Computational Study of the Donor-Acceptor Interactions Underlying the Variable Oxygen Probe

SUPPORTING INFORMATION

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Tables S1-13 and **Figures S1-13**

Structure numbers have been maintained from the papers referenced,[1-9] whilst letter codes refer to entries from the Cambridge Structural Database (CSD).[10] pK_a values for substituents have been made consistent across all systems,[11-17] with generally the same value as originally reported or changed by 0.01-0.02 pK_a units (the majority have been taken from reference 11). The pK_a of water, as mentioned in the main text, was updated to 14 rather than the previously used 15.7 (The authors refer readers to the two references cited for further explanation).[18, 19] Note that the pK_a of 2 for 2,4-$(NO_2)_2$-PhSOH was estimated in the original manuscript for the silyl system **2**.[2] The only substituent removed from the data sets was 2,4,6-trinitrophenol (picric acid) as it was a clear outlier in **3** and **4**, likely due to steric effects of having the dual *ortho* substituents, which the pK_a does not account for. The only other set to have this substituent was the cyclopropyl **10**, hence why the VOP slope changed significantly (- 4.1 x 10^{-3} Å) from that originally reported (- 4.6 x 10^{-3} Å).

Table S1. Experimental C-O bond lengths (Å) determined for derivatives of **1** with updated pK_a values for given parent acids. Adapted from Ref 1

Label	Parent Acid	pK_a	C-O (Å)
5a	PhOH	9.98	1.433
3	4-Cl-PhOH	9.42	1.428
6a	4-NO_2-PhOH	7.16	1.448
3	2,5-$(NO_2)_2$-PhOH	5.22	1.458
6a	2,4-$(NO_2)_2$-PhOH	4.09	1.466
3	3,5-$(NO_2)_2$-$PhCO_2H$	2.82	1.476
DIGRER*	H_2O	14	1.410
DRIBSE01*	H_2O	14	1.397

*new additions

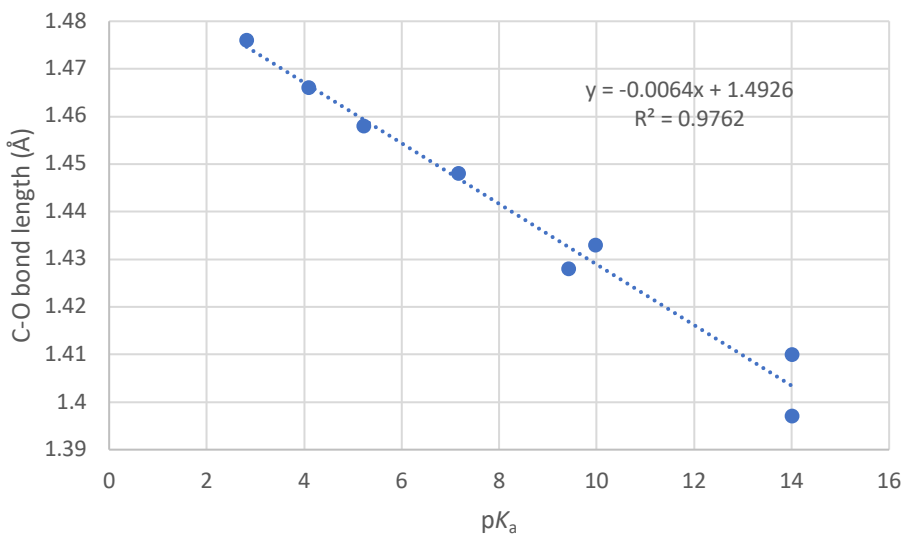


Figure S1. Experimental VOP plot of C-O bonds (Å) for derivatives of **1** adapted from Ref 1

Table S2. Experimental C-O bond lengths (Å) determined for derivatives of **2** with updated pK_a values for given parent acids. Adapted from Ref 2

Label	Parent Acid	pK_a	C-O (Å)
6	4-NO_2-$PhCO_2H$	3.42	1.483
7	3,5-$(NO_2)_2$-$PhCO_2H$	2.82	1.487
8	2,4-$(NO_2)_2$-$PhCO_2H$	1.42	1.497
9	2,4-$(NO_2)_2$-PhSOH	2	1.49
11	4-NO_2-PhOH	7.16	1.465

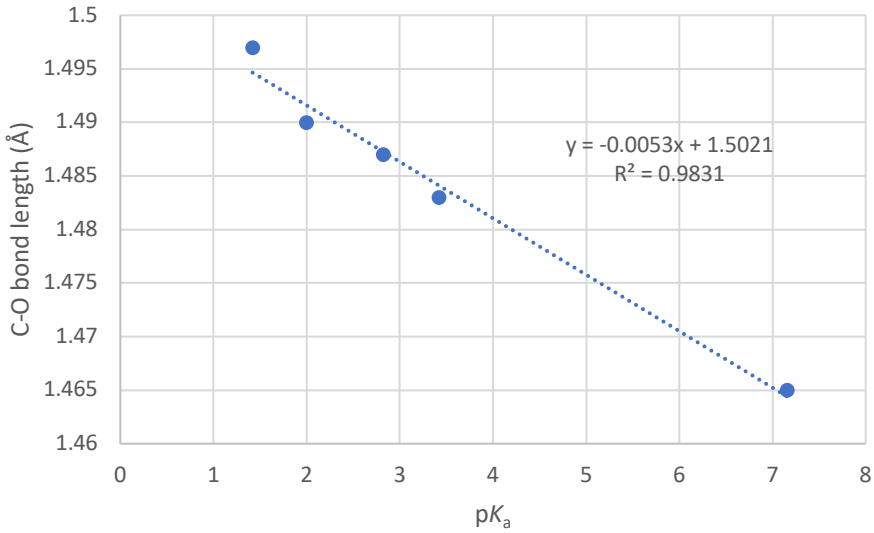


Figure S2. Experimental VOP plot of C-O bonds (Å) for derivatives of **2** adapted from Ref 2

Table S3. Experimental C-O bond lengths (Å) determined for derivatives of **3** with updated pK_a values for given parent acids. Adapted from Ref 3

Label	Parent Acid	pK_a	C-O (Å)
6a	4-NO_2-$PhCO_2H$	3.42	1.466[#]
6b	2,4-$(NO_2)_2$-PhSOH	2	1.473
6d	4-NO_2-$PhSO_3H$	-3.8	1.487
6e	2-NO_2-$PhCO_2H$	2.17	1.471
6f	4-CH_3-$PhSO_3H$	-2.7	1.488
6g	$PhSO_3H$	-2.8	1.490[#]
XIJFEB*	H_2O	14	1.439
YEPWIA*	BnOH	15.4	1.433[#]
LOYSEA*	CH_3CO_2H	4.76	1.458
SUGBII*	$ClCH_2CO_2H$	2.87	1.465
VANZIT*	4-NO_2-$PhSO_3H$	-3.8	1.494
OMIJUQ*	4-CH_3-$PhSO_3H$	-2.7	1.482

*new additions. [#]Averages of two molecules in the unit cell

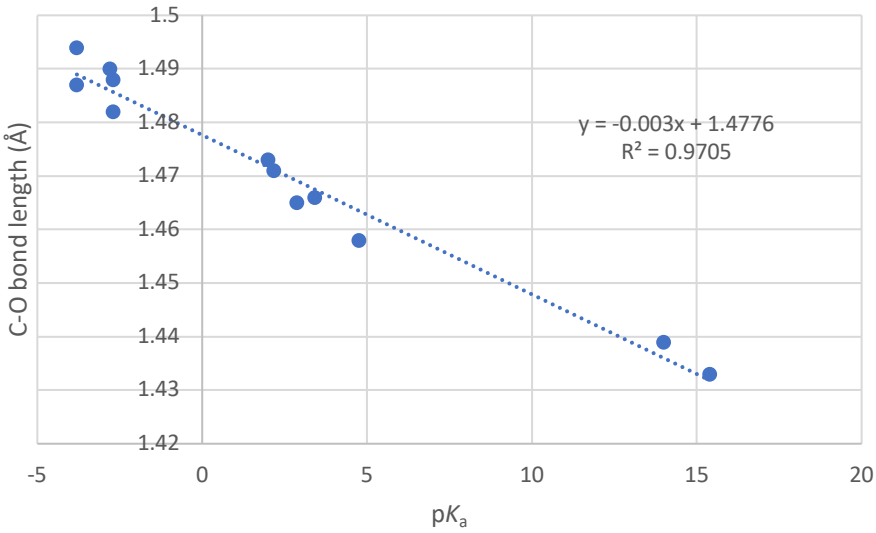


Figure S3. Experimental VOP plot of C-O bonds (Å) for derivatives of **3** adapted from Ref 3

Table S4. Experimental C-O bond lengths (Å) determined for derivatives of **4** with updated pK_a values for given parent acids. Adapted from Ref 3

Label	**Parent Acid**	**pK_a**	**C-O (Å)**
5a	4-NO_2-$PhCO_2H$	3.42	1.473
5b	2,4-$(NO_2)_2$-PhSOH	2	1.476
5d	4-NO_2-$PhSO_3H$	-3.8	1.492
5e	4-NO_2-PhOH	7.16	1.46
5f	4-Cl-3-NO_2-$PhCO_2H$	3.29	1.466
5g	3,5-$(NO_2)_2$-$PhCO_2H$	2.82	1.471
5h	2,4-$(NO_2)_2$-$PhCO_2H$	1.42	1.479
5i	CCl_3CO_2H	0.63	1.478
IDANIL*	H_2O	14	1.43
VOKBEE*	H_2O	14	1.438
BABTOQ*	CH_3CO_2H	4.76	1.465
DECQEH*	CH_3SO_3H	-1.9	1.49

*new additions.

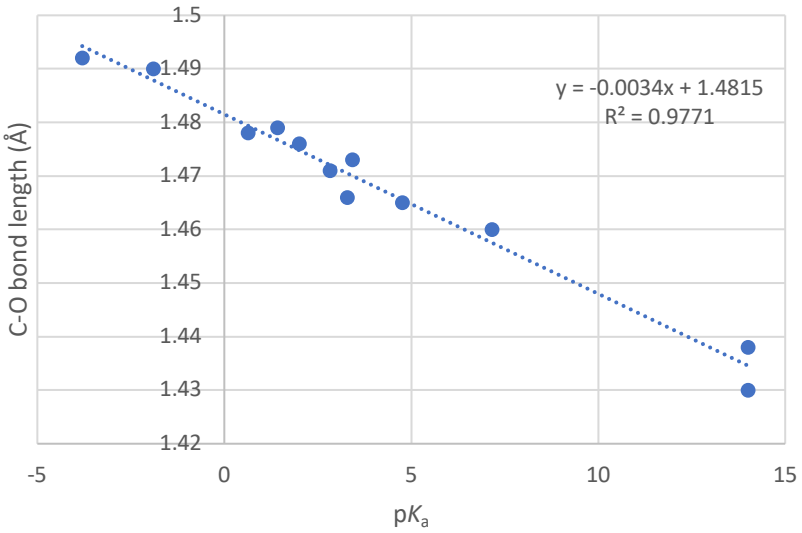


Figure S4. Experimental VOP plot of C-O bonds (Å) for derivatives of **4** adapted from Ref 3

Table S5. Experimental C-O bond lengths (Å) determined for derivatives of **5** with updated pK_a values for given parent acids. Adapted from Ref 4

Label	Parent Acid	pK_a	C-O (Å)
7m	4-NO_2-PhOH	7.16	1.451
4f	4-NO_2-PhCO_2H	3.42	1.468
4g	3,5-$(NO_2)_2$-PhCO_2H	2.82	1.471
4h	2,4-$(NO_2)_2$-PhCO_2H	1.42	1.478*

*Averages of two molecules in the unit cell

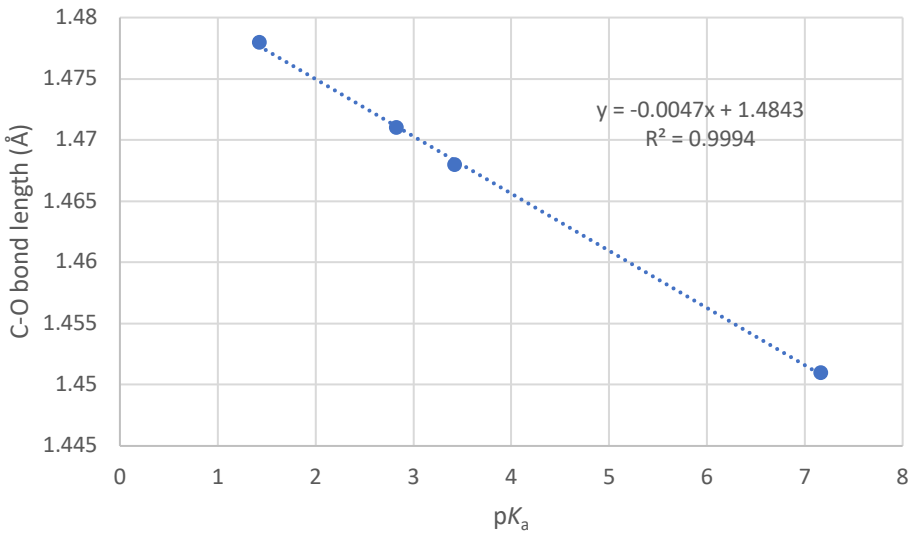


Figure S5. Experimental VOP plot of C-O bonds (Å) for derivatives of **5** adapted from Ref 4

Table S 6. Experimental C-O bond lengths (Å) determined for derivatives of **6** with updated pK_a values for given parent acids. Adapted from Ref 4

Label	Parent Acid	pK_a	C-O (Å)
4i	4-NO_2-PhOH	7.16	1.456*
4j	4-NO_2-$PhCO_2H$	3.42	1.475*
7k	2,4-$(NO_2)_2$-$PhCO_2H$	1.42	1.489

*Averages of two molecules in the unit cell

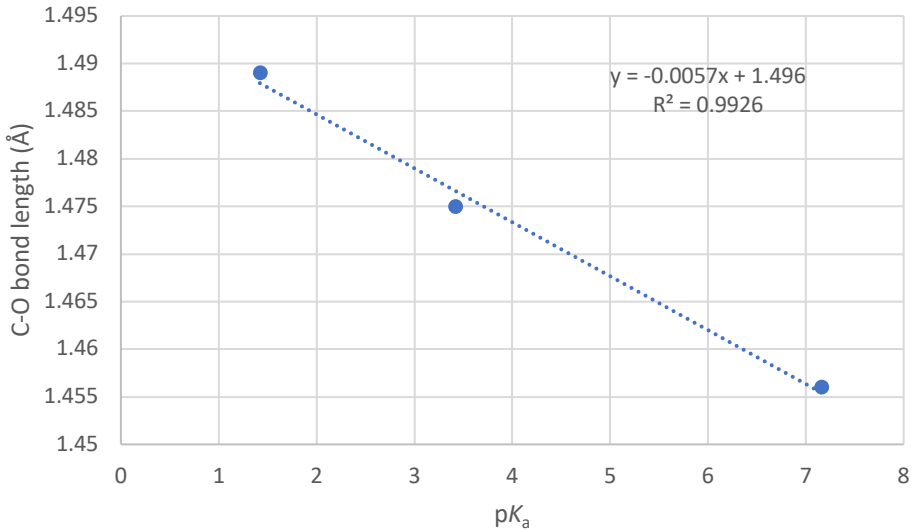


Figure S6. Experimental VOP plot of C-O bonds (Å) for derivatives of **6** adapted from Ref 4

Table S7. Experimental C-O bond lengths (Å) determined for derivatives of **7** with updated pK_a values for given parent acids. Adapted from Ref 5

Structures*	Parent Acid	pK_a	C-O (Å)*
1150	H_2O	14	1.423
57	CH_3OH	15.5	1.414
10	PhOH	9.98	1.426
1	4-NO_2-PhOH	7.16	1.440
263	CH_3CO_2H	4.76	1.443
38	$PhCO_2H$	4.2	1.448
23	4-NO_2-$PhCO_2H$	3.42	1.451
11	CH_3SO_3H	-1.9	1.463
33	4-CH_3-$PhSO_3H$	-2.7	1.461
1	4-NO_2-$PhSO_3H$	-3.8	1.463

*C-O bond lengths presented for **7** are an average of often multiple structures obtained from the Cambridge structural database. The number of structures averaged is provided.

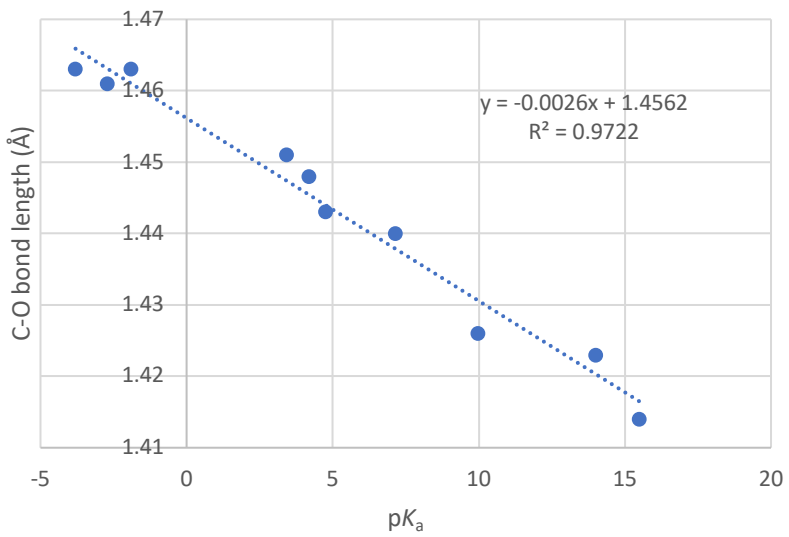


Figure S7. Experimental VOP plot of C-O bonds (Å) for derivatives of **7** adapted from Ref 5

Table S8. Experimental C-O bond lengths (Å) determined for derivatives of **8** with updated pK_a values for given parent acids. Adapted from Ref 5

Label	**Parent Acid**	**pK_a**	**C-O (Å)**
11a	H_2O	14	1.426*
11b	4-NO_2-PhOH	7.16	1.437
11c	3-NO_2-PhCO_2H	3.49	1.462
11d	2-NO_2-PhCO_2H	2.17	1.451
11e	CCl_3CO_2H	0.63	1.473
11f	CH_3SO_3H	-1.9	1.478

*Averages of two molecules in the unit cell

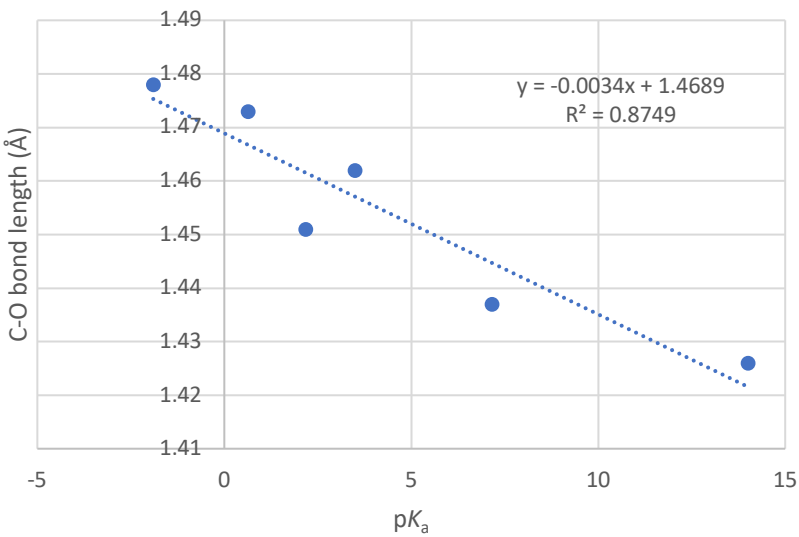


Figure S8. Experimental VOP plot of C-O bonds (Å) for derivatives of **8** adapted from Ref 5

Table S9. Experimental C-O bond lengths (Å) determined for derivatives of **9** with updated pK_a values for given parent acids. Adapted from Ref 6

Label	Parent Acid	pK_a	C-O (Å)
5a	4-NO_2-PhOH	7.16	1.459
5e	3,5-$(NO_2)_2$-$PhCO_2H$	2.82	1.471
5f	3,4-$(NO_2)_2$-$PhCO_2H$	2.82	1.4735
5g	2-NO_2-$PhCO_2H$	2.17	1.475

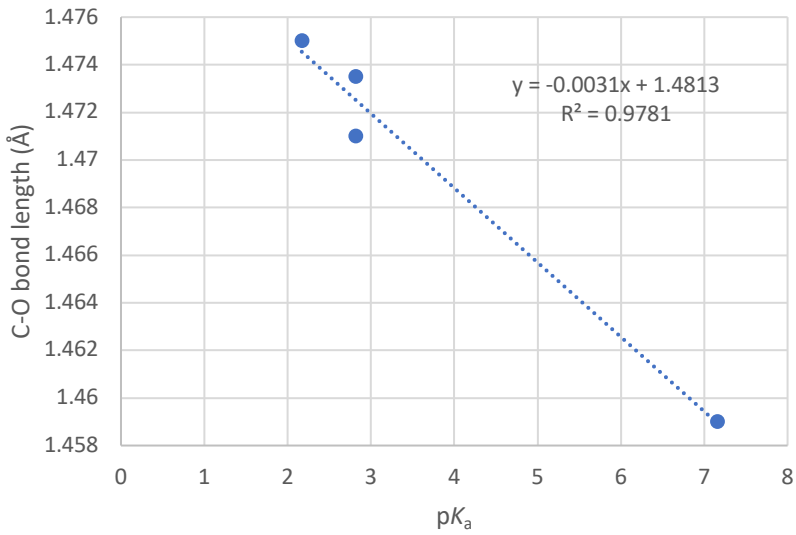


Figure S9. Experimental VOP plot of C-O bonds (Å) for derivatives of **9** adapted from Ref 6

Table S10. Experimental C-O bond lengths (Å) determined for derivatives of **10** with updated pK_a values for given parent acids. Adapted from Ref 7

Label	Parent Acid	pK_a	C-O (Å)
8c	2,4-$(NO_2)_2$-PhSOH	2	1.465
8d	3,5-$(NO_2)_2$-$PhCO_2H$	2.82	1.464
8e	4-NO_2-$PhCO_2H$	3.42	1.458
8f	4-NO_2-PhOH	7.16	1.446
DUSXOF*	4-CH_3CO_2-2-OH-PhOH	8.12	1.439

*new addition

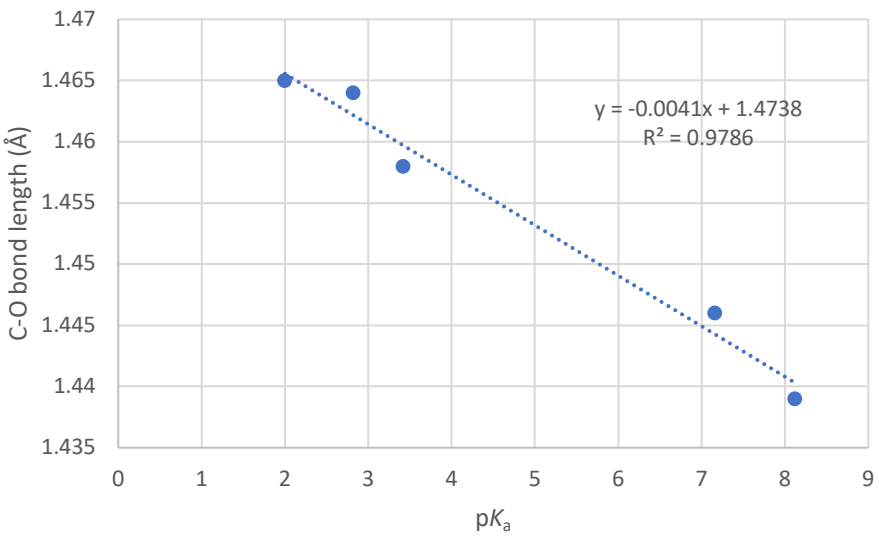


Figure S10. Experimental VOP plot of C-O bonds (Å) for derivatives of **10** adapted from Ref 7

Table S11. Experimental C-O bond lengths (Å) determined for derivatives of **11** with updated pK_a values for given parent acids. Adapted from Ref 7

Label	Parent Acid	pK_a	C-O (Å)
9a	2,4-$(NO_2)_2$-$PhCO_2H$	1.42	1.492
9b	2,4-$(NO_2)_2$-PhSOH	2	1.485
9d	4-NO_2-$PhCO_2H$	3.42	1.476

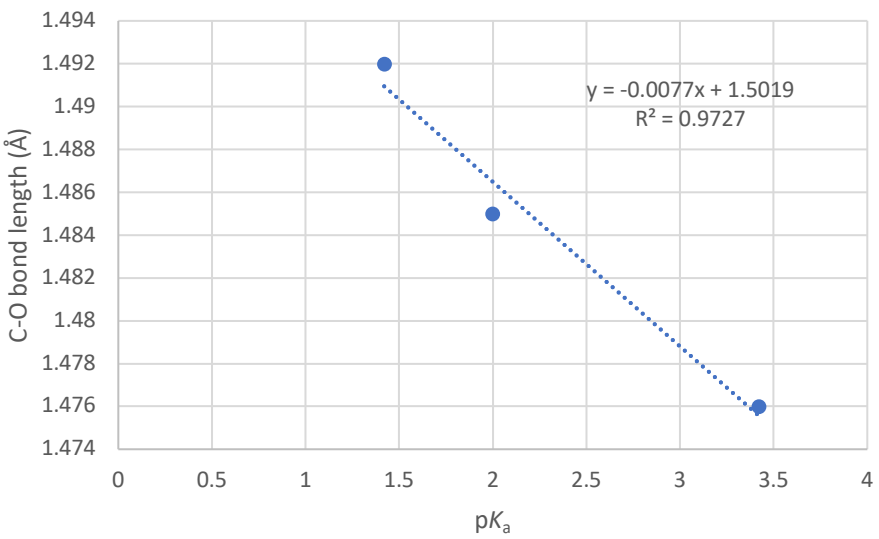


Figure S 11. Experimental VOP plot of C-O bonds (Å) for derivatives of **11** adapted from Ref 7

Table S 12. Experimental C-O bond lengths (Å) determined for derivatives of **12** with updated pK_a values for given parent acids. Adapted from Ref 8

Label	Parent Acid	pK_a	C-O (Å)
HUFTIL	1-Adamantol	18	1.426
PIVHAE	$MeOCH_2CH_2OH$*	14.8	1.415
DUSLEJ	PhOH*	9.98	1.430
SECCIO	4-CH_3CONH-PhOH	9.58	1.436
YUXJEG	4-Ph-PhOH*	9.55	1.434
KERKOI10	2-HCO-PhOH	8.17	1.436
NEQBUI	4-HCO-PhOH	7.61	1.436
1a	3-NC-PhOH	8.61	1.442
1b	4-NO_2-PhOH	7.16	1.437
1c	2,4-$(NO_2)_2$-PhOH	4.09	1.451
1d	3-NO_2-$PhCO_2H$	3.49	1.452
1e	4-NO_2-$PhCO_2H$	3.42	1.452
1f	3,5-$(NO_2)_2$-$PhCO_2H$	2.82	1.451
1g	2-NO_2-$PhCO_2H$	2.17	1.452
1h	4-CH_3-$PhSO_3H$	-2.7	1.460

*structure is approximated to the pK_a of this parent acid

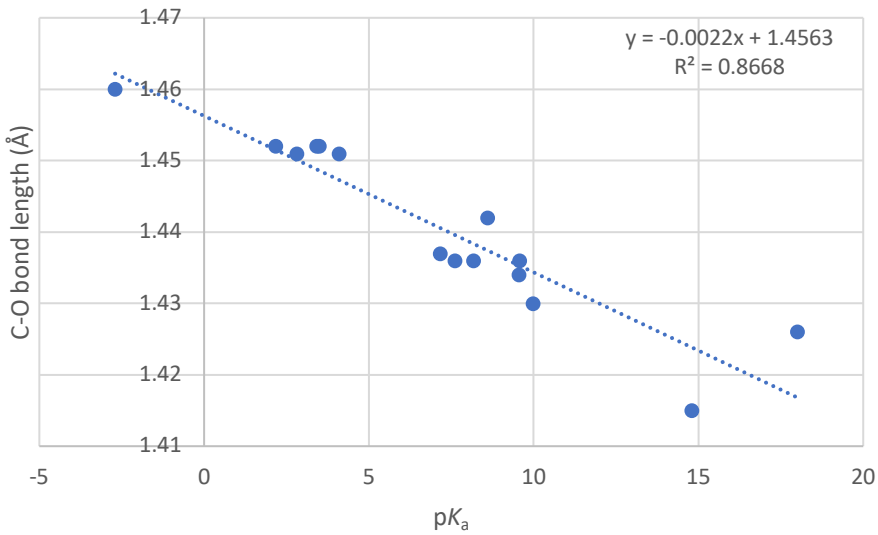


Figure S 12. Experimental VOP plot of C-O bonds (Å) for derivatives of **12** adapted from Ref 8

Table S 13. Experimental C-O bond lengths (Å) determined for derivatives of **13** with updated pK_a values for given parent acids. Adapted from Ref 9

Label	Parent Acid	pK_a	C-O (Å)
10	CH_3CO_2H	4.76	1.456
11	CCl_3CO_2H	0.63	1.466
12	CH_3SO_3H	-1.9	1.476
13	$PhCO_2H$	4.2	1.455
14	4-NO_2-PhOH	7.16	1.438
15	4-NO_2-$PhCO_2H$	3.42	1.46
16	3,5-$(NO_2)_2$-$PhCO_2H$	2.82	1.462

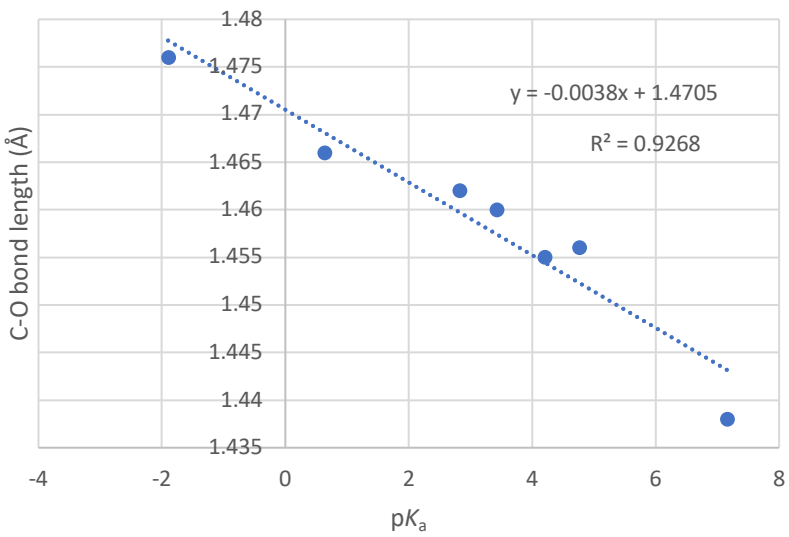


Figure S 13. Experimental VOP plot of C-O bonds (Å) for derivatives of **13** adapted from Ref 9

Table S 14. pK_a values for selected substituents and corresponding C-O bond lengths (Å) in systems **1-13** calculated at B3LYP/6-311++G(d,p)

Substituent	**pK_a**	**1**	**2**	**3**	**4**	**5**	**6**
ROH	14	1.420	1.445	1.433	1.439	1.441	1.442
$ROCOCH_3$	4.76	1.458	1.474	1.458	1.464	1.466	1.469
$ROCOCF_3$	0.23	1.485	1.494	1.472	1.480	1.482	1.486
ROC(O)OH	3.6	1.465	1.481	1.462	1.469	1.471	1.474
ROPh	9.98	1.429	1.452	1.438	1.444	1.445	1.447
$ROCH_2CF_3$	12.4	1.426	1.451	1.437	1.442	1.445	1.447
$ROCOCHCl_2$	1.3	1.477	1.487	1.467	1.474	1.476	1.480
ROPh-p-NO_2	7.16	1.442	1.463	1.447	1.453	1.454	1.457

Substituent	**7**	**8**	**9**	**10**	**11**	**12**	**13**
ROH	1.431	1.432	1.437	1.432	1.437	1.429	1.428
$ROCOCH_3$	1.448	1.451	1.462	1.452	1.469	1.448	1.452
$ROCOCF_3$	1.459	1.464	1.478	1.466	1.488	1.46	1.468
ROC(O)OH	1.451	1.454	1.467	1.456	1.474	1.451	1.457
ROPh	1.428	1.429	1.441	1.431	1.448	1.427	1.432
$ROCH_2CF_3$	1.426	1.428	1.440	1.430	1.442	1.427	1.431
$ROCOCHCl_2$	1.455	1.459	1.472	1.461	1.482	1.455	1.462
ROPh-p-NO_2	1.436	1.438	1.451	1.439	1.458	1.435	1.441

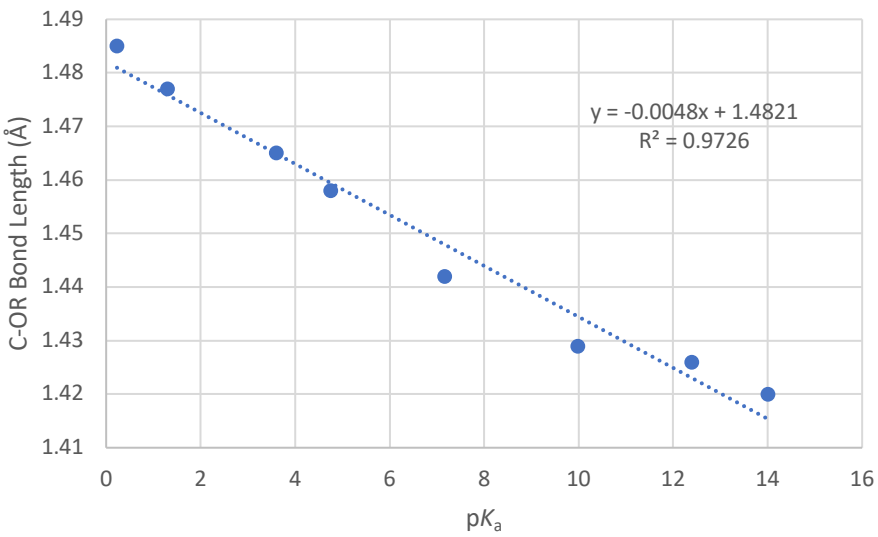


Figure S 14. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **1**, calculated at B3LYP/6-311++G(d,p) in the gas phase.

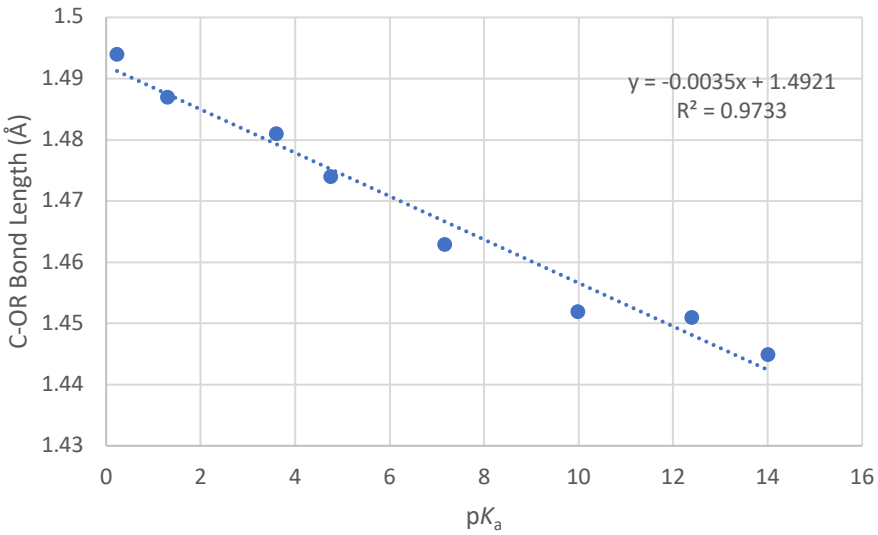


Figure S 15. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **2**, calculated at B3LYP/6-311++G(d,p) in the gas phase.

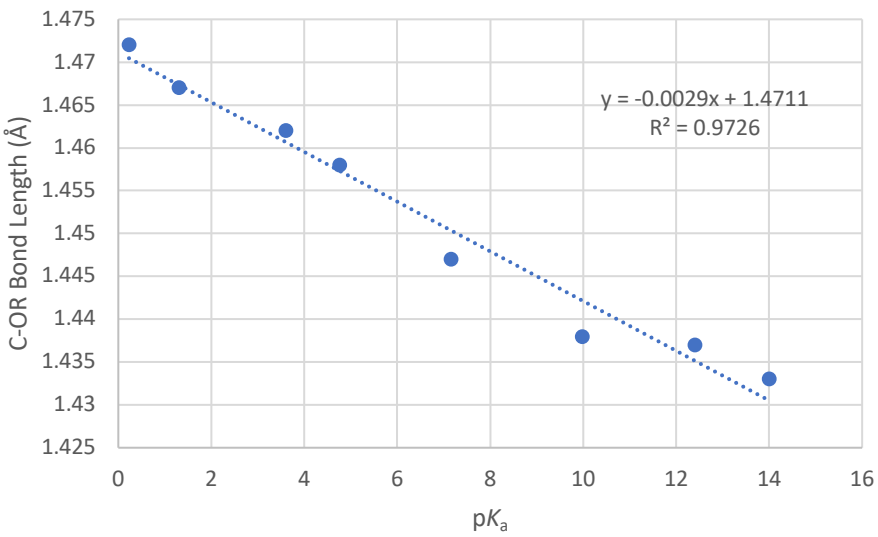


Figure S 16. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **3**, calculated at B3LYP/6-311++G(d,p) in the gas phase.

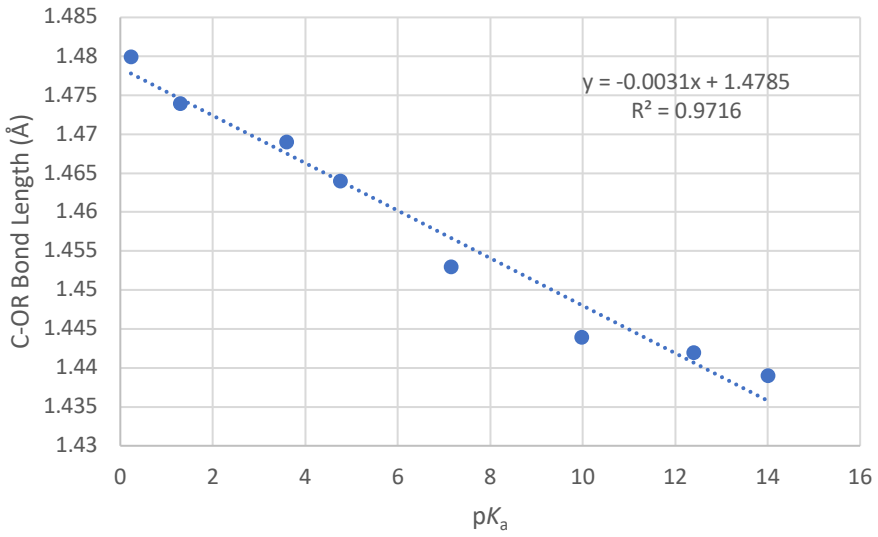


Figure S 17. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **4**, calculated at B3LYP/6-311++G(d,p) in the gas phase.

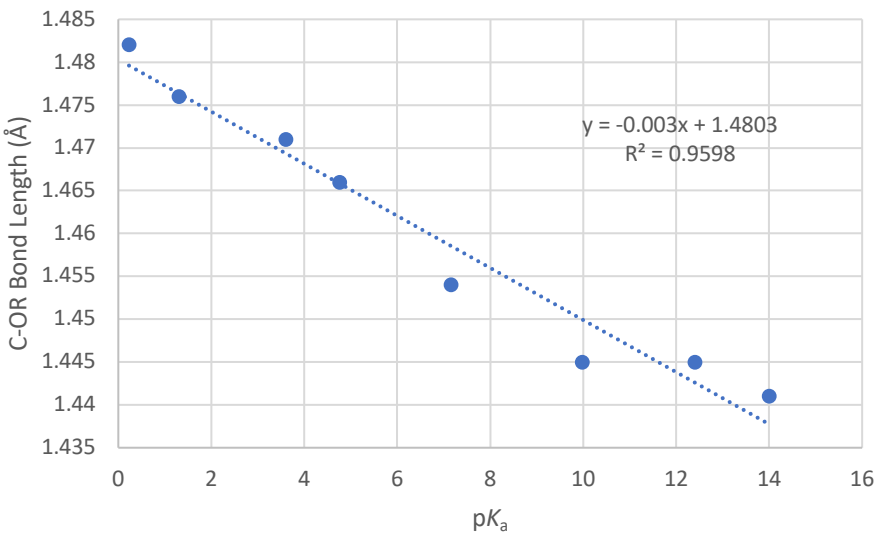


Figure S 18. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **5**, calculated at B3LYP/6-311++G(d,p) in the gas phase.

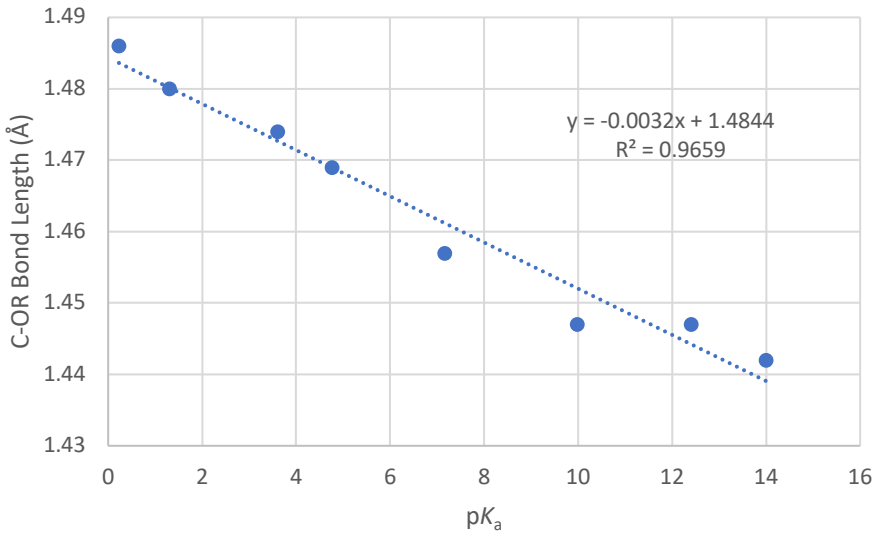


Figure S 19. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **6**, calculated at B3LYP/6-311++G(d,p) in the gas phase.

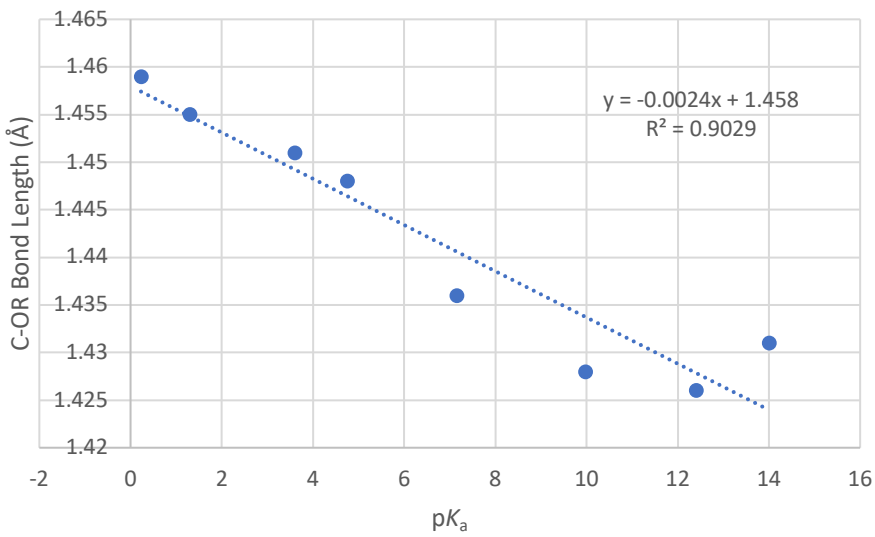


Figure S 20. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **7**, calculated at B3LYP/6-311++G(d,p) in the gas phase.

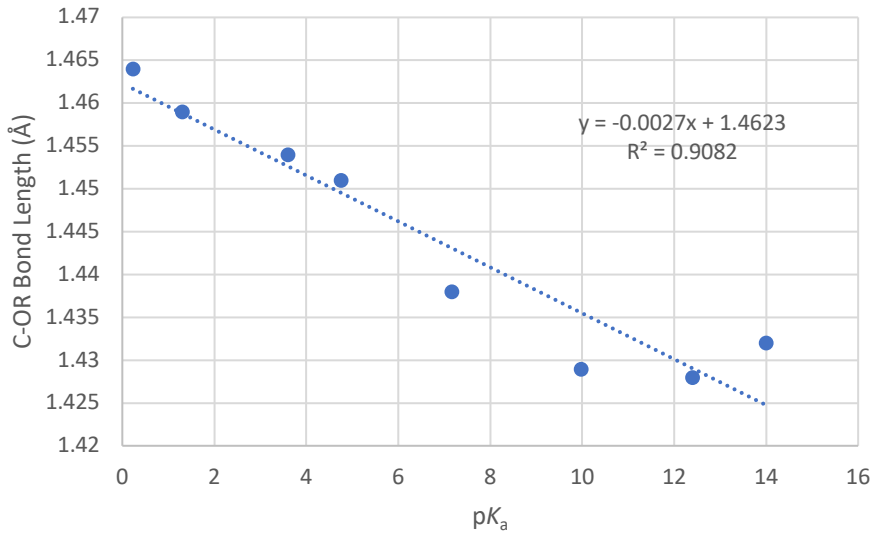


Figure S 21. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **8**, calculated at B3LYP/6-311++G(d,p) in the gas phase.

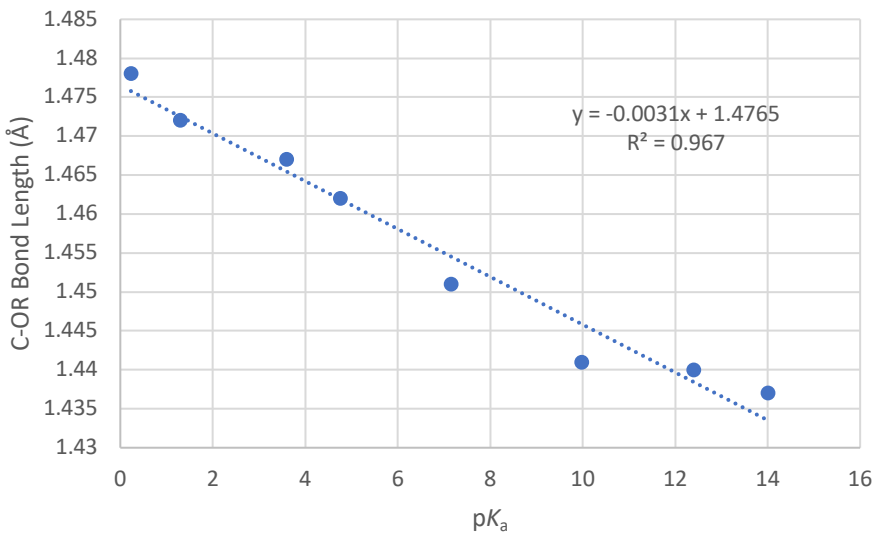


Figure S 22. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **9**, calculated at B3LYP/6-311++G(d,p) in the gas phase.

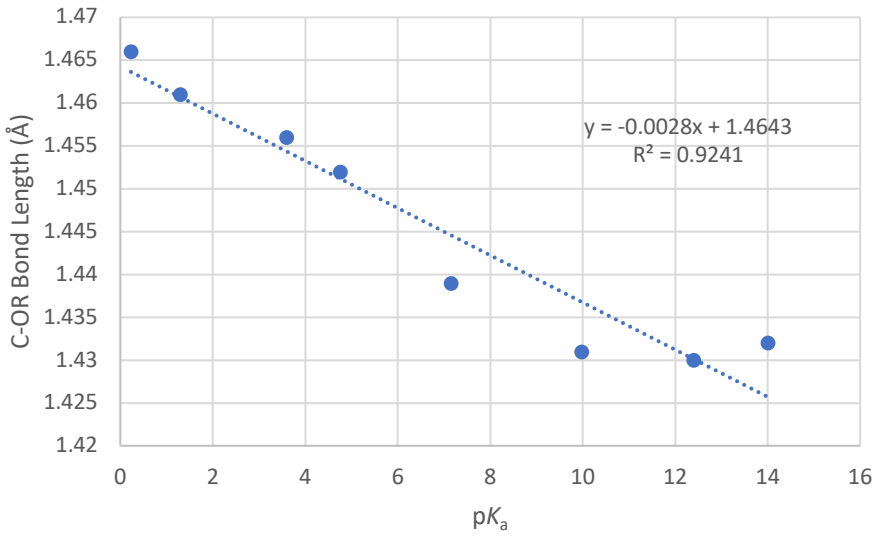


Figure S 23. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **10**, calculated at B3LYP/6-311++G(d,p) in the gas phase.

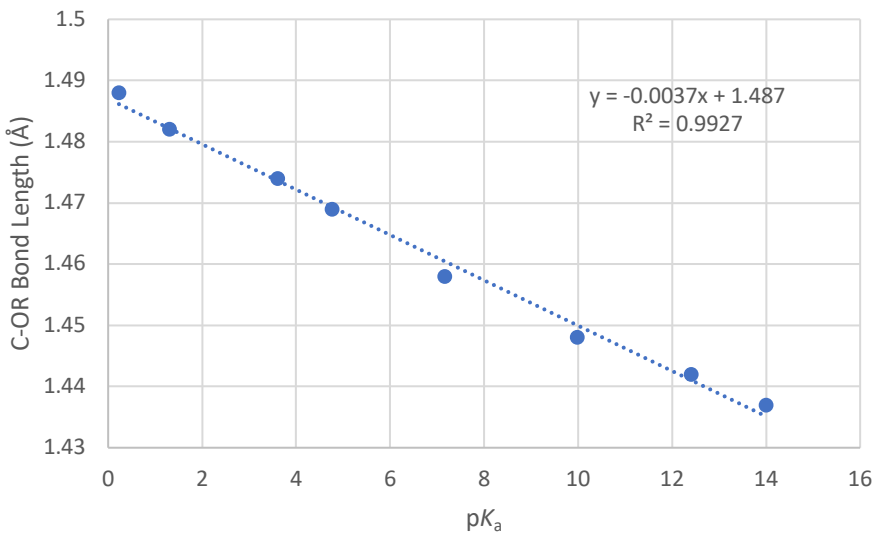


Figure S 24. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **11**, calculated at B3LYP/6-311++G(d,p) in the gas phase.

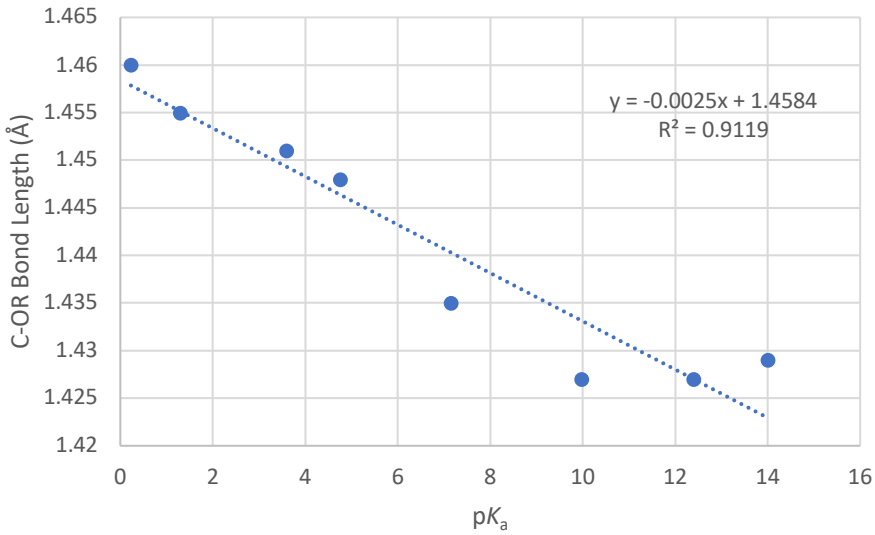


Figure S 25. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **12**, calculated at B3LYP/6-311++G(d,p) in the gas phase.

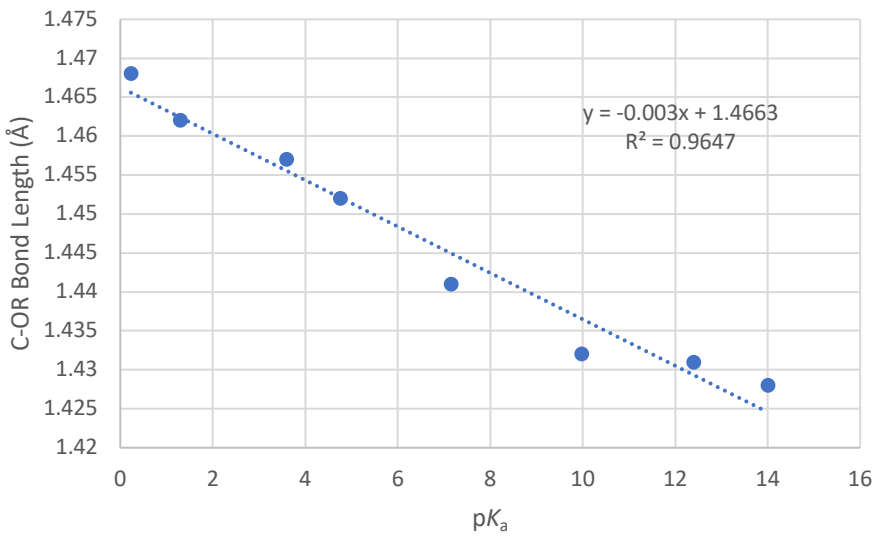


Figure S 26. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **13**, calculated at B3LYP/6-311++G(d,p) in the gas phase.

Table S 15. pK_a values for selected substituents and corresponding C-O bond lengths (Å) in systems **1-13** calculated at M06-2X/6-311++G(d,p)

Substituent	**pK_a**	**1**	**2**	**3**	**4**	**5**	**6**
ROH	14	1.409	1.43	1.421	1.426	1.427	1.429
$ROCOCH_3$	4.76	1.439	1.455	1.442	1.448	1.448	1.450
$ROCOCF_3$	0.23	1.459	1.47	1.454	1.460	1.461	1.463
ROC(O)OH	3.6	1.446	1.461	1.446	1.453	1.453	1.455
ROPh	9.98	1.416	1.436	1.425	1.430	1.431	1.432
$ROCH_2CF_3$	12.4	1.416	1.435	1.424	1.429	1.430	1.432
ROPh-p-NO_2	7.16	1.425	1.444	1.432	1.437	1.437	1.439
$ROCOCHCl_2$	1.3	1.452	1.464	1.449	1.455	1.455	1.458

Substituent	**7**	**8**	**9**	**10**	**11**	**12**	**13**
ROH	1.419	1.42	1.425	1.420	1.422	1.416	1.417
$ROCOCH_3$	1.435	1.436	1.446	1.437	1.449	1.432	1.438
$ROCOCF_3$	1.445	1.447	1.458	1.449	1.464	1.442	1.451
ROC(O)OH	1.438	1.440	1.451	1.441	1.453	1.434	1.443
ROPh	1.417	1.418	1.428	1.419	1.437	1.415	1.421
$ROCH_2CF_3$	1.417	1.417	1.428	1.418	1.426	1.414	1.42
ROPh-p-NO_2	1.423	1.424	1.435	1.426	1.438	1.420	1.428
$ROCOCHCl_2$	1.441	1.442	1.453	1.445	1.458	1.438	1.446

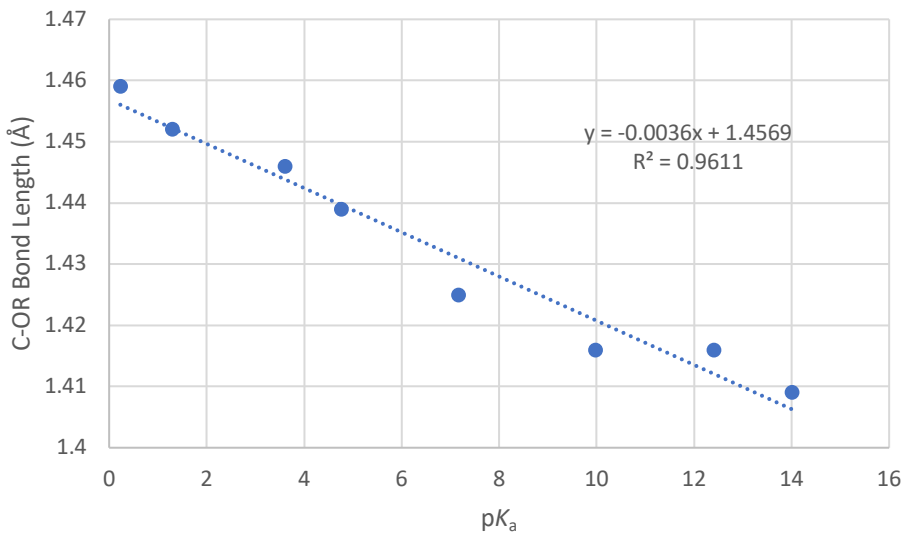


Figure S 27. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **1**, calculated at M06-2X/6-311++G(d,p) in the gas phase.

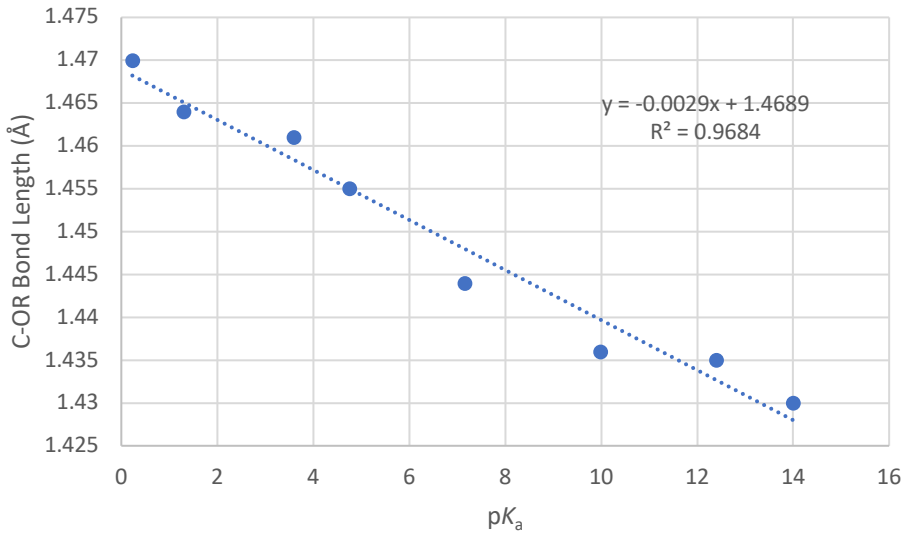


Figure S 28. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **2**, calculated at M06-2X/6-311++G(d,p) in the gas phase.

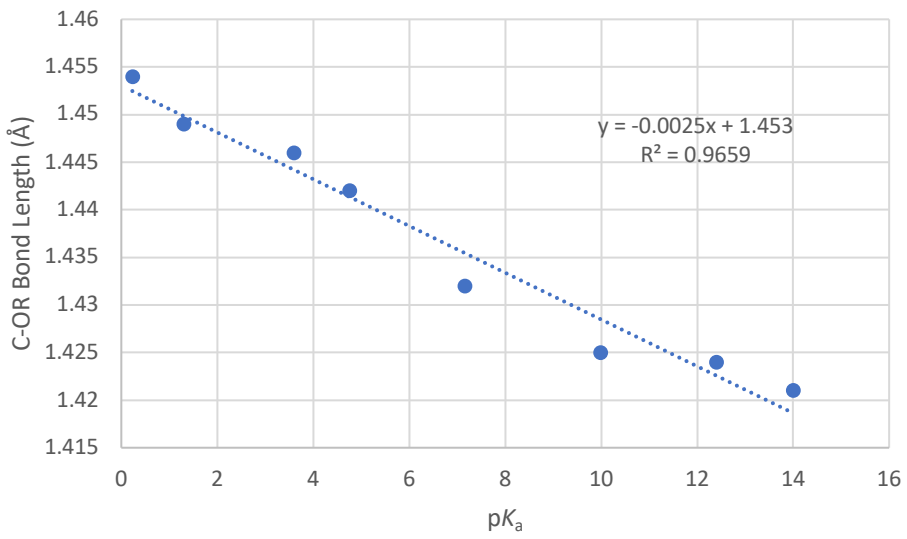


Figure S 29. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **3**, calculated at M06-2X/6-311++G(d,p) in the gas phase.

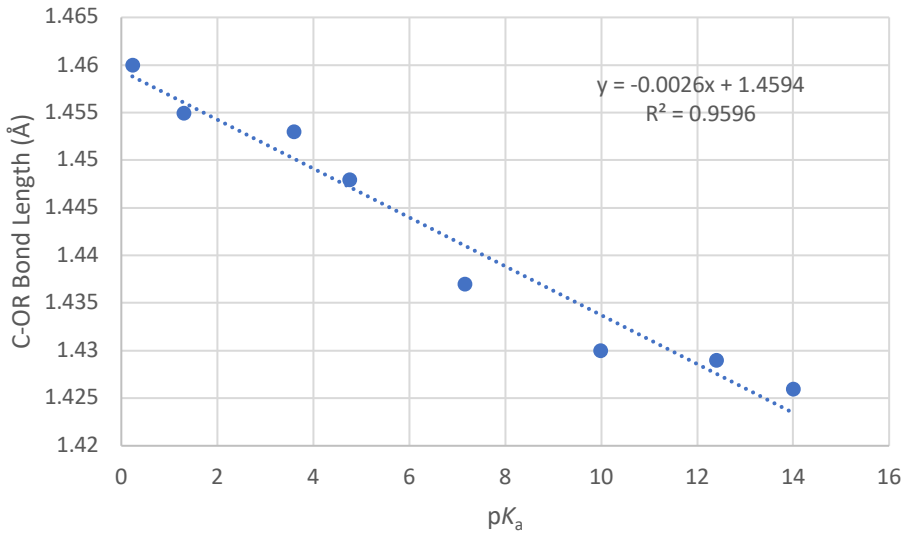


Figure S 30. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **4**, calculated at M06-2X/6-311++G(d,p) in the gas phase.

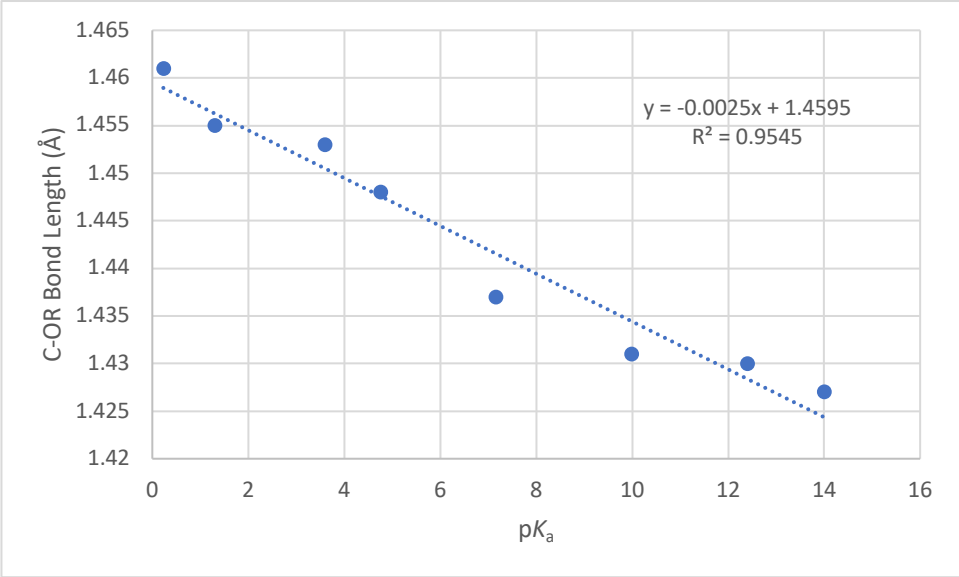


Figure S 31. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **5**, calculated at M06-2X/6-311++G(d,p) in the gas phase.

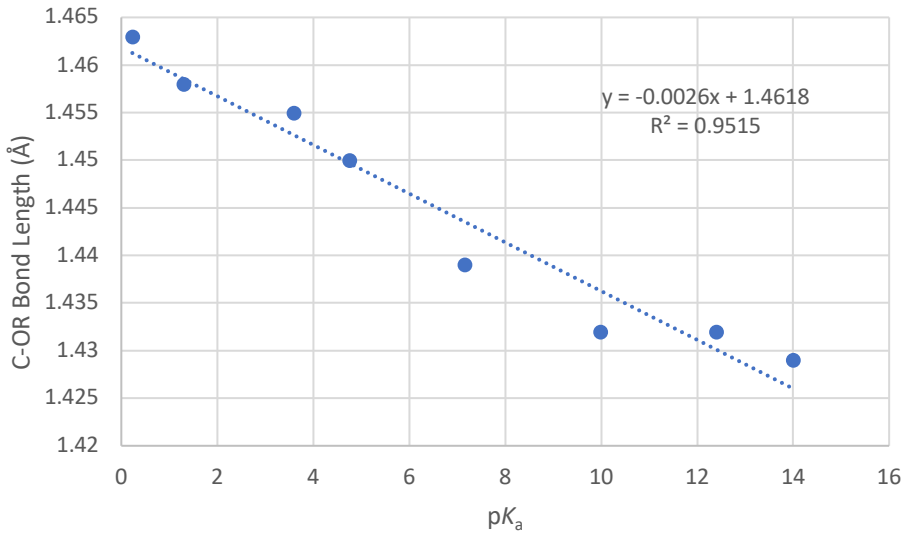


Figure S 32. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **6**, calculated at M06-2X/6-311++G(d,p) in the gas phase.

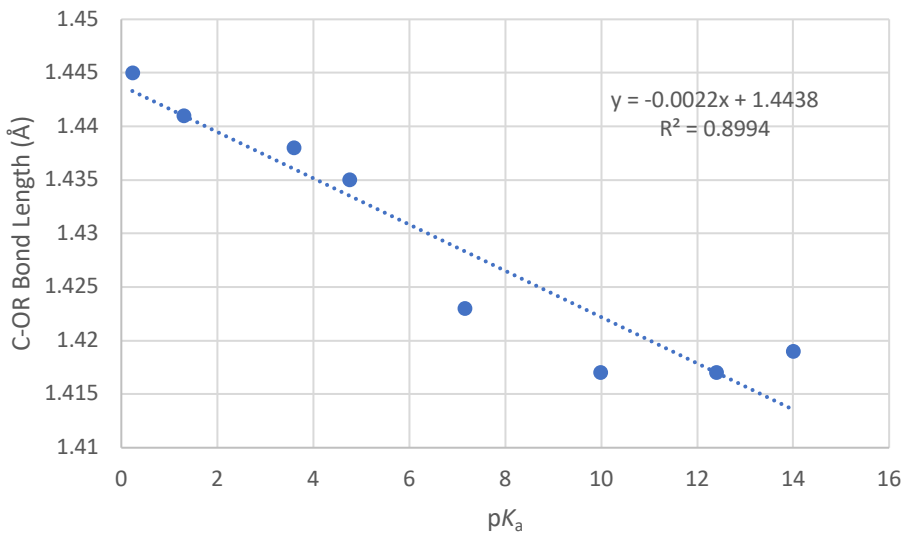


Figure S 33. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **7**, calculated at M06-2X/6-311++G(d,p) in the gas phase.

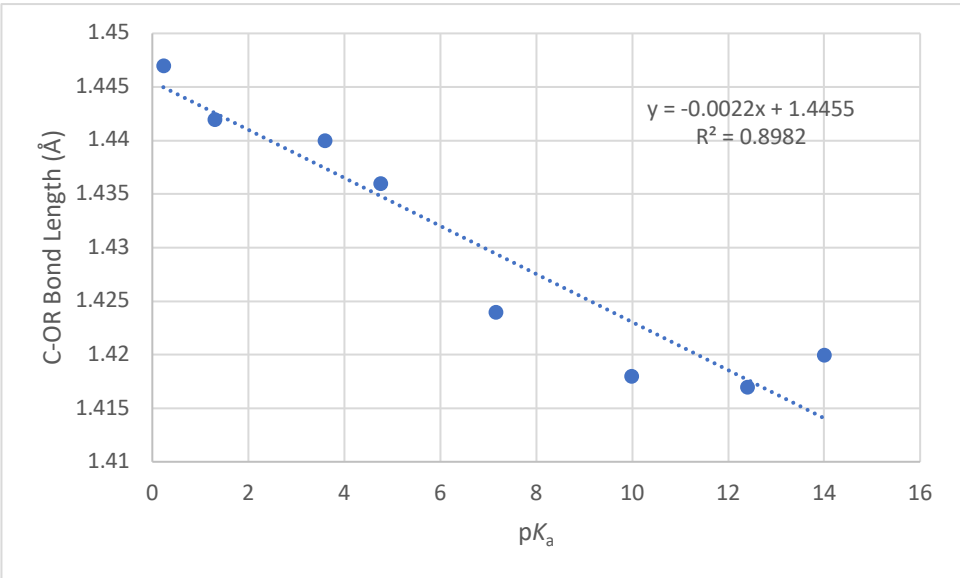


Figure S 34. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **8**, calculated at M06-2X/6-311++G(d,p) in the gas phase.

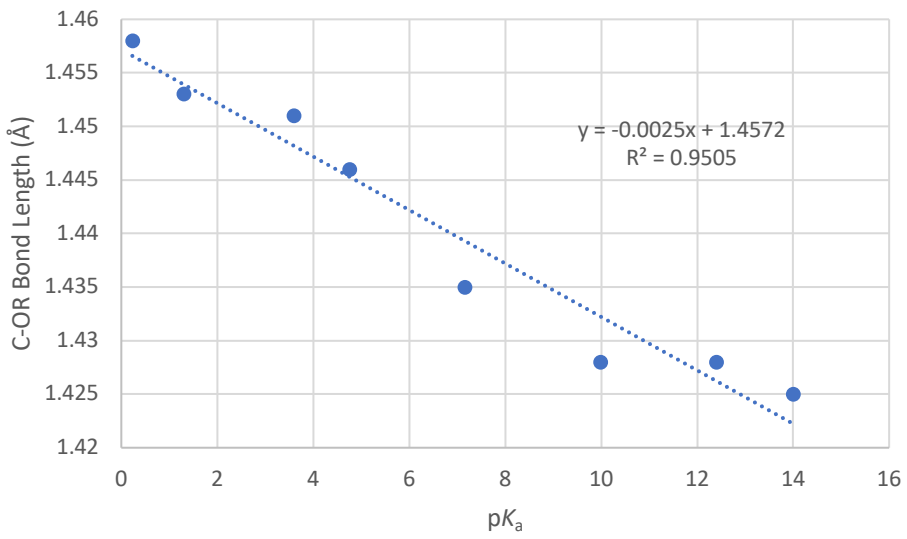


Figure S 35. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **9**, calculated at M06-2X/6-311++G(d,p) in the gas phase.

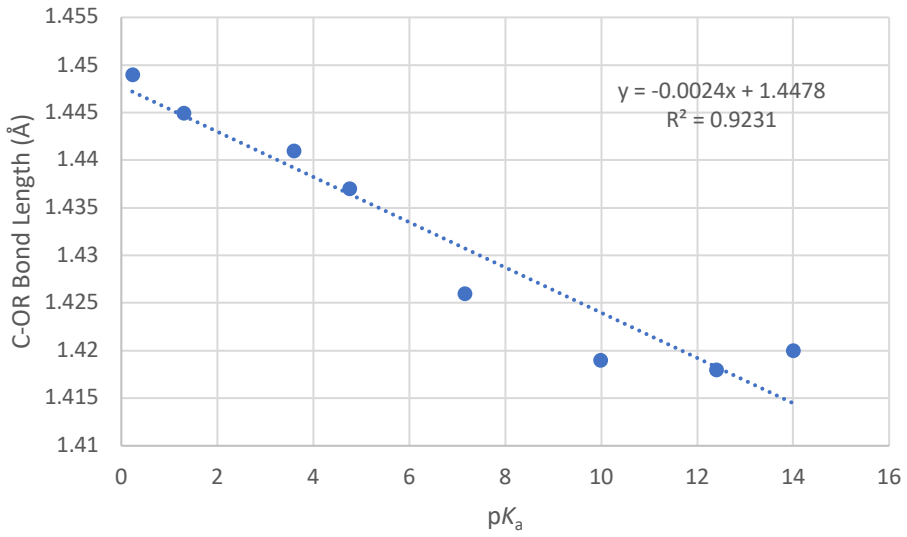


Figure S 36. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **10**, calculated at M06-2X/6-311++G(d,p) in the gas phase.

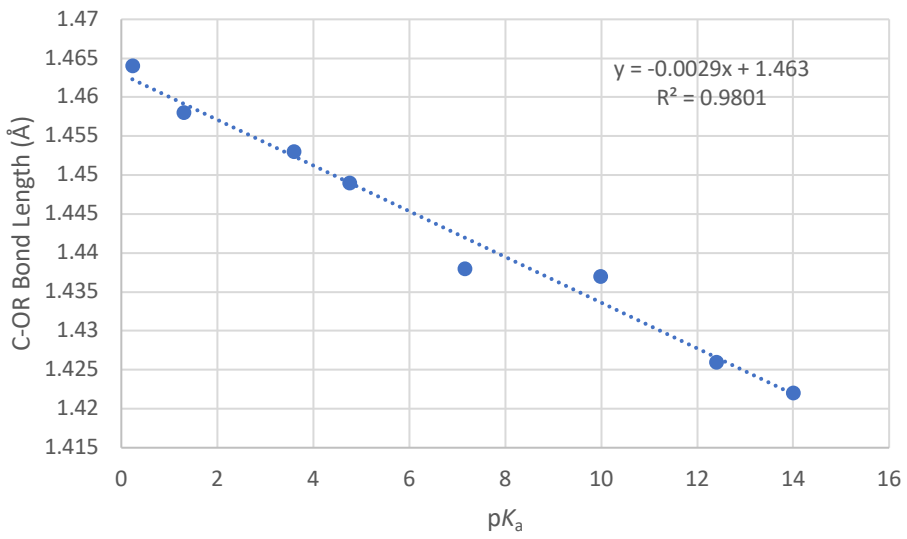


Figure S 37. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **11**, calculated at M06-2X/6-311++G(d,p) in the gas phase.

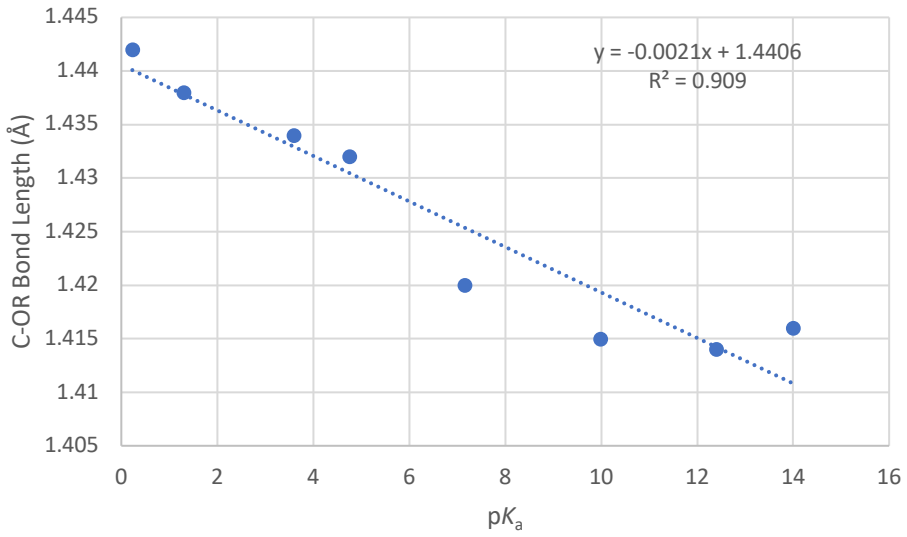


Figure S 38. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **12**, calculated at M06-2X/6-311++G(d,p) in the gas phase.

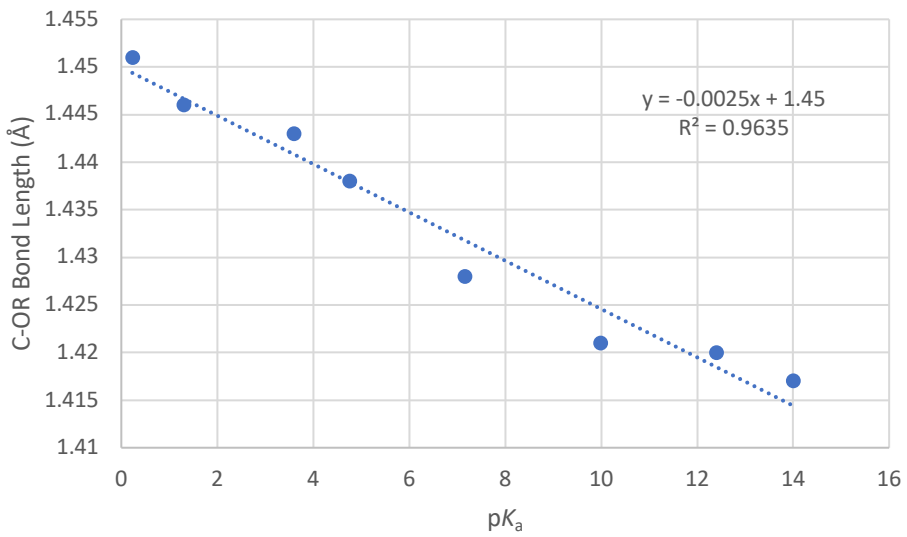


Figure S 39. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **13**, calculated at M06-2X/6-311++G(d,p) in the gas phase.

Table S 16. pK_a values for selected substituents and corresponding C-O bond lengths (Å) in systems **1-13** calculated at MP2/6-31+G(d)

Substituent	**pK_a**	**1**	**2**	**3**	**4**	**5**	**6**
ROH	14	1.423	1.448	1.439	1.442	1.445	1.445
$ROCOCH_3$	4.76	1.453	1.472	1.459	1.463	1.464	1.466
$ROCOCF_3$	0.23	1.475	1.488	1.471	1.476	1.476	1.480
ROC(O)OH	3.6	1.460	1.478	1.463	1.468	1.468	1.471
ROPh	9.98	1.428	1.455	1.443	1.448	1.447	1.449
$ROCH_2CF_3$	12.4	1.428	1.452	1.441	1.444	1.445	1.446
$ROCOCHCl_2$	1.3	1.466	1.481	1.465	1.470	1.470	1.473
ROPh-p-NO_2	7.16	1.436	1.460	1.447	1.451	1.451	1.453

Substituent	**7**	**8**	**9**	**10**	**11**	**12**	**13**
ROH	1.436	1.437	1.442	1.438	1.442	1.435	1.434
$ROCOCH_3$	1.452	1.453	1.462	1.455	1.468	1.453	1.456
$ROCOCF_3$	1.461	1.464	1.475	1.467	1.483	1.463	1.469
ROC(O)OH	1.454	1.456	1.466	1.459	1.472	1.455	1.460
ROPh	1.433	1.434	1.442	1.436	1.456	1.433	1.442
$ROCH_2CF_3$	1.432	1.433	1.444	1.435	1.444	1.433	1.436
$ROCOCHCl_2$	1.457	1.459	1.469	1.462	1.476	1.458	1.463
ROPh-p-NO_2	1.438	1.439	1.449	1.441	1.461	1.438	1.447

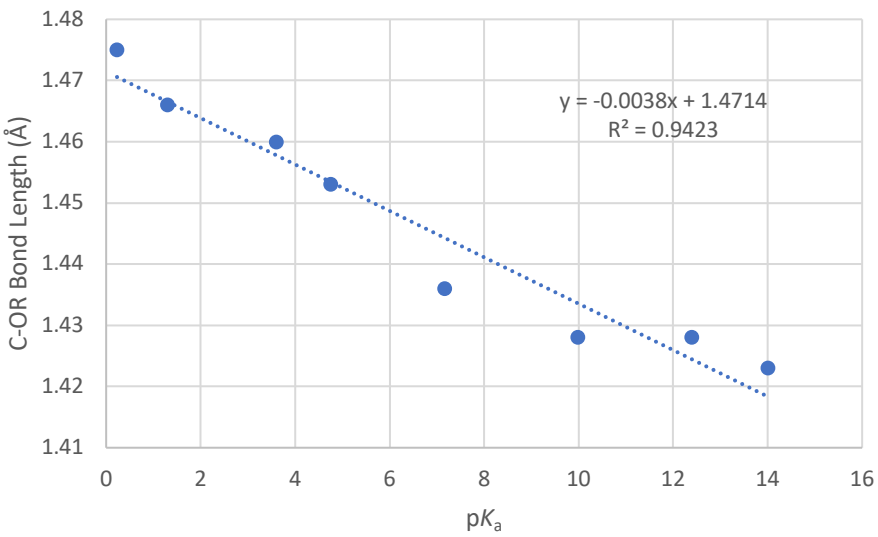


Figure S 40. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **1**, calculated at MP2/6-31+G(d) in the gas phase.

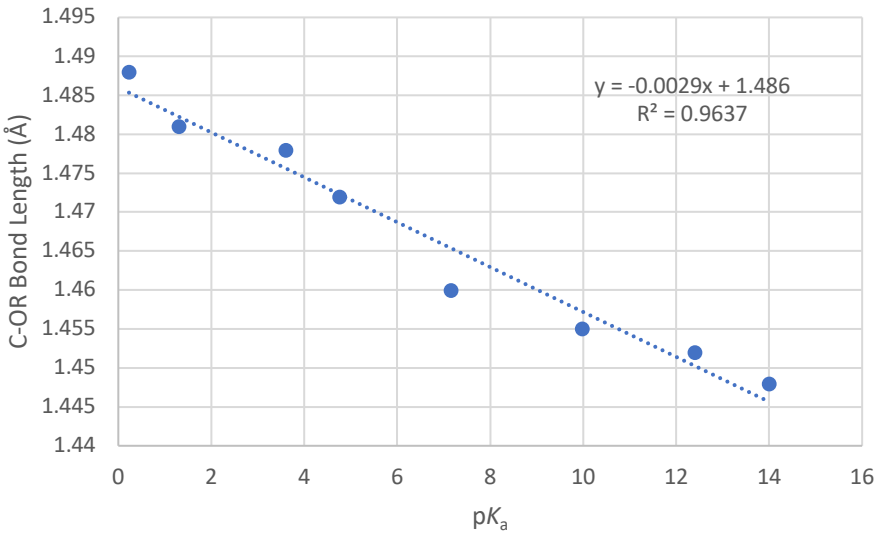


Figure S 41. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **2**, calculated at MP2/6-31+G(d) in the gas phase.

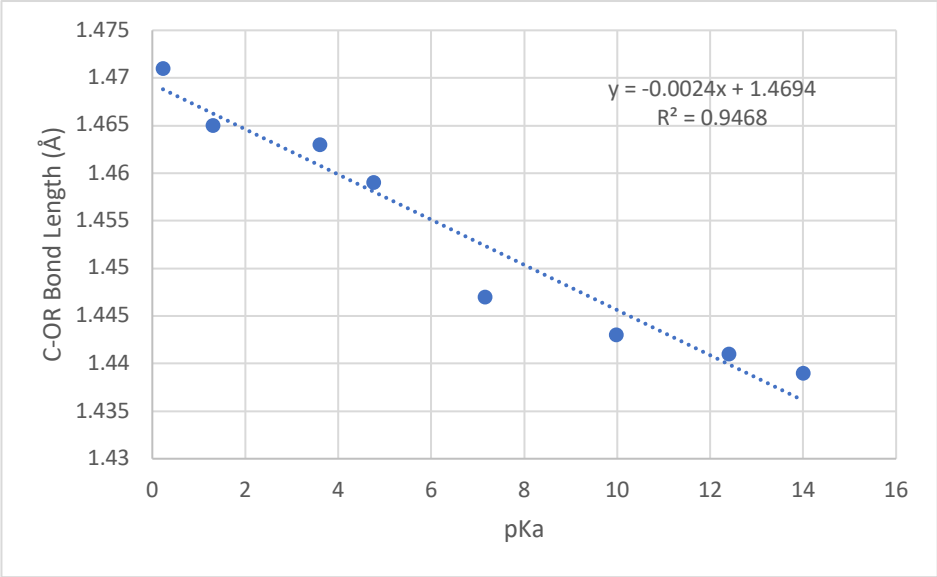


Figure S 42. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **3**, calculated at MP2/6-31+G(d) in the gas phase.

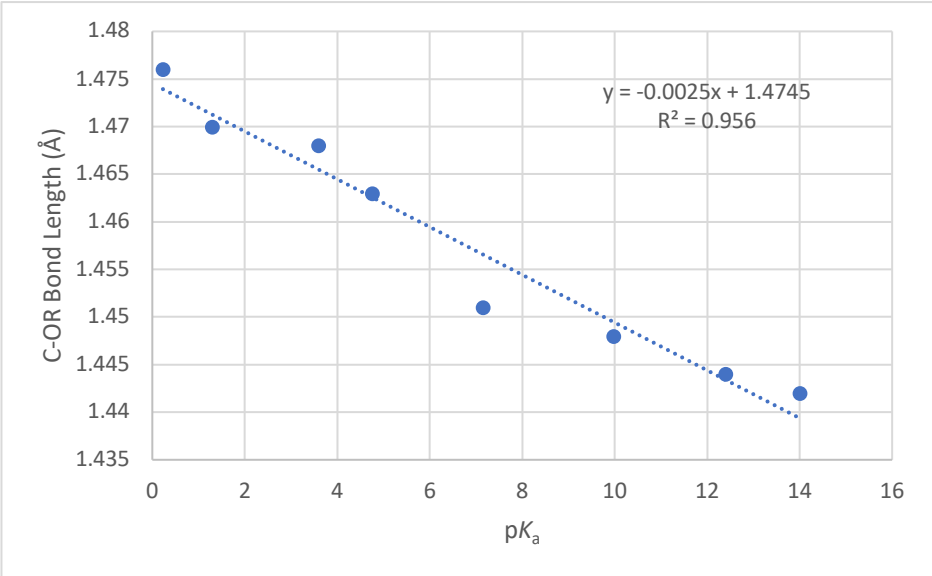


Figure S 43. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **4**, calculated at MP2/6-31+G(d) in the gas phase.

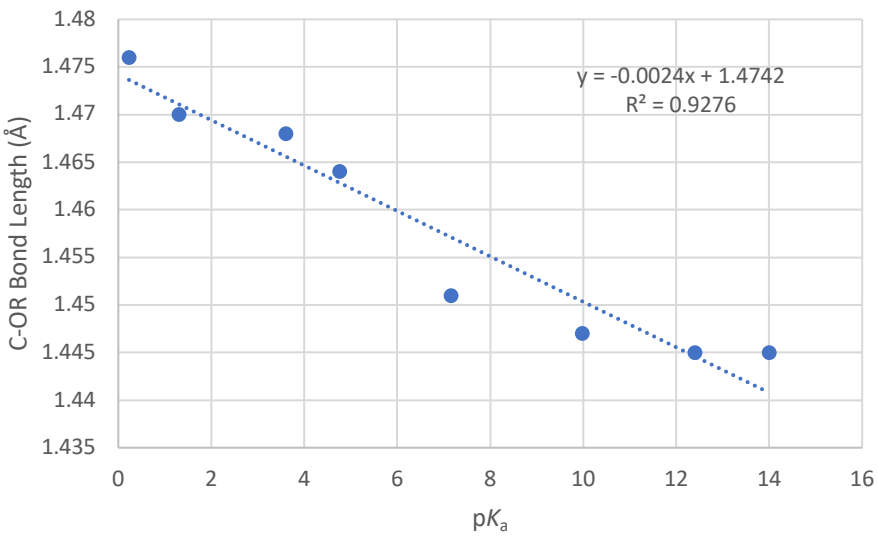


Figure S 44. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **5**, calculated at MP2/6-31+G(d) in the gas phase.

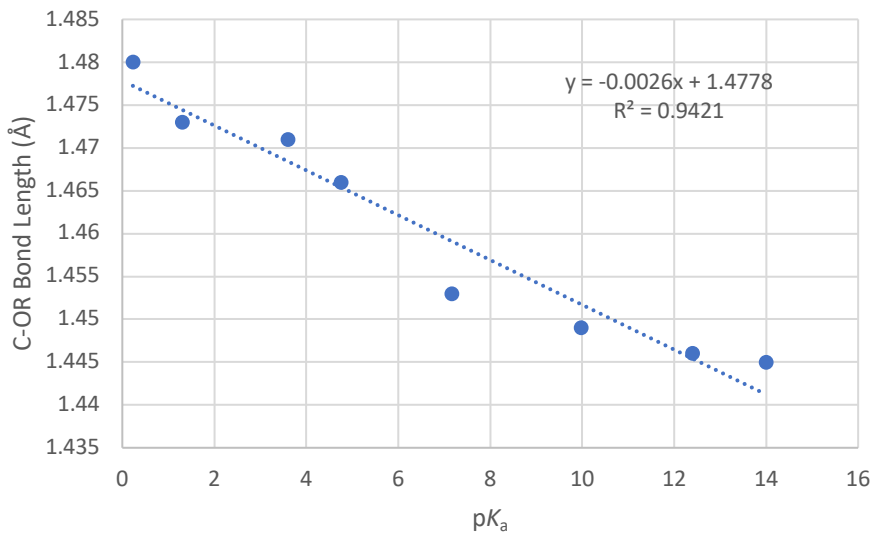


Figure S 45. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **6**, calculated at MP2/6-31+G(d) in the gas phase.

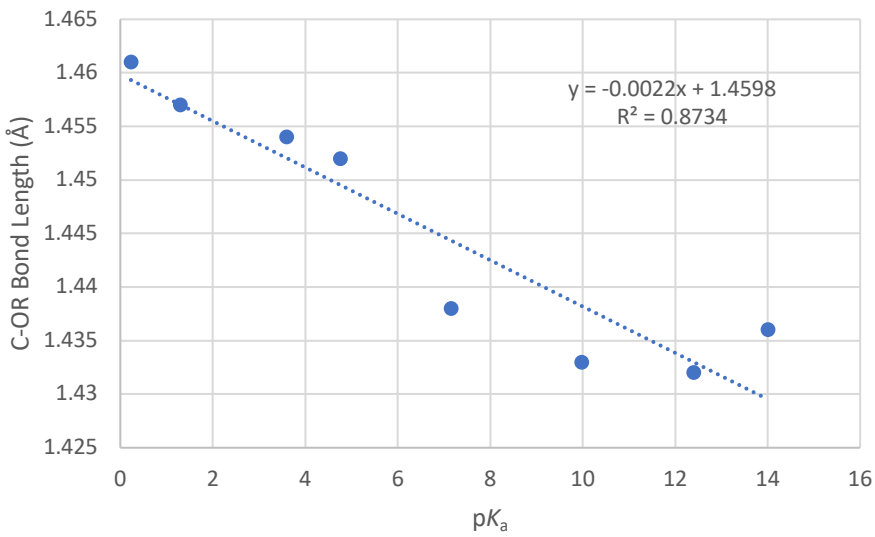


Figure S 46. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **7**, calculated at MP2/6-31+G(d) in the gas phase.

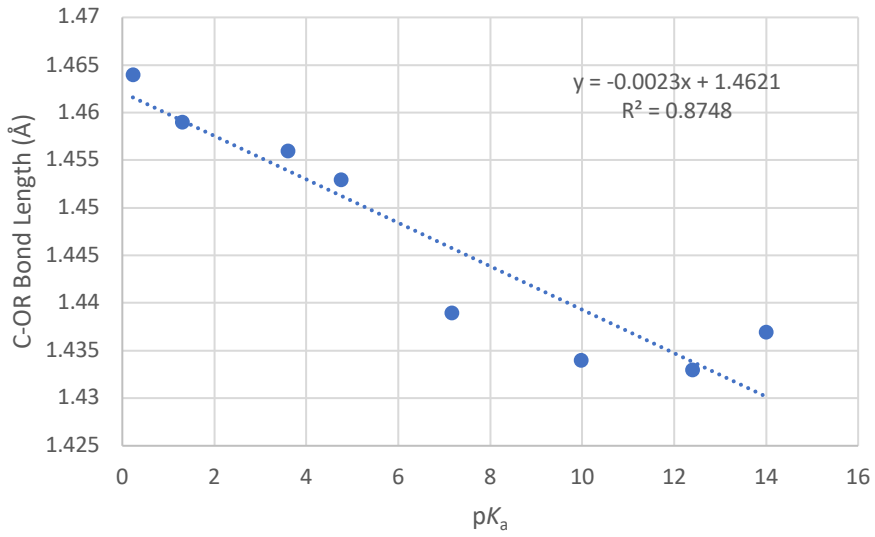


Figure S 47. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **8**, calculated at MP2/6-31+G(d) in the gas phase.

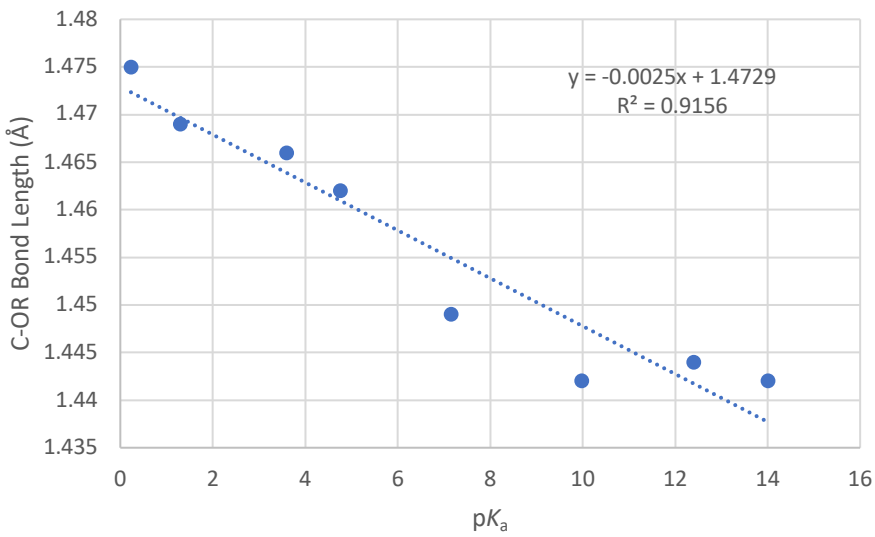


Figure S 48. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **9**, calculated at MP2/6-31+G(d) in the gas phase.

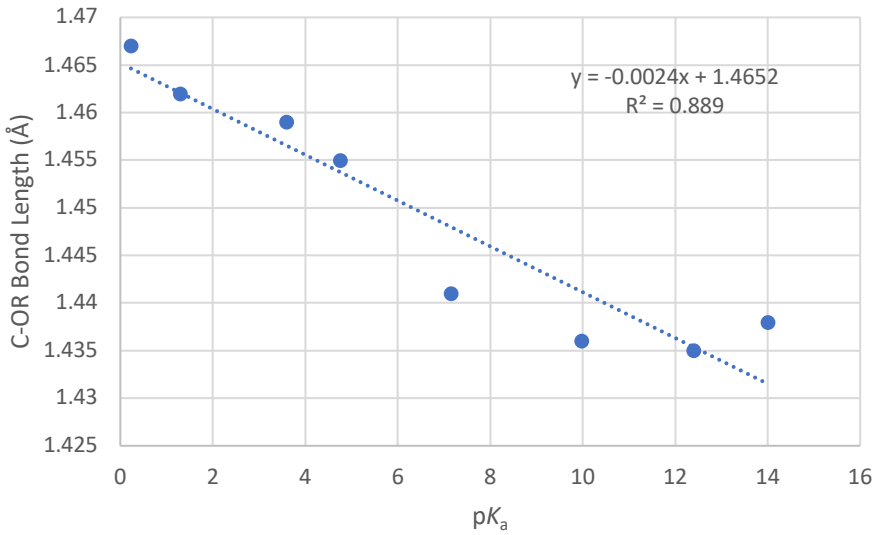


Figure S 49. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **10**, calculated at MP2/6-31+G(d) in the gas phase.

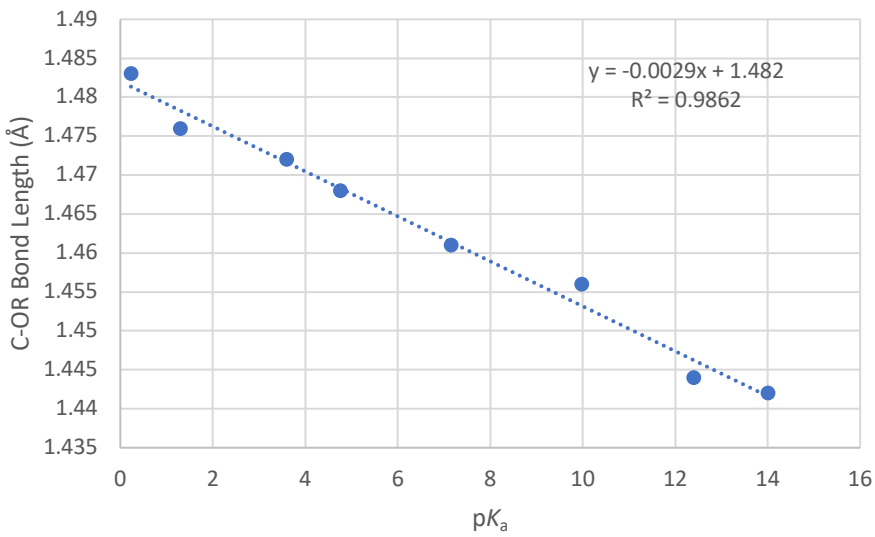


Figure S 50. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **11**, calculated at MP2/6-31+G(d) in the gas phase.

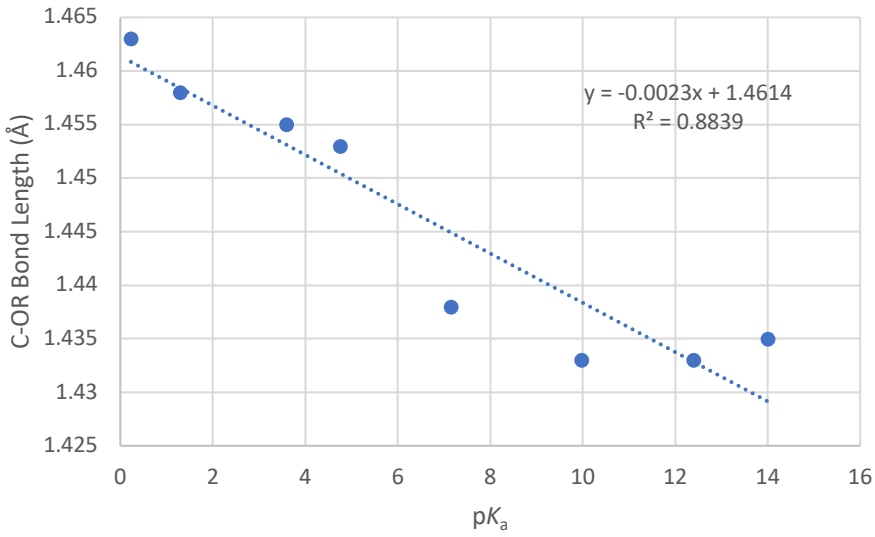


Figure S 51. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **12**, calculated at MP2/6-31+G(d) in the gas phase.

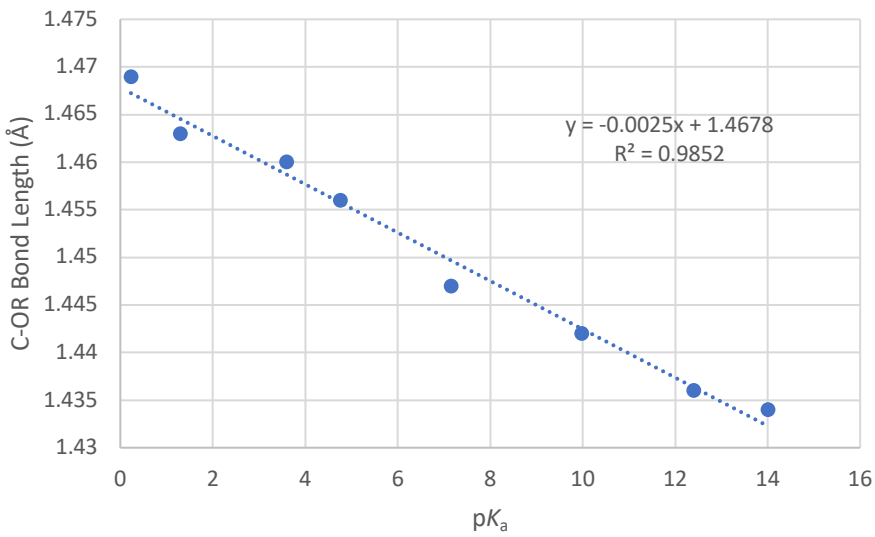


Figure S 52. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **13**, calculated at MP2/6-31+G(d) in the gas phase.

Table S 17. pK_a values for selected substituents and corresponding C-O bond lengths (Å) in systems **1**, **6**, **7** and **11** calculated at B3LYP/6-311++G(d,p) in various solvents with the PCM model

Substituent	pK_a	1-Me_2CO	6-Me_2CO	7-Me_2CO	11-Me_2CO	1-MeCN	6-MeCN
ROH	14	1.422	1.446	1.436	1.446	1.422	1.446
$ROCOCH_3$	4.76	1.461	1.471	1.454	1.476	1.462	1.471
$ROCOCF_3$	0.23	1.500	1.493	1.469	1.502	1.500	1.493
ROC(O)OH	3.6	1.471	1.477	1.458	1.484	1.472	1.477
ROPh	9.98	1.434	1.452	1.435	1.457	1.434	1.452
$ROCH_2CF_3$	12.4	1.430	1.451	1.434	1.451	1.430	1.451
$ROCOCHCl_2$	1.3	1.485	1.484	1.463	1.492	1.485	1.484
ROPh-p-NO_2	7.16	1.451	1.462	1.445	1.470	1.452	1.463

Substituent	7-MeCN	11-MeCN	1-DMSO	6-DMSO	7-DMSO	11-DMSO
ROH	1.436	1.446	1.422	1.446	1.436	1.447
$ROCOCH_3$	1.454	1.477	1.462	1.471	1.454	1.477
$ROCOCF_3$	1.469	1.503	1.500	1.493	1.469	1.503
ROC(O)OH	1.458	1.484	1.472	1.477	1.458	1.484
ROPh	1.436	1.458	1.435	1.452	1.436	1.458
$ROCH_2CF_3$	1.435	1.452	1.430	1.451	1.435	1.452
$ROCOCHCl_2$	1.463	1.493	1.485	1.484	1.463	1.493
ROPh-p-NO_2	1.445	1.470	1.452	1.463	1.445	1.470

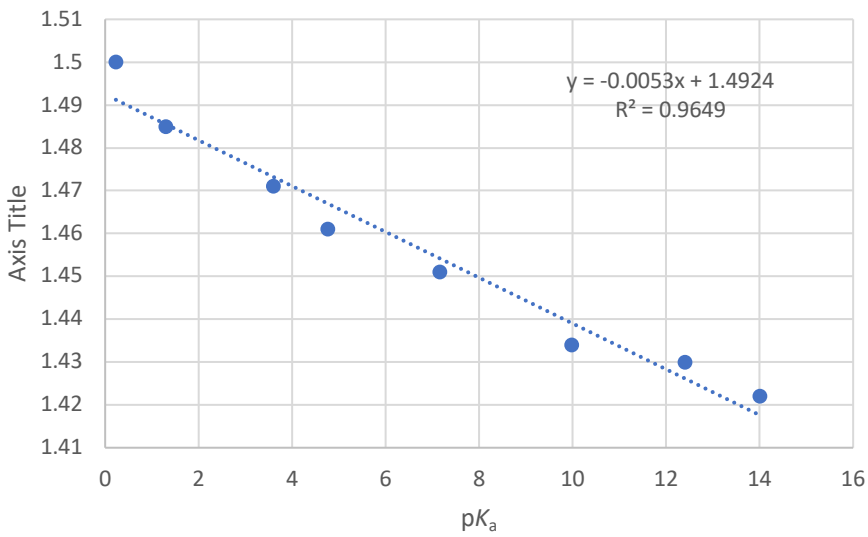


Figure S 53. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **1**, calculated at B3LYP/6-311++G(d,p) in acetone with the PCM model.

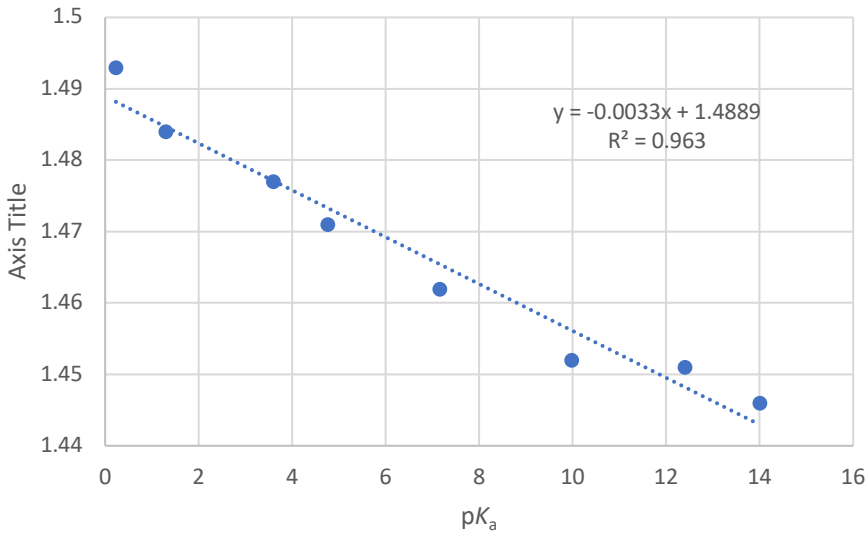


Figure S 54. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **6**, calculated at B3LYP/6-311++G(d,p) in acetone with the PCM model.

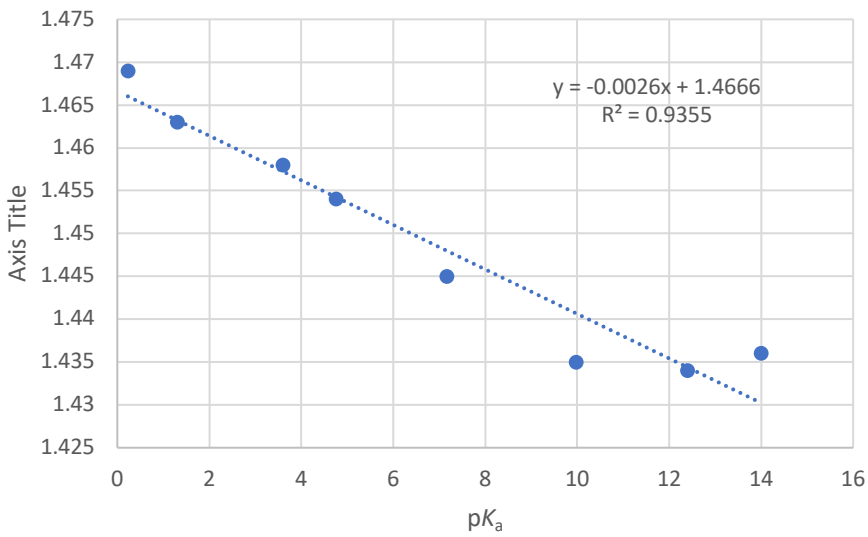


Figure S 55. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **7**, calculated at B3LYP/6-311++G(d,p) in acetone with the PCM model.

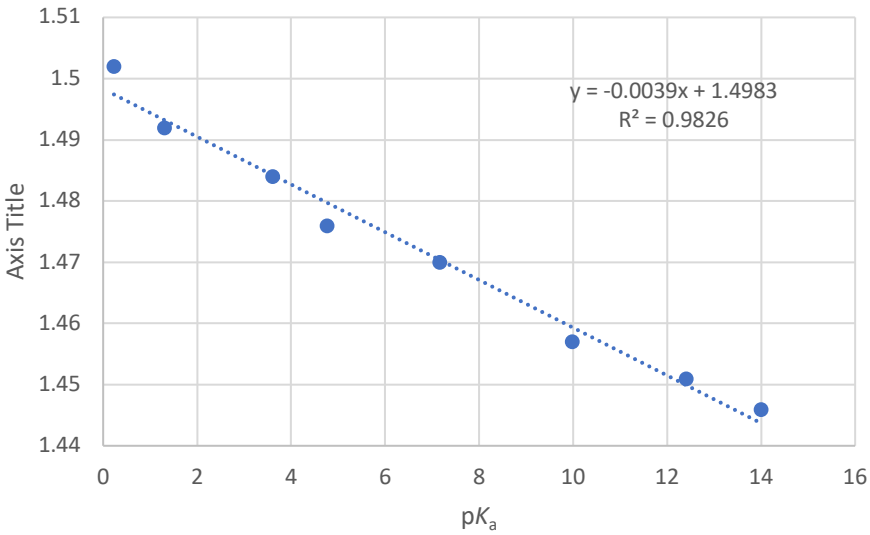


Figure S 56. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **11**, calculated at B3LYP/6-311++G(d,p) in acetone with the PCM model.

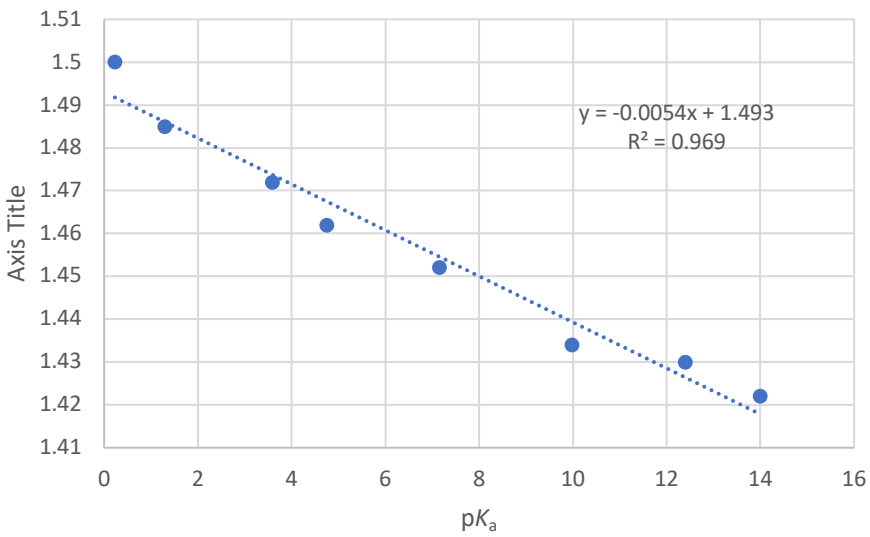


Figure S 57. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **1**, calculated at B3LYP/6-311++G(d,p) in acetonitrile with the PCM model.

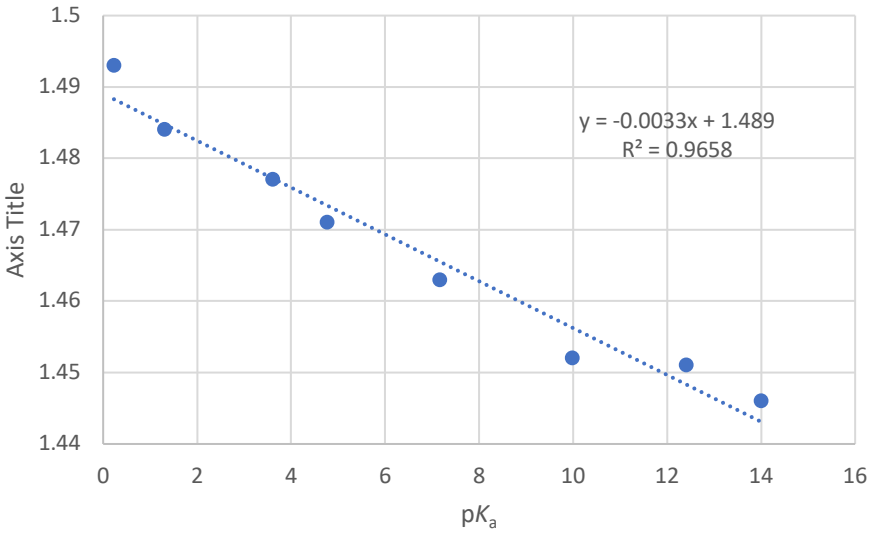


Figure S 58. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **6**, calculated at B3LYP/6-311++G(d,p) in acetonitrile with the PCM model.

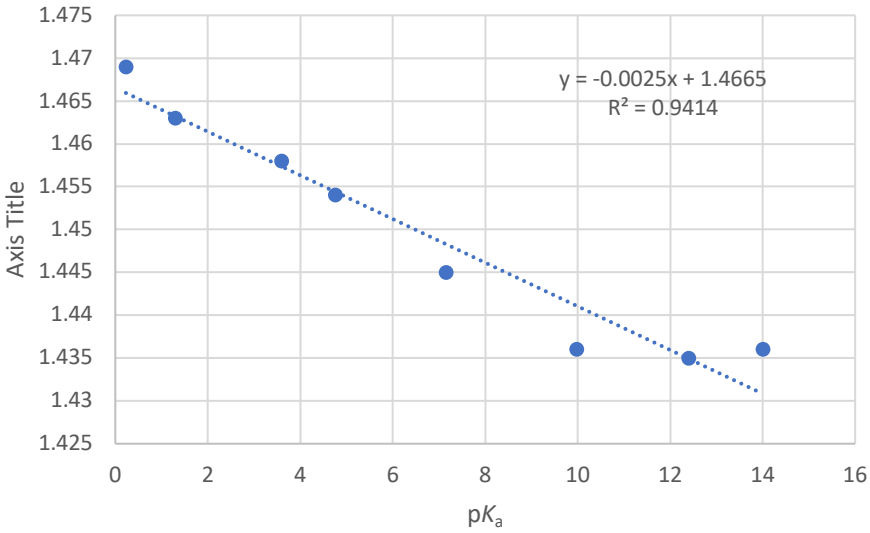


Figure S 59. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **7**, calculated at B3LYP/6-311++G(d,p) in acetonitrile with the PCM model.

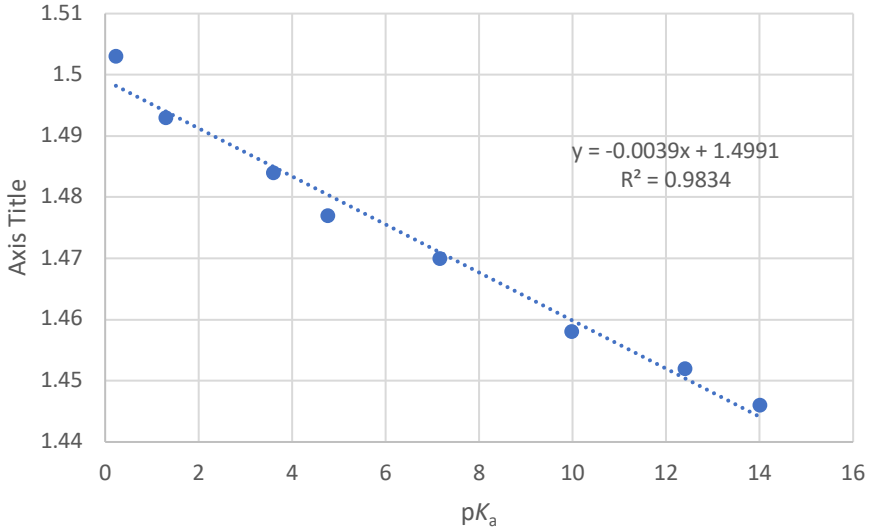


Figure S 60. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **11**, calculated at B3LYP/6-311++G(d,p) in acetonitrile with the PCM model.

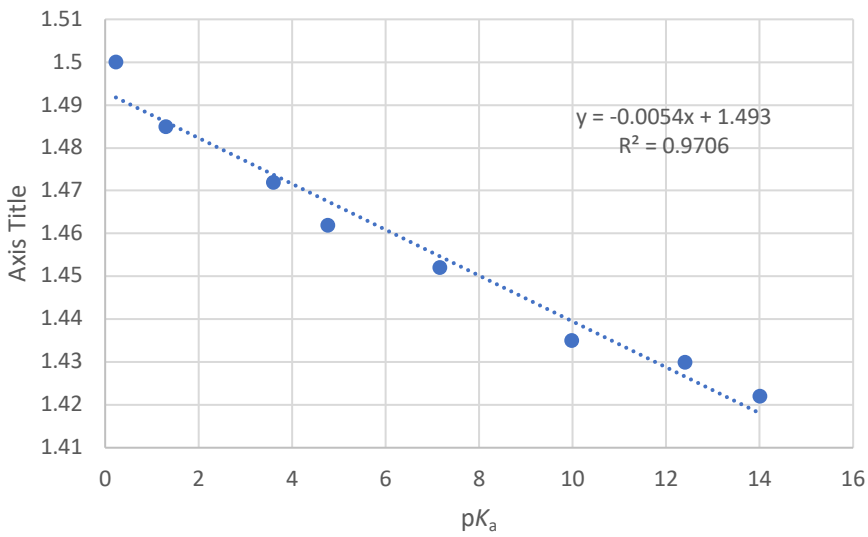


Figure S 61. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **1**, calculated at B3LYP/6-311++G(d,p) in dimethyl sulfoxide with the PCM model.

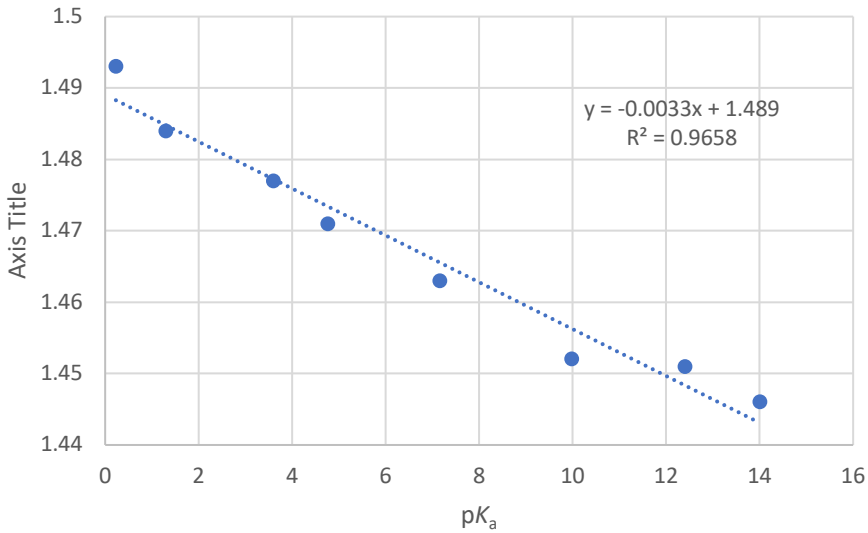


Figure S 62. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **6**, calculated at B3LYP/6-311++G(d,p) in dimethyl sulfoxide with the PCM model.

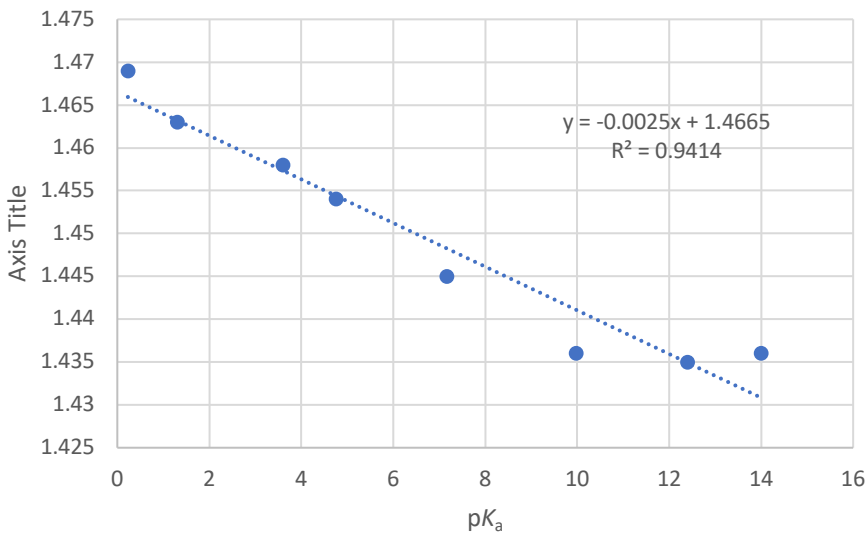


Figure S 63. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **7**, calculated at B3LYP/6-311++G(d,p) in dimethyl sulfoxide with the PCM model.

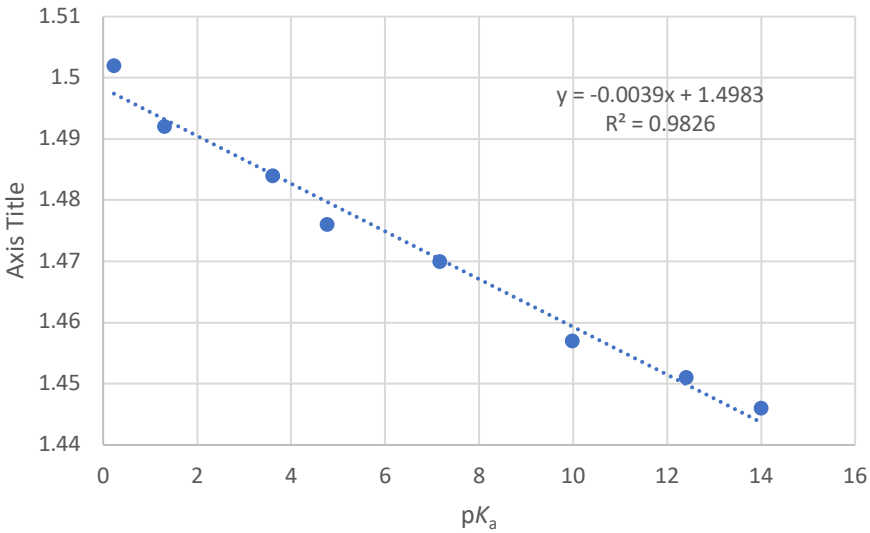


Figure S 64. Theoretical variable oxygen probe plot of C-OR bond length (Å) against pK_a of the corresponding acid (ROH) for **11**, calculated at B3LYP/6-311++G(d,p) in dimethyl sulfoxide with the PCM model.

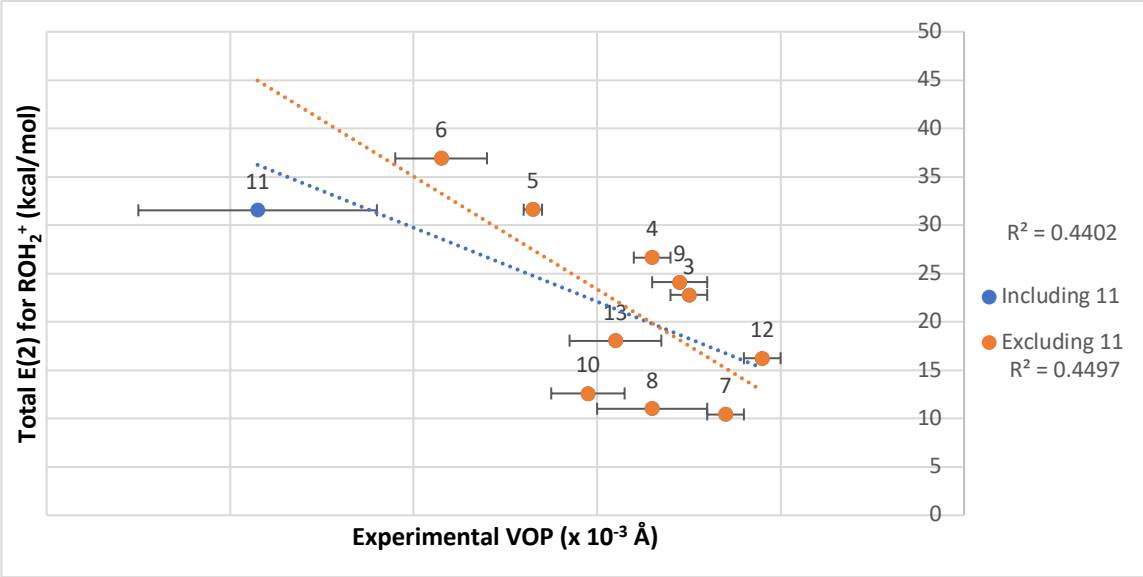


Figure S 65. Plot of total NBO interactions (kcal/mol, M06-2X/6-311++G(d,p)) for **3-13**.OH_2^+ *vs* experimental Variable Oxygen Probe slope ($\times 10^{-3}$ Å) with (blue, R^2=0.44) and without (orange, R^2 = 0.45) **11**.OH_2^+.

NBO Data

Donors into the C-X σ* antibonding orbital (X = OH, $OCOCF_3$, OH_2^+ or NH_3^+) are provided below. Sum of E(2) energies (kcal/mol) of these donor-acceptor interactions give total donations recorded in **Tables 1-3** in the main text. Note that E_j-E_i (a.u) refers to the energy difference between the donor and acceptor orbitals and $F_{i,j}$ (a.u) refers to the Fock matrix overlap of the donor and acceptor orbitals.

<u>For Table 1 (ROH): B3LYP/6-311++G(d,p)</u>

1_OH	Donor	Acceptor	E(2)	Ej-Ei	Fi,j
	8. LP (1) O 15	38. BD*(1) C 3- O 16	0.54	0.77	0.018
	9. LP (2) O 15		13.64	0.58	0.08
	17. BD (1) C 2- H 7		4.16	0.75	0.05
	18. BD (1) C 2- H 8		0.73	0.75	0.021
2_OH	26. BD (1) C 3- H 7	61. BD*(1) C 4- O 30	1.64	0.72	0.031
	27. BD (1) C 3-Si 17		4.05	0.67	0.047
	32. BD (1) C 5- H 13		0.77	0.74	0.021
	33. BD (1) C 5- H 14		4.72	0.74	0.053
3_OH	11. BD (1) C 1- C 6	35. BD*(1) C 2- O 18	2.65	0.8	0.041
	12. BD (1) C 1- H 9		0.69	0.74	0.02
	13. BD (1) C 1- H 10		0.55	0.74	0.018
	17. BD (1) C 3- C 4		3.03	0.81	0.044
	19. BD (1) C 3- H 17		0.63	0.75	0.019

4_OH	15. BD (1) C 2- H 7	37. BD*(1) C 3- O 15	4.33	0.74	0.05
	16. BD (1) C 2- H 8		0.86	0.74	0.022
	27. BD (1) C 17- H 18		0.72	0.75	0.021
	28. BD (1) C 17- H 19		4.87	0.74	0.054
5_OH	20. LP (2) S 17	69. BD*(1) C 4- O 29	1.21	0.51	0.022
	31. BD (1) C 3- H 7		1.02	0.75	0.025
	32. BD (1) C 3- S 17		3	0.77	0.043
	37. BD (1) C 5- H 13		0.73	0.74	0.021
	38. BD (1) C 5- H 14		4.97	0.74	0.054
6_OH	31. LP (2)Se 30	78. BD*(1) C 4- O 28	1.15	0.5	0.021
	40. BD (1) C 3- H 7		1.01	0.75	0.025
	41. BD (1) C 3-Se 30		3.79	0.71	0.046
	46. BD (1) C 5- H 13		0.76	0.74	0.021
	47. BD (1) C 5- H 14		4.94	0.73	0.054
7_OH	7. BD (1) C 1- H 2	24. BD*(1) C 4- O 11	0.63	0.74	0.019
	8. BD (1) C 1- H 3		0.63	0.74	0.019
	10. BD (1) C 1- C 7		2.48	0.81	0.04
8_OH	33. BD (1) C 8- C 9	81. BD*(1) C 22- O 25	2.59	0.75	0.039
9_OH	17. BD (1) C 2- C 3	52. BD*(1) C 4- O 25	1.06	0.79	0.026
	21. BD (1) C 3- H 7		1.04	0.75	0.025
	22. BD (1) C 3- H 15		2.29	0.75	0.037
	26. BD (1) C 5- C 6		3.69	0.76	0.047
	27. BD (1) C 5- H 12		0.57	0.75	0.018
10_OH	9. BD (1) C 1- C 3	32. BD*(1) C 9- O 12	3.19	0.75	0.044
	12. BD (1) C 2- C 3		0.69	0.75	0.02
11_OH	12. BD (1) C 1- C 3	43. BD*(1) C 9- O 19	3.23	0.77	0.044
	15. BD (1) C 2- C 3		0.81	0.76	0.022
	23. BD (1) C 11- C 12		3.03	0.76	0.043
	24. BD (1) C 11- C 13		0.86	0.75	0.023
12_OH	10. BD (3) C 1- C 3	23. BD*(1) C 4- O 7	5.98	0.56	0.052
13_OH	20. BD (1) C 1- C 2	72. BD*(1) C 4- O 30	0.91	0.79	0.024
	22. BD (1) C 1- H 5		0.77	0.75	0.022
	23. BD (1) C 1- H 6		2.26	0.75	0.037
	30. BD (1) C 3- C 20		2.9	0.82	0.043
	47. BD (2) C 20- C 21		0.73	0.54	0.018

For Table 1 (ROH): M06-2X/6-311++G(d,p)

1_OH	Donor	Acceptor	E(2)	Ej-Ei	Fi,j
	8. LP (1) O 15	38. BD*(1) C 3- O 16	0.68	0.94	0.023
	9. LP (2) O 15		15.57	0.74	0.096
	17. BD (1) C 2- H 7		4.6	0.9	0.057
	18. BD (1) C 2- H 8		0.8	0.9	0.024
2_OH	26. BD (1) C 3- H 7	61. BD*(1) C 4- O 30	1.82	0.87	0.036
	27. BD (1) C 3-Si 17		4.87	0.82	0.056
	32. BD (1) C 5- H 13		0.97	0.9	0.026
	33. BD (1) C 5- H 14		5.08	0.89	0.06
3_OH	11. BD (1) C 1- C 6	35. BD*(1) C 2- O 18	2.99	0.96	0.048
	12. BD (1) C 1- H 9		0.8	0.9	0.024
	13. BD (1) C 1- H 10		0.73	0.9	0.023
	17. BD (1) C 3- C 4		3.43	0.96	0.051
	18. BD (1) C 3- H 7		0.6	0.91	0.021
	19. BD (1) C 3- H 17		0.73	0.9	0.023
4_OH	15. BD (1) C 2- H 7	37. BD*(1) C 3- O 15	4.77	0.89	0.058
	16. BD (1) C 2- H 8		0.95	0.89	0.026
	27. BD (1) C 17- H 18		0.8	0.9	0.024
	28. BD (1) C 17- H 19		5.38	0.89	0.062
5_OH	20. LP (2) S 17	69. BD*(1) C 4- O 29	1.14	0.65	0.024
	31. BD (1) C 3- H 7		1.09	0.91	0.028
	32. BD (1) C 3- S 17		3.24	0.93	0.049
	37. BD (1) C 5- H 13		0.81	0.89	0.024
	38. BD (1) C 5- H 14		5.51	0.89	0.062
6_OH	31. LP (2)Se 30	78. BD*(1) C 4- O 28	1.15	0.63	0.024
	40. BD (1) C 3- H 7		1.11	0.91	0.028
	41. BD (1) C 3-Se 30		4.03	0.87	0.053
	46. BD (1) C 5- H 13		0.85	0.89	0.025
	47. BD (1) C 5- H 14		5.45	0.89	0.062
7_OH	7. BD (1) C 1- H 2	24. BD*(1) C 4- O 11	0.76	0.89	0.023
	8. BD (1) C 1- H 3		0.76	0.89	0.023
	10. BD (1) C 1- C 7		2.8	0.96	0.046
8_OH	30. BD (1) C 4- C 8	81. BD*(1) C 22- O 25	0.54	0.9	0.02
	33. BD (1) C 8- C 9		2.61	0.91	0.044
	34. BD (1) C 8- C 13		0.54	0.9	0.02
9_OH	17. BD (1) C 2- C 3	52. BD*(1) C 4- O 25	0.84	0.95	0.025
	21. BD (1) C 3- H 7		1.84	0.9	0.036

	22. BD (1) C 3- H 15		2.68	0.9	0.044
	26. BD (1) C 5- C 6		4.11	0.92	0.055
	27. BD (1) C 5- H 12		0.61	0.9	0.021
	29. BD (1) C 6- H 13		0.51	0.91	0.019
10_OH	9. BD (1) C 1- C 3	32. BD*(1) C 9- O 12	3.61	0.9	0.051
	12. BD (1) C 2- C 3		0.98	0.9	0.027
11_OH	12. BD (1) C 1- C 3	43. BD*(1) C 9- O 19	3.83	0.92	0.053
	15. BD (1) C 2- C 3		1.02	0.92	0.027
	23. BD (1) C 11- C 12		3.62	0.91	0.051
	24. BD (1) C 11- C 13		1.05	0.91	0.028
12_OH	10. BD (3) C 1- C 3	23. BD*(1) C 4- O 7	6.33	0.71	0.06
13_OH	20. BD (1) C 1- C 2	72. BD*(1) C 4- O 30	1.1	0.94	0.029
	22. BD (1) C 1- H 5		1.25	0.91	0.03
	23. BD (1) C 1- H 6		2.51	0.91	0.043
	28. BD (1) C 3- H 8		0.66	0.91	0.022
	30. BD (1) C 3- C 20		2.79	0.97	0.046
	47. BD (2) C 20- C 21		0.78	0.66	0.02

<u>For Table 2 (ROH2+): B3LYP/6-311++G(d,p)</u>

	Donor	Acceptor	E(2)	Ej-Ei	Fi,j
3_OH$_2^+$	10. BD (1) C 1- C 6	35. BD*(1) C 2- O 18	7.81	0.53	0.057
	11. BD (1) C 1- H 9		1.34	0.49	0.023
	12. BD (1) C 1- H 10		0.79	0.5	0.018
	14. BD (1) C 2- H 8		0.75	0.56	0.018
	16. BD (1) C 3- C 4		7.82	0.53	0.057
	17. BD (1) C 3- H 7		0.8	0.5	0.018
	18. BD (1) C 3- H 17		1.34	0.49	0.023
	21. BD (1) C 4- H 12		0.62	0.46	0.015
	26. BD (1) C 6- H 16		0.62	0.46	0.015
4_OH$_2^+$	14. BD (1) C 2- H 7	37. BD*(1) C 3- O 15	11.45	0.48	0.066
	15. BD (1) C 2- H 8		1.69	0.49	0.026
	16. BD (1) C 3- H 6		0.82	0.55	0.019
	27. BD (1) C 17- H 18		1.69	0.49	0.026
	28. BD (1) C 17- H 19		11.45	0.48	0.066
7_OH$_2^+$	6. BD (1) C 1- H 2	24. BD*(1) C 4- O 11	1.05	0.53	0.021
	7. BD (1) C 1- H 3		0.98	0.53	0.02
	9. BD (1) C 1- C 7		6.17	0.57	0.053
	10. BD (1) C 4- H 5		0.58	0.6	0.017
	14. BD (1) C 7- H 9		0.71	0.5	0.017
9_OH$_2^+$	16. BD (1) C 2- C 3	52. BD*(1) C 4- O 25	0.94	0.54	0.02
	20. BD (1) C 3- H 7		5.63	0.5	0.047

	21. BD (1) C 3- H 15		4.14	0.51	0.041
	25. BD (1) C 5- C 6		10.02	0.5	0.063
	27. BD (1) C 5- C 16		1.05	0.51	0.021
	28. BD (1) C 6- H 13		1.11	0.49	0.021
	29. BD (1) C 6- H 14		0.57	0.48	0.015
10_OH$_2^+$	8. BD (1) C 1- C 3	32. BD*(1) C 9- O 12	10.05	0.49	0.062
	11. BD (1) C 2- C 3		2.4	0.5	0.031
	17. BD (1) C 9- H 11		0.71	0.57	0.018
12_OH$_2^+$	9. BD (3) C 1- C 3	23. BD*(1) C 4- O 7	17.31	0.33	0.068
	12. BD (1) C 4- H 6		0.6	0.59	0.017
13_OH$_2^+$	19. BD (1) C 1- C 2	72. BD*(1) C 4- O 30	0.9	0.57	0.02
	21. BD (1) C 1- H 5		3.93	0.54	0.041
	22. BD (1) C 1- H 6		3.68	0.55	0.04
	28. BD (1) C 3- C 10		1.14	0.59	0.023
	29. BD (1) C 3- C 20		5.09	0.58	0.049
	46. BD (2) C 20- C 21		1.93	0.28	0.021

For Table 2 (ROH$_2^+$): M06-2X/6-311++G(d,p)

	Donor	**Acceptor**	**E(2)**	**Ej-Ei**	**Fi,j**
3_OH$_2^+$	10. BD (1) C 1- C 6	35. BD*(1) C 2- O 18	7.9	0.7	0.067
	11. BD (1) C 1- H 9		1.44	0.66	0.028
	12. BD (1) C 1- H 10		1.05	0.67	0.024
	14. BD (1) C 2- H 8		0.66	0.73	0.019
	16. BD (1) C 3- C 4		7.91	0.7	0.067
	17. BD (1) C 3- H 7		1.05	0.67	0.024
	18. BD (1) C 3- H 17		1.43	0.66	0.028
	21. BD (1) C 4- H 12		0.67	0.63	0.018
	26. BD (1) C 6- H 16		0.67	0.63	0.018
4_OH$_2^+$	14. BD (1) C 2- H 7	37. BD*(1) C 3- O 15	11.25	0.65	0.076
	15. BD (1) C 2- H 8		1.7	0.66	0.03
	16. BD (1) C 3- H 6		0.76	0.72	0.021
	27. BD (1) C 17- H 18		1.7	0.66	0.03
	28. BD (1) C 17- H 19		11.24	0.65	0.076
5_OH$_2^+$	20. LP (2) S 17	69. BD*(1) C 4- O 29	5.18	0.37	0.039
	30. BD (1) C 3- H 7		1.93	0.66	0.032
	31. BD (1) C 3- S 17		10.17	0.65	0.072
	33. BD (1) C 4- H 12		0.69	0.7	0.02
	36. BD (1) C 5- H 13		1.95	0.65	0.032
	37. BD (1) C 5- H 14		11.68	0.63	0.077
6_OH$_2^+$	30. LP (2)Se 31	78. BD*(1) C 4- O 28	5.74	0.33	0.039
	39. BD (1) C 3- H 7		2.01	0.64	0.032
	40. BD (1) C 3-Se 31		14.32	0.58	0.081

	42. BD (1) C 4- H 12		0.74	0.68	0.02
	45. BD (1) C 5- H 13		2.14	0.63	0.033
	46. BD (1) C 5- H 14		11.96	0.61	0.076
7_OH$_2^+$	6. BD (1) C 1- H 2	24. BD*(1) C 4- O 11	1.26	0.69	0.026
	7. BD (1) C 1- H 3		1.17	0.69	0.025
	9. BD (1) C 1- C 7		6.65	0.74	0.062
	10. BD (1) C 4- H 5		0.55	0.76	0.018
	14. BD (1) C 7- H 9		0.8	0.66	0.02
8_OH$_2^+$	29. BD (1) C 4- C 8	81. BD*(1) C 22- O 25	1.38	0.68	0.027
	32. BD (1) C 8- C 9		8.27	0.67	0.066
	33. BD (1) C 8- C 13		0.74	0.68	0.02
	48. BD (1) C 22- H 24		0.63	0.74	0.019
9_OH$_2^+$	16. BD (1) C 2- C 3	52. BD*(1) C 4- O 25	1.11	0.72	0.025
	20. BD (1) C 3- H 7		5.07	0.67	0.052
	21. BD (1) C 3- H 15		4.64	0.69	0.05
	25. BD (1) C 5- C 6		9.69	0.68	0.072
	26. BD (1) C 5- H 12		0.67	0.68	0.019
	27. BD (1) C 5- C 16		1.17	0.69	0.025
	28. BD (1) C 6- H 13		1.12	0.67	0.024
	29. BD (1) C 6- H 14		0.63	0.66	0.018
10_OH$_2^+$	8. BD (1) C 1- C 3	32. BD*(1) C 9- O 12	8.81	0.67	0.069
	11. BD (1) C 2- C 3		3.18	0.67	0.041
	17. BD (1) C 9- H 11		0.61	0.75	0.019
11_OH$_2^+$	11. BD (1) C 1- C 3	43. BD*(1) C 9- O 19	11.46	0.61	0.075
	13. BD (1) C 1- H 5		0.53	0.62	0.016
	14. BD (1) C 2- C 3		3.33	0.62	0.041
	19. BD (1) C 9- H 10		0.88	0.68	0.022
	22. BD (1) C 11- C 12		11.48	0.61	0.075
	23. BD (1) C 11- C 13		3.33	0.62	0.041
	26. BD (1) C 12- H 15		0.53	0.62	0.016
12_OH$_2^+$	9. BD (3) C 1- C 3	23. BD*(1) C 4- O 7	15.72	0.49	0.078
	12. BD (1) C 4- H 6		0.52	0.76	0.018
13_OH$_2^+$	19. BD (1) C 1- C 2	72. BD*(1) C 4- O 30	0.84	0.73	0.022
	21. BD (1) C 1- H 5		4.16	0.7	0.048
	22. BD (1) C 1- H 6		4.12	0.71	0.048
	27. BD (1) C 3- H 8		0.58	0.7	0.018
	28. BD (1) C 3- C 10		1.34	0.76	0.028
	29. BD (1) C 3- C 20		5.23	0.75	0.056
	46. BD (2) C 20- C 21		1.79	0.42	0.024

For Table 3 (RNH_3^+): B3LYP/6-311++G(d,p)

1_NH_3^+	9. LP (2) O 15	38. BD*(1) C 3- N 16	25.45	0.44	0.094
	15. BD (1) C 2- H 7		6.51	0.58	0.055
	16. BD (1) C 2- H 8		1.07	0.6	0.023
	19. BD (1) C 3- N 16		0.54	0.77	0.018
2_NH_3^+	24. BD (1) C 3- H 7	61. BD*(1) C 4- N 30	1.68	0.62	0.029
	25. BD (1) C 3-Si 17		7.35	0.54	0.056
	30. BD (1) C 5- H 13		0.91	0.64	0.021
	31. BD (1) C 5- H 14		6.13	0.63	0.055
3_NH_3^+	9. BD (1) C 1- C 6	35. BD*(1) C 2- N 18	4.22	0.69	0.048
	10. BD (1) C 1- H 9		0.73	0.65	0.019
	11. BD (1) C 1- H 10		0.53	0.65	0.017
	15. BD (1) C 3- C 4		4.22	0.69	0.048
	16. BD (1) C 3- H 7		0.53	0.65	0.017
	17. BD (1) C 3- H 17		0.73	0.65	0.019
4_NH_3^+	13. BD (1) C 2- H 7	38. BD*(1) C 3- N 18	6.2	0.64	0.056
	14. BD (1) C 2- H 8		0.9	0.65	0.022
	24. BD (1) C 15- H 16		0.9	0.65	0.022
	25. BD (1) C 15- H 17		6.2	0.64	0.056
5_NH_3^+	20. LP (2) S 17	69. BD*(1) C 4- N 29	2.04	0.38	0.025
	29. BD (1) C 3- H 7		1.09	0.66	0.024
	30. BD (1) C 3- S 17		5.02	0.65	0.051
	35. BD (1) C 5- H 13		0.94	0.64	0.022
	36. BD (1) C 5- H 14		6.33	0.63	0.056
6_NH_3^+	29. LP (2)Se 28	78. BD*(1) C 4- N 29	1.9	0.36	0.023
	38. BD (1) C 3- H 7		1.1	0.65	0.024
	39. BD (1) C 3-Se 28		6.41	0.59	0.055
	44. BD (1) C 5- H 13		0.97	0.64	0.022
	45. BD (1) C 5- H 14		6.33	0.62	0.056
7_NH_3^+	5. BD (1) C 1- H 2	24. BD*(1) C 4- N 11	0.61	0.65	0.018
	6. BD (1) C 1- H 3		0.61	0.65	0.018
	8. BD (1) C 1- C 7		3.9	0.7	0.047
8_NH_3^+	31. BD (1) C 8- C 9	81. BD*(1) C 22- N 25	4.49	0.64	0.048
9_NH_3^+	15. BD (1) C 2- C 3	52. BD*(1) C 4- N 25	1.29	0.69	0.027
	19. BD (1) C 3- H 7		1.29	0.65	0.026
	20. BD (1) C 3- H 15		2.55	0.66	0.037
	24. BD (1) C 5- C 6		5.64	0.66	0.054
	25. BD (1) C 5- H 12		0.55	0.66	0.017

	27. BD (1) C 6- H 13		0.74	0.64	0.019
10_NH_3^+	7. BD (1) C 1- C 3	32. BD*(1) C 9- N 12	4.85	0.64	0.05
	10. BD (1) C 2- C 3		1.1	0.65	0.024
11_NH_3^+	10. BD (1) C 1- C 3	43. BD*(1) C 9- N 19	4.9	0.63	0.05
	13. BD (1) C 2- C 3		1.23	0.64	0.025
	21. BD (1) C 11- C 12		4.9	0.63	0.05
	22. BD (1) C 11- C 13		1.23	0.64	0.025
12_NH_3^+	8. BD (3) C 1- C 3	23. BD*(1) C 4- N 7	8.39	0.46	0.055
13_NH_3^+	18. BD (1) C 1- C 2	72. BD*(1) C 4- N 30	0.9	0.69	0.022
	20. BD (1) C 1- H 5		1.76	0.66	0.03
	21. BD (1) C 1- H 6		2.26	0.67	0.035
	28. BD (1) C 3- C 20		3.7	0.7	0.046
	45. BD (2) C 20- C 21		1.12	0.41	0.019

For Table 3 (RNH_3^+): M06-2X/6-311++G(d,p)

1_NH_3^+	9. LP (2) O 15	38. BD*(1) C 3- N 16	27.29	0.6	0.114
	15. BD (1) C 2- H 7		7.22	0.73	0.065
	16. BD (1) C 2- H 8		1.11	0.75	0.026
2_NH_3^+	24. BD (1) C 3- H 7	61. BD*(1) C 4- N 30	1.92	0.76	0.034
	25. BD (1) C 3-Si 17		8.79	0.68	0.069
	30. BD (1) C 5- H 13		1.16	0.78	0.027
	31. BD (1) C 5- H 14		6.61	0.77	0.064
3_NH_3^+	9. BD (1) C 1- C 6	35. BD*(1) C 2- N 18	4.87	0.83	0.057
	10. BD (1) C 1- H 9		0.83	0.79	0.023
	11. BD (1) C 1- H 10		0.7	0.79	0.021
	15. BD (1) C 3- C 4		4.88	0.83	0.057
	16. BD (1) C 3- H 7		0.7	0.79	0.021
	17. BD (1) C 3- H 17		0.83	0.79	0.023
4_NH_3^+	13. BD (1) C 2- H 7	38. BD*(1) C 3- N 18	6.97	0.78	0.066
	14. BD (1) C 2- H 8		0.99	0.79	0.025
	24. BD (1) C 15- H 16		1	0.79	0.025
	25. BD (1) C 15- H 17		6.98	0.78	0.066
5_NH_3^+	20. LP (2) S 17	69. BD*(1) C 4- N 29	2.15	0.51	0.029
	29. BD (1) C 3- H 7		1.17	0.8	0.027
	30. BD (1) C 3- S 17		5.6	0.8	0.06
	35. BD (1) C 5- H 13		1.05	0.79	0.026

	36. BD (1) C 5- H 14		7.12	0.77	0.066
6_NH$_3^+$	29. LP (2)Se 28	78. BD*(1) C 4- N 29	1.98	0.49	0.028
	38. BD (1) C 3- H 7		1.21	0.8	0.028
	39. BD (1) C 3-Se 28		6.94	0.74	0.064
	44. BD (1) C 5- H 13		1.09	0.78	0.026
	45. BD (1) C 5- H 14		7.07	0.77	0.066
7_NH$_3^+$	5. BD (1) C 1- H 2	24. BD*(1) C 4- N 11	0.74	0.79	0.022
	6. BD (1) C 1- H 3		0.74	0.79	0.022
	8. BD (1) C 1- C 7		4.51	0.84	0.055
	13. BD (1) C 7- H 9		0.54	0.76	0.018
8_NH$_3^+$	28. BD (1) C 4- C 8	81. BD*(1) C 22- N 25	0.63	0.79	0.02
	31. BD (1) C 8- C 9		4.51	0.78	0.053
	32. BD (1) C 8- C 13		0.67	0.79	0.02
9_NH$_3^+$	15. BD (1) C 2- C 3	52. BD*(1) C 4- N 25	1.39	0.83	0.03
	19. BD (1) C 3- H 7		1.54	0.79	0.031
	20. BD (1) C 3- H 15		3.03	0.8	0.044
	24. BD (1) C 5- C 6		6.42	0.8	0.064
	25. BD (1) C 5- H 12		0.68	0.8	0.021
	27. BD (1) C 6- H 13		0.87	0.78	0.023
10_NH$_3^+$	7. BD (1) C 1- C 3	32. BD*(1) C 9- N 12	5.46	0.78	0.058
	10. BD (1) C 2- C 3		1.56	0.79	0.031
11_NH$_3^+$	10. BD (1) C 1- C 3	43. BD*(1) C 9- N 19	5.84	0.78	0.06
	13. BD (1) C 2- C 3		1.54	0.78	0.031
	21. BD (1) C 11- C 12		5.85	0.78	0.06
	22. BD (1) C 11- C 13		1.55	0.78	0.031
12_NH$_3^+$	8. BD (3) C 1- C 3	23. BD*(1) C 4- N 7	8.89	0.59	0.065
13_NH$_3^+$	18. BD (1) C 1- C 2	72. BD*(1) C 4- N 30	0.87	0.83	0.024
	20. BD (1) C 1- H 5		2.09	0.8	0.036
	21. BD (1) C 1- H 6		2.67	0.81	0.041
	27. BD (1) C 3- C 10		0.6	0.85	0.02
	28. BD (1) C 3- C 20		4.18	0.85	0.053
	45. BD (2) C 20- C 21		1.23	0.52	0.023

<u>For Table 6 (ROCOCF$_3$): B3LYP/6-311++G(d,p)</u>

2_OCOCF$_3$	43. BD (1) C 3- H 7	84. BD*(1) C 4- O 30	1.99	0.66	0.032
	44. BD (1) C 3-Si 17		5.82	0.6	0.053
	49. BD (1) C 5- H 13		1.01	0.67	0.023

	50. BD (1) C 5- H 14		5.88	0.67	0.056
	66. BD (1) C 31- C 32		3.66	0.84	0.05
4_OCOCF$_3$	32. BD (1) C 2- H 7	60. BD*(1) C 3- O 15	5.5	0.68	0.054
	33. BD (1) C 2- H 8		1.09	0.68	0.024
	50. BD (1) C 22- H 23		0.97	0.68	0.023
	51. BD (1) C 22- H 24		5.98	0.68	0.057
	44. BD (1) C 16- C 17		3.58	0.86	0.049
5_OCOCF$_3$	26. LP (2) S 17	92. BD*(1) C 4- O 29	1.7	0.44	0.025
	48. BD (1) C 3- H 7		1.27	0.69	0.026
	49. BD (1) C 3- S 17		3.98	0.7	0.047
	54. BD (1) C 5- H 13		1.01	0.67	0.023
	55. BD (1) C 5- H 14		6.11	0.67	0.057
	74. BD (1) C 30- C 31		3.57	0.85	0.049
6_OCOCF$_3$	37. LP (2)Se 29	101. BD*(1) C 4- O 28	1.61	0.43	0.023
	57. BD (1) C 3- H 7		1.25	0.69	0.026
	58. BD (1) C 3-Se 29		4.99	0.65	0.051
	63. BD (1) C 5- H 13		1.04	0.67	0.024
	64. BD (1) C 5- H 14		6.08	0.67	0.057
	83. BD (1) C 30- C 31		3.59	0.85	0.049

For Table 6 (ROCOCF$_3$): M06-2X/6-311++G(d,p)

2_OCOCF$_3$	43. BD (1) C 3- H 7	84. BD*(1) C 4- O 30	2.08	0.81	0.037
	44. BD (1) C 3-Si 17		6.73	0.75	0.063
	49. BD (1) C 5- H 13		0.97	0.82	0.025
	50. BD (1) C 5- H 14		6.56	0.82	0.066
	66. BD (1) C 31- C 32		4.2	1.01	0.058
4_OCOCF$_3$	17. LP (2) O 18		0.58	0.66	0.017
	32. BD (1) C 2- H 7	60. BD*(1) C 3- O 15	5.97	0.83	0.063
	33. BD (1) C 2- H 8		1.2	0.83	0.028
	44. BD (1) C 16- C 17		4.09	1.02	0.058
	50. BD (1) C 22- H 23		1.03	0.83	0.026
	51. BD (1) C 22- H 24		6.61	0.83	0.066
5_OCOCF$_3$	26. LP (2) S 17	92. BD*(1) C 4- O 29	1.64	0.58	0.028
	30. LP (2) O 32		0.6	0.66	0.018
	48. BD (1) C 3- H 7		1.38	0.85	0.03
	49. BD (1) C 3- S 17		4.24	0.86	0.054
	54. BD (1) C 5- H 13		1.08	0.83	0.027
	55. BD (1) C 5- H 14		6.75	0.82	0.067
	74. BD (1) C 30- C 31		4.09	1.02	0.058

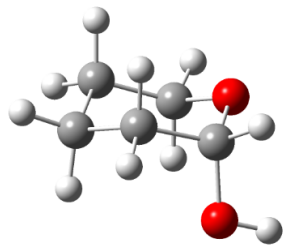
6_OCOCF$_3$	37. LP (2)Se 29	101. BD*(1) C 4- O 28	1.68	0.56	0.027
	39. LP (2) O 32		0.6	0.66	0.018
	57. BD (1) C 3- H 7		1.39	0.84	0.031
	58. BD (1) C 3-Se 29		5.28	0.81	0.058
	63. BD (1) C 5- H 13		1.14	0.82	0.027
	64. BD (1) C 5- H 14		6.68	0.82	0.066
	83. BD (1) C 30- C 31		4.11	1.02	0.058

Cartesian Coordinates and Energies

Structures are presented for **Table 1** (**1-13**.OH), **Table 2** (**1-13**.OH_2^+) and **Table 3** (**1-13**.NH_3^+) initially at both levels of theory (B3LYP/6-311++G(d,p), M06-2X/6-311++G(d,p)), followed by the structures for the theoretical VOP slopes in **Table 5** at each level of theory (B3LYP/6-311++G(d,p), M06-2X/6-311++G(d,p) and MP2/6-31G+(d)) in descending pK_a value of each substituent. The coordinates for the structures contributing to **Table 6** calculated at B3LYP/6-311++G(d,p) are presented last in order of acetone, acetonitrile and then dimethylsulfoxide. Energies (E) are given as electronic energies at 0 K corrected with zero-point vibration energy (ZPVE, unscaled).

For Table 1 (ROH): B3LYP/6-311++G(d,p)

1



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ZPVE = 0.150620

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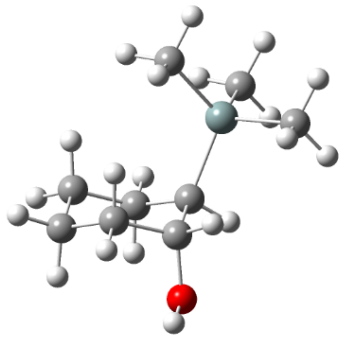
C	1.42851200	0.44483600	-0.01069500
C	-0.55073500	1.30436400	1.04759500
C	-1.17523100	-0.08387900	1.14762800
H	2.50320800	0.43912100	0.19791400
H	1.24652000	-1.48282700	0.87610700
H	1.25331800	-1.50313000	-0.88960600
H	-1.04656100	-0.59367100	-0.95152800
H	-1.04335700	-1.99490800	0.11299800
H	-0.79400000	1.92175400	1.91353200
H	-0.90793300	1.81746000	0.14646300
H	-0.90908400	-0.52961200	2.11319000
H	-2.26619000	0.00760100	1.12113200

O	0.88592100	1.24318800	1.02620100
O	1.18241300	1.01241200	-1.28920900
H	1.55809200	1.90000100	-1.29455500

2



E = -719.640914

ZPVE = 0.274734

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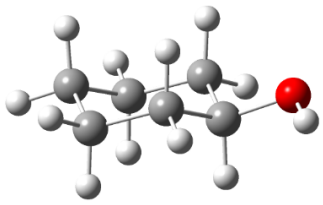
C	0.53689600	0.25005100	-0.22485800
C	0.87667400	1.43945500	0.68922200
C	-0.31380200	2.38547200	0.90969300
C	-1.57272400	1.64998000	1.38749400
H	1.36292800	-0.46209400	-0.08216900
H	-0.55680700	-0.94814400	1.20433400
H	-1.03149000	-1.25517000	-0.45361700
H	-2.24661000	0.92268800	-0.53267900
H	-2.80472300	-0.04276300	0.82185700
H	1.70993500	2.01135700	0.25925200
H	-0.02670400	3.16193200	1.63013900
H	-0.52488900	2.90728200	-0.03055600
H	-1.39500300	1.24111500	2.38793100
H	-2.40407400	2.35675400	1.47717900
Si	0.68236900	0.58691700	-2.10935400
C	-0.51125300	1.87692800	-2.81664000
H	-0.36628800	2.86604300	-2.37308100
H	-0.34384700	1.97703200	-3.89449100
H	-1.55826900	1.59666100	-2.67343600
C	2.44979200	1.16352000	-2.47068600
H	2.61323900	1.24472300	-3.55012900
H	2.66181200	2.14461900	-2.03535100
H	3.18972100	0.45990100	-2.07683900
C	0.38524200	-1.05037700	-3.01017400
H	1.04207900	-1.84056700	-2.63341600
H	-0.64649000	-1.39748500	-2.90298000
H	0.58310500	-0.93924400	-4.08106900
O	1.32178900	0.87766000	1.94354500
H	1.53484300	1.60008000	2.54392800

3

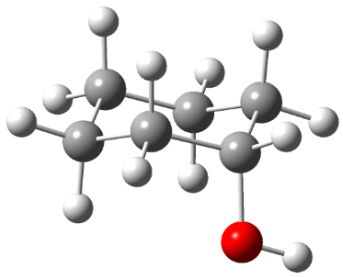


E = -311.015018

ZPVE = 0.173849

Symbol	X	Y	Z
C	-4.36098100	-0.84723000	0.02492400
C	-2.83533500	-0.88904200	0.03570800
C	-2.24085000	0.52290900	0.00819900
C	-2.77617800	1.38222000	1.16455000
C	-4.31113500	1.42314000	1.16502900
C	-4.90812500	0.00833400	1.17730200
H	-1.14600300	0.46697800	0.05193900
H	-2.50455400	-1.39378200	0.95747300
H	-4.68267700	-0.43210100	-0.93781900
H	-4.74971600	-1.86831100	0.07655500
H	-2.42484200	0.96918600	2.11901300
H	-2.36671300	2.39494900	1.09718400
H	-4.67305400	1.99440500	2.02602100
H	-4.65782900	1.95382500	0.26906100
H	-4.67254200	-0.47456900	2.13461300
H	-5.99978400	0.05572400	1.11711800
H	-2.49913600	0.98354800	-0.95302300
O	-2.42542700	-1.66526800	-1.09723900
H	-1.46333300	-1.69631100	-1.11730800

4



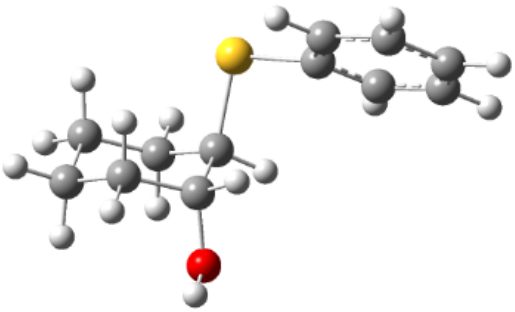
E = -311.013665

ZPVE = 0.173988

Symbol	X	Y	Z

C	-0.65925000	-0.95087900	-0.00756600
C	0.87624600	-0.97854000	-0.02286900
C	1.48436100	0.42566500	-0.04589600
C	-0.61105900	1.32709900	1.10242500
C	-1.19366200	-0.09300800	1.14860000
H	2.57451600	0.34484400	0.06637000
H	1.24551000	-1.49352700	0.87254500
H	1.24492200	-1.53618100	-0.88856000
H	-1.01896000	-0.54475700	-0.95843300
H	-1.04538300	-1.97262600	0.06720800
H	-0.96246300	1.91278600	1.95808800
H	-0.97258700	1.83507300	0.20183000
H	-0.92738500	-0.56354300	2.10498500
H	-2.28726900	-0.05257200	1.11613900
O	1.19029700	0.98421000	-1.33866600
H	1.56149300	1.87126800	-1.38116100
C	0.92435700	1.29938900	1.08679700
H	1.32814100	2.31601900	1.00035200
H	1.29747000	0.90218200	2.03960800

5



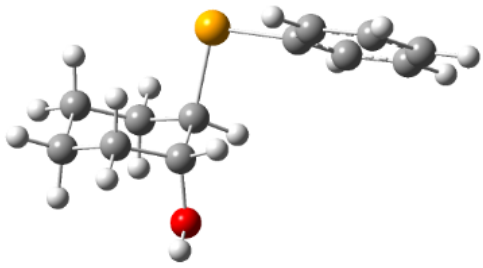
E = -940.248153

ZPVE = 0.255585

Symbol	X	Y	Z
C	-1.81884900	0.09030500	0.20367100
C	-0.43659700	-0.46015300	-0.17795800
C	0.58844300	0.64566500	-0.47613000
C	0.65671800	1.68444800	0.65576700
C	-0.72710400	2.20667600	1.06382800
C	-1.71577700	1.07489500	1.37694600
H	1.57872800	0.20172800	-0.58489300
H	-0.04086600	-1.04405200	0.65969000
H	-0.50835400	-1.13529800	-1.03514300
H	-2.27257900	0.59258800	-0.65896400
H	-2.48264000	-0.74008800	0.46384200
H	1.28476400	2.52191900	0.33019200
H	-0.61568700	2.87348600	1.92750400
H	-1.11418600	2.82198000	0.24461900
H	-1.38322900	0.53692300	2.27139100

H	-2.69917800	1.49630600	1.60777000
S	0.18527500	1.43365200	-2.11430900
C	1.70805300	2.31057800	-2.48766700
C	1.67568400	3.69884900	-2.65431400
C	2.91232900	1.62432000	-2.68378700
C	2.83356900	4.39133800	-3.00823700
H	0.74391000	4.23141200	-2.50488400
C	4.07046500	2.32218300	-3.01625800
H	2.93981400	0.54526900	-2.58679700
C	4.03418800	3.70693400	-3.18291800
H	2.79604500	5.46724300	-3.13850600
H	4.99912000	1.78132300	-3.16125000
H	4.93532300	4.24650600	-3.45129300
O	1.31064700	1.00506700	1.74499400
H	1.42538800	1.62945700	2.46865100

6



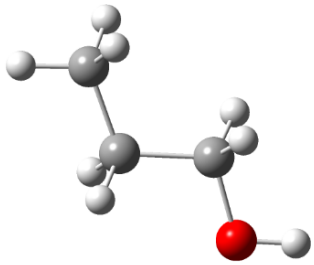
E = -2943.580443

ZPVE = 0.254252

Symbol	X	Y	Z
C	-1.92650700	0.22489800	0.32738600
C	-0.73553300	-0.74464400	0.30924400
C	0.53525200	-0.11613100	-0.27673100
C	0.87856100	1.22474500	0.38707500
C	-0.32092500	2.18053800	0.44774200
C	-1.56719400	1.52527100	1.05975600
H	1.38116000	-0.79086400	-0.14727500
H	-0.50178000	-1.03907000	1.33873600
H	-0.98446600	-1.65884600	-0.23630500
H	-2.23818500	0.45533000	-0.69922400
H	-2.78343400	-0.25641100	0.80883200
H	1.69889600	1.69753900	-0.16524400
H	-0.03597300	3.07419700	1.01613300
H	-0.54004400	2.51799300	-0.57092600
H	-1.38114300	1.30317700	2.11619400
H	-2.40735200	2.22596900	1.02641500
C	2.23273600	0.20708100	-2.72662600
C	2.73547300	1.39787500	-3.25807400
C	3.08083600	-0.89485200	-2.57700200
C	4.07704000	1.48596000	-3.63180300

H	2.07970900	2.25215600	-3.37674800
C	4.42378900	-0.79674100	-2.93562200
H	2.69013400	-1.82883500	-2.19038900
C	4.92400000	0.39231000	-3.46628500
H	4.45876000	2.41268400	-4.04599200
H	5.07595500	-1.65438800	-2.81252100
H	5.96733400	0.46352600	-3.75216600
O	1.34364100	0.87731900	1.70740700
H	1.61828000	1.68405000	2.15546400
Se	0.34939900	0.07647800	-2.27252800

7

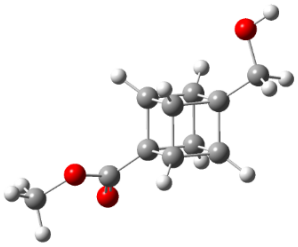


E = -194.311382

ZPVE = 0.107983

Symbol	X	Y	Z
C	-0.90661700	1.59947100	0.01664600
H	-0.56706400	0.55886100	0.04169300
H	-2.00093500	1.57363800	0.04106400
C	-0.41324900	2.29733600	1.27371400
H	-0.76376400	3.33960000	1.28495700
H	0.68625100	2.31323400	1.28566700
C	-0.42147400	2.28420400	-1.26440500
H	0.67170700	2.29883200	-1.32186600
H	-0.79050000	1.76207200	-2.15069800
H	-0.77133100	3.31994900	-1.32259900
O	-0.91675100	1.58685700	2.40880500
H	-0.60947000	2.02084800	3.21007000

8

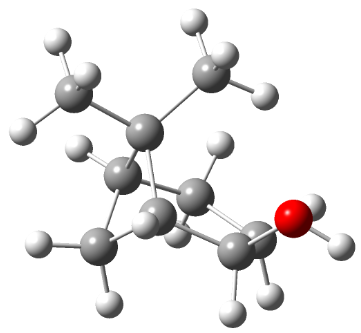


E = -651.842056

ZPVE = 0.207564

Symbol	X	Y	Z
C	-0.86402000	0.32343000	-0.78644800
C	-1.13674900	1.86637500	-0.56796500
H	-1.92364400	2.42620800	-1.06840700
C	-0.99775300	1.67886500	0.98016100
H	-1.65855900	2.11565200	1.72589600
C	-0.73358500	0.14743900	0.77776200
H	-1.19859400	-0.65899100	1.34102800
C	0.54696400	1.95855300	0.86996200
C	0.80744800	0.42014700	0.66182300
H	1.58546000	-0.15805600	1.15927300
C	0.66879900	0.60567700	-0.89202300
H	1.31605400	0.16402700	-1.64593700
C	0.40220300	2.14002700	-0.68630500
H	0.85028000	2.94517800	-1.26497300
C	-1.63352300	-0.56262700	-1.69610100
O	-2.93416600	-0.63297300	-1.32262400
O	-1.18673200	-1.15245600	-2.65313800
C	-3.78271600	-1.45824200	-2.14048200
H	-3.42978600	-2.49067100	-2.13811300
H	-4.77238900	-1.39113600	-1.69353900
H	-3.79981900	-1.08999900	-3.16740200
C	1.34721900	2.83025400	1.78294300
H	2.40411200	2.81274400	1.47682300
H	1.28756900	2.44179100	2.81093200
O	0.82453200	4.16142400	1.71594700
H	1.34116800	4.72850200	2.29604100

9



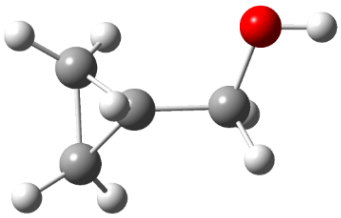
E = -427.667301

ZPVE = 0.235092

Symbol	X	Y	Z
C	-2.19844100	-1.64022000	0.10749800
C	-0.66812000	-1.56672600	0.09799300
C	-0.13847400	-0.12255200	0.37402600
C	-1.23580500	0.97201100	0.57749500

C	-2.64731900	0.41091600	0.43750600
C	-2.72729800	-0.85444300	1.33830100
H	0.51407000	-0.13644700	1.25108600
H	-0.28167300	-2.25266800	0.85883700
H	-0.28572200	-1.92634400	-0.86171700
H	-2.54669400	-2.66735100	-0.03889000
H	-1.15080500	1.37072600	1.59787200
H	-3.38297100	1.20708700	0.57731800
H	-2.10576500	-0.86528400	2.23880100
H	-3.74634300	-1.11576500	1.61866500
H	0.48751100	0.20034300	-0.46089800
C	-2.83269600	-0.53202200	-0.80516100
C	-4.32172400	-0.80048300	-1.07513200
H	-4.88269200	-1.06079800	-0.17533500
H	-4.79371500	0.08376500	-1.51551200
H	-4.43565800	-1.62549200	-1.78624300
C	-2.16224400	-0.19574800	-2.13887900
H	-1.09983600	0.02284000	-2.05148200
H	-2.28329100	-1.03129800	-2.83799600
H	-2.63052500	0.68447300	-2.58842400
O	-1.09769000	2.06756600	-0.34221000
H	-0.27540800	2.52888200	-0.14962300

10

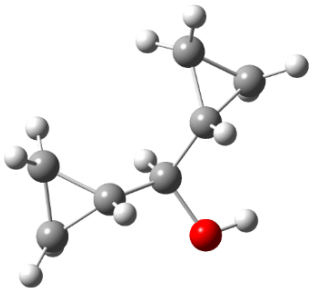


E = -232.381885

ZPVE = 0.114046

Symbol	X	Y	Z
C	-1.98030400	0.96161900	0.01705400
C	-0.47080500	0.98483500	0.00199400
C	-1.24208500	2.27954500	0.00982000
H	-2.50211800	0.66594900	-0.88488000
H	-2.47291500	0.65848200	0.93437700
H	0.03969700	0.70082200	-0.91000400
H	0.05042800	0.70743900	0.91095800
H	-1.25694300	2.83781800	-0.92071900
C	-1.25373300	3.14144000	1.24005700
H	-2.14479000	3.78420300	1.23728000
H	-1.29824600	2.50566900	2.13575200
O	-0.06618400	3.94233400	1.25123600
H	-0.11811400	4.56068200	1.98632300

11

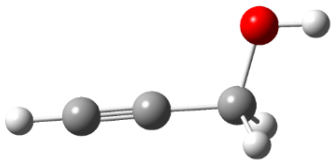


E = -349.050578

ZPVE = 0.176098

Symbol	X	Y	Z
C	-1.54663300	0.93555800	0.47746300
C	-0.07915200	1.27249000	0.36589100
C	-1.12653000	2.34790100	0.16746700
H	-2.00408000	0.35336700	-0.31316600
H	-1.93935200	0.72794100	1.46607400
H	0.46778300	0.91974600	-0.50014000
H	0.49937400	1.28624900	1.28411600
H	-1.27655600	2.68298200	-0.85505900
C	-1.28035900	3.44876800	1.19604100
H	-1.18165300	3.00532100	2.20055800
C	-2.61250400	4.15231900	1.10879000
C	-3.79889000	3.63940300	1.88814100
C	-3.13143500	4.93296600	2.28765500
H	-2.81863000	4.57034500	0.12785100
H	-3.65432100	2.77721100	2.52920500
H	-4.77414700	3.68239300	1.41843800
H	-3.65022900	5.86389900	2.09416200
H	-2.52962600	4.93687500	3.18913900
O	-0.26570500	4.45160400	1.02133800
H	0.57454400	4.00019800	0.88575700

12



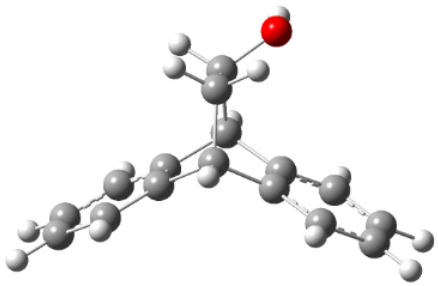
E = -191.862473

ZPVE = 0.060333

Symbol	X	Y	Z
C	-1.81165700	0.44496600	-0.13513800
H	-2.64415900	-0.21526900	-0.12439300

C	-0.86425200	1.18312700	-0.14824600
C	0.26478600	2.10516200	-0.16120100
H	0.14034000	2.80698100	-0.99714300
H	0.25617300	2.68995700	0.76873300
O	1.48323900	1.36943000	-0.28988400
H	2.21202900	1.99862500	-0.29598400

13



E = -693.284256

ZPVE = 0.256576

Symbol	X	Y	Z
C	1.54597400	0.36661100	-0.12404400
C	2.18934600	1.79002500	-0.11915500
C	-0.38751700	2.00124300	0.04121900
C	0.00418900	0.48588800	-0.07126100
H	1.86161300	-0.18101200	-1.01445100
H	1.87406200	-0.19385200	0.75339600
H	-0.44004400	0.09410800	-0.99349200
H	-1.47269700	2.11598300	0.10666200
H	3.27705800	1.73145400	-0.18528600
C	0.33025300	2.57049800	1.24852100
C	1.72619400	2.46641900	1.15769100
C	-0.25673800	3.14345300	2.36977900
C	2.53122500	2.93602000	2.18848500
C	0.55337000	3.62243500	3.40323300
H	-1.33691800	3.22176700	2.44278500
C	1.93998900	3.51917500	3.31305900
H	3.61140800	2.85323700	2.12071700
H	0.10034000	4.07588000	4.27781300
H	2.56378200	3.89315400	4.11731800
C	0.18514100	2.66265000	-1.19915400
C	-0.52840800	3.31231000	-2.19925700
C	1.58148000	2.54913300	-1.28596300
C	0.15550500	3.86101500	-3.28862900
H	-1.60835700	3.40010000	-2.13311200
C	2.25956200	3.09151300	-2.37089800
C	1.54171400	3.75132500	-3.37347000
H	-0.39561600	4.37535100	-4.06797600
H	3.33949500	3.00659600	-2.43934100
H	2.06739900	4.18057900	-4.21916400

O	-0.45471500	-0.28338900	1.04034600
H	-1.41763100	-0.26997400	1.05234300

For Table 1 (ROH): M06-2X/6-311++G(d,p)

1

E = -346.799052

ZPVE = 0.152810

Symbol	X	Y	Z
C	-0.66149900	-0.96145000	-0.00787500
C	0.86765100	-0.97766700	0.00291500
C	1.42034700	0.44015400	-0.00263800
C	-0.53738300	1.29832700	1.03948500
C	-1.16445100	-0.08491300	1.14059300
H	2.49843000	0.44381300	0.18227900
H	1.22847000	-1.47118300	0.91017700
H	1.27087000	-1.51256100	-0.85894700
H	-1.01222500	-0.55430700	-0.96083400
H	-1.05053600	-1.97827800	0.07822100
H	-0.79241700	1.92160900	1.89644800
H	-0.88286300	1.79978400	0.12786300
H	-0.88695300	-0.53370800	2.10027400
H	-2.25347800	0.00820400	1.11921300
O	0.88724000	1.22835100	1.03415100
O	1.13605500	0.99815200	-1.26524000
H	1.49325800	1.89106900	-1.28100100

2

E = -719.389132

ZPVE = 0.277998

Symbol	X	Y	Z
C	-1.80935800	0.25636400	0.36794800
C	-0.49951400	-0.53234300	0.33309300
C	0.67190400	0.32857800	-0.17551800
C	0.80781700	1.60385300	0.66091400
C	-0.51118200	2.37438700	0.78100300
C	-1.65946800	1.48663100	1.26494000
H	1.59978400	-0.23476000	-0.00459200
H	-0.27034300	-0.87244400	1.34863000
H	-0.60693300	-1.42772200	-0.28501100
H	-2.08277600	0.57325100	-0.64731600
H	-2.62282200	-0.37797600	0.73004000
H	1.56593900	2.26172400	0.21074700
H	-0.36774400	3.22160000	1.46187800
H	-0.76389600	2.80074600	-0.19374000
H	-1.45471900	1.15412500	2.28779800

H	-2.58768200	2.06337100	1.29199700
Si	0.70847600	0.61510400	-2.05925100
C	-0.25706300	2.11229400	-2.67822700
H	0.15069600	3.04945400	-2.29011400
H	-0.18191500	2.15157700	-3.76925900
H	-1.31789800	2.06967800	-2.42093100
C	2.50784400	0.86657400	-2.55317600
H	2.59823900	1.05249600	-3.62671300
H	2.94731700	1.72124300	-2.03118700
H	3.10929200	-0.01395500	-2.31294000
C	0.03018000	-0.91940800	-2.90943100
H	0.54905800	-1.82231500	-2.57618600
H	-1.03567800	-1.05083100	-2.70366400
H	0.15415700	-0.84282900	-3.99293200
O	1.26645100	1.19502800	1.95206000
H	1.31051800	1.96801700	2.52152500

3

E = -310.862957

ZPVE = 0.175940

Symbol	X	Y	Z
C	-4.35927500	-0.83900900	0.02422400
C	-2.83920600	-0.88635100	0.04408200
C	-2.24975900	0.52112600	0.00624000
C	-2.77753900	1.37034400	1.16584500
C	-4.30740200	1.41828100	1.15379400
C	-4.89896400	0.00674700	1.17992200
H	-1.15562100	0.46759800	0.03749500
H	-2.51546200	-1.38018100	0.97381300
H	-4.66932600	-0.40858800	-0.93502100
H	-4.74992500	-1.85866200	0.06311200
H	-2.43835700	0.93906600	2.11551000
H	-2.36162700	2.37939000	1.11169800
H	-4.67459800	2.00048300	2.00298700
H	-4.64283900	1.93186700	0.24487700
H	-4.64255900	-0.47274100	2.13243900
H	-5.98979500	0.04896100	1.13319200
H	-2.52656500	0.97810000	-0.95104300
O	-2.42971100	-1.66045400	-1.07468800
H	-1.46968400	-1.66737200	-1.10917600

4

E = -310.862344

ZPVE = 0.176154

Symbol	X	Y	Z
C	-0.65136200	-0.93852400	-0.01436300

C	0.87878300	-0.97975800	-0.00829600
C	1.47716700	0.42256000	-0.04341700
C	-0.60162700	1.32561300	1.08868300
C	-1.18069400	-0.09017900	1.14453100
H	2.56881100	0.35168300	0.04588800
H	1.23243300	-1.48182500	0.89935800
H	1.25558700	-1.54387400	-0.86482700
H	-0.99001200	-0.50900900	-0.96195700
H	-1.04992200	-1.95471900	0.04245000
H	-0.96271400	1.92270900	1.93006300
H	-0.94583500	1.81610700	0.17253200
H	-0.89841300	-0.55885600	2.09601400
H	-2.27292200	-0.05297300	1.12070000
O	1.14370900	0.97337200	-1.31626900
H	1.48968600	1.86811500	-1.36423400
C	0.92867300	1.28779100	1.09377700
H	1.34174200	2.30006600	1.01687300
H	1.28620500	0.87460400	2.04429100

5

E = -939.976200

ZPVE = 0.258686

Symbol	X	Y	Z
C	-1.80324900	0.19098900	0.21888300
C	-0.48376800	-0.49190600	-0.15256500
C	0.60146900	0.51406500	-0.54819100
C	0.78757000	1.58624500	0.52955500
C	-0.53218700	2.24904800	0.92384000
C	-1.58489800	1.21660800	1.33369500
H	1.55355300	-0.00469200	-0.67466200
H	-0.10735600	-1.04161700	0.71553200
H	-0.62876900	-1.21245100	-0.96128400
H	-2.22578000	0.69018800	-0.66004600
H	-2.52773600	-0.56358800	0.53498200
H	1.48966100	2.34338000	0.16081600
H	-0.34469200	2.95666700	1.73887900
H	-0.89354400	2.83336100	0.07163300
H	-1.24968400	0.69745500	2.23745800
H	-2.52352300	1.71975000	1.57860100
S	0.16273600	1.24534300	-2.17866800
C	1.62141600	2.22565400	-2.49089900
C	1.50945700	3.61176400	-2.59521200
C	2.86835500	1.62027600	-2.65569200
C	2.63590400	4.38572500	-2.85974400
H	0.53938400	4.07678400	-2.46384300
C	3.99381600	2.39824200	-2.89988300
H	2.95146900	0.54094300	-2.59946300
C	3.87979700	3.78202500	-3.00552100
H	2.54018100	5.46192400	-2.94310500
H	4.95940300	1.92169200	-3.02178800

H	4.75728000	4.38560300	-3.20421900
O	1.37194300	0.89424700	1.63270300
H	1.54520600	1.52773400	2.33376800

6

E = -2943.341781

ZPVE = 0.257498

Symbol	X	Y	Z
C	-1.88732000	0.32755200	0.31949600
C	-0.80642800	-0.75701200	0.32626800
C	0.49856200	-0.27927300	-0.31341400
C	0.98774700	1.02889200	0.31109400
C	-0.09924600	2.10403800	0.34276600
C	-1.38029400	1.59657300	1.00899500
H	1.27779700	-1.03149400	-0.18493600
H	-0.57511100	-1.02199200	1.36328400
H	-1.15536500	-1.66369800	-0.17380700
H	-2.17737100	0.56223600	-0.71143600
H	-2.78289500	-0.04502700	0.82274500
H	1.85598300	1.39126700	-0.25216100
H	0.28761400	2.98385200	0.86849700
H	-0.30995300	2.41452900	-0.68524300
H	-1.17697400	1.37383700	2.06147300
H	-2.14565400	2.37615700	0.98476800
C	2.10831900	0.17355500	-2.71255400
C	2.52592400	1.40392400	-3.21794300
C	3.03563700	-0.85339000	-2.53511200
C	3.86499300	1.60517000	-3.54232100
H	1.80340200	2.20055800	-3.35070200
C	4.37487200	-0.64226700	-2.84445000
H	2.70632900	-1.81663700	-2.16273800
C	4.79104500	0.58567900	-3.35114600
H	4.18356500	2.56255400	-3.93774300
H	5.09165200	-1.44218400	-2.70047300
H	5.83374600	0.74540800	-3.59842100
O	1.39547300	0.66900000	1.63206700
H	1.74888900	1.44992100	2.06600500
Se	0.25348400	-0.10341500	-2.27393300

7

E = -194.206784

ZPVE = 0.109302

Symbol	X	Y	Z
C	-0.91042000	1.59398000	0.01753200
H	-0.56867200	0.55570900	0.04590900

H	-2.00327200	1.57108600	0.04532000
C	-0.41406300	2.29599200	1.26547400
H	-0.76554800	3.33661000	1.26893000
H	0.68421300	2.31089400	1.26944900
C	-0.42162500	2.28399300	-1.25292000
H	0.67062200	2.29811700	-1.29892600
H	-0.78479100	1.77063300	-2.14445400
H	-0.77125200	3.31884600	-1.29938200
O	-0.91184600	1.59304300	2.39323700
H	-0.60654100	2.02599800	3.19288000

8

E = -651.585947

ZPVE = 0.210963

Symbol	X	Y	Z
C	-0.85489900	0.32758300	-0.77748300
C	-1.13130400	1.85603800	-0.55833700
H	-1.92120900	2.41112300	-1.05651000
C	-0.98752500	1.66414700	0.98230600
H	-1.63841800	2.10215400	1.73418700
C	-0.72534000	0.13972700	0.77294900
H	-1.19178100	-0.67050100	1.32704700
C	0.54622400	1.93715700	0.86443800
C	0.80970000	0.41118900	0.65512800
H	1.58918900	-0.16390700	1.15051700
C	0.66739200	0.60279200	-0.89132500
H	1.30489700	0.16038500	-1.65158500
C	0.40124500	2.12993100	-0.67878200
H	0.84996600	2.94098800	-1.24630000
C	-1.63186300	-0.55515800	-1.68069200
O	-2.92557300	-0.60244700	-1.31343400
O	-1.19254200	-1.15886800	-2.62405800
C	-3.76297100	-1.42394200	-2.12720100
H	-3.41249300	-2.45635200	-2.11154500
H	-4.75851300	-1.35032700	-1.69758500
H	-3.76097400	-1.06516700	-3.15688300
C	1.33363200	2.82332100	1.77014800
H	2.38835900	2.81928700	1.46220000
H	1.27478100	2.44326400	2.79947100
O	0.78259200	4.12877100	1.67862000
H	1.27720200	4.71995400	2.24984300

9

E = -427.471823

ZPVE = 0.238137

Symbol	X	Y	Z

C	-2.20080700	-1.63447800	0.10377400
C	-0.67655800	-1.55458900	0.06481000
C	-0.15909100	-0.12992800	0.41886800
C	-1.24946500	0.97408400	0.55315700
C	-2.65419000	0.40520400	0.44265800
C	-2.71299700	-0.85605500	1.34036800
H	0.39830900	-0.17882800	1.35660500
H	-0.26550200	-2.27687500	0.77538100
H	-0.32176800	-1.85263600	-0.92494100
H	-2.55387100	-2.65814100	-0.04727500
H	-1.16141300	1.42802100	1.54921600
H	-3.39495800	1.19579600	0.58330100
H	-2.07227200	-0.86164000	2.22666000
H	-3.72505600	-1.12439400	1.63465000
H	0.55421600	0.20165600	-0.33958200
C	-2.83183900	-0.52782000	-0.79258400
C	-4.31196200	-0.79692000	-1.06545900
H	-4.86813000	-1.06135400	-0.16446300
H	-4.78169300	0.08942400	-1.50148500
H	-4.41931900	-1.61948100	-1.77880400
C	-2.14847000	-0.18505100	-2.11131500
H	-1.08657200	0.02906300	-2.00335700
H	-2.26640900	-1.01764400	-2.81310600
H	-2.60757200	0.70213700	-2.55427800
O	-1.12165600	2.00332300	-0.42370700
H	-0.29027900	2.46209400	-0.28119500

10

E = -232.270931

ZPVE = 0.115668

Symbol	X	Y	Z
C	-1.97498500	0.96655800	0.02348700
C	-0.47129400	1.00651400	0.00854800
C	-1.25479100	2.28503600	-0.00285900
H	-2.48682200	0.65060100	-0.87532300
H	-2.46313400	0.67734100	0.94621100
H	0.03779900	0.71282800	-0.89919000
H	0.05096700	0.75825000	0.92415700
H	-1.27370000	2.83927600	-0.93404800
C	-1.25989300	3.13682400	1.23076900
H	-2.14079900	3.79072200	1.23203400
H	-1.31468100	2.48750400	2.11518200
O	-0.06737200	3.90823400	1.24720100
H	-0.09740500	4.51114900	1.99307900

11

E = -348.893193

ZPVE = 0.178457

Symbol	X	Y	Z
C	-1.56343600	0.96963900	0.49837500
C	-0.09649400	1.29069800	0.39286600
C	-1.12883400	2.36240100	0.15961200
H	-2.01260100	0.37124200	-0.28242700
H	-1.96608700	0.79830800	1.48896300
H	0.45092400	0.90821600	-0.45795800
H	0.46844500	1.33008600	1.31764800
H	-1.26936200	2.68717700	-0.86640500
C	-1.27684200	3.46217100	1.18225100
H	-1.18665200	3.01425600	2.18615800
C	-2.60760900	4.15623100	1.09075100
C	-3.77312700	3.60802400	1.86233600
C	-3.12368300	4.89759900	2.28671000
H	-2.81456000	4.58899000	0.11773300
H	-3.60216200	2.73267900	2.47694400
H	-4.75220000	3.65285700	1.40502400
H	-3.66245300	5.82044900	2.12076100
H	-2.50704900	4.88443300	3.17682800
O	-0.27094800	4.45249100	1.00899800
H	0.56663000	3.99958600	0.87455200

12

E = -191.774210

ZPVE = 0.061560

Symbol	X	Y	Z
C	-1.80575900	0.44646500	-0.13538400
H	-2.63749100	-0.21673500	-0.12455300
C	-0.86335500	1.18673500	-0.14849300
C	0.26978500	2.10998200	-0.16140600
H	0.14107300	2.80732500	-0.99748100
H	0.25688500	2.68998300	0.76881300
O	1.47048100	1.37034300	-0.28924200
H	2.20488000	1.98888000	-0.29550900

13

E = -692.998348

ZPVE = 0.259396

Symbol	X	Y	Z
C	1.44106800	0.38874300	-0.12378600
C	2.13816500	1.78022000	-0.11787700
C	-0.43146800	2.08257300	0.03273700
C	-0.09856500	0.57072900	-0.05351500

H	1.72674000	-0.15852500	-1.02430900
H	1.76968400	-0.18073100	0.74905200
H	-0.56699000	0.17431800	-0.96094300
H	-1.51044900	2.22524500	0.10033200
H	3.22307800	1.68567300	-0.18082900
C	0.30514400	2.62204900	1.23897100
C	1.69297300	2.47007200	1.15299900
C	-0.26660100	3.19794600	2.36195600
C	2.51015900	2.89940500	2.18757700
C	0.55526800	3.63856600	3.39935400
H	-1.34403500	3.29987600	2.43194100
C	1.93534400	3.49122500	3.31270500
H	3.58632000	2.77842800	2.11992000
H	0.11552400	4.09559300	4.27795300
H	2.56745400	3.83671900	4.12225300
C	0.17116300	2.71090900	-1.20443300
C	-0.51622300	3.37340300	-2.20951800
C	1.55929700	2.54963000	-1.28632300
C	0.18841100	3.88591500	-3.29989800
H	-1.59218200	3.49622400	-2.14442700
C	2.25859200	3.05416900	-2.37175000
C	1.56708500	3.72717800	-3.38032200
H	-0.34179600	4.41111900	-4.08546400
H	3.33462400	2.92974100	-2.43364900
H	2.10836300	4.12929800	-4.22858900
O	-0.67646900	-0.03921800	1.08789900
H	-0.46922000	-0.97679800	1.07869800

For Table 2 (ROH_2^+): B3LYP/6-311++G(d,p)

3

E = -311.324109

ZPVE = 0.185610

Symbol	X	Y	Z
C	-4.44384400	-0.72375500	-0.07857200
C	-2.94952200	-0.82868400	0.03694600
C	-2.20835000	0.47806900	0.05271300
C	-2.72109700	1.29001400	1.27350100
C	-4.24522700	1.45064700	1.23558300
C	-4.94952800	0.09222300	1.14246400
H	-1.12781600	0.32583400	0.13299400
H	-2.61774400	-1.52967500	0.80389100
H	-4.70651900	-0.19891300	-1.00197700
H	-4.91601800	-1.71073100	-0.08922600
H	-2.41715300	0.78948700	2.19932700
H	-2.22097100	2.26029400	1.26511600

H	-4.58140100	1.97808400	2.13132500
H	-4.53017200	2.07441400	0.38080400
H	-4.78390900	-0.48253900	2.06020900
H	-6.02969300	0.21312700	1.04109200
H	-2.41757600	1.03198000	-0.86733600
O	-2.45772200	-1.59348200	-1.33800800
H	-1.49249000	-1.70009300	-1.40886500
H	-2.89183700	-2.45143500	-1.49137600

4

E = -311.323104

ZPVE = 0.185279

Symbol	X	Y	Z
C	-0.70334400	-0.97310600	-0.01631400
C	0.81433700	-1.04483900	0.21879100
C	1.48551500	0.30238900	0.27615000
C	-0.74080700	1.42191300	0.81822200
C	-1.37302600	0.02830200	0.93447200
H	2.55967100	0.25753400	0.45320600
H	1.02209700	-1.48571400	1.20403800
H	1.31976600	-1.70308700	-0.49667800
H	-0.90539200	-0.68895900	-1.05480600
H	-1.12409500	-1.97192800	0.11578700
H	-1.18790300	2.11019700	1.53828600
H	-0.94502300	1.83905900	-0.17390100
H	-1.28718600	-0.33023400	1.96724000
H	-2.44141900	0.08746100	0.71670100
O	1.45769900	0.84801900	-1.29144100
H	1.84158500	1.73476200	-1.40522100
C	0.77648300	1.37431700	1.06161900
H	1.25636400	2.34840100	0.91491300
H	0.98149700	1.11324700	2.10950100
H	1.86534800	0.23503500	-1.92759900

7

E = -194.608584

ZPVE = 0.120445

Symbol	X	Y	Z
C	-0.76254900	1.52173500	-0.03624700
H	-0.18560900	0.59364900	-0.01872900
H	-1.82665400	1.26736000	-0.09852300
C	-0.49222300	2.31153400	1.21288100
H	-1.10557200	3.20314400	1.33463600
H	0.56061700	2.51034800	1.40143400
C	-0.36859400	2.36532600	-1.26561400

H	0.69474900	2.61348000	-1.25709300
H	-0.56928200	1.79025700	-2.16985800
H	-0.94452300	3.29136700	-1.32371000
O	-0.85726500	1.40146200	2.44615800
H	-0.74564900	1.81732800	3.32073100
H	-1.73642500	0.98543200	2.38169200

9

E = -427.983571

ZPVE = 0.247127

Symbol	X	Y	Z
C	-2.50748200	-1.49727300	0.19261400
C	-1.01266300	-1.81469200	0.05911900
C	-0.13147300	-0.58850200	0.44776000
C	-0.90425900	0.72622300	0.57797500
C	-2.39747100	0.61719100	0.51704500
C	-2.72681900	-0.60850200	1.44576000
H	0.33001800	-0.75898500	1.42386500
H	-0.75692400	-2.64507900	0.72087900
H	-0.78357800	-2.15231600	-0.95382800
H	-3.11625800	-2.39655200	0.09030300
H	-0.55599000	1.35440100	1.39595700
H	-2.88791400	1.57168900	0.71343200
H	-2.08915200	-0.77921900	2.31516200
H	-3.75905600	-0.56713700	1.78219200
H	0.71397600	-0.47522900	-0.23743100
C	-2.91036000	-0.26173600	-0.68775800
C	-4.43115800	-0.12235100	-0.84824300
H	-4.97242100	-0.21222700	0.09379000
H	-4.68794000	0.84666800	-1.28608100
H	-4.80737900	-0.90029000	-1.51784800
C	-2.27568200	-0.10507300	-2.07729000
H	-1.19828600	-0.30972300	-2.11197500
H	-2.71619500	-0.81773500	-2.77941300
H	-2.48735700	0.88739100	-2.49901800
O	-0.50208900	1.75466500	-0.64544000
H	0.45054900	1.93984300	-0.70860600
H	-0.82555900	1.40410800	-1.50055200

10

E = -232.687307

ZPVE = 0.125734

Symbol	X	Y	Z
C	-1.94057100	0.89380300	0.08023000
C	-0.47596200	1.05366600	-0.10475700

C	-1.34853500	2.30923500	-0.01662500
H	-2.55108700	0.59646700	-0.76198800
H	-2.30711800	0.56073600	1.04323600
H	-0.04708200	0.84395800	-1.07625600
H	0.16560800	0.81037400	0.73569800
H	-1.55189800	2.84540800	-0.93556800
C	-1.37094800	3.10639900	1.20491800
H	-2.11561500	3.89674900	1.25158100
H	-1.27847000	2.54890700	2.13455000
O	-0.01617300	4.03865400	1.19548600
H	0.18210300	4.52235700	2.01741000
H	0.76775800	3.54265000	0.89842400

12

E = -192.151672

ZPVE = 0.072455

Symbol	X	Y	Z
C	-1.77063000	0.41679600	-0.61872400
H	-2.59914700	-0.25159600	-0.70423400
C	-0.83940000	1.17193600	-0.53038700
C	0.23452200	2.09965400	-0.43815600
H	0.66976000	2.39592700	-1.39105100
H	0.05224800	2.94403700	0.22591200
O	1.46759400	1.32447100	0.23157100
H	2.19358000	1.88952000	0.55813900
H	1.19027300	0.68699600	0.91733700

13

E = -693.601590

ZPVE = 0.268560

Symbol	X	Y	Z
C	1.37560600	0.34313800	-0.25464900
C	2.10614500	1.72345100	-0.16182700
C	-0.47018500	2.08343100	-0.02703300
C	-0.13256600	0.58333500	-0.11422100
H	1.57171200	-0.12324400	-1.22191200
H	1.74326900	-0.34744900	0.51138000
H	-0.76705500	0.01654200	-0.78965700
H	-1.54706400	2.24724700	0.02002200
H	3.18606900	1.59125700	-0.21687500
C	0.27108600	2.57511100	1.21132300
C	1.66297400	2.37685900	1.13629000
C	-0.30896000	3.13291100	2.35099200
C	2.47387000	2.76217400	2.19630900
C	0.51663900	3.52254500	3.41261400

H	-1.38038600	3.29946200	2.40130400
C	1.89487500	3.34102300	3.33152200
H	3.54841800	2.62478100	2.14418100
H	0.08029600	3.97792300	4.29336200
H	2.52718100	3.65337800	4.15413800
C	0.16408300	2.70466500	-1.26402400
C	-0.51368600	3.39597800	-2.26178900
C	1.55462100	2.54589500	-1.31600400
C	0.21767900	3.94456600	-3.31766700
H	-1.59024300	3.52058700	-2.21842200
C	2.27937600	3.08914400	-2.36913500
C	1.60239700	3.79316500	-3.36910300
H	-0.29512800	4.49390800	-4.09790200
H	3.35652500	2.97267900	-2.41673100
H	2.16043100	4.22532100	-4.19120000
O	-0.63937800	0.01806600	1.29128700
H	-0.27364700	-0.85191300	1.52886600
H	-0.38919800	0.69482000	1.97247900

For Table 2 (ROH_2^+): M06-2X/6-311++G(d,p)

3

E = -311.167988

ZPVE = 0.188046

Symbol	X	Y	Z
C	-4.44123500	-0.71821100	-0.08472900
C	-2.94478800	-0.83627900	0.02539800
C	-2.21389000	0.47927500	0.04603800
C	-2.71870500	1.27366600	1.26757500
C	-4.23802400	1.43898100	1.22089700
C	-4.93687800	0.08165800	1.13697800
H	-1.13211900	0.33046900	0.11175300
H	-2.62850100	-1.51155900	0.82310900
H	-4.69323800	-0.18100100	-1.00425600
H	-4.91556400	-1.70364300	-0.10982800
H	-2.42699100	0.75505800	2.18688600
H	-2.21799200	2.24213500	1.27811900
H	-4.57833200	1.97521500	2.10801800
H	-4.51478700	2.04915300	0.35454900
H	-4.74922200	-0.49260400	2.05028000
H	-6.01752400	0.20045300	1.05417000
H	-2.44002500	1.03106500	-0.87155000
O	-2.47423500	-1.56892900	-1.28535000
H	-1.50921600	-1.66115500	-1.37278800
H	-2.91732200	-2.41888200	-1.45466200

4

E = -311.167416

ZPVE = 0.187881

Symbol	X	Y	Z
C	-0.68537100	-0.95989400	-0.03054100
C	0.82231100	-1.04379900	0.22948800
C	1.48912500	0.30977700	0.25451100
C	-0.72242600	1.42092500	0.79879700
C	-1.35230900	0.03254100	0.92339300
H	2.56276000	0.26290200	0.43748800
H	1.00898600	-1.46499100	1.22458700
H	1.33158600	-1.71169600	-0.47326700
H	-0.87171200	-0.65492500	-1.06586100
H	-1.11591300	-1.95552800	0.08255300
H	-1.17942300	2.11851700	1.50162800
H	-0.91032000	1.81998800	-0.20375200
H	-1.25069000	-0.32494200	1.95423000
H	-2.42116000	0.08896900	0.71359400
O	1.40874400	0.82841300	-1.23744000
H	1.75452800	1.72798800	-1.37003600
C	0.78474100	1.36684500	1.06931500
H	1.26862400	2.34052900	0.93843300
H	0.96925500	1.08376600	2.11250500
H	1.78083300	0.21738500	-1.89665800

5

E = -940.283220

ZPVE = 0.270135

Symbol	X	Y	Z
C	-1.85816400	0.26658300	0.28107900
C	-0.70348400	-0.73456400	0.35442400
C	0.57685200	-0.19627800	-0.29091100
C	0.91760700	1.20427800	0.16421600
C	-0.22548800	2.18354400	0.26359600
C	-1.46624900	1.59079500	0.93793900
H	1.41974400	-0.86947700	-0.10825100
H	-0.49187100	-0.96428600	1.40476400
H	-0.96611700	-1.67669900	-0.12906800
H	-2.14031300	0.44032700	-0.76235900
H	-2.73312400	-0.15305100	0.77904100
H	1.80555500	1.60457200	-0.32616400
H	0.11192800	3.10964300	0.74149900
H	-0.45524600	2.45118100	-0.77300400
H	-1.27833600	1.42767000	2.00507600
H	-2.28062100	2.31309300	0.87100800
S	0.39057100	-0.09862500	-2.12113100
C	2.10535400	0.15572300	-2.56676200
C	2.51733900	1.39792800	-3.04982700
C	3.01653000	-0.89676400	-2.46396300
C	3.84686400	1.58921000	-3.41585800

H	1.79611300	2.20065800	-3.15595000
C	4.34535000	-0.69405000	-2.81877600
H	2.67957000	-1.87322200	-2.13340700
C	4.76035000	0.54758200	-3.29388600
H	4.16472800	2.54963200	-3.80297400
H	5.05150400	-1.51233300	-2.74697000
H	5.79318500	0.69737100	-3.58362800
O	1.41938200	1.02133000	1.68180800
H	2.22399600	0.48182800	1.76506900
H	1.52941300	1.86076300	2.16063700

6

E = -2943.651145

ZPVE = 0.268626

Symbol	X	Y	Z
C	-1.89419800	0.24715900	0.36513200
C	-0.72303700	-0.73698900	0.39041800
C	0.52334000	-0.17227000	-0.29319100
C	0.85502400	1.22884800	0.13631300
C	-0.29381100	2.19282000	0.30067600
C	-1.49783200	1.57311800	1.01623100
H	1.38663400	-0.83019300	-0.16861200
H	-0.47248900	-0.96836400	1.43229500
H	-0.98977900	-1.68099200	-0.08699600
H	-2.21846900	0.42349900	-0.66627300
H	-2.74506400	-0.18745400	0.89124100
H	1.72560800	1.64381300	-0.37193800
H	0.05323400	3.11270300	0.78302600
H	-0.56956200	2.47993900	-0.71904700
H	-1.26508600	1.40353900	2.07324400
H	-2.32600500	2.28217400	0.98785200
C	2.15085300	0.17778400	-2.67603300
C	2.62171900	1.42278400	-3.09298000
C	3.01963700	-0.90962900	-2.57637300
C	3.97134100	1.58042100	-3.39769900
H	1.93588300	2.25606500	-3.19555600
C	4.36827200	-0.73992500	-2.87133700
H	2.64002700	-1.88515400	-2.29360200
C	4.84333100	0.50314100	-3.28117300
H	4.33688000	2.54321200	-3.73368600
H	5.04327900	-1.58437700	-2.80212200
H	5.89161200	0.62742100	-3.52383200
O	1.42706100	1.05448500	1.66194100
H	2.23752600	0.52093200	1.71332800
H	1.55606000	1.89559000	2.13191100
Se	0.28093300	-0.04973700	-2.26589600

7

E = -194.501516

ZPVE = 0.121855

Symbol	X	Y	Z
C	-0.76784900	1.51792600	-0.02805300
H	-0.19386100	0.58894100	-0.00672200
H	-1.83294200	1.26987400	-0.08461100
C	-0.49107900	2.30949100	1.21923100
H	-1.09899000	3.20720900	1.32335700
H	0.56481400	2.51241100	1.38547300
C	-0.37253100	2.36030100	-1.24822100
H	0.69121300	2.60198100	-1.23330000
H	-0.57492200	1.79605600	-2.15711800
H	-0.94335400	3.28897500	-1.29504200
O	-0.84942400	1.42131400	2.42113500
H	-0.76508400	1.83392900	3.29916600
H	-1.70497100	0.96401700	2.33246400

8

E = -651.883956

ZPVE = 0.223174

Symbol	X	Y	Z
C	-0.84022500	0.32328800	-0.78527800
C	-1.06703700	1.86673300	-0.65840300
H	-1.82182700	2.42709700	-1.20215700
C	-0.97679500	1.75196900	0.89662900
H	-1.65780400	2.21884600	1.60906200
C	-0.75209600	0.21292700	0.77373600
H	-1.25398600	-0.54153000	1.37095200
C	0.57629800	1.97836400	0.79845900
C	0.79093900	0.42318800	0.67904600
H	1.54245800	-0.13548900	1.23055600
C	0.69385400	0.54079000	-0.87538500
H	1.34021600	0.04036100	-1.58907100
C	0.47849200	2.08463200	-0.75860100
H	0.97001900	2.84025600	-1.36676100
C	-1.61761700	-0.59229400	-1.67046600
O	-2.91481900	-0.56279300	-1.35660200
O	-1.13649600	-1.26058000	-2.54207000
C	-3.76197200	-1.41404000	-2.14608000
H	-3.45162200	-2.45252400	-2.03643100
H	-4.76635600	-1.26734700	-1.76068100
H	-3.70269900	-1.12800900	-3.19559300
C	1.40348600	2.78902300	1.70573000
H	2.43601100	2.92298600	1.38629200
H	1.32264700	2.51129400	2.75718800
O	0.84380300	4.24010900	1.62669600
H	1.19697400	4.87346600	2.27605900

H	-0.13124000	4.24831500	1.62951300

9

E = -427.784198

ZPVE = 0.250619

Symbol	X	Y	Z
C	-2.51490700	-1.48388700	0.19993300
C	-1.02873500	-1.81205100	0.06551200
C	-0.13872000	-0.58221200	0.40441900
C	-0.90471800	0.73824000	0.55570800
C	-2.40166500	0.61858100	0.51599400
C	-2.72291800	-0.59068200	1.44575700
H	0.37050500	-0.75049500	1.35476800
H	-0.77576600	-2.62050200	0.75315000
H	-0.81245600	-2.18139100	-0.93852700
H	-3.13332900	-2.37611900	0.09893300
H	-0.56379100	1.32843600	1.40541500
H	-2.89129700	1.57621600	0.70097100
H	-2.06616800	-0.75729200	2.30192600
H	-3.75016600	-0.55665000	1.79561100
H	0.66501300	-0.47017200	-0.32961600
C	-2.89959900	-0.25769100	-0.68068000
C	-4.41105800	-0.11401300	-0.85567200
H	-4.95416500	-0.19326900	0.08580100
H	-4.65671500	0.85280600	-1.30281000
H	-4.78297400	-0.89730200	-1.52016500
C	-2.24459700	-0.12294600	-2.05723900
H	-1.16668000	-0.32685000	-2.06817900
H	-2.67599000	-0.84977300	-2.74945300
H	-2.45536900	0.86071100	-2.50130700
O	-0.53849600	1.73249500	-0.60537000
H	0.41365400	1.90680900	-0.69617500
H	-0.90781700	1.41855900	-1.45633500

10

E = -232.572632

ZPVE = 0.128007

Symbol	X	Y	Z
C	-1.92619700	0.91923200	0.08401900
C	-0.45920400	1.10459700	-0.08165600
C	-1.36960200	2.32303100	-0.01465100
H	-2.50500700	0.58326300	-0.76435300
H	-2.29076500	0.58528500	1.04669200
H	-0.01505300	0.88574900	-1.04280600
H	0.16592200	0.87898300	0.77589400

H	-1.56274700	2.86232200	-0.93338900
C	-1.36379800	3.13134600	1.21565100
H	-2.11796800	3.91267600	1.26889800
H	-1.30217500	2.54566200	2.13188500
O	-0.04653500	3.96507900	1.17829600
H	0.21314500	4.42384700	1.99667400
H	0.69199500	3.44829100	0.80518600

11

E = -349.207875

ZPVE = 0.189784

Symbol	X	Y	Z
C	-1.45863500	0.89913800	0.44946100
C	-0.03843900	1.34350600	0.38967200
C	-1.14594400	2.35267500	0.15962800
H	-1.86026500	0.32884600	-0.37595300
H	-1.87455600	0.65399300	1.41828300
H	0.55344300	1.06786500	-0.47203200
H	0.50669000	1.38277100	1.32661900
H	-1.31727800	2.70131100	-0.85161400
C	-1.47462700	3.31393700	1.22401800
H	-1.32636500	2.91393900	2.22965000
C	-2.68712600	4.13754800	1.09640800
C	-3.88169200	3.70356400	1.92071500
C	-3.15702700	4.95267900	2.28485400
H	-2.88727200	4.52055300	0.10304000
H	-3.76619200	2.84185700	2.56554000
H	-4.84399100	3.78344700	1.43547900
H	-3.62394900	5.90320000	2.06733100
H	-2.56101100	4.93145400	3.19087600
O	-0.25148700	4.42059300	1.12715800
H	-0.33366800	5.16736100	1.74361200
H	0.64117500	4.03699700	1.14812000

12

E = -192.059359

ZPVE = 0.073956

Symbol	X	Y	Z
C	-1.74844700	0.41703400	-0.60192500
H	-2.57405700	-0.25795600	-0.67796200
C	-0.82527600	1.17700000	-0.52497900
C	0.26674800	2.10487700	-0.43082700
H	0.67890600	2.40284900	-1.39295800
H	0.06284600	2.95507900	0.21896100

O	1.43362200	1.33972800	0.22295900
H	2.16255100	1.88114600	0.57872700
H	1.14190600	0.65798600	0.85841000

13

E = -693.313688

ZPVE = 0.271862

Symbol	X	Y	Z
C	1.37919900	0.36429900	-0.24911600
C	2.10435300	1.73972800	-0.16162100
C	-0.46874800	2.09884900	-0.02676300
C	-0.12807500	0.59784000	-0.08919700
H	1.56739700	-0.09473000	-1.22035300
H	1.75446900	-0.32233000	0.51622100
H	-0.75893300	0.03545300	-0.77259700
H	-1.54606800	2.26013200	0.02354800
H	3.18481100	1.61380100	-0.21658100
C	0.27215400	2.59730700	1.20261200
C	1.65883300	2.38882600	1.13269800
C	-0.31073400	3.13490000	2.34569500
C	2.46551500	2.74789700	2.20105300
C	0.51012200	3.49961600	3.41676000
H	-1.38240000	3.30108000	2.39153500
C	1.88460400	3.31006500	3.34066000
H	3.53863300	2.60058700	2.15057000
H	0.07208900	3.94097800	4.30326700
H	2.51344500	3.60257300	4.17260600
C	0.16253900	2.70920800	-1.26329500
C	-0.51639300	3.38757300	-2.26378300
C	1.54952000	2.55132300	-1.31552100
C	0.21174100	3.92093600	-3.32648500
H	-1.59259600	3.51180400	-2.21679000
C	2.27141300	3.07799500	-2.37457800
C	1.59306500	3.76813800	-3.37962800
H	-0.30225600	4.46027400	-4.11222000
H	3.34808600	2.95891900	-2.42052500
H	2.14865500	4.18936100	-4.20840400
O	-0.59761800	0.06542900	1.28478900
H	-0.26219300	-0.81852100	1.51154500
H	-0.33887400	0.73144600	1.97181900

<u>For Table 3 (RNH_3^+): B3LYP/6-311++G(d,p)</u>

1

E = -327.408763

ZPVE = 0.176736

Symbol	X	Y	Z

C	-0.72664000	-0.99290600	0.05198200
C	0.80635300	-0.99119400	-0.01854000
C	1.39054800	0.41624400	0.03049700
C	-0.62050500	1.29078900	1.07143500
C	-1.18383100	-0.11153700	1.21995000
H	2.46781600	0.41559500	0.20271600
H	1.21204100	-1.50846800	0.85623500
H	1.18578200	-1.52830300	-0.89352200
H	-1.16902600	-0.63220200	-0.88696600
H	-1.08091000	-2.01798800	0.17168800
H	-0.78402500	1.90713500	1.95273300
H	-1.06398500	1.80942200	0.21122900
H	-0.85014000	-0.54297000	2.16868600
H	-2.27406100	-0.04811400	1.26142700
O	0.83442900	1.29247800	0.91203600
N	1.28628400	1.07834200	-1.43019800
H	1.57171500	2.05912900	-1.35990900
H	1.89379900	0.60674500	-2.10496300
H	0.32915300	1.04850700	-1.78924100

2

E = -700.113487

ZPVE = 0.301911

Symbol	X	Y	Z
C	-1.94322800	0.57098800	0.42834600
C	-0.78987800	-0.42571400	0.24238200
C	0.52733000	0.24114200	-0.23320700
C	0.88676700	1.44736700	0.63356200
C	-0.26801900	2.42155600	0.88348800
C	-1.54990400	1.72203400	1.36287500
H	1.33935100	-0.49639000	-0.13196700
H	-0.62963700	-0.95773800	1.19416400
H	-1.07714200	-1.20991500	-0.46116800
H	-2.24135900	0.98217300	-0.54026400
H	-2.81822700	0.05064400	0.82542000
H	1.76434100	1.97356100	0.25325800
H	0.04107100	3.20936900	1.58014700
H	-0.46205200	2.92484700	-0.06686500
H	-1.42549400	1.34141300	2.38778200
H	-2.35379900	2.45841800	1.42926100
Si	0.66917300	0.57765600	-2.15664600
C	-0.60181700	1.79276800	-2.83239200
H	-0.53093800	2.78910500	-2.38743400
H	-0.42762400	1.91529200	-3.90653000
H	-1.62925200	1.43923300	-2.71605100
C	2.40835300	1.25189600	-2.44348800
H	2.60294500	1.31777700	-3.51830300
H	2.55123200	2.25952200	-2.04047400
H	3.18178200	0.60238600	-2.02123500
C	0.46885400	-1.09977300	-2.98251200

H	1.17793000	-1.83791600	-2.59625700
H	-0.53898300	-1.50713800	-2.86515000
H	0.65218700	-1.00562900	-4.05716400
N	1.37482000	0.93587400	2.03201800
H	2.18836600	0.32500700	1.92969800
H	1.62800000	1.71058400	2.65130200
H	0.63459900	0.39637200	2.48835300

3

E = -291.481557

ZPVE = 0.201490

Symbol	X	Y	Z
C	-4.46410400	-0.69691400	-0.05598200
C	-2.94439600	-0.83423800	0.00075100
C	-2.22153900	0.50864600	0.07578700
C	-2.73015200	1.30888900	1.29001900
C	-4.25577400	1.46733900	1.26150300
C	-4.96174300	0.10925900	1.15885800
H	-1.13825700	0.36120900	0.14560300
H	-2.64822400	-1.47645600	0.83480300
H	-4.74774200	-0.17252100	-0.97833000
H	-4.94081700	-1.68300300	-0.07774500
H	-2.42539700	0.79933600	2.21137700
H	-2.23923400	2.28423600	1.29920000
H	-4.58966300	1.99022000	2.16056300
H	-4.54442500	2.09735000	0.41157100
H	-4.78838400	-0.47098600	2.07245000
H	-6.04270600	0.23963800	1.07573000
H	-2.41880800	1.07965700	-0.84135300
N	-2.46220000	-1.59463400	-1.25179100
H	-1.44688100	-1.73028400	-1.23975600
H	-2.90636200	-2.51482600	-1.32526700
H	-2.69519600	-1.06881300	-2.09999600

4

E = -291.479719

ZPVE = 0.201389

Symbol	X	Y	Z
C	-0.68047200	-0.97967100	0.02095200
C	0.85729300	-1.00655100	-0.01706700
C	1.47916000	0.39268400	-0.01675700
C	-0.62814500	1.31514900	1.10472800
C	-1.20279500	-0.10674900	1.17057000
H	2.56777400	0.33842000	0.04549000
H	1.23519700	-1.50788300	0.87936700
H	1.22834300	-1.59318200	-0.86509000

H	-1.08810400	-0.61707600	-0.93468400
H	-1.04891900	-2.00323800	0.11607000
H	-0.95963300	1.90504100	1.96183300
H	-1.03223100	1.83796400	0.22482400
H	-0.92573400	-0.56480900	2.12708600
H	-2.29423300	-0.07171600	1.14912300
C	0.91001700	1.30418900	1.07398300
H	1.31756000	2.31725300	0.98131100
H	1.29065800	0.91636800	2.02395800
N	1.22189200	1.04901500	-1.39457000
H	1.64350700	1.98035500	-1.44611000
H	1.60832200	0.48109500	-2.15349000
H	0.21677900	1.15166600	-1.56209500

5

E = -920.715006

ZPVE = 0.282776

Symbol	X	Y	Z
C	-1.80371500	0.02063300	0.19831100
C	-0.41513600	-0.50397200	-0.19350200
C	0.58794600	0.61892500	-0.51779800
C	0.61942500	1.70659600	0.56787700
C	-0.76155600	2.17888700	1.02716200
C	-1.71491100	1.01967300	1.35931800
H	1.58937600	0.19560300	-0.64408100
H	-0.01419200	-1.11676000	0.62844800
H	-0.47810600	-1.17748800	-1.05040900
H	-2.27419600	0.50400300	-0.66370300
H	-2.44658800	-0.81902300	0.47169100
H	1.24085600	2.54390200	0.24572300
H	-0.66328100	2.87458000	1.86823800
H	-1.17281300	2.76138700	0.19928000
H	-1.39622300	0.49679800	2.27416900
H	-2.70047600	1.42783000	1.59294900
S	0.16773400	1.39589600	-2.15178800
C	1.69467800	2.28379100	-2.49947200
C	1.71719100	3.68057100	-2.42371200
C	2.83657800	1.58776800	-2.91404400
C	2.88417800	4.37475500	-2.74399300
H	0.82172300	4.22050500	-2.13866100
C	4.00208200	2.28710500	-3.21842000
H	2.80451800	0.50963400	-3.02342200
C	4.02711100	3.67970800	-3.13356900
H	2.89478900	5.45744900	-2.69655200
H	4.88260400	1.74652300	-3.54575100
H	4.93090700	4.22125900	-3.38673300
N	1.38052500	1.14301800	1.80083300
H	2.31468300	0.81655800	1.53912400
H	1.48391100	1.85877100	2.52531800
H	0.87370000	0.35402500	2.21183200

6

E = -2924.048447

ZPVE = 0.281391

Symbol	X	Y	Z
C	-1.93728900	0.19540100	0.35049000
C	-0.76970900	-0.80041800	0.30417100
C	0.50657700	-0.20525000	-0.31323400
C	0.87748200	1.15394600	0.28798900
C	-0.29531900	2.12800500	0.42440700
C	-1.53645200	1.49010400	1.06952500
H	1.34170500	-0.90259300	-0.20778900
H	-0.55006100	-1.14381200	1.32762100
H	-1.04580500	-1.70188600	-0.24631000
H	-2.26654700	0.43084400	-0.66708000
H	-2.79134500	-0.26540400	0.85179900
H	1.70791800	1.60266600	-0.25937800
H	0.02084000	3.02841100	0.96321200
H	-0.53845200	2.45270900	-0.59016000
H	-1.36286700	1.28093000	2.13621300
H	-2.35584600	2.21176500	1.05010300
C	2.19335900	0.18729700	-2.72656000
C	2.70105100	1.44027600	-3.08396600
C	3.02652700	-0.93660100	-2.73158700
C	4.04724400	1.56860100	-3.42901300
H	2.04752400	2.30422000	-3.11326900
C	4.37238600	-0.79714400	-3.06614600
H	2.62303900	-1.91566000	-2.50043700
C	4.88291100	0.45368500	-3.41419100
H	4.43718200	2.53787600	-3.71755500
H	5.01582100	-1.66934200	-3.07654000
H	5.92643600	0.55510700	-3.68819500
Se	0.30649800	-0.00318600	-2.30525500
N	1.47514200	0.91276800	1.70944200
H	2.26908500	0.26839300	1.66805800
H	1.79698000	1.79083000	2.12561700
H	0.77268200	0.50914900	2.33518300

7

E = -174.772542

ZPVE = 0.135885

Symbol	X	Y	Z
C	-0.83700100	1.57999500	-0.07517000
H	-0.41678200	0.56938000	-0.13450000
H	-1.92850600	1.47950500	-0.07081600

C	-0.38056600	2.24803200	1.21446200
H	-0.81372300	3.24060200	1.34476000
H	0.70545300	2.32440800	1.28169000
C	-0.39974700	2.39216700	-1.30132100
H	0.68777100	2.48309700	-1.35370700
H	-0.73590800	1.89758300	-2.21314800
H	-0.82958000	3.39656500	-1.28972500
N	-0.82103500	1.43398200	2.43417200
H	-0.52259000	1.86754100	3.31307200
H	-1.84109200	1.33996000	2.46255200
H	-0.42923100	0.48756100	2.40365600

8

E = -632.305183

ZPVE = 0.235172

Symbol	X	Y	Z
C	-0.86714500	0.32321300	-0.80580400
C	-1.09117700	1.88309000	-0.69106600
H	-1.82572800	2.44397000	-1.26368900
C	-1.05033300	1.77495200	0.87255400
H	-1.75391400	2.25339100	1.55528300
C	-0.82846100	0.22687100	0.76604400
H	-1.35143300	-0.52119700	1.35469500
C	0.51504700	1.99451200	0.83646500
C	0.72514900	0.43654900	0.72295200
H	1.45470100	-0.13202600	1.29614100
C	0.67943100	0.54517800	-0.84189100
H	1.35253200	0.04772100	-1.53368800
C	0.46283900	2.09672800	-0.74023400
H	0.97704500	2.83460400	-1.35792800
C	-1.61070300	-0.57387500	-1.74116400
O	-2.89396300	-0.70146900	-1.36449300
O	-1.12199800	-1.09646100	-2.71236800
C	-3.72947700	-1.53260500	-2.20688900
H	-3.33774800	-2.54922400	-2.23594000
H	-4.71378200	-1.51070600	-1.74665600
H	-3.76441500	-1.12708900	-3.21799500
C	1.32252600	2.84650500	1.75869300
H	2.38966700	2.82446300	1.52538500
H	1.17953100	2.58526200	2.80985100
N	0.89458500	4.31804900	1.62836700
H	1.43108200	4.93627000	2.24349400
H	1.02110000	4.63981700	0.66377900
H	-0.09819700	4.42185400	1.85938000

9

E = -408.137544

ZPVE = 0.262989

Symbol	X	Y	Z
C	-2.54452300	-1.50850300	0.21761500
C	-1.05500300	-1.85097400	0.11237800
C	-0.13400300	-0.60353100	0.31700600
C	-0.89697600	0.72736000	0.56915700
C	-2.41397700	0.59499900	0.51450400
C	-2.76265700	-0.59692100	1.45485200
H	0.53719800	-0.77230400	1.16006900
H	-0.81224500	-2.59895400	0.87039400
H	-0.83965000	-2.31347500	-0.85353500
H	-3.16115800	-2.40402100	0.12549700
H	-0.60715400	1.16005900	1.52901400
H	-2.90834100	1.55608700	0.69546600
H	-2.11562900	-0.75939400	2.32031700
H	-3.79322400	-0.56010400	1.79778700
H	0.52172300	-0.49336800	-0.55240300
C	-2.92683600	-0.28416900	-0.68801500
C	-4.44613200	-0.13667400	-0.86017400
H	-4.99334500	-0.20546300	0.08040100
H	-4.69336700	0.82653000	-1.31716800
H	-4.82614700	-0.92190100	-1.51908300
C	-2.28170700	-0.16222600	-2.07473500
H	-1.20288400	-0.34655900	-2.09267500
H	-2.71440200	-0.90068100	-2.75494500
H	-2.49147800	0.81644600	-2.52592400
N	-0.43812300	1.79465700	-0.45280600
H	-0.89146300	2.69398700	-0.26830900
H	0.57491800	1.93674700	-0.42160500
H	-0.69339800	1.50146300	-1.40141700

10

E = -212.846569

ZPVE = 0.141783

Symbol	X	Y	Z
C	-1.98133800	0.88954900	0.03949700
C	-0.51117800	1.07164200	-0.19231500
C	-1.40542500	2.28862700	-0.00407900
H	-2.60579700	0.59295800	-0.79258500
H	-2.29986100	0.49916500	0.99870400
H	-0.11490000	0.89193800	-1.18335100
H	0.15727300	0.78903600	0.61499000
H	-1.64132800	2.86881300	-0.89134600
C	-1.33436400	3.07974800	1.26392300
H	-2.19052900	3.74027600	1.40968000
H	-1.21756200	2.44672800	2.14432900
N	-0.09762000	3.99728400	1.24401700
H	-0.15786700	4.67227100	0.47604600

H	0.01360000	4.52305000	2.11612700
H	0.74908800	3.44027300	1.09159600

11

E = -329.521551

ZPVE = 0.203488

Symbol	X	Y	Z
C	-1.46984800	0.91308700	0.49823300
C	-0.02317700	1.30988600	0.43875600
C	-1.10682500	2.35048500	0.20675800
H	-1.88314900	0.33399000	-0.31683700
H	-1.89048100	0.68030100	1.46903200
H	0.56628800	0.99894800	-0.41425400
H	0.52380300	1.32838100	1.37644200
H	-1.25943300	2.67832600	-0.81818300
C	-1.38542100	3.40571900	1.24066600
H	-1.29496600	2.99397400	2.24952100
C	-2.68139900	4.15113300	1.08289700
C	-3.89872800	3.69245100	1.85141700
C	-3.23539600	4.98605000	2.22612500
H	-2.86728700	4.51522700	0.07584800
H	-3.78841200	2.85349100	2.52782700
H	-4.84919100	3.72700600	1.33572500
H	-3.73061200	5.91553800	1.97595400
H	-2.69090200	5.00912400	3.16516800
N	-0.22731000	4.45440500	1.16668000
H	0.68313900	4.00516500	1.29756900
H	-0.22199400	4.90602000	0.24802000
H	-0.34934500	5.18606400	1.87212500

12

E = -172.317075

ZPVE = 0.088498

Symbol	X	Y	Z
C	-1.88209800	0.50436200	-0.45759000
H	-2.75812600	-0.10285300	-0.41460000
C	-0.90198700	1.19465700	-0.51095200
C	0.27280400	2.03326400	-0.58188100
H	0.63141400	2.16482100	-1.60490500
H	0.11283900	3.01579600	-0.13295100
N	1.42450300	1.38164400	0.20056300
H	2.27590800	1.95246500	0.17079500
H	1.16002500	1.24738400	1.18218200
H	1.64213700	0.45697600	-0.18565600

13

E = -673.756293

ZPVE = 0.284102

Symbol	X	Y	Z
C	1.39325600	0.35138000	-0.22420500
C	2.10894800	1.73931300	-0.15640300
C	-0.46070300	2.09551000	-0.01586200
C	-0.13778900	0.57295800	-0.11308500
H	1.62508400	-0.14410000	-1.16776300
H	1.75956800	-0.29627500	0.57967300
H	-0.68653400	0.10307600	-0.92874900
H	-1.53822300	2.27238800	0.03271200
H	3.18989600	1.61387500	-0.21392800
C	0.27799500	2.59656600	1.21596600
C	1.66783900	2.39878900	1.13913200
C	-0.29391600	3.18134900	2.34383000
C	2.48391400	2.79406000	2.19296300
C	0.53321200	3.58328300	3.39797700
H	-1.36435500	3.35630500	2.39415200
C	1.91090100	3.39030200	3.32085500
H	3.55808700	2.65402800	2.13799300
H	0.10083000	4.05722700	4.27103500
H	2.54571800	3.71197100	4.13796600
C	0.16416400	2.72336300	-1.25129300
C	-0.51230700	3.42191600	-2.24424300
C	1.55296100	2.55116100	-1.31469900
C	0.21483300	3.95883900	-3.30963000
H	-1.58702800	3.56079200	-2.19176400
C	2.27352800	3.08204700	-2.37743900
C	1.59666800	3.79022200	-3.37441200
H	-0.29893200	4.51291900	-4.08600400
H	3.34923700	2.95491500	-2.43272100
H	2.15243700	4.21382600	-4.20251600
N	-0.66114900	-0.10139000	1.16588100
H	-1.68293500	-0.06452300	1.21852800
H	-0.37269100	-1.08066100	1.23070000
H	-0.28757200	0.41315200	1.97709600

<u>For Table 3 (RNH_3^+): M06-2X/6-311++G(d,p)</u>

1

E = -327.252768

ZPVE = 0.178877

Symbol	X	Y	Z
C	-0.71174900	-0.98019600	0.03270100
C	0.81772600	-0.99564800	-0.00868100
C	1.39881800	0.40866800	0.03214400

C	-0.58871200	1.29069900	1.04825800
C	-1.16805300	-0.10223900	1.19731700
H	2.47806000	0.41003100	0.18829400
H	1.19998300	-1.50129400	0.88202600
H	1.21113700	-1.54012700	-0.87172800
H	-1.13614800	-0.60495800	-0.90841500
H	-1.08067700	-2.00031100	0.13909900
H	-0.78065100	1.91987500	1.91397100
H	-1.00885800	1.79675000	0.16758900
H	-0.83395500	-0.53487000	2.14443100
H	-2.25638300	-0.03013300	1.23436300
O	0.85254500	1.27160200	0.93395400
N	1.23712600	1.06558100	-1.38553100
H	1.51099500	2.05088600	-1.32283800
H	1.81948400	0.60347100	-2.08852900
H	0.26410700	1.02291800	-1.70115000

2

E = -699.861362

ZPVE = 0.305212

Symbol	X	Y	Z
C	-1.80941000	0.23853300	0.35234100
C	-0.50268300	-0.55356800	0.30736400
C	0.67571400	0.30589500	-0.19241800
C	0.79995800	1.59648900	0.60779000
C	-0.51185200	2.36135700	0.78251900
C	-1.66401100	1.46658700	1.25220600
H	1.60771100	-0.26581700	-0.06744300
H	-0.30225300	-0.95961000	1.31154700
H	-0.60620900	-1.43177800	-0.33180200
H	-2.08139500	0.55891600	-0.65955700
H	-2.62175700	-0.39575700	0.71098400
H	1.58057000	2.24965300	0.20853400
H	-0.36626100	3.21226200	1.45649000
H	-0.76191800	2.78535700	-0.19116700
H	-1.51364200	1.14037900	2.29135500
H	-2.58376800	2.05327100	1.26427500
Si	0.70394400	0.61267800	-2.11026600
C	-0.27496100	2.12020400	-2.65185500
H	0.13907300	3.05557900	-2.26545500
H	-0.21742000	2.18114700	-3.74287400
H	-1.33439800	2.07244000	-2.39053000
C	2.50981300	0.88022700	-2.53776800
H	2.62118000	1.07406100	-3.60763000
H	2.93828100	1.74025200	-2.01437000
H	3.11567600	0.00199800	-2.30059500
C	0.02779500	-0.93241000	-2.91551900
H	0.55263200	-1.83134200	-2.58174500
H	-1.03858600	-1.06584600	-2.71584000
H	0.15047900	-0.86579100	-3.99961000

N	1.31013900	1.24682200	2.02432100
H	2.21346600	0.76921500	1.97966800
H	1.40879700	2.07983800	2.61096000
H	0.64504500	0.61553200	2.48103700

3

E = -291.329110

ZPVE = 0.203390

Symbol	X	Y	Z
C	-4.45970600	-0.69042600	-0.05938400
C	-2.94569200	-0.83233100	0.00647000
C	-2.22902100	0.50887000	0.07171500
C	-2.73145700	1.29692600	1.28887500
C	-4.25141400	1.46071000	1.24855100
C	-4.95103200	0.10385100	1.15824100
H	-1.14537300	0.36612400	0.12835800
H	-2.65460200	-1.46595200	0.84900500
H	-4.73122400	-0.15029200	-0.97593000
H	-4.93921700	-1.67365700	-0.09416500
H	-2.43891600	0.77149200	2.20444300
H	-2.23653700	2.26854400	1.31105700
H	-4.59041900	1.99426300	2.13776000
H	-4.53083500	2.07524900	0.38537200
H	-4.75734700	-0.47475900	2.06794500
H	-6.03223600	0.22833800	1.08771000
H	-2.44700800	1.07832300	-0.84133800
N	-2.46839000	-1.58512800	-1.23405800
H	-1.45286500	-1.71890400	-1.22444400
H	-2.91402600	-2.50433500	-1.30987900
H	-2.70468400	-1.05380200	-2.07830700

4

E = -291.328273

ZPVE = 0.203415

Symbol	X	Y	Z
C	-0.66816800	-0.96649300	0.00649200
C	0.86466900	-1.00476300	-0.00822400
C	1.48164900	0.39136300	-0.01378300
C	-0.61625900	1.31723300	1.08592000
C	-1.18883800	-0.10001200	1.15511800
H	2.57064000	0.34312900	0.03594400
H	1.22297600	-1.49554400	0.90115900
H	1.24615300	-1.59705400	-0.84612000
H	-1.06332200	-0.59313200	-0.94933400
H	-1.04550300	-1.98637400	0.09193200
H	-0.95655600	1.91207300	1.93455600

H	-1.00837400	1.83324600	0.19761100
H	-0.90101300	-0.55709400	2.10805800
H	-2.27909600	-0.06700600	1.13773200
C	0.91702400	1.29586300	1.07846500
H	1.33476200	2.30440400	0.99635800
H	1.27790300	0.89214300	2.02874600
N	1.19001500	1.03864000	-1.37086300
H	1.59665600	1.97621500	-1.43139100
H	1.56265200	0.47477300	-2.13984500
H	0.17826700	1.12671400	-1.50910200

5

E = -920.442768

ZPVE = 0.285822

Symbol	X	Y	Z
C	-1.78820300	0.09434200	0.19822600
C	-0.43383100	-0.51599900	-0.16999900
C	0.60171900	0.54588000	-0.56464600
C	0.70315700	1.66550300	0.47580400
C	-0.64522800	2.22675800	0.91586400
C	-1.63739300	1.12854900	1.31477700
H	1.58398500	0.08072200	-0.70048100
H	-0.05377800	-1.10034700	0.68087300
H	-0.53408800	-1.22843300	-0.99057100
H	-2.22871300	0.57244900	-0.68181000
H	-2.47391700	-0.69650200	0.50554800
H	1.36974100	2.45427800	0.11984200
H	-0.50515800	2.95786100	1.71856200
H	-1.04072100	2.77762300	0.05923500
H	-1.32451800	0.62785400	2.24297600
H	-2.59907900	1.58822300	1.54642300
S	0.15073900	1.26658000	-2.19199800
C	1.63417100	2.22001000	-2.49137500
C	1.58972000	3.61213000	-2.41515300
C	2.82519600	1.57297400	-2.82566100
C	2.74183900	4.35454400	-2.66061600
H	0.65403700	4.10817200	-2.18274800
C	3.97496300	2.31993300	-3.05570400
H	2.84163000	0.49365500	-2.93093900
C	3.93375600	3.70962800	-2.97297900
H	2.70407700	5.43612500	-2.61438600
H	4.89705200	1.81851100	-3.32379900
H	4.82758300	4.28941400	-3.16814600
N	1.41287400	1.09537800	1.71069000
H	2.32849300	0.70875000	1.46500200
H	1.54923800	1.81875900	2.42213800
H	0.85397700	0.34558700	2.12971600

6

E = -2923.809188

ZPVE = 0.284688

Symbol	X	Y	Z
C	-1.89971600	0.27897800	0.32538000
C	-0.80999600	-0.79575100	0.32257500
C	0.48656500	-0.31575500	-0.34100200
C	0.95929600	1.02887900	0.21082600
C	-0.13691800	2.08608900	0.30524200
C	-1.40146800	1.56144500	0.99413100
H	1.27657100	-1.06340600	-0.22350200
H	-0.60145700	-1.10066700	1.35929900
H	-1.15240600	-1.70121500	-0.18136000
H	-2.20429500	0.50145100	-0.70214200
H	-2.78380400	-0.09747700	0.84194200
H	1.82158400	1.39308900	-0.35220200
H	0.24824400	2.98493100	0.79739100
H	-0.37538200	2.37219800	-0.72175500
H	-1.22339100	1.37426300	2.06337900
H	-2.16901900	2.33582200	0.96177400
C	2.09894400	0.15109100	-2.69743200
C	2.52361900	1.42341300	-3.07990000
C	3.01249000	-0.90018800	-2.61045000
C	3.86905200	1.64416800	-3.36446600
H	1.80498100	2.23011400	-3.16910400
C	4.35669500	-0.66820500	-2.88363100
H	2.67012800	-1.89718000	-2.35637200
C	4.78451900	0.60228600	-3.26019900
H	4.19768600	2.62878300	-3.67447200
H	5.06549500	-1.48543900	-2.82508300
H	5.82941000	0.77557800	-3.48701500
Se	0.23828600	-0.15822700	-2.30153500
N	1.50910600	0.78673200	1.62660800
H	2.25882500	0.08984000	1.61557800
H	1.87856200	1.65172000	2.03067700
H	0.76649300	0.44432200	2.24398700

7

E = -174.667393

ZPVE = 0.137046

Symbol	X	Y	Z
C	-0.84095900	1.57473700	-0.06960600
H	-0.41899200	0.56596200	-0.12564600
H	-1.93148700	1.47715700	-0.06176300
C	-0.38052200	2.24908800	1.21027400
H	-0.81503600	3.24149100	1.33327100
H	0.70552100	2.32572500	1.26871400
C	-0.40178300	2.38902500	-1.28704000

H	0.68508000	2.47855000	-1.33027800
H	-0.73414200	1.90137500	-2.20227500
H	-0.83135800	3.39212100	-1.26638200
N	-0.81680200	1.43929400	2.41974200
H	-0.52042000	1.86788600	3.30134700
H	-1.83685300	1.34468800	2.44324300
H	-0.42478600	0.49328000	2.38237700

8

E = -632.048668

ZPVE = 0.238472

Symbol	X	Y	Z
C	-0.84479800	0.32539500	-0.78924400
C	-1.08731600	1.86633700	-0.65685600
H	-1.83793100	2.41968600	-1.21387200
C	-1.02116000	1.74205900	0.89844900
H	-1.71484800	2.20451100	1.60062000
C	-0.78682000	0.20431100	0.77003900
H	-1.29847700	-0.55716900	1.34983600
C	0.53137200	1.96854700	0.83904000
C	0.75799100	0.42735400	0.70983900
H	1.50053900	-0.13695500	1.26786300
C	0.68870200	0.55273300	-0.84646300
H	1.35026700	0.06609700	-1.55585100
C	0.45844400	2.09480900	-0.72385600
H	0.96072200	2.84482800	-1.33530000
C	-1.59702900	-0.58372800	-1.70139400
O	-2.89667900	-0.59167900	-1.39452900
O	-1.09848800	-1.21705600	-2.58962400
C	-3.71987900	-1.43957200	-2.21149400
H	-3.38795500	-2.47377300	-2.12702500
H	-4.72967000	-1.32501500	-1.82921000
H	-3.66061700	-1.12536800	-3.25297300
C	1.32359200	2.84859500	1.74643900
H	2.38620600	2.86274000	1.49669600
H	1.19756400	2.59306100	2.80019900
N	0.82220700	4.27676700	1.58387100
H	1.32287300	4.94515500	2.17553700
H	0.92321300	4.57122600	0.60705400
H	-0.17526700	4.32445000	1.81549000

9

E = -407.941781

ZPVE = 0.266026

Symbol	X	Y	Z

C	-2.54686400	-1.49941700	0.21435900
C	-1.06316800	-1.84206000	0.09909300
C	-0.14670600	-0.60018200	0.31312200
C	-0.90493700	0.72747000	0.56592100
C	-2.41687200	0.59406400	0.51673900
C	-2.75600300	-0.59603600	1.45214100
H	0.51631400	-0.77343000	1.16066900
H	-0.81788500	-2.59655100	0.84825100
H	-0.85666700	-2.29110000	-0.87445000
H	-3.16885200	-2.38995100	0.11695700
H	-0.61199300	1.16014900	1.52469800
H	-2.91412700	1.55349800	0.69582600
H	-2.09371200	-0.75977900	2.30549000
H	-3.78265600	-0.56399400	1.80454700
H	0.51490200	-0.48520000	-0.55099500
C	-2.91767700	-0.27884600	-0.67983200
C	-4.42871900	-0.12802600	-0.85763700
H	-4.97436400	-0.19343800	0.08360000
H	-4.66764300	0.83530600	-1.31660600
H	-4.80568900	-0.91477600	-1.51515400
C	-2.26147400	-0.16697500	-2.05581000
H	-1.18311400	-0.35473700	-2.05821600
H	-2.69075800	-0.91351900	-2.72842900
H	-2.46898900	0.80726300	-2.51611100
N	-0.46344000	1.77946500	-0.45655900
H	-0.92079500	2.67707200	-0.27375000
H	0.54927600	1.92535200	-0.43578400
H	-0.72736700	1.47749300	-1.40041600

10

E = -212.735383

ZPVE = 0.143258

Symbol	X	Y	Z
C	-1.97000000	0.90151800	0.04260800
C	-0.50542300	1.10818100	-0.17928000
C	-1.42170100	2.30115800	-0.00914000
H	-2.57625200	0.58400900	-0.79358500
H	-2.28565400	0.51822600	1.00450600
H	-0.10216500	0.92392700	-1.16528300
H	0.15728000	0.84749100	0.63942100
H	-1.65892100	2.87847600	-0.89638700
C	-1.34794200	3.08182000	1.26277100
H	-2.19316900	3.75374800	1.41263200
H	-1.24088200	2.43423100	2.13380000
N	-0.10109900	3.96155400	1.23678300
H	-0.15436300	4.63902000	0.47051100
H	0.03759900	4.47975900	2.10892000
H	0.72488200	3.37824000	1.06695600

11

E = -329.363579

ZPVE = 0.205778

Symbol	X	Y	Z
C	-1.48557200	0.94360900	0.51214600
C	-0.03827700	1.32628300	0.46585900
C	-1.10529800	2.36303200	0.19983800
H	-1.88639500	0.35108200	-0.29772400
H	-1.92132300	0.74135100	1.48240200
H	0.55689400	0.99005300	-0.37174000
H	0.49000900	1.36475300	1.41271100
H	-1.24457200	2.68534400	-0.82797000
C	-1.38060000	3.41594700	1.23027500
H	-1.29880100	2.99817000	2.23854500
C	-2.67549200	4.15359800	1.06933100
C	-3.87195400	3.66699800	1.83659000
C	-3.21951300	4.95702100	2.22820000
H	-2.86345600	4.52916200	0.06770300
H	-3.73661600	2.81610800	2.49222500
H	-4.82860100	3.70618700	1.33566700
H	-3.73203300	5.88170100	2.00201500
H	-2.65989000	4.96320800	3.15768000
N	-0.24138400	4.45189200	1.15323200
H	0.67076600	4.00421800	1.28122800
H	-0.24286700	4.89848400	0.23151000
H	-0.36566900	5.18657300	1.85576800

12

E = -172.228051

ZPVE = 0.089496

Symbol	X	Y	Z
C	-1.86177000	0.49726900	-0.44667700
H	-2.73011900	-0.12294000	-0.39859100
C	-0.89499700	1.20094500	-0.50765200
C	0.27987500	2.04856800	-0.57765700
H	0.62761900	2.18798300	-1.60191100
H	0.11415100	3.02249200	-0.11565200
N	1.41276300	1.38100300	0.18842400
H	2.27131000	1.94074900	0.17113700
H	1.14105200	1.23290200	1.16619400
H	1.61753500	0.45954600	-0.21260900

13

E = -673.471620

ZPVE = 0.286952

Symbol	X	Y	Z
C	1.39311800	0.37314300	-0.23447800
C	2.10569500	1.75468700	-0.15968200
C	-0.46158800	2.10946500	-0.02409900
C	-0.13214200	0.59327200	-0.10519400
H	1.61526800	-0.10761100	-1.18709600
H	1.76461200	-0.28119200	0.56088100
H	-0.69306400	0.11110500	-0.90517900
H	-1.53957000	2.28342000	0.02354500
H	3.18710000	1.63457800	-0.21430900
C	0.27358900	2.61211400	1.20275300
C	1.65832200	2.40442400	1.13366100
C	-0.30447900	3.17325900	2.33461400
C	2.46724600	2.76845600	2.20024800
C	0.51508600	3.54521300	3.40225200
H	-1.37489200	3.34928100	2.37784200
C	1.88912800	3.34325800	3.33351400
H	3.54007500	2.61857100	2.14962600
H	0.07891600	4.00217700	4.28187800
H	2.51811300	3.64115400	4.16341000
C	0.16383100	2.72800300	-1.25778700
C	-0.51283700	3.41129100	-2.25618600
C	1.54978800	2.56028100	-1.31612500
C	0.21380400	3.93715000	-3.32402500
H	-1.58783900	3.54560400	-2.20465900
C	2.27003700	3.07898900	-2.38055800
C	1.59328300	3.77254800	-3.38426000
H	-0.29974400	4.48028000	-4.10751800
H	3.34578400	2.95251200	-2.43031600
H	2.14845800	4.18820900	-4.21612200
N	-0.61920700	-0.05143200	1.18742400
H	-1.63342100	0.04209400	1.29358700
H	-0.37949700	-1.04469500	1.23440400
H	-0.17802900	0.43897600	1.97969300

<u>For Table 4 (ROH): MP2/6-31+G(d)</u>

1

E = -345.756157

ZPVE = 0.154109

Symbol	X	Y	Z
C	-0.66341800	-0.96166800	-0.00647900
C	0.86504000	-0.97852400	-0.00325600
C	1.42668700	0.43248800	-0.00386400
C	-0.54333800	1.30110400	1.04089000
C	-1.16482600	-0.08227600	1.13915900
H	2.50722400	0.44069900	0.18137000

H	1.23065100	-1.47893300	0.90221000
H	1.26589500	-1.51563700	-0.86981600
H	-1.02561700	-0.56741400	-0.96336700
H	-1.05039900	-1.98292100	0.09086200
H	-0.78995600	1.92532400	1.90320300
H	-0.88032700	1.81072400	0.12862600
H	-0.88876100	-0.52970300	2.10312400
H	-2.25870800	0.00814900	1.11936200
O	0.89798500	1.22987600	1.04701300
O	1.13728400	0.99795300	-1.27722900
H	1.49510300	1.90615500	-1.27672700

2

E = -717.458472

ZPVE = 0.281421

Symbol	X	Y	Z
C	-1.85432700	0.31862400	0.39896200
C	-0.58038400	-0.52080400	0.30295700
C	0.62305100	0.30175800	-0.19428300
C	0.82025000	1.55045500	0.66347900
C	-0.46087300	2.36876400	0.83090800
C	-1.63381400	1.51896000	1.31974600
H	1.52969100	-0.30628800	-0.03150900
H	-0.34954500	-0.91851000	1.30050200
H	-0.74158000	-1.38861700	-0.34852000
H	-2.15439100	0.66937300	-0.59933400
H	-2.68184700	-0.29737600	0.77463700
H	1.60554800	2.18899000	0.22603800
H	-0.26837700	3.19825600	1.52783000
H	-0.71618600	2.83009700	-0.13109100
H	-1.42844600	1.15774700	2.33547800
H	-2.53970400	2.13630800	1.37573400
Si	0.69869300	0.61740100	-2.07839600
C	-0.33957900	2.06118300	-2.72429600
H	0.00764300	3.02639500	-2.33915500
H	-0.25282800	2.10025300	-3.81770800
H	-1.40334300	1.96343800	-2.48368300
C	2.50166000	0.97512800	-2.51730000
H	2.61833500	1.13552300	-3.59573000
H	2.87309800	1.87311300	-2.01002900
H	3.15327000	0.14083000	-2.23279400
C	0.14655400	-0.95281300	-2.96895500
H	0.68380500	-1.83540200	-2.60258700
H	-0.92592700	-1.13792800	-2.84117200
H	0.34077900	-0.86963900	-4.04496300
O	1.28855000	1.07733200	1.94919400
H	1.38890400	1.84896100	2.53842200

3

E = -309.863011

ZPVE = 0.177863

Symbol	X	Y	Z
C	-4.35743300	-0.83992800	0.02693800
C	-2.83999100	-0.88259900	0.04748500
C	-2.24854400	0.52129800	0.01101000
C	-2.77949600	1.37411900	1.16650900
C	-4.30847200	1.41927600	1.15548000
C	-4.89971800	0.00852600	1.17960200
H	-1.15091000	0.46630900	0.04652500
H	-2.50676000	-1.39325200	0.96745600
H	-4.67031400	-0.41559900	-0.93713200
H	-4.74642300	-1.86397700	0.06957900
H	-2.43537900	0.95218100	2.12217700
H	-2.36449800	2.38769900	1.10551200
H	-4.67652100	2.00069300	2.01032300
H	-4.64879300	1.93982600	0.24870100
H	-4.65254400	-0.47193500	2.13762100
H	-5.99445000	0.05174500	1.12666100
H	-2.51769600	0.97628700	-0.95239000
O	-2.43737800	-1.65953200	-1.09443300
H	-1.46289500	-1.68253400	-1.11832300

4

E = -309.862240

ZPVE = 0.177991

Symbol	X	Y	Z
C	-0.65157000	-0.94079300	-0.01290300
C	0.87766700	-0.97814100	-0.01118400
C	1.47783000	0.42071700	-0.03607700
C	-0.60177900	1.32595300	1.09027700
C	-1.18152500	-0.08879600	1.14199500
H	2.57350500	0.35106100	0.04951600
H	1.23605400	-1.49060700	0.89311500
H	1.25648800	-1.53759400	-0.87465700
H	-1.00083300	-0.52509600	-0.96564100
H	-1.04565200	-1.96272200	0.05575000
H	-0.96091500	1.91920600	1.94089400
H	-0.95215200	1.82715800	0.17936400
H	-0.90834100	-0.55934900	2.09876300
H	-2.27785300	-0.04926200	1.11335200
O	1.14208100	0.97264800	-1.32558300
H	1.50968000	1.87416300	-1.37544700
C	0.92729100	1.28885300	1.09436900
H	1.34187400	2.30448900	1.01541700
H	1.28744400	0.88101600	2.05047400

5

E = -937.737108

ZPVE = 0.259490

Symbol	X	Y	Z
C	-1.80653100	0.16809500	0.21672000
C	-0.47310500	-0.48825200	-0.14783300
C	0.59299300	0.53360600	-0.55420200
C	0.74521100	1.63338500	0.49527800
C	-0.58704300	2.26599500	0.88646300
C	-1.61416400	1.21670300	1.31333900
H	1.56180700	0.02880000	-0.64791400
H	-0.08724100	-1.02996800	0.72504900
H	-0.60339800	-1.22267200	-0.95279900
H	-2.25120500	0.64019000	-0.66990900
H	-2.51323000	-0.60255100	0.54987400
H	1.43335900	2.40441400	0.11985700
H	-0.41323000	2.99211300	1.69389400
H	-0.96804800	2.83558700	0.02820600
H	-1.27395800	0.72275700	2.23242100
H	-2.56880400	1.70533200	1.54592200
S	0.17546800	1.21951700	-2.20587900
C	1.63756600	2.19899200	-2.48444400
C	1.53660100	3.59620400	-2.56642600
C	2.88863000	1.58562000	-2.65731900
C	2.67576600	4.37081700	-2.81093200
H	0.56572700	4.07008200	-2.43477200
C	4.02733400	2.36406600	-2.88257600
H	2.96665000	0.50034700	-2.62560400
C	3.92407300	3.75798100	-2.96090400
H	2.58752000	5.45364300	-2.87614400
H	4.99357800	1.88026200	-3.01216500
H	4.81034700	4.36150500	-3.14528700
O	1.35796600	0.96454200	1.61952400
H	1.54277700	1.63434600	2.30411900

6

E = -2937.833460

ZPVE = 0.258542

Symbol	X	Y	Z
C	-1.89720700	0.34588000	0.29494300
C	-0.84336900	-0.76364200	0.30210200
C	0.47044600	-0.31701400	-0.33622100
C	0.99195200	0.98720300	0.25482300
C	-0.06813100	2.08440300	0.29084200
C	-1.35706400	1.61103000	0.96502600
H	1.24022700	-1.08212500	-0.18466100

H	-0.62284300	-1.04205100	1.34129100
H	-1.21383700	-1.66510300	-0.20234100
H	-2.20005600	0.57778800	-0.73569100
H	-2.79888400	-0.00123700	0.81524500
H	1.86611400	1.32190000	-0.32193000
H	0.34421100	2.95970900	0.81346800
H	-0.27903400	2.40406300	-0.73800000
H	-1.16245600	1.40381900	2.02513000
H	-2.10808000	2.41022100	0.92602300
C	2.09434700	0.17477900	-2.67930300
C	2.49338100	1.38053300	-3.27189000
C	3.04921700	-0.80909400	-2.38727900
C	3.84369100	1.60044800	-3.56566900
H	1.75105400	2.14446400	-3.49432500
C	4.39814800	-0.58030400	-2.67224400
H	2.73741400	-1.76127500	-1.96220600
C	4.79948800	0.62651300	-3.25746800
H	4.14897500	2.53775900	-4.02718600
H	5.13519700	-1.34779800	-2.44339500
H	5.84924000	0.80085000	-3.48400200
O	1.41512300	0.62410000	1.58797200
H	1.81022700	1.41202400	2.00638200
Se	0.24092700	-0.13952900	-2.30051200

7

E = -193.586190

ZPVE = 0.110695

Symbol	X	Y	Z
C	-0.90791100	1.59761700	0.01593700
H	-0.56437900	0.55775300	0.04648700
H	-2.00285100	1.57578300	0.04587600
C	-0.41059800	2.30108000	1.26222000
H	-0.76555600	3.34152600	1.27621000
H	0.68866500	2.31225000	1.27689700
C	-0.42179400	2.28373800	-1.25924800
H	0.67237500	2.29665700	-1.30904600
H	-0.78947100	1.76364600	-2.14860300
H	-0.77349900	3.31989000	-1.30967400
O	-0.91911300	1.58339200	2.39705300
H	-0.60906400	2.02157000	3.20894000

8

E = -649.695298

ZPVE = 0.210007

Symbol	X	Y	Z

C	-0.86821700	0.34794900	-0.78413300
C	-1.09891700	1.89901800	-0.59792500
H	-1.86326900	2.46972000	-1.13230800
C	-1.00456400	1.71662200	0.95234300
H	-1.65778300	2.19398000	1.68757900
C	-0.78628700	0.17629500	0.77029800
H	-1.29898500	-0.61681300	1.32079800
C	0.54356300	1.93775800	0.86734100
C	0.76464300	0.39597200	0.68406200
H	1.52051200	-0.19520500	1.21118100
C	0.66976900	0.57758100	-0.87209800
H	1.30857600	0.10192200	-1.62048200
C	0.44789800	2.11851500	-0.68538600
H	0.94238600	2.91481700	-1.24802700
C	-1.65020500	-0.48824400	-1.71820800
O	-2.87938000	-0.76614400	-1.20448500
O	-1.27882500	-0.86362000	-2.82537300
C	-3.74288900	-1.51981800	-2.08645000
H	-3.29296000	-2.48683400	-2.31826100
H	-4.67065600	-1.64452400	-1.53076900
H	-3.91204200	-0.96560600	-3.01155500
C	1.33796200	2.80163600	1.78404300
H	2.40204500	2.76616300	1.50209500
H	1.23911200	2.43865900	2.81924200
O	0.82321300	4.13809200	1.66234500
H	1.33507400	4.72325300	2.24926700

9

E = -426.095530

ZPVE = 0.240358

Symbol	X	Y	Z
C	-2.19336900	-1.63237700	0.09601000
C	-0.67030400	-1.55098300	0.05208400
C	-0.15578800	-0.13789300	0.44642000
C	-1.24052600	0.97027100	0.55298900
C	-2.64408500	0.40731300	0.43603600
C	-2.70446000	-0.85576500	1.33368600
H	0.35904000	-0.20651800	1.41194600
H	-0.25226800	-2.29493400	0.74308100
H	-0.31653700	-1.82575200	-0.94865500
H	-2.54704000	-2.66226800	-0.05564300
H	-1.15770100	1.45036200	1.54156100
H	-3.38734700	1.20240500	0.58034500
H	-2.06740400	-0.86520500	2.22827100
H	-3.72053700	-1.12378000	1.63143600
H	0.59827100	0.20055900	-0.27399900
C	-2.83071400	-0.52757700	-0.79618700
C	-4.31457700	-0.79479400	-1.05446200
H	-4.86626100	-1.05941800	-0.14756300

H	-4.78755800	0.09528200	-1.48759800
H	-4.42926900	-1.61954000	-1.76916800
C	-2.16682100	-0.19284000	-2.12648600
H	-1.10388800	0.03214100	-2.03533000
H	-2.28824500	-1.03725900	-2.81890700
H	-2.64107600	0.68712200	-2.57564800
O	-1.10438100	1.99285900	-0.45436800
H	-0.29648300	2.50355600	-0.26195900

10

E = -231.540426

ZPVE = 0.116856

Symbol	X	Y	Z
C	-1.97693000	0.96002500	0.02000900
C	-0.47038200	1.00084300	0.00639600
C	-1.25378800	2.28398000	0.00527500
H	-2.49401700	0.65150800	-0.88293300
H	-2.46867400	0.65997600	0.94129900
H	0.04414500	0.71592400	-0.90565500
H	0.05489100	0.74030800	0.92060700
H	-1.27384400	2.84160500	-0.92818800
C	-1.26506300	3.13465000	1.23690200
H	-2.13961100	3.80077200	1.23309900
H	-1.32355600	2.49254600	2.12833000
O	-0.05068700	3.90441200	1.25075800
H	-0.09859400	4.54429100	1.98334800

11

E = -347.780624

ZPVE = 0.180401

Symbol	X	Y	Z
C	-1.55697900	0.95165500	0.47361700
C	-0.08835500	1.27979000	0.38039400
C	-1.12610400	2.35868000	0.16555600
H	-2.00768400	0.36888100	-0.32352300
H	-1.96532200	0.75329700	1.46031700
H	0.46850600	0.91897900	-0.47882500
H	0.47681600	1.29743600	1.30946500
H	-1.26150500	2.69763400	-0.86070600
C	-1.28580800	3.44494300	1.19704500
H	-1.18948400	2.99789300	2.20367900
C	-2.61097800	4.14399300	1.10089900
C	-3.78622700	3.62738300	1.89116900
C	-3.12144000	4.92286900	2.28199300
H	-2.82394400	4.55859400	0.11697300

H	-3.62739300	2.76391400	2.53095900
H	-4.76824200	3.66648200	1.43010800
H	-3.64821500	5.85265400	2.09193300
H	-2.50412000	4.92908000	3.17564300
O	-0.27327600	4.45761600	1.02753200
H	0.57165300	3.99576300	0.86549200

12

E = -191.212904

ZPVE = 0.060220

Symbol	X	Y	Z
C	-1.82422400	0.43629400	-0.13489600
H	-2.65026300	-0.24068500	-0.12561400
C	-0.86364600	1.19067700	-0.14786100
C	0.26303500	2.12207000	-0.15998000
H	0.15104000	2.82035500	-0.99988900
H	0.26721000	2.70288200	0.77180900
O	1.47356100	1.36225200	-0.28973500
H	2.21978600	1.98913400	-0.29709100

13

E = -690.927832

ZPVE = 0.257252

Symbol	X	Y	Z
C	1.54535900	0.38346300	-0.14590600
C	2.18809100	1.79830100	-0.12454000
C	-0.38563000	2.00961400	0.02953100
C	0.01147000	0.50710100	-0.06394700
H	1.84674500	-0.14236200	-1.05930400
H	1.88580700	-0.20025100	0.71707700
H	-0.46605300	0.07843700	-0.95752600
H	-1.47721800	2.12482400	0.09553300
H	3.28224500	1.74380500	-0.18798900
C	0.32424000	2.57352200	1.23142000
C	1.72312700	2.46617700	1.14499300
C	-0.27286800	3.13006900	2.36286800
C	2.52873100	2.91552800	2.19266600
C	0.53606800	3.59464100	3.40818200
H	-1.35816300	3.20747200	2.43055400
C	1.93026200	3.48681900	3.32375400
H	3.61345200	2.82771200	2.12956200
H	0.07979000	4.03824800	4.29118000
H	2.55154200	3.84854900	4.14096500
C	0.18591400	2.66743100	-1.20053200
C	-0.53360400	3.30311000	-2.21398200
C	1.58617200	2.55929200	-1.28093500

C	0.15485600	3.84937400	-3.30588700
H	-1.61879100	3.38527700	-2.15070200
C	2.26974800	3.09513600	-2.37358900
C	1.54944700	3.74608800	-3.38492100
H	-0.39640700	4.35571800	-4.09598400
H	3.35476000	3.01252500	-2.43771800
H	2.07640800	4.17388900	-4.23576100
O	-0.40147800	-0.22196800	1.10010000
H	-1.37356600	-0.16784400	1.16955200

For Table 4 ($ROCH_2CF_3$): B3LYP/6-311++G(d,p)

1

E = -723.381396

ZPVE = 0.183598

Symbol	X	Y	Z
C	-0.58007100	-0.98618500	-0.06125600
C	0.93845100	-0.97133400	0.15677500
C	1.48691800	0.45169200	0.20999800
C	-0.63823800	1.32403500	0.91025500
C	-1.26133000	-0.06657300	0.96070000
H	2.52180600	0.46755600	0.57162700
H	1.18124100	-1.44730600	1.11258800
H	1.46255400	-1.52032900	-0.62899600
H	-0.80808700	-0.64381800	-1.07559700
H	-0.95886100	-2.00846700	0.02437400
H	-1.01326400	1.96751000	1.70694900
H	-0.85391100	1.80314200	-0.05233100
H	-1.14548400	-0.47701600	1.97041300
H	-2.33514700	0.01307500	0.76292000
O	0.78836800	1.27945900	1.11296000
O	1.44881300	0.97304900	-1.11680000
C	2.08419900	2.22139300	-1.25716100
H	1.65334700	2.98025000	-0.59657800
H	3.16236700	2.15235900	-1.06162700
C	1.90375000	2.69175000	-2.68750300
F	2.43049000	1.83727200	-3.58487400
F	2.52592600	3.88473800	-2.85082000
F	0.60644700	2.86730100	-3.00944000

2

E = -1096.069124

ZPVE = 0.307859

Symbol	X	Y	Z
C	-2.05457900	0.48311300	0.60495100
C	-0.83445800	-0.40590100	0.32137900

C	0.37844100	0.38061100	-0.23944000
C	0.70578200	1.59106700	0.64636700
C	-0.52056200	2.46930200	0.93431700
C	-1.68796400	1.66167400	1.51645700
H	1.25625300	-0.27652900	-0.15929900
H	-0.53172600	-0.88890800	1.25697600
H	-1.11085100	-1.21465000	-0.36258400
H	-2.46796200	0.86897100	-0.33378600
H	-2.84517400	-0.11624600	1.06797300
H	1.49216100	2.20136500	0.18089400
H	-0.24651500	3.29030600	1.60522500
H	-0.82715800	2.94101600	-0.00584300
H	-1.40699000	1.28120700	2.50453600
H	-2.55347100	2.31533000	1.66387300
Si	0.36032100	0.71583200	-2.13265000
C	-1.11014200	1.71816000	-2.77957500
H	-1.17237000	2.71344900	-2.33088200
H	-1.00866800	1.85539000	-3.86150400
H	-2.06317400	1.21192700	-2.60387700
C	1.95297800	1.62982400	-2.59425500
H	2.05571900	1.68798000	-3.68256800
H	1.96907500	2.65538300	-2.21312900
H	2.83930700	1.11700200	-2.20788900
C	0.35299900	-0.96783300	-2.99362400
H	1.19910600	-1.58443700	-2.67521200
H	-0.56264800	-1.53028300	-2.78930700
H	0.42456500	-0.84381400	-4.07881800
O	1.26223300	1.05458800	1.87424600
C	1.91474700	1.98458900	2.69099600
H	1.22404200	2.61366800	3.26747000
H	2.58655600	2.63884900	2.11783800
C	2.77129600	1.23050900	3.69363700
F	3.40054200	2.11726300	4.50537600
F	3.72301800	0.48406300	3.10145300
F	2.04519500	0.41281300	4.47943800

3

E = -687.442525

ZPVE = 0.207041

Symbol	X	Y	Z
C	-4.26146600	-0.87504400	0.07702100
C	-2.73785800	-0.78421600	0.08066400
C	-2.26290400	0.67168600	0.00640000
C	-2.87356000	1.51367800	1.13898300
C	-4.40555900	1.42555100	1.14428600
C	-4.87747000	-0.03385800	1.20498200
H	-1.17030400	0.72417200	0.05333500
H	-2.35140300	-1.24369100	1.00518000
H	-4.62138000	-0.51951600	-0.89546300
H	-4.55866600	-1.92374300	0.16252800

H	-2.48712100	1.16080500	2.10398000
H	-2.54980000	2.55416800	1.03974500
H	-4.81313000	1.99100700	1.98825700
H	-4.79794900	1.89558800	0.23358100
H	-4.59908200	-0.46401800	2.17576900
H	-5.96882600	-0.08514800	1.14730600
H	-2.56325800	1.07869100	-0.96654400
O	-2.27636500	-1.56760200	-1.03222000
C	-0.90842300	-1.86814400	-1.02614600
H	-0.28049900	-1.01793200	-1.32073100
H	-0.57034700	-2.23102700	-0.04577600
C	-0.65281600	-2.98049300	-2.02854900
F	0.67224100	-3.27295600	-2.04485300
F	-1.00334400	-2.63623900	-3.28157400
F	-1.30978100	-4.11449900	-1.71964800

4

E = -687.441552

ZPVE = 0.207143

Symbol	X	Y	Z
C	-0.59078000	-0.92680900	-0.09007100
C	0.93779500	-0.91012800	0.06018900
C	1.49610400	0.50958600	0.17022800
C	-0.73323700	1.29158600	1.12948700
C	-1.27531400	-0.14228700	1.03839100
H	2.57627600	0.46525500	0.37264800
H	1.22620700	-1.45407100	0.96790400
H	1.41691700	-1.41450400	-0.78329900
H	-0.86010700	-0.48742100	-1.05593700
H	-0.94633800	-1.96184700	-0.10380600
H	-1.19237700	1.82121900	1.97014300
H	-1.00969600	1.84022300	0.22237900
H	-1.10476200	-0.65501200	1.99471800
H	-2.35871200	-0.12570700	0.88347700
O	1.31561100	1.11982800	-1.12399500
C	2.03308400	2.30323900	-1.33037600
H	1.59830700	3.16720900	-0.81152800
H	3.08487100	2.20631300	-1.02716900
C	2.02046500	2.62265100	-2.81542500
F	2.60880800	1.66366500	-3.55482800
F	2.70157000	3.77563800	-3.03257300
F	0.77383400	2.79652800	-3.29378200
C	0.79483800	1.30271300	1.28353400
H	1.17376700	2.32947300	1.32020300
H	1.07469900	0.84422600	2.24011100

5

E = -1316.676026

ZPVE = 0.288728

Symbol	X	Y	Z
C	-1.77000100	0.02110300	0.21344300
C	-0.35580200	-0.47492400	-0.12209000
C	0.61796700	0.66593400	-0.45733600
C	0.61145700	1.76033200	0.62311000
C	-0.80357000	2.23385200	0.97862400
C	-1.73665200	1.06812600	1.33551900
H	1.63127900	0.26929600	-0.52772700
H	0.05499400	-1.00051400	0.74653800
H	-0.37858700	-1.19103700	-0.94797400
H	-2.23624100	0.45436800	-0.67922700
H	-2.39299100	-0.82883000	0.50809500
H	1.21790400	2.60841100	0.28088100
H	-0.75717200	2.95931200	1.79725200
H	-1.19845500	2.77432900	0.11237200
H	-1.39260900	0.59522500	2.26197800
H	-2.74365400	1.44949800	1.53025400
S	0.20805600	1.35848200	-2.13585800
C	1.68479000	2.31418200	-2.50376500
C	1.57536200	3.69317800	-2.70988800
C	2.93095600	1.69406000	-2.65274900
C	2.69982800	4.44271200	-3.05559900
H	0.61050200	4.17380900	-2.59915000
C	4.05464200	2.44976600	-2.97715100
H	3.01823500	0.62129800	-2.52582200
C	3.94196600	3.82516500	-3.18268200
H	2.60333600	5.51055900	-3.21757700
H	5.01636500	1.96078900	-3.08553400
H	4.81670700	4.40930000	-3.44482200
O	1.27925700	1.16432600	1.75695400
C	1.76208900	2.07492300	2.70548000
H	0.96508400	2.53416100	3.30388100
H	2.35849700	2.87311000	2.24302400
C	2.67085400	1.33034700	3.66818400
F	3.14196700	2.19513800	4.60038900
F	3.73575300	0.78246100	3.05301900
F	2.02868800	0.34395000	4.32266600

6

E = -3320.008359

ZPVE = 0.287413

Symbol	X	Y	Z
C	-1.91284100	0.16869200	0.36449000
C	-0.68810700	-0.75756300	0.37732300
C	0.55147600	-0.11837600	-0.26143600
C	0.85244400	1.27004000	0.31922400
C	-0.37860700	2.18565200	0.34135800

C	-1.58856500	1.52138800	1.01370600
H	1.42317400	-0.75294900	-0.10502300
H	-0.42910700	-0.99069200	1.41658800
H	-0.91132000	-1.70768700	-0.11525200
H	-2.25212200	0.32833900	-0.66655900
H	-2.74158000	-0.31433200	0.89093300
H	1.66076000	1.73791900	-0.25633800
H	-0.12941900	3.12903100	0.83780100
H	-0.62136100	2.44001400	-0.69536400
H	-1.37706300	1.36940800	2.07784000
H	-2.45372200	2.18887400	0.95550700
C	2.20361500	0.20977700	-2.73501700
C	2.60821200	1.40222700	-3.34148300
C	3.13749200	-0.80910400	-2.52122800
C	3.93855700	1.57482200	-3.72590800
H	1.88552700	2.19153200	-3.51102900
C	4.46844600	-0.62476700	-2.89047500
H	2.82372700	-1.74638600	-2.07681200
C	4.87102700	0.56565800	-3.49588200
H	4.24425300	2.50136600	-4.19924600
H	5.18780000	-1.41744400	-2.71715000
H	5.90539400	0.70302500	-3.78987900
O	1.34830300	1.01346600	1.65403800
Se	0.33708200	-0.04131600	-2.26167700
C	2.08854600	2.05900700	2.22057500
H	1.46889800	2.91923100	2.50423500
H	2.88735300	2.40694700	1.55153200
C	2.75022700	1.54816100	3.48865900
F	3.46719300	2.54985800	4.05575000
F	3.59857500	0.52950500	3.25364400
F	1.85481200	1.12749600	4.40247000

7

E = -570.740729

ZPVE = 0.141346

Symbol	X	Y	Z
C	-0.90568600	1.60072700	0.02218100
H	-0.56494900	0.56181600	0.06467000
H	-1.99880000	1.57660300	0.06417400
C	-0.39051400	2.32926200	1.25260500
H	-0.74078500	3.37264200	1.26001400
H	0.70996100	2.34563600	1.26067600
C	-0.43873200	2.25988500	-1.27885100
H	0.65304400	2.27250800	-1.35312100
H	-0.82148700	1.71845300	-2.14689800
H	-0.79006000	3.29362100	-1.35371500
O	-0.86759600	1.65609100	2.41616700
C	-0.44658600	2.25099100	3.61081900
H	0.64792800	2.25255100	3.71083300

H	-0.80822400	3.28408400	3.71034100
C	-1.00807800	1.45892600	4.77828100
F	-0.60422500	2.02923600	5.94061200
F	-0.58134800	0.18236500	4.78708900
F	-2.35392200	1.43836500	4.78669900

8

E = -1028.271218

ZPVE = 0.240728

Symbol	X	Y	Z
C	-0.85994000	0.32688600	-0.78362000
C	-1.11604600	1.87045200	-0.55138300
H	-1.89883300	2.44351700	-1.04268400
C	-0.97246900	1.66853900	0.99460700
H	-1.62595000	2.10568700	1.74653000
C	-0.72428300	0.13642200	0.77826100
H	-1.19415100	-0.66941600	1.33798100
C	0.57388900	1.93403800	0.87907200
C	0.81889400	0.39455400	0.65758500
H	1.59347600	-0.19481700	1.14695600
C	0.67520500	0.59461600	-0.89394800
H	1.31532600	0.15324200	-1.65387200
C	0.42509600	2.12978900	-0.67465600
H	0.87835000	2.93509900	-1.24902500
C	-1.64206600	-0.54446800	-1.69780900
O	-2.94076100	-0.60469200	-1.31923100
O	-1.20298200	-1.13049300	-2.66039700
C	-3.80217000	-1.41463700	-2.14000500
H	-3.45992000	-2.45055200	-2.14718500
H	-4.78883200	-1.34041200	-1.68779300
H	-3.81974600	-1.03755200	-3.16361000
C	1.38883100	2.78519900	1.79691500
H	2.44716600	2.77427400	1.49085100
H	1.33273400	2.40064200	2.82791100
O	0.88757000	4.12198400	1.75318500
C	1.59157700	5.00558500	2.58052800
H	1.54166500	4.71229900	3.63833900
H	2.64784800	5.09294200	2.29057800
C	0.97077200	6.38632700	2.46152000
F	1.64605700	7.25042100	3.25857700
F	-0.31845700	6.40499800	2.84821400
F	1.02630800	6.86847000	1.20615600

9

E = -804.095812

ZPVE = 0.268308

Symbol	X	Y	Z
C	-2.20029700	-1.66832400	0.04725600
C	-0.66958200	-1.61896900	0.01346700
C	-0.10562600	-0.20286100	0.35793400
C	-1.18155700	0.88615600	0.66514700
C	-2.60616900	0.36457000	0.51512000
C	-2.69048800	-0.95422600	1.33591700
H	0.58052500	-0.28057800	1.20472700
H	-0.28204100	-2.35155100	0.72852000
H	-0.30917800	-1.93066900	-0.97095000
H	-2.56824500	-2.67838600	-0.15626300
H	-1.06629200	1.22674900	1.70476500
H	-3.32237300	1.16345900	0.72192700
H	-2.05242700	-1.03370800	2.22126300
H	-3.70893100	-1.21300400	1.61982200
H	0.49323700	0.15832700	-0.48088500
C	-2.83291700	-0.49436500	-0.78049500
C	-4.33228000	-0.71836800	-1.03336000
H	-4.87937100	-1.02561600	-0.13996400
H	-4.79608200	0.20017400	-1.40668500
H	-4.47622100	-1.49419600	-1.79239600
C	-2.18543100	-0.08402900	-2.10475000
H	-1.11657300	0.10756800	-2.03104800
H	-2.33814900	-0.87007400	-2.85280600
H	-2.64662600	0.83093100	-2.48700700
O	-1.04045100	2.04496100	-0.17822200
C	0.03104000	2.87842900	0.16226500
H	1.00985200	2.40894800	-0.00348400
H	-0.02313600	3.21077100	1.20874700
C	-0.02126400	4.11944100	-0.71116200
F	1.00880600	4.94047800	-0.38590600
F	0.09377100	3.83145100	-2.02176700
F	-1.15936000	4.81900300	-0.54754700

10

E = -608.811281

ZPVE = 0.147275

Symbol	X	Y	Z
C	-1.95957100	0.94987600	-0.00343600
C	-0.45241300	0.99455600	0.03432200
C	-1.24008800	2.27878600	0.00047200
H	-2.44618600	0.64072300	-0.92020300
H	-2.48106900	0.64966800	0.89866600
H	0.09452300	0.71169700	-0.85647600
H	0.04116700	0.73245000	0.96303300
H	-1.23145100	2.82886700	-0.93460700
C	-1.31335300	3.14757300	1.22129500
H	-2.20267900	3.79444900	1.18435700
H	-1.38466000	2.52845200	2.12836300

O	-0.14037400	3.96234300	1.28718700
C	-0.14864300	4.84920200	2.37005800
H	-0.99342900	5.55100000	2.32618800
H	-0.17910900	4.32568800	3.33610900
C	1.12721900	5.67203700	2.34009800
F	1.24197000	6.40309700	1.21606900
F	2.23281400	4.91221000	2.44638900
F	1.12668100	6.53526500	3.38669800

11

E = -725.477030

ZPVE = 0.209099

Symbol	X	Y	Z
C	-1.82632300	0.88933300	0.33512900
C	-0.32684300	0.98623700	0.22953200
C	-1.18066300	2.22273400	0.05005500
H	-2.37309200	0.40767900	-0.46602600
H	-2.25227900	0.73272700	1.31918300
H	0.15897300	0.56922500	-0.64458900
H	0.24451400	0.88695300	1.14606300
H	-1.27851100	2.59301100	-0.96650800
C	-1.21755900	3.32437300	1.09085100
H	-1.04636600	2.88596900	2.08819200
C	-2.52938900	4.07126400	1.09537200
C	-3.65272000	3.63457000	2.00491800
C	-2.91063300	4.91920600	2.27949700
H	-2.81733600	4.44979700	0.11941800
H	-3.47613500	2.79764400	2.67084300
H	-4.66520300	3.68984400	1.62383200
H	-3.41364200	5.85936400	2.09017600
H	-2.22717700	4.94227900	3.12036200
O	-0.19835400	4.31596800	0.85222700
C	1.12327300	3.87841200	1.01215200
H	1.26992400	3.34395800	1.96099200
H	1.46341400	3.23502900	0.19272600
C	2.03000700	5.09641600	1.04009100
F	1.75475500	5.92313300	2.06709300
F	1.95899200	5.81927500	-0.09319000
F	3.31825500	4.69263200	1.18202100

12

E = -568.289967

ZPVE = 0.093991

Symbol	X	Y	Z
C	-1.78429000	0.40223900	-0.13947700

H	-2.59326000	-0.28710700	-0.13135000
C	-0.86271400	1.17153700	-0.14969100
C	0.22942800	2.13332800	-0.15743000
H	0.09818000	2.83582300	-0.99362700
H	0.21402400	2.71854200	0.77383000
O	1.47539700	1.45031200	-0.28441600
C	2.56862100	2.33044100	-0.29733300
H	2.64518500	2.90924600	0.63325300
H	2.52884200	3.02766800	-1.14536900
C	3.84387100	1.51668500	-0.43492900
F	4.01939800	0.66135500	0.58730700
F	3.87811300	0.80563600	-1.57537300
F	4.90589300	2.35957700	-0.44807700

13

E = -1069.711943

ZPVE = -1069.711943

Symbol	X	Y	Z
C	1.46384800	0.37421400	-0.18618000
C	2.15876900	1.77145300	-0.14294100
C	-0.41230800	2.07598400	-0.00597700
C	-0.07209500	0.55013500	-0.14097300
H	1.76187100	-0.16346000	-1.08836700
H	1.76380100	-0.22084200	0.67800000
H	-0.53611600	0.17712200	-1.06276300
H	-1.49013300	2.24215400	0.04423700
H	3.24395200	1.67211700	-0.19773800
C	0.31392000	2.59502800	1.21971300
C	1.70563900	2.43876000	1.14242500
C	-0.26487200	3.17151900	2.34350800
C	2.51531900	2.85811700	2.19105300
C	0.55042600	3.59949900	3.39496800
H	-1.34163500	3.29466600	2.40494100
C	1.93280600	3.44299200	3.31917200
H	3.59223200	2.73530600	2.13440200
H	0.10469000	4.05483700	4.27212600
H	2.56036900	3.77711800	4.13777700
C	0.20103400	2.73235900	-1.23053800
C	-0.47837000	3.42386100	-2.22637200
C	1.59325900	2.57333000	-1.30225500
C	0.23735300	3.96824300	-3.29716100
H	-1.55535000	3.54775700	-2.17113600
C	2.30303800	3.11155800	-2.36879000
C	1.62004900	3.81296600	-3.36734900
H	-0.28617900	4.51489000	-4.07339500
H	3.38018700	2.99143500	-2.42600100
H	2.17029600	4.23919900	-4.19872700
O	-0.55878200	-0.23283200	0.95326100
C	-1.95067800	-0.39449600	0.99578800
H	-2.36947800	-0.61912800	0.00564300

H	-2.46814500	0.48094600	1.40732000
C	-2.27423000	-1.57338900	1.89811900
F	-1.82936000	-1.39903100	3.15503400
F	-3.62056300	-1.72993500	1.96140500
F	-1.75658600	-2.72844400	1.43883300

For Table 4 ($ROCH_2CF_3$): M06-2X/6-311++G(d,p)

1

E = -723.109405

ZPVE = 0.186869

Symbol	X	Y	Z
C	-0.52864300	-0.95479700	-0.11319700
C	0.96199200	-0.99583300	0.22719700
C	1.54040400	0.40935700	0.25909700
C	-0.56279200	1.36842000	0.79654800
C	-1.23981600	0.00668000	0.84075700
H	2.56632200	0.42034800	0.64386700
H	1.10882000	-1.43375800	1.21875200
H	1.52486800	-1.58988400	-0.49488300
H	-0.65469800	-0.61027600	-1.14372000
H	-0.95697600	-1.95691200	-0.04712900
H	-0.97368200	2.05064200	1.54012500
H	-0.68323900	1.81815100	-0.19662700
H	-1.19435600	-0.38090500	1.86386900
H	-2.29370300	0.11869600	0.57388600
O	0.82978700	1.26935300	1.10731200
O	1.53165600	0.88774600	-1.07352100
C	2.11452200	2.15194700	-1.21834800
H	1.74501300	2.86103700	-0.47122100
H	3.20906600	2.10575900	-1.16799000
C	1.72902100	2.67498600	-2.58050600
F	2.13928800	1.87523100	-3.56787700
F	2.28385100	3.88116600	-2.77895600
F	0.40357900	2.81640200	-2.70085900

2

E = -1095.699428

ZPVE = 0.312139

Symbol	X	Y	Z
C	-1.98223400	0.72696100	0.61021300
C	-0.88123200	-0.30431900	0.33628200
C	0.39730100	0.32602300	-0.25752900
C	0.86425800	1.49963500	0.59862600
C	-0.24385600	2.53371200	0.80585700
C	-1.46623000	1.88935000	1.46150300

H	1.19932600	-0.42222500	-0.19383100
H	-0.62116200	-0.79621000	1.27906500
H	-1.26078900	-1.08592800	-0.33056700
H	-2.36782200	1.12634000	-0.33248400
H	-2.82191400	0.23898300	1.11210300
H	1.74395800	1.97882600	0.14640000
H	0.12300700	3.37703400	1.39879500
H	-0.51389300	2.94355100	-0.17438600
H	-1.18690100	1.51711100	2.45317700
H	-2.25246600	2.63447500	1.60558900
Si	0.31592500	0.67859700	-2.12885800
C	-1.32044800	1.38154000	-2.74234800
H	-1.57873000	2.33695900	-2.28001600
H	-1.24941700	1.54495300	-3.82201400
H	-2.14601600	0.68622100	-2.57026800
C	1.69447000	1.87365800	-2.59352800
H	1.75383700	1.98108100	-3.67994600
H	1.52666400	2.86926800	-2.17291700
H	2.66714500	1.51907700	-2.24137800
C	0.58855400	-0.96714000	-2.99685300
H	1.57185800	-1.38093900	-2.75912300
H	-0.16371600	-1.70218400	-2.69774900
H	0.52576600	-0.85218100	-4.08212100
O	1.28162900	0.93702800	1.85146600
C	1.83909000	1.85097100	2.74091700
H	1.08520900	2.43977700	3.27858800
H	2.54149500	2.53611000	2.24741700
C	2.62017800	1.07202900	3.77394000
F	3.15699600	1.91916400	4.66912300
F	3.62186000	0.37554600	3.22993800
F	1.84822600	0.21379600	4.44607800

3

E = -687.172070

ZPVE = 0.210213

Symbol	X	Y	Z
C	-4.27663300	-0.86093300	0.04752900
C	-2.75738200	-0.80864800	0.07666700
C	-2.25060400	0.63087500	0.02193900
C	-2.85067900	1.46049500	1.16168200
C	-4.37936900	1.41264500	1.13552800
C	-4.87775400	-0.03309000	1.18537600
H	-1.15825200	0.65762800	0.07869700
H	-2.39564100	-1.28285100	1.00411000
H	-4.60812900	-0.46665000	-0.91958500
H	-4.59807100	-1.90339800	0.10071200
H	-2.49472300	1.06640000	2.12135300
H	-2.49641100	2.49178400	1.09478100
H	-4.78982500	1.98598100	1.97054700
H	-4.73901300	1.88639500	0.21449000

H	-4.59765100	-0.47799800	2.14780800
H	-5.96827000	-0.06496800	1.12982000
H	-2.54049400	1.05544200	-0.94653400
O	-2.30289300	-1.58314800	-1.02894300
C	-0.92576200	-1.79019600	-1.06723200
H	-0.37510300	-0.93341800	-1.47277100
H	-0.51797800	-2.04302300	-0.07961900
C	-0.65996800	-2.96762800	-1.97686200
F	0.66413900	-3.18725100	-2.05428000
F	-1.10553900	-2.75694300	-3.21761100
F	-1.22706500	-4.09028000	-1.52708700

4

E = -687.172264

ZPVE = 0.210396

Symbol	X	Y	Z
C	-0.58625300	-0.88996500	-0.10918100
C	0.93354900	-0.94964900	0.06878400
C	1.53669600	0.44694000	0.15489800
C	-0.63819900	1.33793300	1.07555100
C	-1.24233900	-0.06716100	1.00251100
H	2.61984400	0.38124100	0.32998100
H	1.18157000	-1.48501900	0.99186200
H	1.40087400	-1.48572600	-0.76029000
H	-0.81025300	-0.43486100	-1.07846300
H	-0.99544700	-1.90307100	-0.12533400
H	-1.09075100	1.90900000	1.88990400
H	-0.85899100	1.87220600	0.14475300
H	-1.09239500	-0.57156400	1.96540900
H	-2.32141300	-0.00618700	0.84074000
O	1.33144900	1.04169100	-1.12861600
C	1.89334600	2.30593400	-1.28075800
H	1.28928100	3.09966900	-0.82404100
H	2.91436600	2.35783800	-0.87982000
C	1.97396300	2.59823900	-2.76135800
F	2.75778100	1.72958700	-3.40539600
F	2.48850000	3.82518400	-2.95230600
F	0.77285100	2.57052200	-3.34482400
C	0.87800200	1.26373500	1.26893700
H	1.31828700	2.26374700	1.32730000
H	1.10751100	0.77130200	2.22038000

5

E = -1316.285983

ZPVE = 0.292961

Symbol	X	Y	Z
C	-1.73754500	0.13661800	0.25074200
C	-0.37388600	-0.48466600	-0.06532800
C	0.65980600	0.55877000	-0.50222400
C	0.75268700	1.70281700	0.51066500
C	-0.61265300	2.31330800	0.82330800
C	-1.60156200	1.24591900	1.29700600
H	1.64411700	0.09267600	-0.57396900
H	0.01933700	-0.96569900	0.83542800
H	-0.46356100	-1.25450200	-0.83552100
H	-2.17952600	0.55114800	-0.66190300
H	-2.41662400	-0.64081000	0.60866400
H	1.43867600	2.47403800	0.13527000
H	-0.50518800	3.11074000	1.56439900
H	-0.98273800	2.78571600	-0.09145700
H	-1.24649500	0.81169300	2.23838000
H	-2.57361200	1.70223900	1.49807600
S	0.22489100	1.16682400	-2.18249800
C	1.63499100	2.21389400	-2.50574900
C	1.45237300	3.58731200	-2.66419900
C	2.91529400	1.66955300	-2.61810200
C	2.54351000	4.41013400	-2.92959100
H	0.45591700	4.00424500	-2.57547300
C	4.00446400	2.49717400	-2.86387300
H	3.05303300	0.59881000	-2.51984500
C	3.82057500	3.86827500	-3.02271800
H	2.39408800	5.47598500	-3.05566500
H	4.99653800	2.06892100	-2.94455500
H	4.67021000	4.51017100	-3.22218000
O	1.34409700	1.10257500	1.66633900
C	1.66795400	1.99867500	2.68274100
H	0.79898200	2.29277200	3.28367700
H	2.16080600	2.90061000	2.29717600
C	2.64301700	1.30870100	3.60885400
F	2.96400300	2.13179600	4.62109600
F	3.77683800	0.97269200	2.98825500
F	2.12798700	0.19707500	4.14148600

6

E = -3319.651552

ZPVE = 0.291771

Symbol	X	Y	Z
C	-1.86077200	0.30986500	0.35108800
C	-0.74282300	-0.73363100	0.43022900
C	0.54247000	-0.26965100	-0.25960900
C	0.98068600	1.10726800	0.24013100
C	-0.14318200	2.14092200	0.17039100
C	-1.39047300	1.65474300	0.91157500
H	1.34969400	-0.97568300	-0.06211600

H	-0.49453800	-0.91079600	1.48184300
H	-1.06655300	-1.68774600	0.00739400
H	-2.17794300	0.44201500	-0.68969600
H	-2.73203700	-0.04763500	0.90494600
H	1.85221600	1.45083800	-0.33308900
H	0.20525100	3.09807200	0.56913500
H	-0.37675200	2.31006100	-0.88472500
H	-1.16022500	1.53923600	1.97666100
H	-2.18492500	2.40039100	0.83178100
C	2.11324100	0.13181000	-2.68915600
C	2.40990200	1.33995200	-3.31839900
C	3.13758500	-0.76921200	-2.39808200
C	3.72674000	1.64475700	-3.65314100
H	1.61182300	2.03893700	-3.53936900
C	4.45333700	-0.45191200	-2.71758900
H	2.90357000	-1.71791900	-1.92889500
C	4.74948200	0.75347800	-3.34787400
H	3.95183900	2.58345200	-4.14563200
H	5.24615200	-1.15270000	-2.48403500
H	5.77451300	0.99494700	-3.60239200
O	1.39847500	0.87344700	1.58968000
Se	0.29059700	-0.28372600	-2.22576800
C	1.99362900	1.96989200	2.21002500
H	1.26288500	2.70454200	2.56926400
H	2.71724100	2.47268200	1.55528800
C	2.74928500	1.46068800	3.41590900
F	3.31983100	2.49253300	4.06018300
F	3.72153800	0.60905600	3.07994400
F	1.94731900	0.83784800	4.28401600

7

E = -570.516858

ZPVE = 0.143765

Symbol	X	Y	Z
C	-0.91229400	1.59250800	0.03436200
H	-0.57014200	0.55559600	0.07822400
H	-2.00406500	1.57245800	0.07698800
C	-0.39702400	2.32054300	1.25870000
H	-0.74812300	3.36272200	1.26361100
H	0.70260700	2.33503700	1.26421500
C	-0.43750500	2.26055600	-1.25341400
H	0.65368100	2.27158900	-1.31363300
H	-0.81324100	1.73062400	-2.12933900
H	-0.78711000	3.29423900	-1.31435600
O	-0.87004700	1.65340300	2.41531200
C	-0.44390400	2.25595300	3.59515300
H	0.65002100	2.25482600	3.69014200
H	-0.80931100	3.28702900	3.69014500
C	-1.00273400	1.46552400	4.75550400

F	-0.60679900	2.02554600	5.91132100
F	-0.57658800	0.20046600	4.75481200
F	-2.33747900	1.44514300	4.75482900

8

E = -1027.895755

ZPVE = 0.245197

Symbol	X	Y	Z
C	-0.84393400	0.34474500	-0.76608400
C	-1.09512200	1.87417400	-0.52543300
H	-1.87894600	2.44937600	-1.00975700
C	-0.94447300	1.65981000	1.01160800
H	-1.58431500	2.09783500	1.77293800
C	-0.70679400	0.13467100	0.78069400
H	-1.18127300	-0.67480400	1.32873800
C	0.59197100	1.91142900	0.88616900
C	0.83145400	0.38415800	0.65595300
H	1.60557900	-0.20851800	1.13862500
C	0.68167800	0.59812500	-0.88681000
H	1.30796100	0.15649600	-1.65662500
C	0.44065200	2.12620500	-0.65327500
H	0.89746500	2.93752800	-1.21395800
C	-1.63968800	-0.51536300	-1.67589700
O	-2.93103700	-0.54616100	-1.30202400
O	-1.21290700	-1.11417000	-2.62776000
C	-3.78696900	-1.34393900	-2.12103900
H	-3.45413000	-2.38222600	-2.11859300
H	-4.77876700	-1.25779500	-1.68537300
H	-3.78353300	-0.97308500	-3.14635000
C	1.39966800	2.76966200	1.79881600
H	2.45584200	2.77204800	1.48975000
H	1.34464500	2.39227200	2.83111700
O	0.87678800	4.08579100	1.73867900
C	1.56564900	4.97900500	2.55532900
H	1.51444600	4.69613200	3.61491000
H	2.61874700	5.08102400	2.26227700
C	0.91783800	6.33693000	2.41335500
F	1.56216600	7.22488500	3.18846500
F	-0.36230500	6.32497300	2.79233500
F	0.96580200	6.78772800	1.15776800

9

E = -803.782140

ZPVE = 0.272443

Symbol	X	Y	Z

C	-2.16021800	-1.64589000	-0.02176800
C	-0.63950600	-1.53449100	-0.09221700
C	-0.12623100	-0.15156000	0.40512400
C	-1.23195200	0.88938100	0.74471700
C	-2.63198100	0.31995900	0.60316100
C	-2.64099900	-1.05112700	1.32402500
H	0.50448800	-0.29784100	1.28404500
H	-0.19905800	-2.32609800	0.51967300
H	-0.30761100	-1.70970100	-1.11843500
H	-2.50243000	-2.64651600	-0.29808000
H	-1.10996400	1.21879500	1.78688900
H	-3.37650400	1.07169200	0.87457100
H	-1.97007900	-1.16447600	2.18031100
H	-3.63891200	-1.37299800	1.61214300
H	0.51743600	0.28951700	-0.35989500
C	-2.83688000	-0.44102100	-0.74113900
C	-4.32189100	-0.69764800	-0.99912200
H	-4.84309400	-1.09123600	-0.12484400
H	-4.81813800	0.23042900	-1.29650900
H	-4.44193600	-1.41852800	-1.81301200
C	-2.20575000	0.09287300	-2.02231100
H	-1.14284400	0.30954400	-1.92675500
H	-2.33841100	-0.63670500	-2.82787900
H	-2.69330500	1.02335800	-2.32360800
O	-1.15051700	2.04803600	-0.08643400
C	-0.09998400	2.89983000	0.24369100
H	0.85760600	2.37466400	0.34787200
H	-0.29813200	3.46394000	1.16456500
C	0.06294000	3.88920400	-0.88608300
F	1.05224500	4.75120300	-0.59661900
F	0.38170100	3.28227900	-2.03433900
F	-1.04392500	4.60362200	-1.09955800

10

E = -608.581081

ZPVE = 0.149946

Symbol	X	Y	Z
C	-1.93513700	0.95727800	0.02231600
C	-0.43481000	1.04346200	0.04642800
C	-1.25526800	2.29778300	-0.00926700
H	-2.41410900	0.61368600	-0.88420400
H	-2.43941900	0.66908800	0.93651200
H	0.10822100	0.75449500	-0.84273300
H	0.07060600	0.82586900	0.97904500
H	-1.26776800	2.83616500	-0.94934000
C	-1.32510800	3.16378300	1.20943400
H	-2.21144800	3.81281200	1.17927000
H	-1.39148500	2.53737700	2.11140400
O	-0.15656700	3.96526800	1.27218400

C	-0.16432200	4.83498800	2.35864100
H	-0.99569100	5.55091700	2.31283100
H	-0.20578200	4.30162000	3.31776000
C	1.12166200	5.62789300	2.33492400
F	1.24858900	6.34863300	1.21849100
F	2.19799100	4.84501200	2.43814000
F	1.14119400	6.48181000	3.37274500

11

E = -725.202240

ZPVE = 0.212580

Symbol	X	Y	Z
C	-1.80840100	0.93575400	0.36334700
C	-0.31186700	1.03046700	0.28280400
C	-1.15982700	2.25347400	0.05551400
H	-2.33518800	0.42974000	-0.43383500
H	-2.25070400	0.81701700	1.34471700
H	0.18519700	0.58826500	-0.57048500
H	0.24049300	0.96646300	1.21317600
H	-1.23956100	2.61147900	-0.96615400
C	-1.21769200	3.35074500	1.09173700
H	-1.06381000	2.90497100	2.09015500
C	-2.53282200	4.07916100	1.07810800
C	-3.63881200	3.61221700	1.98095000
C	-2.91704200	4.89956400	2.27126800
H	-2.81817800	4.46155300	0.10412700
H	-3.43933500	2.76752800	2.62885400
H	-4.65268800	3.66379200	1.60804200
H	-3.43923300	5.83076700	2.10028200
H	-2.22183300	4.91481100	3.10144100
O	-0.20841000	4.33489600	0.87561900
C	1.09775300	3.85700000	0.96834200
H	1.25769100	3.26722400	1.88109200
H	1.39583900	3.25658800	0.10185700
C	2.01817500	5.05307000	1.03911200
F	1.78031600	5.81121800	2.11324400
F	1.91585200	5.83419400	-0.03885700
F	3.29396700	4.63507500	1.11595700

12

E = -568.082370

ZPVE = 0.096150

Symbol	X	Y	Z
C	-1.76205300	0.39994600	-0.14268800
H	-2.56934400	-0.29336800	-0.13722000

C	-0.84610200	1.17196500	-0.15003100
C	0.24842400	2.13727600	-0.15655900
H	0.11444500	2.83634700	-0.99271900
H	0.23067400	2.71680900	0.77598100
O	1.48079700	1.45570600	-0.28359200
C	2.56295100	2.33629200	-0.29720200
H	2.63987500	2.91237100	0.63399100
H	2.52262700	3.02888600	-1.14783300
C	3.82579800	1.51661800	-0.43382100
F	3.98658800	0.66997700	0.58393800
F	3.84385800	0.80772100	-1.56319900
F	4.88815000	2.33873800	-0.45172800

13

E = -1069.308876

ZPVE = 0.293643

Symbol	X	Y	Z
C	1.49234300	0.37390200	-0.26945200
C	2.15586100	1.77587100	-0.16306200
C	-0.42107500	2.02433600	-0.07861100
C	-0.04178100	0.51541100	-0.20017600
H	1.79337700	-0.10358800	-1.20262400
H	1.80752600	-0.25716200	0.56253600
H	-0.52028900	0.11016400	-1.10072600
H	-1.50307800	2.16903800	-0.05384900
H	3.24361100	1.70473100	-0.19369300
C	0.26450700	2.53092500	1.16959500
C	1.65644500	2.39520400	1.12452900
C	-0.35365000	3.05755000	2.29234800
C	2.42948800	2.78718200	2.20611700
C	0.42541800	3.45784800	3.37841000
H	-1.43326000	3.16664500	2.32341500
C	1.80817600	3.32248600	3.33515100
H	3.50852900	2.67966200	2.17334900
H	-0.04933400	3.87636600	4.25775700
H	2.40741800	3.63510600	4.18199500
C	0.20511700	2.70455500	-1.27624600
C	-0.46859400	3.38404600	-2.27935500
C	1.59890400	2.58591300	-1.31417700
C	0.25691300	3.95733200	-3.32461600
H	-1.54931000	3.47509500	-2.24747900
C	2.31895200	3.15237500	-2.35430100
C	1.64179800	3.84283000	-3.36077800
H	-0.26177700	4.49555200	-4.10891000
H	3.39953000	3.06084400	-2.38342400
H	2.19927700	4.29248900	-4.17386500
O	-0.47465100	-0.24037700	0.92166300
C	-1.85395700	-0.24072400	1.12193300
H	-2.40980300	-0.35927200	0.18255500
H	-2.20273800	0.66168500	1.63828000

C	-2.19448100	-1.42490300	1.99762500
F	-1.57370400	-1.37616800	3.17700500
F	-3.51764900	-1.44134500	2.23461400
F	-1.87608100	-2.58559500	1.41753200

For Table 4 ($ROCH_2CF_3$): MP2/6-31+G(d)

1

E = -721.161987

ZPVE = 0.188284

Symbol	X	Y	Z
C	-0.53787100	-0.95974900	-0.10169300
C	0.95689400	-0.99249200	0.21641500
C	1.53286500	0.41099000	0.25042400
C	-0.58356000	1.36097100	0.81277500
C	-1.24309500	-0.00658300	0.86348200
H	2.56511900	0.42983200	0.62613900
H	1.12156000	-1.43856000	1.20552700
H	1.51529800	-1.58366700	-0.51764400
H	-0.68738100	-0.62104200	-1.13400300
H	-0.95855600	-1.96929800	-0.02692600
H	-0.98424500	2.04229800	1.56707200
H	-0.71057200	1.81502700	-0.17924900
H	-1.18127800	-0.39518000	1.88842400
H	-2.30677000	0.09454400	0.61259200
O	0.82727600	1.27456300	1.12145600
O	1.50408400	0.89355300	-1.09366200
C	2.10904900	2.16704200	-1.22526000
H	1.72530100	2.87999300	-0.48754500
H	3.20288700	2.10658500	-1.14436000
C	1.76375700	2.68246000	-2.59970400
F	2.20571700	1.86760900	-3.58471500
F	2.33715900	3.90275600	-2.78933200
F	0.42664700	2.83190100	-2.76363700

2

E = -1092.865101

ZPVE = 0.315705

Symbol	X	Y	Z
C	-2.00977600	0.65672500	0.61146400
C	-0.87000100	-0.32919900	0.33735600
C	0.38437900	0.35285900	-0.24804600
C	0.80069200	1.53743100	0.61469200
C	-0.34096800	2.52309900	0.85099100
C	-1.54300600	1.82251600	1.48426000
H	1.21979800	-0.36480600	-0.17369400

H	-0.59586300	-0.82002800	1.28098700
H	-1.21821500	-1.12540000	-0.33533100
H	-2.40460300	1.05287700	-0.33213700
H	-2.83915200	0.13000300	1.10122200
H	1.66810800	2.05531800	0.17355200
H	-0.00197700	3.36116100	1.47444100
H	-0.62532400	2.96225800	-0.11558500
H	-1.26249700	1.44674600	2.47711200
H	-2.35974900	2.54067500	1.63159500
Si	0.32881400	0.69297000	-2.12929500
C	-1.25840900	1.48992000	-2.77584800
H	-1.48185200	2.45199000	-2.30298800
H	-1.15247000	1.67154400	-3.85303700
H	-2.12773600	0.83716500	-2.64103000
C	1.78840900	1.80015000	-2.59157000
H	1.90014900	1.85240400	-3.68128300
H	1.65694500	2.82627500	-2.22859800
H	2.73134900	1.41832800	-2.18226100
C	0.52109200	-0.97980900	-2.98173400
H	1.46851000	-1.45888600	-2.70910200
H	-0.28880900	-1.66694500	-2.71115100
H	0.50669300	-0.86818400	-4.07232200
O	1.24499500	0.96077100	1.87058700
C	1.84722900	1.89083400	2.73972800
H	1.11715500	2.47223500	3.31874200
H	2.51762800	2.58093000	2.20691400
C	2.68712700	1.10993100	3.72212200
F	3.27249800	1.96630000	4.60705700
F	3.67804500	0.41776600	3.11405600
F	1.95071500	0.22872400	4.43729400

3

E = -685.267308

ZPVE = 0.212295

Symbol	X	Y	Z
C	-4.27301700	-0.85217500	0.03499200
C	-2.75622000	-0.79032700	0.06345900
C	-2.25512200	0.64844100	0.02257000
C	-2.85545300	1.46402400	1.17255700
C	-4.38320600	1.40744200	1.15390300
C	-4.87573700	-0.03999500	1.18378900
H	-1.15925900	0.68037600	0.07396700
H	-2.38360000	-1.28734400	0.97810500
H	-4.61173800	-0.45134600	-0.93015500
H	-4.58951200	-1.90060500	0.07888900
H	-2.48878600	1.06782100	2.13098000
H	-2.50697600	2.50217000	1.11076300
H	-4.79340200	1.96721400	2.00380400
H	-4.75376600	1.89874300	0.24274100
H	-4.59844100	-0.49899100	2.14407400

H	-5.97041300	-0.07459200	1.12660900
H	-2.54868800	1.08211000	-0.94408000
O	-2.30652300	-1.55457300	-1.07182300
C	-0.91556400	-1.78330400	-1.08686700
H	-0.35013400	-0.94193400	-1.50725900
H	-0.52560800	-2.01813000	-0.08629200
C	-0.66028300	-2.98757800	-1.96204300
F	0.68084400	-3.22654400	-2.02663300
F	-1.10166600	-2.80676500	-3.22714800
F	-1.24680100	-4.10691800	-1.47838900

4

E = -685.267605

ZPVE = 0.212457

Symbol	X	Y	Z
C	-0.58614600	-0.89374600	-0.10792300
C	0.93409400	-0.93516700	0.06175700
C	1.52096000	0.46504400	0.16365300
C	-0.66042800	1.32229400	1.09477700
C	-1.24662700	-0.08886800	1.01316700
H	2.61062900	0.41097700	0.32689900
H	1.19543100	-1.48410500	0.97786200
H	1.40814100	-1.45593100	-0.77845400
H	-0.82687900	-0.43949300	-1.07681600
H	-0.98224100	-1.91682900	-0.12626300
H	-1.11608500	1.88030800	1.92246500
H	-0.89804800	1.86730400	0.17155000
H	-1.09016000	-0.60176300	1.97414000
H	-2.33132900	-0.03957100	0.85579900
O	1.29537300	1.06722700	-1.12937700
C	1.91985100	2.31872000	-1.29105500
H	1.35727000	3.14068700	-0.82906700
H	2.94851900	2.32116700	-0.90267100
C	1.99304000	2.59596200	-2.77378500
F	2.73615000	1.67737000	-3.43217900
F	2.57013100	3.81323600	-2.98297100
F	0.76911700	2.62276600	-3.34961200
C	0.85707000	1.27005900	1.27895900
H	1.28312100	2.28012200	1.33507000
H	1.10087300	0.78379900	2.23469900

5

E = -1313.143899

ZPVE = 0.294011

Symbol	X	Y	Z
C	-1.77819500	0.12752200	0.23991100

C	-0.41831400	-0.50659100	-0.06234700
C	0.62627500	0.51906700	-0.51340900
C	0.71548100	1.68659700	0.46697100
C	-0.64271000	2.30913200	0.77091200
C	-1.63846700	1.25758600	1.26175200
H	1.61284700	0.04132300	-0.54918500
H	-0.03139800	-0.98241700	0.84812400
H	-0.51218200	-1.29338500	-0.82171700
H	-2.22643700	0.52147100	-0.68210800
H	-2.46181300	-0.64287400	0.61826500
H	1.41252700	2.44786800	0.08268500
H	-0.52807500	3.11714700	1.50555800
H	-1.01432200	2.77845300	-0.14960300
H	-1.29365600	0.84331900	2.21883900
H	-2.61268400	1.72691600	1.44765100
S	0.23423000	1.08897100	-2.21487900
C	1.62930900	2.16914700	-2.46612600
C	1.42848900	3.55272600	-2.58731200
C	2.92946900	1.64774400	-2.56081200
C	2.51847400	4.40607000	-2.79125400
H	0.41912700	3.95427600	-2.51879900
C	4.01786100	2.50567200	-2.74304600
H	3.08575600	0.57229500	-2.49673700
C	3.81521500	3.88602900	-2.85972900
H	2.35375500	5.47753700	-2.88787500
H	5.02307700	2.09398200	-2.80930800
H	4.66301400	4.55097500	-3.01047800
O	1.30623000	1.09718000	1.64660300
C	1.74544400	2.04897400	2.58905900
H	0.93081900	2.43667700	3.21474400
H	2.26865500	2.88914400	2.11069200
C	2.73047900	1.35505500	3.49927100
F	3.16932600	2.22840600	4.44881400
F	3.81617900	0.90375300	2.83029500
F	2.17701700	0.30044600	4.14129200

6

E = -3313.241913

ZPVE = 0.293020

Symbol	X	Y	Z
C	-1.92415700	0.31578600	0.31483900
C	-0.82875900	-0.74766000	0.41446200
C	0.46843000	-0.31112800	-0.26370600
C	0.93431700	1.06194600	0.20093000
C	-0.16692900	2.11581600	0.13579000
C	-1.42835200	1.65403200	0.86724500
H	1.26558600	-1.02980300	-0.04163400
H	-0.59705000	-0.92596800	1.47350800
H	-1.16475800	-1.70372500	-0.00689600

H	-2.23853400	0.44478000	-0.73006100
H	-2.80916800	-0.01845100	0.87073700
H	1.80694800	1.37867000	-0.39095500
H	0.20074300	3.06434500	0.54867000
H	-0.39450300	2.30656300	-0.92111700
H	-1.21377300	1.54761900	1.93930100
H	-2.21008200	2.41784800	0.77012400
C	2.07555200	0.16082900	-2.61066700
C	2.34650500	1.32596600	-3.34064100
C	3.13101100	-0.64358600	-2.15883500
C	3.67137700	1.68433800	-3.61435200
H	1.52526100	1.95054800	-3.68675000
C	4.45266600	-0.27192100	-2.42060500
H	2.92362600	-1.56674700	-1.62102500
C	4.72661000	0.89533600	-3.14379700
H	3.87802400	2.58868700	-4.18371200
H	5.26866100	-0.89799000	-2.06455800
H	5.75596400	1.17982000	-3.35135800
O	1.37424200	0.83796100	1.56030800
Se	0.25867000	-0.32993100	-2.23604300
C	2.14477000	1.90003800	2.07633800
H	1.53212000	2.73802200	2.43368200
H	2.87552900	2.26970200	1.34292500
C	2.91528600	1.36144200	3.25753700
F	3.66971900	2.35607000	3.80385500
F	3.75547500	0.36034000	2.90824800
F	2.09805300	0.89122600	4.22812700

7

E = -568.991102

ZPVE = 0.145219

Symbol	X	Y	Z
C	-0.90975600	1.59513400	0.02783300
H	-0.56512400	0.55631100	0.07044500
H	-2.00408800	1.57501400	0.06995500
C	-0.39489500	2.32299500	1.25212200
H	-0.74961700	3.36565600	1.26622100
H	0.70638400	2.33481000	1.26676900
C	-0.43654000	2.26295000	-1.26245200
H	0.65683700	2.27403100	-1.32496500
H	-0.81472300	1.72829000	-2.13842100
H	-0.78940500	3.29785000	-1.32547700
O	-0.87975500	1.63878400	2.41324000
C	-0.44424600	2.25435100	3.60173500
H	0.65144500	2.25171300	3.69264000
H	-0.81048200	3.28707400	3.69209500
C	-1.00210900	1.46727300	4.76299600
F	-0.59792400	2.03857600	5.93295900
F	-0.57173300	0.18522700	4.76777000

F	-2.35432700	1.44772400	4.76711100

8

E = -1025.100353

ZPVE = 0.244475

Symbol	X	Y	Z
C	-0.85917900	0.36250400	-0.77401100
C	-1.08161600	1.91003800	-0.55460500
H	-1.84819700	2.49670300	-1.06770400
C	-0.97185500	1.69681000	0.99091000
H	-1.61685300	2.16142300	1.74162500
C	-0.76122000	0.15968400	0.77599600
H	-1.27028400	-0.64153400	1.31776600
C	0.57578300	1.91377700	0.89292700
C	0.78962700	0.37457600	0.67762200
H	1.54845300	-0.22997600	1.18470900
C	0.67879400	0.58750300	-0.87348600
H	1.30897700	0.12491500	-1.63702100
C	0.46525700	2.12544700	-0.65457100
H	0.95647900	2.93045700	-1.20789700
C	-1.65459700	-0.45286700	-1.71622300
O	-2.88360600	-0.72319500	-1.20018600
O	-1.29060300	-0.81718600	-2.82927600
C	-3.76091800	-1.45555100	-2.08743100
H	-3.32389200	-2.42506000	-2.33283500
H	-4.68741700	-1.57533600	-1.52872300
H	-3.92715800	-0.88755500	-3.00458000
C	1.38233100	2.75621300	1.81680900
H	2.44772100	2.74076900	1.52977300
H	1.29579000	2.39172100	2.85479700
O	0.87374400	4.09329400	1.72737600
C	1.57886900	4.97992900	2.56589100
H	1.49927100	4.69840900	3.62554700
H	2.64029400	5.05423100	2.28973800
C	0.96315500	6.34923800	2.40544000
F	1.61991000	7.23800600	3.20257900
F	-0.34086500	6.36874200	2.76309500
F	1.04795500	6.80281300	1.13449600

9

E = -801.502167

ZPVE = 0.274723

Symbol	X	Y	Z
C	-2.17222900	-1.65095500	-0.00535900
C	-0.65073800	-1.56430700	-0.07270400

C	-0.11929000	-0.18793800	0.42114100
C	-1.20785000	0.87963300	0.71646800
C	-2.61464500	0.33491400	0.57412000
C	-2.64880200	-1.02113200	1.32539800
H	0.48205100	-0.33867300	1.32520700
H	-0.22176100	-2.36237000	0.54724100
H	-0.31539600	-1.75493500	-1.09910800
H	-2.52945100	-2.65819000	-0.26240400
H	-1.09090300	1.24754200	1.75102500
H	-3.35146100	1.10778800	0.82938700
H	-1.98503400	-1.12924900	2.19403900
H	-3.65631700	-1.32155100	1.62111600
H	0.56250800	0.23059200	-0.32831600
C	-2.83195100	-0.45374300	-0.75116300
C	-4.32208300	-0.69389500	-0.99928200
H	-4.84982600	-1.06006700	-0.11371100
H	-4.80572300	0.23775700	-1.31776700
H	-4.45510100	-1.43373300	-1.79845300
C	-2.20260700	0.03673200	-2.04992200
H	-1.13559100	0.24743000	-1.96495900
H	-2.34418000	-0.71904700	-2.83459100
H	-2.68509400	0.96372000	-2.38072500
O	-1.10227800	2.02176700	-0.16069700
C	-0.05559000	2.88902600	0.20821600
H	0.92266600	2.38994900	0.23800700
H	-0.24354900	3.37011900	1.17922900
C	0.02657200	3.97078700	-0.84120800
F	1.01479800	4.85085000	-0.51425100
F	0.31845800	3.47050600	-2.06481700
F	-1.12343700	4.67316600	-0.94897500

10

E = -606.945658

ZPVE = 0.151296

Symbol	X	Y	Z
C	-1.93659700	0.94372100	0.02003500
C	-0.43389100	1.04197200	0.03700900
C	-1.26380200	2.29521200	-0.00379400
H	-2.42329000	0.60371100	-0.88840900
H	-2.43696200	0.64077900	0.93562900
H	0.11144200	0.76393400	-0.85901600
H	0.08186300	0.81757200	0.96618300
H	-1.28789300	2.83614300	-0.94665500
C	-1.33501700	3.15967800	1.21387500
H	-2.21552700	3.82063100	1.18107900
H	-1.40297100	2.53937500	2.12231700
O	-0.14335000	3.95712700	1.26743400
C	-0.16274700	4.84470000	2.36080300
H	-0.99299500	5.56278900	2.29837300

H	-0.21549600	4.31614100	3.32366700
C	1.12619200	5.63061800	2.34058700
F	1.26908800	6.35253600	1.20643500
F	2.21347600	4.83613200	2.46258700
F	1.13982400	6.50516800	3.38644200

11

E = -723.185189

ZPVE = 0.214627

Symbol	X	Y	Z
C	-1.81105800	0.91877900	0.32468500
C	-0.31025100	1.00918400	0.26727400
C	-1.15103100	2.24662100	0.05620900
H	-2.33391900	0.43460000	-0.49401500
H	-2.27078900	0.77465200	1.29813500
H	0.20114600	0.58396300	-0.59140700
H	0.23186400	0.91680800	1.20496700
H	-1.21424000	2.62090200	-0.96521900
C	-1.22527600	3.33135700	1.10071000
H	-1.06056700	2.88996100	2.10338500
C	-2.54249800	4.05220800	1.08264400
C	-3.63659600	3.62876600	2.03165800
C	-2.91000800	4.93121700	2.24571000
H	-2.85477900	4.38968300	0.09596400
H	-3.42615100	2.81339700	2.71820300
H	-4.66094700	3.65733900	1.67306600
H	-3.43555800	5.85786700	2.03792100
H	-2.19818700	4.99158000	3.06399100
O	-0.22148800	4.34625300	0.88277100
C	1.09954500	3.86078600	0.97729500
H	1.25698900	3.27062600	1.89189200
H	1.39736700	3.26287100	0.10782400
C	2.01371400	5.05977600	1.05205500
F	1.77229100	5.82473100	2.14195300
F	1.91137200	5.85415700	-0.03760200
F	3.30893900	4.63894900	1.13034300

12

E = -566.616270

ZPVE = 0.095003

Symbol	X	Y	Z
C	-1.79617300	0.39966800	-0.14023500
H	-2.59784100	-0.30652100	-0.13270200
C	-0.84708700	1.16817700	-0.14985200
C	0.23890400	2.14244500	-0.15718300

H	0.12003400	2.84166400	-0.99827800
H	0.23657400	2.72518700	0.77603800
O	1.48053300	1.43814700	-0.28495400
C	2.56893800	2.33666000	-0.29679200
H	2.64101400	2.91177900	0.63709700
H	2.52384100	3.03019000	-1.14831300
C	3.83268900	1.52118300	-0.43385500
F	4.00036500	0.66158400	0.59477700
F	3.85767300	0.80596300	-1.57969500
F	4.90722500	2.35915500	-0.44873300

13

E = -1066.334599

ZPVE = 0.291849

Symbol	X	Y	Z
C	1.48122800	0.37852500	-0.29071500
C	2.15099200	1.77534200	-0.16964100
C	-0.42466800	2.03739800	-0.09159900
C	-0.04936900	0.53060000	-0.20755100
H	1.77462600	-0.08767900	-1.23846800
H	1.80307400	-0.27363800	0.52948400
H	-0.54931200	0.10342100	-1.09258400
H	-1.51199800	2.18862300	-0.06770900
H	3.24533100	1.69933300	-0.19641700
C	0.25633900	2.53762100	1.15498400
C	1.65377400	2.39056700	1.11492500
C	-0.36969800	3.05632300	2.28910000
C	2.42903300	2.76011900	2.21534400
C	0.41037000	3.44234500	3.38703600
H	-1.45310200	3.17862800	2.31500500
C	1.80240900	3.28978500	3.35150100
H	3.51230900	2.64154600	2.19018900
H	-0.06707000	3.85560800	4.27342500
H	2.40090900	3.58743200	4.21037300
C	0.20445600	2.71826200	-1.28024800
C	-0.47111700	3.39889200	-2.29491800
C	1.60509700	2.59674600	-1.31198800
C	0.26315800	3.97181200	-3.34224900
H	-1.55687300	3.49290100	-2.26758100
C	2.33432900	3.16005900	-2.36028700
C	1.65856300	3.85436300	-3.37356500
H	-0.25282100	4.51159900	-4.13395300
H	3.41985800	3.06571100	-2.38838500
H	2.22089600	4.30330800	-4.19010000
O	-0.46074800	-0.21266700	0.95041400
C	-1.86014300	-0.24859000	1.12497300
H	-2.39018800	-0.41831800	0.17666400
H	-2.24726300	0.66028100	1.60357400
C	-2.17174600	-1.41320300	2.03474200
F	-1.56032200	-1.30440700	3.23443300

F	-3.51545800	-1.46467900	2.26065000
F	-1.80687600	-2.59796600	1.49220600

For Table 4 (ROPh): B3LYP/6-311++G(d,p)

1

E = -577.971275

ZPVE = 0.230881

Symbol	X	Y	Z
C	-0.87610300	-0.81422100	-0.03079800
C	0.59373500	-0.87988300	-0.46662100
C	1.34209000	0.40302500	-0.11050800
C	-0.17619400	0.88109900	1.68130600
C	-0.96617900	-0.40236500	1.44490200
H	2.42048200	0.29167200	-0.25385700
H	1.09868800	-1.70223900	0.05105400
H	0.68634700	-1.05778400	-1.54061000
H	-1.40817200	-0.08493300	-0.65007300
H	-1.35777100	-1.78282500	-0.19240500
H	-0.11135700	1.12871500	2.74149600
H	-0.64332600	1.72391800	1.15822100
H	-0.55873600	-1.19723400	2.08024800
H	-2.00735600	-0.24681400	1.74604100
O	1.18958600	0.75168700	1.24657000
O	0.85957800	1.42286000	-0.98680800
C	1.58375300	2.58116600	-1.14272600
C	1.23254800	3.36837200	-2.24426800
C	2.60565600	2.99468400	-0.28399200
C	1.90719500	4.55803900	-2.49109100
H	0.43564500	3.02735400	-2.89442200
C	3.28025100	4.18762000	-0.55197800
H	2.85213200	2.41579400	0.59513600
C	2.94000000	4.97403300	-1.64858200
H	1.62903600	5.16007400	-3.34911500
H	4.07280900	4.50427000	0.11722000
H	3.46707600	5.90052200	-1.84371800

2

E = -950.659970

ZPVE = 0.355170

Symbol	X	Y	Z
C	-2.20293700	0.76436100	0.11599900
C	-1.03501700	-0.22587700	0.23346300
C	0.33345600	0.40072300	-0.13527400
C	0.57276200	1.70770300	0.63889100
C	-0.60527200	2.68770800	0.54151100

C	-1.93813100	2.03525000	0.93293600
H	1.11301100	-0.28921800	0.21888400
H	-0.98601600	-0.58306700	1.26833700
H	-1.22657100	-1.10926100	-0.38407700
H	-2.36447200	1.03570500	-0.93353700
H	-3.12650800	0.28499900	0.45698800
H	1.49118400	2.18268000	0.28116900
H	-0.41180900	3.55948600	1.17234100
H	-0.66020000	3.05432300	-0.48997500
H	-1.91376200	1.78398500	1.99860900
H	-2.75258000	2.75395900	0.79760200
Si	0.74935700	0.46483000	-2.01137500
C	-0.42791300	1.48418700	-3.08851300
H	-0.47093800	2.53442800	-2.78711200
H	-0.08400600	1.45800600	-4.12814500
H	-1.44757100	1.09002700	-3.07283300
C	2.49601900	1.16790100	-2.21151900
H	2.83113300	1.06285800	-3.24839400
H	2.54732800	2.23190700	-1.96161000
H	3.21780200	0.64302500	-1.57804600
C	0.73590100	-1.31734700	-2.64556200
H	1.41740400	-1.95251900	-2.07133900
H	-0.26037500	-1.76570400	-2.59134000
H	1.05377700	-1.35387000	-3.69238400
O	0.78512300	1.32185800	2.02285300
C	1.46308800	2.13520800	2.88282000
C	1.58787200	1.65112900	4.19334900
C	2.03539500	3.36859600	2.55101300
C	2.27535100	2.38522200	5.14996000
H	1.14039800	0.69390000	4.43338900
C	2.72598000	4.09483700	3.52444800
H	1.95050000	3.77518500	1.55272400
C	2.85196300	3.61540900	4.82354700
H	2.36317500	1.99435700	6.15783500
H	3.16475800	5.04912900	3.25365300
H	3.38762200	4.18779700	5.57144600

3

E = -542.033585

ZPVE = 0.254431

Symbol	X	Y	Z
C	-4.20133900	-0.57457700	-0.29737600
C	-2.70333200	-0.51130500	-0.00352700
C	-2.29046400	0.88231300	0.48169600
C	-3.10712200	1.30264100	1.71418500
C	-4.61593800	1.23312800	1.44039900
C	-5.02633200	-0.15509300	0.92874400
H	-1.21994100	0.90958700	0.70161100
H	-2.46644300	-1.26070900	0.76256400
H	-4.41486500	0.09265600	-1.14048000

H	-4.46375400	-1.58702500	-0.61697000
H	-2.86121000	0.64465100	2.55805800
H	-2.82027500	2.31364700	2.01931900
H	-5.17715900	1.48358400	2.34631100
H	-4.88090100	1.98800000	0.68914200
H	-4.88763800	-0.89168300	1.73081900
H	-6.09146200	-0.16998300	0.67844700
H	-2.46367800	1.58833600	-0.33900900
O	-2.03135700	-0.86330800	-1.22559700
C	-0.75145500	-1.33917200	-1.21309600
C	-0.20232700	-1.61421400	-2.47321400
C	0.01183700	-1.57504600	-0.06478400
C	1.08575900	-2.12047700	-2.58024200
H	-0.80826700	-1.42570700	-3.35142500
C	1.30601000	-2.08636400	-0.18858900
H	-0.38073700	-1.36600400	0.92087200
C	1.85230600	-2.36191500	-1.43729600
H	1.49469500	-2.32924700	-3.56278000
H	1.88758300	-2.26495400	0.70937700
H	2.85782200	-2.75637200	-1.52250600

4

E = -542.032590

ZPVE = 0.254516

Symbol	X	Y	Z
C	-0.64543100	-1.24364500	-0.60085900
C	0.88575900	-1.23436000	-0.71321600
C	1.49558700	0.12152700	-0.34649200
C	-0.52491600	0.59590800	1.13628800
C	-1.10718600	-0.78132900	0.78813600
H	2.58703500	0.03196600	-0.35311700
H	1.30914500	-1.98305700	-0.03236000
H	1.20399600	-1.50410500	-1.72407100
H	-1.06522400	-0.58031800	-1.36425100
H	-1.02300100	-2.24882100	-0.81379900
H	-0.82141000	0.89159700	2.14760900
H	-0.93899000	1.34735400	0.45537000
H	-0.78516200	-1.51313600	1.54142700
H	-2.20057700	-0.75044600	0.83235800
O	1.10212200	1.03691500	-1.39129400
C	1.80832600	2.18157200	-1.62285100
C	1.31041300	2.99596800	-2.64983100
C	2.96413600	2.57065300	-0.93717100
C	1.96079200	4.17520600	-2.98626200
H	0.41530400	2.67836600	-3.17131600
C	3.60867300	3.75924600	-1.28887300
H	3.36919400	1.96851300	-0.13558500
C	3.11780900	4.56751900	-2.30828000
H	1.56312800	4.79240900	-3.78446100
H	4.50425600	4.04935200	-0.75016700

H	3.62410100	5.48849200	-2.57169000
C	1.00730300	0.60768500	1.02633500
H	1.39572100	1.60926400	1.22951300
H	1.43810900	-0.05687500	1.78615000

5

E = -1171.266933

ZPVE = 0.336042

Symbol	X	Y	Z
C	-2.00970300	0.11691300	-0.03626600
C	-0.57728600	-0.42857800	-0.12871800
C	0.46537600	0.66762900	-0.39742700
C	0.33843100	1.84164100	0.59047100
C	-1.09893700	2.36269500	0.71425300
C	-2.10475000	1.23959300	1.00573100
H	1.46752400	0.24918800	-0.29738700
H	-0.31074800	-0.89710400	0.82479700
H	-0.50168100	-1.20229300	-0.89767100
H	-2.32991300	0.49445300	-1.01450200
H	-2.69346500	-0.69786700	0.22124000
H	1.01414000	2.63966800	0.27209500
H	-1.14167000	3.12607700	1.49556400
H	-1.35693300	2.85608700	-0.22863000
H	-1.91018100	0.82832300	2.00224600
H	-3.11766300	1.65312800	1.02814800
S	0.31299200	1.24179400	-2.16239100
C	1.85445500	2.13696400	-2.38939200
C	1.81629200	3.49899400	-2.70467400
C	3.08978700	1.48195400	-2.32262900
C	2.99950600	4.19740400	-2.94526000
H	0.86046200	4.00643300	-2.76065800
C	4.26954400	2.18800700	-2.54277100
H	3.12602900	0.41989700	-2.10969100
C	4.22788700	3.54649900	-2.85782400
H	2.95854500	5.25237100	-3.19271100
H	5.22176800	1.67267600	-2.48345500
H	5.14752500	4.09155100	-3.03752600
O	0.80701300	1.30986700	1.84971300
C	1.29620000	2.13878200	2.82042200
C	1.70391200	1.50303300	4.00102100
C	1.41946600	3.52718000	2.70780900
C	2.23027400	2.24563200	5.04930600
H	1.60181000	0.42651500	4.06988400
C	1.95277200	4.26026300	3.77065300
H	1.10798500	4.04685000	1.81223100
C	2.35992000	3.63254300	4.94279300
H	2.54266900	1.73848500	5.95559100
H	2.04430500	5.33641300	3.67151000
H	2.77021100	4.21094600	5.76194000

6

E = -3174.599222

ZPVE = 0.334774

Symbol	X	Y	Z
C	-2.13689600	0.26457200	0.08653700
C	-0.90986600	-0.62656100	0.32662800
C	0.38280500	-0.02263100	-0.23545600
C	0.60368300	1.42479000	0.23031200
C	-0.63460600	2.31004600	0.03575900
C	-1.90284500	1.68046800	0.63042400
H	1.24162600	-0.61936000	0.07059700
H	-0.76507700	-0.74828200	1.40644300
H	-1.06409400	-1.62608900	-0.08857800
H	-2.35985200	0.31458600	-0.98662100
H	-3.01387600	-0.18434800	0.56297800
H	1.46444400	1.83854300	-0.30100900
H	-0.45203100	3.29154500	0.48101600
H	-0.76702500	2.46759500	-1.03972600
H	-1.80953300	1.63852900	1.72108500
H	-2.76428000	2.31919700	0.41258600
C	2.28930200	0.04848800	-2.54448200
C	2.77579800	1.18294400	-3.19985400
C	3.17723700	-0.95973400	-2.15595400
C	4.14122100	1.30953100	-3.45829000
H	2.08896600	1.96326900	-3.50537500
C	4.54190700	-0.82070400	-2.40097100
H	2.80186700	-1.85395400	-1.67224500
C	5.02620700	0.31232300	-3.05459800
H	4.51096500	2.19164600	-3.96930200
H	5.22499900	-1.60429400	-2.09225900
H	6.08752600	0.41462200	-3.25049000
O	0.93697100	1.30915400	1.63386800
Se	0.38022800	-0.14451600	-2.24596500
C	1.66108100	2.28294700	2.26278300
C	1.91907300	2.05443000	3.62136400
C	2.14928200	3.44406500	1.65509800
C	2.65706000	2.97172000	4.35708900
H	1.53392000	1.14900300	4.07512300
C	2.89222200	4.35635900	2.40827100
H	1.96114200	3.65174900	0.61080100
C	3.15134400	4.13190200	3.75590200
H	2.84928500	2.77936100	5.40694700
H	3.26626400	5.25283500	1.92583300
H	3.72678900	4.84710600	4.33143100

7

E = -425.332717

ZPVE = 0.188836

Symbol	X	Y	Z
C	-0.44262500	1.56008800	-0.05042700
H	0.59976000	1.26454600	-0.20409500
H	-1.00471800	0.64298700	0.15079800
C	-0.51836000	2.45588200	1.17613300
H	-1.55799200	2.74399100	1.38015600
H	0.06505800	3.37295700	1.02099700
C	-0.98770400	2.25172200	-1.30330200
H	-0.42353100	3.15971800	-1.53776800
H	-0.92363100	1.59095700	-2.17088000
H	-2.03785800	2.53434100	-1.18071400
O	0.00895100	1.72921000	2.28650700
C	0.05066200	2.32733900	3.51300100
C	-0.39464800	3.62575900	3.77766400
C	0.58340000	1.55066200	4.55062500
C	-0.30229500	4.13372500	5.07641700
H	-0.80973500	4.24391800	2.99315700
C	0.66827700	2.06959900	5.83492600
H	0.92256600	0.54691800	4.32380600
C	0.22566400	3.36694700	6.10876200
H	-0.65034800	5.14211300	5.27218200
H	1.08275800	1.45840100	6.62912100
H	0.29319100	3.76940900	7.11251300

8

E = -882.863241

ZPVE = 0.288158

Symbol	X	Y	Z
C	-0.91475300	0.42842300	-0.87581600
C	-1.29748000	1.80209300	-0.19234100
H	-2.26995000	2.28088600	-0.28167300
C	-0.63666200	1.32861100	1.14602100
H	-1.06748400	1.45435700	2.13712300
C	-0.25785600	-0.03964600	0.48256600
H	-0.40449200	-1.02306700	0.92405100
C	0.73656700	1.93538400	0.67586000
C	1.11159000	0.56047800	0.00655200
H	2.07719400	0.06327600	0.09125000
C	0.44969400	1.03332700	-1.33726700
H	0.86680400	0.90087200	-2.33254000
C	0.06955900	2.40354600	-0.66967800
H	0.19674500	3.38530500	-1.12136100
C	-1.81672600	-0.39038300	-1.72564000
O	-2.91357600	-0.78209800	-1.03427000
O	-1.62324800	-0.68185200	-2.88345900
C	-3.86662500	-1.58016800	-1.75954300
H	-3.40444000	-2.50503500	-2.10792100
H	-4.66513000	-1.79403700	-1.05227400
H	-4.25210000	-1.02866400	-2.61836600

C	1.67871500	2.73569000	1.51596600
H	2.56885600	3.01163200	0.93316400
H	2.00714700	2.14946300	2.38587600
O	0.99617100	3.91362200	1.95154500
C	1.65841500	4.81215500	2.73961300
C	2.98289000	4.66922200	3.16276200
C	0.92212100	5.93919000	3.12688800
C	3.55739800	5.65542200	3.96921600
H	3.57091400	3.80787800	2.87615200
C	1.50721600	6.90988600	3.92813600
H	-0.10282000	6.03018300	2.78758100
C	2.83087100	6.77570400	4.35630800
H	4.58561700	5.53658500	4.29290600
H	0.92708200	7.77791900	4.22127700
H	3.28489500	7.53512100	4.98163500

9

E = -658.687123

ZPVE = 0.315718

Symbol	X	Y	Z
C	-2.35711800	-1.70276700	0.04791600
C	-0.83042000	-1.81888800	0.09439600
C	-0.14244600	-0.48864200	0.53753400
C	-1.09604000	0.73732300	0.69484500
C	-2.55976300	0.37089300	0.46686800
C	-2.83932700	-0.91521700	1.29704500
H	0.37231000	-0.65354000	1.48726300
H	-0.55830300	-2.61652900	0.79297100
H	-0.45445400	-2.12834400	-0.88476700
H	-2.82359700	-2.66889900	-0.16704200
H	-1.01584200	1.13462300	1.71334900
H	-3.19575700	1.24644900	0.61931800
H	-2.27015500	-1.04835800	2.22168100
H	-3.89577200	-1.05452400	1.51937500
H	0.63680300	-0.21681900	-0.17661300
C	-2.80411200	-0.48165200	-0.82969300
C	-4.30071400	-0.54156500	-1.17342800
H	-4.93177500	-0.77104200	-0.31256600
H	-4.63580800	0.41649100	-1.58381700
H	-4.48474400	-1.30930700	-1.93216200
C	-2.03234000	-0.17672700	-2.11531600
H	-0.95668200	-0.09190200	-1.97092200
H	-2.21591100	-0.96511000	-2.85421300
H	-2.37152400	0.76847200	-2.54856400
O	-0.77536100	1.80835400	-0.21447300
C	0.28097600	2.63301900	0.04114300
C	0.44403600	3.70043800	-0.85333400
C	1.17779000	2.48375600	1.10447000
C	1.48313700	4.60452300	-0.68123700
H	-0.25977300	3.80065200	-1.67096400

C	2.21617200	3.40439700	1.26670100
H	1.08630400	1.66137900	1.80053300
C	2.37842700	4.46525300	0.38262400
H	1.59440400	5.42584400	-1.38071700
H	2.90481300	3.27844000	2.09515800
H	3.18861500	5.17228000	0.51549400

10

E = -463.403264

ZPVE = 0.194748

Symbol	X	Y	Z
C	-1.44016000	0.61645000	0.12478300
C	-0.45033000	1.52832200	-0.55781400
C	-1.58701500	2.11561000	0.23807100
H	-2.15746500	0.08107700	-0.48497200
H	-1.10550700	0.06940900	0.99922400
H	-0.48753500	1.61367600	-1.63681000
H	0.54644300	1.60071800	-0.13807400
H	-2.39354500	2.56773800	-0.32972900
C	-1.31901600	2.77791500	1.55857500
H	-2.22373500	2.78364900	2.17980200
H	-0.53246300	2.23910900	2.10317000
O	-0.90241500	4.12448000	1.31139700
C	-0.63131600	4.93823600	2.37323000
C	-0.25986700	6.25107200	2.05343700
C	-0.69895200	4.54448600	3.71336100
C	0.03917700	7.15513500	3.06303900
H	-0.21346600	6.53530600	1.00896700
C	-0.39516500	5.46705000	4.71814000
H	-0.98191000	3.53678600	3.98574800
C	-0.02634700	6.77039500	4.40518200
H	0.32535800	8.16804800	2.80199600
H	-0.45053300	5.15253400	5.75458400
H	0.20717700	7.47863200	5.19118500

11

E = -580.065702

ZPVE = 0.256211

Symbol	X	Y	Z
C	-2.34247800	0.64975200	0.66701000
C	-0.91540300	0.53282300	0.19245400
C	-1.65749900	1.83773900	0.03539000
H	-3.12256400	0.15201600	0.10392500
H	-2.51604500	0.67230000	1.73683500
H	-0.71414900	-0.04224200	-0.70323800

H	-0.13575900	0.47045400	0.94095900
H	-1.96821200	2.08442200	-0.97561200
C	-1.32163800	3.06264400	0.85845500
H	-1.03094200	2.76799900	1.87233300
C	-2.48038900	4.02846300	0.95260300
C	-3.48165500	3.90667200	2.07505900
C	-2.51487500	5.06571500	2.04368600
H	-2.87160800	4.33337200	-0.01321700
H	-3.32231100	3.13618700	2.82072800
H	-4.52465200	4.09370900	1.84992400
H	-2.89463800	6.04997800	1.79859600
H	-1.70245700	5.06899000	2.76156200
O	-0.24421200	3.79506100	0.22702000
C	1.07010500	3.56257500	0.51474700
C	1.98530800	4.18504500	-0.34582600
C	1.54917800	2.81136400	1.59288100
C	3.35105500	4.05767300	-0.13057400
H	1.59807000	4.76584700	-1.17443400
C	2.92545400	2.69142400	1.79719400
H	0.87392000	2.31898500	2.27899000
C	3.83464000	3.30779100	0.94397500
H	4.04327000	4.54653700	-0.80742600
H	3.28175500	2.10571300	2.63776900
H	4.90050700	3.20679600	1.11008500

12

E = -422.882646

ZPVE = 0.141442

Symbol	X	Y	Z
C	-1.81500600	0.42550800	-0.10207400
H	-2.65350200	-0.15507000	0.19671000
C	-0.86317900	1.07999800	-0.42957400
C	0.27119700	1.88145300	-0.86802100
H	0.70774000	1.44005300	-1.77326900
H	-0.06673800	2.89593500	-1.11600700
O	1.24241300	1.92649000	0.17649100
C	2.39170600	2.63844400	-0.04421000
C	3.30476600	2.64617700	1.01734000
C	2.68674700	3.32750900	-1.22302700
C	4.50133100	3.33835800	0.89649500
H	3.05309200	2.10446800	1.92101800
C	3.89679500	4.01985500	-1.32844200
H	1.99843200	3.33741800	-2.05744000
C	4.80701400	4.03130000	-0.27845500
H	5.20144100	3.33792700	1.72448200
H	4.11894000	4.55247400	-2.24647600
H	5.74220100	4.57072000	-0.36929300

13

E = -924.303323

ZPVE = 0.337028

Symbol	X	Y	Z
C	1.40317300	0.44364200	-0.01388200
C	2.17131200	1.80227000	-0.06449800
C	-0.38456600	2.24656900	-0.08731300
C	-0.12277200	0.70045500	-0.07748000
H	1.71822200	-0.19422800	-0.84217900
H	1.62660700	-0.07634900	0.91903100
H	-0.54001700	0.26400900	-0.98827700
H	-1.45251900	2.46511600	-0.09555800
H	3.25088400	1.64346900	-0.05597500
C	0.31291600	2.83080600	1.12629800
C	1.69687600	2.60487200	1.13248200
C	-0.28832700	3.52439300	2.16931700
C	2.47846600	3.07579200	2.18075100
C	0.49891200	4.00439600	3.21971200
H	-1.36040400	3.69207700	2.16880400
C	1.87457700	3.78177900	3.22528000
H	3.54950400	2.89957400	2.18799400
H	0.03636000	4.55188500	4.03333200
H	2.48004400	4.15794800	4.04242600
C	0.32126200	2.76226800	-1.32871900
C	-0.27073700	3.39861300	-2.41339700
C	1.70426500	2.52373700	-1.31687600
C	0.52307000	3.80721300	-3.48967000
H	-1.34000200	3.58516100	-2.42236400
C	2.49153600	2.92674400	-2.38871300
C	1.89623300	3.57240900	-3.47706200
H	0.06770900	4.31075600	-4.33504700
H	3.56161500	2.74517800	-2.38097600
H	2.50734600	3.89345100	-4.31324600
O	-0.71143800	0.06225400	1.06098200
C	-2.05532200	-0.19144600	1.09905100
C	-2.52432800	-0.73930300	2.30036300
C	-2.94979700	0.03425900	0.04803100
C	-3.86703800	-1.06061900	2.44402100
H	-1.81571000	-0.90434500	3.10304700
C	-4.29814800	-0.29608400	0.20745400
H	-2.61866200	0.45916500	-0.88969000
C	-4.76649700	-0.84189700	1.39732000
H	-4.21474700	-1.48504000	3.37943700
H	-4.98273100	-0.11856700	-0.61482300
H	-5.81438300	-1.09243600	1.51167000

<u>For Table 4 (ROPh): M06-2X/6-311++G(d,p)</u>

1

E = -577.722091

ZPVE = 0.233946

Symbol	X	Y	Z
C	-0.85340800	-0.77329900	-0.04883900
C	0.61892200	-0.92612800	-0.43605300
C	1.38529900	0.35247700	-0.13236200
C	-0.12243900	0.96135200	1.59241900
C	-0.95300000	-0.30015700	1.40294900
H	2.46244000	0.22794400	-0.27765000
H	1.07848200	-1.72864900	0.14819900
H	0.73495200	-1.16496200	-1.49464800
H	-1.32496800	-0.03823700	-0.70773400
H	-1.37895500	-1.72069400	-0.18588600
H	-0.07781800	1.26379700	2.63823000
H	-0.54204300	1.78859600	1.00802100
H	-0.57506700	-1.07846200	2.07416400
H	-1.99060700	-0.09709800	1.68034500
O	1.23455900	0.75070300	1.20292500
O	0.90268800	1.33467300	-1.03016300
C	1.58417800	2.51541900	-1.14435200
C	1.18588600	3.33773100	-2.19936500
C	2.61280900	2.91521000	-0.29263800
C	1.82018200	4.55236400	-2.40788700
H	0.38339800	2.99876600	-2.84304300
C	3.24499000	4.13623400	-0.52228300
H	2.89800800	2.30477000	0.55282000
C	2.85836100	4.95878500	-1.57150300
H	1.50573900	5.18339800	-3.23088600
H	4.04418600	4.44497500	0.14148000
H	3.35463700	5.90709900	-1.73563700

2

E = -950.312959

ZPVE = 0.359299

Symbol	X	Y	Z
C	-2.09708100	0.97659900	0.14197300
C	-1.04509900	-0.13341900	0.24096700
C	0.36723500	0.34740800	-0.15295600
C	0.75047000	1.60928500	0.61965600
C	-0.29794300	2.71402000	0.47222800
C	-1.67337200	2.21998900	0.92557200
H	1.08437100	-0.42234800	0.16424500
H	-1.01549300	-0.49524400	1.27407300
H	-1.34017700	-0.98580100	-0.38060600
H	-2.25448400	1.25420700	-0.90444700
H	-3.05532100	0.60583500	0.51596700
H	1.73327000	1.95677800	0.28440900
H	-0.00362900	3.59485200	1.04750200
H	-0.33282800	3.01516500	-0.58189500

H	-1.62736600	1.98368300	1.99352600
H	-2.41214100	3.01609900	0.80430600
Si	0.67979900	0.43987900	-2.03082500
C	-0.73631100	1.14246000	-3.05477000
H	-1.00334000	2.16354000	-2.77325800
H	-0.43515100	1.15666600	-4.10674100
H	-1.63364200	0.52307700	-2.97927800
C	2.21910300	1.47639800	-2.34975600
H	2.50272900	1.42054300	-3.40419800
H	2.05371000	2.53036700	-2.10856800
H	3.06892200	1.12507600	-1.75791100
C	0.97865200	-1.32414400	-2.61204600
H	1.85908900	-1.75568700	-2.12902300
H	0.12398700	-1.96672300	-2.38317600
H	1.13785400	-1.35808000	-3.69303300
O	0.85807200	1.21424800	1.99620800
C	1.46472500	2.03557700	2.89232800
C	1.36993700	1.63905900	4.23030800
C	2.17354400	3.19340700	2.56728200
C	1.97801000	2.38623000	5.22532600
H	0.81633900	0.73621000	4.45787600
C	2.78037800	3.93452500	3.58038800
H	2.26079400	3.52839300	1.54281800
C	2.68980000	3.54262700	4.90815300
H	1.89643600	2.06446300	6.25705200
H	3.32883000	4.83140000	3.31645800
H	3.16360500	4.12719600	5.68659800

3

E = -541.786121

ZPVE = 0.257454

Symbol	X	Y	Z
C	-4.22618500	-0.56347200	-0.30846700
C	-2.73131400	-0.55725100	-0.02295600
C	-2.27260300	0.82104100	0.44750800
C	-3.04975200	1.24735700	1.69602900
C	-4.55752700	1.23549300	1.43414400
C	-5.01511500	-0.13595000	0.93150300
H	-1.19657400	0.82658500	0.63573000
H	-2.52327300	-1.30941900	0.75024200
H	-4.41817000	0.12903800	-1.13557600
H	-4.52353800	-1.56033200	-0.64201700
H	-2.82073300	0.56014400	2.52002600
H	-2.72419600	2.24006200	2.01589700
H	-5.10295800	1.50847600	2.34118600
H	-4.79514800	1.99297000	0.67787000
H	-4.87045000	-0.87745200	1.72659200
H	-6.08385300	-0.12312800	0.70486800
H	-2.46005700	1.52800900	-0.36875100
O	-2.08397500	-0.93583400	-1.23437700

C	-0.79223400	-1.35897500	-1.20892300
C	-0.22432700	-1.62376300	-2.45904700
C	-0.03554600	-1.55632600	-0.05323200
C	1.07886600	-2.08269600	-2.55039800
H	-0.83255200	-1.46343400	-3.34076200
C	1.27528500	-2.01965100	-0.16204900
H	-0.44474200	-1.35436500	0.92716300
C	1.84139400	-2.28499900	-1.40026200
H	1.50418200	-2.28477600	-3.52654000
H	1.85436700	-2.16938400	0.74186600
H	2.86074400	-2.64258000	-1.47261500

4

E = -541.785970

ZPVE = 0.257682

Symbol	X	Y	Z
C	-0.62871400	-1.21160500	-0.60833100
C	0.89805500	-1.29601100	-0.67141800
C	1.55239000	0.04969200	-0.37488000
C	-0.45135800	0.70211600	1.02016700
C	-1.09178200	-0.65924900	0.74157400
H	2.64101500	-0.07261500	-0.38056500
H	1.26015200	-2.01626500	0.07076000
H	1.22944000	-1.64056500	-1.65374400
H	-0.98113200	-0.55494600	-1.40957900
H	-1.06018100	-2.19972800	-0.78705300
H	-0.76416200	1.08101600	1.99629300
H	-0.79323700	1.42392300	0.27096700
H	-0.80922500	-1.36065200	1.53690300
H	-2.18149700	-0.57675100	0.76334400
O	1.17546100	0.91195900	-1.45208000
C	1.81543600	2.09792100	-1.62784900
C	1.26517100	2.93861900	-2.60025800
C	2.96118300	2.49880500	-0.93946600
C	1.85434200	4.16017200	-2.88112400
H	0.37736000	2.60384900	-3.12275900
C	3.54244100	3.73154500	-1.23353100
H	3.40709100	1.87136300	-0.17999400
C	2.99971000	4.56793400	-2.19820100
H	1.41677700	4.80018900	-3.63839700
H	4.43204900	4.03344700	-0.69294900
H	3.45840100	5.52401400	-2.41657500
C	1.07602200	0.61548500	0.96579800
H	1.51799900	1.59877300	1.14207100
H	1.43980700	-0.04901400	1.75811800

5

E = -1170.899694

ZPVE = 0.340190

Symbol	X	Y	Z
C	-1.96663100	0.21284900	0.00828900
C	-0.58913900	-0.45021100	-0.07428500
C	0.51707100	0.54792200	-0.42856600
C	0.50564000	1.75898900	0.51019600
C	-0.87511100	2.40677400	0.61426700
C	-1.94482900	1.38055000	0.99664700
H	1.49184300	0.06411000	-0.34287000
H	-0.33640700	-0.87526200	0.90209900
H	-0.58871100	-1.26875400	-0.79828500
H	-2.26589500	0.57632000	-0.98085200
H	-2.70946900	-0.52843000	0.31291900
H	1.25458200	2.47719600	0.16218400
H	-0.84383800	3.21586500	1.34762600
H	-1.11362300	2.85255100	-0.35638100
H	-1.73378100	1.00134500	2.00216800
H	-2.92274000	1.86622200	1.03505600
S	0.31887800	1.05216900	-2.18720000
C	1.77948400	2.05953800	-2.38672200
C	1.64661900	3.42547600	-2.63464200
C	3.05233800	1.49178100	-2.31212200
C	2.77895000	4.21747700	-2.80349700
H	0.65557200	3.86065500	-2.69039600
C	4.18049300	2.28942400	-2.46264300
H	3.15389100	0.42573300	-2.14360600
C	4.04616500	3.65290000	-2.71095500
H	2.66852700	5.27748100	-2.99963200
H	5.16592000	1.84335700	-2.39835100
H	4.92715400	4.27105600	-2.83521300
O	0.91527300	1.22966600	1.77456600
C	1.34278700	2.07452200	2.75235100
C	1.58519000	1.48013200	3.99398500
C	1.56338800	3.44186500	2.58588600
C	2.04637700	2.24357900	5.05375100
H	1.40755300	0.41656600	4.09666600
C	2.02797700	4.19624500	3.66240700
H	1.38090900	3.92876000	1.63761000
C	2.27173800	3.61050400	4.89626700
H	2.23156000	1.76896000	6.01028800
H	2.19735500	5.25769800	3.52345700
H	2.63080900	4.20702500	5.72536600

6

E = -3174.265305

ZPVE = 0.338945

Symbol	X	Y	Z
C	-2.08891100	0.39325400	0.07590200

C	-0.98732100	-0.62147100	0.39314900
C	0.36520900	-0.21558000	-0.19549500
C	0.75169600	1.21300300	0.19476000
C	-0.35831400	2.22506300	-0.09126200
C	-1.68314700	1.79293200	0.54251800
H	1.14724000	-0.88881500	0.15742000
H	-0.85883500	-0.67954700	1.47921000
H	-1.25922100	-1.62080100	0.04425900
H	-2.28436200	0.41011100	-1.00231900
H	-3.01823100	0.08596500	0.56174300
H	1.67644900	1.48121300	-0.32499500
H	-0.06040200	3.20684700	0.28395100
H	-0.47102700	2.30907500	-1.17642400
H	-1.57568100	1.79413900	1.63240800
H	-2.46222600	2.51801500	0.29569500
C	2.16860000	0.00046300	-2.48655700
C	2.49404700	1.17087000	-3.17093800
C	3.18278600	-0.84190600	-2.03108400
C	3.82890900	1.49704400	-3.39567100
H	1.70299100	1.82420000	-3.51996100
C	4.51489000	-0.50298200	-2.24286300
H	2.92789500	-1.76176800	-1.51748500
C	4.83973600	0.66497400	-2.92696900
H	4.07681000	2.40623700	-3.93074600
H	5.29941400	-1.15736000	-1.88154200
H	5.87818000	0.92356700	-3.09591200
O	1.01129200	1.13517500	1.60113500
Se	0.32067800	-0.43814900	-2.16658100
C	1.70575400	2.13221500	2.21441000
C	1.78441100	2.03838200	3.60686800
C	2.33556300	3.18898100	1.55655100
C	2.48704300	2.98748400	4.33082300
H	1.28837600	1.20738500	4.09334600
C	3.03884900	4.13601100	2.29980400
H	2.28912900	3.28883400	0.48066600
C	3.12081300	4.04636800	3.68186700
H	2.54064700	2.90102500	5.40978500
H	3.52533900	4.95319800	1.77998500
H	3.66816700	4.78920000	4.24825400

7

E = -425.131681

ZPVE = 0.191126

Symbol	X	Y	Z
C	-0.43904600	1.55632100	-0.03856000
H	0.60168200	1.26295400	-0.19738900
H	-1.00447000	0.64183600	0.15745500
C	-0.50959700	2.44087400	1.19007600
H	-1.54859000	2.72787100	1.39785500

H	0.07476000	3.35760100	1.03777700
C	-0.98788800	2.27210400	-1.27002000
H	-0.41930100	3.18057300	-1.48428300
H	-0.93510800	1.63140500	-2.15105700
H	-2.03336800	2.55707100	-1.12758400
O	0.01646000	1.71094100	2.28475900
C	0.05350600	2.31363500	3.50173500
C	-0.39461500	3.61013600	3.75126900
C	0.58355900	1.54747800	4.54423800
C	-0.30722200	4.12722700	5.04415200
H	-0.80802200	4.22062900	2.96018000
C	0.66330500	2.07562100	5.82129900
H	0.92400800	0.54364600	4.32183300
C	0.21772900	3.37208700	6.08194300
H	-0.65771200	5.13571200	5.23065000
H	1.07593400	1.47250500	6.62159800
H	0.28083600	3.78296300	7.08165300

8

E = -882.510570

ZPVE = 0.292574

Symbol	X	Y	Z
C	-0.89654500	0.44753900	-0.85993000
C	-1.26914100	1.81216200	-0.18226900
H	-2.23922000	2.29311900	-0.27052100
C	-0.60874800	1.33506500	1.14743300
H	-1.02648400	1.46929500	2.14164800
C	-0.24681900	-0.03031800	0.48348700
H	-0.40522700	-1.01310600	0.91913300
C	0.75701500	1.92244300	0.66897800
C	1.12113900	0.55548400	0.00450800
H	2.08318000	0.05453300	0.08815600
C	0.46026500	1.03363600	-1.33069200
H	0.86401200	0.89388700	-2.32936900
C	0.09558300	2.40052200	-0.66245700
H	0.23430000	3.38337200	-1.10532700
C	-1.81239000	-0.36361800	-1.69860600
O	-2.89823300	-0.74048900	-0.99979100
O	-1.63408600	-0.65870400	-2.85099900
C	-3.84815800	-1.52589800	-1.72105100
H	-3.38739000	-2.44928200	-2.07308100
H	-4.64951100	-1.74046300	-1.01906800
H	-4.22671500	-0.96946300	-2.57890200
C	1.68934900	2.72963900	1.50760500
H	2.57721700	3.01472700	0.92690300
H	2.01602000	2.15123800	2.38260400
O	0.98667200	3.88837100	1.92471600
C	1.63614600	4.78564200	2.71371300
C	2.95701200	4.64713300	3.13686500

C	0.89290600	5.90383000	3.10185700
C	3.52207000	5.63236100	3.94708600
H	3.55041800	3.79035300	2.84814300
C	1.46869100	6.87239300	3.90616700
H	-0.13094900	5.98534300	2.75815500
C	2.78992900	6.74387000	4.33599900
H	4.54950700	5.51861700	4.27258600
H	0.88351700	7.73538700	4.20148700
H	3.23778800	7.50266000	4.96513500

9

E = -658.396978

ZPVE = 0.319856

Symbol	X	Y	Z
C	-2.31746700	-1.68232400	0.02590300
C	-0.79314800	-1.74379900	0.08402200
C	-0.17116100	-0.41362600	0.59690500
C	-1.16260800	0.77547700	0.74654400
C	-2.60383000	0.35949700	0.50360300
C	-2.83805000	-0.95493700	1.28975800
H	0.29662300	-0.59453300	1.56731300
H	-0.49555200	-2.55912400	0.74876900
H	-0.40038000	-1.98876300	-0.90574900
H	-2.75089100	-2.65269100	-0.22988700
H	-1.10141700	1.17639600	1.76587300
H	-3.27566200	1.20527900	0.66629400
H	-2.26331400	-1.09080700	2.21000700
H	-3.88848100	-1.14311900	1.49873600
H	0.63626700	-0.09572100	-0.06616400
C	-2.78328300	-0.45534800	-0.81262600
C	-4.26070300	-0.55610900	-1.19301200
H	-4.89773000	-0.83318800	-0.35142700
H	-4.61612000	0.40272400	-1.58113100
H	-4.39627600	-1.30700800	-1.97687800
C	-1.98504700	-0.08342400	-2.05725400
H	-0.91699700	0.02103900	-1.87183600
H	-2.12893500	-0.84958200	-2.82633600
H	-2.33540700	0.87054600	-2.45914200
O	-0.88175900	1.84369600	-0.15838200
C	0.21398800	2.61774800	0.04918900
C	0.40009100	3.65792500	-0.86729100
C	1.12757300	2.44264700	1.08931300
C	1.48100200	4.51347600	-0.73948300
H	-0.32283000	3.77191600	-1.66581000
C	2.20977700	3.31486900	1.20541800
H	1.01536800	1.63740300	1.80247900
C	2.39596600	4.34947900	0.30068600
H	1.61157300	5.31638100	-1.45563900
H	2.91390400	3.17122100	2.01680500

H	3.24096500	5.01914000	0.39928700

10

E = -463.195888

ZPVE = 0.197309

Symbol	X	Y	Z
C	-1.41164100	0.63568200	0.15372800
C	-0.44882500	1.56889800	-0.52684300
C	-1.60880700	2.12277600	0.24580400
H	-2.09951000	0.07162900	-0.46110800
H	-1.06950200	0.11704600	1.04091700
H	-0.47926200	1.63595800	-1.60563500
H	0.53525900	1.68724300	-0.09061600
H	-2.42328500	2.54897400	-0.32772900
C	-1.34350000	2.79650300	1.55693900
H	-2.24637000	2.81239000	2.17944400
H	-0.55672000	2.25741600	2.10147200
O	-0.92271400	4.12599200	1.29479000
C	-0.64189700	4.92866000	2.35410000
C	-0.25893300	6.23649400	2.04073200
C	-0.71062900	4.52651700	3.68753000
C	0.05116400	7.12917600	3.05203800
H	-0.21386000	6.52141100	0.99680500
C	-0.39511600	5.43908300	4.69481000
H	-1.00334400	3.52037500	3.95472100
C	-0.01471100	6.73697200	4.38974100
H	0.34663200	8.14020600	2.79705400
H	-0.45102700	5.11917800	5.72882500
H	0.22801300	7.43725500	5.17897300

11

E = -579.814270

ZPVE = 0.259368

Symbol	X	Y	Z
C	-1.97296100	0.88651300	0.27375200
C	-0.51253900	1.02428000	-0.05224400
C	-1.41086800	2.22802600	-0.10406500
H	-2.61612600	0.38697600	-0.43785100
H	-2.24346200	0.73324500	1.31138100
H	-0.15499100	0.62065000	-0.99011000
H	0.19791000	0.96665500	0.76377600
H	-1.66595400	2.60688600	-1.08865400
C	-1.29925500	3.29781300	0.95211900
H	-1.06175800	2.82228700	1.91626900
C	-2.56202800	4.09849300	1.10075200

C	-3.60856000	3.63106000	2.07090100
C	-2.79156600	4.85869700	2.37103800
H	-2.90939300	4.55768700	0.18157300
H	-3.40003800	2.73508500	2.64244100
H	-4.64734100	3.75962800	1.79863800
H	-3.27449200	5.82416600	2.30788900
H	-2.02636000	4.78300700	3.13417200
O	-0.25682200	4.23227400	0.62606900
C	1.02131300	3.74284600	0.71581200
C	1.76527000	3.56886500	-0.44623700
C	1.58225500	3.45627300	1.95827400
C	3.06943300	3.09340200	-0.36476300
H	1.30399000	3.80430200	-1.39780500
C	2.88408000	2.97334800	2.03156700
H	0.99784600	3.62346800	2.85628900
C	3.63070400	2.78694900	0.87153600
H	3.64780000	2.95748200	-1.27116300
H	3.32020700	2.75229100	2.99876400
H	4.64548200	2.41314800	0.93173100

12

E = -422.697931

ZPVE = 0.143479

Symbol	X	Y	Z
C	-1.80016200	0.43666200	-0.10967200
H	-2.64078200	-0.14429700	0.18706100
C	-0.84952100	1.08942300	-0.43459900
C	0.29297000	1.89124900	-0.86387500
H	0.73301900	1.44870300	-1.76519400
H	-0.04261500	2.90613100	-1.10731000
O	1.24455700	1.92541900	0.18224500
C	2.38741800	2.63437200	-0.03951200
C	3.30078100	2.64408300	1.01755600
C	2.67513600	3.31935500	-1.21798700
C	4.49315300	3.33560500	0.89265000
H	3.04780700	2.10219300	1.92029600
C	3.88221600	4.01156100	-1.32696200
H	1.98461800	3.32693700	-2.05042200
C	4.79334100	4.02569500	-0.28253300
H	5.19551300	3.33758200	1.71780000
H	4.10111300	4.54260500	-2.24582600
H	5.72682800	4.56573900	-0.37746700

13

E = -923.923268

ZPVE = 0.340908

Symbol	X	Y	Z
C	1.48417800	0.43182000	-0.11453200
C	2.17728500	1.82407300	-0.08859600
C	-0.39496400	2.13132800	-0.17429400
C	-0.04872700	0.61022000	-0.17781700
H	1.83900900	-0.13903700	-0.97356600
H	1.72361800	-0.12156800	0.79438300
H	-0.44497600	0.15108600	-1.08776500
H	-1.47179200	2.29750700	-0.20624300
H	3.26298400	1.72674900	-0.05245500
C	0.23349500	2.70130000	1.07669200
C	1.62297200	2.54804000	1.11881900
C	-0.44055100	3.29313400	2.13296800
C	2.34206700	2.99906400	2.21494600
C	0.28383700	3.75358000	3.23282900
H	-1.52042700	3.39382300	2.10221600
C	1.66639100	3.60943700	3.27231700
H	3.41976100	2.87829700	2.24889600
H	-0.23360800	4.22479500	4.06005200
H	2.22241800	3.97091800	4.12930400
C	0.31562400	2.71205900	-1.37590600
C	-0.28205500	3.33170200	-2.46269500
C	1.70566300	2.55451700	-1.32777200
C	0.51547900	3.80606100	-3.50527500
H	-1.35974600	3.45341500	-2.49653500
C	2.49725000	3.02247200	-2.36513400
C	1.89625300	3.65273800	-3.45597300
H	0.05635700	4.29760600	-4.35472100
H	3.57471600	2.90137800	-2.32710400
H	2.50987200	4.02540600	-4.26762500
O	-0.59042500	-0.04190800	0.96249500
C	-1.94164400	-0.16705700	1.08314300
C	-2.39824700	-0.53511500	2.35118700
C	-2.85463900	0.01584900	0.04440700
C	-3.75224300	-0.72407000	2.57468600
H	-1.66744700	-0.66482400	3.13991900
C	-4.21434800	-0.17689400	0.28546400
H	-2.52726700	0.30288400	-0.94605900
C	-4.67236900	-0.54559400	1.54220700
H	-4.09346600	-1.01017300	3.56269200
H	-4.91690100	-0.03421200	-0.52740400
H	-5.73064400	-0.69086000	1.71890700

<u>For Table 4 (ROPh): MP2/6-31+G(d)</u>

1

E = -575.986115

ZPVE = 0.233985

Symbol	X	Y	Z

C	-0.85873300	-0.77230100	-0.04366200
C	0.60863100	-0.93633200	-0.44201700
C	1.38936900	0.33200600	-0.14598200
C	-0.11005800	0.96262300	1.59208300
C	-0.94820600	-0.29181800	1.40566000
H	2.46806700	0.20843700	-0.30388700
H	1.06860800	-1.74607900	0.13873100
H	0.71516800	-1.17972000	-1.50489500
H	-1.33981500	-0.04341300	-0.70712900
H	-1.38937600	-1.72365900	-0.16907700
H	-0.05193500	1.26816800	2.63956600
H	-0.51198300	1.79768400	1.00255200
H	-0.57404100	-1.07164000	2.08197000
H	-1.98808200	-0.08214500	1.68806700
O	1.26148100	0.72990600	1.20645600
O	0.88645800	1.32378900	-1.04116600
C	1.58171300	2.51544800	-1.14553900
C	1.18920100	3.33431000	-2.21296800
C	2.60040500	2.92152200	-0.27360900
C	1.82697700	4.55713600	-2.42005900
H	0.39644100	2.98882600	-2.87272000
C	3.23613500	4.14956400	-0.50248800
H	2.87544600	2.31579400	0.58301000
C	2.85667200	4.97173600	-1.56559300
H	1.52015800	5.18638300	-3.25321600
H	4.02747400	4.46584600	0.17451300
H	3.35523700	5.92453600	-1.72797800

2

E = -947.691143

ZPVE = 0.361619

Symbol	X	Y	Z
C	-2.02451600	0.90107200	0.26328400
C	-0.95007800	-0.19060500	0.26450900
C	0.42783800	0.32773500	-0.19597600
C	0.82466100	1.57778700	0.58189700
C	-0.24736500	2.66353800	0.54924200
C	-1.58144000	2.12498600	1.06561900
H	1.18000400	-0.43376400	0.07506800
H	-0.85494000	-0.58842900	1.28408600
H	-1.27023700	-1.03166500	-0.36679100
H	-2.24859800	1.21057200	-0.76510500
H	-2.95753400	0.49655300	0.67751200
H	1.78342900	1.95942600	0.20729900
H	0.07331800	3.52715500	1.14441900
H	-0.35586600	3.01785300	-0.48619800
H	-1.47334700	1.85652200	2.12467500
H	-2.34477000	2.91201200	1.01265600
Si	0.66428700	0.45509900	-2.08933000
C	-0.74813600	1.27255800	-3.04263200

H	-0.96059600	2.29248500	-2.70548100
H	-0.47711600	1.32789000	-4.10476800
H	-1.67595800	0.69405800	-2.97421600
C	2.25708700	1.40922900	-2.44293100
H	2.52529400	1.32760800	-3.50327100
H	2.15519800	2.47678500	-2.21465000
H	3.10040900	1.02083100	-1.85933600
C	0.84462300	-1.31190600	-2.72951900
H	1.70930300	-1.81190300	-2.27790700
H	-0.04266400	-1.91536800	-2.50585200
H	0.98455700	-1.32342000	-3.81691700
O	1.01916300	1.12493900	1.95093200
C	1.51519100	2.02152100	2.87033200
C	1.20170700	1.74703800	4.20947900
C	2.33060900	3.11784300	2.55384200
C	1.70158500	2.56078500	5.22676100
H	0.57150000	0.88767600	4.42858400
C	2.81848900	3.93183700	3.58374300
H	2.59808200	3.34254800	1.52542700
C	2.50931600	3.66279400	4.91943600
H	1.45177300	2.33761700	6.26228000
H	3.44866900	4.78275700	3.33128400
H	2.89335000	4.30176500	5.71124500

3

E = -540.092644

ZPVE = 0.258241

Symbol	X	Y	Z
C	-4.27938500	-0.63188200	-0.23540500
C	-2.78350400	-0.66198600	0.02753100
C	-2.25450100	0.72114400	0.38369500
C	-2.99525000	1.28274000	1.60065600
C	-4.50560900	1.31228200	1.36160700
C	-5.02768900	-0.07340100	0.97799500
H	-1.17433100	0.68513600	0.56640000
H	-2.58456900	-1.37201300	0.84561900
H	-4.46092400	-0.00119900	-1.11654700
H	-4.62314500	-1.64301900	-0.48338500
H	-2.77796900	0.66036100	2.48166500
H	-2.62272000	2.28857400	1.83048300
H	-5.02543700	1.68016200	2.25533000
H	-4.72912300	2.02088800	0.55100500
H	-4.90514300	-0.75721100	1.83093400
H	-6.10276100	-0.03262200	0.76397300
H	-2.41196300	1.37162400	-0.48851200
O	-2.17993200	-1.15483700	-1.18671600
C	-0.83698300	-1.46211800	-1.17320500
C	-0.21979100	-1.50214000	-2.43175300
C	-0.09979000	-1.77583600	-0.02269200
C	1.12683900	-1.84887300	-2.53999300

H	-0.81498700	-1.25708100	-3.30850600
C	1.25494000	-2.11103900	-0.14479500
H	-0.55579600	-1.76094400	0.96262800
C	1.87483800	-2.15306500	-1.39557400
H	1.59475600	-1.87560000	-3.52220400
H	1.82310900	-2.34690800	0.75319400
H	2.92683600	-2.41574900	-1.47877400

4

E = -540.093053

ZPVE = 0.258338

Symbol	X	Y	Z
C	-0.58568200	-1.23535400	-0.61780400
C	0.93762600	-1.36747400	-0.56958700
C	1.61487700	-0.02324400	-0.33825400
C	-0.44949500	0.81793000	0.84045300
C	-1.11913100	-0.54261300	0.63751600
H	2.70137900	-0.17285300	-0.26211300
H	1.22879300	-2.03898600	0.25122700
H	1.32361900	-1.80268300	-1.49921100
H	-0.86893500	-0.65564600	-1.50487200
H	-1.03780400	-2.22943600	-0.72690000
H	-0.81463100	1.29173600	1.76056800
H	-0.71581800	1.48640300	0.01109100
H	-0.92414600	-1.17671300	1.51579700
H	-2.20814000	-0.42420600	0.57126800
O	1.32424000	0.75070500	-1.52669900
C	1.88231400	2.00497100	-1.64016300
C	1.16612600	2.91699500	-2.42772500
C	3.10926300	2.37901900	-1.07487900
C	1.67349600	4.19805400	-2.64934300
H	0.21952800	2.59899300	-2.85937800
C	3.60127400	3.67151400	-1.29422800
H	3.68589900	1.68207600	-0.47356400
C	2.89231500	4.58504900	-2.07877800
H	1.11007100	4.89836400	-3.26292500
H	4.55263500	3.95806200	-0.84975300
H	3.28405300	5.58595000	-2.24439200
C	1.07215200	0.67794300	0.90453700
H	1.54628700	1.65945200	1.02255800
H	1.35684900	0.07941400	1.78279300

5

E = -1167.970520

ZPVE = 0.339943

Symbol	X	Y	Z

C	-1.95051400	0.21896000	0.06968200
C	-0.59566400	-0.47743500	-0.07774300
C	0.52398700	0.48864900	-0.47539000
C	0.56953000	1.70694100	0.44495200
C	-0.78495200	2.38822300	0.60295800
C	-1.85769300	1.39272100	1.04605500
H	1.49178800	-0.02269200	-0.40037000
H	-0.31223300	-0.92252500	0.88498700
H	-0.65144800	-1.29620800	-0.80686600
H	-2.29723600	0.58246000	-0.90710300
H	-2.69599700	-0.50745000	0.41768200
H	1.32574800	2.40714000	0.07077200
H	-0.69895200	3.21000200	1.32454100
H	-1.06054800	2.83418800	-0.36245200
H	-1.61401700	1.01952600	2.04989400
H	-2.82610400	1.90327300	1.12169500
S	0.30568400	0.98528200	-2.23220700
C	1.73092200	2.04343100	-2.38988700
C	1.56017900	3.42702800	-2.55271700
C	3.02733400	1.50540200	-2.35914300
C	2.67526400	4.26408800	-2.67024400
H	0.55397900	3.84124700	-2.58069900
C	4.13909500	2.34742100	-2.45498500
H	3.16186700	0.42945800	-2.26141500
C	3.96603000	3.72782400	-2.61165800
H	2.53411300	5.33553400	-2.79949600
H	5.14085700	1.92342500	-2.42194100
H	4.83268900	4.38042300	-2.69365000
O	1.01504400	1.16119900	1.70857300
C	1.39695000	2.04523800	2.69495400
C	1.41176300	1.51898500	3.99459800
C	1.79916700	3.36920300	2.46911600
C	1.82604600	2.31184600	5.06493900
H	1.09875500	0.48742200	4.14083200
C	2.20343600	4.15648700	3.55506200
H	1.80523500	3.79796400	1.47131000
C	2.22161400	3.63846100	4.85207000
H	1.83354800	1.89309800	6.06941700
H	2.51080600	5.18497900	3.37470700
H	2.53780000	4.25938900	5.68700700

6

E = -3168.069659

ZPVE = 0.339146

Symbol	X	Y	Z
C	-2.10325700	0.38551200	0.10484200
C	-1.02344500	-0.66868300	0.35821400
C	0.32547400	-0.27164900	-0.23758300
C	0.75202800	1.13332500	0.16468300

C	-0.33576100	2.18143600	-0.04344700
C	-1.65187000	1.75751800	0.60978500
H	1.10317500	-0.97478900	0.08303900
H	-0.87889900	-0.78129600	1.44165800
H	-1.32881100	-1.64946900	-0.02888000
H	-2.32959200	0.44852900	-0.96865700
H	-3.03242100	0.08345700	0.60471800
H	1.66352400	1.39458800	-0.38355500
H	0.00731300	3.14065500	0.36452200
H	-0.48002800	2.32299400	-1.12300300
H	-1.52282100	1.72379500	1.70005400
H	-2.42246100	2.51051900	0.40165200
C	2.10998800	0.09294600	-2.47254000
C	2.42821900	1.24503700	-3.20466200
C	3.13334600	-0.69342500	-1.92519900
C	3.76762600	1.61129700	-3.38047700
H	1.63106100	1.85572200	-3.62428000
C	4.46881100	-0.31526400	-2.09011400
H	2.88886600	-1.60348800	-1.38025600
C	4.78846700	0.84013200	-2.81372300
H	4.01168100	2.50597200	-3.95035300
H	5.25981500	-0.92508100	-1.65777200
H	5.82863300	1.13077900	-2.94529100
O	1.06746500	1.00584600	1.57317600
Se	0.27320500	-0.40189400	-2.21881500
C	1.77274700	2.03186600	2.16454600
C	1.67183700	2.09963900	3.56130700
C	2.58311500	2.94447400	1.47387600
C	2.37231700	3.07854800	4.26618600
H	1.03920500	1.37674600	4.07188200
C	3.27005200	3.92962100	2.19476100
H	2.68563800	2.91070200	0.39336700
C	3.17568300	4.00256200	3.58637200
H	2.28552800	3.12232700	5.35015700
H	3.89258800	4.63972200	1.65334500
H	3.71519100	4.77162300	4.13416400

7

E = -423.815774

ZPVE = 0.191113

Symbol	X	Y	Z
C	-0.45554700	1.55163400	-0.04466200
H	0.58122300	1.22611900	-0.18317000
H	-1.05498600	0.65379000	0.14131600
C	-0.52458500	2.44078300	1.18036900
H	-1.56008100	2.75722200	1.36943000
H	0.09745600	3.33778600	1.05025900
C	-0.95725900	2.27980500	-1.29076400
H	-0.35276800	3.16885600	-1.49986100

H	-0.90782000	1.62910600	-2.16866900
H	-1.99795700	2.59918700	-1.17026600
O	-0.04047200	1.67644500	2.29166300
C	0.02010900	2.30285800	3.51390100
C	-0.45920700	3.59402400	3.77129000
C	0.58212300	1.54158300	4.55003900
C	-0.31857700	4.13240700	5.05843700
H	-0.90148600	4.20065300	2.98750400
C	0.70437400	2.08640700	5.82648400
H	0.93761800	0.53891000	4.32413500
C	0.24371400	3.38332500	6.09244800
H	-0.68056500	5.14073800	5.25026800
H	1.14754600	1.49007600	6.62158700
H	0.34398800	3.80947500	7.08784100

8

E = -879.926141

ZPVE = 0.290088

Symbol	X	Y	Z
C	-0.91613700	0.46083700	-0.85633500
C	-1.26912300	1.85656000	-0.20765500
H	-2.23294600	2.35831500	-0.32961800
C	-0.64866700	1.37284900	1.14448800
H	-1.07894500	1.53904600	2.13592100
C	-0.30738400	-0.01596400	0.50529500
H	-0.50542700	-0.99509500	0.94887100
C	0.74327000	1.91890200	0.68015200
C	1.08815300	0.52902600	0.03941000
H	2.04427200	0.00778800	0.15173600
C	0.46523900	1.01315900	-1.31766300
H	0.87791300	0.84800800	-2.31597700
C	0.12232700	2.40116200	-0.67378500
H	0.30030300	3.38231700	-1.12247200
C	-1.84820800	-0.29976000	-1.71498100
O	-2.79059200	-0.93093300	-0.96400300
O	-1.81796200	-0.34150500	-2.94040800
C	-3.79275000	-1.64059900	-1.72885300
H	-3.32379000	-2.42031300	-2.33160200
H	-4.45994400	-2.07131900	-0.98434200
H	-4.32822800	-0.94811300	-2.38093900
C	1.67968300	2.71025400	1.52355700
H	2.58923000	2.96569600	0.95722300
H	1.96847700	2.14188500	2.42184000
O	0.98145500	3.90426900	1.90010100
C	1.64838400	4.79996700	2.70439800
C	2.96341600	4.63456100	3.15769100
C	0.91543800	5.94064600	3.06436900
C	3.53321000	5.62025400	3.97630700
H	3.54966300	3.76091500	2.89079800

C	1.49650500	6.91164400	3.87724800
H	-0.10320000	6.04241600	2.69699200
C	2.81096800	6.75754100	4.33912700
H	4.55482900	5.48807100	4.32746600
H	0.92055000	7.79314900	4.15177800
H	3.26313300	7.51564400	4.97416200

9

E = -656.328667

ZPVE = 0.320722

Symbol	X	Y	Z
C	-2.30767700	-1.68393700	0.01474800
C	-0.78396100	-1.73592900	0.06811100
C	-0.16996400	-0.40500900	0.58753300
C	-1.16922700	0.77129000	0.75148100
C	-2.60559400	0.35250800	0.50436500
C	-2.82736000	-0.96888900	1.28530600
H	0.30873600	-0.59170300	1.55644000
H	-0.47863900	-2.55738100	0.72958800
H	-0.38827100	-1.97624900	-0.92604200
H	-2.73660500	-2.66215300	-0.24547200
H	-1.11159900	1.17527300	1.77472500
H	-3.28570800	1.19693800	0.67804500
H	-2.24802300	-1.10823400	2.20803900
H	-3.87918000	-1.16550200	1.50454000
H	0.63271300	-0.07220900	-0.07997000
C	-2.79028200	-0.45728100	-0.81325600
C	-4.27170700	-0.56767300	-1.17775400
H	-4.90011500	-0.85490200	-0.32957900
H	-4.63922500	0.39355900	-1.55797900
H	-4.40989800	-1.31796200	-1.96638800
C	-2.01471800	-0.07629200	-2.06921700
H	-0.94387800	0.04704000	-1.89954000
H	-2.15714900	-0.85033200	-2.83594200
H	-2.38713100	0.87258500	-2.47264200
O	-0.89910400	1.85277900	-0.16404200
C	0.21568100	2.62462600	0.05542200
C	0.42895700	3.64140100	-0.88888200
C	1.11043300	2.46361400	1.12315900
C	1.51928100	4.49942400	-0.75845000
H	-0.28074800	3.74632700	-1.70656000
C	2.20125200	3.33637300	1.24237300
H	0.97600100	1.68099000	1.86274700
C	2.41670000	4.35012200	0.30769800
H	1.67174300	5.28543900	-1.49557200
H	2.89188600	3.20539600	2.07344500
H	3.26843000	5.01870800	0.40837900

10

E = -461.770878

ZPVE = 0.196922

Symbol	X	Y	Z
C	-1.46175800	0.62855100	0.13393700
C	-0.45616100	1.52931700	-0.53456600
C	-1.59681100	2.12822100	0.24102600
H	-2.17554000	0.09780300	-0.48794200
H	-1.14576600	0.08198400	1.01819100
H	-0.47667700	1.61153600	-1.61653500
H	0.53476300	1.60117600	-0.09541700
H	-2.39397600	2.58852500	-0.33791100
C	-1.31825300	2.78469700	1.55606200
H	-2.22950300	2.85751200	2.16657900
H	-0.56577100	2.20827300	2.11435300
O	-0.81924800	4.10246500	1.28176400
C	-0.58157900	4.92189100	2.36003700
C	-0.24821400	6.24752800	2.04255700
C	-0.63683500	4.51244100	3.69910300
C	0.00868400	7.16336700	3.06053700
H	-0.20976600	6.53656900	0.99481900
C	-0.38663500	5.44904700	4.71233500
H	-0.88762000	3.49178900	3.97021800
C	-0.05503100	6.76875500	4.40416000
H	0.26295600	8.18988900	2.80398800
H	-0.43942200	5.12857200	5.75113300
H	0.13957500	7.48592300	5.19806400

11

E = -578.010730

ZPVE = 0.260434

Symbol	X	Y	Z
C	-1.93482800	0.86336400	0.30850700
C	-0.45794400	1.00384500	0.05182700
C	-1.35610200	2.21148700	-0.04682200
H	-2.54806800	0.36102300	-0.43337500
H	-2.25842900	0.70948800	1.33426200
H	-0.05147900	0.59797800	-0.86989600
H	0.21616700	0.94585700	0.90175800
H	-1.56279800	2.57909700	-1.05154400
C	-1.30850200	3.29385200	0.99729400
H	-1.08819700	2.84481200	1.98246300
C	-2.58675500	4.07532300	1.08055500
C	-3.64786800	3.65850700	2.06842400

C	-2.85292300	4.91879000	2.29645200
H	-2.93468400	4.46892400	0.12694100
H	-3.43873600	2.80423800	2.70616300
H	-4.68735700	3.74752300	1.76773900
H	-3.34687900	5.87534200	2.15734000
H	-2.09813400	4.91138100	3.07809000
O	-0.26964400	4.26561100	0.68588700
C	1.01575500	3.74693300	0.73381100
C	1.73878800	3.61949000	-0.45534900
C	1.60101500	3.41205000	1.96066500
C	3.04734000	3.12755100	-0.41905200
H	1.26389800	3.90200200	-1.39219500
C	2.90638000	2.91122200	1.98833200
H	1.04005800	3.55477400	2.88253600
C	3.63094000	2.76242200	0.79970200
H	3.61022400	3.02608300	-1.34505400
H	3.36308800	2.65100100	2.94145900
H	4.64744800	2.37583300	0.82493200

12

E = -421.441545

ZPVE = 0.140860

Symbol	X	Y	Z
C	-1.83777000	0.43726700	-0.10382500
H	-2.67605600	-0.14552100	0.21067500
C	-0.86414600	1.10353600	-0.42006300
C	0.27464300	1.89925000	-0.86789500
H	0.67313600	1.49099900	-1.80632500
H	-0.02710300	2.94130800	-1.04062300
O	1.27501600	1.84544400	0.15721300
C	2.41175700	2.59485000	-0.05993900
C	3.31317600	2.62540200	1.01402100
C	2.70774800	3.26964700	-1.25083800
C	4.49189300	3.36020800	0.90834900
H	3.05824100	2.08538900	1.92276100
C	3.89262700	4.01533600	-1.33602600
H	2.02997700	3.25733000	-2.09865000
C	4.79340500	4.05424700	-0.27172600
H	5.18361400	3.38323900	1.74791600
H	4.11424500	4.54880000	-2.25827700
H	5.71098700	4.63228600	-0.35049900

13

E = -921.163318

ZPVE = 0.338064

Symbol	X	Y	Z

C	1.54816300	0.39278800	-0.30073600
C	2.16158000	1.81037700	-0.11842700
C	-0.41543600	1.99767300	-0.32101100
C	0.01140300	0.50067200	-0.35144400
H	1.93827300	-0.05450300	-1.22263800
H	1.81886300	-0.25541600	0.54062700
H	-0.38842400	0.01399000	-1.25202500
H	-1.50256400	2.11314900	-0.40500300
H	3.25448600	1.76597900	-0.02798400
C	0.11505300	2.52851200	0.98468600
C	1.51200300	2.42184500	1.09835300
C	-0.64935500	3.02569100	2.04108400
C	2.15114400	2.81555800	2.27559200
C	-0.00485100	3.43823900	3.21486100
H	-1.73322100	3.09639300	1.95008700
C	1.38736100	3.32862100	3.33323900
H	3.23367400	2.72845300	2.37092600
H	-0.58866400	3.83891500	4.04170600
H	1.87897600	3.64769600	4.25055200
C	0.31981200	2.67814500	-1.44549700
C	-0.26154100	3.32702600	-2.53679800
C	1.71886400	2.60462500	-1.32254100
C	0.56420200	3.91665400	-3.50366900
H	-1.34638600	3.38553600	-2.62752800
C	2.54042900	3.18189600	-2.29203000
C	1.95786700	3.84532000	-3.38112900
H	0.12108900	4.43307700	-4.35310100
H	3.62504600	3.12372800	-2.19993100
H	2.59161700	4.30659000	-4.13628700
O	-0.46302500	-0.18402600	0.82577200
C	-1.82166200	-0.16107400	1.07045400
C	-2.19404800	-0.15502800	2.42077900
C	-2.79924500	-0.18717000	0.06705500
C	-3.54601600	-0.17782900	2.76808100
H	-1.41075200	-0.12892500	3.17498900
C	-4.15220300	-0.19900500	0.42847300
H	-2.52191900	-0.21327300	-0.98378700
C	-4.53256000	-0.19070500	1.77375800
H	-3.82921800	-0.17221900	3.81894400
H	-4.91026400	-0.21763200	-0.35240800
H	-5.58580600	-0.20039800	2.04501300

<u>For Table 4 (ROPh-p-NO_2): B3LYP/6-311++G(d,p)</u>

1

E = -782.535454

ZPVE = 0.233245

Symbol	X	Y	Z
C	-0.97672100	-0.70931000	0.15217700
C	0.31685100	-0.82130000	-0.66522400

C	1.25990000	0.34625100	-0.38995800
C	0.29806500	0.71518800	1.77604300
C	-0.64068700	-0.47727000	1.63137800
H	2.24759200	0.17610000	-0.82627700
H	0.85269400	-1.73574500	-0.39044800
H	0.11371000	-0.86749200	-1.73760900
H	-1.57851300	0.12372800	-0.22522300
H	-1.57470100	-1.61630300	0.02865400
H	0.66265400	0.82625000	2.79741700
H	-0.20803600	1.64387500	1.48746100
H	-0.15877100	-1.36797900	2.05008900
H	-1.54783400	-0.29347500	2.21579900
O	1.48817200	0.55778100	0.97635500
O	0.67678200	1.50401600	-1.02209600
C	1.42361800	2.62616300	-1.20390300
C	0.85129300	3.60232200	-2.03429100
C	2.68214900	2.84531800	-0.62612100
C	1.52836900	4.77933600	-2.29773500
H	-0.12265500	3.41065000	-2.46685300
C	3.36403000	4.02530400	-0.89807000
H	3.10998900	2.12231200	0.05303400
C	2.78666200	4.97952700	-1.72893300
H	1.10456900	5.54030600	-2.93832800
H	4.33532100	4.21696200	-0.46302900
N	3.51179000	6.22549300	-2.00710800
O	2.97087700	7.05212800	-2.73530900
O	4.61846100	6.37167900	-1.49742200

2

E = -1155.224889

ZPVE = 0.357670

Symbol	X	Y	Z
C	-1.96731900	0.82966900	-0.12171000
C	-0.88987700	-0.22645300	0.16444300
C	0.54948700	0.28572200	-0.09576100
C	0.80347500	1.61876700	0.62166200
C	-0.28688000	2.66599000	0.36221400
C	-1.69450000	2.12623600	0.65072000
H	1.24094500	-0.43089900	0.37030200
H	-0.96916800	-0.52743900	1.21530600
H	-1.08152700	-1.12906300	-0.42389700
H	-2.00671000	1.04902000	-1.19455800
H	-2.95104200	0.43294100	0.14891500
H	1.78549300	2.00864000	0.34079900
H	-0.09317500	3.56018100	0.96123600
H	-0.21548100	2.97319500	-0.68713600
H	-1.79455400	1.93803200	1.72503000
H	-2.43725800	2.88815100	0.39538700
Si	1.15086900	0.20911000	-1.92389100
C	0.15633600	1.23787300	-3.16217200

H	0.15765800	2.30479600	-2.92249100
H	0.59667000	1.12926200	-4.15912400
H	-0.88476400	0.91123300	-3.22967000
C	2.95265900	0.78662900	-1.97724900
H	3.38156700	0.59670300	-2.96627300
H	3.05354400	1.85896000	-1.78411000
H	3.57031900	0.25665900	-1.24553000
C	1.07184700	-1.60390600	-2.45261800
H	1.64937800	-2.24448900	-1.77913000
H	0.04596500	-1.98272300	-2.47295400
H	1.48456200	-1.72668400	-3.45890000
O	0.85278900	1.30523600	2.04975100
C	1.50457400	2.09920400	2.92408200
C	1.47053100	1.67234400	4.26510900
C	2.20050200	3.27343700	2.59221400
C	2.11617800	2.39371900	5.25034900
H	0.93025800	0.76449400	4.50252200
C	2.85139200	3.99704800	3.58384700
H	2.23802400	3.63321300	1.57420500
C	2.80661900	3.55672800	4.90173200
H	2.09767100	2.07411700	6.28317000
H	3.39166500	4.90292500	3.34502300
N	3.49269000	4.32774700	5.94205500
O	4.08799700	5.34732900	5.60420100
O	3.43513100	3.91164000	7.09571400

3

E = -746.598362

ZPVE = 0.256862

Symbol	X	Y	Z
C	-4.18370600	-0.57961500	-0.30504700
C	-2.69130000	-0.50703700	0.00856600
C	-2.28594700	0.88750600	0.49249000
C	-3.11886900	1.30681800	1.71488500
C	-4.62399200	1.23012900	1.42398600
C	-5.02295800	-0.16114200	0.91207300
H	-1.21823300	0.91906900	0.72623600
H	-2.45468300	-1.25820200	0.77158900
H	-4.39071700	0.08557100	-1.15109500
H	-4.43811100	-1.59388000	-0.62494000
H	-2.87894500	0.65279700	2.56329700
H	-2.83860700	2.31960700	2.01886200
H	-5.19545900	1.47992500	2.32321800
H	-4.88438300	1.98222100	0.66859600
H	-4.89025300	-0.89565500	1.71683800
H	-6.08455300	-0.18176800	0.64908000
H	-2.45181300	1.59147800	-0.33115800
O	-1.99966300	-0.85577900	-1.21370600
C	-0.73675200	-1.33550200	-1.19889200
C	-0.18657200	-1.61695600	-2.46254700

C	0.02528900	-1.57355500	-0.04426500
C	1.09219300	-2.12776500	-2.57408400
H	-0.79012400	-1.42660700	-3.34106400
C	1.31072900	-2.08886300	-0.15740400
H	-0.36745800	-1.35945400	0.93928100
C	1.83558900	-2.36233500	-1.41532100
H	1.52551800	-2.34952900	-3.53959100
H	1.91167900	-2.27841100	0.72146700
N	3.19353400	-2.90334400	-1.52642600
O	3.82237600	-3.09574500	-0.48946800
O	3.62765500	-3.13495400	-2.65104400

4

E = -746.597253

ZPVE = 0.256983

Symbol	X	Y	Z
C	-0.96731400	-0.98565100	-0.37635400
C	0.45717400	-1.09171400	-0.93966900
C	1.30997500	0.13905600	-0.62504700
C	-0.13488300	0.58233400	1.43020700
C	-0.95369500	-0.68037200	1.12783800
H	2.33366700	-0.03780200	-0.96914200
H	0.96296500	-1.96055500	-0.50141500
H	0.43955500	-1.24530400	-2.02214700
H	-1.50574100	-0.19221200	-0.90521100
H	-1.50745300	-1.91687200	-0.57258200
H	-0.09089900	0.76080300	2.50885200
H	-0.63298100	1.45254800	0.98908400
H	-0.52131600	-1.53250200	1.66915100
H	-1.97660600	-0.56327900	1.49873000
O	0.75006200	1.22776600	-1.40707900
C	1.48403400	2.31593600	-1.72377700
C	0.81269200	3.29509600	-2.47880700
C	2.82819600	2.51622100	-1.37125500
C	1.46533500	4.44593300	-2.87649100
H	-0.22308800	3.12205800	-2.74257300
C	3.48425500	3.67322900	-1.77362100
H	3.36818200	1.78603700	-0.78596100
C	2.80333000	4.62797400	-2.52008800
H	0.96052800	5.20494400	-3.45808100
H	4.51945900	3.84351800	-1.51120800
N	3.50149000	5.84767300	-2.93734000
O	2.87206200	6.67139900	-3.59477200
O	4.67679300	5.97880900	-2.60712400
C	1.29241500	0.47880300	0.87119600
H	1.84267400	1.40563800	1.05529800
H	1.83754600	-0.31728300	1.39352200

5

E = -1375.831357

ZPVE = 0.338497

Symbol	X	Y	Z
C	-2.01801800	0.10390600	-0.04838500
C	-0.58337600	-0.43694100	-0.13060200
C	0.45773900	0.66150000	-0.39640400
C	0.31788500	1.84151000	0.58065900
C	-1.12098400	2.35445300	0.70240700
C	-2.12373700	1.22779500	0.99108200
H	1.46105700	0.24785700	-0.28735500
H	-0.32195600	-0.90512500	0.82467900
H	-0.49998900	-1.21115800	-0.89789300
H	-2.33345600	0.47852100	-1.02906100
H	-2.70049800	-0.71232800	0.20662100
H	0.99371700	2.63955800	0.26526200
H	-1.17108700	3.12130900	1.48027000
H	-1.37595600	2.84404300	-0.24298400
H	-1.93550200	0.81899400	1.98994900
H	-3.13745600	1.63879000	1.00631200
S	0.31860700	1.23263500	-2.16268300
C	1.85955400	2.13500900	-2.36987200
C	1.82200900	3.50548600	-2.64612800
C	3.09360100	1.47597400	-2.32307800
C	3.00621600	4.20920200	-2.86590500
H	0.86662800	4.01494700	-2.69072400
C	4.27416800	2.18677200	-2.52329600
H	3.12787500	0.40779400	-2.14260400
C	4.23360400	3.55409400	-2.79765100
H	2.96681900	5.27064400	-3.08375400
H	5.22581000	1.66886800	-2.48090100
H	5.15373900	4.10297300	-2.96206700
O	0.78648100	1.32062600	1.85490200
C	1.28407300	2.14075000	2.80776800
C	1.70551900	1.50313500	3.98841500
C	1.40772500	3.53373000	2.69060700
C	2.24270200	2.23632400	5.02908000
H	1.60236900	0.42763500	4.05946800
C	1.94992800	4.26978800	3.73710300
H	1.08598800	4.05178500	1.79874300
C	2.36250300	3.62103100	4.89525300
H	2.57193100	1.75811200	5.94125000
H	2.05349900	5.34374900	3.66418500
N	2.93114600	4.40536400	5.99606800
O	3.02006200	5.62103000	5.84950000
O	3.28768900	3.80251000	7.00414700

6

E = -3379.163719

ZPVE = 0.337231

Symbol	X	Y	Z
C	-2.15265000	0.26214100	0.07881300
C	-0.92966300	-0.63126200	0.33020100
C	0.36832800	-0.03609300	-0.22950900
C	0.58929700	1.41540800	0.21827400
C	-0.64513400	2.30275300	0.02078300
C	-1.91713400	1.68048900	0.61525800
H	1.22401300	-0.63147300	0.08795600
H	-0.79224000	-0.74985600	1.41146200
H	-1.08448700	-1.63228800	-0.08063900
H	-2.37080000	0.30641000	-0.99530200
H	-3.03281000	-0.18075300	0.55435500
H	1.45431700	1.82168600	-0.31029600
H	-0.46094100	3.28783100	0.45808600
H	-0.77351900	2.45285300	-1.05597900
H	-1.83035100	1.64567900	1.70681600
H	-2.77468500	2.32099200	0.38912500
C	2.28928600	0.05178200	-2.52061500
C	2.76450700	1.20128400	-3.15795400
C	3.18747900	-0.94888400	-2.13625000
C	4.13044600	1.35099900	-3.40108500
H	2.06905600	1.97396300	-3.46354000
C	4.55222300	-0.78690500	-2.36674400
H	2.82046000	-1.85493100	-1.66838400
C	5.02578900	0.36159100	-3.00093100
H	4.49219400	2.24394000	-3.89866500
H	5.24380200	-1.56464900	-2.06244500
H	6.08717900	0.48159500	-3.18562900
O	0.92359700	1.31711400	1.63282600
Se	0.38080100	-0.17247600	-2.23819300
C	1.65756600	2.27142600	2.24762100
C	1.92101000	2.04208500	3.61016400
C	2.15905100	3.42795200	1.63053300
C	2.67090600	2.94283800	4.34180900
H	1.52618900	1.14392300	4.06820700
C	2.91498100	4.33196400	2.36685400
H	1.96668300	3.63480900	0.58771400
C	3.16590300	4.08654500	3.71193200
H	2.88171800	2.77734000	5.38933500
H	3.30981200	5.22792800	1.90773000
N	3.96197500	5.04691700	4.48256200
O	4.16667600	4.80065400	5.66760600
O	4.38054200	6.04401000	3.90118600

7

E = -629.896920

ZPVE = 0.191257

Symbol	X	Y	Z
C	-0.51477600	1.54220300	-0.03677500

H	0.46017700	1.05736600	-0.14416800
H	-1.24457200	0.74901000	0.15131300
C	-0.47122900	2.46056500	1.17330700
H	-1.44589400	2.93602600	1.33700800
H	0.28021600	3.24793600	1.03826000
C	-0.87408500	2.30088600	-1.31772300
H	-0.14271900	3.08404900	-1.53929400
H	-0.90000200	1.62298000	-2.17356700
H	-1.85781800	2.77399000	-1.24174400
O	-0.12934200	1.66556600	2.31861900
C	-0.02587800	2.25066200	3.53269700
C	-0.23090800	3.61652300	3.77626400
C	0.31209500	1.39393700	4.59460500
C	-0.09851100	4.11445800	5.06752400
H	-0.49135500	4.29314800	2.97474400
C	0.44325300	1.89021300	5.87723600
H	0.46570500	0.34323100	4.38314200
C	0.23605800	3.25273700	6.10516400
H	-0.25229200	5.16422100	5.27671600
H	0.70258400	1.24480800	6.70506500
N	0.37417100	3.78475900	7.46557600
O	0.67006700	2.99840600	8.36008600
O	0.18632300	4.98599500	7.63430800

8

E = -1087.426977

ZPVE = 0.290600

Symbol	X	Y	Z
C	-0.91504600	0.43674000	-0.87010400
C	-1.29000100	1.81058100	-0.18354400
H	-2.26058500	2.29378000	-0.26790600
C	-0.62628700	1.33229600	1.15183300
H	-1.05374200	1.45693700	2.14461000
C	-0.25469300	-0.03607600	0.48467300
H	-0.40246400	-1.01912700	0.92609100
C	0.74721800	1.93503300	0.67706700
C	1.11508400	0.55953300	0.00431600
H	2.07929700	0.05922300	0.08489500
C	0.44990700	1.03710600	-1.33601700
H	0.86319100	0.90492200	-2.33273100
C	0.07740600	2.40787700	-0.66550300
H	0.20635400	3.38934700	-1.11747000
C	-1.82291900	-0.37759200	-1.71946400
O	-2.91830500	-0.76570100	-1.02588300
O	-1.63143200	-0.66630400	-2.87794100
C	-3.87741200	-1.55965900	-1.74936600
H	-3.41938900	-2.48559500	-2.10002100
H	-4.67415100	-1.77111800	-1.03956700
H	-4.26314800	-1.00512100	-2.60597000

C	1.69887800	2.72571500	1.51352600
H	2.58531000	3.00531400	0.92902500
H	2.02509000	2.14151600	2.38414400
O	1.02159600	3.91332600	1.95816300
C	1.67568400	4.80368800	2.73853300
C	3.00459300	4.66138800	3.16289600
C	0.93406900	5.93266000	3.12652000
C	3.58034200	5.63942000	3.96609200
H	3.59347900	3.80167100	2.87613900
C	1.50768200	6.90383400	3.92463800
H	-0.09014800	6.02144400	2.78681100
C	2.83205500	6.74890700	4.34017600
H	4.60344700	5.54931100	4.30450000
H	0.95134000	7.77847800	4.23212600
N	3.44584600	7.77747800	5.18865500
O	2.75956900	8.74552500	5.50091800
O	4.61041500	7.61235900	5.53896300

9

E = -863.251746

ZPVE = 0.318208

Symbol	X	Y	Z
C	-2.35748200	-1.70460000	0.04484500
C	-0.83118400	-1.82230600	0.09612200
C	-0.14166400	-0.48932700	0.52942900
C	-1.09940000	0.72839900	0.70498100
C	-2.56167600	0.36817400	0.46872500
C	-2.84252100	-0.92059000	1.29481500
H	0.39122300	-0.65200700	1.46928100
H	-0.56194800	-2.61370900	0.80231100
H	-0.45169600	-2.13946900	-0.87894700
H	-2.82315200	-2.66997100	-0.17318200
H	-1.01930800	1.12101300	1.72436400
H	-3.19715900	1.24354300	0.62377100
H	-2.27630400	-1.05676300	2.22078100
H	-3.89946900	-1.05863700	1.51402600
H	0.62289500	-0.21422500	-0.19929700
C	-2.80233600	-0.48115000	-0.83078400
C	-4.29822300	-0.53885600	-1.17768700
H	-4.93150500	-0.76885100	-0.31877800
H	-4.63164600	0.41972000	-1.58791800
H	-4.48082300	-1.30554600	-1.93746700
C	-2.02791400	-0.17231700	-2.11398700
H	-0.95125000	-0.09620200	-1.97035400
H	-2.21475600	-0.95524700	-2.85729300
H	-2.36259900	0.77639300	-2.54306400
O	-0.77591200	1.81671000	-0.19773600
C	0.27049300	2.63211000	0.05146900
C	0.43430100	3.69917400	-0.85088300

C	1.16954600	2.48475700	1.11951700
C	1.46684800	4.60267200	-0.68956800
H	-0.26885000	3.79586400	-1.66848300
C	2.20575100	3.39633800	1.28281100
H	1.07687400	1.66555800	1.81789100
C	2.34842900	4.44558600	0.38231800
H	1.60249000	5.42811100	-1.37469800
H	2.90752100	3.29839300	2.09976700
N	3.44635000	5.40114900	0.55906600
O	4.20433200	5.23625600	1.51085700
O	3.54722500	6.31469700	-0.25469400

10

E = -667.967525

ZPVE = 0.197174

Symbol	X	Y	Z
C	-1.44160900	0.61671800	0.11729000
C	-0.46373400	1.53879100	-0.56626100
C	-1.59777600	2.11458000	0.24282700
H	-2.16245600	0.08317700	-0.48950300
H	-1.09697800	0.06478200	0.98461100
H	-0.51151400	1.63355400	-1.64388700
H	0.53661700	1.61304900	-0.15549200
H	-2.41271600	2.56554100	-0.31343800
C	-1.32330100	2.76430600	1.56619300
H	-2.22379100	2.77544300	2.19143600
H	-0.53210500	2.22710800	2.10301300
O	-0.90236400	4.11949100	1.32486900
C	-0.62154300	4.92613600	2.37193800
C	-0.24451400	6.24019600	2.04357500
C	-0.68174500	4.53394700	3.71751300
C	0.06670100	7.14685900	3.03833700
H	-0.20469500	6.52077700	0.99861300
C	-0.36858600	5.44776000	4.71747700
H	-0.96805500	3.52923100	3.99432700
C	0.00184000	6.74220800	4.37380100
H	0.35818900	8.16097600	2.80227700
H	-0.40872700	5.16534200	5.76056800
N	0.33119000	7.70151100	5.43411700
O	0.65329700	8.83710700	5.09834900
O	0.26688000	7.31602800	6.59775600

11

E = -784.630610

ZPVE = 0.258790

Symbol	X	Y	Z
C	-2.42585600	0.63163100	0.69538200
C	-1.01502500	0.46191600	0.19107900
C	-1.71883700	1.78809100	0.03088500
H	-3.23407900	0.15273500	0.15662000
H	-2.57426400	0.67397800	1.76824500
H	-0.85209800	-0.13129600	-0.70032300
H	-0.22284900	0.38066500	0.92487500
H	-2.04515000	2.03133800	-0.97579300
C	-1.32941800	3.00972300	0.83061900
H	-1.01540700	2.72358500	1.83883500
C	-2.44589100	4.02035000	0.93698300
C	-3.41402800	3.95763800	2.09339700
C	-2.40993500	5.08021100	2.00739700
H	-2.85714000	4.31752900	-0.02269700
H	-3.25845800	3.19771500	2.85051800
H	-4.45613400	4.17580600	1.89482900
H	-2.76226600	6.07177800	1.75174600
H	-1.57740200	5.07006000	2.70183200
O	-0.23475100	3.69385100	0.15266900
C	1.06365800	3.51187800	0.47071400
C	1.97640500	4.21358200	-0.33948200
C	1.54839000	2.72179400	1.52507000
C	3.33523500	4.13152700	-0.10559500
H	1.58517800	4.81923600	-1.14715100
C	2.91479800	2.64165000	1.76177000
H	0.87872200	2.16565500	2.16458000
C	3.79891800	3.34250700	0.94925300
H	4.04377800	4.66656700	-0.72278600
H	3.30261500	2.03775600	2.57075700
N	5.23855500	3.24934900	1.20341300
O	5.99258400	3.88033900	0.46804100
O	5.61348600	2.54589500	2.13780000

12

E = -627.445606

ZPVE = 0.143825

Symbol	X	Y	Z
C	-1.78861200	0.41945000	-0.06807300
H	-2.61875400	-0.16581100	0.24560700
C	-0.84725300	1.07874000	-0.41413500
C	0.27304300	1.88462900	-0.87348600
H	0.70828800	1.44018500	-1.77661300
H	-0.06996700	2.89686800	-1.11908900
O	1.26058700	1.94331400	0.16548500
C	2.39618900	2.65114800	-0.05738700
C	3.31378400	2.66250200	1.00574300
C	2.68625700	3.34056700	-1.24224400
C	4.50511700	3.35255500	0.88875900

H	3.06557600	2.12182900	1.91017900
C	3.88624300	4.03469000	-1.35815900
H	1.99616000	3.34664100	-2.07423800
C	4.78249300	4.03577300	-0.29730100
H	5.22356100	3.37264900	1.69651500
H	4.13119700	4.57363100	-2.26303700
N	6.04807800	4.77085900	-0.42633900
O	6.81797100	4.75351700	0.52826000
O	6.26335900	5.36005800	-1.48069500

13

E = -1128.867445

ZPVE = 0.339467

Symbol	X	Y	Z
C	1.38936700	0.44312200	-0.02324600
C	2.16637800	1.79678700	-0.06530000
C	-0.38607700	2.25867600	-0.09834600
C	-0.13312600	0.71391200	-0.08992800
H	1.69982700	-0.19226800	-0.85493200
H	1.60775000	-0.08462700	0.90648000
H	-0.55820400	0.27163100	-0.99331100
H	-1.45237500	2.48645700	-0.11222600
H	3.24437400	1.62939100	-0.05219100
C	0.31002600	2.83706600	1.11947400
C	1.69193500	2.59990500	1.13156100
C	-0.29125400	3.53654300	2.15847900
C	2.47200200	3.06437600	2.18379200
C	0.49483700	4.01016100	3.21260000
H	-1.36133300	3.71680400	2.15131700
C	1.86836700	3.77531600	3.22506200
H	3.54157400	2.88041700	2.19622100
H	0.03323000	4.56304000	4.02292800
H	2.47278500	4.14687000	4.04494100
C	0.32852400	2.76968400	-1.33760500
C	-0.25583000	3.41146700	-2.42310800
C	1.70972000	2.52332400	-1.31884900
C	0.54557700	3.81759500	-3.49449500
H	-1.32371000	3.60533700	-2.43661300
C	2.50434900	2.92381500	-2.38612700
C	1.91728500	3.57484900	-3.47563100
H	0.09728100	4.32566300	-4.34076200
H	3.57330600	2.73666800	-2.37391200
H	2.53397800	3.89426200	-4.30819700
O	-0.72943600	0.08174100	1.05951400
C	-2.05599100	-0.18224300	1.10277500
C	-2.51355700	-0.74557700	2.30702900
C	-2.96150400	0.04675000	0.05551700
C	-3.84529200	-1.07822700	2.46403800
H	-1.79843100	-0.91147400	3.10277000
C	-4.30076000	-0.28999000	0.21409800

H	-2.63957300	0.48211100	-0.87962000
C	-4.73346900	-0.84754600	1.41134400
H	-4.21033100	-1.51259400	3.38447100
H	-5.01300900	-0.12280900	-0.58228600
N	-6.14912400	-1.19642500	1.57219700
O	-6.49910700	-1.68989900	2.63998300
O	-6.90555700	-0.97609500	0.63073000

For Table 4 (ROPh-p-NO_2): M06-2X/6-311++G(d,p)

1

E = -782.212066

ZPVE = 0.236819

Symbol	X	Y	Z
C	-0.95777300	-0.65643400	0.13946100
C	0.33753100	-0.86021700	-0.64824500
C	1.28624500	0.30718500	-0.43011900
C	0.34392900	0.80381900	1.68988200
C	-0.62219800	-0.36815900	1.60393400
H	2.26854300	0.12373200	-0.87453700
H	0.84940200	-1.76216400	-0.30066500
H	0.14922800	-0.96703900	-1.71785700
H	-1.51107800	0.18701200	-0.28419800
H	-1.59265400	-1.54021800	0.05214100
H	0.69492300	0.96848700	2.70774300
H	-0.13503300	1.72341400	1.33357100
H	-0.15609900	-1.24795500	2.05934800
H	-1.52369700	-0.13616100	2.17639400
O	1.52533700	0.56134800	0.92146500
O	0.69308700	1.43225700	-1.07373100
C	1.42067900	2.56649500	-1.21975200
C	0.82749700	3.56017900	-2.00742600
C	2.68003000	2.77431100	-0.64884800
C	1.48619200	4.75176200	-2.23685300
H	-0.14872600	3.36714400	-2.43323200
C	3.34396300	3.97033000	-0.88608800
H	3.12416600	2.03140400	-0.00226500
C	2.74360600	4.93845900	-1.67358400
H	1.04977300	5.53253700	-2.84468900
H	4.31885500	4.16069000	-0.45805700
N	3.45244200	6.20347900	-1.91444900
O	2.89642800	7.03823300	-2.59729200
O	4.55103200	6.33788500	-1.41758100

2

E = -1154.803430

ZPVE = 0.362239

Symbol	X	Y	Z
C	-1.85579300	1.03589200	-0.09775900
C	-0.89774900	-0.12919900	0.17176200
C	0.57587300	0.23560700	-0.10352800
C	0.96842300	1.51852700	0.62475300
C	0.01552600	2.67491600	0.32028800
C	-1.42837700	2.29557200	0.65663600
H	1.20540500	-0.55530800	0.32712700
H	-0.99626900	-0.42707000	1.22106900
H	-1.18724700	-0.99908700	-0.42715500
H	-1.88770000	1.25785000	-1.16833400
H	-2.86972100	0.75028100	0.19435000
H	2.00078500	1.78104000	0.37339900
H	0.31139900	3.56904000	0.87441300
H	0.10441000	2.91560300	-0.74579000
H	-1.50715300	2.12258300	1.73481900
H	-2.09408800	3.12801900	0.41675700
Si	1.07820700	0.18620200	-1.94443600
C	-0.17441400	0.92273200	-3.14108700
H	-0.39235800	1.97451200	-2.94253100
H	0.22869200	0.85444800	-4.15607700
H	-1.11767600	0.37088800	-3.12609100
C	2.71577600	1.09101200	-2.15286600
H	3.10200500	0.94571500	-3.16528900
H	2.60814700	2.16807400	-1.99524000
H	3.47168700	0.72121200	-1.45440000
C	1.29672900	-1.62791500	-2.38605500
H	2.08827100	-2.08832200	-1.78931900
H	0.37648300	-2.19246500	-2.21286300
H	1.56129400	-1.74321200	-3.44038000
O	0.92065900	1.20834400	2.03429800
C	1.52210400	2.01186500	2.92960600
C	1.31961900	1.66793900	4.27519500
C	2.32400200	3.11432200	2.60847200
C	1.90541400	2.40462400	5.28332600
H	0.69707800	0.81028300	4.49555900
C	2.91495700	3.85454600	3.62317100
H	2.49364400	3.40505300	1.58181600
C	2.70040300	3.49469400	4.94261700
H	1.76022100	2.15308700	6.32512600
H	3.53912500	4.70908300	3.39907800
N	3.32556500	4.28571700	6.00939700
O	4.00993200	5.23355800	5.68284700
O	3.12125000	3.94503000	7.15612900

3

E = -746.276599

ZPVE = 0.260295

Symbol	X	Y	Z

C	-4.20857200	-0.56080400	-0.32058700
C	-2.71805400	-0.55592500	-0.01746100
C	-2.25867500	0.81894500	0.45850800
C	-3.04825500	1.24364200	1.70015900
C	-4.55307500	1.23494800	1.42247100
C	-5.00807400	-0.13479300	0.91337400
H	-1.18468800	0.82261000	0.65939700
H	-2.51511300	-1.31451500	0.74975800
H	-4.39110700	0.13447300	-1.14729500
H	-4.50421400	-1.55643000	-0.65898000
H	-2.82827700	0.55523600	2.52542800
H	-2.72323300	2.23502600	2.02358100
H	-5.10639200	1.50674600	2.32470900
H	-4.78223600	1.99451700	0.66587100
H	-4.87282500	-0.87847900	1.70792100
H	-6.07399500	-0.12022000	0.67533000
H	-2.43596000	1.52845200	-0.35755200
O	-2.05539300	-0.93069700	-1.22992900
C	-0.78172500	-1.36673000	-1.20281000
C	-0.21772400	-1.64503100	-2.45680300
C	-0.02710200	-1.56683500	-0.04087700
C	1.07442300	-2.11720700	-2.55425700
H	-0.82449700	-1.48173800	-3.33806500
C	1.27317100	-2.04320100	-0.13903000
H	-0.43455000	-1.35473900	0.93712900
C	1.80739600	-2.31184400	-1.38744600
H	1.52493100	-2.33798900	-3.51237900
H	1.87569500	-2.20610300	0.74439200
N	3.18418000	-2.81253000	-1.48219800
O	3.79991800	-2.97096500	-0.44824400
O	3.62548300	-3.03879700	-2.58970200

4

E = -746.276269

ZPVE = 0.260588

Symbol	X	Y	Z
C	-0.95452700	-0.94401200	-0.37599100
C	0.46518700	-1.14673500	-0.91011100
C	1.34061300	0.07931900	-0.67582800
C	-0.07957500	0.69676800	1.32284200
C	-0.93292600	-0.55402300	1.10326300
H	2.35584800	-0.13027000	-1.02808000
H	0.93601800	-1.99354000	-0.39877300
H	0.45317400	-1.37401000	-1.97852100
H	-1.44361600	-0.15346800	-0.95341700
H	-1.53602500	-1.85709400	-0.52401500
H	-0.04412900	0.95697000	2.38332000
H	-0.53689900	1.54382500	0.80071900
H	-0.51837500	-1.38221900	1.69155800
H	-1.95005700	-0.38555200	1.46541600

O	0.77842400	1.12122600	-1.49058000
C	1.48453900	2.23646100	-1.75364400
C	0.79432700	3.22861400	-2.46606000
C	2.82034900	2.44366000	-1.38976500
C	1.42163400	4.40752500	-2.81127700
H	-0.23657500	3.04050200	-2.73713300
C	3.45207700	3.62964200	-1.73838200
H	3.37400700	1.69740900	-0.83849100
C	2.74983000	4.59400600	-2.44073200
H	0.90511800	5.18322000	-3.36010200
H	4.48355800	3.81240700	-1.46882700
N	3.42387100	5.84758900	-2.80110100
O	2.78260400	6.67453200	-3.41542800
O	4.58194900	5.98315600	-2.46411400
C	1.34386300	0.49417300	0.79669000
H	1.93354000	1.40330900	0.93677200
H	1.84058700	-0.30116300	1.36392600

5

E = -1375.389814

ZPVE = 0.343079

Symbol	X	Y	Z
C	-1.98567300	0.20811800	-0.01056900
C	-0.60795900	-0.45602100	-0.07638000
C	0.50297800	0.54018700	-0.42121500
C	0.48034200	1.75656300	0.50900100
C	-0.90067500	2.40235100	0.60512500
C	-1.97441900	1.37630200	0.97713100
H	1.47700900	0.05720100	-0.32238100
H	-0.36742500	-0.88200900	0.90286700
H	-0.59956000	-1.27526000	-0.79925500
H	-2.27346300	0.57068600	-1.00320900
H	-2.73237500	-0.53188600	0.28673400
H	1.23352200	2.47224800	0.16697000
H	-0.87695300	3.21309700	1.33744100
H	-1.12983800	2.84768300	-0.36777800
H	-1.77646200	0.99724600	1.98541600
H	-2.95172200	1.86336300	1.00426400
S	0.32667600	1.04241100	-2.18223400
C	1.78398400	2.06007800	-2.35635100
C	1.64609400	3.42823000	-2.58925700
C	3.05855300	1.49766900	-2.27240900
C	2.77621200	4.22851000	-2.73219700
H	0.65348100	3.85846300	-2.65556300
C	4.18411500	2.30351900	-2.39755300
H	3.16375500	0.42982900	-2.11774000
C	4.04515400	3.66945500	-2.62931800
H	2.66271000	5.29009000	-2.91745600
H	5.17115800	1.86209000	-2.32710700
H	4.92419700	4.29391400	-2.73383000

O	0.88306100	1.23711400	1.78730900
C	1.34180700	2.07132000	2.74134800
C	1.63080000	1.46922800	3.97452700
C	1.55078600	3.44442700	2.56961000
C	2.12438600	2.22030900	5.02107600
H	1.46031600	0.40538200	4.07838400
C	2.04904400	4.19956100	3.62251900
H	1.33178800	3.93348900	1.63124400
C	2.32853400	3.58321800	4.83013100
H	2.35420700	1.77358600	5.97882500
H	2.22081300	5.26197600	3.51422200
N	2.85237400	4.39016700	5.93946700
O	3.01771900	5.57672300	5.74546500
O	3.08957100	3.82202000	6.98510900

6

E = -3378.755476

ZPVE = 0.341856

Symbol	X	Y	Z
C	-2.11097600	0.38638900	0.05439500
C	-1.01114900	-0.62340300	0.39221700
C	0.34760200	-0.21986200	-0.18371500
C	0.72559800	1.21352500	0.19260700
C	-0.38356900	2.22145600	-0.10509300
C	-1.71433800	1.78988200	0.51678300
H	1.12765300	-0.88690300	0.18513200
H	-0.89737100	-0.67560600	1.48039100
H	-1.27620200	-1.62559800	0.04680100
H	-2.29342400	0.39554800	-1.02594300
H	-3.04514200	0.08071200	0.53132700
H	1.65526300	1.47839200	-0.31856200
H	-0.09200000	3.20706100	0.26599900
H	-0.48511700	2.29887600	-1.19168900
H	-1.62163200	1.79866800	1.60803400
H	-2.49114800	2.51198400	0.25563300
C	2.17471500	0.01474100	-2.44941500
C	2.48794400	1.19616800	-3.12066500
C	3.19701300	-0.81267300	-1.98479600
C	3.81978700	1.54927100	-3.32160600
H	1.69026600	1.83608600	-3.47950500
C	4.52567100	-0.44704300	-2.17356700
H	2.95168600	-1.74176100	-1.48323800
C	4.83865600	0.73265300	-2.84290400
H	4.05897200	2.46635000	-3.84700800
H	5.31691400	-1.08989200	-1.80636400
H	5.87446100	1.01197000	-2.99377400
O	0.97902700	1.15610700	1.60823400
Se	0.33058100	-0.45696400	-2.15339400
C	1.70143700	2.12508900	2.20437900

C	1.82180000	2.01077200	3.59707800
C	2.32400500	3.18525500	1.53549900
C	2.55284000	2.93479300	4.31448500
H	1.33096700	1.18009000	4.08764800
C	3.06066400	4.11408400	2.25775700
H	2.24433000	3.29898600	0.46382800
C	3.16618000	3.98031000	3.63155300
H	2.65758900	2.86245100	5.38848000
H	3.55197800	4.94146400	1.76379600
N	3.94418400	4.96970900	4.38771300
O	4.02188100	4.82449700	5.58993100
O	4.46377600	5.87369700	3.76658700

7

E = -629.621697

ZPVE = 0.193947

Symbol	X	Y	Z
C	-0.51226400	1.54005500	-0.02186000
H	0.46132000	1.05723600	-0.13639800
H	-1.24493700	0.74981800	0.15933300
C	-0.46466500	2.44362100	1.19289600
H	-1.43896500	2.91885400	1.36023400
H	0.28759700	3.23087800	1.06072000
C	-0.87205800	2.32658200	-1.27971900
H	-0.13661400	3.10967400	-1.47996300
H	-0.90618000	1.67217200	-2.15120600
H	-1.85108700	2.80212600	-1.18187200
O	-0.12465100	1.64383400	2.31971200
C	-0.02352000	2.23366900	3.52583700
C	-0.23122000	3.59759600	3.75383800
C	0.31339200	1.38601100	4.59087600
C	-0.10179700	4.10549100	5.04023900
H	-0.49126700	4.26678100	2.94620100
C	0.44174200	1.89084700	5.86769700
H	0.46788900	0.33520600	4.38253100
C	0.23127000	3.25113100	6.07642100
H	-0.25702300	5.15630200	5.24436600
H	0.70053600	1.25539700	6.70369200
N	0.36660500	3.79483600	7.43447100
O	0.65988400	3.02193000	8.32248000
O	0.17728100	4.98362700	7.58784000

8

E = -1087.000085

ZPVE = 0.295416

Symbol	X	Y	Z
C	-0.89589300	0.46166800	-0.85499700
C	-1.26342100	1.82044700	-0.16416300
H	-2.23499800	2.30059600	-0.23797900
C	-0.58795600	1.33502200	1.15509600
H	-0.99588800	1.46014900	2.15465400
C	-0.23029600	-0.02470500	0.47748300
H	-0.38127200	-1.01049200	0.90858400
C	0.77130800	1.92863400	0.66554900
C	1.13114500	0.56699400	-0.01231600
H	2.09511300	0.06781800	0.05750400
C	0.45480400	1.05330600	-1.33657700
H	0.84842700	0.92156400	-2.34024200
C	0.09488700	2.41496400	-0.65543100
H	0.22673700	3.40062200	-1.09434200
C	-1.81878700	-0.34639600	-1.69021400
O	-2.89945300	-0.72372600	-0.98540900
O	-1.64580200	-0.63757500	-2.84407500
C	-3.85470100	-1.50817800	-1.70196800
H	-3.39601200	-2.43100300	-2.05789300
H	-4.65139200	-1.72330500	-0.99502300
H	-4.23823600	-0.95003500	-2.55639300
C	1.71414700	2.72784300	1.49856100
H	2.59280600	3.02390900	0.91099000
H	2.04882200	2.14741500	2.36810200
O	1.01301400	3.88822000	1.93538200
C	1.65609000	4.77765300	2.71718100
C	2.98487200	4.64316500	3.13038900
C	0.90385200	5.89141600	3.11586500
C	3.55338700	5.61959200	3.93852400
H	3.58072000	3.79215000	2.83272000
C	1.46887900	6.86048300	3.91821800
H	-0.12202700	5.96685400	2.77914200
C	2.79289700	6.71033800	4.32087800
H	4.57905600	5.54093100	4.27287800
H	0.90750700	7.72772200	4.23819800
N	3.40041700	7.73895000	5.17651400
O	2.70916700	8.68293100	5.49711100
O	4.55620700	7.58317300	5.51132000

9

E = -862.887245

ZPVE = 0.322821

Symbol	X	Y	Z
C	-2.30582500	-1.68215000	0.01766600
C	-0.78180300	-1.73670700	0.08611500
C	-0.16948400	-0.40466900	0.60616500
C	-1.17069400	0.77358200	0.76261800

C	-2.60751600	0.35551100	0.50511400
C	-2.83900500	-0.96509400	1.28201800
H	0.29938600	-0.58668700	1.57574100
H	-0.48459600	-2.55116400	0.75161200
H	-0.37990700	-1.97698900	-0.90092700
H	-2.73193300	-2.65319400	-0.24630300
H	-1.11700100	1.17258200	1.78246900
H	-3.28445400	1.19682800	0.66944600
H	-2.27097300	-1.10362300	2.20596800
H	-3.88990600	-1.15868000	1.48223700
H	0.63591700	-0.07937400	-0.05601300
C	-2.77266000	-0.45291300	-0.81709400
C	-4.24690500	-0.55859900	-1.20815200
H	-4.88850400	-0.84351300	-0.37283700
H	-4.60459400	0.40025400	-1.59387600
H	-4.37288000	-1.30596800	-1.99670000
C	-1.96792700	-0.06913600	-2.05404700
H	-0.90050700	0.03469200	-1.86341800
H	-2.10489500	-0.82970000	-2.82948600
H	-2.31921000	0.88612700	-2.45214500
O	-0.88808200	1.85605600	-0.13630600
C	0.19142400	2.63015000	0.07209800
C	0.36874000	3.67731700	-0.84497300
C	1.10737200	2.45520100	1.11617700
C	1.43679000	4.54088300	-0.72167100
H	-0.35450500	3.78756400	-1.64270600
C	2.18096300	3.32674900	1.24147100
H	0.99956800	1.64684700	1.82526000
C	2.33305100	4.35442900	0.32681300
H	1.58945300	5.35477100	-1.41736500
H	2.90192900	3.21306800	2.03976800
N	3.47331400	5.26910400	0.46417000
O	4.23806900	5.08349900	1.38819000
O	3.58329200	6.15779000	-0.35477200

10

E = -667.685932

ZPVE = 0.200146

Symbol	X	Y	Z
C	-1.41065600	0.63818400	0.15087100
C	-0.45823100	1.58013600	-0.53019300
C	-1.61621600	2.12376100	0.25364100
H	-2.10161500	0.07586900	-0.46180900
H	-1.05978000	0.11503500	1.03188900
H	-0.49752400	1.65559700	-1.60802100
H	0.52891900	1.69948400	-0.10119200
H	-2.43786900	2.54871400	-0.31028000
C	-1.34611300	2.78760800	1.56710000
H	-2.24554300	2.80742900	2.19299400

H	-0.55471300	2.25077000	2.10516900
O	-0.92316200	4.12440300	1.30887900
C	-0.63424700	4.92218100	2.35397400
C	-0.24829100	6.23102700	2.02989700
C	-0.69617300	4.52092100	3.69236100
C	0.07167500	7.12892900	3.02621300
H	-0.20980600	6.51118000	0.98516500
C	-0.37397100	5.42615600	4.69564800
H	-0.99051600	3.51719500	3.96363600
C	0.00406200	6.71219800	4.35297300
H	0.37135900	8.14289500	2.79882700
H	-0.41361500	5.14200400	5.73854800
N	0.34339100	7.66413100	5.41907200
O	0.66874300	8.78531600	5.08877100
O	0.27839500	7.27349500	6.56617500

11

E = -784.303062

ZPVE = 0.262521

Symbol	X	Y	Z
C	-2.28008200	0.74928000	0.62950500
C	-0.80367100	0.60278400	0.39347000
C	-1.49067300	1.90423000	0.08364900
H	-2.96570000	0.24359200	-0.03635500
H	-2.61574500	0.81612700	1.65702000
H	-0.47277400	-0.00032800	-0.44111900
H	-0.16328400	0.55302300	1.26359300
H	-1.63451200	2.13351900	-0.96716600
C	-1.30173100	3.13740600	0.93023900
H	-1.07281100	2.86061600	1.96729400
C	-2.52164800	4.01762900	0.93417900
C	-3.54740200	3.83503200	2.01530800
C	-2.66505800	5.05309300	2.00821200
H	-2.88568500	4.27655500	-0.05407900
H	-3.35757500	3.08182200	2.77014800
H	-4.58906600	3.95262600	1.74973300
H	-3.10513600	6.00397700	1.74141100
H	-1.87629600	5.11018400	2.74848900
O	-0.24180600	3.94518900	0.38866100
C	1.05460700	3.63239100	0.58283600
C	1.95784600	4.26366700	-0.28414600
C	1.53567300	2.79072100	1.59129600
C	3.31615800	4.05496500	-0.15631400
H	1.55953600	4.91489500	-1.05138000
C	2.90042400	2.57904700	1.72130600
H	0.86397100	2.30437900	2.28291900
C	3.77229100	3.20792500	0.84780800
H	4.02616300	4.53115200	-0.81878900
H	3.29479100	1.93390300	2.49480500

N	5.21485800	2.97485500	0.98795900
O	5.95490900	3.54466500	0.21327500
O	5.58276300	2.22611900	1.86971400

12

E = -627.186715

ZPVE = 0.146267

Symbol	X	Y	Z
C	-1.77203300	0.43328700	-0.07847100
H	-2.60556400	-0.15143000	0.23158800
C	-0.83050500	1.09022400	-0.41967600
C	0.29964400	1.89614100	-0.86816200
H	0.73715000	1.45039600	-1.76841300
H	-0.04169800	2.90872100	-1.11047600
O	1.26533800	1.94270000	0.17172400
C	2.39586900	2.64818800	-0.05171300
C	3.31226300	2.66065900	1.00798200
C	2.67760800	3.33292900	-1.23628500
C	4.50041600	3.35032000	0.88815300
H	3.06165600	2.11959200	1.91112500
C	3.87545300	4.02780200	-1.35606400
H	1.98520700	3.33650900	-2.06617700
C	4.76640200	4.02765700	-0.29856300
H	5.22358200	3.37498100	1.69194700
H	4.12067100	4.56688700	-2.26109900
N	6.03162900	4.76500600	-0.43216000
O	6.79337200	4.74674200	0.51125300
O	6.23685400	5.34648400	-1.47676100

13

E = -1128.413017

ZPVE = 0.343829

Symbol	X	Y	Z
C	1.47606100	0.43844100	-0.11270700
C	2.16953900	1.83002800	-0.08077400
C	-0.40165100	2.13993200	-0.17820400
C	-0.05526800	0.62076100	-0.18452000
H	1.83266300	-0.13122900	-0.97158800
H	1.71117700	-0.11790700	0.79551600
H	-0.45108200	0.15585700	-1.09105100
H	-1.47803500	2.30985700	-0.21554700
H	3.25467100	1.73065000	-0.03971600
C	0.22135900	2.70866800	1.07662600
C	1.61014700	2.55256400	1.12528900
C	-0.45708800	3.30510000	2.12746400
C	2.32440600	3.00287900	2.22481700

C	0.26265700	3.76494100	3.23058700
H	-1.53597300	3.41426500	2.08928800
C	1.64439200	3.61594400	3.27779000
H	3.40164900	2.88065200	2.26435100
H	-0.25757900	4.24058400	4.05337000
H	2.19671300	3.97727200	4.13711400
C	0.31492000	2.72083200	-1.37707400
C	-0.27823300	3.34290200	-2.46481300
C	1.70425200	2.56223800	-1.32171000
C	0.52475800	3.81849400	-3.50245900
H	-1.35548800	3.46689800	-2.50338400
C	2.50105200	3.03137600	-2.35446400
C	1.90512200	3.66381300	-3.44672700
H	0.07014800	4.31231800	-4.35286600
H	3.57821200	2.91001600	-2.31170600
H	2.52266100	4.03764000	-4.25475200
O	-0.60610300	-0.03215800	0.95947400
C	-1.94058000	-0.19889700	1.06265700
C	-2.39201900	-0.63928300	2.31471700
C	-2.85502100	0.01100900	0.02444100
C	-3.73468500	-0.87139600	2.53060900
H	-1.66092200	-0.78792200	3.09882000
C	-4.20622600	-0.22321500	0.24165800
H	-2.53153000	0.35059600	-0.94942100
C	-4.62873600	-0.65863600	1.48581400
H	-4.10291200	-1.21017000	3.48942300
H	-4.93294400	-0.07142500	-0.54500600
N	-6.06047400	-0.89872500	1.70914300
O	-6.40088100	-1.28563700	2.80742400
O	-6.81770700	-0.69596100	0.78273700

<u>For Table 4 (ROPh-p-NO_2): MP2/6-31+G(d)</u>

1

E = -780.010029

ZPVE = 0.236578

Symbol	X	Y	Z
C	-0.95953400	-0.65948700	0.14482800
C	0.33269800	-0.88144300	-0.64191400
C	1.28945600	0.27974800	-0.44448800
C	0.34602300	0.82165000	1.67494700
C	-0.62484700	-0.34487600	1.60346900
H	2.27341700	0.09323800	-0.89215200
H	0.84169400	-1.78524200	-0.28351600
H	0.14074300	-1.00542500	-1.71332300
H	-1.52156300	0.17294800	-0.29593500
H	-1.59534700	-1.54991200	0.07685800
H	0.70302500	1.00212400	2.69142500
H	-0.11447600	1.74319200	1.29386000
H	-0.16416900	-1.22019600	2.07965100

H	-1.53092300	-0.09970800	2.17218400
O	1.54567600	0.54621800	0.91636500
O	0.68119300	1.40552800	-1.09667000
C	1.42338500	2.55453100	-1.22945600
C	0.83401300	3.54893100	-2.02578600
C	2.67775200	2.77080400	-0.63932200
C	1.48981900	4.75498500	-2.24730800
H	-0.13645600	3.35151200	-2.47454900
C	3.34541800	3.97682900	-0.86883000
H	3.11981400	2.03227600	0.01990900
C	2.74420900	4.94847700	-1.66431700
H	1.04614100	5.53256600	-2.86100200
H	4.31765400	4.16443200	-0.42364800
N	3.44568400	6.21521900	-1.89212300
O	2.80712000	7.14257000	-2.42559100
O	4.63801100	6.29032100	-1.53909800

2

E = -1151.715620

ZPVE = 0.363999

Symbol	X	Y	Z
C	-1.83564200	0.99511200	-0.01951200
C	-0.85840900	-0.16584800	0.18751100
C	0.60105300	0.21890400	-0.13000900
C	0.99981400	1.49242400	0.60451800
C	0.02751500	2.64533200	0.37309400
C	-1.39717300	2.24007700	0.75198600
H	1.25463300	-0.57132200	0.27884900
H	-0.91958100	-0.49388600	1.23443700
H	-1.16438000	-1.02694300	-0.42299400
H	-1.90948900	1.24293500	-1.08543200
H	-2.84031900	0.68916000	0.30015200
H	2.02589100	1.77237600	0.33430400
H	0.33836300	3.52735000	0.94632400
H	0.07101200	2.92969400	-0.68818200
H	-1.43965800	2.04281700	1.83119600
H	-2.08330200	3.07317800	0.55345100
Si	1.07305700	0.19238800	-1.98582800
C	-0.15271800	1.02991000	-3.15392700
H	-0.33117700	2.08249300	-2.91041800
H	0.24713400	0.99373200	-4.17536600
H	-1.12073100	0.51710700	-3.16680100
C	2.76172100	1.01533100	-2.19158300
H	3.15120700	0.84063400	-3.20181600
H	2.71153900	2.10125200	-2.04787900
H	3.49779400	0.61621500	-1.48332500
C	1.19851600	-1.62484700	-2.47786500
H	1.96641500	-2.14360800	-1.89241800
H	0.25001700	-2.15222700	-2.32423900
H	1.46322200	-1.72705300	-3.53686100

O	0.99328700	1.13607000	2.01999600
C	1.55841900	1.99147200	2.92124200
C	1.26971300	1.71296800	4.26895300
C	2.41113600	3.06086400	2.60053300
C	1.81366300	2.48618200	5.28793000
H	0.60946100	0.87881100	4.49444300
C	2.95629900	3.84601900	3.61865400
H	2.66608000	3.29462400	1.57218500
C	2.65203900	3.54977000	4.94455600
H	1.59550100	2.27693500	6.33045100
H	3.61312900	4.67848300	3.38556300
N	3.22494200	4.37836200	6.00786100
O	3.83148700	5.41453900	5.67463700
O	3.07306200	3.99750700	7.18444500

3

E = -744.116968

ZPVE = 0.260621

Symbol	X	Y	Z
C	-4.24729600	-0.59289800	-0.27623800
C	-2.75596200	-0.61084300	0.00966800
C	-2.25044100	0.76548800	0.41983200
C	-3.01481200	1.27108200	1.64710500
C	-4.52193400	1.28826200	1.38775500
C	-5.01916700	-0.08933500	0.94673800
H	-1.17185500	0.74275100	0.61434400
H	-2.55536900	-1.35242300	0.79806500
H	-4.42587600	0.06716800	-1.13607200
H	-4.57326200	-1.59907200	-0.56466800
H	-2.79970400	0.62035200	2.50783100
H	-2.65926900	2.27271200	1.91732900
H	-5.05833600	1.61516200	2.28725700
H	-4.74502900	2.02359900	0.60135200
H	-4.89920700	-0.80270600	1.77538100
H	-6.09124000	-0.05564400	0.71830600
H	-2.40900800	1.44417300	-0.42999800
O	-2.12378200	-1.04821900	-1.21636900
C	-0.81368300	-1.43658400	-1.18608900
C	-0.21708600	-1.61265300	-2.44650400
C	-0.07193000	-1.69809800	-0.02302700
C	1.10187400	-2.03723300	-2.55522900
H	-0.81258400	-1.41064900	-3.33342700
C	1.25571100	-2.12028100	-0.12434500
H	-0.50232500	-1.57382400	0.96502300
C	1.82327000	-2.28524300	-1.38469800
H	1.57088600	-2.17110700	-3.52485300
H	1.84203000	-2.32429300	0.76626500
N	3.21750600	-2.72409100	-1.48516300
O	3.79373000	-3.07460200	-0.43757400
O	3.74561400	-2.72192400	-2.61358700

4

E = -744.117136

ZPVE = 0.260722

Symbol	X	Y	Z
C	-0.94087700	-0.95824000	-0.37429600
C	0.48772100	-1.20742300	-0.86118200
C	1.37123000	0.01874500	-0.67819400
C	-0.08513000	0.78498400	1.23353500
C	-0.95102100	-0.46591000	1.07387000
H	2.39420700	-0.21811300	-1.00221400
H	0.93800400	-2.03304300	-0.29135300
H	0.49920200	-1.49818100	-1.91837200
H	-1.41831000	-0.21048700	-1.01967700
H	-1.52626500	-1.88140900	-0.46882900
H	-0.07181500	1.11171200	2.28082000
H	-0.51756700	1.60803300	0.64938000
H	-0.56733200	-1.25931100	1.73288800
H	-1.97898800	-0.25926500	1.39679900
O	0.81715000	1.01712800	-1.57385700
C	1.51190100	2.17305500	-1.79173200
C	0.77434400	3.20858100	-2.39066700
C	2.87291200	2.36360400	-1.50472900
C	1.37676500	4.42296200	-2.69909500
H	-0.27758800	3.03755600	-2.60651400
C	3.48283700	3.58430600	-1.80187600
H	3.47235300	1.57757800	-1.05745100
C	2.72907300	4.59448700	-2.39363300
H	0.81503100	5.22777100	-3.16266200
H	4.53296700	3.74854000	-1.58078900
N	3.37307200	5.87344400	-2.70354500
O	2.73044800	6.69532200	-3.38450700
O	4.52524900	6.06407400	-2.26943200
C	1.34683400	0.52852800	0.76037900
H	1.95205500	1.43782200	0.85515400
H	1.81995300	-0.23462200	1.39591500

5

E = -1371.994786

ZPVE = 0.342357

Symbol	X	Y	Z
C	-2.01910900	0.20480400	-0.02464400
C	-0.65847000	-0.49172200	-0.09797200
C	0.47857500	0.47112300	-0.45079700
C	0.47875200	1.70034100	0.45495600
C	-0.88198100	2.37969700	0.54917000

C	-1.97436600	1.38559000	0.94631600
H	1.44252900	-0.03742000	-0.32450500
H	-0.42343200	-0.92818700	0.88196100
H	-0.67703100	-1.31802300	-0.82020600
H	-2.31706500	0.55992600	-1.02016200
H	-2.78061200	-0.51870200	0.29259400
H	1.25315100	2.39462600	0.11023000
H	-0.83257800	3.20581800	1.26976500
H	-1.11255200	2.82014700	-0.43039200
H	-1.78101900	1.01943300	1.96361200
H	-2.94475900	1.89683700	0.97078600
S	0.34559700	0.95495300	-2.21977500
C	1.75986200	2.03662000	-2.30334900
C	1.57461000	3.41677400	-2.47965400
C	3.06102700	1.52080100	-2.19369300
C	2.68017500	4.27314600	-2.53090100
H	0.56502300	3.81308900	-2.57268700
C	4.16164900	2.38234800	-2.22364300
H	3.20838800	0.44725800	-2.08784800
C	3.97406100	3.75959100	-2.39163800
H	2.52881300	5.34164800	-2.67209300
H	5.16694000	1.97614300	-2.13044600
H	4.83252800	4.42717100	-2.42225500
O	0.86950700	1.17700000	1.75034700
C	1.36304000	2.04640600	2.68318600
C	1.57375500	1.49087600	3.95702500
C	1.68846100	3.39165400	2.44627000
C	2.09328400	2.26114600	4.99050300
H	1.31610800	0.44645200	4.11588300
C	2.20439600	4.17323100	3.48277100
H	1.54373100	3.85144300	1.47416500
C	2.40393400	3.59926700	4.73513900
H	2.26040600	1.83979300	5.97675900
H	2.45459200	5.21663500	3.31733900
N	2.94585200	4.42426500	5.81763600
O	3.05516100	5.64894200	5.61626200
O	3.26769700	3.85170900	6.87636700

6

E = -3372.094142

ZPVE = 0.341727

Symbol	X	Y	Z
C	-2.14344800	0.36617000	0.03894900
C	-1.06455600	-0.67157300	0.35603800
C	0.30009000	-0.27921600	-0.20652300
C	0.70212700	1.13918200	0.17049700
C	-0.38561800	2.17314600	-0.09731100
C	-1.71983100	1.75443100	0.52237200
H	1.07364900	-0.96854200	0.15207200

H	-0.95649300	-0.75587200	1.44652000
H	-1.34880400	-1.66481800	-0.01462100
H	-2.33521300	0.39886100	-1.04227400
H	-3.08570500	0.06985300	0.51678500
H	1.63294000	1.39113300	-0.34779800
H	-0.06651300	3.14664400	0.29655700
H	-0.49496200	2.28548400	-1.18422000
H	-1.62916200	1.75089500	1.61703000
H	-2.48766400	2.49556100	0.26788900
C	2.13064600	0.10449300	-2.40151600
C	2.42295400	1.27655900	-3.11274200
C	3.16874200	-0.65280600	-1.84090200
C	3.75202200	1.69244800	-3.25375000
H	1.61399300	1.86180400	-3.54599600
C	4.49311400	-0.22389000	-1.96930600
H	2.94359500	-1.57807400	-1.31325100
C	4.78662900	0.95171200	-2.67128500
H	3.97705200	2.60131100	-3.80871600
H	5.29608100	-0.81053000	-1.52716400
H	5.81826300	1.28109600	-2.77536600
O	0.97310000	1.05753400	1.59612000
Se	0.30639700	-0.45199200	-2.18611700
C	1.74681000	2.03181400	2.16251600
C	1.77478900	2.02617500	3.56767900
C	2.48438600	2.99464400	1.45416200
C	2.53289500	2.95751200	4.26739900
H	1.19974600	1.26793600	4.09393100
C	3.24019900	3.93978600	2.15157600
H	2.48298700	3.03269900	0.36979000
C	3.24973100	3.91337300	3.54328500
H	2.55801700	2.96145800	5.35251400
H	3.81491300	4.69109200	1.61867700
N	4.04479700	4.90746700	4.26856100
O	3.90741100	4.96824100	5.50541500
O	4.81126600	5.63412900	3.60757100

7

E = -627.839818

ZPVE = 0.193580

Symbol	X	Y	Z
C	-0.50477800	1.54215700	-0.03755700
H	0.48215700	1.08473900	-0.16603500
H	-1.21668900	0.73140800	0.15127600
C	-0.46523200	2.44561300	1.17741600
H	-1.45003200	2.89441300	1.36630000
H	0.27064000	3.24979000	1.04127100
C	-0.90091900	2.31879900	-1.29253500
H	-0.18913000	3.12446200	-1.50122600
H	-0.92334000	1.65980100	-2.16504300

H	-1.89553200	2.76436900	-1.18542000
O	-0.08624000	1.63389800	2.30218900
C	0.00207400	2.23864700	3.52353600
C	-0.19336100	3.60875100	3.75288900
C	0.33890800	1.38923500	4.59150700
C	-0.09260700	4.11601400	5.05132700
H	-0.45605400	4.28584700	2.94698900
C	0.44504800	1.88815400	5.88368300
H	0.49552200	0.33324000	4.38609500
C	0.23911500	3.25494500	6.09244300
H	-0.24765300	5.17227500	5.24821500
H	0.69524700	1.24008300	6.71758200
N	0.34044500	3.79122700	7.45234100
O	0.43029900	2.97649200	8.39049600
O	0.33338000	5.02931500	7.59062500

8

E = -1083.949682

ZPVE = 0.292691

Symbol	X	Y	Z
C	-0.92163100	0.47817300	-0.85534200
C	-1.27697000	1.85969500	-0.17907400
H	-2.24749000	2.35381100	-0.27567700
C	-0.62793000	1.36135200	1.15444100
H	-1.04325100	1.50632600	2.15562700
C	-0.28383700	-0.01357600	0.48737600
H	-0.46346000	-1.00111400	0.91962700
C	0.74981800	1.92923200	0.67387300
C	1.09758800	0.55296500	0.00553600
H	2.06087800	0.04038600	0.09293800
C	0.44568800	1.05173700	-1.33242800
H	0.84253700	0.90673600	-2.34010400
C	0.10040200	2.42616700	-0.66137300
H	0.26002800	3.41544000	-1.09921200
C	-1.86078700	-0.27887700	-1.71055800
O	-2.77995900	-0.93524700	-0.95394900
O	-1.85167400	-0.29618300	-2.93669900
C	-3.78778700	-1.64490700	-1.71254600
H	-3.31991300	-2.40750200	-2.33749100
H	-4.43485500	-2.09726300	-0.96324500
H	-4.34415500	-0.94792900	-2.34182400
C	1.69658100	2.71248700	1.51188800
H	2.59150300	2.98997500	0.93398900
H	2.00463800	2.13534500	2.39729400
O	0.99404300	3.89889300	1.92331300
C	1.66194000	4.78904300	2.71709800
C	2.98539400	4.63154300	3.15342700
C	0.92712300	5.92593900	3.09397200
C	3.56747100	5.60751600	3.96708600

H	3.57566400	3.76568900	2.87221500
C	1.50106200	6.90092300	3.90031100
H	-0.09795600	6.02233400	2.74472300
C	2.82046100	6.72473600	4.32687200
H	4.58942000	5.50113000	4.31750300
H	0.94504400	7.78498700	4.19576100
N	3.43564300	7.74666900	5.17857000
O	2.81905700	8.81797300	5.33336600
O	4.53780200	7.48451200	5.69653800

9

E = -860.352661

ZPVE = 0.323302

Symbol	X	Y	Z
C	-2.30364000	-1.68656000	0.01244000
C	-0.78031300	-1.73946700	0.07264400
C	-0.16741000	-0.40578700	0.58693600
C	-1.16997900	0.76566900	0.75567200
C	-2.60481500	0.35017100	0.50056700
C	-2.82845300	-0.97157200	1.28080900
H	0.31795600	-0.58983400	1.55301500
H	-0.47829500	-2.55663400	0.74045900
H	-0.37945900	-1.98504600	-0.91795400
H	-2.73113800	-2.66472100	-0.24889800
H	-1.11450400	1.17165200	1.77772700
H	-3.28536800	1.19445000	0.67280700
H	-2.25347300	-1.11106300	2.20620400
H	-3.88111700	-1.16732400	1.49557500
H	0.62972700	-0.07306200	-0.08742400
C	-2.78320500	-0.46004400	-0.81778000
C	-4.26322600	-0.57010000	-1.18804100
H	-4.89531600	-0.85629100	-0.34240000
H	-4.62907600	0.39058500	-1.57099500
H	-4.39813000	-1.32118300	-1.97620800
C	-2.00302000	-0.07891600	-2.07098500
H	-0.93164100	0.03927200	-1.89980100
H	-2.14517000	-0.85121000	-2.83911400
H	-2.37230900	0.87088800	-2.47517500
O	-0.89546300	1.85460800	-0.15954000
C	0.19979200	2.63467000	0.06857200
C	0.39416300	3.67512900	-0.85725900
C	1.10673800	2.46591300	1.12722500
C	1.46496100	4.55061000	-0.72590000
H	-0.32249900	3.78841600	-1.66709100
C	2.18204600	3.34694300	1.26895300
H	0.99140700	1.66567200	1.85022300
C	2.35177800	4.36841200	0.33903000
H	1.62152900	5.35715800	-1.43515100

H	2.88879500	3.23239200	2.08503400
N	3.48511000	5.28498700	0.48744900
O	4.17992500	5.18905900	1.51714800
O	3.68859300	6.10700400	-0.42644700

10

E = -665.795088

ZPVE = 0.199228

Symbol	X	Y	Z
C	-1.44733300	0.62476100	0.13031400
C	-0.47677000	1.55196600	-0.55194600
C	-1.61382400	2.12051600	0.25216300
H	-2.16391500	0.08433700	-0.47965100
H	-1.10051000	0.07817800	1.00284800
H	-0.52296300	1.64314500	-1.63230400
H	0.52202600	1.64070600	-0.13422400
H	-2.43400500	2.56662800	-0.30512400
C	-1.32356400	2.77045000	1.56646000
H	-2.22570800	2.82726700	2.19073600
H	-0.54884400	2.21016100	2.10926400
O	-0.85062300	4.10350100	1.29169300
C	-0.58622100	4.91398900	2.35862200
C	-0.20976400	6.22890000	2.03412900
C	-0.67180800	4.52146500	3.70307300
C	0.08748200	7.14556100	3.03472100
H	-0.14938900	6.50758400	0.98506000
C	-0.37408400	5.43913100	4.71441100
H	-0.96107400	3.51384900	3.98242700
C	-0.00465900	6.73474900	4.36770100
H	0.37603300	8.16432200	2.79613500
H	-0.43128400	5.15148800	5.75964400
N	0.30495200	7.69389300	5.43115300
O	0.43724000	8.89040300	5.11030600
O	0.41711300	7.25766700	6.59269500

11

E = -782.034001

ZPVE = 0.262794

Symbol	X	Y	Z
C	-1.86262500	0.84288400	0.33601200
C	-0.38635900	1.01864500	0.09972400
C	-1.31562900	2.20154400	-0.02663500
H	-2.45131200	0.31653400	-0.40887200
H	-2.19595600	0.69087500	1.35885600
H	0.04438000	0.61194600	-0.81055200

H	0.27292100	0.98189700	0.96237700
H	-1.51793400	2.55097500	-1.03862100
C	-1.31472800	3.29742500	1.00295200
H	-1.09189400	2.87333100	1.99774300
C	-2.61090900	4.04886600	1.05971400
C	-3.67009700	3.62174800	2.04564000
C	-2.91108900	4.90580400	2.25871500
H	-2.95965700	4.41547600	0.09582300
H	-3.44531200	2.78466000	2.70060600
H	-4.70809700	3.67762000	1.73257400
H	-3.42803200	5.84644400	2.09719700
H	-2.16548900	4.93216100	3.04881000
O	-0.29511300	4.29305500	0.67941100
C	1.00053400	3.82776500	0.75331100
C	1.76783500	3.79124300	-0.41615800
C	1.56965600	3.46882600	1.98308900
C	3.09546000	3.36520900	-0.37270300
H	1.30772600	4.08913900	-1.35505400
C	2.89063000	3.02540500	2.04042500
H	0.98174900	3.54585200	2.89511800
C	3.62892000	2.97789400	0.85687300
H	3.70702600	3.32627900	-1.26883200
H	3.35047400	2.73800700	2.98095900
N	5.02004600	2.51240200	0.91084500
O	5.72946900	2.68858100	-0.09750100
O	5.40674000	1.96654600	1.96163600

12

E = -625.464647

ZPVE = 0.143261

Symbol	X	Y	Z
C	-1.81626600	0.43197600	-0.07785100
H	-2.64898500	-0.15435300	0.24548700
C	-0.84946300	1.10079000	-0.40842200
C	0.27824300	1.90120100	-0.87067300
H	0.69767300	1.47348200	-1.79061100
H	-0.03715300	2.93338900	-1.07206000
O	1.27269200	1.89265300	0.16839300
C	2.40958300	2.62116300	-0.06263600
C	3.32739500	2.63950800	1.00072000
C	2.69925100	3.29900300	-1.25522600
C	4.51413000	3.35351500	0.89308800
H	3.08076400	2.09733800	1.91004200
C	3.88956200	4.02376700	-1.36703700
H	2.00916800	3.30320700	-2.09251800
C	4.78205600	4.03024900	-0.30034800
H	5.22779900	3.38346200	1.71020700
H	4.12912800	4.56027300	-2.27983400
N	6.02771600	4.79399500	-0.42195300
O	6.70782700	4.95749000	0.60860000

O	6.33219500	5.23168500	-1.54761700

13

E = -1125.186593

ZPVE = 0.340590

Symbol	X	Y	Z
C	1.57631400	0.40634100	-0.31796400
C	2.14820500	1.83619300	-0.09952300
C	-0.42503100	1.96225000	-0.37794700
C	0.03933600	0.47701800	-0.39988800
H	1.99513600	-0.01421500	-1.23965400
H	1.84715400	-0.25072000	0.51646600
H	-0.33454700	-0.03071400	-1.29973300
H	-1.51101400	2.05820400	-0.49478000
H	3.23846100	1.81633900	0.02375100
C	0.05237900	2.49625200	0.94705300
C	1.44708300	2.41916200	1.10306500
C	-0.75659400	2.96565600	1.98273200
C	2.03922300	2.81578400	2.30363900
C	-0.15904200	3.38184400	3.17995300
H	-1.83805700	3.02072700	1.85595700
C	1.23091600	3.30247100	3.34057900
H	3.12001400	2.75452400	2.43210600
H	-0.77708200	3.76427600	3.99025900
H	1.68611700	3.62423100	4.27544700
C	0.32700500	2.66771900	-1.47646100
C	-0.23870500	3.31144900	-2.57893500
C	1.72266000	2.63093100	-1.30957500
C	0.60072400	3.92984200	-3.51547400
H	-1.32138100	3.34366300	-2.70260700
C	2.55806400	3.23697700	-2.24906800
C	1.99127700	3.89462100	-3.34989900
H	0.17053100	4.44272700	-4.37348100
H	3.64040600	3.20744200	-2.12370600
H	2.63533500	4.37831300	-4.08181500
O	-0.43626500	-0.21384200	0.77932800
C	-1.78658200	-0.24425700	1.00883800
C	-2.16690700	-0.34111600	2.35630100
C	-2.76295800	-0.22042700	0.00181000
C	-3.51182600	-0.41894300	2.70528800
H	-1.38859600	-0.34838600	3.11551800
C	-4.11537700	-0.28559600	0.34340100
H	-2.48513200	-0.17406500	-1.04745100
C	-4.46868100	-0.37614400	1.68844900
H	-3.82084100	-0.49269400	3.74333600
H	-4.88595400	-0.26619700	-0.42121300
N	-5.88910300	-0.44117400	2.04471500
O	-6.17810200	-0.72343300	3.22316900
O	-6.72313800	-0.20906600	1.14864800

For Table 4 ($ROCOCH_3$): B3LYP/6-311++G(d,p)

1

E = -499.618067

ZPVE = 0.187750

Symbol	X	Y	Z
C	-0.59319600	-0.94148500	-0.10020800
C	0.93063800	-0.76969600	-0.05487900
C	1.33323600	0.67922200	0.20507300
C	-0.75584600	1.14677500	1.27802700
C	-1.22397900	-0.29855500	1.14208500
H	2.39682100	0.78887800	0.40433400
H	1.34667700	-1.36787400	0.76299800
H	1.40216100	-1.10932800	-0.98049800
H	-0.99025500	-0.46542900	-1.00299600
H	-0.84931200	-2.00298100	-0.16045700
H	-1.08268200	1.59258700	2.21805500
H	-1.14602700	1.75632200	0.45405600
H	-0.93409900	-0.85683400	2.03959500
H	-2.31714400	-0.32039300	1.08440800
O	0.67928900	1.24680800	1.30241300
O	1.02168100	1.43935300	-0.99905500
C	1.88419600	2.42188100	-1.37578000
C	1.33914700	3.17786900	-2.56074000
H	1.02350000	2.48533900	-3.34329400
H	0.45933100	3.74852700	-2.25200700
H	2.09903600	3.85819100	-2.93963600
O	2.93607700	2.64338400	-0.83320800

2

E = -872.311750

ZPVE = 0.312165

Symbol	X	Y	Z
C	-2.05187900	0.44923200	0.35480700
C	-0.78710300	-0.41990100	0.30940900
C	0.47479600	0.36728200	-0.12420300
C	0.64893100	1.64341200	0.70923500
C	-0.62267000	2.49151200	0.81320400
C	-1.84609500	1.67606300	1.25281000
H	1.34668600	-0.26166100	0.10710600
H	-0.61489300	-0.83108900	1.31120300
H	-0.94235100	-1.27989200	-0.34890200
H	-2.31927200	0.77920200	-0.65622200
H	-2.89574300	-0.14623500	0.71844900
H	1.47039400	2.25735600	0.33847000
H	-0.43736700	3.32476700	1.49601500
H	-0.81179600	2.93372800	-0.17074200

H	-1.70954400	1.34581800	2.28865900
H	-2.73587200	2.31345600	1.24205200
Si	0.71611600	0.61201700	-2.01892600
C	-0.44195500	1.86323000	-2.84195300
H	-0.30102900	2.87599000	-2.45416100
H	-0.23504600	1.89676700	-3.91702000
H	-1.49629500	1.60101300	-2.72031100
C	2.49832300	1.18152900	-2.30020000
H	2.71034900	1.26254100	-3.37110400
H	2.69539000	2.16112100	-1.85470600
H	3.21737600	0.47449400	-1.87498100
C	0.47134600	-1.06918500	-2.85043000
H	1.09607100	-1.84130700	-2.39071300
H	-0.56758800	-1.40719300	-2.79796500
H	0.74341800	-1.01264900	-3.90920800
O	1.03991500	1.21043900	2.06310600
C	1.84161500	2.02453500	2.77915400
C	2.15404100	1.42171800	4.12759500
H	1.23034400	1.27511800	4.69242200
H	2.61909400	0.44151400	4.00145000
H	2.82134100	2.08357200	4.67582100
O	2.25367000	3.09076500	2.38590000

3

E = -463.685226

ZPVE = 0.211489

Symbol	X	Y	Z
C	-4.15399500	-0.72484400	-0.13504300
C	-2.64294800	-0.55086000	-0.02174100
C	-2.24721200	0.91216800	0.17591900
C	-2.95493400	1.50561900	1.40492300
C	-4.47811200	1.33658900	1.31547400
C	-4.86430600	-0.13280900	1.09276800
H	-1.16211400	0.98767600	0.28309000
H	-2.24987100	-1.15102600	0.80291200
H	-4.49871000	-0.21941500	-1.04492200
H	-4.39347900	-1.78633600	-0.24781100
H	-2.58640000	1.00776800	2.31069700
H	-2.69260900	2.56314000	1.50557900
H	-4.95494300	1.71820700	2.22390500
H	-4.86120900	1.94116400	0.48331400
H	-4.59779900	-0.71593700	1.98350000
H	-5.94766300	-0.22943100	0.97298300
H	-2.53014000	1.47291600	-0.72325600
O	-2.06143300	-1.06565100	-1.25511100
C	-0.81980800	-1.59505100	-1.19916800
O	-0.16335400	-1.67633900	-0.18860700
C	-0.37601400	-2.06443500	-2.56252900
H	-1.10281900	-2.76805700	-2.97382300
H	-0.32155200	-1.21349000	-3.24588700

H	0.60091000	-2.53691600	-2.48406200

4

E = -463.683950

ZPVE = 0.211561

Symbol	X	Y	Z
C	-0.63691600	-0.87720600	-0.09754100
C	0.89630000	-0.78506600	-0.10528100
C	1.40398500	0.63557200	0.13852300
C	-0.75424200	1.17356100	1.38781200
C	-1.22947800	-0.27238000	1.18351000
H	2.49167000	0.65223500	0.21799800
H	1.30635900	-1.41927000	0.69033200
H	1.30496800	-1.15763600	-1.04907500
H	-1.03408300	-0.34472500	-0.96857200
H	-0.94279800	-1.92293400	-0.20238700
H	-1.14536500	1.57465600	2.32807600
H	-1.15837600	1.80334700	0.58722200
H	-0.92527900	-0.87949600	2.04675700
H	-2.32294400	-0.30941800	1.14749000
O	1.04596800	1.41569500	-1.04781100
C	1.83719900	2.45794300	-1.38026400
C	1.33047500	3.13948800	-2.62765100
H	1.28546500	2.42497500	-3.45255700
H	0.31706700	3.51271800	-2.46245600
H	1.99137400	3.96457100	-2.88498300
O	2.81803600	2.78921200	-0.75801300
C	0.77856600	1.26870100	1.38504900
H	1.11265400	2.30578200	1.47119900
H	1.18168400	0.73807600	2.25677100

5

E = -1092.917844

ZPVE = 0.293024

Symbol	X	Y	Z
C	-1.85162300	-0.02191300	0.14923600
C	-0.39878300	-0.46581900	-0.07617500
C	0.54832500	0.70895300	-0.36773700
C	0.41841000	1.82898700	0.67530200
C	-1.03009800	2.23919900	0.94901800
C	-1.93822500	1.03971700	1.25455800
H	1.58065800	0.35587500	-0.37094300
H	-0.03177600	-0.95962300	0.83066100
H	-0.33458800	-1.19713700	-0.88625300
H	-2.26662300	0.38207800	-0.78173700
H	-2.46230400	-0.89204800	0.40925500

H	1.00979500	2.69647700	0.38392000
H	-1.04176300	2.96553600	1.76531500
H	-1.39566800	2.75986600	0.05791800
H	-1.64509100	0.59175000	2.21095500
H	-2.97058100	1.38268000	1.37287200
S	0.22687500	1.35417200	-2.08732900
C	1.74649000	2.25872800	-2.41203500
C	1.72721100	3.65546300	-2.47159300
C	2.94181100	1.57518100	-2.66379400
C	2.89300000	4.36030100	-2.77061300
H	0.80113400	4.18503700	-2.28284300
C	4.10663000	2.28351900	-2.94824000
H	2.95343700	0.49144000	-2.64711900
C	4.08432700	3.67728600	-3.00406800
H	2.86866700	5.44338800	-2.81361800
H	5.02883900	1.74617600	-3.13978900
H	4.99073600	4.22659000	-3.23191800
O	1.02192700	1.28242000	1.89421600
C	1.60929500	2.15037900	2.74928500
C	2.19910900	1.42087800	3.93102200
H	1.42033500	0.85763300	4.45011200
H	2.94949500	0.70411500	3.58962200
H	2.65399200	2.13878600	4.61030600
O	1.65138300	3.34407800	2.57675000

6

E = -3096.250286

ZPVE = 0.291759

Symbol	X	Y	Z
C	-2.00569100	0.12910700	0.30603700
C	-0.72721500	-0.71556000	0.40730100
C	0.49568100	-0.01971200	-0.20397900
C	0.68035600	1.40824100	0.32120500
C	-0.60265800	2.24202100	0.28458100
C	-1.79748100	1.51935900	0.92269800
H	1.39947200	-0.59341700	0.00091600
H	-0.50353600	-0.89446500	1.46601300
H	-0.86751800	-1.69496200	-0.05734300
H	-2.30210800	0.23401800	-0.74514400
H	-2.82812700	-0.39008700	0.80764600
H	1.48033000	1.91884600	-0.21345700
H	-0.41248900	3.20157800	0.77149400
H	-0.82100600	2.45957300	-0.76605900
H	-1.62960600	1.41436800	2.00065600
H	-2.69939300	2.12752800	0.80410500
C	2.25029400	0.17118300	-2.61846200
C	2.75004800	1.40473400	-3.04434500
C	3.10848000	-0.92903600	-2.52357000
C	4.10181600	1.53787900	-3.36300500

H	2.08549800	2.25640400	-3.12448100
C	4.45981400	-0.78862700	-2.83469000
H	2.71795400	-1.89193600	-2.21581000
C	4.95805900	0.44417600	-3.25543800
H	4.48342800	2.49852500	-3.69037800
H	5.12053800	-1.64507600	-2.75744000
H	6.00867200	0.55022300	-3.50105400
O	1.12558000	1.24582500	1.71120600
Se	0.36023800	-0.02594400	-2.21607400
C	1.93648400	2.19713200	2.22699900
C	2.32208300	1.85972200	3.64628000
H	1.42678800	1.74124400	4.26058800
H	2.86268300	0.91059500	3.66840500
H	2.94894300	2.65202000	4.05011700
O	2.29885400	3.17672900	1.62202200

7

E = -346.982544

ZPVE = 0.145793

Symbol	X	Y	Z
C	-0.85883600	1.58913400	0.10436100
H	-0.44751200	0.57658300	0.16510100
H	-1.94459100	1.49541200	0.20676000
C	-0.32275500	2.40987300	1.26434600
H	-0.73771400	3.42141500	1.27238900
H	0.76655000	2.49759300	1.23113400
C	-0.50963700	2.21945600	-1.24753100
H	0.57305500	2.30027000	-1.38358900
H	-0.90227000	1.61709000	-2.06996000
H	-0.93245000	3.22426700	-1.34161500
O	-0.69919300	1.74241900	2.49325300
C	-0.30336600	2.32642300	3.64546600
C	-0.75967000	1.52807300	4.84053300
H	-1.84803300	1.43526500	4.83440400
H	-0.34499300	0.51846500	4.79480600
H	-0.43366500	2.02223600	5.75326100
O	0.33185100	3.35195900	3.68806800

8

E = -804.513053

ZPVE = 0.245163

Symbol	X	Y	Z
C	-0.83677300	0.35491100	-0.76205900
C	-1.03665400	1.90831200	-0.53802400
H	-1.79436500	2.50647000	-1.03924400

C	-0.91313100	1.70705000	1.00999600
H	-1.55762800	2.16824900	1.75573800
C	-0.72089400	0.16597600	0.80101300
H	-1.22522700	-0.61890600	1.36034800
C	0.64352200	1.91506600	0.90697100
C	0.83153300	0.36595600	0.69199100
H	1.57984100	-0.24895500	1.19006700
C	0.70814700	0.56531000	-0.86108100
H	1.33758700	0.09828200	-1.61449000
C	0.51426200	2.10937600	-0.64936200
H	1.00323900	2.89268400	-1.22539400
C	-1.64514700	-0.48454900	-1.68321600
O	-2.94239500	-0.52118500	-1.29587900
O	-1.22738500	-1.06283600	-2.65978800
C	-3.82796400	-1.29674200	-2.12416800
H	-3.50912500	-2.33971600	-2.15242800
H	-4.80930500	-1.20877200	-1.66289400
H	-3.84474600	-0.90122600	-3.14082900
C	1.48940200	2.72531700	1.83148500
H	2.54530400	2.69151800	1.54512800
H	1.41153900	2.37089500	2.86412500
O	1.03055600	4.10022000	1.77123100
C	1.68315200	4.98775200	2.55562000
C	1.11157700	6.37362400	2.39551000
H	1.20471000	6.69692400	1.35615700
H	0.04781700	6.37077800	2.64345300
H	1.64407000	7.06299500	3.04725300
O	2.60018000	4.68529400	3.27925000

9

E = -580.338212

ZPVE = 0.272727

Symbol	X	Y	Z
C	-2.25113300	-1.64593100	0.10220200
C	-0.71978600	-1.70223400	0.11889400
C	-0.06878800	-0.31247500	0.40907500
C	-1.07484600	0.85445400	0.62332900
C	-2.52755000	0.43334400	0.44285100
C	-2.73136400	-0.82783600	1.33180300
H	0.57687000	-0.37695500	1.28609400
H	-0.40729800	-2.41983300	0.88408800
H	-0.35279600	-2.09274000	-0.83481000
H	-2.68345300	-2.63798800	-0.05895000
H	-0.94962500	1.26234700	1.62769700
H	-3.19437900	1.28830100	0.58243000
H	-2.12913500	-0.89874600	2.24204500
H	-3.77430600	-0.99960200	1.59214600
H	0.58828500	-0.03539100	-0.41677000
C	-2.77459300	-0.48112800	-0.81026500

C	-4.27671700	-0.61680700	-1.10488300
H	-4.87193100	-0.83316200	-0.21573200
H	-4.66383300	0.30772100	-1.54556100
H	-4.45092000	-1.42416500	-1.82369600
C	-2.05651500	-0.19404400	-2.13091300
H	-0.97951800	-0.07401900	-2.02697700
H	-2.23770500	-1.01068100	-2.83869700
H	-2.44149600	0.72505100	-2.58257600
O	-0.81306300	1.95537900	-0.30202800
C	0.15997200	2.82876500	0.03364000
C	0.27681100	3.92703100	-0.99449000
H	0.45607700	3.49882500	-1.98313500
H	-0.65956400	4.48768700	-1.04607900
H	1.09239900	4.59399100	-0.72283800
O	0.83663700	2.73474800	1.03010400

10

E = -385.053370

ZPVE = 0.151718

Symbol	X	Y	Z
C	-1.92378800	1.00983300	-0.07510200
C	-0.43457100	0.99819800	0.16469200
C	-1.16495000	2.31146100	0.04025700
H	-2.29313600	0.72362000	-1.05209100
H	-2.57185100	0.72464200	0.74596800
H	0.21567000	0.69876800	-0.64803900
H	-0.08205200	0.71006400	1.14848200
H	-1.01341300	2.86361500	-0.88157900
C	-1.38345500	3.16958700	1.24965600
H	-2.22542600	3.85404300	1.11816700
H	-1.57783500	2.56703400	2.14083600
O	-0.18375700	3.95784000	1.47070600
C	-0.19421200	4.78098100	2.54101700
C	1.09769300	5.55217100	2.64342000
H	1.94444800	4.86353600	2.68174200
H	1.22576800	6.17917000	1.75782000
H	1.07989100	6.17355900	3.53629000
O	-1.12726400	4.87239900	3.30217200

11

E = -501.720264

ZPVE = 0.213567

Symbol	X	Y	Z
C	-1.47961600	1.04388300	0.40462300
C	-0.02194200	1.42563200	0.47701600

C	-1.06797400	2.48883100	0.25422500
H	-1.83694400	0.52354600	-0.47566500
H	-1.96940200	0.74749800	1.32476900
H	0.62217500	1.16406100	-0.35364200
H	0.46115900	1.38962800	1.44687000
H	-1.12659300	2.90391900	-0.74754000
C	-1.38820700	3.47425900	1.34896900
H	-1.33741700	2.98780500	2.32555800
C	-2.72319200	4.15591900	1.17948600
C	-3.95800500	3.55323300	1.80621400
C	-3.38433500	4.83623700	2.35354800
H	-2.85752900	4.62827400	0.21075800
H	-3.83950200	2.65536100	2.40146300
H	-4.88356600	3.59475800	1.24497100
H	-3.92000600	5.75925800	2.16727900
H	-2.87570600	4.79408800	3.30926200
O	-0.33964600	4.50265800	1.31861600
C	0.27143200	4.83591100	2.47364300
C	1.29916800	5.91573100	2.24053700
H	1.99901900	5.60811300	1.46097000
H	0.80239600	6.82546600	1.89449300
H	1.83238700	6.11759600	3.16725400
O	0.02500000	4.33622900	3.54663000

12

E = -344.533291

ZPVE = 0.098419

Symbol	X	Y	Z
C	-1.63856800	0.33355900	-0.10867200
H	-2.39501700	-0.41191300	-0.06907700
C	-0.77855200	1.17049100	-0.15276800
C	0.22812700	2.21775300	-0.20804500
H	0.14119200	2.79780000	-1.13046800
H	0.11899700	2.91226500	0.62898500
O	1.53990200	1.60632700	-0.15186800
C	2.58466100	2.46945000	-0.19057200
C	3.89418400	1.72872900	-0.12503300
H	3.94677700	1.14764900	0.79833800
H	3.96730200	1.02657600	-0.95838400
H	4.71494200	2.44161000	-0.16412100
O	2.44890600	3.66534400	-0.26691600

13

E = -845.954564

ZPVE = 0.294093

Symbol X Y Z

C	1.36377900	0.37065100	-0.14527000
C	2.10892200	1.74378700	-0.11184200
C	-0.45383500	2.14136000	-0.00892600
C	-0.16345900	0.61059200	-0.11646700
H	1.64653500	-0.18225600	-1.04340300
H	1.64564100	-0.22733300	0.72307600
H	-0.65842800	0.22220100	-1.00559900
H	-1.52724800	2.32354900	0.02690100
H	3.19037900	1.60437600	-0.15303700
C	0.27998600	2.65555100	1.21520000
C	1.66606300	2.44689000	1.15792300
C	-0.28996100	3.27162500	2.32268200
C	2.47898700	2.85380700	2.20922100
C	0.52900100	3.68798500	3.37631800
H	-1.36222500	3.43358200	2.36689800
C	1.90568900	3.47949400	3.32021900
H	3.55145300	2.69166400	2.16708800
H	0.09080400	4.17684800	4.23931300
H	2.53606700	3.80630800	4.13973400
C	0.19817000	2.75549100	-1.23607000
C	-0.44640600	3.45180300	-2.25146300
C	1.58474500	2.54809500	-1.28895100
C	0.30051900	3.95484900	-3.32097300
H	-1.51977300	3.60606100	-2.21289900
C	2.32551700	3.04415700	-2.35495800
C	1.67820100	3.75272700	-3.37195400
H	-0.19534700	4.50464800	-4.11303400
H	3.39849700	2.88597800	-2.39762600
H	2.25203500	4.14688100	-4.20329100
O	-0.69575600	-0.10457100	1.03016300
C	-2.01479500	-0.40396500	1.02763400
C	-2.39020900	-1.17295500	2.26883800
H	-1.87720100	-2.13790700	2.27247000
H	-2.07044200	-0.62901000	3.15986900
H	-3.46672100	-1.32961800	2.28752900
O	-2.77267900	-0.09702500	0.13887300

<u>For Table 4 ($ROCOCH_3$): M06-2X/6-311++G(d,p)</u>

1

E = -499.402654

ZPVE = 0.190602

Symbol	X	Y	Z
C	-0.60125700	-0.91176800	-0.11629800
C	0.92387500	-0.82125400	-0.05164200
C	1.37629300	0.61329100	0.17198700
C	-0.66629800	1.18718700	1.22850300
C	-1.19778700	-0.23470300	1.11878200
H	2.44641600	0.69334500	0.35325300
H	1.29601600	-1.41167000	0.79094400

H	1.39157400	-1.20130700	-0.96186300
H	-0.95764100	-0.40694600	-1.01966500
H	-0.91535700	-1.95558700	-0.18015000
H	-0.98551300	1.66920900	2.15193600
H	-1.01978200	1.78919600	0.38272800
H	-0.91790400	-0.79078700	2.01952700
H	-2.28941700	-0.21124000	1.06838900
O	0.75933000	1.21528300	1.26525100
O	1.05977300	1.33943100	-1.02926000
C	1.80576500	2.43666300	-1.30156700
C	1.27833700	3.14513500	-2.51817600
H	1.21483300	2.44769600	-3.35394400
H	0.27053800	3.50948100	-2.31199700
H	1.93264500	3.97725900	-2.76371800
O	2.75481300	2.77464900	-0.65473400

2

E = -871.999223

ZPVE = 0.316184

Symbol	X	Y	Z
C	-1.89582400	0.25883400	0.32080000
C	-0.57955800	-0.51963300	0.33780100
C	0.60511400	0.34907100	-0.12457600
C	0.69100500	1.63630300	0.69284700
C	-0.63335200	2.39602600	0.77093400
C	-1.78902000	1.49669100	1.21373000
H	1.53120700	-0.20580100	0.08004900
H	-0.39026000	-0.86057200	1.36206900
H	-0.65448400	-1.41634000	-0.28292800
H	-2.13420000	0.56636600	-0.70572600
H	-2.71584000	-0.38137700	0.65662300
H	1.47468000	2.29856300	0.31466400
H	-0.50984600	3.24600600	1.44546900
H	-0.85015500	2.80606700	-0.21900300
H	-1.62396200	1.17449800	2.24763500
H	-2.72232800	2.06513500	1.20160800
Si	0.72008500	0.63101200	-2.01015300
C	-0.25323800	2.09889200	-2.67912000
H	0.11816800	3.04798500	-2.28389700
H	-0.13437200	2.13017600	-3.76651500
H	-1.32245000	2.03503500	-2.46501400
C	2.53464200	0.92519500	-2.41254600
H	2.67245400	1.11020900	-3.48116700
H	2.92642200	1.79313300	-1.87472400
H	3.14596400	0.06076900	-2.14074600
C	0.12245300	-0.92928500	-2.87248100
H	0.64548500	-1.81557300	-2.50305300
H	-0.94919300	-1.08448200	-2.72060800
H	0.29986500	-0.86104200	-3.94906300
O	1.08308700	1.24131500	2.03700900

C	1.67208100	2.17060600	2.80444600
C	2.00632000	1.61546500	4.16287600
H	1.08935800	1.29493100	4.65962200
H	2.64788100	0.74029500	4.05441500
H	2.50496100	2.38020100	4.75243200
O	1.89956700	3.29440500	2.44141100

3

E = -463.472521

ZPVE = 0.214300

Symbol	X	Y	Z
C	-4.17950700	-0.71471500	-0.14631400
C	-2.67022900	-0.58507000	-0.02379300
C	-2.24281600	0.86449400	0.16854200
C	-2.92792500	1.45964000	1.40228800
C	-4.44991200	1.33671600	1.30141300
C	-4.86718100	-0.12011900	1.08585100
H	-1.15638900	0.91574500	0.26381700
H	-2.30316700	-1.18793000	0.81287200
H	-4.50101600	-0.18106800	-1.04790200
H	-4.44607400	-1.76639700	-0.27658400
H	-2.58020500	0.93074600	2.29755300
H	-2.63423600	2.50526700	1.52059500
H	-4.92369400	1.73668500	2.20153000
H	-4.80492100	1.94095600	0.45798900
H	-4.59503300	-0.70718800	1.97109200
H	-5.95167800	-0.19675500	0.97773300
H	-2.53262000	1.42775100	-0.72637400
O	-2.10556500	-1.11875000	-1.23870500
C	-0.82643000	-1.52658600	-1.19433100
O	-0.14535200	-1.48289700	-0.20499200
C	-0.37801300	-2.03929400	-2.53553700
H	-1.03492500	-2.84785200	-2.85794300
H	-0.45155500	-1.23863200	-3.27281600
H	0.64792700	-2.39009900	-2.46288000

4

E = -463.472148

ZPVE = 0.214373

Symbol	X	Y	Z
C	-0.62821600	-0.85559900	-0.11176500
C	0.90201700	-0.82021900	-0.08556900
C	1.43313900	0.59145000	0.12517200
C	-0.70437700	1.21183500	1.32699900
C	-1.21338600	-0.22110600	1.15215200

H	2.52241100	0.59423500	0.19525500
H	1.27124400	-1.43969800	0.73941800
H	1.31862300	-1.22678800	-1.01030500
H	-0.98258600	-0.30636800	-0.98997600
H	-0.97229100	-1.88744900	-0.21754100
H	-1.10554700	1.65275300	2.24285500
H	-1.06389500	1.82518300	0.49360400
H	-0.92032300	-0.81693500	2.02572700
H	-2.30558000	-0.23368000	1.11124500
O	1.06813900	1.33834000	-1.06044300
C	1.76772100	2.45379700	-1.32288800
C	1.26719500	3.12073900	-2.57529600
H	1.33491200	2.42549800	-3.41283800
H	0.21686700	3.38796600	-2.45036800
H	1.86043100	4.00961600	-2.77249600
O	2.67320800	2.85124500	-0.63968400
C	0.82533500	1.25227400	1.36035800
H	1.19803500	2.27524000	1.44238700
H	1.18921200	0.70607100	2.23814300

5

E = -1092.585183

ZPVE = 0.296868

Symbol	X	Y	Z
C	-1.83252100	0.08131600	0.17250900
C	-0.42672800	-0.48996700	-0.03265100
C	0.59028400	0.59067200	-0.41260700
C	0.56685100	1.75889500	0.57501300
C	-0.83596300	2.30507200	0.82253800
C	-1.81333500	1.19664300	1.22027100
H	1.59664900	0.16685900	-0.42276600
H	-0.08411900	-0.94216500	0.90387400
H	-0.42755600	-1.27415100	-0.79340900
H	-2.21556100	0.47668700	-0.77475200
H	-2.50988600	-0.71908100	0.48005300
H	1.23562600	2.55554100	0.24344700
H	-0.77810300	3.08289800	1.58630900
H	-1.17425600	2.78130800	-0.10271700
H	-1.51429000	0.77726600	2.18726200
H	-2.81366000	1.61628900	1.34995100
S	0.24173000	1.16115500	-2.12778300
C	1.68864800	2.17026400	-2.40916400
C	1.56674900	3.55790000	-2.47063000
C	2.93953800	1.57712900	-2.58584600
C	2.68983900	4.34668800	-2.70216700
H	0.59283900	4.01229900	-2.33099400
C	4.06090300	2.36911700	-2.80356900
H	3.02612800	0.49672100	-2.56045300
C	3.93729900	3.75457000	-2.86406600
H	2.58879100	5.42448200	-2.74747100

H	5.03013600	1.90345100	-2.93771300
H	4.81164200	4.36996000	-3.03891100
O	1.10730000	1.20949700	1.80094900
C	1.62555500	2.08002900	2.68581500
C	2.14320700	1.36341600	3.90302300
H	1.32310900	0.83133800	4.38741700
H	2.88832700	0.62488600	3.60531600
H	2.57847200	2.08577800	4.58830400
O	1.66111400	3.26738500	2.51013900

6

E = -3095.950759

ZPVE = 0.295786

Symbol	X	Y	Z
C	-1.96554100	0.21174700	0.29848600
C	-0.75707400	-0.71593900	0.44844800
C	0.49850600	-0.14208800	-0.21042900
C	0.78978400	1.28169400	0.26163800
C	-0.42238500	2.20477900	0.17272300
C	-1.64920700	1.60011700	0.85950100
H	1.36381600	-0.76945200	0.00805200
H	-0.53593000	-0.84071100	1.51438400
H	-0.96789700	-1.70752600	0.04150700
H	-2.24180100	0.29882400	-0.75902200
H	-2.82592100	-0.22111400	0.81461000
H	1.63547100	1.70399800	-0.28431900
H	-0.15690400	3.17097500	0.60606700
H	-0.63603000	2.37187800	-0.88711600
H	-1.46074200	1.51712100	1.93557700
H	-2.50585200	2.26681800	0.73599200
C	2.16564500	0.12106100	-2.58704400
C	2.58134900	1.38557200	-3.00166000
C	3.09616000	-0.91097000	-2.46444500
C	3.92434000	1.61701900	-3.28602800
H	1.85512200	2.18435200	-3.09554400
C	4.43797900	-0.67286000	-2.74257200
H	2.76589300	-1.89682700	-2.15817000
C	4.85281600	0.59030200	-3.15438400
H	4.24334400	2.60217100	-3.60490500
H	5.15800200	-1.47683500	-2.64486600
H	5.89804400	0.77299600	-3.37354900
O	1.19060500	1.13117900	1.64683500
Se	0.30905400	-0.20177700	-2.18548100
C	1.93532400	2.11671200	2.17894800
C	2.27687100	1.81665600	3.61294900
H	1.35824200	1.71345900	4.19223600
H	2.81423900	0.86939200	3.67086500
H	2.88614200	2.62205800	4.01421600
O	2.27379800	3.09742500	1.57404100

7

E = -346.816785

ZPVE = 0.147887

Symbol	X	Y	Z
C	-0.86398000	1.58006600	0.11063400
H	-0.45161900	0.56932000	0.16790000
H	-1.94867400	1.49035600	0.21230300
C	-0.32880700	2.39473000	1.26924400
H	-0.74255000	3.40683100	1.27628400
H	0.76054900	2.48169800	1.23291800
C	-0.50595900	2.22635600	-1.22557800
H	0.57713300	2.30655700	-1.34630700
H	-0.89232700	1.63970400	-2.05987600
H	-0.92591600	3.23235000	-1.30114400
O	-0.70305200	1.72989600	2.48423500
C	-0.30802500	2.32103800	3.62394400
C	-0.75560900	1.53646600	4.82610700
H	-1.84224400	1.44306500	4.81796600
H	-0.33610300	0.53058200	4.78238800
H	-0.42694000	2.04292600	5.72955300
O	0.32089400	3.34399200	3.65061600

8

E = -804.195671

ZPVE = 0.249324

Symbol	X	Y	Z
C	-0.82373900	0.36761600	-0.74810800
C	-1.02197000	1.90800300	-0.52360800
H	-1.78001300	2.50508200	-1.02287300
C	-0.89654200	1.70198900	1.01663500
H	-1.53202300	2.16579600	1.76662700
C	-0.71145500	0.16775700	0.80119400
H	-1.22077900	-0.61829300	1.35190700
C	0.64985500	1.89898400	0.90784600
C	0.83545200	0.36160400	0.69166300
H	1.58298900	-0.25269600	1.18847300
C	0.71119700	0.56720600	-0.85388300
H	1.33067600	0.09826100	-1.61291400
C	0.52288500	2.10429600	-0.63587200
H	1.01510700	2.89110400	-1.20192800
C	-1.64179300	-0.46256800	-1.66567000
O	-2.92884700	-0.48593300	-1.27559400
O	-1.23628800	-1.03974600	-2.63971800
C	-3.80695700	-1.24916300	-2.10445800

H	-3.48820100	-2.29131200	-2.13562300
H	-4.79131200	-1.16242300	-1.65236500
H	-3.81282400	-0.84998500	-3.11902900
C	1.48871800	2.71654200	1.82780400
H	2.54413000	2.69032200	1.54019300
H	1.41069100	2.36659600	2.86160800
O	1.01261800	4.06954400	1.75104400
C	1.65457600	4.96142600	2.52619700
C	1.07515100	6.33907400	2.36361100
H	1.16506800	6.65157100	1.32245300
H	0.01392100	6.32175000	2.61442800
H	1.60547100	7.03150400	3.01163900
O	2.56993900	4.66616300	3.24480300

9

E = -580.082615

ZPVE = 0.276511

Symbol	X	Y	Z
C	-2.23161200	-1.62912400	0.07924900
C	-0.70466500	-1.64424500	0.09081900
C	-0.10355900	-0.26654700	0.49052100
C	-1.13333900	0.88007100	0.66639900
C	-2.56797000	0.42067400	0.48477600
C	-2.73220800	-0.86737800	1.33072400
H	0.45446100	-0.36157000	1.42232600
H	-0.36630600	-2.40595800	0.79819400
H	-0.33601800	-1.94644800	-0.89280700
H	-2.64324300	-2.62159800	-0.12168000
H	-1.02184100	1.31051600	1.66439700
H	-3.26157500	1.25057400	0.63997700
H	-2.12014100	-0.94634100	2.23313400
H	-3.76805000	-1.07911900	1.58536500
H	0.63017100	0.05212600	-0.25155900
C	-2.76675600	-0.45248300	-0.79027500
C	-4.25180600	-0.61534300	-1.11451100
H	-4.85012700	-0.87501700	-0.23972200
H	-4.65168600	0.31412700	-1.53011700
H	-4.38985300	-1.40358900	-1.86031300
C	-2.02380800	-0.10174300	-2.07469100
H	-0.95187200	0.02803900	-1.93142300
H	-2.17637500	-0.89330300	-2.81553100
H	-2.41074800	0.83146300	-2.49230600
O	-0.90815200	1.95367900	-0.27524800
C	0.15836700	2.73432100	-0.04384400
C	0.26599800	3.82467000	-1.07456300
H	0.30780800	3.38363500	-2.07135000
H	-0.62211900	4.45655200	-1.02915800
H	1.15753800	4.41592700	-0.88351100
O	0.91622200	2.56734000	0.87472600

10

E = -384.881369

ZPVE = 0.153985

Symbol	X	Y	Z
C	-1.91015200	1.01725200	-0.04975200
C	-0.42388900	1.03838600	0.17430700
C	-1.17774000	2.32759800	0.02639000
H	-2.27761800	0.69953300	-1.01580900
H	-2.54266500	0.74605100	0.78642400
H	0.21925600	0.73003900	-0.63848000
H	-0.05927600	0.79015400	1.16338700
H	-1.04481600	2.86925500	-0.90269900
C	-1.38630000	3.18301400	1.23576900
H	-2.22541800	3.87200000	1.11392100
H	-1.57942100	2.57126600	2.12165400
O	-0.18954300	3.94978100	1.45074300
C	-0.19892700	4.75785500	2.52297000
C	1.09262900	5.51882200	2.64161900
H	1.92698900	4.81869400	2.69601600
H	1.23438700	6.13484900	1.75261500
H	1.06277100	6.14289100	3.53068400
O	-1.13250700	4.84308300	3.27465500

11

E = -501.501972

ZPVE = 0.216706

Symbol	X	Y	Z
C	-1.52736100	1.06307200	0.39481300
C	-0.06141200	1.39600400	0.44902300
C	-1.07042100	2.48352100	0.22728200
H	-1.90401300	0.54548800	-0.47687000
H	-2.01772700	0.80013700	1.32376500
H	0.56100000	1.10151900	-0.38489200
H	0.42617500	1.36351900	1.41588200
H	-1.12912400	2.90520300	-0.77039300
C	-1.34066900	3.45955500	1.33701600
H	-1.29926200	2.94736800	2.30341600
C	-2.66222000	4.16387300	1.19473900
C	-3.88301300	3.53453300	1.80318900
C	-3.30652700	4.78793500	2.40071500
H	-2.79503600	4.67290000	0.24569000
H	-3.74901300	2.61135500	2.35325200
H	-4.81355000	3.60375700	1.25644200
H	-3.84933300	5.71280500	2.25859300

H	-2.77752300	4.70058800	3.34079600
O	-0.27188700	4.43704300	1.30232200
C	0.18235000	4.91463200	2.47104500
C	1.26155500	5.93821600	2.24625500
H	2.05190100	5.51119600	1.62839300
H	0.84192500	6.78899600	1.70724600
H	1.65847000	6.26154900	3.20481600
O	-0.22213100	4.56312800	3.54777400

12

E = -344.383941

ZPVE = 0.100201

Symbol	X	Y	Z
C	-1.62566200	0.33792500	-0.10960300
H	-2.38280000	-0.40871200	-0.07032900
C	-0.76863600	1.17420700	-0.15274200
C	0.24616900	2.22022300	-0.20681200
H	0.15803100	2.79800800	-1.12952200
H	0.13420600	2.91208600	0.63090100
O	1.53731300	1.60370700	-0.14948700
C	2.57538600	2.46265100	-0.19084300
C	3.88388800	1.72886400	-0.12515600
H	3.93082500	1.15040400	0.79822400
H	3.95144400	1.02915500	-0.95893600
H	4.69961500	2.44551800	-0.16465000
O	2.43307400	3.65160400	-0.26964500

13

E = -845.609295

ZPVE = 0.297788

Symbol	X	Y	Z
C	1.38675700	0.37217200	-0.22122400
C	2.10824400	1.74847400	-0.13609100
C	-0.46021600	2.10306900	-0.06800700
C	-0.14030700	0.58414300	-0.16952000
H	1.67158400	-0.13168600	-1.14578300
H	1.67985100	-0.25618600	0.62086000
H	-0.64513400	0.17370400	-1.04459500
H	-1.53652400	2.26769500	-0.04568600
H	3.19222400	1.63096000	-0.16151400
C	0.24413900	2.59700100	1.17533300
C	1.62997800	2.40717300	1.13962800
C	-0.35907000	3.15346600	2.29219800
C	2.41349400	2.77974700	2.22098700
C	0.43049800	3.53544400	3.37754600
H	-1.43478100	3.29467100	2.31624800

C	1.80810900	3.35008300	3.34162100
H	3.48794800	2.63129200	2.19405600
H	-0.03164900	3.98041000	4.25084200
H	2.41543900	3.65080800	4.18715400
C	0.20111800	2.73926700	-1.27109100
C	-0.44051500	3.42855600	-2.28854300
C	1.58892900	2.56271100	-1.30181000
C	0.31263100	3.95545400	-3.33855900
H	-1.51716900	3.55807100	-2.26389000
C	2.33649000	3.08194700	-2.34740700
C	1.69207300	3.78414800	-3.36700500
H	-0.18057600	4.50072600	-4.13441300
H	3.41248200	2.94497200	-2.37064200
H	2.27054600	4.19756600	-4.18472700
O	-0.62224900	-0.10974600	0.99428600
C	-1.95072300	-0.28567500	1.10078500
C	-2.29623300	-0.98095100	2.38784100
H	-1.76873100	-1.93367700	2.44482300
H	-1.96324000	-0.36693200	3.22620100
H	-3.37040600	-1.13783900	2.43664800
O	-2.73850600	0.07528000	0.26763700

<u>For Table 4 ($ROCOCH_3$): MP2/6-31+G(d)</u>

1

E = -497.944110

ZPVE = 0.192382

Symbol	X	Y	Z
C	-0.59646100	-0.92107200	-0.11311600
C	0.92780400	-0.83223300	-0.04391400
C	1.38590000	0.59895700	0.17027200
C	-0.67344600	1.19193300	1.21194100
C	-1.19942000	-0.23030900	1.11023800
H	2.45800700	0.68692300	0.35242100
H	1.29791800	-1.42021000	0.80591300
H	1.40037400	-1.22393900	-0.95164100
H	-0.95440800	-0.43375600	-1.02876800
H	-0.91045900	-1.97034100	-0.16218500
H	-0.99051300	1.68439700	2.13409300
H	-1.01249100	1.79433200	0.35799500
H	-0.92593700	-0.77734000	2.02192200
H	-2.29546600	-0.21050600	1.05425700
O	0.76815000	1.21997100	1.26858700
O	1.06161700	1.31691500	-1.05058400
C	1.80785600	2.43882400	-1.30465500
C	1.26736200	3.15725600	-2.50974500
H	1.13700400	2.45863900	-3.33997400
H	0.28655400	3.57875600	-2.26940000
H	1.95243200	3.95811500	-2.78879400
O	2.76687000	2.78724700	-0.63657700

2

E = -869.654448

ZPVE = 0.320025

Symbol	X	Y	Z
C	-1.94874500	0.30536900	0.34561700
C	-0.64833600	-0.49861900	0.33264800
C	0.55399800	0.34599600	-0.12710100
C	0.66415400	1.62940900	0.68710100
C	-0.64035800	2.41343600	0.78857000
C	-1.80623700	1.53523000	1.24313200
H	1.47097900	-0.22901400	0.08979100
H	-0.45718500	-0.86564000	1.35148000
H	-0.75213800	-1.38790100	-0.30131900
H	-2.20902700	0.62174400	-0.67495500
H	-2.77515400	-0.32619100	0.69692900
H	1.46654400	2.27820500	0.31790300
H	-0.48992700	3.25977400	1.46895600
H	-0.86502400	2.83956400	-0.19682200
H	-1.63856200	1.20788400	2.27806400
H	-2.73229600	2.12430900	1.24278300
Si	0.71717200	0.62647200	-2.01556300
C	-0.31117600	2.04003800	-2.73446600
H	0.00567000	3.01704600	-2.35289300
H	-0.17427200	2.05958900	-3.82329700
H	-1.38372500	1.93202800	-2.54206900
C	2.53526900	1.00885700	-2.35546000
H	2.70874100	1.17398600	-3.42545300
H	2.86551600	1.91105500	-1.82728800
H	3.18253900	0.18281600	-2.03841400
C	0.23765900	-0.97295000	-2.89486100
H	0.77259200	-1.83715300	-2.48396400
H	-0.83634200	-1.17555700	-2.81542800
H	0.48272100	-0.90884400	-3.96173900
O	1.05508600	1.21166900	2.04356000
C	1.74166100	2.12340000	2.77852500
C	2.04867900	1.57775900	4.14722900
H	1.12092600	1.49599800	4.72179500
H	2.48269800	0.57807200	4.06872500
H	2.73580100	2.25334200	4.65746600
O	2.05281900	3.23790400	2.37593500

3

E = -462.057158

ZPVE = 0.216736

Symbol	X	Y	Z

C	-4.17610400	-0.72998700	-0.12608000
C	-2.67034800	-0.57760700	-0.01581700
C	-2.25506500	0.87488700	0.15487400
C	-2.93760900	1.47933600	1.38574600
C	-4.45795800	1.33482500	1.30146900
C	-4.86021300	-0.12800600	1.10494100
H	-1.16484300	0.93896600	0.24207300
H	-2.27830700	-1.18092500	0.81231400
H	-4.51543500	-0.21454000	-1.03525600
H	-4.43048800	-1.79065000	-0.23954800
H	-2.57149500	0.97170700	2.28992200
H	-2.65624700	2.53484500	1.48457700
H	-4.92909400	1.73898300	2.20633100
H	-4.83272400	1.93049900	0.45644200
H	-4.57943500	-0.70531200	1.99788100
H	-5.94886600	-0.21720300	1.00471100
H	-2.55255100	1.42577700	-0.74884100
O	-2.11323000	-1.11179700	-1.25379600
C	-0.83111000	-1.55922900	-1.19324000
O	-0.15269500	-1.55762400	-0.17403000
C	-0.36976300	-2.03201800	-2.54496200
H	-1.12247400	-2.68085500	-2.99865000
H	-0.23155100	-1.16803200	-3.20212300
H	0.57709100	-2.56138800	-2.43583400

4

E = -462.056812

ZPVE = 0.216753

Symbol	X	Y	Z
C	-0.61593400	-0.86633000	-0.11257800
C	0.91290100	-0.81677700	-0.07882500
C	1.43088700	0.59601700	0.14122600
C	-0.71784800	1.20388500	1.32257100
C	-1.21511000	-0.23211600	1.14428100
H	2.52372900	0.61366600	0.20611000
H	1.28657400	-1.44159300	0.74536500
H	1.34080600	-1.21665200	-1.00610200
H	-0.97644600	-0.33046300	-1.00001100
H	-0.94919100	-1.90710000	-0.21208900
H	-1.12818500	1.64054000	2.24181500
H	-1.08098500	1.82055500	0.48963800
H	-0.93006900	-0.82709000	2.02499600
H	-2.31104500	-0.25162000	1.09287700
O	1.05042900	1.34269200	-1.05858400
C	1.78688300	2.44911200	-1.33970900
C	1.26546500	3.12963300	-2.57637300
H	1.15941300	2.40731100	-3.38942500
H	0.27626700	3.54971900	-2.37079500
H	1.95041500	3.92797700	-2.86291300
O	2.73415800	2.83183800	-0.66533500

C	0.81026800	1.25702200	1.36599200
H	1.17469100	2.28706000	1.44704500
H	1.17421700	0.72111200	2.25497200

5

E = -1089.932722

ZPVE = 0.298264

Symbol	X	Y	Z
C	-1.87690300	0.09928300	0.17569600
C	-0.48807900	-0.50903400	-0.03313100
C	0.55657600	0.53469100	-0.43918200
C	0.56041800	1.72899400	0.51034600
C	-0.82250300	2.31282100	0.76104600
C	-1.82235000	1.23969500	1.19377300
H	1.55532200	0.08047200	-0.41976800
H	-0.14900900	-0.96213800	0.90826600
H	-0.51716300	-1.31043800	-0.78239100
H	-2.27174200	0.47657900	-0.77718100
H	-2.56870900	-0.68177300	0.51577400
H	1.25215200	2.50371700	0.16586400
H	-0.73715000	3.10780500	1.51081700
H	-1.16276500	2.78494100	-0.17029400
H	-1.53101300	0.83996200	2.17470700
H	-2.81563400	1.68924700	1.31726800
S	0.24643400	1.06930400	-2.17036500
C	1.66737000	2.12516700	-2.37848100
C	1.50297600	3.51665000	-2.45215800
C	2.95365300	1.57274500	-2.48435200
C	2.61649400	4.34737600	-2.61585400
H	0.50468700	3.94235400	-2.37094600
C	4.06522500	2.40733800	-2.63208600
H	3.07913400	0.49153300	-2.45662700
C	3.89901300	3.79564500	-2.69888000
H	2.48125400	5.42587300	-2.66726400
H	5.05993600	1.97244400	-2.70903200
H	4.76491600	4.44350500	-2.81745700
O	1.09712700	1.18522900	1.75870400
C	1.72977700	2.07491900	2.57245600
C	2.25292900	1.38200600	3.80107700
H	1.42881000	0.90129600	4.33546700
H	2.96340600	0.60233100	3.51276500
H	2.74138000	2.11351800	4.44515000
O	1.84879000	3.26609100	2.32079400

6

E = -3090.030600

ZPVE = 0.297379

Symbol	X	Y	Z
C	-2.06575100	0.28159000	0.24841200
C	-0.92130200	-0.71769000	0.43158900
C	0.37605800	-0.23793100	-0.21454400
C	0.74529100	1.18251100	0.18336200
C	-0.40545000	2.17306100	0.07824500
C	-1.66585100	1.66092700	0.77674100
H	1.20452600	-0.90369700	0.05580800
H	-0.72542700	-0.84224300	1.50631000
H	-1.19029500	-1.70629600	0.03822300
H	-2.33673100	0.36067100	-0.81355600
H	-2.95724700	-0.08324000	0.77405500
H	1.61212700	1.53321100	-0.38238900
H	-0.07569900	3.13078500	0.49948900
H	-0.61227600	2.34412300	-0.98643300
H	-1.48723700	1.59874400	1.85890300
H	-2.48455000	2.37651700	0.62971600
C	2.08891100	0.14949500	-2.48176800
C	2.40583600	1.35205100	-3.12719500
C	3.11229100	-0.69571400	-2.03123500
C	3.74565800	1.71243500	-3.30774300
H	1.60864700	2.01113000	-3.46498600
C	4.44892100	-0.32654900	-2.20625200
H	2.86588100	-1.64540600	-1.55932300
C	4.76799500	0.87940900	-2.84140200
H	3.98919500	2.65113600	-3.80149500
H	5.24139900	-0.98386200	-1.85319000
H	5.80873500	1.16643600	-2.97532000
O	1.15491600	1.07778100	1.58698100
Se	0.25439600	-0.33531300	-2.19624000
C	2.22329400	1.84126400	1.94979300
C	2.59556400	1.57963100	3.38361100
H	1.70773900	1.62298000	4.01926200
H	3.02175400	0.57553000	3.47014800
H	3.33083000	2.31808300	3.70423300
O	2.80311500	2.61064700	1.19573000

7

E = -345.779930

ZPVE = 0.149573

Symbol	X	Y	Z
C	-0.86291400	1.58290700	0.10517800
H	-0.44849500	0.57031000	0.16289700
H	-1.95029700	1.49364400	0.20546700
C	-0.32775700	2.40000200	1.26159600
H	-0.74643900	3.41148900	1.27681500
H	0.76357000	2.48286000	1.23422900
C	-0.50534000	2.22625000	-1.23423600
H	0.57988700	2.30589900	-1.35686600

H	-0.89351700	1.63315500	-2.06729600
H	-0.92839500	3.23309300	-1.31417200
O	-0.71268800	1.71809600	2.48416700
C	-0.30841600	2.31970700	3.63368300
C	-0.75698000	1.53267200	4.83411400
H	-1.84637600	1.44104600	4.83212200
H	-0.33779100	0.52373500	4.79372000
H	-0.42501000	2.04000800	5.73988500
O	0.33373000	3.36106000	3.65988500

8

E = -801.889479

ZPVE = 0.248749

Symbol	X	Y	Z
C	-0.83989900	0.39042100	-0.75443900
C	-1.00791100	1.94616700	-0.54546200
H	-1.74952600	2.55386900	-1.07120800
C	-0.92007400	1.73667200	1.00243700
H	-1.55530200	2.22580200	1.74631000
C	-0.76342000	0.19179600	0.79677600
H	-1.30691200	-0.58756200	1.33686300
C	0.63581300	1.89762800	0.91834100
C	0.79484200	0.35022300	0.71161700
H	1.52739500	-0.27655000	1.22965600
C	0.70617900	0.55903500	-0.84130700
H	1.32508700	0.07018600	-1.59763400
C	0.54703900	2.10471600	-0.63176900
H	1.07405000	2.88660400	-1.18583700
C	-1.65594600	-0.39793500	-1.70195100
O	-2.88888600	-0.64837800	-1.18509800
O	-1.30362000	-0.75621100	-2.82071000
C	-3.78296800	-1.35388600	-2.07737500
H	-3.36489200	-2.32840500	-2.33553200
H	-4.70950100	-1.46297600	-1.51651700
H	-3.94191500	-0.77251800	-2.98744500
C	1.47261300	2.69912700	1.85005100
H	2.53601200	2.65729000	1.58351300
H	1.36333200	2.36431400	2.88908800
O	1.00960600	4.07231700	1.74229300
C	1.66708000	4.96356100	2.53330800
C	1.11655300	6.35002100	2.34479200
H	1.22835800	6.65409100	1.30051800
H	0.04958200	6.36144000	2.58296200
H	1.65366400	7.04037600	2.99525400
O	2.57926500	4.64883400	3.28498600

9

E = -578.291665

ZPVE = 0.279120

Symbol	X	Y	Z
C	-2.23263700	-1.62994000	0.07789300
C	-0.70679200	-1.65202700	0.08450400
C	-0.09901600	-0.27456100	0.47353200
C	-1.12408000	0.87056100	0.65975800
C	-2.55852100	0.42230300	0.47482500
C	-2.72408200	-0.86216000	1.32849400
H	0.47541400	-0.36991200	1.40055100
H	-0.36887500	-2.41441500	0.79849500
H	-0.33835300	-1.96642100	-0.89973100
H	-2.64975900	-2.62806200	-0.11706900
H	-1.01019800	1.30888100	1.65841900
H	-3.25096900	1.26006600	0.63308500
H	-2.10861600	-0.94133700	2.23455400
H	-3.76281000	-1.06868600	1.59566900
H	0.62496200	0.04496000	-0.28301800
C	-2.77221400	-0.45691700	-0.79240900
C	-4.26225300	-0.61701600	-1.09806800
H	-4.85415700	-0.87215800	-0.21425100
H	-4.66498700	0.31484100	-1.51431400
H	-4.41087700	-1.41043400	-1.84118900
C	-2.05069700	-0.11875800	-2.09190400
H	-0.97532700	0.01904800	-1.96795600
H	-2.21054500	-0.92366600	-2.82209900
H	-2.45023800	0.80873800	-2.51900800
O	-0.89595900	1.95216900	-0.29710200
C	0.15621800	2.76433500	-0.01858100
C	0.28649300	3.84161700	-1.06056800
H	0.51764900	3.38806100	-2.02894400
H	-0.65840200	4.38150600	-1.16296400
H	1.08463700	4.52609600	-0.77236600
O	0.89172900	2.61719500	0.94975900

10

E = -383.734737

ZPVE = 0.155708

Symbol	X	Y	Z
C	-1.91281300	1.00591600	-0.05431400
C	-0.42603600	1.02550300	0.18598600
C	-1.17555600	2.32056000	0.02930800
H	-2.27564700	0.68828600	-1.02652400
H	-2.55824700	0.73307000	0.77580700
H	0.23033900	0.71509400	-0.62060800
H	-0.06887000	0.77384700	1.18054700
H	-1.03358100	2.85648600	-0.90630500
C	-1.39699100	3.18587200	1.22721200
H	-2.22229000	3.89141400	1.08590000

H	-1.60587300	2.58820800	2.12111000
O	-0.17344600	3.94304300	1.44505300
C	-0.19099900	4.76233800	2.52850200
C	1.09991900	5.52553400	2.64256600
H	1.94873900	4.83910000	2.59487400
H	1.18681000	6.22300300	1.80442400
H	1.10874000	6.07710300	3.58274400
O	-1.14643900	4.85614200	3.28813300

11

E = -499.974937

ZPVE = 0.219050

Symbol	X	Y	Z
C	-1.48862200	1.03219600	0.41783000
C	-0.03170400	1.41504700	0.46388000
C	-1.07890200	2.47216300	0.23495400
H	-1.85609200	0.49321500	-0.44998000
H	-1.96994700	0.75880200	1.35242500
H	0.60282300	1.13496200	-0.37123300
H	0.46371400	1.40740400	1.43117800
H	-1.15274100	2.87685900	-0.77311600
C	-1.37234900	3.45358700	1.33017300
H	-1.32279000	2.96058100	2.30936700
C	-2.68732100	4.15943500	1.16945700
C	-3.92056900	3.56765500	1.80518100
C	-3.32322000	4.83591500	2.35760300
H	-2.82268400	4.64337400	0.20323800
H	-3.80127800	2.65932600	2.38885300
H	-4.85501800	3.62803400	1.25583000
H	-3.85176400	5.76873400	2.18575800
H	-2.79681000	4.77531000	3.30531700
O	-0.30232300	4.45688600	1.28327700
C	0.22362000	4.85367700	2.46990300
C	1.25732100	5.92549900	2.25503300
H	1.92601400	5.65118200	1.43599200
H	0.75489300	6.85842200	1.98124200
H	1.81956600	6.07316500	3.17748000
O	-0.11066100	4.40646400	3.56066600

12

E = -343.406628

ZPVE = 0.099287

Symbol	X	Y	Z
C	-1.65384300	0.33050300	-0.10904900
H	-2.40482700	-0.42832700	-0.07095800

C	-0.76947200	1.17181500	-0.15251600
C	0.23451300	2.22764600	-0.20714300
H	0.16059200	2.80641500	-1.13281200
H	0.13741100	2.91987900	0.63468400
O	1.53814400	1.58938200	-0.14909400
C	2.58333900	2.46312200	-0.19095200
C	3.89148900	1.72739600	-0.12508700
H	3.94477000	1.15000600	0.80166100
H	3.96422200	1.02562700	-0.96005800
H	4.70859200	2.44745300	-0.16652200
O	2.43792300	3.67472300	-0.27075500

13

E = -843.124677

ZPVE = 0.296354

Symbol	X	Y	Z
C	1.38126800	0.36285000	-0.29342300
C	2.09866800	1.73676900	-0.15731500
C	-0.47082800	2.08717700	-0.12090400
C	-0.14249800	0.57205000	-0.21268400
H	1.65758100	-0.09668900	-1.24969700
H	1.69006200	-0.31111000	0.51397000
H	-0.67968800	0.12573600	-1.05650900
H	-1.55310100	2.25221100	-0.11021700
H	3.18998400	1.62156700	-0.16715100
C	0.21064800	2.56898100	1.13304700
C	1.60253600	2.37097600	1.11882700
C	-0.41930100	3.09811600	2.26034200
C	2.37049400	2.71008100	2.23450300
C	0.35417500	3.45463000	3.37338900
H	-1.49965400	3.24588300	2.26610200
C	1.74142000	3.25710700	3.36142600
H	3.44949600	2.55454100	2.22884800
H	-0.12418300	3.88165300	4.25302000
H	2.33458300	3.53450800	4.23088900
C	0.20342500	2.73945000	-1.30079900
C	-0.43259100	3.43990400	-2.32765300
C	1.59992300	2.57539800	-1.30827000
C	0.33818900	3.98929800	-3.36117400
H	-1.51551000	3.56218100	-2.32039600
C	2.36569400	3.11326800	-2.34386500
C	1.72987000	3.82884900	-3.36807700
H	-0.14665600	4.54374600	-4.16241000
H	3.44809500	2.98443800	-2.35291300
H	2.32017500	4.25955600	-4.17472100
O	-0.57423700	-0.09939900	1.00490200
C	-1.91537000	-0.24813800	1.17053000
C	-2.21181500	-0.87229400	2.50574800
H	-1.63085800	-1.78958300	2.63185000
H	-1.91694800	-0.17863300	3.29928600

H	-3.27883400	-1.08552300	2.57463100
O	-2.74770900	0.09676700	0.34105200

For Table 4 (ROC(O)OH): B3LYP/6-311++G(d,p)

1

E = -535.574128

ZPVE = 0.165853

Symbol	X	Y	Z
C	-0.59151200	-0.94517700	-0.09710200
C	0.93394700	-0.78907500	-0.05235500
C	1.35052100	0.65858000	0.18505900
C	-0.73684300	1.17215700	1.23751200
C	-1.21728300	-0.27094000	1.13108800
H	2.41590500	0.76624500	0.37708700
H	1.34374700	-1.37525300	0.77713500
H	1.40376400	-1.14852900	-0.97102800
H	-0.98132100	-0.48367000	-1.01022300
H	-0.85758100	-2.00503400	-0.13606300
H	-1.05692400	1.64089800	2.16829600
H	-1.11755300	1.76910400	0.40082800
H	-0.93512100	-0.81352100	2.04060300
H	-2.31030800	-0.28264700	1.07135400
O	0.70238000	1.25933900	1.26023800
O	1.04403500	1.39163500	-1.04633700
C	1.86762300	2.38794200	-1.38059000
O	2.90827800	2.68553900	-0.85203300
O	1.34664000	3.01893100	-2.45168500
H	1.96792300	3.72227500	-2.68275400

2

E = -908.267708

ZPVE = 0.290314

Symbol	X	Y	Z
C	-2.08247100	0.62492200	0.35633900
C	-0.88984700	-0.34105300	0.28577400
C	0.43233400	0.35232500	-0.13134600
C	0.69957500	1.59795900	0.71825400
C	-0.49714700	2.54471300	0.82666800
C	-1.77798800	1.82273600	1.26547400
H	1.25355200	-0.34290700	0.09518700
H	-0.75009400	-0.79257600	1.27468800
H	-1.11529800	-1.16768900	-0.39529100
H	-2.33424900	0.98744500	-0.64667000
H	-2.96486700	0.09047800	0.72291500
H	1.57871300	2.14128800	0.37249900

H	-0.24713400	3.35947900	1.51144300
H	-0.64850100	3.00318800	-0.15708300
H	-1.66115900	1.47502200	2.29759600
H	-2.61579700	2.52688500	1.26427300
Si	0.69630200	0.59378000	-2.02370500
C	-0.60929200	1.64162600	-2.90632400
H	-0.67146700	2.65844900	-2.50911700
H	-0.35215400	1.72277400	-3.96791800
H	-1.60618000	1.19673500	-2.84595100
C	2.39031900	1.39281400	-2.28966100
H	2.64180400	1.40324700	-3.35504200
H	2.42195700	2.42855000	-1.93890500
H	3.18210900	0.84335200	-1.77104300
C	0.70155000	-1.12973500	-2.80183000
H	1.45615100	-1.77517700	-2.34190400
H	-0.26676800	-1.62902900	-2.70420100
H	0.92940700	-1.06576200	-3.87053400
O	1.03157100	1.10758100	2.07534400
C	1.85928200	1.84890600	2.79838300
O	2.39043500	2.88535700	2.47559300
O	2.03593400	1.24974700	3.99602500
H	2.64556900	1.81199700	4.49181900

3

E = -499.640710

ZPVE = 0.189589

Symbol	X	Y	Z
C	-4.15923300	-0.73442300	-0.13441800
C	-2.64826000	-0.57073800	-0.02047000
C	-2.23760800	0.88835400	0.16518300
C	-2.93928000	1.49506500	1.39147900
C	-4.46390900	1.33868700	1.30389000
C	-4.86287900	-0.12862700	1.09068800
H	-1.15169200	0.95490700	0.27124100
H	-2.25743400	-1.17394500	0.80275300
H	-4.49850500	-0.23134000	-1.04720300
H	-4.40670900	-1.79439200	-0.24128600
H	-2.57421700	1.00026400	2.30030700
H	-2.66717100	2.55063200	1.48426900
H	-4.93636900	1.72972000	2.21046300
H	-4.84241400	1.94149700	0.46854600
H	-4.60147500	-0.70878100	1.98484700
H	-5.94674900	-0.21705800	0.97115700
H	-2.51649300	1.44471400	-0.73753000
O	-2.07580900	-1.09788200	-1.25797800
C	-0.85285100	-1.61202300	-1.18922600
O	-0.15660300	-1.71611800	-0.20794000
O	-0.49350400	-2.02157000	-2.42301200
H	0.39464000	-2.39226600	-2.33765200

4

E = -499.639681

ZPVE = 0.189676

Symbol	X	Y	Z
C	-0.59680100	-0.90486000	-0.12385300
C	0.93478300	-0.80030200	-0.07216300
C	1.42038700	0.63004000	0.15195000
C	-0.79057900	1.18931200	1.29124300
C	-1.24583200	-0.26643900	1.11275400
H	2.50449500	0.66274100	0.26567000
H	1.31848600	-1.40557100	0.75816500
H	1.38499200	-1.19519900	-0.98726400
H	-0.96119700	-0.40325700	-1.02662500
H	-0.88909300	-1.95610700	-0.20850000
H	-1.22220400	1.61580700	2.20197300
H	-1.16507600	1.79076000	0.45561700
H	-0.97403400	-0.84434500	2.00635300
H	-2.33634900	-0.31324300	1.03208700
O	1.09474000	1.36945100	-1.07499200
C	1.87540900	2.39694200	-1.38588700
O	2.84237800	2.79214300	-0.77989000
O	1.41420600	2.95256400	-2.52595500
H	2.00349400	3.69194200	-2.72492800
C	0.74032100	1.29755000	1.34904100
H	1.06356100	2.33971900	1.41641000
H	1.11284700	0.79773900	2.25187700

5

E = -1128.873501

ZPVE = 0.271134

Symbol	X	Y	Z
C	-1.85547700	-0.01981300	0.15465100
C	-0.40370100	-0.46725800	-0.07067400
C	0.54617400	0.70481700	-0.36369900
C	0.41574600	1.82701300	0.67597300
C	-1.02969800	2.24023500	0.95300400
C	-1.93952700	1.04223600	1.25978400
H	1.57783700	0.35025800	-0.36328400
H	-0.03710000	-0.96151700	0.83586800
H	-0.34079700	-1.19848900	-0.88079700
H	-2.27065400	0.38385700	-0.77640300
H	-2.46724000	-0.88843800	0.41646900
H	1.01532800	2.69037000	0.38967900
H	-1.03865600	2.96718800	1.76919200
H	-1.39328300	2.76262000	0.06225000
H	-1.64626100	0.59482000	2.21606000

H	-2.97076700	1.38806600	1.37828100
S	0.22871500	1.35370000	-2.08112600
C	1.74823500	2.26081800	-2.39985000
C	1.72095700	3.65624300	-2.48242300
C	2.95061400	1.58055100	-2.62533600
C	2.88604000	4.36339000	-2.77887400
H	0.78930400	4.18301300	-2.31411100
C	4.11457000	2.29163000	-2.90608100
H	2.96921700	0.49734300	-2.59106600
C	4.08440700	3.68412600	-2.98552400
H	2.85552300	5.44541100	-2.84063700
H	5.04244600	1.75703400	-3.07651600
H	4.99030100	4.23522700	-3.21096900
O	1.01477300	1.27145600	1.89876700
C	1.58481800	2.13287000	2.73548600
O	1.67001600	3.32967400	2.60703600
O	2.07392200	1.44231300	3.78627200
H	2.48234300	2.09311500	4.37224800

6

E = -3132.205953

ZPVE = 0.269862

Symbol	X	Y	Z
C	-2.01217700	0.13783000	0.30724700
C	-0.73857400	-0.71391500	0.41095400
C	0.48910900	-0.02583500	-0.19936900
C	0.67799000	1.40222200	0.32183100
C	-0.59838100	2.24349900	0.28599500
C	-1.79733300	1.52716200	0.92373400
H	1.38994900	-0.60211300	0.01057400
H	-0.51684500	-0.89391800	1.46968400
H	-0.88304500	-1.69251500	-0.05391300
H	-2.30763500	0.24329200	-0.74415500
H	-2.83733500	-0.37625900	0.80929400
H	1.48734100	1.90627000	-0.20457600
H	-0.40271200	3.20233300	0.77283100
H	-0.81276700	2.46265200	-0.76497300
H	-1.63033800	1.42226000	2.00154100
H	-2.69529600	2.14059700	0.80351700
C	2.25107600	0.17843900	-2.60621200
C	2.73736800	1.40499100	-3.06638900
C	3.12223300	-0.90755700	-2.47370800
C	4.08897900	1.54544400	-3.38271800
H	2.06260600	2.24542900	-3.17522700
C	4.47344900	-0.75896500	-2.78103200
H	2.74252400	-1.86606800	-2.13982500
C	4.95834400	0.46668600	-3.23693600
H	4.46019300	2.50035700	-3.73765100
H	5.14455000	-1.60397300	-2.67376300

H	6.00891100	0.57859800	-3.48002500
O	1.11398500	1.23331500	1.71931600
Se	0.36074200	-0.02912300	-2.21032500
C	1.90957700	2.17294800	2.21957900
O	2.32059900	3.15884900	1.65772400
O	2.20186300	1.84608400	3.49570000
H	2.78136600	2.54403400	3.82851200

7

E = -382.937501

ZPVE = 0.123867

Symbol	X	Y	Z
C	-0.85944300	1.58718600	0.12084100
H	-0.44780400	0.57518100	0.18262100
H	-1.94481300	1.49455700	0.22481200
C	-0.32212000	2.40900400	1.27816200
H	-0.74004600	3.41876300	1.28999100
H	0.76712600	2.49271300	1.24794700
C	-0.50972000	2.21868700	-1.23036100
H	0.57287300	2.29867900	-1.36728700
H	-0.90306100	1.61593100	-2.05188700
H	-0.93275200	3.22331500	-1.32480100
O	-0.70112800	1.73648700	2.50694000
C	-0.30751200	2.32217700	3.63398200
O	0.32556200	3.34456300	3.73320200
O	-0.73520700	1.57952400	4.67365100
H	-0.43426900	2.03032900	5.47343100

8

E = -840.467981

ZPVE = 0.223262

Symbol	X	Y	Z
C	-0.83542200	0.36211600	-0.75849100
C	-1.03642100	1.91573900	-0.53652200
H	-1.79352000	2.51423200	-1.03777100
C	-0.91388400	1.71659000	1.01173000
H	-1.55856900	2.17964400	1.75591700
C	-0.72016100	0.17535500	0.80487800
H	-1.22354800	-0.60921800	1.36539800
C	0.64227300	1.92535700	0.90833000
C	0.83219900	0.37616600	0.69608100
H	1.58092000	-0.23713500	1.19555200
C	0.70941500	0.57359000	-0.85728900
H	1.33980000	0.10585500	-1.60940300
C	0.51421100	2.11785700	-0.64794300

H	1.00199000	2.90177800	-1.22384600
C	-1.64206700	-0.48006300	-1.67899600
O	-2.93930300	-0.51704700	-1.29299200
O	-1.22189800	-1.06014400	-2.65342300
C	-3.82391000	-1.29407400	-2.12117600
H	-3.50452100	-2.33690800	-2.14780500
H	-4.80563700	-1.20581100	-1.66085500
H	-3.83984400	-0.89961100	-3.13823000
C	1.48883900	2.73357400	1.83221900
H	2.54381300	2.70509000	1.54355800
H	1.40800800	2.38413900	2.86588500
O	1.02500500	4.11001700	1.76790900
C	1.67531900	4.97490700	2.54222800
O	2.59739700	4.72928200	3.28025500
O	1.13119200	6.19482900	2.37003200
H	1.62355100	6.79736600	2.94288500

9

E = -616.293919

ZPVE = 0.250792

Symbol	X	Y	Z
C	-2.24020800	-1.64005300	0.09495300
C	-0.70862200	-1.68515500	0.10821300
C	-0.06946700	-0.29568200	0.42461400
C	-1.08443300	0.86282500	0.63396100
C	-2.53323100	0.43480900	0.45121200
C	-2.72539300	-0.83481300	1.33115800
H	0.55831600	-0.36728900	1.31402800
H	-0.38758500	-2.41350400	0.85944800
H	-0.34053300	-2.05388900	-0.85339800
H	-2.66533600	-2.63390800	-0.07307100
H	-0.96209400	1.28336400	1.63310600
H	-3.20531200	1.28422500	0.59731600
H	-2.12328600	-0.90835000	2.24133700
H	-3.76711700	-1.01496400	1.58997100
H	0.60258400	-0.00657900	-0.38503700
C	-2.77221700	-0.47221300	-0.80884400
C	-4.27341700	-0.61563000	-1.10402600
H	-4.86748600	-0.84197800	-0.21652300
H	-4.66601400	0.30919500	-1.53875700
H	-4.44166300	-1.41928200	-1.82822900
C	-2.05562200	-0.16862300	-2.12648500
H	-0.97866300	-0.04700800	-2.02336100
H	-2.23574100	-0.97810900	-2.84258100
H	-2.44119700	0.75506900	-2.56729500
O	-0.83154900	1.96105800	-0.30453300
C	0.12036100	2.82278300	0.03275400
O	0.80690000	2.80158300	1.02617500
O	0.20902800	3.76144600	-0.93267000

H	0.90775200	4.36902400	-0.65662900

10

E = -421.008333

ZPVE = 0.129812

Symbol	X	Y	Z
C	-1.91205000	1.01208500	-0.05515600
C	-0.42187400	1.01676800	0.17427800
C	-1.16442100	2.32222500	0.04256800
H	-2.28614100	0.71609000	-1.02729100
H	-2.55219200	0.72811900	0.77250600
H	0.22635000	0.71895600	-0.64042200
H	-0.05869500	0.74141200	1.15772500
H	-1.02445100	2.86908400	-0.88395000
C	-1.38486400	3.18633800	1.24529800
H	-2.22340600	3.87326900	1.10889100
H	-1.57294800	2.59063400	2.14182500
O	-0.18062800	3.97689700	1.45743400
C	-0.20588400	4.79236600	2.50660500
O	-1.11010400	4.92711000	3.29493200
O	0.96267000	5.46139700	2.55825300
H	0.91133100	6.04098500	3.32957800

11

E = -537.675670

ZPVE = 0.191668

Symbol	X	Y	Z
C	-1.47837300	1.03985100	0.40136700
C	-0.01916500	1.41531700	0.46503200
C	-1.06145100	2.48351400	0.25056600
H	-1.84463500	0.52456600	-0.47808800
H	-1.96407300	0.74347000	1.32370300
H	0.61902000	1.15556500	-0.37050200
H	0.47078600	1.37519000	1.43123800
H	-1.12472700	2.90221400	-0.74908600
C	-1.37335900	3.46518400	1.34896300
H	-1.31958300	2.97824300	2.32498200
C	-2.69966100	4.16204400	1.18575000
C	-3.93756400	3.56991500	1.81696400
C	-3.35148500	4.84733700	2.36259100
H	-2.83171700	4.63564800	0.21763600
H	-3.82547700	2.67075300	2.41152900
H	-4.86328800	3.61896300	1.25681200
H	-3.87748400	5.77569600	2.17621800
H	-2.84131400	4.80089500	3.31716800

O	-0.31010100	4.48593700	1.31354900
C	0.25027200	4.83137600	2.46406500
O	0.01215100	4.38684700	3.56313800
O	1.17060600	5.78706400	2.22030400
H	1.56097400	6.01079200	3.07532500

12

E = -380.486904

ZPVE = 0.076388

Symbol	X	Y	Z
C	-1.61843400	0.33757800	-0.10866600
H	-2.37586300	-0.40709300	-0.06967900
C	-0.75542500	1.17080300	-0.15195100
C	0.25082000	2.21713300	-0.20727800
H	0.16748700	2.79444100	-1.13138600
H	0.14519100	2.90920900	0.63179500
O	1.56256100	1.60063800	-0.15062900
C	2.58164300	2.46188500	-0.19101200
O	2.49911600	3.66253300	-0.26758000
O	3.72772800	1.76435400	-0.13158100
H	4.44653400	2.40962500	-0.16241000

13

E = -881.909510

ZPVE = 0.272128

Symbol	X	Y	Z
C	1.38706900	0.36489900	-0.14872300
C	2.11640800	1.74618000	-0.11254000
C	-0.45052300	2.11415000	-0.00825100
C	-0.14154100	0.59018600	-0.12688100
H	1.67753700	-0.18603100	-1.04541200
H	1.66992800	-0.23026300	0.72103000
H	-0.63044600	0.19663600	-1.01684000
H	-1.52611000	2.28469900	0.02773800
H	3.19911500	1.61808100	-0.15431300
C	0.27763100	2.63182800	1.21822700
C	1.66592400	2.44103500	1.15910400
C	-0.29994800	3.23631800	2.32788900
C	2.47450200	2.85513000	2.21082300
C	0.51444800	3.65984300	3.38187300
H	-1.37439900	3.38126700	2.37520200
C	1.89367700	3.47004300	3.32374900
H	3.54877200	2.70604900	2.16793700
H	0.07034700	4.13788500	4.24777500
H	2.52011900	3.80144300	4.14438100
C	0.19432100	2.73966900	-1.23414000

C	-0.45853900	3.43242700	-2.24656200
C	1.58304200	2.54772300	-1.28758200
C	0.28260700	3.94802500	-3.31408100
H	-1.53349400	3.57495200	-2.20711100
C	2.31791800	3.05609300	-2.35185300
C	1.66241400	3.76128500	-3.36591100
H	-0.21937600	4.49557900	-4.10379300
H	3.39256200	2.91023100	-2.39528600
H	2.23167600	4.16506800	-4.19574000
O	-0.66722700	-0.14221900	1.01814400
C	-1.96429900	-0.43734100	0.99657100
O	-2.76069600	-0.15695600	0.13322700
O	-2.26237100	-1.12270100	2.11707500
H	-3.20742800	-1.31933700	2.07305900

<u>For Table 4 (ROC(O)OH): M06-2X/6-311++G(d,p)</u>

1

E = -535.358427

ZPVE = 0.168587

Symbol	X	Y	Z
C	-0.58539100	-0.93242200	-0.10793700
C	0.93869700	-0.83452100	-0.03261200
C	1.38305600	0.60517100	0.16545500
C	-0.67333500	1.19846500	1.18330800
C	-1.19443700	-0.22880300	1.10599400
H	2.45208500	0.69808500	0.34757500
H	1.30742800	-1.40321000	0.82614000
H	1.41625300	-1.23106800	-0.93037900
H	-0.93594000	-0.45132900	-1.02618200
H	-0.89349100	-1.97900100	-0.14893500
H	-0.99939100	1.70193900	2.09250300
H	-1.02188900	1.77703400	0.32011000
H	-0.91923000	-0.76094000	2.02251700
H	-2.28554800	-0.21205600	1.04609000
O	0.75475500	1.23653400	1.22903600
O	1.07018900	1.29770000	-1.06439900
C	1.79493600	2.38244900	-1.32861700
O	2.75254000	2.77296500	-0.72438900
O	1.28423200	2.97505700	-2.41454800
H	1.83480000	3.74675100	-2.59170000

2

E = -907.954889

ZPVE = 0.294086

Symbol	X	Y	Z

C	-2.02989800	0.83488700	0.32536300
C	-0.95788200	-0.25905200	0.26697700
C	0.42659700	0.28563100	-0.14268900
C	0.82217600	1.47946500	0.71705500
C	-0.24803700	2.56482300	0.76129700
C	-1.59300100	1.99700100	1.21922200
H	1.17190600	-0.49568200	0.06132700
H	-0.87528900	-0.71983900	1.25726700
H	-1.26871500	-1.05243000	-0.42092100
H	-2.23308500	1.21708400	-0.67928700
H	-2.96614000	0.40843900	0.69518800
H	1.77903500	1.89980700	0.40258300
H	0.08758500	3.37527000	1.41199200
H	-0.34103300	2.98286400	-0.24815200
H	-1.50069400	1.64695900	2.25248200
H	-2.34903600	2.78590100	1.21537400
Si	0.65103200	0.56400700	-2.01730700
C	-0.81166300	1.36301500	-2.89323900
H	-1.06551500	2.34709600	-2.49297800
H	-0.55938400	1.49061100	-3.95038000
H	-1.70399900	0.73398700	-2.84309300
C	2.17867200	1.62548800	-2.29686100
H	2.41722600	1.67422800	-3.36273500
H	2.03154900	2.65025900	-1.94454100
H	3.05103700	1.21629500	-1.77975500
C	0.91253100	-1.13646900	-2.77715300
H	1.81041600	-1.61454600	-2.37726000
H	0.06453600	-1.79674200	-2.57585300
H	1.02548300	-1.06526800	-3.86213200
O	1.01747900	0.95701200	2.06697100
C	1.76836500	1.68308100	2.87494200
O	2.32170000	2.71808100	2.61265200
O	1.83237500	1.07617400	4.06840600
H	2.38982000	1.62999300	4.62698600

3

E = -499.427811

ZPVE = 0.192222

Symbol	X	Y	Z
C	-4.18561100	-0.73401700	-0.13276900
C	-2.67658100	-0.60905700	-0.01463300
C	-2.23809600	0.83904100	0.15286000
C	-2.91560300	1.45512200	1.38067400
C	-4.43861800	1.33954800	1.28637700
C	-4.86486200	-0.11780600	1.09354900
H	-1.15093700	0.88484900	0.24429100
H	-2.30764100	-1.20640300	0.82489800
H	-4.50582400	-0.21141200	-1.04093100
H	-4.45709900	-1.78595600	-0.24764900
H	-2.56773200	0.93776800	2.28260800

H	-2.61516800	2.50045500	1.48192300
H	-4.90659900	1.75498600	2.18237600
H	-4.79307300	1.93378600	0.43576300
H	-4.59378700	-0.69387500	1.98633800
H	-5.94982700	-0.19008700	0.98917400
H	-2.52752100	1.39029700	-0.74929700
O	-2.12324600	-1.16360500	-1.23023300
C	-0.86080100	-1.55406700	-1.17603400
O	-0.13600100	-1.51777500	-0.21783100
O	-0.50021700	-2.01553300	-2.37997000
H	0.42032100	-2.29158300	-2.30337700

4

E = -499.427560

ZPVE = 0.192370

Symbol	X	Y	Z
C	-0.58625900	-0.89254800	-0.13146100
C	0.94126200	-0.83680000	-0.04680800
C	1.44608100	0.58644700	0.14275500
C	-0.74490800	1.21806900	1.23557100
C	-1.22818500	-0.22674400	1.08795000
H	2.53212600	0.60916100	0.24774500
H	1.28660900	-1.42443300	0.81095900
H	1.39941700	-1.26430900	-0.94172600
H	-0.91203200	-0.37663400	-1.04018000
H	-0.91212800	-1.93197000	-0.21729000
H	-1.18613700	1.68243900	2.12076700
H	-1.07900300	1.79924500	0.36958600
H	-0.96327700	-0.79068300	1.99120800
H	-2.31745500	-0.25474700	1.00397200
O	1.11201900	1.28850100	-1.08422400
C	1.79672200	2.39082900	-1.33556900
O	2.67961000	2.85926700	-0.66803000
O	1.35195700	2.92244600	-2.48175400
H	1.87284400	3.71917600	-2.63472800
C	0.78175200	1.28074000	1.32767600
H	1.13886700	2.31091200	1.39047900
H	1.11905200	0.76902200	2.23618500

5

E = -1128.540522

ZPVE = 0.274848

Symbol	X	Y	Z
C	-1.84860400	0.08815800	0.16535100
C	-0.44683700	-0.49361500	-0.03766400
C	0.57932900	0.57949100	-0.41424600

C	0.55989200	1.74790800	0.57231100
C	-0.83729300	2.30314600	0.82240500
C	-1.82326900	1.20068000	1.21589800
H	1.58269400	0.14894200	-0.41927500
H	-0.10921700	-0.95054800	0.89823300
H	-0.45151100	-1.27578800	-0.80035700
H	-2.22744600	0.48766300	-0.78183600
H	-2.53191300	-0.70768300	0.47103700
H	1.23964600	2.53790500	0.24778700
H	-0.77404700	3.07905300	1.58816500
H	-1.16912100	2.78563400	-0.10186400
H	-1.52940900	0.77709900	2.18231000
H	-2.82024200	1.62841700	1.34403500
S	0.24131700	1.15809100	-2.12760100
C	1.68872900	2.17052900	-2.39472900
C	1.55895700	3.55590200	-2.48385300
C	2.94696800	1.58274900	-2.53283100
C	2.68176000	4.34808800	-2.70529500
H	0.57925700	4.00609700	-2.37422700
C	4.06765600	2.37860400	-2.73908700
H	3.04067900	0.50364700	-2.48646800
C	3.93640300	3.76187000	-2.82791200
H	2.57458600	5.42410300	-2.77318100
H	5.04266500	1.91725300	-2.84244400
H	4.81045400	4.37995800	-2.99437100
O	1.09323200	1.18579200	1.80093100
C	1.60115100	2.04771100	2.66793700
O	1.67458900	3.23933100	2.53904400
O	2.03588400	1.37188900	3.73916100
H	2.40118600	2.02580500	4.34628600

6

E = -3131.906100

ZPVE = 0.273762

Symbol	X	Y	Z
C	-1.97696500	0.21698500	0.29005100
C	-0.77361400	-0.71655100	0.44478800
C	0.48716700	-0.14928400	-0.20978700
C	0.78104500	1.27393000	0.25992300
C	-0.42457800	2.20320700	0.17086000
C	-1.65647800	1.60353600	0.85323800
H	1.34936300	-0.77858200	0.01475000
H	-0.55681000	-0.84328300	1.51126100
H	-0.98700400	-1.70679600	0.03615500
H	-2.24980100	0.30521800	-0.76824800
H	-2.84055700	-0.21165700	0.80401700
H	1.63498900	1.69091200	-0.27689500
H	-0.15501100	3.16792400	0.60579000
H	-0.63212500	2.37298100	-0.88964600

H	-1.47239900	1.51937000	1.92968800
H	-2.50895300	2.27471000	0.72606700
C	2.16587700	0.12673000	-2.57510100
C	2.57407200	1.38743500	-3.00829600
C	3.10403100	-0.89475300	-2.42537800
C	3.91757500	1.62568900	-3.28470800
H	1.84172900	2.17787600	-3.12318500
C	4.44627300	-0.64925700	-2.69456100
H	2.77982800	-1.87823100	-2.10524600
C	4.85378200	0.60999100	-3.12540700
H	4.23087300	2.60762800	-3.61879800
H	5.17242400	-1.44469500	-2.57515600
H	5.89943400	0.79809900	-3.33779000
O	1.17247600	1.11705800	1.65215800
Se	0.30832700	-0.20480000	-2.18486200
C	1.90479600	2.09130100	2.16827000
O	2.28298300	3.08291700	1.60595300
O	2.17119200	1.79625600	3.44712900
H	2.70637700	2.52118400	3.79020500

7

E = -382.771573

ZPVE = 0.125753

Symbol	X	Y	Z
C	-0.86400200	1.57849600	0.12525500
H	-0.45070900	0.56849800	0.18374600
H	-1.94832200	1.48909500	0.22820500
C	-0.32824000	2.39490900	1.28111900
H	-0.74541600	3.40504800	1.29144100
H	0.76097800	2.47873700	1.24786800
C	-0.50565300	2.22590200	-1.21035100
H	0.57732400	2.30599000	-1.33184900
H	-0.89221200	1.63836200	-2.04369700
H	-0.92652100	3.23142000	-1.28665500
O	-0.70487400	1.72531800	2.49640500
C	-0.31107600	2.31823800	3.61213300
O	0.31635300	3.33915300	3.69093200
O	-0.72600700	1.59408800	4.65750100
H	-0.42393600	2.05384100	5.44919000

8

E = -840.150437

ZPVE = 0.227198

Symbol	X	Y	Z
C	-0.82209300	0.37039800	-0.74627800

C	-1.02579600	1.90902600	-0.51921900
H	-1.78658900	2.50510300	-1.01499900
C	-0.89579600	1.70154700	1.02075900
H	-1.52939000	2.16360000	1.77324500
C	-0.70521500	0.16799000	0.80292000
H	-1.21005400	-0.62111200	1.35335500
C	0.64930100	1.90325000	0.90736100
C	0.84098900	0.36707600	0.68990800
H	1.59188400	-0.24493800	1.18445900
C	0.71194100	0.57412900	-0.85533600
H	1.33098900	0.10740400	-1.61603300
C	0.51844900	2.11075600	-0.63531400
H	1.00658400	2.90117300	-1.19966500
C	-1.63827100	-0.46834100	-1.65822700
O	-2.93034500	-0.46667200	-1.28576900
O	-1.22572400	-1.07555900	-2.61087600
C	-3.80553300	-1.24136100	-2.10678200
H	-3.49848800	-2.28754700	-2.10621300
H	-4.79503400	-1.13155400	-1.67123100
H	-3.79248200	-0.86869200	-3.13135200
C	1.48625000	2.72450200	1.82463000
H	2.54044900	2.70927100	1.53339900
H	1.40903200	2.38099900	2.86021300
O	0.99691600	4.07574300	1.74168000
C	1.63233000	4.95063400	2.50680000
O	2.55303800	4.71374900	3.23990300
O	1.08158900	6.15668300	2.33413600
H	1.56629700	6.76621400	2.90264100

9

E = -616.037888

ZPVE = 0.254491

Symbol	X	Y	Z
C	-2.22555600	-1.62649800	0.07996400
C	-0.69857600	-1.63223200	0.08619300
C	-0.10600100	-0.25125400	0.48692500
C	-1.14306000	0.88676100	0.66368500
C	-2.57489600	0.42159700	0.48499000
C	-2.72702100	-0.86710600	1.33249400
H	0.45114100	-0.34357100	1.41950800
H	-0.35193300	-2.39222000	0.79128200
H	-0.33119900	-1.92925200	-0.89924200
H	-2.63129000	-2.62173300	-0.11850500
H	-1.03137800	1.32743100	1.65678700
H	-3.27174400	1.24814200	0.64189500
H	-2.11278300	-0.94190900	2.23385700
H	-3.76098200	-1.08402700	1.58975600
H	0.62639600	0.07250400	-0.25459300
C	-2.77062000	-0.45378500	-0.78905100

C	-4.25582700	-0.62543000	-1.10786800
H	-4.85033600	-0.88689200	-0.23096800
H	-4.66155100	0.30093500	-1.52434100
H	-4.39108800	-1.41582000	-1.85176500
C	-2.03398800	-0.09746300	-2.07534500
H	-0.96135200	0.03319800	-1.93849600
H	-2.18928600	-0.88685500	-2.81778700
H	-2.42191000	0.83727000	-2.48769000
O	-0.92886900	1.95969700	-0.28865400
C	0.12185200	2.72645500	-0.05489500
O	0.90166500	2.61605900	0.85341200
O	0.19197400	3.66894900	-1.00373700
H	0.96697200	4.20540200	-0.80100500

10

E = -420.836067

ZPVE = 0.131949

Symbol	X	Y	Z
C	-1.90284800	1.01889600	-0.03298400
C	-0.41673700	1.04999900	0.18673800
C	-1.17659400	2.33405500	0.02695500
H	-2.27198300	0.69165000	-0.99512000
H	-2.53231900	0.75299900	0.80716500
H	0.22666800	0.73947100	-0.62481600
H	-0.04684000	0.81457300	1.17689300
H	-1.04888600	2.86869900	-0.90665200
C	-1.38752900	3.19783800	1.22810800
H	-2.21904600	3.89362600	1.09732700
H	-1.58139700	2.59478100	2.11911800
O	-0.18289600	3.96063200	1.43861900
C	-0.20586200	4.76162500	2.49123600
O	-1.11417600	4.89002000	3.26698900
O	0.95770000	5.41774400	2.56362900
H	0.90543800	5.98712700	3.33987000

11

E = -537.457172

ZPVE = 0.194674

Symbol	X	Y	Z
C	-1.52804600	1.05384000	0.40259300
C	-0.06009000	1.37655300	0.45295800
C	-1.06131300	2.47083200	0.23084000
H	-1.91127100	0.53902400	-0.46776300
H	-2.01870700	0.79575600	1.33278000
H	0.55895800	1.07898800	-0.38216100

H	0.43023200	1.34247600	1.41827600
H	-1.11916400	2.89274800	-0.76653100
C	-1.32483400	3.44827900	1.33922500
H	-1.28657900	2.93882300	2.30705300
C	-2.63397600	4.17225400	1.19427500
C	-3.86437500	3.55723300	1.79808600
C	-3.27549900	4.80271900	2.39893500
H	-2.75567000	4.68379300	0.24536500
H	-3.74406600	2.63189900	2.34769200
H	-4.79088600	3.63766800	1.24625200
H	-3.80437900	5.73504200	2.25394100
H	-2.75328300	4.70821100	3.34207300
O	-0.23972600	4.41438900	1.30133600
C	0.18069300	4.89140100	2.45903600
O	-0.19971600	4.57650900	3.55611200
O	1.13669400	5.79963700	2.22798900
H	1.42535600	6.11830700	3.09086200

12

E = -380.337282

ZPVE = 0.078054

Symbol	X	Y	Z
C	-1.60957700	0.34315900	-0.11005900
H	-2.36825600	-0.40211300	-0.07166800
C	-0.74881500	1.17500700	-0.15213200
C	0.26606300	2.21961100	-0.20564000
H	0.18240700	2.79496300	-1.12986400
H	0.15797400	2.90905600	0.63411800
O	1.55707400	1.59700200	-0.14752000
C	2.57151300	2.45358900	-0.19113500
O	2.47980200	3.64755200	-0.27157800
O	3.71384300	1.76876500	-0.13052900
H	4.42933100	2.41451600	-0.16437000

13

E = -881.563699

ZPVE = 0.275680

Symbol	X	Y	Z
C	1.41081000	0.37685100	-0.18967100
C	2.12129500	1.75941100	-0.12606300
C	-0.44926000	2.09413300	-0.04203000
C	-0.11691000	0.58081900	-0.14897000
H	1.70068700	-0.14322000	-1.10347500
H	1.70341600	-0.23405500	0.66523800
H	-0.61344800	0.16815200	-1.02750600

H	-1.52701600	2.25036800	-0.01371200
H	3.20575300	1.64934700	-0.15868700
C	0.26052100	2.60253400	1.19287100
C	1.64769500	2.42704100	1.14666900
C	-0.33852200	3.16707100	2.30768200
C	2.43733200	2.82115300	2.21571600
C	0.45687900	3.57080800	3.38041500
H	-1.41534900	3.29559400	2.34152400
C	1.83588000	3.39950900	3.33414800
H	3.51286300	2.68291700	2.18094100
H	-0.00235500	4.01950300	4.25318900
H	2.44735000	3.71614200	4.17079300
C	0.19829600	2.72811100	-1.25476400
C	-0.45615800	3.40613500	-2.27145600
C	1.58686600	2.55939800	-1.29518400
C	0.28531000	3.93064500	-3.33095100
H	-1.53333500	3.52932600	-2.23895900
C	2.32253100	3.07597600	-2.35045900
C	1.66543500	3.76727200	-3.36942500
H	-0.21758100	4.46777500	-4.12624200
H	3.39911000	2.94561800	-2.38150900
H	2.23474500	4.17867100	-4.19454400
O	-0.60165700	-0.13019700	1.00906000
C	-1.91020500	-0.32169200	1.07441000
O	-2.72849300	0.03254200	0.26811200
O	-2.19114000	-0.99108200	2.19708200
H	-3.14772500	-1.11070100	2.21454200

<u>For Table 4 (ROC(O)OH): MP2/6-31+G(d)</u>

1

E = -533.852306

ZPVE = 0.169247

Symbol	X	Y	Z
C	-0.58544800	-0.93655800	-0.10523800
C	0.93834000	-0.84673400	-0.02894300
C	1.39477300	0.58706400	0.16324400
C	-0.67260500	1.20502600	1.17195200
C	-1.19511600	-0.21974800	1.09970100
H	2.46670400	0.68239300	0.34247500
H	1.30536000	-1.41685200	0.83409900
H	1.41663300	-1.25402900	-0.92648400
H	-0.93769800	-0.46986400	-1.03350300
H	-0.89806100	-1.98683000	-0.13291200
H	-0.99225500	1.71787000	2.08168000
H	-1.00506500	1.78820400	0.30302900
H	-0.92709300	-0.74635300	2.02492600
H	-2.29061800	-0.20162300	1.03660200
O	0.77173900	1.23603100	1.23529500
O	1.07263100	1.27453100	-1.08385900

C	1.79123000	2.38719500	-1.32198600
O	2.75591200	2.79344700	-0.69930900
O	1.25910800	2.98747600	-2.41330400
H	1.81184700	3.77815100	-2.57843500

2

E = -905.562396

ZPVE = 0.296899

Symbol	X	Y	Z
C	-2.04382100	0.77418100	0.34455300
C	-0.93557900	-0.28119700	0.27831400
C	0.42549600	0.31006600	-0.14189700
C	0.78087700	1.51869100	0.70916800
C	-0.32329900	2.56385300	0.78072000
C	-1.64420600	1.94665000	1.24122700
H	1.20234100	-0.44482100	0.07116600
H	-0.83145100	-0.74293500	1.27020500
H	-1.22582600	-1.08913500	-0.40748900
H	-2.26901800	1.15092900	-0.66060800
H	-2.96628300	0.31201700	0.71953100
H	1.72747600	1.97171800	0.40052300
H	-0.00826300	3.37644800	1.44581300
H	-0.44153000	3.00438300	-0.21945700
H	-1.53972500	1.59856900	2.27705000
H	-2.43025900	2.71239600	1.24124200
Si	0.66026800	0.57525800	-2.02414200
C	-0.75942700	1.44770400	-2.91460700
H	-0.98471000	2.43573900	-2.49992300
H	-0.48515200	1.58960300	-3.96775600
H	-1.68035200	0.85487100	-2.89611000
C	2.24598400	1.56291600	-2.29846500
H	2.51621500	1.56504900	-3.36130400
H	2.13895800	2.60856800	-1.98733700
H	3.09092500	1.13598700	-1.74513300
C	0.85112200	-1.14210200	-2.78346900
H	1.71258000	-1.67146600	-2.36018400
H	-0.03690200	-1.76160800	-2.61365900
H	1.00249300	-1.07527800	-3.86728500
O	0.99893100	0.98784200	2.07120200
C	1.79413900	1.72356900	2.85108200
O	2.36698000	2.76430200	2.56067200
O	1.87738900	1.11171300	4.05896500
H	2.46978000	1.67294500	4.59914000

3

E = -497.964740

ZPVE = 0.193591

Symbol	X	Y	Z
C	-4.17836100	-0.73081300	-0.13352700
C	-2.67298900	-0.59143500	-0.01399800
C	-2.24207700	0.85555000	0.15435000
C	-2.92340200	1.46695900	1.38272300
C	-4.44475900	1.33750700	1.29244000
C	-4.86070800	-0.12129800	1.09492000
H	-1.15156200	0.90894700	0.24584100
H	-2.28916600	-1.20186600	0.81227700
H	-4.50695400	-0.21224500	-1.04443000
H	-4.44181500	-1.78879300	-0.24817900
H	-2.56570800	0.95695500	2.28890600
H	-2.63136000	2.51942800	1.48088700
H	-4.91495700	1.74632300	2.19554700
H	-4.81045300	1.93676300	0.44615000
H	-4.59029400	-0.70123200	1.98933900
H	-5.94942500	-0.20001400	0.98914900
H	-2.53074300	1.40764900	-0.75103900
O	-2.12002800	-1.13318700	-1.25538200
C	-0.86014800	-1.57369800	-1.17646500
O	-0.14357200	-1.59834700	-0.18660700
O	-0.49294900	-2.00965800	-2.40546700
H	0.42690600	-2.32881800	-2.30932500

4

E = -497.964574

ZPVE = 0.193631

Symbol	X	Y	Z
C	-0.58455600	-0.89257800	-0.13153900
C	0.94179600	-0.82808500	-0.04854900
C	1.43868500	0.59358400	0.15614100
C	-0.75339700	1.21170400	1.24652200
C	-1.23061800	-0.23344700	1.08870400
H	2.52883500	0.62683400	0.24829800
H	1.29537000	-1.42759800	0.80259800
H	1.40429100	-1.24434500	-0.95140700
H	-0.91955800	-0.38305200	-1.04390200
H	-0.90388500	-1.93887100	-0.21564700
H	-1.19695500	1.66689200	2.14083100
H	-1.09423900	1.80368100	0.38707400
H	-0.97052400	-0.80359400	1.99327100
H	-2.32378200	-0.26443900	1.00074500
O	1.08240700	1.30426000	-1.07773300
C	1.81379500	2.38930100	-1.34765200
O	2.74923800	2.83482500	-0.69969000
O	1.34203200	2.93323000	-2.49615100
H	1.90078100	3.71818800	-2.66689800
C	0.77194100	1.28135700	1.33960300
H	1.12450900	2.31691500	1.40531500

H	1.11276600	0.77262400	2.25314800

5

E = -1125.840212

ZPVE = 0.275199

Symbol	X	Y	Z
C	-1.87989400	0.10168300	0.17469500
C	-0.49232100	-0.50910900	-0.03543500
C	0.55431400	0.53279100	-0.44105100
C	0.55845000	1.72616800	0.50894400
C	-0.82131000	2.31237100	0.76358900
C	-1.82292700	1.24009900	1.19486800
H	1.55230600	0.07746000	-0.42035200
H	-0.15320800	-0.96487300	0.90451500
H	-0.52268800	-1.30860800	-0.78649800
H	-2.27529800	0.48044400	-0.77737800
H	-2.57218600	-0.67859400	0.51506300
H	1.25782100	2.49695900	0.17199000
H	-0.73365100	3.10620600	1.51472900
H	-1.15908900	2.78761700	-0.16683800
H	-1.53240100	0.83855400	2.17494800
H	-2.81479700	1.69235500	1.31862300
S	0.24585600	1.07453900	-2.16915900
C	1.66789800	2.12988200	-2.37359400
C	1.50185300	3.52030100	-2.46216100
C	2.95567700	1.57817000	-2.46353500
C	2.61545800	4.35103000	-2.62576500
H	0.50222800	3.94527200	-2.39418000
C	4.06709100	2.41308400	-2.61019800
H	3.08304600	0.49756400	-2.42456300
C	3.89935700	3.80037600	-2.69271600
H	2.47900800	5.42868600	-2.69012600
H	5.06296100	1.97888900	-2.67443800
H	4.76524200	4.44818500	-2.81156000
O	1.08884800	1.16954100	1.75930500
C	1.70597900	2.05001700	2.55639000
O	1.87127900	3.24314900	2.35500300
O	2.13343300	1.38285600	3.65579900
H	2.57979200	2.05081200	4.21473600

6

E = -3125.938014

ZPVE = 0.274200

Symbol	X	Y	Z
C	-2.03528200	0.29372700	0.25729800

C	-0.90863600	-0.73051100	0.41102500
C	0.39392500	-0.26218600	-0.23398400
C	0.79047700	1.14248100	0.19047200
C	-0.34030700	2.15713100	0.11154900
C	-1.60504000	1.65442300	0.80927100
H	1.21194000	-0.94663400	0.01979700
H	-0.70837300	-0.88311000	1.48107000
H	-1.19759700	-1.70492500	-0.00282000
H	-2.31524800	0.39884800	-0.80002800
H	-2.92804200	-0.06468800	0.78493600
H	1.66827200	1.48634600	-0.36311100
H	0.00815300	3.10258600	0.54447900
H	-0.54888500	2.34872100	-0.94905600
H	-1.42075900	1.56852000	1.88860500
H	-2.41012600	2.38850000	0.68054300
C	2.08899700	0.15496000	-2.51705000
C	2.40905900	1.35539300	-3.16503200
C	3.10978000	-0.70306000	-2.08509100
C	3.74987800	1.70060400	-3.36700500
H	1.61422700	2.02371700	-3.48999600
C	4.44747000	-0.34910100	-2.28192100
H	2.86121300	-1.65185800	-1.61271200
C	4.77011600	0.85469900	-2.91949500
H	3.99599100	2.63697200	-3.86393600
H	5.23770400	-1.01671400	-1.94360700
H	5.81178500	1.12899100	-3.07168300
O	1.19625900	0.98664900	1.59546600
Se	0.25310500	-0.31294600	-2.21454800
C	2.14448800	1.83936000	2.00174600
O	2.69153600	2.70831200	1.34012200
O	2.41000000	1.57515500	3.30421700
H	3.10423700	2.21268900	3.56771500

7

E = -381.687151

ZPVE = 0.126492

Symbol	X	Y	Z
C	-0.86324700	1.58109300	0.12084900
H	-0.44808300	0.56921900	0.18048900
H	-1.95018900	1.49205900	0.22299700
C	-0.32710400	2.40062900	1.27411400
H	-0.74888200	3.41024800	1.29172400
H	0.76399700	2.48056400	1.24908200
C	-0.50572000	2.22472700	-1.21844500
H	0.57935800	2.30413800	-1.34229500
H	-0.89433800	1.63037100	-2.05011800
H	-0.92960600	3.23108900	-1.29964200
O	-0.71373100	1.71543500	2.49716900
C	-0.30924000	2.31997100	3.61992900

O	0.33116400	3.35666900	3.70374600
O	-0.73437000	1.58053400	4.67112600
H	-0.42232400	2.05034900	5.47051900

8

E = -837.796447

ZPVE = 0.225705

Symbol	X	Y	Z
C	-0.83735700	0.39133000	-0.75251600
C	-1.00526000	1.94809100	-0.55147900
H	-1.74495800	2.55518100	-1.08010400
C	-0.92052700	1.74663600	0.99750000
H	-1.55675200	2.24100400	1.73679700
C	-0.76373600	0.20072500	0.80010300
H	-1.30783300	-0.57573900	1.34365300
C	0.63524900	1.90647400	0.91447600
C	0.79468500	0.35795600	0.71652000
H	1.52625100	-0.26609600	1.23923900
C	0.70895300	0.55909900	-0.83748300
H	1.32951400	0.06599300	-1.58959800
C	0.54967400	2.10590300	-0.63659800
H	1.07657100	2.88571700	-1.19339100
C	-1.65157400	-0.40343200	-1.69643400
O	-2.88973700	-0.63846300	-1.18554900
O	-1.29270100	-0.77906800	-2.80733400
C	-3.78281800	-1.34857400	-2.07539000
H	-3.37069100	-2.32974300	-2.31735900
H	-4.71439600	-1.44262700	-1.52024500
H	-3.92996300	-0.77786800	-2.99410900
C	1.47297400	2.70762300	1.84417000
H	2.53545200	2.66888400	1.57599500
H	1.36007600	2.37986300	2.88447000
O	1.00724900	4.08271800	1.72982400
C	1.66606300	4.95073000	2.50853100
O	2.58364100	4.69547300	3.27260600
O	1.13745400	6.17952900	2.30555600
H	1.63972600	6.78615100	2.88626300

9

E = -614.199237

ZPVE = 0.256059

Symbol	X	Y	Z
C	-2.22554800	-1.62674200	0.07875300
C	-0.69971000	-1.64091500	0.08645300
C	-0.10113600	-0.26161600	0.48255600

C	-1.13254300	0.87744300	0.65983400
C	-2.56395600	0.42457900	0.47229400
C	-2.72271500	-0.85981500	1.32759600
H	0.46217200	-0.35607000	1.41642100
H	-0.35689400	-2.40345400	0.79780800
H	-0.32871000	-1.94811400	-0.89878600
H	-2.63699600	-2.62732000	-0.11483000
H	-1.02280100	1.32980800	1.65221300
H	-3.25979200	1.25952900	0.62865800
H	-2.10987400	-0.93509100	2.23582000
H	-3.76108300	-1.07031600	1.59227600
H	0.63059800	0.06051800	-0.26560800
C	-2.76957300	-0.45756600	-0.79440500
C	-4.25852700	-0.62465500	-1.10162600
H	-4.85116300	-0.88073400	-0.21853000
H	-4.66403900	0.30453500	-1.52071700
H	-4.40182200	-1.42017500	-1.84338500
C	-2.04797900	-0.11644400	-2.09312800
H	-0.97247400	0.02152700	-1.97119900
H	-2.20825100	-0.92054000	-2.82396200
H	-2.44608500	0.81210900	-2.51848400
O	-0.91022200	1.95272200	-0.31195100
C	0.12596300	2.74848900	-0.03175700
O	0.88116300	2.66806900	0.92619200
O	0.20867100	3.68749900	-1.00539700
H	0.97208100	4.25109000	-0.76630400

10

E = -419.641926

ZPVE = 0.132574

Symbol	X	Y	Z
C	-1.90469800	1.00862200	-0.03980100
C	-0.41587700	1.04398200	0.18044200
C	-1.17999900	2.33145600	0.03296900
H	-2.27790300	0.68911400	-1.00734900
H	-2.53654500	0.72902600	0.79846500
H	0.23364900	0.74325100	-0.63511000
H	-0.04146600	0.79695900	1.16969900
H	-1.05607100	2.87006500	-0.90336300
C	-1.39632100	3.19189600	1.23350200
H	-2.21814200	3.90155700	1.09767200
H	-1.59560000	2.59323100	2.12832200
O	-0.16628100	3.94767000	1.44421300
C	-0.20454700	4.77117900	2.49727400
O	-1.13430100	4.92259600	3.27557700
O	0.97985500	5.42328700	2.56506000
H	0.91694200	6.00984300	3.34550300

11

E = -535.882263

ZPVE = 0.195883

Symbol	X	Y	Z
C	-1.48739900	1.03642200	0.41115000
C	-0.02955000	1.41419100	0.45277100
C	-1.07366200	2.47613300	0.23348500
H	-1.86146300	0.50515800	-0.45846000
H	-1.96620500	0.75910700	1.34591700
H	0.60067700	1.13929500	-0.38711200
H	0.47098000	1.39930300	1.41723900
H	-1.15057300	2.88784000	-0.77123400
C	-1.36319700	3.45007300	1.33479100
H	-1.30989100	2.95351800	2.31168800
C	-2.67247000	4.16533400	1.17989000
C	-3.90644900	3.57631500	1.81700800
C	-3.30439700	4.84114500	2.37083100
H	-2.80643600	4.65198500	0.21513400
H	-3.78975200	2.66628900	2.39859800
H	-4.84054300	3.64043300	1.26769100
H	-3.82833000	5.77655100	2.19976200
H	-2.77864400	4.77772700	3.31864000
O	-0.28416700	4.45064600	1.28644600
C	0.20762600	4.83898700	2.46468900
O	-0.09604500	4.42516900	3.57558500
O	1.14222300	5.79192200	2.23225200
H	1.48802000	6.04283700	3.11246300

12

E = -379.312454

ZPVE = 0.076156

Symbol	X	Y	Z
C	-1.63599000	0.33441100	-0.10894300
H	-2.38733500	-0.42411100	-0.06931900
C	-0.74841100	1.17179700	-0.15172500
C	0.25482000	2.22699800	-0.20739700
H	0.18411800	2.80236200	-1.13489900
H	0.16146400	2.91733400	0.63581700
O	1.55913600	1.58449500	-0.14904500
C	2.57733000	2.45815000	-0.19141000
O	2.48707500	3.67326800	-0.26986800
O	3.72933300	1.75751700	-0.13065600
H	4.44982000	2.41888500	-0.16293000

13

E = -879.031112

ZPVE = 0.273145

Symbol	X	Y	Z
C	1.41082400	0.37729300	-0.23544000
C	2.11866400	1.75870800	-0.14050800
C	-0.45294200	2.09046900	-0.07758500
C	-0.11408000	0.58064400	-0.16840800
H	1.69121100	-0.11343400	-1.17471800
H	1.71955000	-0.26773000	0.59518600
H	-0.64102800	0.12983800	-1.01581200
H	-1.53643400	2.24857000	-0.05676400
H	3.21037800	1.65033400	-0.16232500
C	0.24082900	2.59479700	1.16108600
C	1.63446300	2.41338300	1.12959100
C	-0.37865600	3.13860000	2.28695900
C	2.41511400	2.78423600	2.22593700
C	0.40715300	3.52671300	3.38014100
H	-1.46070400	3.26968800	2.30901600
C	1.79634700	3.34715600	3.35049300
H	3.49556700	2.64072700	2.20701200
H	-0.06380100	3.96120600	4.25989100
H	2.39876100	3.64789500	4.20563500
C	0.20168200	2.73036700	-1.27614900
C	-0.45260000	3.40997700	-2.30536300
C	1.59866200	2.57208100	-1.30046300
C	0.30100400	3.94690200	-3.35791600
H	-1.53590400	3.52713700	-2.28496400
C	2.34705700	3.09784700	-2.35480200
C	1.69320300	3.79302700	-3.38167000
H	-0.19774800	4.48574400	-4.16122100
H	3.42990300	2.97481500	-2.37672000
H	2.27003100	4.21398000	-4.20304400
O	-0.55303200	-0.10400300	1.04445500
C	-1.87553500	-0.27831300	1.15430600
O	-2.73402700	0.05470200	0.35023300
O	-2.11483300	-0.90775900	2.32785800
H	-3.08546000	-1.02372100	2.37485900

<u>For Table 4 (ROCOCHCl$_2$): B3LYP/6-311++G(d,p)</u>

1

E = -1418.864034

ZPVE = 0.170165

Symbol	X	Y	Z
C	-0.58720900	-0.95238600	-0.10131700
C	0.93659100	-0.78228100	-0.05482700
C	1.33808700	0.66138600	0.22326400
C	-0.75552000	1.13010200	1.28439800
C	-1.21740400	-0.31570000	1.14444200

H	2.40290500	0.77686800	0.41373000
H	1.35469800	-1.38650900	0.75747900
H	1.40884900	-1.11110100	-0.98360100
H	-0.98338300	-0.47281400	-1.00213100
H	-0.84193300	-2.01359600	-0.16630700
H	-1.07544900	1.57180700	2.22812100
H	-1.14569700	1.74385100	0.46501500
H	-0.92679400	-0.87675800	2.03991300
H	-2.31023800	-0.33881900	1.08686000
O	0.68470500	1.23581500	1.30357600
O	1.02446800	1.42428100	-1.00159200
C	1.82339900	2.43657800	-1.33104500
C	1.32545500	3.18421500	-2.57241000
O	2.83717300	2.77088900	-0.77630600
Cl	1.31252100	2.10632800	-4.00975100
Cl	-0.28517000	3.92277600	-2.27466700
H	2.01580000	3.99244200	-2.78273600

2

E = -1791.558514

ZPVE = 0.294652

Symbol	X	Y	Z
C	-2.08500000	0.61988900	0.34753400
C	-0.88356400	-0.33556400	0.28534000
C	0.43205700	0.36583500	-0.13868200
C	0.68619000	1.62145900	0.69750200
C	-0.51788200	2.55830900	0.80382200
C	-1.79253600	1.82793900	1.24696700
H	1.26007900	-0.31951300	0.09277500
H	-0.73969500	-0.77745100	1.27791500
H	-1.10088100	-1.17009600	-0.38843000
H	-2.34027200	0.97144800	-0.65843900
H	-2.96214000	0.08036400	0.71885200
H	1.56259700	2.16932100	0.35179000
H	-0.27574200	3.37957500	1.48356200
H	-0.67219100	3.00880100	-0.18307900
H	-1.67501400	1.49132100	2.28248100
H	-2.63592000	2.52516400	1.23773200
Si	0.69438600	0.59464700	-2.03418500
C	-0.61453900	1.63426300	-2.92077500
H	-0.67636700	2.65433100	-2.53185100
H	-0.36015600	1.70725000	-3.98360200
H	-1.61094700	1.18925700	-2.85454600
C	2.38598500	1.39737400	-2.30326000
H	2.63762400	1.40280400	-3.36860800
H	2.41447800	2.43544300	-1.95898700
H	3.17967300	0.85327200	-1.78192800
C	0.70410400	-1.13428800	-2.79848500
H	1.45955100	-1.77472200	-2.33306800

H	-0.26327300	-1.63484400	-2.69848500
H	0.93308700	-1.07757200	-3.86733500
O	1.02375400	1.14482600	2.06515200
C	1.85796100	1.87034400	2.78971200
C	2.14123800	1.24217500	4.15928600
H	2.83261200	1.88450300	4.69167200
O	2.38065400	2.91173500	2.47424200
Cl	0.64094400	1.14454100	5.14483700
Cl	2.93193200	-0.36187800	3.98560000

3

E = -1382.931022

ZPVE = 0.193970

Symbol	X	Y	Z
C	-4.16501100	-0.71016200	-0.13443200
C	-2.65588600	-0.54084600	-0.01221000
C	-2.24897000	0.91655200	0.19162300
C	-2.95724700	1.50391800	1.42386000
C	-4.48096900	1.34306400	1.32949700
C	-4.87408700	-0.12279800	1.09672100
H	-1.16379000	0.98681500	0.30174800
H	-2.26187800	-1.15621100	0.80038200
H	-4.50284200	-0.19603000	-1.04139000
H	-4.40807200	-1.76941000	-0.25588100
H	-2.59272100	0.99904100	2.32729900
H	-2.68894600	2.55903600	1.53035700
H	-4.95717900	1.72076000	2.23961000
H	-4.85929000	1.95514800	0.50094700
H	-4.61361800	-0.71375800	1.98399200
H	-5.95703900	-0.21385300	0.97217300
H	-2.52703500	1.48331700	-0.70446900
O	-2.07460800	-1.04801300	-1.26015500
C	-0.85937000	-1.57404600	-1.21700700
O	-0.15463900	-1.69031500	-0.24519200
C	-0.38607900	-2.06373700	-2.58941200
Cl	-0.26325600	-0.69986000	-3.75248000
Cl	-1.44380600	-3.37797500	-3.20685000
H	0.60831800	-2.47894100	-2.47580900

4

E = -1382.930149

ZPVE = 0.194047

Symbol	X	Y	Z
C	-0.62172200	-0.89019200	-0.10653400
C	0.91088900	-0.78933500	-0.10030000
C	1.40586800	0.63080000	0.16063400

C	-0.76800300	1.15304700	1.38678700
C	-1.22965900	-0.29569300	1.17201800
H	2.49325500	0.66169800	0.23796000
H	1.32031200	-1.42376000	0.69526800
H	1.33143700	-1.15187700	-1.04240000
H	-1.01397800	-0.35721800	-0.97903200
H	-0.91801000	-1.93754300	-0.21917300
H	-1.16763100	1.54626000	2.32650100
H	-1.17016600	1.78454500	0.58724600
H	-0.93035100	-0.90480500	2.03552900
H	-2.32212100	-0.33933800	1.12452100
O	1.04217400	1.41711700	-1.03231100
C	1.81019600	2.44442600	-1.36026500
C	1.32036700	3.15815300	-2.62455900
O	2.79616700	2.82710000	-0.78048300
Cl	1.34693700	2.05774400	-4.04369300
Cl	-0.30732700	3.87558800	-2.36380400
H	1.99957800	3.97490700	-2.83814800
C	0.76407700	1.26068900	1.39819200
H	1.08896500	2.30044800	1.48993200
H	1.16635300	0.73148000	2.27094800

5

E = -2012.164089

ZPVE = 0.275484

Symbol	X	Y	Z
C	-1.86632400	-0.01111500	0.14020500
C	-0.41862200	-0.46953500	-0.08884300
C	0.53975300	0.69479600	-0.38503400
C	0.41816800	1.81941100	0.65180500
C	-1.02222500	2.24264500	0.93779600
C	-1.93995900	1.05097800	1.24595300
H	1.56861000	0.33238700	-0.38498500
H	-0.05356700	-0.96727200	0.81632600
H	-0.36305300	-1.20112300	-0.89908300
H	-2.28116000	0.39545100	-0.78963800
H	-2.48345300	-0.87518000	0.40402300
H	1.02526300	2.67789700	0.36653100
H	-1.02371000	2.96828300	1.75518500
H	-1.38394500	2.76905100	0.04868700
H	-1.64909900	0.60182600	2.20192700
H	-2.96795600	1.40550100	1.36596800
S	0.22469100	1.34608700	-2.10144400
C	1.74039400	2.26220400	-2.41287400
C	1.69911500	3.65566300	-2.51980300
C	2.95310200	1.59127300	-2.60886000
C	2.86082100	4.37035500	-2.81142700
H	0.75941400	4.17500700	-2.37443600
C	4.11346200	2.31040600	-2.88367000
H	2.98341600	0.50905200	-2.55654700

C	4.06948900	3.70090800	-2.98780400
H	2.81954500	5.45070500	-2.89283500
H	5.04956300	1.78328100	-3.03045700
H	4.97277700	4.25797700	-3.20882100
O	1.01819700	1.26048200	1.87927300
C	1.62040100	2.09565000	2.71433600
C	2.22059100	1.37455900	3.92576500
O	1.72224100	3.29063400	2.59521700
Cl	0.93197500	0.60566100	4.91526700
Cl	3.47341400	0.19013900	3.42210900
H	2.70845300	2.11194000	4.55212600

6

E = -4015.496559

ZPVE = 0.274210

Symbol	X	Y	Z
C	-2.01891700	0.14635900	0.29093500
C	-0.75493000	-0.71954700	0.39423200
C	0.48062900	-0.04578700	-0.21624300
C	0.68350400	1.38045900	0.30161800
C	-0.58247300	2.23687100	0.27153600
C	-1.78918500	1.53279600	0.90843700
H	1.37499100	-0.63122400	-0.00418100
H	-0.53558100	-0.90335500	1.45269500
H	-0.91007900	-1.69625600	-0.07106000
H	-2.31366300	0.25546800	-0.76018900
H	-2.84921000	-0.35876500	0.79337300
H	1.50007500	1.87593200	-0.22195000
H	-0.37654900	3.19263700	0.76007000
H	-0.79392000	2.45988200	-0.77917400
H	-1.62475300	1.42661600	1.98632400
H	-2.67972800	2.15654500	0.78707400
C	2.24274200	0.17718700	-2.62074500
C	2.71003600	1.39686600	-3.11742000
C	3.13112500	-0.88951800	-2.45146400
C	4.06025500	1.54979300	-3.43402700
H	2.02180000	2.22221000	-3.25430000
C	4.48094100	-0.72746700	-2.75773200
H	2.76652400	-1.84401000	-2.09026800
C	4.94700700	0.49115200	-3.25069800
H	4.41682300	2.49900500	-3.81804100
H	5.16572000	-1.55708000	-2.62120200
H	5.99655200	0.61309400	-3.49319400
O	1.12037900	1.20882500	1.70468200
Se	0.35400900	-0.04757200	-2.22683900
C	1.93686600	2.11775400	2.21803400
C	2.33002000	1.79639500	3.66382800
O	2.36096800	3.10341700	1.66873300
Cl	0.89020300	1.82423100	4.73967700

Cl	3.21074400	0.23442800	3.76567500
H	3.00488200	2.56943200	4.01175400

7

E = -1266.227665

ZPVE = 0.128306

Symbol	X	Y	Z
C	-0.85505400	1.59206400	0.08458400
H	-0.44061100	0.58122400	0.14437700
H	-1.94015400	1.49654600	0.18738500
C	-0.32144000	2.41176900	1.24447900
H	-0.74196000	3.42026600	1.26429600
H	0.76777600	2.49748900	1.22197700
C	-0.50508100	2.22886600	-1.26411600
H	0.57740100	2.31202700	-1.39955500
H	-0.89582900	1.62686800	-2.08728900
H	-0.93123500	3.23230800	-1.35642900
O	-0.70117700	1.73437400	2.47497000
C	-0.32023000	2.30046600	3.61239000
C	-0.77087900	1.50978500	4.84275800
O	0.31041100	3.32137100	3.72361300
Cl	-2.56312400	1.43629700	4.93953100
Cl	-0.02951900	-0.12631100	4.86420100
H	-0.42251600	2.03210900	5.72590100

8

E = -1723.758289

ZPVE = 0.227634

Symbol	X	Y	Z
C	-0.83736200	0.34546100	-0.76417000
C	-1.03278200	1.89971800	-0.54201200
H	-1.78686100	2.50176300	-1.04335200
C	-0.91267300	1.69948500	1.00628200
H	-1.55624600	2.16484800	1.74990000
C	-0.72421400	0.15770700	0.79914400
H	-1.23087300	-0.62486700	1.35938400
C	0.64427200	1.90266700	0.90425900
C	0.82904400	0.35256900	0.69194700
H	1.57504300	-0.26360200	1.19189400
C	0.70837000	0.55122600	-0.86143300
H	1.33796400	0.08166500	-1.61299400
C	0.51868600	2.09609900	-0.65206900
H	1.00989200	2.87843300	-1.22710600
C	-1.64593900	-0.49383800	-1.68602800
O	-2.94303200	-0.52751500	-1.30060900

O	-1.22617600	-1.07342500	-2.66081000
C	-3.83001800	-1.30076700	-2.13021200
H	-3.51416800	-2.34463300	-2.15742200
H	-4.81164200	-1.20936400	-1.67037500
H	-3.84375600	-0.90517900	-3.14682000
C	1.49076500	2.70955900	1.82829700
H	2.54640100	2.68704600	1.54202700
H	1.40882500	2.36708300	2.86408800
O	1.02646000	4.09091300	1.76335800
C	1.66232500	4.97040100	2.52694600
C	1.09848200	6.38630500	2.38747600
O	2.58469700	4.73539000	3.26564200
Cl	-0.61170600	6.45273500	2.93373000
Cl	1.29152400	6.99417800	0.70849000
H	1.66825000	7.04247700	3.03476700

9

E = -1499.584524

ZPVE = 0.255191

Symbol	X	Y	Z
C	-2.25234900	-1.65529500	0.09902800
C	-0.72093800	-1.71062600	0.10190200
C	-0.06937200	-0.32446200	0.40772100
C	-1.07732400	0.83603300	0.63279900
C	-2.53010100	0.42131500	0.45767800
C	-2.72379200	-0.84764100	1.33889700
H	0.57218500	-0.39859500	1.28713700
H	-0.39964100	-2.43768400	0.85410900
H	-0.36136200	-2.08515800	-0.86054200
H	-2.68457400	-2.64643900	-0.06593900
H	-0.94390300	1.25598200	1.63070000
H	-3.19492100	1.27524100	0.60966400
H	-2.11603800	-0.92538800	2.24497800
H	-3.76484000	-1.02047500	1.60484100
H	0.58983100	-0.03910500	-0.41361200
C	-2.78375600	-0.48398900	-0.80070700
C	-4.28815600	-0.61737000	-1.08419000
H	-4.87717800	-0.83956400	-0.19233200
H	-4.67771200	0.30977800	-1.51648900
H	-4.46680100	-1.42011600	-1.80675800
C	-2.07582400	-0.18405800	-2.12372100
H	-0.99688600	-0.07169400	-2.03138200
H	-2.26848500	-0.99124900	-2.83898500
H	-2.45830700	0.74246500	-2.56103800
O	-0.81746200	1.93988300	-0.30632900
C	0.11439700	2.82006600	0.02535500
C	0.26843900	3.93178300	-1.01773200
O	0.80061600	2.80813400	1.01739900
Cl	-1.25945000	4.85121200	-1.22797700

Cl	0.86706700	3.26141700	-2.57511800
H	1.01750300	4.62910200	-0.66184600

10

E = -1304.298559

ZPVE = 0.134210

Symbol	X	Y	Z
C	-1.93354100	0.99006300	-0.06956200
C	-0.44030200	1.00149000	0.13471200
C	-1.19256700	2.30426400	0.03169800
H	-2.32244800	0.70504900	-1.03908500
H	-2.55816400	0.69176300	0.76484700
H	0.19615400	0.71939600	-0.69462400
H	-0.05836300	0.71595900	1.10803900
H	-1.07219900	2.86393300	-0.88975900
C	-1.39749000	3.15030600	1.24870800
H	-2.23408300	3.84371000	1.13646700
H	-1.57068800	2.54530700	2.14197900
O	-0.18712200	3.94043700	1.45962400
C	-0.18820200	4.76141900	2.50023000
C	1.11510800	5.55409500	2.62725000
O	-1.08563000	4.90789700	3.29196000
Cl	1.37084700	6.60767700	1.19508200
Cl	2.50929000	4.45776300	2.91234200
H	1.03353500	6.20155900	3.49227300

11

E = -1420.966081

ZPVE = 0.196009

Symbol	X	Y	Z
C	-1.48397500	1.03413200	0.39082500
C	-0.02987500	1.42819300	0.44092000
C	-1.08761400	2.48406400	0.23970100
H	-1.85319400	0.51801200	-0.48680900
H	-1.95702000	0.72883400	1.31681100
H	0.60345800	1.18099300	-0.40192100
H	0.47099500	1.39123500	1.40158300
H	-1.16653900	2.90526900	-0.75763200
C	-1.40354600	3.45647700	1.34351600
H	-1.33402300	2.96970900	2.31855900
C	-2.73362100	4.14690000	1.19499600
C	-3.96320300	3.53893200	1.82835000
C	-3.38502400	4.81610400	2.38140900
H	-2.87432200	4.62732700	0.23167000
H	-3.84054400	2.63538500	2.41404600

H	-4.89150100	3.58470600	1.27235700
H	-3.91826200	5.74217800	2.20537400
H	-2.87027100	4.76618900	3.33335000
O	-0.34511600	4.49252100	1.30031000
C	0.23083600	4.86108000	2.43175300
C	1.30048000	5.93813800	2.21797200
O	0.00060900	4.44003500	3.53965300
Cl	0.58410600	7.43337200	1.52711200
Cl	2.64954400	5.31391700	1.20875100
H	1.71686800	6.19807200	3.18393400

12

E = -1263.776407

ZPVE = 0.080889

Symbol	X	Y	Z
C	-1.67420300	0.34834800	-0.10935500
H	-2.43517400	-0.39288100	-0.07062400
C	-0.80770800	1.17777100	-0.15245600
C	0.20378700	2.21706100	-0.20762000
H	0.13104600	2.79429100	-1.13263600
H	0.10756100	2.91079600	0.63119400
O	1.51659100	1.59257000	-0.14889800
C	2.55114700	2.42927700	-0.18935100
C	3.89559700	1.70390000	-0.12294700
O	2.48366100	3.62893700	-0.26885200
Cl	4.07161700	0.82360700	1.43094400
Cl	4.11230600	0.62509400	-1.54040600
H	4.68003500	2.45060600	-0.16203100

13

E = -1765.199626

ZPVE = 0.276460

Symbol	X	Y	Z
C	1.36505400	0.37664800	-0.13570800
C	2.11499400	1.74699000	-0.11483300
C	-0.44534900	2.15553900	0.00604100
C	-0.15863900	0.62790700	-0.11078400
H	1.64202800	-0.18725200	-1.02853100
H	1.64266800	-0.21522900	0.73798300
H	-0.65835200	0.23711200	-0.99582900
H	-1.51792200	2.34377900	0.04941500
H	3.19514500	1.60179400	-0.16389500
C	0.30017800	2.66973800	1.22399600
C	1.68477200	2.45728800	1.15530700
C	-0.25970200	3.29287700	2.33228100

C	2.50804000	2.86838800	2.19674200
C	0.56968400	3.71369500	3.37543300
H	-1.33141000	3.45315900	2.38771500
C	1.94532000	3.50214500	3.30830800
H	3.57953600	2.70283900	2.14664800
H	0.13986600	4.20620600	4.24037500
H	2.58317300	3.83141100	4.12092800
C	0.19988400	2.76357200	-1.22894000
C	-0.44991500	3.46123000	-2.23988200
C	1.58491500	2.54895600	-1.29132900
C	0.29131800	3.95911900	-3.31566800
H	-1.52199300	3.62197400	-2.19286900
C	2.31951700	3.03960200	-2.36403500
C	1.66745400	3.74965700	-3.37689800
H	-0.20773600	4.51068000	-4.10438500
H	3.39130900	2.87650200	-2.41482000
H	2.23669500	4.13974600	-4.21321600
O	-0.69966100	-0.09372600	1.04022100
C	-1.98469500	-0.42362400	1.01406600
C	-2.40627800	-1.23019700	2.24557200
O	-2.77868900	-0.15793000	0.14620000
Cl	-1.50717000	-2.78314300	2.33575600
Cl	-2.22352100	-0.26090400	3.74497200
H	-3.45731900	-1.47381500	2.14506200

<u>For Table 4 (ROCOCHCl$_2$): M06-2X/6-311++G(d,p)</u>

1

E = -1418.605344

ZPVE = 0.173028

Symbol	X	Y	Z
C	-0.59080000	-0.91436300	-0.12527400
C	0.93456000	-0.84211900	-0.04325400
C	1.39532900	0.58627200	0.18893300
C	-0.65434500	1.18871500	1.21297900
C	-1.19321200	-0.22940500	1.10260400
H	2.46664800	0.66685300	0.36605200
H	1.29344300	-1.43547900	0.80282900
H	1.40912000	-1.22357000	-0.94919300
H	-0.93053900	-0.40676200	-1.03341700
H	-0.91469600	-1.95472000	-0.19147000
H	-0.97246600	1.67547800	2.13379700
H	-0.99324700	1.79305500	0.36369100
H	-0.92815500	-0.78550300	2.00779800
H	-2.28370900	-0.19630600	1.04014300
O	0.77604100	1.20695700	1.25999700
O	1.08497500	1.30719100	-1.03272300
C	1.75738800	2.42894100	-1.26154800
C	1.23143900	3.15486200	-2.49749200
O	2.67051700	2.86015300	-0.62263900

Cl	1.43358000	2.14598400	-3.94428300
Cl	-0.46665800	3.62012500	-2.25251300
H	1.81064100	4.06101600	-2.63490900

2

E = -1791.202650

ZPVE = 0.298522

Symbol	X	Y	Z
C	-1.98271200	0.82169700	0.36478900
C	-0.89620500	-0.25690700	0.29050600
C	0.46896800	0.30312500	-0.16179000
C	0.86502400	1.51080400	0.67575000
C	-0.21713100	2.58353100	0.73624200
C	-1.54163500	2.00074900	1.23414500
H	1.23129000	-0.46454500	0.03129800
H	-0.78093000	-0.70484900	1.28360400
H	-1.21239700	-1.06276000	-0.38001800
H	-2.21827200	1.18879200	-0.63839200
H	-2.90191500	0.38536800	0.76431800
H	1.81439900	1.93763100	0.34666800
H	0.12172500	3.40506800	1.37153800
H	-0.33954100	2.98997900	-0.27463500
H	-1.41819200	1.66601500	2.26940400
H	-2.30878100	2.77871300	1.23936900
Si	0.64224700	0.56729400	-2.04462400
C	-0.85427200	1.33644100	-2.88873200
H	-1.11375800	2.31959800	-2.48983400
H	-0.63030300	1.45974600	-3.95272800
H	-1.73498800	0.69395700	-2.81187900
C	2.14512200	1.65140700	-2.36769100
H	2.35730200	1.69702100	-3.43921300
H	1.98952200	2.67620100	-2.01889700
H	3.03647400	1.25995500	-1.86952200
C	0.91203500	-1.13594800	-2.79366700
H	1.82832100	-1.59485900	-2.41361500
H	0.08099700	-1.80790300	-2.56261300
H	0.99428300	-1.07445300	-3.88195800
O	1.08371200	1.00404200	2.03152700
C	1.81722000	1.73514200	2.84472700
C	1.90347300	1.11926900	4.24008700
H	2.54749700	1.74197000	4.85069900
O	2.36854000	2.76901600	2.58599100
Cl	0.28828200	1.10821200	4.98530700
Cl	2.60738500	-0.50825600	4.17686700

3

E = -1382.674369

ZPVE = 0.196770

Symbol	X	Y	Z
C	-4.19692800	-0.71730300	-0.12926200
C	-2.68874900	-0.59563500	-0.00539400
C	-2.24409400	0.84954900	0.17066300
C	-2.92432200	1.46134000	1.39924200
C	-4.44730100	1.34971400	1.29934000
C	-4.87697100	-0.10562500	1.09895100
H	-1.15689200	0.89256800	0.26561400
H	-2.31978700	-1.20385000	0.82630800
H	-4.51255200	-0.18841400	-1.03525100
H	-4.47063800	-1.76787200	-0.25091900
H	-2.58042400	0.93935000	2.29997100
H	-2.62136500	2.50534600	1.50544400
H	-4.91669000	1.76238700	2.19576300
H	-4.79765200	1.94859800	0.45040000
H	-4.60956200	-0.68694400	1.98938200
H	-5.96173100	-0.17477700	0.99151000
H	-2.52744200	1.40545000	-0.73039600
O	-2.12922700	-1.13604300	-1.22824600
C	-0.87134400	-1.53290900	-1.19486600
O	-0.14572000	-1.53460900	-0.24007000
C	-0.38399100	-2.00877100	-2.56137500
Cl	-0.34784200	-0.63667100	-3.69126900
Cl	-1.38716700	-3.33819300	-3.17211100
H	0.63037200	-2.37498900	-2.45050700

4

E = -1382.674989

ZPVE = 0.196859

Symbol	X	Y	Z
C	-0.60297700	-0.86632500	-0.13091000
C	0.92642900	-0.84002000	-0.06509500
C	1.45481200	0.57005800	0.15157700
C	-0.70807000	1.21373400	1.28839800
C	-1.21758900	-0.21880200	1.11218300
H	2.54352200	0.58114800	0.22898800
H	1.27368000	-1.45346100	0.77354300
H	1.36567000	-1.25301600	-0.97619800
H	-0.93079500	-0.32277500	-1.02281900
H	-0.94830200	-1.89735400	-0.23770200
H	-1.12881400	1.66340100	2.19085900
H	-1.04271000	1.82304400	0.44196800
H	-0.95193000	-0.80896400	1.99827800
H	-2.30798700	-0.22576000	1.04096500
O	1.09801400	1.30992100	-1.04982600
C	1.75991300	2.42236300	-1.29948200
C	1.22057900	3.13691800	-2.53645000

O	2.67171300	2.87385600	-0.66495300
Cl	1.29824700	2.09036400	-3.96643900
Cl	-0.43887100	3.69380300	-2.21768300
H	1.83478000	4.01066300	-2.72273600
C	0.82072400	1.24867100	1.36197500
H	1.19433200	2.27196600	1.44327400
H	1.16323800	0.71080900	2.25311800

5

E =

ZPVE =

Symbol	X	Y	Z

6

E = -4015.153748

ZPVE = 0.278138

Symbol	X	Y	Z
C	-1.94969700	0.24395500	0.30487000
C	-0.76940100	-0.72065700	0.44827400
C	0.49942700	-0.19014500	-0.22233000
C	0.83162100	1.22672600	0.23781000
C	-0.34827300	2.18899300	0.15574700
C	-1.58657400	1.62457300	0.85672400
H	1.34736700	-0.83918600	0.00090200
H	-0.54398400	-0.85052100	1.51270000
H	-1.01367800	-1.70625700	0.04565800
H	-2.23474800	0.33412400	-0.74984300
H	-2.81644600	-0.15963400	0.83340900
H	1.69909000	1.61927400	-0.29622800
H	-0.05000900	3.14874000	0.58356400
H	-0.56155600	2.35842900	-0.90358900
H	-1.39066300	1.54306400	1.93149900
H	-2.42253700	2.31716100	0.73571800
C	2.14758100	0.11758600	-2.60428200
C	2.51508600	1.36964000	-3.09497500
C	3.11770500	-0.86559700	-2.40942500
C	3.85026900	1.63761700	-3.38431100
H	1.75804700	2.13066200	-3.24355800
C	4.45166500	-0.58908900	-2.68948900
H	2.82545200	-1.84415900	-2.04619600
C	4.81872300	0.66138000	-3.17833200
H	4.13197500	2.61256100	-3.76392900
H	5.20294600	-1.35435900	-2.53408800
H	5.85795500	0.87319100	-3.39953600
O	1.21496400	1.06481500	1.63471900

Se	0.30133500	-0.25148500	-2.19455300
C	1.94994700	2.01692400	2.17814300
C	2.20773900	1.75477100	3.66012300
O	2.37637900	2.99455900	1.63191900
Cl	0.67082100	1.85631100	4.55011200
Cl	3.00675100	0.19031400	3.90606600
H	2.86252900	2.53249500	4.03665600

7

E = -1266.017833

ZPVE = 0.130367

Symbol	X	Y	Z
C	-0.85650700	1.57979300	0.09498500
H	-0.43281500	0.57417300	0.15341300
H	-1.93986700	1.47936400	0.19712200
C	-0.33076000	2.39937700	1.25265700
H	-0.75682400	3.40587500	1.26842100
H	0.75805300	2.49172800	1.22785100
C	-0.50296900	2.23281500	-1.23911200
H	0.57917100	2.32546600	-1.35874600
H	-0.88118000	1.64092200	-2.07311100
H	-0.93593200	3.23310300	-1.31573500
O	-0.70564000	1.72510900	2.46920800
C	-0.31963100	2.29884200	3.59425800
C	-0.76600200	1.51667900	4.82599900
O	0.30757600	3.31562600	3.68795900
Cl	-2.53933300	1.46036000	4.91032800
Cl	-0.05477700	-0.10994200	4.82202800
H	-0.40578600	2.03823000	5.70554700

8

E =

ZPVE =

Symbol	X	Y	Z

9

E = -1499.285885

ZPVE = 0.259003

Symbol	X	Y	Z
C	-2.21501500	-1.63135700	0.05203500
C	-0.68802500	-1.62204500	0.05582900

C	-0.10896100	-0.25119300	0.50791700
C	-1.15821100	0.87003900	0.71585400
C	-2.58571100	0.39686700	0.53104000
C	-2.72168600	-0.92271600	1.33202200
H	0.44126300	-0.37154500	1.44154000
H	-0.33176500	-2.40378700	0.73159700
H	-0.31882300	-1.87727800	-0.94035800
H	-2.61079800	-2.62299000	-0.18086400
H	-1.04212800	1.30113200	1.71280100
H	-3.29053700	1.21015700	0.71853800
H	-2.10546900	-1.02347600	2.22946200
H	-3.75294100	-1.15901700	1.58266600
H	0.62560100	0.10283800	-0.21845700
C	-2.77361500	-0.43372600	-0.77409700
C	-4.25770900	-0.60803900	-1.09647100
H	-4.84871700	-0.90342000	-0.22801400
H	-4.67182600	0.32791000	-1.48199400
H	-4.38682900	-1.37469200	-1.86573100
C	-2.04294000	-0.02274600	-2.04812400
H	-0.96807800	0.09608000	-1.91585200
H	-2.20825500	-0.77674300	-2.82432600
H	-2.42676100	0.93264300	-2.41572700
O	-0.95697500	1.95696900	-0.22720600
C	0.09388600	2.72643900	-0.02840000
C	0.26345900	3.75634700	-1.14221700
O	0.87310700	2.65169600	0.88054100
Cl	-1.19911100	4.73421800	-1.35874900
Cl	0.71436400	2.90621100	-2.63978000
H	1.08007200	4.41872900	-0.87796400

10

E = -1304.082433

ZPVE = 0.136488

Symbol	X	Y	Z
C	-1.91112700	0.99614400	-0.03868700
C	-0.42251100	1.05049400	0.15511100
C	-1.20572400	2.32311900	0.01618800
H	-2.29184300	0.66935900	-0.99641200
H	-2.52162900	0.71497100	0.81040400
H	0.21170700	0.75662000	-0.66969100
H	-0.03060600	0.81569700	1.13695000
H	-1.10320100	2.86603100	-0.91563800
C	-1.40686500	3.17442300	1.22688300
H	-2.24081500	3.87085700	1.11616100
H	-1.58265100	2.56546500	2.11776000
O	-0.20158900	3.94389800	1.43140500
C	-0.19739300	4.73822000	2.48543000
C	1.11043500	5.51211600	2.62342600
O	-1.09091400	4.86865800	3.27406500

Cl	1.36289800	6.56139300	1.21359700
Cl	2.46771900	4.39181100	2.86293600
H	1.03824600	6.14280900	3.50229400

11

E = -1420.704001

ZPVE = 0.199154

Symbol	X	Y	Z
C	-1.51324700	1.04791400	0.39158100
C	-0.05592400	1.41634700	0.41748300
C	-1.09438000	2.47942500	0.21373700
H	-1.89512100	0.52326500	-0.47341700
H	-1.98055100	0.77371900	1.32918900
H	0.55783500	1.14064800	-0.42888500
H	0.45266000	1.39717100	1.37383800
H	-1.18236800	2.90144200	-0.78126900
C	-1.36610600	3.44468900	1.32917000
H	-1.31058900	2.93223300	2.29464500
C	-2.67959700	4.16179000	1.20258600
C	-3.89878500	3.53960100	1.82128800
C	-3.30585200	4.78458900	2.41915100
H	-2.81454500	4.67820600	0.25826500
H	-3.76735400	2.61186400	2.36426200
H	-4.83296500	3.61947400	1.28259700
H	-3.83842500	5.71642600	2.28602700
H	-2.77195800	4.68747700	3.35563000
O	-0.29271300	4.43045800	1.28987200
C	0.16203900	4.89850900	2.43416200
C	1.24587000	5.95410500	2.22568500
O	-0.18441000	4.57678400	3.53729100
Cl	0.56268100	7.36661400	1.39208500
Cl	2.62631100	5.27088500	1.34271100
H	1.59673900	6.27814100	3.19890800

12

E = -1263.582845

ZPVE = 0.082688

Symbol	X	Y	Z
C	-1.65533400	0.34968500	-0.10997400
H	-2.41617600	-0.39349500	-0.07081600
C	-0.79253000	1.17916100	-0.15286300
C	0.22588200	2.21857300	-0.20680300
H	0.15018800	2.79413100	-1.13173600
H	0.12621800	2.90912700	0.63325700
O	1.51816400	1.59105300	-0.14830300

C	2.54502400	2.42806400	-0.18974800
C	3.88487700	1.70409700	-0.12303200
O	2.46849400	3.62038500	-0.26965000
Cl	4.03588000	0.82763500	1.41194000
Cl	4.07596400	0.62965400	-1.52236300
H	4.66961200	2.45130500	-0.16294600

13

E = -1764.811212

ZPVE = 0.280124

Symbol	X	Y	Z
C	1.39579400	0.37447100	-0.24595900
C	2.11041600	1.75294100	-0.14472700
C	-0.45962200	2.09789900	-0.08648600
C	-0.12993700	0.58338300	-0.19167700
H	1.67930200	-0.11694500	-1.17736400
H	1.68951800	-0.26492400	0.58747200
H	-0.64269000	0.15692400	-1.05444100
H	-1.53671800	2.26027200	-0.06821900
H	3.19467600	1.63883400	-0.16587100
C	0.23722400	2.58894500	1.16303100
C	1.62326000	2.40124300	1.13339300
C	-0.37513900	3.13597800	2.27884000
C	2.39912400	2.76598700	2.22262200
C	0.40693200	3.51080700	3.37163600
H	-1.45195600	3.26808000	2.30080000
C	1.78469000	3.32678500	3.34321100
H	3.47369600	2.61800800	2.20262900
H	-0.06194600	3.94559600	4.24639500
H	2.38571600	3.61985000	4.19585100
C	0.20440200	2.74006800	-1.28556300
C	-0.43611500	3.43165500	-2.30204400
C	1.59327200	2.57165300	-1.30843700
C	0.32006200	3.96943800	-3.34423700
H	-1.51344700	3.55635900	-2.28221200
C	2.34356500	3.10159400	-2.34659800
C	1.70059600	3.80615200	-3.36543300
H	-0.17153100	4.51713600	-4.13933600
H	3.42043600	2.97144700	-2.36441400
H	2.28133200	4.22817600	-4.17708000
O	-0.59914600	-0.10996900	0.98740900
C	-1.90261100	-0.27013100	1.12351600
C	-2.25467700	-0.96855500	2.43414100
O	-2.74938600	0.07118900	0.34563700
Cl	-1.54777800	-2.59700200	2.47871600
Cl	-1.72525300	0.01948900	3.81048300
H	-3.33286100	-1.07010200	2.48571200

<u>For Table 4 (ROCOCHCl$_2$): MP2/6-31+G(d)</u>

1

E = -1416.011492

ZPVE = 0.174511

Symbol	X	Y	Z
C	-0.59142800	-0.91811800	-0.12316900
C	0.93318900	-0.84372300	-0.04624500
C	1.39778300	0.58077600	0.18503200
C	-0.66373000	1.18842000	1.21088100
C	-1.19282300	-0.23137200	1.10324200
H	2.47189700	0.66796800	0.35846300
H	1.29713500	-1.44098300	0.79971100
H	1.40785500	-1.22796700	-0.95593900
H	-0.94095500	-0.42115100	-1.03677600
H	-0.91284600	-1.96440100	-0.18113000
H	-0.97509200	1.67851100	2.13584300
H	-0.99659400	1.79658300	0.35988900
H	-0.92457700	-0.78436200	2.01288700
H	-2.28834900	-0.20544700	1.04449100
O	0.78264600	1.21208800	1.26789800
O	1.07307700	1.29989000	-1.05063000
C	1.75237600	2.43947200	-1.26434200
C	1.23368500	3.15775800	-2.50324800
O	2.67027900	2.88225800	-0.59529700
Cl	1.42270200	2.13498300	-3.93737300
Cl	-0.45208900	3.64942000	-2.25086700
H	1.83171300	4.05677300	-2.64321400

2

E = -1787.722893

ZPVE = 0.302159

Symbol	X	Y	Z
C	-2.01661800	0.77452900	0.36802600
C	-0.89787500	-0.26963400	0.29921700
C	0.44977100	0.33011000	-0.15157000
C	0.80101600	1.55312600	0.67808800
C	-0.31070500	2.58944300	0.75504000
C	-1.61730100	1.96306200	1.24360600
H	1.23878100	-0.41268500	0.06002700
H	-0.77271900	-0.71581500	1.29595100
H	-1.18979100	-1.09055900	-0.37015800
H	-2.26100600	1.13505200	-0.63861500
H	-2.92804300	0.30734600	0.76304600
H	1.74356200	2.01003900	0.36086500
H	0.00486600	3.41382200	1.40531200
H	-0.44794100	3.01603400	-0.24880900
H	-1.49364800	1.63074100	2.28239700

H	-2.41160500	2.72021000	1.24504000
Si	0.65529200	0.57563900	-2.04051900
C	-0.78895500	1.41819400	-2.91938000
H	-1.02169500	2.40795800	-2.51302100
H	-0.53213300	1.55145400	-3.97804200
H	-1.70127900	0.81318300	-2.88055300
C	2.22283400	1.58349100	-2.34404100
H	2.48110900	1.57794500	-3.40981700
H	2.10380000	2.63105900	-2.04364900
H	3.08057600	1.17516900	-1.79627800
C	0.86088900	-1.14831200	-2.77945500
H	1.73681000	-1.65856500	-2.36243900
H	-0.01481900	-1.77867000	-2.58708000
H	0.99442500	-1.09461700	-3.86632300
O	1.03255500	1.03792600	2.04667700
C	1.81787300	1.77147500	2.83392600
C	1.98032400	1.12543800	4.20450900
H	2.63486200	1.76077900	4.79897200
O	2.36761100	2.82809600	2.55140000
Cl	0.40798400	1.03417100	5.02073900
Cl	2.74398500	-0.46637100	4.04994200

3

E = -1380.123776

ZPVE = 0.198885

Symbol	X	Y	Z
C	-4.18952300	-0.71729600	-0.12870900
C	-2.68492300	-0.58107500	-0.00454100
C	-2.24758600	0.86312400	0.16953500
C	-2.93067300	1.47179300	1.39842900
C	-4.45215500	1.34624300	1.30412500
C	-4.87200100	-0.11079400	1.10123800
H	-1.15703200	0.91362800	0.26380500
H	-2.30018500	-1.20060600	0.81491900
H	-4.51410000	-0.19307700	-1.03785400
H	-4.45534500	-1.77410200	-0.24911200
H	-2.57610700	0.95836500	2.30391900
H	-2.63621500	2.52319700	1.49997700
H	-4.92290400	1.75340000	2.20760800
H	-4.81454100	1.94926000	0.45912900
H	-4.60474400	-0.69487300	1.99389800
H	-5.96063800	-0.18624100	0.99308300
H	-2.53155500	1.41892400	-0.73493500
O	-2.12854900	-1.11029800	-1.25247400
C	-0.86966300	-1.55109300	-1.20066800
O	-0.14715500	-1.59322600	-0.21437100
C	-0.38633000	-2.01533400	-2.56851500
Cl	-0.32156400	-0.63414700	-3.67951800
Cl	-1.40922900	-3.32286600	-3.18651900
H	0.62469700	-2.40120800	-2.44952900

4

E = -1380.124337

ZPVE = 0.198934

Symbol	X	Y	Z
C	-0.60580100	-0.86395000	-0.12985900
C	0.92290600	-0.82530400	-0.07657400
C	1.44175100	0.58283100	0.15948500
C	-0.71613400	1.20131600	1.31157900
C	-1.21657000	-0.23221600	1.12264400
H	2.53489600	0.60630600	0.21892500
H	1.28531000	-1.45496100	0.74875700
H	1.36089500	-1.22028600	-1.00107000
H	-0.95131500	-0.32208100	-1.01952900
H	-0.94274300	-1.90232100	-0.23879200
H	-1.13399000	1.63626100	2.22803100
H	-1.06601200	1.82304900	0.47730200
H	-0.94609000	-0.83233500	2.00450800
H	-2.31156300	-0.24543400	1.05675200
O	1.05542300	1.33453600	-1.04346400
C	1.76094900	2.43390900	-1.31269300
C	1.23434000	3.13414600	-2.55883200
O	2.70990900	2.87280700	-0.67797700
Cl	1.32479400	2.06051000	-3.96461600
Cl	-0.41705600	3.71306700	-2.26525500
H	1.86756400	3.99929200	-2.74833000
C	0.81173600	1.24820100	1.37516300
H	1.17899400	2.27713300	1.46205900
H	1.16541400	0.70976400	2.26662000

5

E = -2008.000805

ZPVE = 0.280468

Symbol	X	Y	Z
C	-1.87609200	0.10669300	0.18096500
C	-0.49102500	-0.50767200	-0.03520100
C	0.55528600	0.52925300	-0.45440800
C	0.56274200	1.72907900	0.48582100
C	-0.81311300	2.31983000	0.74848200
C	-1.81039700	1.24991200	1.19528700
H	1.55285900	0.07271200	-0.43119300
H	-0.14644700	-0.95865000	0.90528000
H	-0.52777400	-1.31174000	-0.78107500
H	-2.27728500	0.48135700	-0.77034500
H	-2.56719200	-0.67073900	0.52996000
H	1.26575800	2.49635500	0.14690200

H	-0.72024300	3.11930000	1.49314800
H	-1.15697900	2.78831300	-0.18334100
H	-1.51069200	0.85428500	2.17505200
H	-2.80095800	1.70317600	1.32539600
S	0.24655900	1.06066900	-2.18532400
C	1.66275700	2.12523600	-2.38461000
C	1.48672100	3.51349800	-2.48668800
C	2.95592400	1.58295800	-2.45201600
C	2.59604500	4.35176800	-2.64117700
H	0.48281700	3.93095200	-2.43690900
C	4.06273700	2.42573900	-2.58848100
H	3.09151400	0.50373300	-2.40317100
C	3.88521800	3.81100200	-2.68405400
H	2.45204400	5.42771300	-2.71676400
H	5.06286500	1.99910800	-2.63414200
H	4.74761300	4.46484700	-2.79474600
O	1.09467300	1.17421400	1.73843800
C	1.72349400	2.03351700	2.54509300
C	2.25484700	1.32803200	3.78583800
O	1.88356200	3.23124300	2.36059800
Cl	0.91118300	0.63731400	4.71433100
Cl	3.44947000	0.10128900	3.32782600
H	2.75129100	2.07168800	4.40716600

6

E = -4008.101080

ZPVE = 0.279548

Symbol	X	Y	Z
C	-2.00940300	0.19035300	0.26725200
C	-0.78458100	-0.68053500	0.55575200
C	0.47811300	-0.15067900	-0.12131000
C	0.70996600	1.32621700	0.16337600
C	-0.51330700	2.19828500	-0.05497800
C	-1.74399800	1.64392200	0.66512000
H	1.35590700	-0.72479900	0.19499400
H	-0.60152500	-0.69089900	1.63990100
H	-0.95430800	-1.72104900	0.25085100
H	-2.26869100	0.14163600	-0.79926400
H	-2.87335600	-0.20088300	0.81893100
H	1.57687100	1.69723600	-0.39310500
H	-0.28098900	3.21472600	0.28544200
H	-0.70135100	2.24921000	-1.13468100
H	-1.59233400	1.70500300	1.75103700
H	-2.61579800	2.26688000	0.42955200
C	2.15426700	0.20495900	-2.44205000
C	2.34565300	1.41778600	-3.11830200
C	3.25860100	-0.54581600	-2.01824500
C	3.64344600	1.87715400	-3.36741600
H	1.48405800	1.99934700	-3.44059700

C	4.55237100	-0.07493300	-2.25741700
H	3.10744000	-1.49541000	-1.50835400
C	4.74727100	1.13902400	-2.92621800
H	3.79083800	2.81902800	-3.89266500
H	5.40811000	-0.65419800	-1.91646200
H	5.75564500	1.50222400	-3.11340000
O	1.02658300	1.45550100	1.59650100
Se	0.37226000	-0.41503200	-2.08522000
C	2.27721100	1.14029600	1.94311000
C	2.49188900	1.29426100	3.44210600
O	3.17217300	0.76825300	1.19637100
Cl	2.17899300	2.96114400	3.95101400
Cl	1.47600200	0.12748500	4.31251700
H	3.53377900	1.06107500	3.65580600

7

E = -1263.845258

ZPVE = 0.131824

Symbol	X	Y	Z
C	-0.86075500	1.58444800	0.09327300
H	-0.44409800	0.57313600	0.15161300
H	-1.94768000	1.49430000	0.19439800
C	-0.32696000	2.40209900	1.24797100
H	-0.75049900	3.41095000	1.27332400
H	0.76435900	2.48276500	1.23030300
C	-0.50228300	2.23168300	-1.24408000
H	0.58279400	2.31233200	-1.36669800
H	-0.88954000	1.63819300	-2.07689600
H	-0.92750700	3.23755000	-1.32375200
O	-0.71499400	1.71215500	2.47150000
C	-0.32273800	2.29829600	3.60578800
C	-0.76991200	1.51163400	4.82995600
O	0.31671100	3.33608100	3.69862400
Cl	-2.53926000	1.43789600	4.89976500
Cl	-0.03378400	-0.10047200	4.82671500
H	-0.41707600	2.04447200	5.71127000

8

E = -1719.955320

ZPVE = 0.231045

Symbol	X	Y	Z
C	-0.83239100	0.38709600	-0.75085200
C	-0.99142300	1.94217800	-0.52980600
H	-1.73005100	2.56144900	-1.04552900
C	-0.89878400	1.72130100	1.01588300

H	-1.52882200	2.20931900	1.76482400
C	-0.75057100	0.17723900	0.79895600
H	-1.29507600	-0.60243300	1.33735300
C	0.65725100	1.87361400	0.92616100
C	0.80843400	0.32696700	0.70904700
H	1.53899300	-0.30873600	1.21888200
C	0.71420000	0.54790300	-0.84202300
H	1.32904400	0.06171700	-1.60320200
C	0.56369100	2.09296000	-0.62161600
H	1.09176600	2.87663300	-1.17209500
C	-1.65575900	-0.39295000	-1.69945800
O	-2.89415900	-0.62172100	-1.18689800
O	-1.30249400	-0.76215100	-2.81421400
C	-3.79599400	-1.31709300	-2.07985300
H	-3.39332300	-2.30010300	-2.33009400
H	-4.72696100	-1.40683000	-1.52302700
H	-3.94012300	-0.73806900	-2.99380000
C	1.49294800	2.67641600	1.85519700
H	2.55588200	2.65569500	1.58579900
H	1.38538700	2.35537800	2.89839600
O	1.00723400	4.04676900	1.73582000
C	1.63430000	4.94593600	2.50065600
C	1.05620700	6.34032500	2.30502600
O	2.55592400	4.72099300	3.27096100
Cl	-0.64689400	6.36869600	2.79534300
Cl	1.27760500	6.86346900	0.62632800
H	1.60751000	7.02257100	2.95005700

9

E = -1496.359696

ZPVE = 0.261365

Symbol	X	Y	Z
C	-2.22092100	-1.63310200	0.06071100
C	-0.69480300	-1.63917400	0.06061200
C	-0.10225500	-0.26738300	0.49001700
C	-1.14065600	0.86058700	0.69186700
C	-2.57051700	0.40572600	0.50589100
C	-2.71694800	-0.90007300	1.33049600
H	0.45866700	-0.38102500	1.42340400
H	-0.34365500	-2.41754400	0.75033900
H	-0.32673000	-1.91772400	-0.93406200
H	-2.62763700	-2.63092100	-0.15526100
H	-1.02275800	1.30813700	1.68583200
H	-3.26998700	1.23298500	0.68581000
H	-2.09966900	-0.99351500	2.23401000
H	-3.75290500	-1.12286100	1.59443300
H	0.62914900	0.07600600	-0.24952500
C	-2.77568600	-0.44592600	-0.78153300
C	-4.26488900	-0.61340200	-1.08684700

H	-4.85336500	-0.88952800	-0.20697900
H	-4.67543200	0.32234000	-1.48597800
H	-4.40732600	-1.39451800	-1.84382400
C	-2.06040900	-0.06728900	-2.07353000
H	-0.98310500	0.06099200	-1.95608000
H	-2.22971200	-0.84712200	-2.82827600
H	-2.45508300	0.87670400	-2.46731900
O	-0.92707800	1.94434800	-0.27585400
C	0.10243600	2.75227300	-0.01972900
C	0.26910700	3.79930500	-1.11267800
O	0.86064600	2.69035100	0.93871200
Cl	-1.21259600	4.74526800	-1.32085100
Cl	0.76696500	2.99479600	-2.61512400
H	1.06801900	4.47478900	-0.81117400

10

E = -1301.800307

ZPVE = 0.137891

Symbol	X	Y	Z
C	-1.90880000	0.98637000	-0.04186500
C	-0.41774400	1.05286500	0.15290800
C	-1.21119300	2.32449400	0.02140600
H	-2.29178300	0.66180800	-1.00387300
H	-2.52043400	0.69199800	0.80625900
H	0.22398000	0.76824900	-0.67448900
H	-0.02068900	0.81224700	1.13493800
H	-1.11486000	2.86854400	-0.91502100
C	-1.41991300	3.17553100	1.22881200
H	-2.24651600	3.88334200	1.11164800
H	-1.59859200	2.57332600	2.12589800
O	-0.19089800	3.94139000	1.42755000
C	-0.19138700	4.74712800	2.49213700
C	1.11967100	5.51053200	2.62060100
O	-1.10500600	4.88591300	3.29338600
Cl	1.36689800	6.54986500	1.20667400
Cl	2.46454000	4.38198900	2.86400600
H	1.04686100	6.14649500	3.50120800

11

E = -1418.042092

ZPVE = 0.201128

Symbol	X	Y	Z
C	-1.46996000	1.02803300	0.40798000
C	-0.02438400	1.45066000	0.42400200
C	-1.10420700	2.47987300	0.22011300

H	-1.84215300	0.48397000	-0.45447200
H	-1.92483900	0.73880600	1.35109300
H	0.59978300	1.19422300	-0.42611900
H	0.49376500	1.45473400	1.37935800
H	-1.21073700	2.88805300	-0.78325100
C	-1.39899000	3.44464000	1.32637400
H	-1.33200300	2.94697100	2.30223100
C	-2.70854800	4.16002500	1.18825600
C	-3.93716000	3.56314600	1.82925800
C	-3.33070100	4.82148900	2.39234700
H	-2.84967000	4.65750000	0.23014900
H	-3.81549600	2.64594100	2.39846300
H	-4.87522800	3.63345800	1.28760800
H	-3.85465300	5.75943400	2.23645800
H	-2.79765800	4.74715000	3.33538000
O	-0.32582400	4.45681400	1.27280300
C	0.19020500	4.85703400	2.43381000
C	1.25905600	5.92216800	2.22377200
O	-0.10571300	4.45924400	3.55348400
Cl	0.53907400	7.36699500	1.49111900
Cl	2.59409500	5.27420300	1.25497500
H	1.65119000	6.19721100	3.20139800

12

E = -1261.470132

ZPVE = 0.081565

Symbol	X	Y	Z
C	-1.67752400	0.34100600	-0.10823100
H	-2.43125700	-0.41531000	-0.06951000
C	-0.78801100	1.17624600	-0.15256100
C	0.21857900	2.22626300	-0.20784300
H	0.15693200	2.80174900	-1.13632100
H	0.13260500	2.91830600	0.63520700
O	1.52281500	1.57761100	-0.14725200
C	2.55626000	2.42952500	-0.18938100
C	3.88917800	1.69935500	-0.12267900
O	2.47647400	3.64601700	-0.27089200
Cl	4.03216100	0.82644400	1.41166700
Cl	4.07228800	0.63104100	-1.52328600
H	4.67576400	2.45112400	-0.16195700

13

E = -1761.192493

ZPVE = 0.278505

Symbol	X	Y	Z
C	1.38164100	0.36687000	-0.29188300

C	2.09881300	1.73958800	-0.15232400
C	-0.47073900	2.09323000	-0.11694900
C	-0.13992900	0.58183800	-0.21388100
H	1.65585800	-0.09220100	-1.24884400
H	1.68646600	-0.31065500	0.51413600
H	-0.68238800	0.12633300	-1.04957900
H	-1.55309400	2.26095100	-0.10673700
H	3.18982100	1.62278000	-0.16178400
C	0.21121200	2.57716900	1.13672900
C	1.60257300	2.37589000	1.12305700
C	-0.41730800	3.12806700	2.25361900
C	2.37068200	2.72045700	2.23665800
C	0.35715500	3.49188800	3.36294800
H	-1.49729100	3.27615900	2.26067400
C	1.74275900	3.28486800	3.35578900
H	3.44893100	2.56008600	2.23396100
H	-0.11993200	3.93314900	4.23612000
H	2.33573900	3.56559800	4.22426200
C	0.20439900	2.74307800	-1.29856200
C	-0.43152200	3.44338700	-2.32534600
C	1.60089500	2.57857600	-1.30402600
C	0.34003000	3.99114100	-3.35910400
H	-1.51428900	3.56708900	-2.31828800
C	2.36687000	3.11434600	-2.34043800
C	1.73158700	3.82998300	-3.36497200
H	-0.14397600	4.54612300	-4.16039400
H	3.44919100	2.98542100	-2.34899400
H	2.32237600	4.25947200	-4.17184000
O	-0.56793100	-0.09230300	1.01164600
C	-1.88343200	-0.24761800	1.18030900
C	-2.18891300	-0.93709600	2.50348300
O	-2.76641300	0.09513200	0.40585300
Cl	-1.49428100	-2.56855600	2.51513400
Cl	-1.60181400	0.05107100	3.85164700
H	-3.27054700	-1.02857500	2.58932100

<u>For Table 4 ($ROCOCF_3$): B3LYP/6-311++G(d,p)</u>

1

E = -797.446283

ZPVE = 0.164848

Symbol	X	Y	Z
C	-0.58803700	-0.93616400	-0.11943900
C	0.93693100	-0.78110000	-0.06266400
C	1.35204500	0.65473600	0.23162700
C	-0.74697100	1.14005700	1.27615600
C	-1.21937200	-0.30091000	1.12635900
H	2.41654500	0.75791900	0.43085300
H	1.34420600	-1.39565100	0.74733400
H	1.41278300	-1.10719000	-0.99050100

H	-0.97511700	-0.44847300	-1.01999500
H	-0.85178500	-1.99449400	-0.19199500
H	-1.06653600	1.58005200	2.22054100
H	-1.12835400	1.76168800	0.45839600
H	-0.93826700	-0.86886400	2.02036200
H	-2.31189700	-0.31434700	1.06301700
O	0.69494800	1.23525700	1.30197000
O	1.06263300	1.43237500	-1.00024600
C	1.86574100	2.44986600	-1.29487500
C	1.32100800	3.17652800	-2.55708800
O	2.86389200	2.79692800	-0.73344000
F	1.25892900	2.33263500	-3.60557900
F	2.10644600	4.20037100	-2.89063600
F	0.07972800	3.65127200	-2.33319600

2

E = -1170.141035

ZPVE = 0.289385

Symbol	X	Y	Z
C	-2.07338900	0.63511300	0.36302800
C	-0.87407400	-0.32292200	0.29891000
C	0.44076100	0.37358700	-0.13560800
C	0.70070300	1.63452900	0.68800100
C	-0.50051900	2.57362300	0.79835000
C	-1.77374200	1.84807400	1.25339300
H	1.26955700	-0.31122100	0.09436300
H	-0.72647800	-0.76198000	1.29236400
H	-1.09641000	-1.15968100	-0.37027700
H	-2.33410700	0.98116000	-0.64328600
H	-2.94903700	0.09938100	0.74285800
H	1.57780500	2.17735200	0.33643900
H	-0.25310000	3.39980900	1.47014000
H	-0.65973800	3.01748000	-0.19071700
H	-1.65212400	1.51765900	2.29060100
H	-2.61549800	2.54698700	1.24472300
Si	0.69279400	0.59081200	-2.03567200
C	-0.63423800	1.60688800	-2.92163900
H	-0.70991800	2.62808800	-2.53818600
H	-0.38452500	1.67799300	-3.98566700
H	-1.62365400	1.14737500	-2.85001600
C	2.37313900	1.41182100	-2.31719200
H	2.62199600	1.40759700	-3.38316100
H	2.38965600	2.45446200	-1.98615700
H	3.17531500	0.88398500	-1.79211800
C	0.71931200	-1.14484200	-2.78274900
H	1.48804600	-1.77021200	-2.31868000
H	-0.24000700	-1.65779700	-2.66910300
H	0.93751100	-1.09515700	-3.85416500
O	1.04825100	1.16729600	2.06360800
C	1.87460600	1.90907900	2.77831500

C	2.11711200	1.22730500	4.15490200
O	2.39700100	2.94707600	2.47641000
F	2.65777800	0.00337200	3.99570300
F	0.95813000	1.08369500	4.82805500
F	2.94656400	1.95476300	4.90463200

3

E = -761.513526

ZPVE = 0.188687

Symbol	X	Y	Z
C	-4.14781100	-0.72511200	-0.13306800
C	-2.64147800	-0.54872700	0.00527800
C	-2.23923100	0.91114000	0.19643000
C	-2.96252300	1.50938800	1.41486500
C	-4.48458800	1.34270600	1.30595800
C	-4.87094400	-0.12671700	1.08486800
H	-1.15552100	0.98580100	0.31781100
H	-2.25352300	-1.15624100	0.82645100
H	-4.47772200	-0.22115500	-1.04853600
H	-4.38655400	-1.78635100	-0.24526100
H	-2.60570000	1.01586200	2.32748400
H	-2.69808000	2.56622900	1.51189600
H	-4.97120200	1.72814700	2.20710600
H	-4.85627200	1.94508600	0.46743800
H	-4.61808100	-0.70774300	1.98074500
H	-5.95203400	-0.22272800	0.94957600
H	-2.50963000	1.46769100	-0.70833800
O	-2.04061400	-1.06836800	-1.23405000
C	-0.82396000	-1.58558500	-1.16602500
O	-0.11861000	-1.70010300	-0.20273400
C	-0.38957900	-2.06408800	-2.57985200
F	-0.36328600	-1.03160600	-3.44481500
F	-1.24572000	-2.98637900	-3.05937700
F	0.82849800	-2.60615100	-2.53991200

4

E = -761.512576

ZPVE = 0.188754

Symbol	X	Y	Z
C	-0.60838000	-0.87873800	-0.13800100
C	0.92433400	-0.78239100	-0.11159700
C	1.42106100	0.63181300	0.17337700
C	-0.76874100	1.15095600	1.37223600
C	-1.23107400	-0.29450700	1.13812900
H	2.50746400	0.65880000	0.26408400
H	1.32203200	-1.42630300	0.68218200

H	1.35663600	-1.13623100	-1.05167200
H	-0.98913600	-0.33760600	-1.01075400
H	-0.90516300	-1.92424200	-0.26406500
H	-1.17944200	1.53701600	2.30990900
H	-1.15943100	1.79108000	0.57360500
H	-0.94430000	-0.91219100	1.99964800
H	-2.32278600	-0.33487200	1.07626100
O	1.07851000	1.43578300	-1.02059400
C	1.84996800	2.46960200	-1.31328100
C	1.31338800	3.16176700	-2.59776800
O	2.82076400	2.86204500	-0.72811600
F	1.29291200	2.30273200	-3.63474200
F	2.08099000	4.20014000	-2.93074500
F	0.05699300	3.61073200	-2.40598300
C	0.76329800	1.25414200	1.40564000
H	1.09067400	2.29165600	1.51256800
H	1.15183500	0.71544500	2.27867300

5

E = -1390.746364

ZPVE = 0.270173

Symbol	X	Y	Z
C	-1.85140200	-0.01483100	0.15946500
C	-0.40086800	-0.46589000	-0.06591600
C	0.55000200	0.70167400	-0.37370000
C	0.41969700	1.83740700	0.64885900
C	-1.02264600	2.25211400	0.93488200
C	-1.93166900	1.05700800	1.25521500
H	1.58153900	0.34679200	-0.37047900
H	-0.03259100	-0.95443900	0.84314300
H	-0.34063700	-1.20398800	-0.86973400
H	-2.26910400	0.38036500	-0.77389100
H	-2.46280900	-0.88021700	0.43159000
H	1.02171000	2.69652600	0.35505100
H	-1.02921700	2.98698800	1.74393600
H	-1.38857400	2.76657700	0.04060500
H	-1.63824400	0.61848000	2.21553200
H	-2.96164000	1.40604900	1.37277500
S	0.23124100	1.33549000	-2.09593400
C	1.74401300	2.25436700	-2.41494900
C	1.70235700	3.64849800	-2.51267800
C	2.95456800	1.58366100	-2.62443100
C	2.86251500	4.36439700	-2.80747000
H	0.76383100	4.16746900	-2.35859000
C	4.11328000	2.30399100	-2.90321300
H	2.98425500	0.50107200	-2.57973700
C	4.06931900	3.69519800	-2.99714900
H	2.82146200	5.44523900	-2.88153000
H	5.04788800	1.77741300	-3.06080000
H	4.97132000	4.25320900	-3.22086400

O	1.02886400	1.29848200	1.88787000
C	1.60937500	2.15496300	2.71444800
C	2.19634600	1.37778200	3.92627600
O	1.70386900	3.34493100	2.60471800
F	1.22231700	0.72426600	4.59003900
F	2.79432200	2.21185100	4.77741000
F	3.10284000	0.46826600	3.51929900

6

E = -3394.078896

ZPVE = 0.268902

Symbol	X	Y	Z
C	-2.00892600	0.15070300	0.30970500
C	-0.74315200	-0.71215200	0.41616100
C	0.48902100	-0.04301900	-0.20638500
C	0.69043300	1.38984400	0.29091300
C	-0.57681200	2.24347300	0.26192500
C	-1.77881800	1.54361100	0.91216600
H	1.38564600	-0.62393800	0.00869500
H	-0.51988600	-0.88680100	1.47552800
H	-0.89844000	-1.69335700	-0.03929600
H	-2.30834800	0.24880500	-0.74106600
H	-2.83612200	-0.35047400	0.82085000
H	1.50420800	1.88051800	-0.24129000
H	-0.37025600	3.20531500	0.73815700
H	-0.79425800	2.45474000	-0.78990700
H	-1.61006500	1.44867500	1.99060400
H	-2.67062700	2.16487600	0.78889600
C	2.24242900	0.16722900	-2.61675400
C	2.70218100	1.38862200	-3.11630700
C	3.13614600	-0.89507800	-2.44794200
C	4.05106400	1.54796400	-3.43540600
H	2.00943700	2.21004500	-3.25408700
C	4.48449100	-0.72653500	-2.75724000
H	2.77704700	-1.85101200	-2.08505900
C	4.94337100	0.49397000	-3.25225100
H	4.40215800	2.49835000	-3.82143300
H	5.17372800	-1.55248600	-2.62121800
H	5.99182900	0.62097400	-3.49667500
O	1.14009700	1.23934600	1.69893300
Se	0.35604800	-0.06637600	-2.21633800
C	1.94996500	2.16377800	2.19091300
C	2.31154200	1.79856700	3.65829400
O	2.37425100	3.14510400	1.64814300
F	2.91088700	0.59392200	3.72001900
F	3.13918700	2.70426300	4.18038000
F	1.20286900	1.74986500	4.42334800

7

E = -644.809923

ZPVE = 0.123007

Symbol	X	Y	Z
C	-0.85664700	1.59148900	0.10611000
H	-0.44291300	0.58105600	0.17576000
H	-1.94109400	1.49975800	0.21818500
C	-0.31187600	2.42712000	1.24858300
H	-0.73193200	3.43559600	1.26015900
H	0.77708500	2.50959800	1.21800700
C	-0.51571100	2.21029800	-1.25344900
H	0.56575200	2.28925900	-1.39843100
H	-0.91412900	1.59790100	-2.06501400
H	-0.94100800	3.21302700	-1.35577200
O	-0.68164500	1.76789300	2.49710200
C	-0.28793900	2.35349800	3.61881000
C	-0.76689100	1.51674600	4.83711200
O	0.34029300	3.36787700	3.73226000
F	-2.10910500	1.41070700	4.84617900
F	-0.38437800	2.08972100	5.97870700
F	-0.25150600	0.27347800	4.79453700

8

E = -1102.340292

ZPVE = 0.222330

Symbol	X	Y	Z
C	-0.83358200	0.35447000	-0.75854900
C	-1.02897800	1.90602100	-0.52605100
H	-1.78633900	2.51077500	-1.01896100
C	-0.89946100	1.69750300	1.02060900
H	-1.53963600	2.15721100	1.77078700
C	-0.71062400	0.15719700	0.80375400
H	-1.21318500	-0.62891900	1.36260800
C	0.65674400	1.90258100	0.91028200
C	0.84153200	0.35347900	0.68835300
H	1.59097300	-0.26431900	1.18092000
C	0.71158900	0.56057900	-0.86289700
H	1.33739300	0.09527100	-1.62012400
C	0.52200100	2.10432000	-0.64425600
H	1.00939600	2.88956900	-1.21876200
C	-1.64538500	-0.48776900	-1.67558300
O	-2.94892100	-0.48220200	-1.31290200
O	-1.22060700	-1.10281900	-2.62596100
C	-3.83841400	-1.26152800	-2.13472900
H	-3.54425100	-2.31198200	-2.12549500
H	-4.82530900	-1.13593500	-1.69479700
H	-3.82653400	-0.89601700	-3.16249600
C	1.51105500	2.69941500	1.83466400

H	2.56444800	2.67983000	1.54107400
H	1.43391100	2.35231700	2.86897000
O	1.05067100	4.08798700	1.78528500
C	1.69502200	4.95407900	2.55458600
C	1.07397100	6.36706200	2.37726300
O	2.61572300	4.73446300	3.28940600
F	-0.22655500	6.36276800	2.72720000
F	1.15867100	6.76818100	1.09470500
F	1.70962200	7.25810600	3.13806100

9

E = -878.166905

ZPVE = 0.249894

Symbol	X	Y	Z
C	-2.25183700	-1.64841900	0.09204400
C	-0.72075200	-1.70914100	0.10687000
C	-0.06718900	-0.32800200	0.43062700
C	-1.07370900	0.83312200	0.65426100
C	-2.52591600	0.42680400	0.46298600
C	-2.73091200	-0.84802500	1.33363000
H	0.56361300	-0.41090600	1.31692200
H	-0.40745900	-2.44335200	0.85527700
H	-0.35436000	-2.07607600	-0.85579700
H	-2.68599100	-2.63671700	-0.08347300
H	-0.94655500	1.25061400	1.65401100
H	-3.18906700	1.28178600	0.61627600
H	-2.13175200	-0.93433700	2.24457000
H	-3.77488800	-1.01817000	1.58911800
H	0.60331800	-0.03957600	-0.38038800
C	-2.77176500	-0.46904300	-0.80388500
C	-4.27420500	-0.59469800	-1.10076500
H	-4.87141300	-0.82110900	-0.21551400
H	-4.65697500	0.33679700	-1.52966000
H	-4.44959100	-1.39162100	-1.83039500
C	-2.05170400	-0.16291100	-2.11911100
H	-0.97281000	-0.05639300	-2.01767900
H	-2.24134900	-0.96452800	-2.84113700
H	-2.42771300	0.76749300	-2.55409600
O	-0.80089300	1.94628200	-0.27893300
C	0.14798700	2.80389000	0.05812500
C	0.25849300	3.90525800	-1.03301300
O	0.84809400	2.79017400	1.03237900
F	-0.91638500	4.54196600	-1.19846200
F	0.60837300	3.36459300	-2.21741800
F	1.18014600	4.80974500	-0.69946600

10

E = -682.880876

ZPVE = 0.128913

Symbol	X	Y	Z
C	-1.91114800	0.99723900	-0.07613100
C	-0.42229600	1.01967200	0.15357500
C	-1.18212000	2.31744000	0.03853600
H	-2.28161800	0.71164800	-1.05258200
H	-2.54780600	0.69339100	0.74702300
H	0.23054100	0.74390100	-0.66499500
H	-0.05506200	0.73532100	1.13291600
H	-1.05123600	2.87900000	-0.88026700
C	-1.41603400	3.15922000	1.25204700
H	-2.25022400	3.85248400	1.12471500
H	-1.60251500	2.55332600	2.14158800
O	-0.21005400	3.95719100	1.49203200
C	-0.23547400	4.76439500	2.54145000
C	1.10959700	5.53653300	2.63630100
O	-1.12772000	4.91408300	3.32839100
F	1.32231800	6.26488000	1.52401800
F	2.14098300	4.68255800	2.77842000
F	1.10347300	6.36297900	3.68286600

11

E = -799.548841

ZPVE = 0.190706

Symbol	X	Y	Z
C	-1.47268300	1.03885200	0.38720100
C	-0.01955700	1.43106800	0.46117500
C	-1.07340100	2.48981400	0.25161100
H	-1.83004900	0.53010200	-0.49948600
H	-1.95935900	0.72752300	1.30403000
H	0.62579200	1.18955700	-0.37410900
H	0.46688800	1.38565200	1.42895600
H	-1.13838800	2.91807200	-0.74365500
C	-1.40624100	3.45258700	1.35753900
H	-1.35303700	2.95875500	2.32981800
C	-2.72673500	4.15538800	1.19401600
C	-3.96912000	3.55621700	1.81104900
C	-3.38719100	4.82660400	2.37463600
H	-2.85177700	4.63892300	0.23015700
H	-3.86145600	2.65016500	2.39575900
H	-4.88950100	3.61116700	1.24303900
H	-3.90981500	5.75787500	2.19458100
H	-2.88649000	4.76937900	3.33377300
O	-0.33829000	4.48917000	1.34396600
C	0.23374400	4.82142000	2.48686700
C	1.30638200	5.91624600	2.22386600
O	0.01802000	4.38847100	3.58596100
F	0.74763700	7.01145800	1.67419200

F	2.25438500	5.46516600	1.38013900
F	1.90029100	6.27827200	3.36255300

12

E = -642.358185

ZPVE = 0.075570

Symbol	X	Y	Z
C	-1.62777200	0.32124600	-0.10810500
H	-2.37137600	-0.43758400	-0.06874200
C	-0.78246200	1.17198600	-0.15203700
C	0.20497300	2.23243300	-0.20810700
H	0.12252100	2.80767300	-1.13323600
H	0.09952900	2.92247900	0.63229600
O	1.53564500	1.63412700	-0.15190500
C	2.54940200	2.49300500	-0.19344300
C	3.89218600	1.71465400	-0.12417400
O	2.48476300	3.68631800	-0.27108600
F	4.92108200	2.56080700	-0.16950300
F	3.99929500	0.85922100	-1.15615600
F	3.97254400	1.00820900	1.01733400

13

E = -1143.782037

ZPVE = 0.271166

Symbol	X	Y	Z
C	1.35320100	0.36841800	-0.15851800
C	2.10524000	1.73743400	-0.11922800
C	-0.45529500	2.15011600	-0.01717700
C	-0.16935300	0.62340900	-0.13853000
H	1.63258700	-0.18564800	-1.05663600
H	1.62634100	-0.23423600	0.70922000
H	-0.66992300	0.22987200	-1.02178500
H	-1.52769900	2.34113000	0.01789000
H	3.18533600	1.58996600	-0.16007200
C	0.28062200	2.65397900	1.21097500
C	1.66517700	2.43824200	1.15295700
C	-0.28872200	3.26758100	2.31982500
C	2.47941900	2.83705200	2.20617600
C	0.53182400	3.67537700	3.37512400
H	-1.36036100	3.43185800	2.36623000
C	1.90746700	3.46104200	3.31859900
H	3.55091900	2.66934700	2.16485800
H	0.09497600	4.15982500	4.24098100
H	2.53829700	3.78029800	4.14057300
C	0.20143700	2.76366100	-1.24345400

C	-0.43936400	3.46843700	-2.25521100
C	1.58664500	2.54843900	-1.29463800
C	0.31185000	3.97279700	-3.32091000
H	-1.51162700	3.62998300	-2.21650300
C	2.33117800	3.04571000	-2.35738100
C	1.68838700	3.76289500	-3.37108400
H	-0.17971700	4.52999200	-4.11029700
H	3.40325600	2.88238900	-2.39978600
H	2.26524200	4.15823700	-4.19963100
O	-0.71656500	-0.09827400	1.01681100
C	-2.00773400	-0.39557700	0.99943600
C	-2.37629400	-1.16858900	2.29659200
O	-2.81415300	-0.13821500	0.14972900
F	-1.61650600	-2.27089000	2.43493300
F	-3.65630800	-1.54380800	2.27023500
F	-2.18616300	-0.39208100	3.37994300

For Table 4 ($ROCOCF_3$): M06-2X/6-311++G(d,p)

1

E = -797.153933

ZPVE = 0.168066

Symbol	X	Y	Z
C	-0.58398300	-0.91000000	-0.13867700
C	0.94064500	-0.83785400	-0.04609500
C	1.40329700	0.58708900	0.19856800
C	-0.65801300	1.19237300	1.19969700
C	-1.19510500	-0.22567300	1.08510900
H	2.47278600	0.66289000	0.38844000
H	1.29302600	-1.43466200	0.80029100
H	1.42277400	-1.21648700	-0.94910300
H	-0.91897800	-0.40395300	-1.04929800
H	-0.90622500	-1.95057900	-0.20698500
H	-0.98208900	1.67943300	2.11801900
H	-0.99109100	1.79742600	0.34838800
H	-0.93614500	-0.78151800	1.99206000
H	-2.28501000	-0.19286100	1.01511300
O	0.77273400	1.21176700	1.25699600
O	1.11714000	1.31916900	-1.03116900
C	1.79739300	2.43909400	-1.23149900
C	1.24045000	3.14493700	-2.48730600
O	2.69652600	2.87927100	-0.58902700
F	1.31760300	2.34604500	-3.55344200
F	1.91608100	4.25318500	-2.74126900
F	-0.04431900	3.46339800	-2.30185100

2

E = -1169.751566

ZPVE = 0.293537

Symbol	X	Y	Z
C	-1.98831700	0.83141800	0.36287000
C	-0.89986600	-0.24567900	0.29734500
C	0.46611400	0.31380100	-0.15289900
C	0.85771500	1.52954200	0.67300700
C	-0.22784900	2.59831900	0.72966600
C	-1.55204700	2.01536700	1.22784400
H	1.22980300	-0.45067400	0.04663000
H	-0.78876100	-0.69081800	1.29210600
H	-1.21221200	-1.05453100	-0.37115200
H	-2.22053500	1.19372500	-0.64273200
H	-2.90826300	0.39573100	0.76101400
H	1.80519700	1.95733300	0.33981800
H	0.10755900	3.42634800	1.35801700
H	-0.35021100	2.99683200	-0.28425700
H	-1.43287600	1.68615800	2.26552300
H	-2.32022800	2.79207100	1.22715000
Si	0.64571500	0.56325400	-2.03884800
C	-0.84859100	1.32746800	-2.89025200
H	-1.10791500	2.31405100	-2.49976300
H	-0.62311600	1.44238400	-3.95483200
H	-1.72990300	0.68621000	-2.81005100
C	2.15096300	1.64303000	-2.36337300
H	2.36735100	1.67885900	-3.43442300
H	1.99552400	2.67142300	-2.02524600
H	3.04032100	1.25491900	-1.85906000
C	0.91532500	-1.14694400	-2.77048100
H	1.82831800	-1.60502200	-2.38168800
H	0.08121000	-1.81483100	-2.53883500
H	1.00386200	-1.09490600	-3.85874400
O	1.08916700	1.03595900	2.03811300
C	1.82402900	1.78356800	2.83214100
C	1.91676700	1.11198600	4.22044300
O	2.35892800	2.82226900	2.58454600
F	2.43694600	-0.11301900	4.12143100
F	0.69987700	1.00150800	4.76197100
F	2.67547700	1.82543900	5.03740300

3

E = -761.223756

ZPVE = 0.191815

Symbol	X	Y	Z
C	-4.17622400	-0.71679900	-0.14370100
C	-2.67097700	-0.58654300	0.00035700
C	-2.23474900	0.85953900	0.18535800
C	-2.93271500	1.46200900	1.40893500
C	-4.45368700	1.34333000	1.29054400

C	-4.87355400	-0.11321200	1.07913300
H	-1.14922100	0.90879400	0.29392300
H	-2.30841500	-1.19636700	0.83365400
H	-4.48421500	-0.18576100	-1.05099700
H	-4.44312000	-1.76827700	-0.27169900
H	-2.59633700	0.93805800	2.31126700
H	-2.63567900	2.50679200	1.52250200
H	-4.93530900	1.74927200	2.18338800
H	-4.79745800	1.94451000	0.44061400
H	-4.61415700	-0.69715400	1.97011800
H	-5.95636200	-0.18773200	0.95774000
H	-2.51170900	1.41848400	-0.71560800
O	-2.08941800	-1.12632600	-1.21822300
C	-0.83326000	-1.52004400	-1.16023700
O	-0.10159200	-1.50829300	-0.21749800
C	-0.39307500	-2.03330900	-2.54914500
F	-0.46941700	-1.05280800	-3.45222100
F	-1.17910200	-3.03222100	-2.95493100
F	0.85559100	-2.47094600	-2.50933300

4

E = -761.223744

ZPVE = 0.191922

Symbol	X	Y	Z
C	-0.59709400	-0.85721800	-0.15337600
C	0.93213300	-0.82652400	-0.08607900
C	1.45846500	0.57934700	0.15752500
C	-0.71109600	1.20168800	1.29575600
C	-1.21597400	-0.22953800	1.09766100
H	2.54674500	0.58949200	0.24074000
H	1.28039100	-1.45221600	0.74296300
H	1.37448400	-1.22393200	-1.00248200
H	-0.92759300	-0.30435700	-1.03839800
H	-0.93747100	-1.88815200	-0.27454400
H	-1.13451700	1.63713100	2.20368600
H	-1.04738000	1.82271000	0.45835500
H	-0.95024000	-0.83133500	1.97568400
H	-2.30606100	-0.23870300	1.02420900
O	1.11417000	1.34304700	-1.03879800
C	1.78378700	2.45583900	-1.25587000
C	1.23546900	3.13839700	-2.52834700
O	2.67489300	2.91767300	-0.61022300
F	1.32355700	2.32297700	-3.58063900
F	1.91230500	4.24393000	-2.79476900
F	-0.05077400	3.45938700	-2.36023500
C	0.81725000	1.23933000	1.37383300
H	1.18947200	2.26105900	1.47575900
H	1.15748400	0.68659500	2.25658400

5

E = -1390.336650

ZPVE = 0.274385

Symbol	X	Y	Z
C	-1.82281000	0.09505900	0.19125900
C	-0.42247800	-0.48650600	-0.02146100
C	0.59868900	0.58322000	-0.42139000
C	0.58400600	1.76391200	0.54848400
C	-0.81025200	2.31951900	0.81139200
C	-1.78868900	1.21910200	1.22906800
H	1.60293200	0.15469200	-0.42997300
H	-0.07473500	-0.93590800	0.91449200
H	-0.43404700	-1.27587800	-0.77639000
H	-2.21342400	0.48312700	-0.75575100
H	-2.50053300	-0.69855700	0.51391400
H	1.26507100	2.54970000	0.21581100
H	-0.74301300	3.10637200	1.56563800
H	-1.15165800	2.78887700	-0.11597500
H	-1.48507200	0.80804500	2.19821200
H	-2.78445400	1.64727800	1.36281000
S	0.24494900	1.14449900	-2.13670700
C	1.68287700	2.16701700	-2.41880400
C	1.53950500	3.55006700	-2.52262300
C	2.94612900	1.58899200	-2.55174200
C	2.65495100	4.35021100	-2.75285200
H	0.55555100	3.99237200	-2.41876300
C	4.05924700	2.39325300	-2.76636500
H	3.05022500	0.51130300	-2.49537900
C	3.91494500	3.77425900	-2.86923900
H	2.53781200	5.42432400	-2.83284300
H	5.03845200	1.94005600	-2.86539400
H	4.78317900	4.39862900	-3.04223700
O	1.12874500	1.21771000	1.78907700
C	1.62454900	2.07722400	2.65723500
C	2.11314200	1.31029900	3.90574200
O	1.70616800	3.26259600	2.55505900
F	1.09402600	0.66385700	4.47889900
F	2.63360900	2.14337400	4.79216600
F	3.03993300	0.40906400	3.57467800

6

E = -3393.702416

ZPVE = 0.273147

Symbol	X	Y	Z
C	-1.95670700	0.23986600	0.30765800
C	-0.76608800	-0.71060600	0.45823800

C	0.49772100	-0.17032900	-0.21390600
C	0.81371700	1.25408100	0.23228500
C	-0.37754500	2.20149000	0.14923000
C	-1.60978600	1.62725900	0.85263100
H	1.35290300	-0.80828500	0.01323900
H	-0.54217100	-0.83398800	1.52369300
H	-0.99841300	-1.70073600	0.06004700
H	-2.24059300	0.32148200	-0.74801000
H	-2.82002500	-0.17024600	0.83653200
H	1.67387900	1.65261800	-0.30909900
H	-0.09109600	3.16868700	0.56771200
H	-0.59312800	2.35998800	-0.91129000
H	-1.41636900	1.55368400	1.92851600
H	-2.45276500	2.31015300	0.72680000
C	2.15385900	0.11325400	-2.59140500
C	2.53141600	1.36564500	-3.07364900
C	3.11583300	-0.87882400	-2.40110800
C	3.86927800	1.62541700	-3.35813500
H	1.78035000	2.13295700	-3.22041100
C	4.45233000	-0.61063400	-2.67705800
H	2.81537800	-1.85752400	-2.04501900
C	4.82972800	0.64037200	-3.15658500
H	4.15924100	2.60051700	-3.73098200
H	5.19746300	-1.38263500	-2.52559200
H	5.87097100	0.84575500	-3.37423200
O	1.21529200	1.11304900	1.63241000
Se	0.30438100	-0.24521100	-2.18634000
C	1.94552500	2.08175600	2.14790100
C	2.23763000	1.76163400	3.63054800
O	2.34277400	3.07005500	1.61108600
F	2.86968200	0.59224600	3.74682200
F	2.99215900	2.70381100	4.17260900
F	1.09550200	1.68457100	4.31984100

7

E = -644.567165

ZPVE = 0.125388

Symbol	X	Y	Z
C	-0.86071000	1.58070500	0.11299200
H	-0.44218900	0.57352700	0.17968800
H	-1.94408200	1.48859500	0.22178900
C	-0.32246300	2.41163600	1.25609300
H	-0.74471700	3.41949900	1.26532400
H	0.76644300	2.49747800	1.22405000
C	-0.51035400	2.21739500	-1.23004200
H	0.57160700	2.30087500	-1.35707900
H	-0.89775300	1.61881100	-2.05481600
H	-0.93711900	3.21957700	-1.31508700
O	-0.69013100	1.75417800	2.48882000

C	-0.29289500	2.34643300	3.59810700
C	-0.76197000	1.52603700	4.81921400
O	0.33182400	3.35744400	3.69619300
F	-2.09296100	1.43175900	4.83576500
F	-0.36659200	2.10043200	5.94373700
F	-0.25958400	0.29063900	4.77409500

8

E = -1101.945813

ZPVE = 0.226771

Symbol	X	Y	Z
C	-0.81889100	0.36957500	-0.74476700
C	-1.01069100	1.90829700	-0.51121500
H	-1.76721900	2.51290000	-1.00295300
C	-0.88088900	1.69316000	1.02794900
H	-1.51079600	2.15631600	1.78294800
C	-0.70151100	0.15917100	0.80329300
H	-1.21116700	-0.62801900	1.35174900
C	0.66553700	1.88388500	0.91291800
C	0.84602700	0.34702700	0.68913000
H	1.59326000	-0.27184400	1.18052300
C	0.71655700	0.56172300	-0.85500600
H	1.33136500	0.09369100	-1.61817500
C	0.53508300	2.09903300	-0.62880900
H	1.02843100	2.88771800	-1.19118900
C	-1.64217100	-0.46057200	-1.65914700
O	-2.93425100	-0.44391600	-1.28993600
O	-1.23202800	-1.07240100	-2.60961900
C	-3.81677300	-1.20974800	-2.11219300
H	-3.52190600	-2.25938700	-2.10877900
H	-4.80593000	-1.08736400	-1.67936200
H	-3.79632500	-0.83867500	-3.13716700
C	1.51029700	2.69191700	1.83307600
H	2.56380800	2.68076300	1.53980500
H	1.43273400	2.34999600	2.86902800
O	1.02913900	4.05458700	1.76325200
C	1.66406700	4.92761200	2.52203600
C	1.03266600	6.32495300	2.34090200
O	2.58423600	4.71880300	3.25073800
F	-0.25327800	6.30502800	2.69757300
F	1.10294000	6.70869200	1.06490400
F	1.66261900	7.21877300	3.08545700

9

E = -877.834257

ZPVE = 0.254024

Symbol	X	Y	Z
C	-2.22652200	-1.62914600	0.06498600
C	-0.69973000	-1.64197300	0.08198700
C	-0.10423900	-0.27285800	0.51743500
C	-1.13965200	0.86381300	0.70523000
C	-2.57192400	0.41188800	0.50891500
C	-2.73430800	-0.89342600	1.32898200
H	0.43902600	-0.38659600	1.45588400
H	-0.36042700	-2.41757100	0.77315500
H	-0.32571300	-1.91817100	-0.90672200
H	-2.63456000	-2.61830600	-0.15630700
H	-1.02853200	1.30117900	1.70006800
H	-3.26611400	1.23804800	0.67854300
H	-2.12846500	-0.98925600	2.23395200
H	-3.77129200	-1.10989300	1.57328100
H	0.63991500	0.05945200	-0.20852300
C	-2.76034800	-0.43692500	-0.78454000
C	-4.24389700	-0.59491100	-1.11775400
H	-4.84656200	-0.87059500	-0.25095600
H	-4.64203600	0.34110800	-1.51944300
H	-4.37660100	-1.37002300	-1.87776700
C	-2.01291500	-0.05831300	-2.05870500
H	-0.93936900	0.06070700	-1.91602700
H	-2.16919100	-0.83113400	-2.81782900
H	-2.39279500	0.88638300	-2.45601200
O	-0.90976300	1.95100200	-0.23929900
C	0.14410700	2.70687700	-0.01593500
C	0.24068800	3.78610100	-1.11608700
O	0.93768200	2.61440900	0.87131400
F	-0.86137500	4.53779800	-1.14121300
F	0.37665000	3.21112300	-2.31447500
F	1.28309400	4.57471200	-0.90823300

10

E = -682.631776

ZPVE = 0.131502

Symbol	X	Y	Z
C	-1.89802000	1.00741900	-0.05101000
C	-0.41344700	1.05605700	0.16986700
C	-1.19025400	2.33236800	0.02491200
H	-2.26294300	0.68943600	-1.01771600
H	-2.52443900	0.72224000	0.78501600
H	0.23501700	0.76646400	-0.64525000
H	-0.04069400	0.81203200	1.15687900
H	-1.07077600	2.88092500	-0.90152700
C	-1.41489300	3.17589300	1.23588400
H	-2.24608700	3.87351000	1.11437700
H	-1.60307400	2.56324200	2.12134100
O	-0.21293300	3.95071200	1.46873300

C	-0.23712300	4.73944100	2.52439500
C	1.10054600	5.50333000	2.63114700
O	-1.12721100	4.87722500	3.30669500
F	1.30698400	6.23999700	1.53780300
F	2.11875400	4.64968400	2.75440300
F	1.09419600	6.30528400	3.68395400

11

E = -799.253385

ZPVE = 0.194175

Symbol	X	Y	Z
C	-1.51833200	1.05973100	0.38337600
C	-0.05720700	1.40813500	0.43205500
C	-1.07857000	2.48753300	0.22520100
H	-1.89678800	0.54987900	-0.49181500
H	-2.00094400	0.78223200	1.31217000
H	0.56433400	1.13347200	-0.40887800
H	0.43773200	1.37037600	1.39493200
H	-1.14890700	2.91970300	-0.76681900
C	-1.35852500	3.44440300	1.34489500
H	-1.31232300	2.92604000	2.30775600
C	-2.66674100	4.16834700	1.21088200
C	-3.89545500	3.53756800	1.80240100
C	-3.31375500	4.77460800	2.42543700
H	-2.78851400	4.69483300	0.27039600
H	-3.77218900	2.60335700	2.33602400
H	-4.82009800	3.62287700	1.24845200
H	-3.84448300	5.70785500	2.29516500
H	-2.79665600	4.66594800	3.36997000
O	-0.27464700	4.42832600	1.32552100
C	0.15017800	4.89625200	2.47924100
C	1.26884200	5.93208500	2.22699000
O	-0.21576100	4.60658300	3.57859600
F	0.80489700	6.95269700	1.50243300
F	2.28307200	5.37759700	1.56009200
F	1.73089000	6.40746900	3.37316300

12

E = -642.131635

ZPVE = 0.077707

Symbol	X	Y	Z
C	-1.61510900	0.32716900	-0.10050500
H	-2.36098300	-0.43090000	-0.05497000
C	-0.77066300	1.17467300	-0.15048300
C	0.22694600	2.23217500	-0.21296700

H	0.14328000	2.79891700	-1.14246800
H	0.11863700	2.92609900	0.62298800
O	1.53467900	1.62813300	-0.15140600
C	2.54180800	2.48509800	-0.19234600
C	3.87877300	1.71593900	-0.12325900
O	2.47081300	3.67177600	-0.27197100
F	4.89532000	2.56208300	-0.14510300
F	3.99105800	0.88686400	-1.16093700
F	3.94577100	0.99654800	0.99656300

13

E = -1143.359728

ZPVE = 0.275152

Symbol	X	Y	Z
C	1.38480500	0.37009700	-0.23591800
C	2.10664600	1.74553700	-0.14351200
C	-0.46115800	2.10446300	-0.07986100
C	-0.13917800	0.58999700	-0.19357100
H	1.66932700	-0.13293500	-1.16072600
H	1.67149200	-0.26242200	0.60522900
H	-0.64740200	0.17142900	-1.06257300
H	-1.53746200	2.27337600	-0.06018700
H	3.19005900	1.62486100	-0.16715700
C	0.24089300	2.58955700	1.16933200
C	1.62627400	2.39863600	1.13454500
C	-0.36645900	3.13580400	2.28861300
C	2.40747800	2.76285200	2.22016400
C	0.42101200	3.50854600	3.37823000
H	-1.44249600	3.27305900	2.31461900
C	1.79861800	3.32447100	3.34315500
H	3.48173100	2.61343100	2.19541200
H	-0.04374300	3.94199100	4.25560900
H	2.40346300	3.61677800	4.19327500
C	0.20368100	2.74367800	-1.28039900
C	-0.43568300	3.43988100	-2.29438200
C	1.59101900	2.56486700	-1.30757700
C	0.32104600	3.97192700	-3.33901400
H	-1.51196600	3.57254400	-2.27093700
C	2.34168900	3.08908400	-2.34839400
C	1.70024100	3.79820300	-3.36493700
H	-0.16911700	4.52340300	-4.13232400
H	3.41750200	2.95130700	-2.36988000
H	2.28121600	4.21581500	-4.17864900
O	-0.63362900	-0.10895700	0.97811000
C	-1.93846500	-0.27130700	1.07283100
C	-2.27389000	-0.95969600	2.41421200
O	-2.77697900	0.05374200	0.28788200
F	-1.56591100	-2.07821300	2.57143500
F	-3.56129200	-1.26512800	2.46843200
F	-1.98974500	-0.14050900	3.42915800

For Table 4 ($ROCOCF_3$): MP2/6-31+G(d)

1

E = -795.060588

ZPVE = 0.168653

Symbol	X	Y	Z
C	-0.58729000	-0.90899300	-0.13716500
C	0.93699800	-0.84175000	-0.04863000
C	1.40822400	0.57745400	0.19820800
C	-0.66178300	1.19297100	1.20351000
C	-1.19566600	-0.22404400	1.08676900
H	2.48118900	0.65748200	0.38146000
H	1.29211800	-1.44558700	0.79634000
H	1.41755900	-1.22303800	-0.95634200
H	-0.92861000	-0.40860600	-1.05199900
H	-0.91192200	-1.95373400	-0.20120600
H	-0.97702700	1.68208000	2.12737900
H	-0.98565100	1.80625300	0.35218100
H	-0.93751300	-0.78087200	1.99681000
H	-2.29035900	-0.19278700	1.01899500
O	0.78515300	1.21095400	1.27133300
O	1.10599500	1.31061000	-1.04495600
C	1.79254400	2.44829900	-1.23013400
C	1.24542800	3.14593400	-2.48987700
O	2.69851900	2.90092300	-0.56067100
F	1.35001500	2.33689000	-3.56978400
F	1.91565800	4.27925800	-2.74323600
F	-0.06407900	3.45279400	-2.32202400

2

E = -1166.772090

ZPVE = 0.296351

Symbol	X	Y	Z
C	-2.01059100	0.77974400	0.37491300
C	-0.89076800	-0.26319200	0.30615500
C	0.45547000	0.33597100	-0.14956600
C	0.80766300	1.56443400	0.66957800
C	-0.30601000	2.59801100	0.74991400
C	-1.60997000	1.97154500	1.24528500
H	1.24627900	-0.40490700	0.06129400
H	-0.76403800	-0.70775700	1.30343100
H	-1.18286400	-1.08595200	-0.36057400
H	-2.25826100	1.13697500	-0.63193300
H	-2.92009200	0.31286800	0.77425600
H	1.74802300	2.02117000	0.34629600

H	0.01038900	3.42649700	1.39444000
H	-0.44740500	3.01955700	-0.25529100
H	-1.48436200	1.64305100	2.28540300
H	-2.40448600	2.72816600	1.24685200
Si	0.65523800	0.57275700	-2.04217400
C	-0.79427100	1.40862500	-2.91781300
H	-1.02806100	2.39977900	-2.51547000
H	-0.54158100	1.53794700	-3.97791800
H	-1.70499900	0.80162300	-2.87355700
C	2.22015500	1.58150000	-2.35408300
H	2.47479100	1.57094600	-3.42065600
H	2.10108500	2.63067000	-2.05933700
H	3.08071000	1.17700300	-1.80791700
C	0.86080100	-1.15518100	-2.77030600
H	1.73922900	-1.66160900	-2.35402500
H	-0.01306300	-1.78599900	-2.57142900
H	0.99014500	-1.10734900	-3.85790900
O	1.05370100	1.05993600	2.04719900
C	1.83381500	1.81379100	2.81812900
C	1.96983600	1.13559500	4.19472900
O	2.38189700	2.86734900	2.54403700
F	2.52240300	-0.09400600	4.06901000
F	0.75287100	0.99017000	4.77245300
F	2.74180000	1.86282000	5.01698800

3

E = -759.173522

ZPVE = 0.193073

Symbol	X	Y	Z
C	-4.16997900	-0.71812500	-0.13920300
C	-2.66825100	-0.57259600	0.00441900
C	-2.23957200	0.87329700	0.18331800
C	-2.94013600	1.47512500	1.40618700
C	-4.45964100	1.34177800	1.29408500
C	-4.86917000	-0.11709400	1.08441400
H	-1.15060700	0.93029200	0.29069500
H	-2.28929100	-1.19127700	0.82700600
H	-4.48760800	-0.19423400	-1.05083900
H	-4.42887100	-1.77613800	-0.26302800
H	-2.59266700	0.96194800	2.31445800
H	-2.65182700	2.52758400	1.51252800
H	-4.94258500	1.74463900	2.19286300
H	-4.81575100	1.94443400	0.44625900
H	-4.60922300	-0.70148000	1.97893200
H	-5.95581400	-0.19879000	0.96308600
H	-2.51732400	1.42981500	-0.72248000
O	-2.08964600	-1.10372100	-1.23917100
C	-0.83432200	-1.54682200	-1.15991200
O	-0.10834400	-1.58544800	-0.18281900
C	-0.39009400	-2.03621000	-2.55150500

F	-0.43091400	-1.01910800	-3.44439600
F	-1.20610400	-3.01923700	-2.99757800
F	0.86357700	-2.51363600	-2.51338400

4

E = -759.173746

ZPVE = 0.193126

Symbol	X	Y	Z
C	-0.59495900	-0.85708100	-0.15384200
C	0.93323700	-0.81683100	-0.08893800
C	1.45052900	0.58724500	0.17093400
C	-0.72015400	1.19254200	1.30828300
C	-1.21713500	-0.23945300	1.10001200
H	2.54287800	0.60956300	0.24148700
H	1.29043900	-1.45514400	0.73188900
H	1.37953800	-1.20126500	-1.01379100
H	-0.93566400	-0.30766700	-1.04075300
H	-0.92841800	-1.89487000	-0.27632200
H	-1.14573300	1.61773100	2.22549100
H	-1.06519700	1.82328100	0.47830000
H	-0.95335400	-0.84811300	1.97784300
H	-2.31133000	-0.25329400	1.02455800
O	1.08246800	1.35876100	-1.03213100
C	1.79623400	2.45871600	-1.26884300
C	1.24711700	3.13776000	-2.53774900
O	2.73133800	2.90588800	-0.62963800
F	1.30546700	2.29669000	-3.59614200
F	1.94957600	4.24131100	-2.83553800
F	-0.04775700	3.49356900	-2.35620700
C	0.80697800	1.23982900	1.38609300
H	1.17364000	2.26730500	1.49038900
H	1.15266700	0.69015400	2.27361100

5

E = -1387.049548

ZPVE = 0.274657

Symbol	X	Y	Z
C	-1.86621200	0.10203600	0.18956700
C	-0.47719500	-0.50499900	-0.02147400
C	0.56382000	0.53606100	-0.44367600
C	0.56321300	1.74136900	0.48899500
C	-0.81635900	2.32317700	0.75144400
C	-1.80867400	1.24924200	1.19975800
H	1.56417600	0.08571500	-0.42048500
H	-0.13255400	-0.95150900	0.92113700
H	-0.50735200	-1.31194200	-0.76429700

H	-2.26777800	0.47079300	-0.76373300
H	-2.55338100	-0.67780300	0.54048000
H	1.26110600	2.51106600	0.14546900
H	-0.72944500	3.12614700	1.49304400
H	-1.16137300	2.78675500	-0.18217900
H	-1.51105100	0.85808700	2.18217600
H	-2.80133800	1.69849600	1.32609100
S	0.25028200	1.06151500	-2.17569100
C	1.66684100	2.12391700	-2.38568700
C	1.49251300	3.51290300	-2.48138500
C	2.95781400	1.57870900	-2.46933200
C	2.60198200	4.34922100	-2.64515200
H	0.49008100	3.93245400	-2.42043200
C	4.06485100	2.41959700	-2.61567700
H	3.09144300	0.49898300	-2.42622000
C	3.88928000	3.80555700	-2.70436900
H	2.45963200	5.42567400	-2.71584000
H	5.06339700	1.99100300	-2.67458600
H	4.75182200	4.45781500	-2.82258100
O	1.10434400	1.20295700	1.75211000
C	1.71663100	2.08429500	2.54543200
C	2.22667200	1.34598600	3.79711300
O	1.87862200	3.27703800	2.36508400
F	1.19635600	0.76308800	4.45529400
F	2.84018600	2.19213600	4.63797400
F	3.10517800	0.37562100	3.45167500

6

E = -3387.149543

ZPVE = 0.273730

Symbol	X	Y	Z
C	-2.02053900	0.20892300	0.28035800
C	-0.80009200	-0.66650000	0.57381200
C	0.46612100	-0.14740400	-0.10556700
C	0.70458400	1.33119700	0.16266400
C	-0.51549000	2.20712600	-0.05608600
C	-1.74769900	1.66340900	0.66907000
H	1.34178400	-0.72228900	0.21547700
H	-0.61919600	-0.67405700	1.65860200
H	-0.97432500	-1.70748500	0.27362600
H	-2.28017700	0.15504400	-0.78565700
H	-2.88603600	-0.17464900	0.83471400
H	1.56992700	1.69320000	-0.40191100
H	-0.27773200	3.22514800	0.27552500
H	-0.70433200	2.25081500	-1.13590900
H	-1.59529800	1.73075500	1.75458000
H	-2.61624800	2.28949900	0.43062800
C	2.14130100	0.18794400	-2.43264300
C	2.33655100	1.39335500	-3.12105100

C	3.24314000	-0.56362400	-2.00377300
C	3.63596700	1.84517900	-3.37565100
H	1.47713300	1.97510100	-3.44889700
C	4.53853800	-0.10009900	-2.24827400
H	3.08921800	-1.50886100	-1.48662600
C	4.73722000	1.10747300	-2.92739500
H	3.78658400	2.78128500	-3.91014000
H	5.39222200	-0.67925700	-1.90228100
H	5.74678100	1.46536400	-3.11809600
O	1.03993400	1.48011800	1.59661100
Se	0.35755400	-0.42205900	-2.06853800
C	2.30072000	1.18778800	1.91961400
C	2.50595600	1.44959700	3.42286100
O	3.19163200	0.79205200	1.18882600
F	1.65288400	0.69594600	4.15749500
F	3.76017300	1.15086000	3.79434900
F	2.27356600	2.75043800	3.71465700

7

E = -642.895462

ZPVE = 0.125982

Symbol	X	Y	Z
C	-0.86117000	1.58411300	0.10909200
H	-0.44416400	0.57351400	0.17579900
H	-1.94739800	1.49580600	0.21848100
C	-0.31829000	2.41617900	1.24905300
H	-0.74199600	3.42489800	1.26778500
H	0.77283300	2.49522200	1.22500100
C	-0.51147900	2.21640100	-1.23795200
H	0.57265100	2.29488100	-1.36936800
H	-0.90492400	1.61305700	-2.06057900
H	-0.93731500	3.22117800	-1.32655700
O	-0.69667600	1.74262200	2.48966100
C	-0.29200100	2.34778200	3.60806500
C	-0.76152400	1.52598200	4.82262100
O	0.34533200	3.37996800	3.70676700
F	-2.11070500	1.42085400	4.83210300
F	-0.37446300	2.10567800	5.96913600
F	-0.24235500	0.27689000	4.77973800

8

E = -1099.004757

ZPVE = 0.225143

Symbol	X	Y	Z
C	-0.83523000	0.39300300	-0.75132800

C	-0.99599700	1.94786600	-0.53273200
H	-1.73562000	2.56411900	-1.05059800
C	-0.90454800	1.72917900	1.01367500
H	-1.53562100	2.21734200	1.76166800
C	-0.75435000	0.18495100	0.79865100
H	-1.29851300	-0.59470400	1.33730100
C	0.65146300	1.88369300	0.92406100
C	0.80433200	0.33657000	0.70892000
H	1.53613400	-0.29570300	1.22115700
C	0.71130000	0.55532000	-0.84232000
H	1.32662900	0.06857300	-1.60269500
C	0.55927400	2.10058600	-0.62429800
H	1.08673800	2.88388600	-1.17590000
C	-1.65725500	-0.38917300	-1.70002100
O	-2.89310900	-0.62432900	-1.18551100
O	-1.30337100	-0.75395600	-2.81589400
C	-3.79394600	-1.32264400	-2.07782300
H	-3.38694200	-2.30322600	-2.33038200
H	-4.72314200	-1.41762200	-1.51900100
H	-3.94267100	-0.74265300	-2.99037400
C	1.49537400	2.67240900	1.85696900
H	2.55739400	2.64464000	1.58576400
H	1.38521300	2.34680500	2.89815700
O	1.02963900	4.05691000	1.75523000
C	1.67573100	4.92762300	2.53477800
C	1.07827500	6.33062200	2.31972500
O	2.59040000	4.69980700	3.30413200
F	-0.23859100	6.33775800	2.63211900
F	1.20545900	6.70661400	1.02596900
F	1.70049200	7.23742800	3.08756400

9

E = -875.408617

ZPVE = 0.255553

Symbol	X	Y	Z
C	-2.22863600	-1.62994100	0.06399900
C	-0.70279400	-1.65248200	0.07215600
C	-0.09774900	-0.28610000	0.50152200
C	-1.12565600	0.85250000	0.69418800
C	-2.55906300	0.41523400	0.49683600
C	-2.72381400	-0.88534500	1.32719500
H	0.45482400	-0.40252200	1.43950400
H	-0.36308300	-2.43208800	0.76596500
H	-0.33200300	-1.93736400	-0.91958300
H	-2.64469300	-2.62428700	-0.14929600
H	-1.01053300	1.30137600	1.68769300
H	-3.25062100	1.25044600	0.66973400
H	-2.11347400	-0.98122100	2.23509600
H	-3.76378000	-1.09444600	1.58593400

H	0.64387500	0.04462400	-0.23346300
C	-2.76610300	-0.44142600	-0.78720200
C	-4.25549300	-0.59475300	-1.09931200
H	-4.85082600	-0.86373400	-0.22197600
H	-4.65556100	0.34377000	-1.50230500
H	-4.40148300	-1.37598300	-1.85535400
C	-2.04081800	-0.07884300	-2.07829400
H	-0.96381300	0.04889300	-1.95513500
H	-2.20447200	-0.86785800	-2.82442200
H	-2.43388400	0.85895900	-2.48817000
O	-0.88825800	1.94149700	-0.27142500
C	0.13893600	2.74125600	0.01188200
C	0.26170400	3.80254100	-1.09700200
O	0.89913100	2.68203400	0.96220500
F	-0.89885900	4.47965000	-1.25249500
F	0.56026800	3.20564400	-2.27676400
F	1.23156500	4.68547100	-0.81380500

10

E = -680.850407

ZPVE = 0.132049

Symbol	X	Y	Z
C	-1.89459800	0.99346200	-0.05226200
C	-0.40683700	1.06257200	0.16103500
C	-1.20177600	2.33359200	0.02796600
H	-2.26538600	0.67574600	-1.02120900
H	-2.51574300	0.69157300	0.78619100
H	0.24589500	0.78600300	-0.66036800
H	-0.02137400	0.81532700	1.14603100
H	-1.09669500	2.88384500	-0.90377900
C	-1.43208900	3.17492800	1.23729400
H	-2.25750700	3.88257000	1.11383700
H	-1.61793500	2.56850600	2.12969800
O	-0.20678000	3.94942900	1.46252200
C	-0.23745000	4.75085900	2.52820400
C	1.10470400	5.49870200	2.63459200
O	-1.14855300	4.90038700	3.32199700
F	1.33841700	6.22060600	1.51435500
F	2.12401800	4.62188800	2.79006300
F	1.10329300	6.33526600	3.68373500

11

E = -797.091703

ZPVE = 0.195320

Symbol	X	Y	Z

C	-1.46557000	1.03784800	0.40003300
C	-0.01869100	1.45213800	0.44436000
C	-1.08931000	2.48945000	0.22986500
H	-1.82632600	0.50371600	-0.47331100
H	-1.93804600	0.74331400	1.33275100
H	0.61852500	1.19938300	-0.39707000
H	0.48260100	1.44366800	1.40868700
H	-1.17739500	2.90597900	-0.77177000
C	-1.40370200	3.44510400	1.33780500
H	-1.34833300	2.94275800	2.31168500
C	-2.71021500	4.16166300	1.18559600
C	-3.94320100	3.56766800	1.82145800
C	-3.34116000	4.82843200	2.38248100
H	-2.84471200	4.65351100	0.22379900
H	-3.82544000	2.65334300	2.39600900
H	-4.87702400	3.63512000	1.27233100
H	-3.86414000	5.76544100	2.21856100
H	-2.81615100	4.75888200	3.33057000
O	-0.32709900	4.46464800	1.31039900
C	0.19172300	4.82334900	2.48215500
C	1.27210800	5.89391800	2.23582500
O	-0.08408700	4.41241200	3.59633500
F	0.73765800	6.97474500	1.62083000
F	2.25633900	5.40491500	1.44563800
F	1.82169700	6.29649700	3.39261200

12

E = -640.519753

ZPVE = 0.075762

Symbol	X	Y	Z
C	-1.64110200	0.31759500	-0.10707900
H	-2.38044700	-0.45295100	-0.06778600
C	-0.76892500	1.17067500	-0.15208600
C	0.21606600	2.23966800	-0.20830300
H	0.14657900	2.81366300	-1.13688500
H	0.12279600	2.92878400	0.63607700
O	1.53712900	1.61463500	-0.14999500
C	2.54961900	2.48856200	-0.19340000
C	3.88159200	1.71888400	-0.12460700
O	2.47496900	3.69996200	-0.27349800
F	4.91951800	2.56727600	-0.16844900
F	3.98540100	0.86014900	-1.16340600
F	3.95713600	1.00767200	1.02255100

13

E = -1140.240385

ZPVE = 0.272654

Symbol	X	Y	Z
C	1.37467200	0.36518600	-0.30299100
C	2.09359200	1.73718900	-0.15911300
C	-0.47545100	2.09557800	-0.13476600
C	-0.14635900	0.58400900	-0.23311000
H	1.65124000	-0.09405300	-1.25911200
H	1.67549100	-0.31331000	0.50370700
H	-0.68675900	0.12647900	-1.06863100
H	-1.55748500	2.26648500	-0.13091100
H	3.18423200	1.61757900	-0.16370000
C	0.20121400	2.57177000	1.12504600
C	1.59224200	2.36844600	1.11677900
C	-0.43518600	3.09632200	2.25056100
C	2.35451100	2.69890000	2.23870500
C	0.33313300	3.44326400	3.36964600
H	-1.51539000	3.24419100	2.25434300
C	1.71947700	3.24084100	3.36467100
H	3.43273600	2.53868400	2.23956800
H	-0.15026700	3.86045600	4.25087700
H	2.30764100	3.50853600	4.24039500
C	0.20643900	2.74539300	-1.31264900
C	-0.42413000	3.44870900	-2.34078000
C	1.60245800	2.57863800	-1.31155500
C	0.35358100	3.99953700	-3.36818900
H	-1.50665200	3.57460200	-2.33847100
C	2.37450900	3.11799700	-2.34160200
C	1.74495800	3.83658800	-3.36752200
H	-0.12572200	4.55712100	-4.17043500
H	3.45671700	2.98825200	-2.34493700
H	2.34032800	4.26867700	-4.16957400
O	-0.58745400	-0.08833800	0.99570300
C	-1.90457100	-0.22696700	1.15169200
C	-2.17371600	-0.87703500	2.52243100
O	-2.79219500	0.09480300	0.38191600
F	-1.53188600	-2.06337200	2.62723300
F	-3.48754000	-1.09021200	2.69881700
F	-1.73479100	-0.07077600	3.51620100

<u>For Table 5, Acetone (ROH): B3LYP/6-311++G(d,p)</u>

1

E = -346.959456

ZPVE = 0.150217

Symbol	X	Y	Z
C	-0.67201500	-0.97413100	0.00593800
C	0.86229900	-0.97027600	-0.01885100
C	1.42826700	0.44762000	-0.01393600
C	-0.55850400	1.30276600	1.05051200
C	-1.17786000	-0.08659200	1.15068600

H	2.50241400	0.44139200	0.19186900
H	1.24664600	-1.47853800	0.87143700
H	1.25116800	-1.50168200	-0.89102100
H	-1.05969000	-0.59976300	-0.94718400
H	-1.03941700	-1.99778400	0.11938800
H	-0.80381900	1.91936600	1.91613000
H	-0.91396300	1.81664900	0.15005700
H	-0.90997000	-0.53304100	2.11535300
H	-2.26840400	0.00418400	1.12563300
O	0.88320700	1.24473100	1.02777300
O	1.18515300	1.02598600	-1.29022500
H	1.60500700	1.89451000	-1.30847800

6

E = -2943.587970

ZPVE = 0.253987

Symbol	X	Y	Z
C	-1.93220500	0.22697400	0.32644700
C	-0.74394200	-0.74509800	0.29793800
C	0.53069300	-0.11507000	-0.27807400
C	0.87724900	1.22529900	0.38630400
C	-0.32247300	2.17825400	0.46830900
C	-1.56946900	1.51794500	1.07291800
H	1.37378200	-0.79485900	-0.15593000
H	-0.51520400	-1.05433900	1.32436400
H	-0.99438400	-1.65375900	-0.25593400
H	-2.24271100	0.46989400	-0.69767800
H	-2.78971200	-0.25861600	0.80197800
H	1.68758100	1.70585100	-0.17271000
H	-0.03240500	3.06275800	1.04638300
H	-0.54546700	2.53068000	-0.54447200
H	-1.38708500	1.28527800	2.12790700
H	-2.40729300	2.22130700	1.04610900
C	2.23901100	0.21138300	-2.73021400
C	2.73935300	1.39545800	-3.27983400
C	3.08779600	-0.88797800	-2.56133700
C	4.08144900	1.47876600	-3.65567000
H	2.08581800	2.24962400	-3.41049800
C	4.43123700	-0.79388400	-2.92274700
H	2.70224500	-1.81596900	-2.15549700
C	4.92983400	0.38773000	-3.47357100
H	4.46189300	2.39975300	-4.08315700
H	5.08434900	-1.64838700	-2.78496400
H	5.97288900	0.45555100	-3.76083900
O	1.36926900	0.87981400	1.70090500
H	1.60222700	1.69629300	2.15781500
Se	0.35409300	0.08766200	-2.27532800

7

E = -194.316923

ZPVE = 0.107729

Symbol	X	Y	Z
C	-0.90917100	1.59751100	0.01404700
H	-0.56829300	0.55665500	0.03360300
H	-2.00422300	1.57394700	0.03180500
C	-0.41547600	2.29610600	1.27134400
H	-0.76782000	3.33544100	1.28841200
H	0.68184400	2.31264500	1.28707800
C	-0.42065500	2.28423500	-1.26432700
H	0.67235700	2.29750200	-1.31643300
H	-0.78863400	1.76298800	-2.15130800
H	-0.76997200	3.31987600	-1.31881200
O	-0.91421900	1.58737800	2.41640800
H	-0.59893400	2.03061800	3.21123000

11

E = -349.057351

ZPVE = 0.175800

Symbol	X	Y	Z
C	-1.54332400	0.93128100	0.48541400
C	-0.07879900	1.27560800	0.35598000
C	-1.13196400	2.34590700	0.16542800
H	-2.00671600	0.34762000	-0.30073300
H	-1.92396000	0.72738800	1.47957300
H	0.45803300	0.92719600	-0.51798900
H	0.51094300	1.29892100	1.26642800
H	-1.29656400	2.67529300	-0.85670400
C	-1.28335700	3.44436600	1.19502500
H	-1.18104400	3.00541900	2.19858300
C	-2.61119600	4.15535500	1.10661400
C	-3.79904100	3.64249600	1.88360700
C	-3.13358100	4.93665400	2.28686900
H	-2.82165300	4.57045600	0.12503100
H	-3.65263700	2.77998800	2.52352000
H	-4.77216900	3.68827400	1.40981900
H	-3.65498700	5.86616000	2.09218600
H	-2.53765100	4.93571500	3.19265600
O	-0.25584400	4.44658000	1.01907900
H	0.58740800	3.98685700	0.92933400

<u>For Table 5, Acetone ($ROCH_2CF_3$): B3LYP/6-311++G(d,p)</u>

1

E = -723.388255

ZPVE = 0.183084

Symbol	X	Y	Z
C	-0.60242900	-0.98141400	-0.04188400
C	0.92395700	-0.96008500	0.11155400
C	1.47127100	0.46203100	0.17593100
C	-0.63528300	1.30842600	0.97761600
C	-1.24657000	-0.08642000	1.02456100
H	2.51887900	0.47476500	0.49435300
H	1.20915000	-1.45576700	1.04499700
H	1.41945300	-1.49133800	-0.70440300
H	-0.88033400	-0.62366600	-1.03868500
H	-0.96877400	-2.00797800	0.04220400
H	-0.98314600	1.93375400	1.80024800
H	-0.88836200	1.80687600	0.03480000
H	-1.08846600	-0.51702000	2.01991000
H	-2.32731600	-0.00782600	0.87144600
O	0.80253700	1.26871800	1.12297800
O	1.38358600	1.01922500	-1.13785900
C	1.99871800	2.28179800	-1.26429800
H	1.46381400	3.06250300	-0.71544000
H	3.04183000	2.26250200	-0.92686900
C	1.99372500	2.65801700	-2.73145900
F	2.67443400	1.77792500	-3.49818500
F	2.57462500	3.86931900	-2.90283500
F	0.74498600	2.73921100	-3.24210500

6

E = -3320.016535

ZPVE = 0.286937

Symbol	X	Y	Z
C	-1.90871800	0.15033300	0.36591800
C	-0.67237900	-0.75990600	0.36456800
C	0.55959400	-0.09572900	-0.26302000
C	0.84357000	1.29162900	0.32988600
C	-0.40074300	2.18755700	0.37387800
C	-1.60166000	1.49698200	1.03513200
H	1.43910300	-0.72318800	-0.12280400
H	-0.41250800	-1.00711000	1.40054900
H	-0.88279600	-1.70619700	-0.14052500
H	-2.24963000	0.32152100	-0.66284400
H	-2.73067200	-0.35226500	0.88427300
H	1.63916100	1.78003000	-0.24439000
H	-0.16272400	3.12558600	0.88375100
H	-0.64982800	2.45717300	-0.65746600
H	-1.39091400	1.33285200	2.09781300
H	-2.47467500	2.15446300	0.98533200
C	2.21627800	0.21724000	-2.74695200
C	2.64958200	1.41447100	-3.32423500

C	3.12090300	-0.83488500	-2.56761400
C	3.98167600	1.55805300	-3.71710800
H	1.95198500	2.23151200	-3.46400100
C	4.45367000	-0.68032300	-2.94721400
H	2.78688300	-1.77281000	-2.13959800
C	4.88565900	0.51436800	-3.52536500
H	4.31055300	2.48849900	-4.16627500
H	5.15058800	-1.49813800	-2.80189800
H	5.92067100	0.62894100	-3.82654900
O	1.35996600	1.02891300	1.66013200
Se	0.34589100	0.00632300	-2.26439900
C	2.06618600	2.09851000	2.23549500
H	1.41753100	2.93099400	2.53109400
H	2.84897400	2.48133200	1.56883500
C	2.74481400	1.58964100	3.49207400
F	3.43050800	2.59354200	4.08961600
F	3.62763800	0.59773800	3.24317700
F	1.86494100	1.11316300	4.40065200

7

E = -570.747062

ZPVE = 0.140943

Symbol	X	Y	Z
C	-0.90629300	1.59871200	0.02127600
H	-0.56195900	0.56030500	0.05936600
H	-2.00010300	1.57507500	0.05813600
C	-0.39136900	2.32985300	1.24958800
H	-0.74491000	3.36995100	1.26062800
H	0.70700500	2.34495400	1.26187000
C	-0.43894600	2.25945500	-1.27923600
H	0.65279800	2.27290800	-1.34969600
H	-0.82113500	1.71673700	-2.14681900
H	-0.79216400	3.29248200	-1.35097400
O	-0.86935500	1.65423600	2.42126400
C	-0.44084800	2.25790300	3.61414400
H	0.65242400	2.25737100	3.70936100
H	-0.80173500	3.28987600	3.70943200
C	-1.00339800	1.46592100	4.77733800
F	-0.60954700	2.01748200	5.95077000
F	-0.58614900	0.18076100	4.78215900
F	-2.35437500	1.43977900	4.78396900

11

E = -725.484691

ZPVE = 0.208764

Symbol	X	Y	Z

C	-1.82247600	0.89558400	0.33541400
C	-0.32355600	0.99918400	0.22315300
C	-1.18217500	2.23366700	0.05331600
H	-2.37098500	0.41976900	-0.46820600
H	-2.24157300	0.73357600	1.32155900
H	0.15924000	0.59352300	-0.65787300
H	0.25160200	0.89967700	1.13696200
H	-1.28800000	2.60592100	-0.96171700
C	-1.22010400	3.32675300	1.10071400
H	-1.04889600	2.88825500	2.09523600
C	-2.52736600	4.08106300	1.10267800
C	-3.66290100	3.62651900	1.98729900
C	-2.92661500	4.90664200	2.29973600
H	-2.80653600	4.47626000	0.13049200
H	-3.49198000	2.77631400	2.63720700
H	-4.66888600	3.69133300	1.59077200
H	-3.43061200	5.84882400	2.12145500
H	-2.25862500	4.90828000	3.15368000
O	-0.18921900	4.32076100	0.86570900
C	1.13015400	3.87018600	1.04089900
H	1.27204500	3.37227500	2.00842800
H	1.45977800	3.19369400	0.24557000
C	2.04291300	5.08023100	1.01525700
F	1.77042000	5.96355800	2.00113400
F	1.97159400	5.76064500	-0.15080300
F	3.33264000	4.69453800	1.17234200

For Table 5, Acetone (ROPh): B3LYP/6-311++G(d,p)

1

E = -577.976869

ZPVE = 0.230536

Symbol	X	Y	Z
C	-0.86547500	-0.83286100	-0.03429200
C	0.61297400	-0.88782600	-0.44043600
C	1.34778700	0.40273000	-0.08826800
C	-0.22364700	0.89889200	1.66190700
C	-0.98802700	-0.39941800	1.43221700
H	2.42814300	0.28963800	-0.20503900
H	1.11482100	-1.69854300	0.09754300
H	0.73144700	-1.08199600	-1.50896300
H	-1.39925100	-0.12218300	-0.67378400
H	-1.32926100	-1.81082200	-0.18834800
H	-0.18456400	1.16651100	2.71814700
H	-0.69113100	1.72503300	1.11416100
H	-0.58152900	-1.17835800	2.08731600
H	-2.03560100	-0.25194500	1.71255400
O	1.15812100	0.78507900	1.25551800
O	0.88600400	1.41161100	-0.99705200
C	1.60201300	2.57345400	-1.14750700

C	1.20607300	3.39194100	-2.21246300
C	2.66220200	2.96515600	-0.32391800
C	1.87177600	4.58819200	-2.45696700
H	0.38119000	3.07257600	-2.83873200
C	3.32621200	4.16591700	-0.58755200
H	2.95604000	2.36204900	0.52349200
C	2.94028900	4.98265000	-1.64763600
H	1.55722900	5.21227300	-3.28611400
H	4.14797300	4.46278900	0.05487200
H	3.45960400	5.91406500	-1.84003200

6

E = -3174.606135

ZPVE = 0.334464

Symbol	X	Y	Z
C	-2.14916300	0.25964300	0.07652200
C	-0.92012600	-0.62997000	0.30975700
C	0.37325200	-0.01631600	-0.23944100
C	0.58856600	1.43008000	0.23259400
C	-0.65447900	2.31082300	0.05412300
C	-1.92133700	1.66925100	0.63837800
H	1.23295600	-0.61431200	0.06101000
H	-0.78017900	-0.76599100	1.38857900
H	-1.06942600	-1.62573700	-0.11564500
H	-2.36895500	0.32270900	-0.99661200
H	-3.02528000	-0.19844100	0.54505200
H	1.44315400	1.85303700	-0.30004000
H	-0.47511300	3.28813500	0.50937000
H	-0.78819600	2.48408100	-1.01860400
H	-1.83314800	1.61360800	1.72908000
H	-2.78360000	2.30798200	0.42517100
C	2.29729100	0.06111200	-2.54258200
C	2.78943800	1.18324400	-3.21551000
C	3.17917100	-0.94348300	-2.12966300
C	4.15716600	1.29983900	-3.47081000
H	2.10962600	1.96365600	-3.53580900
C	4.54605400	-0.81370700	-2.37218200
H	2.80185500	-1.82602300	-1.62638400
C	5.03713600	0.30579100	-3.04583100
H	4.53184900	2.17187000	-3.99504100
H	5.22471700	-1.59362700	-2.04536900
H	6.09944800	0.40038100	-3.23978000
O	0.93637800	1.30891600	1.63681700
Se	0.38458300	-0.11961300	-2.25218600
C	1.66497500	2.28193700	2.26152200
C	1.94075900	2.04812300	3.61691400
C	2.14220400	3.44805800	1.65245500
C	2.68618100	2.96474000	4.34838100
H	1.56461000	1.14094200	4.07543000

C	2.89236500	4.35936700	2.40102800
H	1.93951100	3.66232600	0.61231200
C	3.16993400	4.12954100	3.74552300
H	2.89157100	2.76787300	5.39487400
H	3.25676200	5.25910800	1.91743700
H	3.75072700	4.84389700	4.31685900

7

E = -425.337494

ZPVE = 0.188634

Symbol	X	Y	Z
C	-0.44420900	1.55904400	-0.05447000
H	0.59743200	1.26281100	-0.21438800
H	-1.01120800	0.64353300	0.14211400
C	-0.51706400	2.45424100	1.17212600
H	-1.55440900	2.74193800	1.38022800
H	0.06916600	3.36825200	1.01994200
C	-0.98970800	2.25676300	-1.30372100
H	-0.42236700	3.16355800	-1.53387300
H	-0.92788100	1.59685500	-2.17207400
H	-2.03849800	2.54111400	-1.17591800
O	0.01262800	1.72389000	2.28844500
C	0.05304500	2.32281200	3.51469000
C	-0.39480700	3.62234400	3.77544500
C	0.58640200	1.54887600	4.55566700
C	-0.30434800	4.13349000	5.07381600
H	-0.80983400	4.23757300	2.98899500
C	0.66950600	2.07133400	5.84043500
H	0.92868400	0.54403000	4.33652800
C	0.22426700	3.36957000	6.11025000
H	-0.65411900	5.14187100	5.26602200
H	1.08403500	1.46247500	6.63629800
H	0.29012800	3.77481600	7.11302000

11

E = -580.072259

ZPVE = 0.255996

Symbol	X	Y	Z
C	-2.33967000	0.65106100	0.67467300
C	-0.91494000	0.53377300	0.19181800
C	-1.65914300	1.83950700	0.03814500
H	-3.12202800	0.15500400	0.11324800
H	-2.50387300	0.67540200	1.74582100
H	-0.72090100	-0.04073200	-0.70601400
H	-0.13514000	0.47052700	0.94018800

H	-1.97974800	2.08307000	-0.97063800
C	-1.32487000	3.06292900	0.86211700
H	-1.02950600	2.77245000	1.87396200
C	-2.48201500	4.03003300	0.95211400
C	-3.48711500	3.90408500	2.07084300
C	-2.52359900	5.06653100	2.04654200
H	-2.87522000	4.33374100	-0.01347300
H	-3.32663100	3.13260700	2.81487900
H	-4.52850800	4.09047300	1.83790100
H	-2.90710200	6.04933300	1.80054600
H	-1.71614300	5.06686800	2.77026300
O	-0.24056600	3.79877700	0.22498200
C	1.07408300	3.56531900	0.51240500
C	1.99191800	4.18800600	-0.34726200
C	1.55095000	2.81051100	1.59017500
C	3.35890200	4.05819300	-0.13147600
H	1.61119600	4.77134200	-1.17765600
C	2.92753700	2.68764300	1.79439400
H	0.87523800	2.31738800	2.27474300
C	3.83998000	3.30477900	0.94265000
H	4.05197200	4.54704700	-0.80742400
H	3.28114800	2.09887800	2.63383700
H	4.90557100	3.20125900	1.10954800

<u>For Table 5, Acetone (ROPh-p-NO_2): B3LYP/6-311++G(d,p)</u>

1

E = -782.546540

ZPVE = 0.232771

Symbol	X	Y	Z
C	-0.96939800	-0.71903700	0.14276400
C	0.34089100	-0.83448700	-0.64646800
C	1.27646500	0.33714000	-0.37132300
C	0.25599600	0.74511600	1.76681900
C	-0.66428500	-0.45999600	1.62358400
H	2.27097000	0.16058200	-0.78540500
H	0.87554200	-1.74180000	-0.34796500
H	0.16282700	-0.89969300	-1.72214000
H	-1.57373200	0.10135400	-0.25806000
H	-1.55478100	-1.63415900	0.02264800
H	0.59734600	0.87936600	2.79307300
H	-0.25248800	1.66220300	1.44922800
H	-0.18143100	-1.33865700	2.06570800
H	-1.58317900	-0.27447300	2.18788000
O	1.46971400	0.58858800	0.99268700
O	0.70471300	1.49005100	-1.04247500
C	1.44111800	2.61128100	-1.21683800
C	0.83936500	3.61303400	-1.99931200
C	2.72337200	2.81546800	-0.68127300
C	1.50633200	4.79504300	-2.25486100

H	-0.15062300	3.43773400	-2.40084800
C	3.39483700	4.00072100	-0.94270100
H	3.18493700	2.07185800	-0.04892000
C	2.78717700	4.98129500	-1.72548500
H	1.05261000	5.56827900	-2.85852400
H	4.38199400	4.17103100	-0.53647000
N	3.49599300	6.22380900	-1.99158900
O	2.93924300	7.07993900	-2.68101500
O	4.62410500	6.37022400	-1.51824600

6

E = -3379.176326

ZPVE = 0.336736

Symbol	X	Y	Z
C	-2.15056300	0.25566700	0.08095600
C	-0.91828800	-0.62787500	0.31972000
C	0.37285300	-0.01475400	-0.23561000
C	0.58021000	1.43698900	0.21834600
C	-0.66479400	2.31242200	0.04294200
C	-1.92810100	1.66970400	0.63349700
H	1.23549300	-0.60540600	0.07078200
H	-0.77765600	-0.75715900	1.39932700
H	-1.06365300	-1.62675900	-0.09914800
H	-2.37152400	0.31069800	-0.99221400
H	-3.02430000	-0.20221500	0.55361600
H	1.43660500	1.85912100	-0.30993700
H	-0.48749900	3.29400800	0.49001300
H	-0.79963300	2.47759500	-1.03061400
H	-1.83978600	1.62251200	1.72458900
H	-2.79180400	2.30444000	0.41571400
C	2.29981100	0.06049000	-2.53271800
C	2.78925400	1.19303100	-3.18996900
C	3.18346500	-0.94711500	-2.13120800
C	4.15719700	1.31725500	-3.44041200
H	2.10744700	1.97485400	-3.50241300
C	4.55038800	-0.80996000	-2.36942500
H	2.80749700	-1.83726800	-1.64050800
C	5.03915000	0.32015400	-3.02681200
H	4.53036800	2.19706400	-3.95250700
H	5.23085900	-1.59215100	-2.05205400
H	6.10151900	0.42049500	-3.21744100
O	0.92927900	1.33037000	1.63456300
Se	0.38728000	-0.13086300	-2.24670300
C	1.65701500	2.28042800	2.25134100
C	1.93216100	2.03876100	3.61195000
C	2.14457900	3.44898300	1.64074400
C	2.67815200	2.93700600	4.34686000
H	1.54891700	1.13407600	4.06661600
C	2.89618800	4.35042400	2.37968500

H	1.94350400	3.66671100	0.60211300
C	3.15995500	4.09404000	3.72414500
H	2.89286100	2.75527300	5.39048500
H	3.27559000	5.25171400	1.91900100
N	3.94524800	5.04523300	4.49184000
O	4.16578200	4.80050600	5.67977100
O	4.36034400	6.05882900	3.92612300

7

E = -629.907456

ZPVE = 0.190954

Symbol	X	Y	Z
C	-0.51399700	1.54258200	-0.03630400
H	0.46265900	1.06155500	-0.14691000
H	-1.24473900	0.74947300	0.14939900
C	-0.47307100	2.46449600	1.16996000
H	-1.44749800	2.93446700	1.33834100
H	0.27920600	3.24908600	1.03889600
C	-0.87499700	2.30211900	-1.31665100
H	-0.14447300	3.08674300	-1.53446700
H	-0.89855100	1.62291600	-2.17160500
H	-1.85957100	2.77233800	-1.23744100
O	-0.12795600	1.66708000	2.32433400
C	-0.02479000	2.24918500	3.53351000
C	-0.22868900	3.61798100	3.77553000
C	0.31182200	1.39138300	4.59835700
C	-0.09734400	4.11574100	5.06417700
H	-0.48688500	4.29400300	2.97345000
C	0.44271900	1.88728800	5.87941800
H	0.46481200	0.33965800	4.39221400
C	0.23633100	3.25306600	6.10647400
H	-0.25181700	5.16694400	5.26263500
H	0.70058600	1.23510900	6.70169100
N	0.37237100	3.78148500	7.45435600
O	0.67534400	3.00371200	8.36150600
O	0.17979700	4.98526200	7.63749300

11

E = -784.642757

ZPVE = 0.258603

Symbol	X	Y	Z
C	-2.42041900	0.61596400	0.69959200
C	-1.02151100	0.46035600	0.15720800
C	-1.73941100	1.78303800	0.02513000
H	-3.23817800	0.13812700	0.17434000

H	-2.53869600	0.65054600	1.77631100
H	-0.87984000	-0.12263100	-0.74467600
H	-0.21212300	0.37993600	0.87228500
H	-2.09694700	2.03019800	-0.96986500
C	-1.33829300	2.99627700	0.82860000
H	-1.01572400	2.70826100	1.83118700
C	-2.43974400	4.02095600	0.93868700
C	-3.39793800	3.96997200	2.10451000
C	-2.38408400	5.08336400	2.00800400
H	-2.86047000	4.31821900	-0.01688400
H	-3.24072300	3.20913800	2.86003400
H	-4.43854100	4.19883200	1.90991800
H	-2.73107900	6.07671400	1.75110100
H	-1.54642200	5.06315200	2.69615200
O	-0.23112100	3.67210900	0.13754500
C	1.06074600	3.50361100	0.46502900
C	1.97731400	4.20079600	-0.34987800
C	1.54270000	2.72553400	1.53293500
C	3.33317600	4.12725600	-0.10820800
H	1.59267700	4.79592200	-1.16838800
C	2.90534800	2.65289400	1.77668200
H	0.87295200	2.17578400	2.17702400
C	3.79526300	3.34973200	0.96002600
H	4.03617000	4.66092200	-0.73218100
H	3.28141600	2.05719900	2.59660800
N	5.22004700	3.26645300	1.22110100
O	5.98888700	3.89914700	0.49325000
O	5.60790300	2.56726200	2.16030100

<u>For Table 5, Acetone ($ROCOCH_3$): B3LYP/6-311++G(d,p)</u>

1

E = -499.627067

ZPVE = 0.187361

Symbol	X	Y	Z
C	-0.62601800	-0.93025900	-0.09410900
C	0.90265700	-0.80378900	-0.08496100
C	1.35825300	0.62865400	0.16744600
C	-0.70218300	1.16286900	1.28221500
C	-1.20893600	-0.26868900	1.16109500
H	2.42857700	0.69653700	0.34925500
H	1.31966200	-1.41503900	0.72216000
H	1.34423100	-1.15577300	-1.02024400
H	-1.03375800	-0.44666200	-0.98804300
H	-0.91086500	-1.98435300	-0.14412000
H	-0.99436800	1.62020800	2.22754800
H	-1.09057000	1.78147300	0.46536400
H	-0.91498300	-0.83366000	2.05289100
H	-2.30267000	-0.25750200	1.12837700
O	0.74310200	1.22633500	1.27294900

O	1.06105900	1.39146700	-1.04311200
C	1.81797500	2.47847000	-1.31617900
C	1.34868300	3.15992600	-2.57286300
H	1.35445600	2.45321100	-3.40533800
H	0.32032600	3.50463700	-2.44127900
H	1.99424500	4.00601500	-2.79829200
O	2.75037700	2.83848600	-0.63247400

6

E = -3096.259165

ZPVE = 0.291324

Symbol	X	Y	Z
C	-2.03458300	0.17182800	0.28857800
C	-0.78212500	-0.70969200	0.39689000
C	0.46768700	-0.04942100	-0.19875900
C	0.68653400	1.37663700	0.31967200
C	-0.57321500	2.24445700	0.28236200
C	-1.79125100	1.55331800	0.91134900
H	1.35219500	-0.64710100	0.01945900
H	-0.57360800	-0.90064000	1.45636600
H	-0.94641500	-1.68405800	-0.07023100
H	-2.32141000	0.28875700	-0.76390100
H	-2.87354000	-0.32525400	0.78435300
H	1.50132300	1.86078600	-0.21634900
H	-0.36193100	3.19624400	0.77637800
H	-0.78116100	2.47446900	-0.76760500
H	-1.63371500	1.44102000	1.98997900
H	-2.67387200	2.18760500	0.78754400
C	2.24636200	0.18568200	-2.60491400
C	2.68051100	1.37302500	-3.20140800
C	3.16508700	-0.83546000	-2.33927200
C	4.02810300	1.53792500	-3.52706600
H	1.97178800	2.16606000	-3.40738100
C	4.51232600	-0.65914600	-2.65248100
H	2.83103700	-1.76595900	-1.89534100
C	4.94553100	0.52580800	-3.24940100
H	4.35817900	2.46074200	-3.99077200
H	5.22027100	-1.45255400	-2.44045000
H	5.99234900	0.65742200	-3.49827200
O	1.12519500	1.20920500	1.71333900
Se	0.35894700	-0.05800000	-2.21214300
C	1.99839400	2.09778400	2.22240200
C	2.35145900	1.75706400	3.64617300
H	1.44620200	1.71523600	4.25546600
H	2.82026900	0.77113500	3.68447300
H	3.03318600	2.50451600	4.04631700
O	2.43915800	3.04276800	1.60218700

7

E = -346.989159

ZPVE = 0.145489

Symbol	X	Y	Z
C	-0.85881700	1.59033300	0.10511400
H	-0.44620400	0.57845000	0.16646900
H	-1.94478500	1.50082400	0.20801100
C	-0.31884600	2.41590900	1.25933400
H	-0.73859300	3.42465400	1.26535100
H	0.77012300	2.49699700	1.22330100
C	-0.51039500	2.21742600	-1.24877200
H	0.57235400	2.29420900	-1.38535600
H	-0.90700500	1.61221200	-2.06705800
H	-0.93232500	3.22243800	-1.34263900
O	-0.69284500	1.75106700	2.49677400
C	-0.30571100	2.32428800	3.64858400
C	-0.76035100	1.52569600	4.84065300
H	-1.84849100	1.43186300	4.83271100
H	-0.34259700	0.51756700	4.79331500
H	-0.43899600	2.01498400	5.75757500
O	0.33025500	3.35701500	3.69781900

11

E = -501.727597

ZPVE = 0.213051

Symbol	X	Y	Z
C	-1.46423600	1.05179400	0.42870800
C	-0.01115500	1.45143300	0.50547000
C	-1.07003400	2.50182300	0.27524700
H	-1.81089800	0.52793900	-0.45370000
H	-1.95384800	0.75390700	1.34846000
H	0.63750600	1.19769700	-0.32412100
H	0.46786900	1.42246100	1.47758000
H	-1.13170600	2.91089000	-0.72871100
C	-1.41212000	3.48592300	1.36416000
H	-1.36733600	3.00380400	2.34193200
C	-2.74619800	4.16136800	1.17310800
C	-3.98626700	3.55038100	1.78176400
C	-3.43071300	4.83969400	2.33501200
H	-2.87081900	4.62986000	0.20146300
H	-3.86849900	2.65424200	2.37975200
H	-4.90169700	3.58682400	1.20393300
H	-3.96853800	5.75888400	2.13688500
H	-2.94026400	4.80247300	3.30084400
O	-0.37295200	4.53429600	1.34383900
C	0.32872600	4.79265800	2.45915900
C	1.32179900	5.90213800	2.22819600
H	1.95816000	5.66555500	1.37327200

H	0.78869700	6.82732200	1.99624400
H	1.93095500	6.04521800	3.11823300
O	0.17672300	4.20930800	3.51357800

For Table 5, Acetone (ROC(O)OH): B3LYP/6-311++G(d,p)

1

E = -535.584938

ZPVE = 0.165281

Symbol	X	Y	Z
C	-0.60191900	-0.95081500	-0.09123800
C	0.92529900	-0.81353500	-0.06012400
C	1.36810800	0.62624300	0.16462000
C	-0.71801800	1.18130600	1.21974600
C	-1.20927200	-0.25761500	1.13483300
H	2.43516300	0.70930200	0.35837700
H	1.33323700	-1.39851700	0.77052400
H	1.38651100	-1.18646300	-0.97737400
H	-0.99818700	-0.49687800	-1.00556200
H	-0.87760700	-2.00806100	-0.11496300
H	-1.02554100	1.66464000	2.14675600
H	-1.09822700	1.77194300	0.37918200
H	-0.92443800	-0.79294000	2.04750000
H	-2.30226200	-0.25667900	1.08515900
O	0.72903700	1.25923500	1.22836400
O	1.08939800	1.35123300	-1.08445500
C	1.84434600	2.41569300	-1.35291700
O	2.78632100	2.82185800	-0.71369800
O	1.38956600	2.97644800	-2.48569200
H	1.94880400	3.74240000	-2.68000900

6

E = -3132.216694

ZPVE = 0.269290

Symbol	X	Y	Z
C	-2.04120800	0.17065000	0.28740800
C	-0.79034600	-0.71310400	0.39590800
C	0.46155000	-0.05373500	-0.19632100
C	0.67901500	1.37146400	0.32225500
C	-0.57733000	2.24157500	0.28958700
C	-1.79718500	1.54999400	0.91457300
H	1.34558300	-0.65132400	0.02357100
H	-0.58424400	-0.90793800	1.45513700
H	-0.95459200	-1.68569900	-0.07461700
H	-2.32627700	0.29061500	-0.76512700
H	-2.88143000	-0.32633900	0.78084100

H	1.50003500	1.85443000	-0.20477500
H	-0.36420500	3.19168600	0.78641900
H	-0.78184800	2.47598700	-0.75987500
H	-1.64183700	1.43489400	1.99313200
H	-2.67802000	2.18641100	0.79058900
C	2.24798200	0.19061800	-2.59383900
C	2.68535500	1.38177200	-3.18021400
C	3.16394900	-0.83422100	-2.33317200
C	4.03414500	1.54681400	-3.50075600
H	1.97839400	2.17729800	-3.38257600
C	4.51229500	-0.65769700	-2.64129300
H	2.82704900	-1.76742300	-1.89718500
C	4.94899300	0.53104400	-3.22805600
H	4.36705800	2.47242700	-3.95675800
H	5.21836200	-1.45379100	-2.43324400
H	5.99669900	0.66273300	-3.47308300
O	1.11370000	1.19785800	1.72321000
Se	0.35892200	-0.05323800	-2.20877100
C	1.97234700	2.08317900	2.21319900
O	2.45274900	3.03229600	1.63588000
O	2.23872800	1.75166500	3.48909400
H	2.86592700	2.40215000	3.83609800

7

E = -382.946336

ZPVE = 0.123454

Symbol	X	Y	Z
C	-0.85872600	1.58724700	0.12045200
H	-0.44366000	0.57657800	0.18156600
H	-1.94433200	1.49744800	0.22465800
C	-0.31814500	2.41476200	1.27131100
H	-0.74148800	3.42131000	1.28138600
H	0.77065500	2.49147500	1.23995300
C	-0.51140400	2.21689600	-1.23246300
H	0.57102800	2.29543800	-1.36961700
H	-0.90764100	1.61049200	-2.04976100
H	-0.93591200	3.22075600	-1.32563200
O	-0.69519200	1.74617700	2.51072900
C	-0.30520400	2.32543100	3.63867500
O	0.32979800	3.35045800	3.74226000
O	-0.73579800	1.58061100	4.67057000
H	-0.44629200	2.01201600	5.48715700

11

E = -537.685322

ZPVE = 0.191047

Symbol	X	Y	Z
C	-1.46253300	1.04849600	0.41797900
C	-0.00833300	1.44371500	0.48113100
C	-1.06609900	2.49828400	0.26482400
H	-1.82094900	0.53097200	-0.46331100
H	-1.94392600	0.74850100	1.34131500
H	0.63124000	1.19319700	-0.35628700
H	0.48089200	1.40967900	1.44795800
H	-1.13828500	2.91170900	-0.73636400
C	-1.39791000	3.47544600	1.36046100
H	-1.34541500	2.99199700	2.33701600
C	-2.72452800	4.16515400	1.18192600
C	-3.96397500	3.56420000	1.80241800
C	-3.39480000	4.84934400	2.34938100
H	-2.85320000	4.63262800	0.21058200
H	-3.84802700	2.66788600	2.40041800
H	-4.88242200	3.60592400	1.23000800
H	-3.92553500	5.77278800	2.15255700
H	-2.89794400	4.80971700	3.31164300
O	-0.34225800	4.51761100	1.33577800
C	0.29432100	4.79895300	2.46179600
O	0.13368100	4.28773300	3.54852200
O	1.18756000	5.77473200	2.21041800
H	1.64879700	5.96771700	3.03905600

<u>For Table 5, Acetone ($ROCOCHCl_2$): B3LYP/6-311++G(d,p)</u>

1

E = -1418.872309

ZPVE = 0.169766

Symbol	X	Y	Z
C	-0.62058800	-0.94594400	-0.09059300
C	0.90662300	-0.80705200	-0.08665900
C	1.35193300	0.62212700	0.18688800
C	-0.71533600	1.13800500	1.29653100
C	-1.20241800	-0.29893900	1.17243800
H	2.42317400	0.70263000	0.35698500
H	1.33397900	-1.42310300	0.71118900
H	1.34950500	-1.14198600	-1.02716700
H	-1.03654600	-0.46010500	-0.97926200
H	-0.89496200	-2.00216600	-0.14672800
H	-1.00072800	1.58727300	2.24720300
H	-1.11585300	1.75687100	0.48674800
H	-0.89590300	-0.86464900	2.05929100
H	-2.29614900	-0.30023300	1.14696000
O	0.73309100	1.22325700	1.27362500
O	1.05052900	1.39496900	-1.04465100
C	1.77353900	2.47780400	-1.29163800
C	1.33777100	3.18971000	-2.57753800

O	2.68773400	2.90658000	-0.63074000
Cl	1.56044200	2.12205500	-4.00710800
Cl	-0.35866400	3.76975800	-2.44018600
H	1.96468300	4.06051300	-2.72548100

6

E = -4015.504845

ZPVE = 0.273787

Symbol	X	Y	Z
C	-2.04163400	0.16523900	0.27746900
C	-0.79312200	-0.72127300	0.38997700
C	0.46021900	-0.06934000	-0.20731700
C	0.67991200	1.35858700	0.29942300
C	-0.57282400	2.23299400	0.26869000
C	-1.79404000	1.54717600	0.89738700
H	1.34293700	-0.66729200	0.01646300
H	-0.58674000	-0.91110100	1.44994600
H	-0.96016800	-1.69600300	-0.07499700
H	-2.32744400	0.28026400	-0.77530800
H	-2.88244600	-0.32687800	0.77459600
H	1.50388700	1.83721800	-0.22674800
H	-0.35627600	3.18440800	0.76140000
H	-0.77682300	2.46369100	-0.78163300
H	-1.63952200	1.43790000	1.97650100
H	-2.67278200	2.18551100	0.76929100
C	2.24292500	0.18641100	-2.60597400
C	2.66357000	1.37841700	-3.20278400
C	3.17297600	-0.82298000	-2.33529500
C	4.01011100	1.55971800	-3.52386100
H	1.94546500	2.16186900	-3.41290500
C	4.51894800	-0.62983400	-2.64382000
H	2.84916200	-1.75701700	-1.89127100
C	4.93908300	0.55964600	-3.24106100
H	4.33019400	2.48574100	-3.98811100
H	5.23616200	-1.41375300	-2.42792200
H	5.98503100	0.70409100	-3.48638600
O	1.11595600	1.19404500	1.70820700
Se	0.35709600	-0.07970900	-2.21961600
C	2.00218900	2.04298700	2.19706700
C	2.36993900	1.73002000	3.65208400
O	2.50524300	2.98001200	1.62327200
Cl	0.94311700	1.96148700	4.72396100
Cl	3.05586400	0.07676100	3.81140800
H	3.13164300	2.42776200	3.97781400

7

E = -1266.234173

ZPVE = 0.128034

Symbol	X	Y	Z
C	-0.85730800	1.59373600	0.08624900
H	-0.44592800	0.58156500	0.14435500
H	-1.94294000	1.50785600	0.19175200
C	-0.31291500	2.41550400	1.23851200
H	-0.73221100	3.42343500	1.25885500
H	0.77623800	2.48819400	1.21372400
C	-0.50871500	2.22677100	-1.26478700
H	0.57382000	2.30133900	-1.40290900
H	-0.90838300	1.62427900	-2.08323800
H	-0.92956400	3.23245200	-1.35429500
O	-0.69256400	1.74276600	2.48062100
C	-0.31816800	2.30518700	3.61535700
C	-0.77223200	1.51200100	4.84443800
O	0.31290900	3.32866900	3.73467300
Cl	-2.56620800	1.41402200	4.91797800
Cl	-0.01725800	-0.12031300	4.86539600
H	-0.44179500	2.03005500	5.73639100

11

E = -1420.973452

ZPVE = 0.195583

Symbol	X	Y	Z
C	-1.47291800	1.03582900	0.40890300
C	-0.02138000	1.43911700	0.46556600
C	-1.08571500	2.48863800	0.25550300
H	-1.83349800	0.51912700	-0.47189700
H	-1.94854500	0.73188900	1.33387400
H	0.61560600	1.19494300	-0.37557400
H	0.47279500	1.40642500	1.42986300
H	-1.16561000	2.90389900	-0.74413600
C	-1.42058600	3.45906800	1.35424100
H	-1.35750100	2.97735400	2.33085500
C	-2.74669500	4.14933200	1.18511700
C	-3.98191500	3.54212700	1.80910100
C	-3.41423300	4.82603500	2.35880500
H	-2.88020500	4.61986900	0.21612200
H	-3.86092700	2.64344600	2.40240400
H	-4.90184800	3.58339600	1.23919000
H	-3.94733700	5.74915200	2.16741800
H	-2.91348500	4.78358400	3.31888700
O	-0.36271100	4.51099200	1.32232000
C	0.26993600	4.82806200	2.43382500
C	1.32014400	5.92503500	2.21466800
O	0.10401900	4.35481800	3.53479800
Cl	0.54915000	7.44674300	1.64485600
Cl	2.60183300	5.36936300	1.08156300

H	1.80086900	6.14353000	3.16032100

For Table 5, Acetone ($ROCOCF_3$): B3LYP/6-311++G(d,p)

1

E = -797.454592

ZPVE = 0.164296

Symbol	X	Y	Z
C	-0.61418800	-0.93192900	-0.11050400
C	0.91360800	-0.80357300	-0.08673000
C	1.36594800	0.61801400	0.20707700
C	-0.71549900	1.14613500	1.28384900
C	-1.20675000	-0.28784400	1.14890600
H	2.43579400	0.69255400	0.38781500
H	1.32733400	-1.42830400	0.71155000
H	1.36741700	-1.13332900	-1.02368400
H	-1.01638900	-0.43903900	-1.00170800
H	-0.89406100	-1.98600100	-0.17554900
H	-1.00662000	1.59354300	2.23333900
H	-1.10380000	1.77061700	0.47246400
H	-0.91270500	-0.85842100	2.03670900
H	-2.29998000	-0.28349200	1.11134900
O	0.73516600	1.22633300	1.27531300
O	1.09209500	1.40435100	-1.04019200
C	1.81175700	2.48866500	-1.25443700
C	1.33792600	3.16770200	-2.57208200
O	2.70647800	2.94150200	-0.59362900
F	1.45864600	2.32963500	-3.61934900
F	2.06273100	4.26095500	-2.82966000
F	0.04459000	3.53441600	-2.48388400

6

E = -3394.087111

ZPVE = 0.268332

Symbol	X	Y	Z
C	-2.02641400	0.16679100	0.29890400
C	-0.76961900	-0.70796600	0.41079900
C	0.47426200	-0.05047500	-0.20016300
C	0.68285800	1.38374400	0.28995800
C	-0.57639900	2.24738600	0.26410800
C	-1.78725000	1.55574800	0.90618600
H	1.36416300	-0.63805600	0.02254100
H	-0.55522300	-0.88847100	1.47094500
H	-0.93052500	-1.68745900	-0.04589600
H	-2.31969800	0.27072000	-0.75293100
H	-2.85974400	-0.32839000	0.80524900

H	1.50294600	1.86505600	-0.23974800
H	-0.36477100	3.20516300	0.74625500
H	-0.78842700	2.46718200	-0.78690100
H	-1.62566200	1.45700100	1.98538900
H	-2.67177400	2.18578800	0.77819800
C	2.24627000	0.17854800	-2.60798200
C	2.67292600	1.36949400	-3.20257500
C	3.16928200	-0.83966400	-2.34651500
C	4.01915000	1.54112700	-3.53021500
H	1.95995600	2.15934200	-3.40603300
C	4.51496800	-0.65631700	-2.66211000
H	2.84010600	-1.77266500	-1.90429300
C	4.94134900	0.53223000	-3.25675100
H	4.34425500	2.46630800	-3.99260200
H	5.22694500	-1.44697600	-2.45365700
H	5.98703000	0.66909400	-3.50745100
O	1.13163600	1.23466800	1.70556300
Se	0.36069300	-0.07483300	-2.21161700
C	1.98769900	2.11106900	2.18607700
C	2.32985300	1.73976200	3.65745900
O	2.47356700	3.06613200	1.64102500
F	2.85992600	0.50413900	3.73474700
F	3.21251500	2.60276700	4.17030200
F	1.22547800	1.76334500	4.42871200

7

E = -644.816429

ZPVE = 0.122561

Symbol	X	Y	Z
C	-0.85528800	1.59178300	0.10714000
H	-0.43653800	0.58366400	0.17832200
H	-1.93964000	1.50206500	0.22056800
C	-0.30764400	2.43637000	1.24018500
H	-0.73499800	3.44053800	1.25133000
H	0.78063000	2.51238700	1.21110600
C	-0.51804100	2.20694100	-1.25532700
H	0.56313400	2.28515000	-1.40100900
H	-0.91948500	1.58931200	-2.06136500
H	-0.94547800	3.20852400	-1.35726700
O	-0.67577400	1.78080000	2.50208800
C	-0.28520200	2.35577200	3.61896600
C	-0.76900200	1.51414500	4.83315900
O	0.34718500	3.36920800	3.75265500
F	-2.11148000	1.40749300	4.84361500
F	-0.38884800	2.08181400	5.98222100
F	-0.25717500	0.26905600	4.79245700

11

E = -799.556178

ZPVE = 0.190095

Symbol	X	Y	Z
C	-1.46192300	1.03937900	0.39528500
C	-0.01218900	1.44458000	0.46570500
C	-1.07664600	2.49513900	0.26017100
H	-1.81698500	0.53370700	-0.49400800
H	-1.94312300	0.72427800	1.31357800
H	0.63058200	1.21249400	-0.37438300
H	0.47608500	1.40148600	1.43261200
H	-1.15190600	2.92176100	-0.73485300
C	-1.42302500	3.44909700	1.36748200
H	-1.37069600	2.95680500	2.33919500
C	-2.73791700	4.15579700	1.19293600
C	-3.98404400	3.55569800	1.80319700
C	-3.40922400	4.82980800	2.36640000
H	-2.85893900	4.63349900	0.22599000
H	-3.87647800	2.65171000	2.39090600
H	-4.89767200	3.60913200	1.22440100
H	-3.93093200	5.75957600	2.17616200
H	-2.91790300	4.77588400	3.33075200
O	-0.34929500	4.49987600	1.36443000
C	0.25299700	4.80576200	2.49012600
C	1.31811400	5.90714200	2.21770800
O	0.07925200	4.35516300	3.59256700
F	0.75266600	7.00913300	1.68816900
F	2.25432200	5.46893800	1.35313600
F	1.93492900	6.26205900	3.34997100

<u>For Table 5, Acetonitrile (ROH): B3LYP/6-311++G(d,p)</u>

1

E = -346.959683

ZPVE = 0.150205

Symbol	X	Y	Z
C	-0.67210500	-0.97416400	0.00601500
C	0.86220800	-0.97007900	-0.01895300
C	1.42822000	0.44778300	-0.01404800
C	-0.55882700	1.30269300	1.05069700
C	-1.17798000	-0.08671200	1.15079800
H	2.50235700	0.44160900	0.19156100
H	1.24663400	-1.47834000	0.87129000
H	1.25116900	-1.50162100	-0.89101300
H	-1.06019100	-0.59994900	-0.94701900
H	-1.03925700	-1.99787400	0.11957700
H	-0.80420300	1.91921100	1.91634800
H	-0.91425700	1.81667800	0.15032400

H	-0.91006000	-0.53324700	2.11541400
H	-2.26850600	0.00403300	1.12578100
O	0.88307400	1.24481000	1.02785900
O	1.18509400	1.02654600	-1.29025900
H	1.60714700	1.89402000	-1.30928900

6

E = -2943.588280

ZPVE = 0.253968

Symbol	X	Y	Z
C	-1.93229300	0.22677600	0.32678400
C	-0.74390100	-0.74510500	0.29795300
C	0.53064600	-0.11491400	-0.27808400
C	0.87708400	1.22580100	0.38570900
C	-0.32288500	2.17833200	0.46839900
C	-1.56959100	1.51773700	1.07325700
H	1.37379300	-0.79467000	-0.15608200
H	-0.51511700	-1.05457300	1.32431200
H	-0.99427500	-1.65379000	-0.25590600
H	-2.24302700	0.46974400	-0.69726300
H	-2.78959400	-0.25904000	0.80243100
H	1.68676200	1.70672400	-0.17388700
H	-0.03274900	3.06282700	1.04636400
H	-0.54632600	2.53080800	-0.54427000
H	-1.38705600	1.28512900	2.12824400
H	-2.40750500	2.22097900	1.04663200
C	2.23917300	0.21110100	-2.73033900
C	2.73971700	1.39550000	-3.27913200
C	3.08774300	-0.88855600	-2.56204200
C	4.08188100	1.47879800	-3.65485400
H	2.08646800	2.24996900	-3.40919700
C	4.43124000	-0.79449000	-2.92342600
H	2.70214900	-1.81668800	-2.15656000
C	4.93006000	0.38743000	-3.47349100
H	4.46251900	2.40002900	-4.08161500
H	5.08419500	-1.64918300	-2.78613700
H	5.97313000	0.45525700	-3.76067900
O	1.37055000	0.88098800	1.70009400
H	1.60143700	1.69802200	2.15718100
Se	0.35418900	0.08737300	-2.27547200

7

E = -194.317129

ZPVE = 0.107725

Symbol	X	Y	Z

C	-0.90913300	1.59748400	0.01398300
H	-0.56812800	0.55662800	0.03333300
H	-2.00422000	1.57395200	0.03156000
C	-0.41545500	2.29609800	1.27127500
H	-0.76772200	3.33537200	1.28854200
H	0.68178200	2.31251700	1.28733400
C	-0.42068200	2.28424100	-1.26439600
H	0.67231700	2.29749900	-1.31645000
H	-0.78874600	1.76295100	-2.15132000
H	-0.77003900	3.31986200	-1.31872300
O	-0.91434500	1.58742200	2.41661400
H	-0.59882700	2.03087600	3.21129700

11

E = -349.057638

ZPVE = 0.175780

Symbol	X	Y	Z
C	-1.54319300	0.93100600	0.48563200
C	-0.07881500	1.27567400	0.35531600
C	-1.13222600	2.34576100	0.16528800
H	-2.00690600	0.34733300	-0.30032500
H	-1.92319200	0.72722700	1.48005900
H	0.45749600	0.92750900	-0.51907100
H	0.51146500	1.29930400	1.26538400
H	-1.29754100	2.67495400	-0.85680400
C	-1.28340100	3.44413000	1.19495600
H	-1.18073000	3.00544900	2.19847200
C	-2.61113100	4.15535500	1.10653700
C	-3.79902000	3.64267700	1.88358300
C	-3.13370700	4.93698200	2.28667100
H	-2.82191400	4.57009800	0.12484900
H	-3.65253300	2.78036700	2.52372800
H	-4.77206300	3.68842400	1.40961700
H	-3.65530800	5.86633800	2.09171800
H	-2.53811300	4.93600700	3.19270000
O	-0.25546100	4.44637300	1.01868400
H	0.58819400	3.98656800	0.93272800

<u>For Table 5, Acetonitrile ($ROCH_2CF_3$): B3LYP/6-311++G(d,p)</u>

1

E = -723.388513

ZPVE = 0.183069

Symbol	X	Y	Z
C	-0.61026900	-0.97815500	-0.05241300
C	0.91642000	-0.96433500	0.09880400

C	1.47009700	0.45489100	0.17239600
C	-0.63205700	1.30469900	0.98283000
C	-1.24898800	-0.08787700	1.02119100
H	2.51814200	0.46075800	0.48938500
H	1.20084200	-1.46777300	1.02830300
H	1.40855700	-1.49206600	-0.72146300
H	-0.88840800	-0.61239300	-1.04626800
H	-0.98076200	-2.00372600	0.02518900
H	-0.97606900	1.92580900	1.81025200
H	-0.88448100	1.81075600	0.04392000
H	-1.09101100	-0.52601600	2.01326500
H	-2.32962200	-0.00372100	0.87043100
O	0.80596300	1.25800400	1.12560700
O	1.38330200	1.02173400	-1.13756900
C	2.00401600	2.28244400	-1.25598300
H	1.47268400	3.06199200	-0.70210900
H	3.04711000	2.25637200	-0.91910000
C	2.00026000	2.66793200	-2.72068100
F	2.67667300	1.78928400	-3.49327700
F	2.58628000	3.87746400	-2.88535800
F	0.75160300	2.75747600	-3.23077700

6

E = -3320.016864

ZPVE = 0.286923

Symbol	X	Y	Z
C	-1.90781800	0.14939000	0.36650600
C	-0.67090100	-0.76004800	0.36461800
C	0.56053600	-0.09490600	-0.26300400
C	0.84380200	1.29258000	0.33002000
C	-0.40111000	2.18760100	0.37462200
C	-1.60148200	1.49611500	1.03587800
H	1.44045600	-0.72197800	-0.12357700
H	-0.41075900	-1.00748800	1.40049400
H	-0.88079500	-1.70637600	-0.14061900
H	-2.24905400	0.32058300	-0.66215000
H	-2.72931200	-0.35390000	0.88491300
H	1.63886000	1.78173100	-0.24425500
H	-0.16361400	3.12565300	0.88458100
H	-0.65055900	2.45733600	-0.65659900
H	-1.39057700	1.33205800	2.09855300
H	-2.47489400	2.15306300	0.98626500
C	2.21668100	0.21693100	-2.74779200
C	2.65158900	1.41522500	-3.32168700
C	3.11959900	-0.83733100	-2.57222500
C	3.98367400	1.55769600	-3.71509100
H	1.95543600	2.23401600	-3.45828100
C	4.45235200	-0.68397500	-2.95251900
H	2.78438900	-1.77585400	-2.14644700

C	4.88596400	0.51177100	-3.52735600
H	4.31385900	2.48901100	-4.16146200
H	5.14796500	-1.50342100	-2.81020700
H	5.92093800	0.62547200	-3.82898700
O	1.36098100	1.02982800	1.66012700
Se	0.34628500	0.00761500	-2.26438800
C	2.06471200	2.10085300	2.23644200
H	1.41413200	2.93177700	2.53189500
H	2.84714300	2.48551700	1.57053100
C	2.74309900	1.59245900	3.49322400
F	3.42637500	2.59663100	4.09269200
F	3.62798500	0.60200600	3.24460200
F	1.86314100	1.11317700	4.40059700

7

E = -570.747307

ZPVE = 0.140938

Symbol	X	Y	Z
C	-0.90657700	1.59871500	0.02120400
H	-0.56242900	0.56021100	0.05923700
H	-2.00044400	1.57550100	0.05754300
C	-0.39169200	2.32986900	1.24950100
H	-0.74515400	3.36988900	1.26063700
H	0.70658400	2.34470700	1.26211500
C	-0.43865400	2.25931200	-1.27920800
H	0.65311000	2.27242100	-1.34921300
H	-0.82079800	1.71666700	-2.14686400
H	-0.79153200	3.29244400	-1.35090200
O	-0.86993100	1.65430500	2.42149700
C	-0.44089300	2.25837800	3.61427200
H	0.65235600	2.25803300	3.70888000
H	-0.80194000	3.29022100	3.70948100
C	-1.00291000	1.46616200	4.77739600
F	-0.60934700	2.01682500	5.95117500
F	-0.58569100	0.18072300	4.78165000
F	-2.35411700	1.43937900	4.78417500

11

E = -725.485022

ZPVE = 0.208755

Symbol	X	Y	Z
C	-1.82235800	0.89513300	0.33506200
C	-0.32362300	0.99973400	0.22085900
C	-1.18320600	2.23371900	0.05235800
H	-2.37160300	0.41928000	-0.46804900

H	-2.23993500	0.73269000	1.32177900
H	0.15823300	0.59481200	-0.66101800
H	0.25279700	0.90048000	1.13388400
H	-1.29060500	2.60595000	-0.96252800
C	-1.22035500	3.32654000	1.09994700
H	-1.04863800	2.88814600	2.09425500
C	-2.52732100	4.08139400	1.10274800
C	-3.66253400	3.62659700	1.98763700
C	-2.92599400	4.90647000	2.30054900
H	-2.80710700	4.47700600	0.13088000
H	-3.49128900	2.77606400	2.63701000
H	-4.66865000	3.69191300	1.59152100
H	-3.43015100	5.84873700	2.12304200
H	-2.25778900	4.90724700	3.15435000
O	-0.18880100	4.32027100	0.86415000
C	1.13030000	3.86990800	1.04373800
H	1.27002200	3.37589600	2.01349800
H	1.46123400	3.19025900	0.25172800
C	2.04301500	5.07976500	1.01488100
F	1.76749000	5.96808600	1.99573300
F	1.97433800	5.75507500	-0.15463300
F	3.33241200	4.69586100	1.17703300

<u>For Table 5, Acetonitrile (ROPh): B3LYP/6-311++G(d,p)</u>

1

E = -577.977096

ZPVE = 0.230523

Symbol	X	Y	Z
C	-0.86475200	-0.83382300	-0.03456800
C	0.61422800	-0.88845700	-0.43873600
C	1.34826100	0.40260900	-0.08701900
C	-0.22624800	0.90021300	1.66043800
C	-0.98931400	-0.39889200	1.43129700
H	2.42873100	0.28935600	-0.20205100
H	1.11569500	-1.69841600	0.10070700
H	0.73433700	-1.08380800	-1.50686100
H	-1.39832400	-0.12419000	-0.67541700
H	-1.32769800	-1.81223800	-0.18809800
H	-0.18872600	1.16910400	2.71640300
H	-0.69366500	1.72533700	1.11112400
H	-0.58302900	-1.17684000	2.08769500
H	-2.03727000	-0.25177500	1.71029400
O	1.15635000	0.78709200	1.25587400
O	0.88775000	1.41055800	-0.99783100
C	1.60314200	2.57279200	-1.14784200
C	1.20438100	3.39318900	-2.21035200
C	2.66556900	2.96316800	-0.32644300
C	1.86938000	4.58994100	-2.45455300
H	0.37786400	3.07504000	-2.83510400

C	3.32877100	4.16451300	-0.58965700
H	2.96242200	2.35845600	0.51875600
C	2.93997100	4.98313400	-1.64728400
H	1.55258900	5.21540900	-3.28178900
H	4.15229600	4.46020500	0.05104200
H	3.45869900	5.91492900	-1.83940200

6

E = -3174.606422

ZPVE = 0.334453

Symbol	X	Y	Z
C	-2.14996600	0.25914000	0.07609500
C	-0.92074100	-0.63023000	0.30913500
C	0.37260300	-0.01609400	-0.23956700
C	0.58751000	1.43038000	0.23244200
C	-0.65586700	2.31071600	0.05458100
C	-1.92254600	1.66856000	0.63854800
H	1.23237300	-0.61403200	0.06079300
H	-0.78099300	-0.76674200	1.38793200
H	-1.06969900	-1.62590500	-0.11658400
H	-2.36962100	0.32263700	-0.99704100
H	-3.02599500	-0.19938200	0.54433100
H	1.44170700	1.85380900	-0.30038900
H	-0.47674600	3.28796400	0.51003800
H	-0.78969000	2.48446200	-1.01804500
H	-1.83451800	1.61244600	1.72925500
H	-2.78493600	2.30716000	0.42552500
C	2.29770600	0.06131200	-2.54194200
C	2.79062500	1.18440000	-3.21274600
C	3.17890200	-0.94447100	-2.13033800
C	4.15853500	1.30069600	-3.46740100
H	2.11144700	1.96586700	-3.53178600
C	4.54596100	-0.81504600	-2.37229700
H	2.80109200	-1.82754800	-1.62837200
C	5.03784000	0.30536000	-3.04393300
H	4.53384500	2.17347400	-3.98992100
H	5.22409000	-1.59588200	-2.04657700
H	6.10025100	0.39968900	-3.23744900
O	0.93612800	1.30925500	1.63667600
Se	0.38475900	-0.11896500	-2.25239300
C	1.66519000	2.28227900	2.26087700
C	1.94276600	2.04798500	3.61586700
C	2.14119700	3.44887100	1.65166200
C	2.68876700	2.96461400	4.34683700
H	1.56760100	1.14050500	4.07463600
C	2.89194400	4.36017000	2.39973000
H	1.93703500	3.66364600	0.61191300
C	3.17131300	4.12988000	3.74383200
H	2.89551800	2.76736400	5.39298600

H	3.25531500	5.26027100	1.91605100
H	3.75253200	4.84423300	4.31474000

7

E = -425.337691

ZPVE = 0.188626

Symbol	X	Y	Z
C	-0.44417100	1.55902700	-0.05463400
H	0.59753500	1.26305200	-0.21476000
H	-1.01114500	0.64341600	0.14171600
C	-0.51721500	2.45417600	1.17197000
H	-1.55455300	2.74154200	1.38022200
H	0.06883100	3.36824300	1.01991600
C	-0.98978200	2.25686400	-1.30376500
H	-0.42244300	3.16368900	-1.53373200
H	-0.92795900	1.59698300	-2.17214000
H	-2.03853900	2.54117000	-1.17573000
O	0.01276000	1.72377400	2.28849500
C	0.05316900	2.32273900	3.51474900
C	-0.39464600	3.62235600	3.77534900
C	0.58644300	1.54880400	4.55584200
C	-0.30426200	4.13354300	5.07374600
H	-0.80955400	4.23760500	2.98885500
C	0.66947000	2.07132500	5.84066400
H	0.92874300	0.54388000	4.33698100
C	0.22423700	3.36962900	6.11033800
H	-0.65399300	5.14195300	5.26582600
H	1.08389800	1.46248100	6.63658500
H	0.29001700	3.77493700	7.11308800

11

E = -580.072555

ZPVE = 0.255997

Symbol	X	Y	Z
C	-2.33944600	0.65139700	0.67270500
C	-0.91430100	0.53468800	0.19089500
C	-1.65872500	1.84043400	0.03750500
H	-3.12119200	0.15566500	0.11014000
H	-2.50436700	0.67497700	1.74373300
H	-0.71957100	-0.03925800	-0.70716400
H	-0.13530700	0.47110800	0.94010900
H	-1.97886300	2.08453000	-0.97131500
C	-1.32507800	3.06326200	0.86256600
H	-1.02956400	2.77221700	1.87410600
C	-2.48231700	4.03014400	0.95298200

C	-3.48749200	3.90305600	2.07151900
C	-2.52440900	5.06588700	2.04826300
H	-2.87570600	4.33436300	-0.01239100
H	-3.32667800	3.13109700	2.81497400
H	-4.52887200	4.08933700	1.83843700
H	-2.90836300	6.04869100	1.80291300
H	-1.71718600	5.06577300	2.77225900
O	-0.24052600	3.79978300	0.22564600
C	1.07419000	3.56596000	0.51284400
C	1.99216000	4.18573200	-0.34886200
C	1.55085300	2.81343100	1.59233500
C	3.35922000	4.05524400	-0.13344000
H	1.61176800	4.76728200	-1.18068900
C	2.92745900	2.68977800	1.79609200
H	0.87503200	2.32282100	2.27859400
C	3.84009900	3.30398600	0.94231200
H	4.05237900	4.54175500	-0.81098100
H	3.28090200	2.10280000	2.63684200
H	4.90567700	3.19986300	1.10892200

<u>For Table 5, Acetonitrile (ROPh-p-NO_2): B3LYP/6-311++G(d,p)</u>

1

E = -782.546940

ZPVE = 0.232749

Symbol	X	Y	Z
C	-0.96895800	-0.71959400	0.14221100
C	0.34221300	-0.83503400	-0.64552900
C	1.27724900	0.33691800	-0.37025200
C	0.25383400	0.74644900	1.76642700
C	-0.66554200	-0.45928400	1.62313600
H	2.27213400	0.16016500	-0.78315200
H	0.87686000	-1.74196600	-0.34590700
H	0.16546200	-0.90108100	-1.72136100
H	-1.57339500	0.10016100	-0.25977600
H	-1.55366500	-1.63514200	0.02218400
H	0.59389900	0.88176300	2.79296500
H	-0.25476100	1.66295700	1.44742100
H	-0.18270300	-1.33735700	2.06644000
H	-1.58508700	-0.27372900	2.18632500
O	1.46872100	0.59000100	0.99373600
O	0.70593600	1.48948900	-1.04298200
C	1.44192100	2.61072300	-1.21721200
C	0.83870100	3.61360500	-1.99728300
C	2.72536200	2.81412600	-0.68397300
C	1.50523800	4.79580500	-2.25264500
H	-0.15211000	3.43906100	-2.39709200
C	3.39638000	3.99957900	-0.94509600
H	3.18860800	2.06947000	-0.05411300
C	2.78721300	4.98135700	-1.72543700

H	1.05012100	5.56965900	-2.85444100
H	4.38440700	4.16889500	-0.54060700
N	3.49535700	6.22372000	-1.99116800
O	2.93785400	7.08100800	-2.67889100
O	4.62438000	6.37009100	-1.51945700

6

E = -3379.176795

ZPVE = 0.336719

Symbol	X	Y	Z
C	-2.15097500	0.25518700	0.08075200
C	-0.91834900	-0.62789500	0.31931400
C	0.37260800	-0.01413900	-0.23569200
C	0.57933300	1.43772400	0.21821100
C	-0.66609800	2.31258300	0.04334900
C	-1.92910100	1.66914100	0.63372000
H	1.23544100	-0.60455900	0.07054800
H	-0.77774100	-0.75744600	1.39889300
H	-1.06324600	-1.62677300	-0.09972700
H	-2.37190600	0.31048600	-0.99241700
H	-3.02450700	-0.20323100	0.55326000
H	1.43537700	1.86043000	-0.31009600
H	-0.48916200	3.29412300	0.49061000
H	-0.80102300	2.47815100	-1.03013100
H	-1.84081700	1.62163600	1.72480700
H	-2.79304400	2.30359100	0.41608600
C	2.30034600	0.06069400	-2.53244400
C	2.79049200	1.19365600	-3.18846800
C	3.18335900	-0.94778100	-2.13160400
C	4.15857300	1.31731800	-3.43861700
H	2.10931000	1.97640100	-3.49992900
C	4.55041600	-0.81122500	-2.36960200
H	2.80697100	-1.83798200	-1.64132200
C	5.03990200	0.31922700	-3.02594800
H	4.53231600	2.19750700	-3.94962600
H	5.23038400	-1.59404900	-2.05272500
H	6.10235300	0.41914200	-3.21634500
O	0.92890500	1.33105300	1.63450600
Se	0.38761600	-0.12988000	-2.24686400
C	1.65680000	2.28087100	2.25105300
C	1.93327400	2.03850100	3.61136700
C	2.14334800	3.45001500	1.64057500
C	2.67959100	2.93652900	4.34605900
H	1.55079500	1.13346900	4.06597500
C	2.89523600	4.35124500	2.37928700
H	1.94116300	3.66839200	0.60230600
C	3.16044500	4.09419200	3.72349500
H	2.89520100	2.75403100	5.38935400
H	3.27367700	5.25287800	1.91851600

N	3.94585600	5.04489100	4.49066100
O	4.16805000	4.79991000	5.67845900
O	4.36020200	6.05931600	3.92544200

7

E = -629.907840

ZPVE = 0.190939

Symbol	X	Y	Z
C	-0.51430900	1.54279800	-0.03599900
H	0.46217900	1.06133000	-0.14605400
H	-1.24558100	0.75009900	0.14927800
C	-0.47364400	2.46483000	1.17008500
H	-1.44801100	2.93475800	1.33856900
H	0.27878200	3.24927800	1.03948300
C	-0.87413600	2.30217300	-1.31672900
H	-0.14284600	3.08612300	-1.53432800
H	-0.89782900	1.62270500	-2.17148900
H	-1.85836700	2.77314100	-1.23797500
O	-0.12863400	1.66699500	2.32471200
C	-0.02536600	2.24894800	3.53355800
C	-0.22947900	3.61781800	3.77563600
C	0.31171300	1.39128600	4.59853300
C	-0.09789400	4.11552700	5.06395100
H	-0.48807000	4.29386500	2.97364900
C	0.44291200	1.88723500	5.87925900
H	0.46485800	0.33951600	4.39257200
C	0.23637100	3.25309300	6.10655200
H	-0.25249200	5.16676800	5.26247700
H	0.70122300	1.23518600	6.70159500
N	0.37291300	3.78129600	7.45346000
O	0.67756800	3.00400500	8.36055000
O	0.17940700	4.98490100	7.63702000

11

E = -784.643248

ZPVE = -784.643248

Symbol	X	Y	Z
C	-2.42115700	0.61547300	0.69823400
C	-1.02234000	0.46009700	0.15548800
C	-1.74016900	1.78296000	0.02437900
H	-3.23900600	0.13820300	0.17259000
H	-2.53910400	0.64934100	1.77499700
H	-0.88097800	-0.12226700	-0.74686400
H	-0.21300700	0.37914800	0.87057800
H	-2.09807600	2.03071700	-0.97033800

C	-1.33864300	2.99546400	0.82863700
H	-1.01573000	2.70699900	1.83085100
C	-2.43941400	4.02074100	0.93919000
C	-3.39691500	3.97006600	2.10565800
C	-2.38271300	5.08309400	2.00860800
H	-2.86075500	4.31817500	-0.01606900
H	-3.23942000	3.20908600	2.86096800
H	-4.43750000	4.19941700	1.91151400
H	-2.72964000	6.07652800	1.75186100
H	-1.54466800	5.06241400	2.69627700
O	-0.23086500	3.67110400	0.13716700
C	1.06076300	3.50328700	0.46507300
C	1.97745400	4.19935000	-0.35089100
C	1.54263200	2.72678500	1.53431100
C	3.33320300	4.12632800	-0.10899500
H	1.59302700	4.79317200	-1.17045200
C	2.90513800	2.65462200	1.77823400
H	0.87294100	2.17810000	2.17933500
C	3.79527200	3.35036500	0.96055900
H	4.03599500	4.65917700	-0.73387900
H	3.28081200	2.06017100	2.59922900
N	5.21946800	3.26768300	1.22183400
O	5.98884400	3.89959100	0.49347100
O	5.60788600	2.56964700	2.16192700

<u>For Table 5, Acetonitrile ($ROCOCH_3$): B3LYP/6-311++G(d,p)</u>

1

E = -499.627420

ZPVE = 0.187355

Symbol	X	Y	Z
C	-0.62693900	-0.92973500	-0.09400800
C	0.90183300	-0.80449300	-0.08594400
C	1.35887000	0.62739500	0.16653000
C	-0.70093500	1.16316800	1.28263700
C	-1.20844900	-0.26804700	1.16176500
H	2.42938600	0.69399500	0.34780500
H	1.31894000	-1.41631700	0.72067300
H	1.34256800	-1.15652100	-1.02158700
H	-1.03510200	-0.44568500	-0.98750200
H	-0.91250700	-1.98361000	-0.14397600
H	-0.99209200	1.62061200	2.22822500
H	-1.08932700	1.78209400	0.46609600
H	-0.91412600	-0.83333100	2.05324100
H	-2.30217100	-0.25610800	1.12992500
O	0.74471800	1.22578000	1.27230100
O	1.06212200	1.39051700	-1.04413100
C	1.81574400	2.47995200	-1.31464600
C	1.34934000	3.15924400	-2.57343600
H	1.36355900	2.45273400	-3.40599200

H	0.31837800	3.49810300	-2.44726100
H	1.99133100	4.00894200	-2.79545700
O	2.74411000	2.84387200	-0.62697300

6

E = -3096.259519

ZPVE = 0.291299

Symbol	X	Y	Z
C	-2.03651600	0.17451000	0.28741500
C	-0.78575800	-0.70933400	0.39632800
C	0.46577500	-0.05139400	-0.19826900
C	0.68669300	1.37454300	0.31964300
C	-0.57151800	2.24454000	0.28190900
C	-1.79101000	1.55551500	0.91039200
H	1.34898600	-0.65052700	0.02107800
H	-0.57828300	-0.90095800	1.45587300
H	-0.95154500	-1.68337000	-0.07095200
H	-2.32267600	0.29203500	-0.76517300
H	-2.87653200	-0.32108600	0.78284900
H	1.50245500	1.85697900	-0.21638500
H	-0.35886900	3.19589500	0.77623200
H	-0.77872700	2.47508400	-0.76808600
H	-1.63409300	1.44293500	1.98907000
H	-2.67242000	2.19138300	0.78619700
C	2.24599500	0.18659000	-2.60368800
C	2.67619000	1.37025200	-3.21036900
C	3.16840100	-0.82853500	-2.32780800
C	4.02348900	1.53739400	-3.53625800
H	1.96470900	2.15876100	-3.42411700
C	4.51533800	-0.64970400	-2.64104700
H	2.83778200	-1.75636400	-1.87578700
C	4.94460800	0.53144100	-3.24836300
H	4.35043000	2.45720300	-4.00809000
H	5.22610900	-1.43835500	-2.42093100
H	5.99116800	0.66484400	-3.49734800
O	1.12459600	1.20715300	1.71355100
Se	0.35880600	-0.06044700	-2.21170500
C	2.00313200	2.09083700	2.22126600
C	2.35377100	1.75059500	3.64560800
H	1.44810400	1.71529800	4.25468400
H	2.81660500	0.76192000	3.68570700
H	3.03990500	2.49451800	4.04479300
O	2.45016400	3.03205900	1.59932200

7

E = -346.989396

ZPVE = 0.145474

Symbol	X	Y	Z
C	-0.85885600	1.59049000	0.10521100
H	-0.44626900	0.57859000	0.16679100
H	-1.94487000	1.50117700	0.20800000
C	-0.31888200	2.41633200	1.25911400
H	-0.73873300	3.42505600	1.26505700
H	0.77012300	2.49727900	1.22321800
C	-0.51027800	2.21719200	-1.24865000
H	0.57251000	2.29372800	-1.38512700
H	-0.90698200	1.61173200	-2.06669300
H	-0.93211800	3.22223100	-1.34272700
O	-0.69301200	1.75155300	2.49668400
C	-0.30613800	2.32451700	3.64856500
C	-0.76030600	1.52545600	4.84053400
H	-1.84844500	1.43164000	4.83299400
H	-0.34256200	0.51735100	4.79268300
H	-0.43854400	2.01448600	5.75743600
O	0.33013300	3.35712200	3.69809700

11

E = -501.727879

ZPVE = 0.213020

Symbol	X	Y	Z
C	-1.46344500	1.05232100	0.43025000
C	-0.01062700	1.45285100	0.50752800
C	-1.07006300	2.50256900	0.27651600
H	-1.80941600	0.52818900	-0.45226500
H	-1.95330800	0.75445100	1.34988000
H	0.63849200	1.19930100	-0.32176600
H	0.46800500	1.42449100	1.47985300
H	-1.13156100	2.91121900	-0.72761600
C	-1.41344500	3.48670800	1.36492700
H	-1.36897400	3.00499200	2.34286700
C	-2.74744800	4.16186000	1.17273300
C	-3.98787100	3.55021300	1.78002000
C	-3.43326000	4.83952500	2.33426900
H	-2.87137200	4.63058000	0.20112000
H	-3.87029700	2.65381600	2.37765800
H	-4.90272800	3.58670000	1.20128700
H	-3.97116600	5.75863400	2.13599400
H	-2.94370700	4.80207300	3.30057200
O	-0.37479500	4.53614200	1.34501500
C	0.33192900	4.79017200	2.45790000
C	1.32303100	5.90142200	2.22731700
H	1.95514500	5.66951100	1.36799300
H	0.78805700	6.82734900	2.00276200
H	1.93674600	6.04068700	3.11481800
O	0.18522900	4.20211800	3.51067400

For Table 5, Acetonitrile (ROC(O)OH): B3LYP/6-311++G(d,p)

1

E = -535.585342

ZPVE = 0.165267

Symbol	X	Y	Z
C	-0.60289900	-0.95159100	-0.09061700
C	0.92477900	-0.81926000	-0.06032800
C	1.37241800	0.61938400	0.16124400
C	-0.71204700	1.18407300	1.21506700
C	-1.20758700	-0.25343800	1.13393500
H	2.43982900	0.69913800	0.35455300
H	1.33100300	-1.40369600	0.77151000
H	1.38474800	-1.19566300	-0.97673200
H	-0.99820000	-0.49872900	-1.00589800
H	-0.88199800	-2.00796700	-0.11146200
H	-1.01732600	1.67065900	2.14106900
H	-1.09073300	1.77390000	0.37330100
H	-0.92414200	-0.78739200	2.04781900
H	-2.30056100	-0.24908600	1.08466900
O	0.73568500	1.25776200	1.22253000
O	1.09726500	1.34113100	-1.09158200
C	1.83685500	2.41911300	-1.34706400
O	2.75824700	2.84371700	-0.68981300
O	1.39364900	2.97006900	-2.48903200
H	1.94133000	3.74667600	-2.67414100

6

E = -3132.217097

ZPVE =

Symbol	X	Y	Z
C	-2.04286900	0.17258400	0.28638700
C	-0.79339200	-0.71306400	0.39531300
C	0.45991700	-0.05553500	-0.19597300
C	0.67904600	1.36954600	0.32225100
C	-0.57604900	2.24140200	0.28926600
C	-1.79710300	1.55151300	0.91376200
H	1.34291800	-0.65432500	0.02469300
H	-0.58819600	-0.90859500	1.45459000
H	-0.95884600	-1.68534600	-0.07542700
H	-2.32735900	0.29309700	-0.76623200
H	-2.88396700	-0.32322800	0.77948000
H	1.50084100	1.85115600	-0.20475800
H	-0.36184200	3.19115000	0.78635400
H	-0.77992900	2.47625800	-0.76021500
H	-1.64234400	1.43616800	1.99238200

H	-2.67694100	2.18921500	0.78944700
C	2.24764200	0.19115300	-2.59285100
C	2.68223600	1.38012400	-3.18576000
C	3.16618200	-0.82968700	-2.32548700
C	4.03083200	1.54690100	-3.50640400
H	1.97337600	2.17266700	-3.39314000
C	4.51431400	-0.65125000	-2.63359000
H	2.83171400	-1.76127900	-1.88421100
C	4.94826100	0.53521300	-3.22706800
H	4.36154100	2.47070900	-3.96763500
H	5.22236000	-1.44417600	-2.42027700
H	5.99578200	0.66827300	-3.47212000
O	1.11320300	1.19604600	1.72346700
Se	0.35873200	-0.05523800	-2.20847900
C	1.97640900	2.07756000	2.21223200
O	2.46193700	3.02325100	1.63333300
O	2.24072400	1.74665800	3.48851200
H	2.87118900	2.39413000	3.83539600

7

E = -382.946648

ZPVE = 0.123434

Symbol	X	Y	Z
C	-0.85869100	1.58731900	0.12045400
H	-0.44342200	0.57673700	0.18164900
H	-1.94431500	1.49759700	0.22460400
C	-0.31811500	2.41512900	1.27108300
H	-0.74168100	3.42154800	1.28101900
H	0.77067300	2.49155300	1.23984400
C	-0.51142600	2.21676900	-1.23259700
H	0.57100100	2.29531900	-1.36967300
H	-0.90766300	1.61010100	-2.04969800
H	-0.93607000	3.22054900	-1.32584200
O	-0.69530200	1.74669000	2.51083900
C	-0.30523400	2.32554000	3.63887400
O	0.33022900	3.35040800	3.74261200
O	-0.73589100	1.58064500	4.67048400
H	-0.44640700	2.01119000	5.48759200

11

E = -537.685682

ZPVE = 0.191014

Symbol	X	Y	Z
C	-1.46248100	1.04821000	0.41816200
C	-0.00830300	1.44361400	0.48076500

C	-1.06632900	2.49810400	0.26498900
H	-1.82112100	0.53090200	-0.46316100
H	-1.94346200	0.74810400	1.34167700
H	0.63087800	1.19329000	-0.35701900
H	0.48127200	1.40952600	1.44741600
H	-1.13912700	2.91148600	-0.73617600
C	-1.39800800	3.47504900	1.36080700
H	-1.34553900	2.99158900	2.33731300
C	-2.72431300	4.16525100	1.18213400
C	-3.96412100	3.56429200	1.80194400
C	-3.39495200	4.84917000	2.34958500
H	-2.85266600	4.63296000	0.21086100
H	-3.84851000	2.66771400	2.39960500
H	-4.88224400	3.60652200	1.22905800
H	-3.92546900	5.77274900	2.15279100
H	-2.89851200	4.80908900	3.31204600
O	-0.34179800	4.51717300	1.33622900
C	0.29448800	4.79928300	2.46221000
O	0.13337800	4.28889900	3.54931600
O	1.18788200	5.77465100	2.21019400
H	1.64940900	5.96875600	3.03847700

For Table 5, Acetonitrile (ROCOCHCl$_2$): B3LYP/6-311++G(d,p)

1

E = -1418.872626

ZPVE = 0.169755

Symbol	X	Y	Z
C	-0.62125400	-0.94580700	-0.09039700
C	0.90600600	-0.80762400	-0.08736900
C	1.35233100	0.62117200	0.18604800
C	-0.71456100	1.13811200	1.29674300
C	-1.20199300	-0.29866800	1.17303700
H	2.42370000	0.70076300	0.35573300
H	1.33349900	-1.42394900	0.71016800
H	1.34838000	-1.14269400	-1.02805400
H	-1.03773200	-0.45978200	-0.97874200
H	-0.89602900	-2.00190900	-0.14636100
H	-0.99915800	1.58749700	2.24758300
H	-1.11536900	1.75707400	0.48720800
H	-0.89499700	-0.86447900	2.05964500
H	-2.29571700	-0.29955500	1.14835600
O	0.73413400	1.22308300	1.27279300
O	1.05146200	1.39423100	-1.04583200
C	1.77210500	2.47890700	-1.29067300
C	1.33837600	3.18972600	-2.57787400
O	2.68285500	2.91050600	-0.62660300
Cl	1.56436000	2.12166500	-4.00658400
Cl	-0.35904400	3.76792700	-2.44351500
H	1.96450000	4.06117700	-2.72520200

6

E = -4015.505163

ZPVE = 0.273769

Symbol	X	Y	Z
C	-2.04279100	0.16635000	0.27679300
C	-0.79513600	-0.72127400	0.38995400
C	0.45916800	-0.07060500	-0.20668600
C	0.67975800	1.35743200	0.29940300
C	-0.57221600	2.23285300	0.26816700
C	-1.79425000	1.54819700	0.89651800
H	1.34123400	-0.66919100	0.01786400
H	-0.58947500	-0.91130400	1.45003300
H	-0.96283200	-1.69593800	-0.07491600
H	-2.32810000	0.28144800	-0.77610300
H	-2.88419100	-0.32494100	0.77371800
H	1.50424400	1.83506800	-0.22680500
H	-0.35510000	3.18415100	0.76087200
H	-0.77569400	2.46362100	-0.78223800
H	-1.64029300	1.43906500	1.97573000
H	-2.67236200	2.18726700	0.76788000
C	2.24286300	0.18685600	-2.60498900
C	2.66089500	1.37686800	-3.20763700
C	3.17524600	-0.81883500	-2.32851200
C	4.00718200	1.55979600	-3.52902100
H	1.94106900	2.15758100	-3.42203100
C	4.52094600	-0.62391000	-2.63725200
H	2.85370600	-1.75136600	-1.87969200
C	4.93849600	0.56348300	-3.24052000
H	4.32520700	2.48418700	-3.99791300
H	5.23995800	-1.40490200	-2.41680700
H	5.98421500	0.70921400	-3.48604600
O	1.11532100	1.19341700	1.70849800
Se	0.35725100	-0.08167000	-2.21903400
C	2.00585400	2.03853800	2.19588700
C	2.37190100	1.72625600	3.65149300
O	2.51382400	2.97202000	1.62045500
Cl	0.94621000	1.96763600	4.72279200
Cl	3.04815400	0.06927600	3.81389500
H	3.13754400	2.42012900	3.97619900

7

E = -1266.234413

ZPVE = 0.128018

Symbol	X	Y	Z

C	-0.85770900	1.59406600	0.08634500
H	-0.44705300	0.58158600	0.14431300
H	-1.94341500	1.50924900	0.19206900
C	-0.31228500	2.41550900	1.23831800
H	-0.73084700	3.42370700	1.25872800
H	0.77692000	2.48695200	1.21340800
C	-0.50895900	2.22671600	-1.26482900
H	0.57360500	2.30031500	-1.40315200
H	-0.90941000	1.62442900	-2.08305000
H	-0.92902200	3.23272600	-1.35417600
O	-0.69237700	1.74311900	2.48078800
C	-0.31812200	2.30537900	3.61549300
C	-0.77248700	1.51219200	4.84450000
O	0.31328600	3.32873400	3.73502400
Cl	-2.56639500	1.41115700	4.91601500
Cl	-0.01506600	-0.11911400	4.86648600
H	-0.44388700	2.03079600	5.73679200

11

E = -1420.973747

ZPVE = 0.195554

Symbol	X	Y	Z
C	-1.47267600	1.03557300	0.40908700
C	-0.02121000	1.43919800	0.46506700
C	-1.08594100	2.48853100	0.25563600
H	-1.83351400	0.51906300	-0.47172100
H	-1.94776600	0.73145100	1.33427300
H	0.61532300	1.19525800	-0.37649900
H	0.47339100	1.40655000	1.42914900
H	-1.16661900	2.90374000	-0.74396600
C	-1.42069700	3.45867000	1.35461100
H	-1.35757500	2.97693300	2.33116000
C	-2.74649700	4.14942300	1.18536400
C	-3.98206300	3.54218300	1.80867200
C	-3.41439600	4.82580300	2.35908700
H	-2.87973000	4.62020100	0.21644800
H	-3.86139200	2.64322900	2.40161600
H	-4.90168900	3.58395200	1.23830300
H	-3.94731100	5.74905300	2.16777900
H	-2.91401100	4.78284800	3.31933900
O	-0.36222000	4.51058800	1.32281300
C	0.26967500	4.82863700	2.43439300
C	1.32051600	5.92496200	2.21470400
O	0.10263300	4.35681700	3.53585100
Cl	0.54975800	7.44674100	1.64434500
Cl	2.60149800	5.36855800	1.08108400
H	1.80175700	6.14381300	3.15999300

For Table 5, Acetonitrile ($ROCOCF_3$): B3LYP/6-311++G(d,p)

1

E = -797.454910

ZPVE = 0.164280

Symbol	X	Y	Z
C	-0.61497800	-0.93157000	-0.11035300
C	0.91289600	-0.80405000	-0.08764600
C	1.36632200	0.61701900	0.20638800
C	-0.71463800	1.14609000	1.28457600
C	-1.20627400	-0.28769300	1.14972300
H	2.43635000	0.69051100	0.38646100
H	1.32685700	-1.42918700	0.71014900
H	1.36608600	-1.13369100	-1.02491800
H	-1.01776600	-0.43822500	-1.00105300
H	-0.89530900	-1.98549100	-0.17545000
H	-1.00478200	1.59336200	2.23441100
H	-1.10333400	1.77088500	0.47367500
H	-0.91163000	-0.85861300	2.03709400
H	-2.29950300	-0.28290700	1.11309400
O	0.73632900	1.22596000	1.27476500
O	1.09322300	1.40356700	-1.04150000
C	1.80957300	2.49015400	-1.25313900
C	1.33883500	3.16714500	-2.57300400
O	2.69969500	2.94704800	-0.58858200
F	1.46395900	2.32863000	-3.61927400
F	2.06286400	4.26141500	-2.82927100
F	0.04472400	3.53213300	-2.48918600

6

E = -3394.087428

ZPVE = 0.268307

Symbol	X	Y	Z
C	-2.02745900	0.16820200	0.29818000
C	-0.77142000	-0.70756600	0.41057100
C	0.47333300	-0.05110100	-0.19969600
C	0.68271300	1.38311200	0.29009700
C	-0.57583900	2.24770500	0.26398900
C	-1.78745900	1.55696400	0.90556500
H	1.36266400	-0.63927600	0.02356700
H	-0.55764100	-0.88834400	1.47078900
H	-0.93288100	-1.68695100	-0.04615100
H	-2.32027500	0.27239400	-0.75375500
H	-2.86132500	-0.32634300	0.80424500
H	1.50338100	1.86363300	-0.23937700
H	-0.36368400	3.20523100	0.74639800
H	-0.78734300	2.46783500	-0.78705200
H	-1.62637600	1.45813200	1.98483100

H	-2.67140900	2.18770300	0.77715400
C	2.24627500	0.17913400	-2.60732300
C	2.67085200	1.36786400	-3.20786600
C	3.17116700	-0.83590500	-2.34010600
C	4.01687900	1.54035800	-3.53602100
H	1.95652500	2.15540100	-3.41548500
C	4.51665000	-0.65154700	-2.65610900
H	2.84385100	-1.76720600	-1.89294100
C	4.94096800	0.53467800	-3.25693000
H	4.34033000	2.46373600	-4.00314700
H	5.23007200	-1.43968400	-2.44312600
H	5.98647000	0.67222500	-3.50799300
O	1.13096600	1.23401800	1.70606400
Se	0.36080300	-0.07561900	-2.21119000
C	1.98985600	2.10760400	2.18592400
C	2.33100800	1.73593700	3.65747500
O	2.47939100	3.06066400	1.64037200
F	2.86137600	0.50041200	3.73454500
F	3.21341200	2.59896900	4.17109700
F	1.22649200	1.75896200	4.42837900

7

E = -644.816668

ZPVE = 0.122542

Symbol	X	Y	Z
C	-0.85530900	1.59190500	0.10718800
H	-0.43686800	0.58362400	0.17798700
H	-1.93965400	1.50250500	0.22102100
C	-0.30701700	2.43601700	1.24021000
H	-0.73355800	3.44054200	1.25155600
H	0.78132700	2.51131100	1.21127100
C	-0.51848500	2.20716700	-1.25528600
H	0.56264700	2.28542700	-1.40125600
H	-0.92013800	1.58960500	-2.06128200
H	-0.94600000	3.20874200	-1.35697800
O	-0.67579100	1.78047900	2.50201400
C	-0.28511500	2.35554300	3.61898100
C	-0.76925600	1.51422100	4.83312900
O	0.34773100	3.36871200	3.75261200
F	-2.11158400	1.40588300	4.84196400
F	-0.39105600	2.08345200	5.98199600
F	-0.25551900	0.26988800	4.79371800

11

E = -799.556460

ZPVE = 0.190063

Symbol	X	Y	Z
C	-1.46199900	1.03849700	0.39516600
C	-0.01224700	1.44386200	0.46425000
C	-1.07702900	2.49437200	0.25994000
H	-1.81782100	0.53317900	-0.49402500
H	-1.94230500	0.72321600	1.31386100
H	0.62966100	1.21204600	-0.37658400
H	0.47690800	1.40082600	1.43071300
H	-1.15349100	2.92106100	-0.73496100
C	-1.42245600	3.44796300	1.36777600
H	-1.36998200	2.95549900	2.33935600
C	-2.73668900	4.15587600	1.19365200
C	-3.98342700	3.55566700	1.80264300
C	-3.40835600	4.82893900	2.36750700
H	-2.85717100	4.63450500	0.22710300
H	-3.87649000	2.65097000	2.38936600
H	-4.89660100	3.61021200	1.22323500
H	-3.92954200	5.75912200	2.17783000
H	-2.91750400	4.77371000	3.33200300
O	-0.34700200	4.49775100	1.36445700
C	0.25022600	4.80905100	2.49112300
C	1.31831600	5.90728200	2.21757600
O	0.07031100	4.36561400	3.59556500
F	0.75503500	7.01056800	1.68815500
F	2.25298200	5.46701900	1.35251300
F	1.93672200	6.26109400	3.34941500

<u>For Table 5, DMSO (ROH): B3LYP/6-311++G(d,p)</u>

1

E = -346.959757

ZPVE = 0.150201

Symbol	X	Y	Z
C	-0.67213400	-0.97417500	0.00604100
C	0.86217800	-0.97001400	-0.01898600
C	1.42820400	0.44783800	-0.01408500
C	-0.55893300	1.30266900	1.05076000
C	-1.17802100	-0.08675100	1.15083400
H	2.50233800	0.44168300	0.19145700
H	1.24663100	-1.47827500	0.87124100
H	1.25117100	-1.50160100	-0.89100900
H	-1.06035600	-0.60001200	-0.94696400
H	-1.03920300	-1.99790400	0.11964100
H	-0.80432800	1.91915900	1.91642200
H	-0.91435300	1.81669000	0.15041500
H	-0.91009400	-0.53331600	2.11543300
H	-2.26854000	0.00398500	1.12582600
O	0.88303100	1.24483600	1.02788800
O	1.18507000	1.02673300	-1.29027000

H	1.60785800	1.89385400	-1.30956100

6

E = -2943.588383

ZPVE = 0.253961

Symbol	X	Y	Z
C	-1.93231800	0.22670600	0.32690500
C	-0.74388000	-0.74510700	0.29797200
C	0.53063300	-0.11486200	-0.27808500
C	0.87702700	1.22597600	0.38549700
C	-0.32302800	2.17836200	0.46840700
C	-1.56963000	1.51767300	1.07336300
H	1.37380200	-0.79460400	-0.15612200
H	-0.51507700	-1.05463900	1.32431200
H	-0.99423000	-1.65380600	-0.25587300
H	-2.24313400	0.46967700	-0.69711800
H	-2.78954800	-0.25918400	0.80259900
H	1.68648400	1.70702100	-0.17430100
H	-0.03287200	3.06286300	1.04632100
H	-0.54662300	2.53083800	-0.54423000
H	-1.38703800	1.28509700	2.12835000
H	-2.40757700	2.22087100	1.04679500
C	2.23922400	0.21099300	-2.73037900
C	2.73984000	1.39551700	-3.27885500
C	3.08772000	-0.88877200	-2.56231200
C	4.08202700	1.47882000	-3.65453400
H	2.08668900	2.25009200	-3.40869200
C	4.43123500	-0.79470700	-2.92368400
H	2.70210700	-1.81696200	-2.15697900
C	4.93013400	0.38733100	-3.47345500
H	4.46273500	2.40014500	-4.08102200
H	5.08413500	-1.64947100	-2.78658900
H	5.97320900	0.45516700	-3.76061300
O	1.37098100	0.88140400	1.69981200
H	1.60117200	1.69862600	2.15695100
Se	0.35421900	0.08724900	-2.27551900

7

E = -194.317197

ZPVE = 0.107724

Symbol	X	Y	Z
C	-0.90911600	1.59747700	0.01396200
H	-0.56806700	0.55662200	0.03324500
H	-2.00421500	1.57395300	0.03148200
C	-0.41544500	2.29609600	1.27125400

H	-0.76768200	3.33535200	1.28858600
H	0.68176500	2.31247200	1.28742600
C	-0.42069200	2.28424300	-1.26442100
H	0.67230200	2.29750000	-1.31646400
H	-0.78878900	1.76293600	-2.15132300
H	-0.77006400	3.31985600	-1.31869800
O	-0.91439400	1.58743700	2.41667900
H	-0.59880000	2.03095700	3.21131900

11

E = -349.057733

ZPVE = 0.175773

Symbol	X	Y	Z
C	-1.54314300	0.93090700	0.48570700
C	-0.07881800	1.27569900	0.35508300
C	-1.13232000	2.34570900	0.16524200
H	-2.00696600	0.34722800	-0.30018400
H	-1.92291700	0.72716200	1.48022700
H	0.45731400	0.92762200	-0.51944900
H	0.51164900	1.29943900	1.26501900
H	-1.29788600	2.67483800	-0.85683400
C	-1.28341700	3.44404800	1.19493600
H	-1.18062600	3.00545400	2.19843700
C	-2.61110900	4.15535500	1.10651200
C	-3.79901600	3.64274400	1.88357400
C	-3.13375100	4.93709800	2.28660200
H	-2.82199800	4.56997700	0.12478800
H	-3.65250900	2.78050200	2.52380200
H	-4.77202900	3.68848100	1.40954600
H	-3.65541500	5.86640300	2.09155400
H	-2.53827300	4.93611200	3.19271500
O	-0.25533100	4.44629400	1.01855500
H	0.58845800	3.98646400	0.93389100

<u>For Table 5, DMSO ($ROCH_2CF_3$): B3LYP/6-311++G(d,p)</u>

1

E = -723.388595

ZPVE = 0.183067

Symbol	X	Y	Z
C	-0.59905300	-0.98537000	-0.04786500
C	0.92784600	-0.96149400	0.10019600
C	1.47256000	0.46128300	0.17113300
C	-0.63342300	1.29847300	0.98499600
C	-1.24137800	-0.09794400	1.02596100
H	2.52119000	0.47425500	0.48592300

H	1.21736500	-1.46203200	1.02968600
H	1.42172700	-1.48708800	-0.72040700
H	-0.88168900	-0.62269600	-1.04158700
H	-0.96270100	-2.01322700	0.03179100
H	-0.97983800	1.91824300	1.81241600
H	-0.89067100	1.80197600	0.04604800
H	-1.07880400	-0.53402000	2.01819500
H	-2.32280300	-0.02079800	0.87711200
O	0.80521900	1.26101700	1.12520200
O	1.37932100	1.02641500	-1.13905700
C	1.99157300	2.29113300	-1.25999600
H	1.45354600	3.06864500	-0.70975200
H	3.03403000	2.27335000	-0.92079900
C	1.98819400	2.67189300	-2.72591000
F	2.67260700	1.79575100	-3.49432600
F	2.56554200	3.88517300	-2.89345500
F	0.73992400	2.75061400	-3.23892700

6

E = -3320.016974

ZPVE = 0.286918

Symbol	X	Y	Z
C	-1.90753800	0.14913200	0.36669600
C	-0.67046200	-0.76008400	0.36465800
C	0.56082700	-0.09468200	-0.26298400
C	0.84389900	1.29285300	0.33004300
C	-0.40117900	2.18762000	0.37480600
C	-1.60139800	1.49589400	1.03607700
H	1.44086100	-0.72165100	-0.12378800
H	-0.41024400	-1.00758700	1.40050600
H	-0.88021300	-1.70642900	-0.14060400
H	-2.24887400	0.32030600	-0.66193200
H	-2.72889600	-0.35434300	0.88513300
H	1.63880700	1.78220900	-0.24423200
H	-0.16382700	3.12568800	0.88476300
H	-0.65072900	2.45736500	-0.65638700
H	-1.39045100	1.33189200	2.09875600
H	-2.47491900	2.15269300	0.98650100
C	2.21680500	0.21679800	-2.74804500
C	2.65218100	1.41543200	-3.32088400
C	3.11921700	-0.83810400	-2.57365000
C	3.98425900	1.55759100	-3.71445700
H	1.95646100	2.23475100	-3.45648100
C	4.45196100	-0.68509100	-2.95416500
H	2.78366300	-1.77681800	-2.14856100
C	4.88604800	0.51099300	-3.52797200
H	4.31482900	2.48918400	-4.15995100
H	5.14718900	-1.50502200	-2.81278700

H	5.92100600	0.62445000	-3.82974300
O	1.36131000	1.03009700	1.66011500
Se	0.34641200	0.00793400	-2.26437300
C	2.06419500	2.10159500	2.23677500
H	1.41295200	2.93195100	2.53226000
H	2.84645500	2.48694400	1.57109600
C	2.74258500	1.59330900	3.49356100
F	3.42505200	2.59755600	4.09369200
F	3.62817300	0.60337900	3.24492800
F	1.86266000	1.11301300	4.40054700

7

E = -570.747388

ZPVE = 0.140937

Symbol	X	Y	Z
C	-0.90668100	1.59872000	0.02117800
H	-0.56260900	0.56017900	0.05919300
H	-2.00056700	1.57566400	0.05733700
C	-0.39180500	2.32987000	1.24947400
H	-0.74522800	3.36986800	1.26064200
H	0.70644000	2.34460800	1.26220100
C	-0.43854800	2.25926300	-1.27919800
H	0.65322300	2.27224100	-1.34904500
H	-0.82068100	1.71665000	-2.14688200
H	-0.79129600	3.29243600	-1.35087700
O	-0.87013600	1.65432700	2.42157500
C	-0.44092000	2.25854000	3.61431300
H	0.65232300	2.25827200	3.70870900
H	-0.80203100	3.29033600	3.70949600
C	-1.00273900	1.46624100	4.77741900
F	-0.60927400	2.01661200	5.95130800
F	-0.58550800	0.18071500	4.78148300
F	-2.35402200	1.43922100	4.78425200

11

E = -725.485131

ZPVE = 0.208753

Symbol	X	Y	Z
C	-1.82232100	0.89496600	0.33493200
C	-0.32365200	0.99991100	0.22003900
C	-1.18357000	2.23372500	0.05200900
H	-2.37183100	0.41909500	-0.46799200
H	-2.23935700	0.73237500	1.32185300
H	0.15786600	0.59524000	-0.66213600
H	0.25321500	0.90073700	1.13278400

H	-1.29152300	2.60594700	-0.96282500
C	-1.22044100	3.32645800	1.09966200
H	-1.04855100	2.88809700	2.09389400
C	-2.52730700	4.08149900	1.10276200
C	-3.66239300	3.62663200	1.98777600
C	-2.92575300	4.90642000	2.30081600
H	-2.80732200	4.47724200	0.13100400
H	-3.49102800	2.77599800	2.63697600
H	-4.66856300	3.69212000	1.59182500
H	-3.42996200	5.84871700	2.12357200
H	-2.25745100	4.90691200	3.15454900
O	-0.18866000	4.32008900	0.86358700
C	1.13034400	3.86982400	1.04473900
H	1.26929600	3.37719000	2.01528400
H	1.46175600	3.18907100	0.25390600
C	2.04303600	5.07961900	1.01477000
F	1.76645100	5.96966000	1.99387100
F	1.97528700	5.75314800	-0.15593600
F	3.33231600	4.69633900	1.17869000

<u>For Table 5, DMSO (ROPh): B3LYP/6-311++G(d,p)</u>

1

E = -577.977171

ZPVE = 0.230519

Symbol	X	Y	Z
C	-0.86450800	-0.83414600	-0.03466000
C	0.61465100	-0.88866800	-0.43816100
C	1.34841900	0.40257000	-0.08660000
C	-0.22712500	0.90065900	1.65993900
C	-0.98974500	-0.39871400	1.43098700
H	2.42892700	0.28926200	-0.20104300
H	1.11599000	-1.69837100	0.10177600
H	0.73531100	-1.08442000	-1.50615100
H	-1.39800900	-0.12486500	-0.67596600
H	-1.32717100	-1.81271400	-0.18801200
H	-0.19012800	1.16998000	2.71581100
H	-0.69452200	1.72543900	1.11009600
H	-0.58352900	-1.17632700	2.08782200
H	-2.03782900	-0.25172100	1.70953500
O	1.15575000	0.78777600	1.25599000
O	0.88833800	1.41020000	-0.99809800
C	1.60352300	2.57256700	-1.14795700
C	1.20381100	3.39360900	-2.20963900
C	2.66670200	2.96249700	-0.32729700
C	1.86857400	4.59053000	-2.45373500
H	0.37674500	3.07586800	-2.83387700
C	3.32963100	4.16404000	-0.59036600
H	2.96457200	2.35724300	0.51715200
C	2.93986300	4.98329600	-1.64716200

H	1.55102800	5.21646500	-3.28032500
H	4.15375000	4.45933300	0.04974800
H	3.45839300	5.91521900	-1.83918500

6

E = -3174.606517

ZPVE = 0.334449

Symbol	X	Y	Z
C	-2.15055800	0.25892900	0.07553100
C	-0.92126700	-0.63025300	0.30893500
C	0.37216600	-0.01589000	-0.23939800
C	0.58669600	1.43069600	0.23255400
C	-0.65683100	2.31076600	0.05441800
C	-1.92356700	1.66837300	0.63804400
H	1.23191200	-0.61370500	0.06126900
H	-0.78183800	-0.76680100	1.38776200
H	-1.06992900	-1.62594500	-0.11682000
H	-2.36990200	0.32240300	-0.99767000
H	-3.02663000	-0.19975000	0.54351900
H	1.44084800	1.85431100	-0.30018800
H	-0.47800600	3.28805300	0.50987200
H	-0.79041100	2.48449900	-1.01822300
H	-1.83586700	1.61227300	1.72878900
H	-2.78599400	2.30681700	0.42475200
C	2.29800300	0.06147800	-2.54131200
C	2.79095700	1.18449300	-3.21228400
C	3.17920400	-0.94416400	-2.12930200
C	4.15890500	1.30081800	-3.46674600
H	2.11180600	1.96589300	-3.53154000
C	4.54631200	-0.81469000	-2.37107600
H	2.80142900	-1.82713400	-1.62711400
C	5.03822800	0.30561000	-3.04291000
H	4.53423800	2.17350800	-3.98938100
H	5.22443600	-1.59540200	-2.04506700
H	6.10066200	0.39996000	-3.23627100
O	0.93515100	1.30981300	1.63686600
Se	0.38499200	-0.11879800	-2.25217200
C	1.66507600	2.28241700	2.26069800
C	1.94423300	2.04735400	3.61527400
C	2.14030100	3.44938900	1.65154800
C	2.69101500	2.96364300	4.34591400
H	1.56965800	1.13958700	4.07398200
C	2.89188100	4.36031500	2.39928300
H	1.93485300	3.66478300	0.61218500
C	3.17281500	4.12928800	3.74296500
H	2.89900000	2.76583700	5.39170800
H	3.25461900	5.26071400	1.91569800
H	3.75464100	4.84336300	4.31360400

7

E = -425.337756

ZPVE = 0.188623

Symbol	X	Y	Z
C	-0.44415200	1.55902300	-0.05468900
H	0.59758000	1.26314800	-0.21488600
H	-1.01110400	0.64337000	0.14158200
C	-0.51727000	2.45415400	1.17191900
H	-1.55460900	2.74139800	1.38022000
H	0.06870500	3.36824700	1.01990800
C	-0.98981000	2.25689400	-1.30378000
H	-0.42248200	3.16373500	-1.53368500
H	-0.92798200	1.59702300	-2.17216300
H	-2.03855800	2.54117400	-1.17566500
O	0.01280500	1.72373800	2.28851100
C	0.05321100	2.32271800	3.51476800
C	-0.39458400	3.62236600	3.77531600
C	0.58645100	1.54878000	4.55590000
C	-0.30422500	4.13356400	5.07372300
H	-0.80944600	4.23762700	2.98880700
C	0.66945200	2.07131800	5.84074100
H	0.92875100	0.54382800	4.33713000
C	0.22422700	3.36964700	6.11036800
H	-0.65393700	5.14198600	5.26576100
H	1.08384000	1.46247600	6.63668100
H	0.28997900	3.77497400	7.11311200

11

E = -580.072651

ZPVE = 0.255999

Symbol	X	Y	Z
C	-2.33937800	0.65152600	0.67193500
C	-0.91406000	0.53503000	0.19056700
C	-1.65855600	1.84078100	0.03725500
H	-3.12087600	0.15591400	0.10891900
H	-2.50461600	0.67482300	1.74290800
H	-0.71903700	-0.03870800	-0.70756600
H	-0.13538700	0.47133000	0.94011600
H	-1.97847600	2.08508200	-0.97159000
C	-1.32515600	3.06338800	0.86272400
H	-1.02959000	2.77212900	1.87415500
C	-2.48243300	4.03017700	0.95330900
C	-3.48761600	3.90266800	2.07179700
C	-2.52469200	5.06564100	2.04889900
H	-2.87590200	4.33458300	-0.01198000
H	-3.32666400	3.13053200	2.81503400

H	-4.52899700	4.08891000	1.83869400
H	-2.90881500	6.04844500	1.80379100
H	-1.71753400	5.06536900	2.77297200
O	-0.24051800	3.80016200	0.22589600
C	1.07422000	3.56619800	0.51301000
C	1.99223400	4.18487000	-0.34945900
C	1.55081400	2.81453200	1.59314700
C	3.35932000	4.05413200	-0.13417300
H	1.61195600	4.76574500	-1.18181700
C	2.92742500	2.69058800	1.79673200
H	0.87495500	2.32486900	2.28004300
C	3.84013100	3.30369300	0.94218700
H	4.05250900	4.53976200	-0.81231300
H	3.28081300	2.10428800	2.63797400
H	4.90570500	3.19934700	1.10868800

<u>For Table 5, DMSO (ROPh-p-NO_2): B3LYP/6-311++G(d,p)</u>

1

E = -782.547071

ZPVE = 0.232742

Symbol	X	Y	Z
C	-0.96883100	-0.71976200	0.14198700
C	0.34261800	-0.83515700	-0.64528900
C	1.27749300	0.33687200	-0.36991200
C	0.25314900	0.74676600	1.76633900
C	-0.66595000	-0.45914500	1.62296200
H	2.27249900	0.16011600	-0.78247700
H	0.87726000	-1.74199700	-0.34538000
H	0.16627500	-0.90138600	-1.72117500
H	-1.57328300	0.09982400	-0.26032200
H	-1.55334400	-1.63542900	0.02193900
H	0.59280800	0.88234400	2.79297700
H	-0.25548700	1.66311100	1.44695000
H	-0.18311500	-1.33705800	2.06658600
H	-1.58570100	-0.27361700	2.18581600
O	1.46839500	0.59038900	0.99407400
O	0.70628200	1.48935000	-1.04310300
C	1.44214900	2.61057800	-1.21729300
C	0.83851100	3.61380800	-1.99663900
C	2.72594900	2.81373800	-0.68475700
C	1.50493100	4.79605700	-2.25193700
H	-0.15254700	3.43949200	-2.39593600
C	3.39684200	3.99924300	-0.94579000
H	3.18967500	2.06875600	-0.05563800
C	2.78724900	4.98139700	-1.72539600
H	1.04942300	5.57011200	-2.85317600
H	4.38513900	4.16826500	-0.54184200
N	3.49521700	6.22371100	-1.99103600
O	2.93750500	7.08136700	-2.67824000

O	4.62451900	6.37007100	-1.51982300

6

E = -3379.176950

ZPVE = 0.336714

Symbol	X	Y	Z
C	-2.15122600	0.25504500	0.08056100
C	-0.91851500	-0.62789800	0.31917100
C	0.37243600	-0.01397300	-0.23565000
C	0.57893400	1.43794800	0.21817400
C	-0.66661000	2.31262800	0.04339400
C	-1.92956300	1.66898300	0.63363900
H	1.23529900	-0.60431200	0.07064100
H	-0.77799200	-0.75750300	1.39875500
H	-1.06323700	-1.62678400	-0.09990600
H	-2.37206900	0.31039600	-0.99262500
H	-3.02473000	-0.20352100	0.55297300
H	1.43491000	1.86081200	-0.31008000
H	-0.48980600	3.29416200	0.49070400
H	-0.80149600	2.47830700	-1.03007300
H	-1.84136500	1.62141500	1.72473200
H	-2.79355700	2.30334700	0.41596600
C	2.30057500	0.06080400	-2.53221100
C	2.79078900	1.19372000	-3.18827200
C	3.18352400	-0.94765300	-2.13116500
C	4.15889700	1.31730100	-3.43836200
H	2.10970200	1.97655400	-3.49970600
C	4.55060800	-0.81117600	-2.36912300
H	2.80714000	-1.83773600	-1.64067100
C	5.04017100	0.31918800	-3.02558700
H	4.53270200	2.19746900	-3.94935900
H	5.23052700	-1.59397300	-2.05207500
H	6.10263500	0.41905000	-3.21593000
O	0.92857700	1.33131900	1.63454500
Se	0.38779000	-0.12966900	-2.24683900
C	1.65666400	2.28097900	2.25097200
C	1.93370800	2.03829700	3.61114500
C	2.14286800	3.45032500	1.64054600
C	2.68025700	2.93618600	4.34574000
H	1.55148600	1.13314100	4.06571700
C	2.89497500	4.35141800	2.37915400
H	1.94020300	3.66897900	0.60243400
C	3.16078100	4.09405400	3.72322600
H	2.89626800	2.75336900	5.38888900
H	3.27308800	5.25316900	1.91836300
N	3.94636700	5.04453100	4.49019200
O	4.16917600	4.79941800	5.67792200
O	4.36048500	6.05921400	3.92512900

7

E = -629.907969

ZPVE = 0.190932

Symbol	X	Y	Z
C	-0.51440500	1.54280100	-0.03595000
H	0.46206200	1.06123500	-0.14580300
H	-1.24584900	0.75021900	0.14917300
C	-0.47389300	2.46491200	1.17006700
H	-1.44827100	2.93477200	1.33853000
H	0.27854100	3.24933700	1.03958100
C	-0.87384600	2.30216100	-1.31679900
H	-0.14232500	3.08592200	-1.53428400
H	-0.89754100	1.62260600	-2.17149400
H	-1.85797400	2.77335600	-1.23820100
O	-0.12891600	1.66703300	2.32481800
C	-0.02556200	2.24894900	3.53359900
C	-0.22974200	3.61783700	3.77569300
C	0.31169500	1.39128100	4.59855500
C	-0.09802800	4.11553400	5.06395800
H	-0.48849000	4.29385600	2.97374000
C	0.44303000	1.88721900	5.87924200
H	0.46488600	0.33951300	4.39262200
C	0.23643900	3.25310300	6.10657000
H	-0.25268500	5.16677700	5.26240800
H	0.70148900	1.23511700	6.70148600
N	0.37311400	3.78123800	7.45329400
O	0.67801800	3.00403500	8.36047900
O	0.17952200	4.98486400	7.63707900

11

E = -784.643410

ZPVE = 0.258562

Symbol	X	Y	Z
C	-2.42146900	0.61534000	0.69775100
C	-1.02265300	0.45996400	0.15497100
C	-1.74038700	1.78292000	0.02413600
H	-3.23934300	0.13829500	0.17193700
H	-2.53936000	0.64898300	1.77452200
H	-0.88136800	-0.12220700	-0.74752400
H	-0.21339500	0.37879500	0.87012400
H	-2.09834400	2.03088000	-0.97051500
C	-1.33872300	2.99519700	0.82864200
H	-1.01569400	2.70658800	1.83073600
C	-2.43930700	4.02063800	0.93936300
C	-3.39652500	3.97009400	2.10608600
C	-2.38224200	5.08302900	2.00876000

H	-2.86090300	4.31807600	-0.01578600
H	-3.23887600	3.20910700	2.86135400
H	-4.43712100	4.19956700	1.91213200
H	-2.72918400	6.07646700	1.75203100
H	-1.54404500	5.06224100	2.69623900
O	-0.23078900	3.67077300	0.13703300
C	1.06077500	3.50319200	0.46508500
C	1.97749400	4.19891300	-0.35120500
C	1.54261000	2.72719200	1.53474000
C	3.33321200	4.12605100	-0.10923700
H	1.59313400	4.79233100	-1.17109000
C	2.90507400	2.65518200	1.77872500
H	0.87292900	2.17884600	2.18005400
C	3.79527300	3.35057900	0.96072900
H	4.03593900	4.65864800	-0.73440500
H	3.28061900	2.06112500	2.60005800
N	5.21928700	3.26807900	1.22206200
O	5.98883700	3.89965800	0.49346800
O	5.60787500	2.57049400	2.16250600

<u>For Table 5, DMSO ($ROCOCH_3$): B3LYP/6-311++G(d,p)</u>

1

E = -499.627537

ZPVE = 0.187353

Symbol	X	Y	Z
C	-0.62718700	-0.92957200	-0.09399800
C	0.90161300	-0.80468200	-0.08621800
C	1.35906100	0.62704300	0.16628700
C	-0.70059900	1.16324900	1.28276400
C	-1.20831400	-0.26787000	1.16193800
H	2.42963000	0.69326400	0.34742300
H	1.31873700	-1.41667600	0.72025600
H	1.34212500	-1.15671600	-1.02195800
H	-1.03546000	-0.44538000	-0.98736400
H	-0.91295500	-1.98338400	-0.14397100
H	-0.99148200	1.62071000	2.22842400
H	-1.08897300	1.78227300	0.46631000
H	-0.91389600	-0.83325400	2.05332000
H	-2.30203100	-0.25571900	1.13033100
O	0.74517300	1.22562200	1.27214900
O	1.06244500	1.39026300	-1.04438500
C	1.81511100	2.48037200	-1.31421700
C	1.34951600	3.15902900	-2.57360200
H	1.36592400	2.45252700	-3.40612300
H	0.31789300	3.49639600	-2.44886700
H	1.99058800	4.00963900	-2.79478900
O	2.74233200	2.84542800	-0.62542500

6

E = -3096.259634

ZPVE = 0.291292

Symbol	X	Y	Z
C	-2.03716300	0.17542100	0.28702600
C	-0.78699800	-0.70923000	0.39616200
C	0.46513100	-0.05210900	-0.19808500
C	0.68677100	1.37378800	0.31963600
C	-0.57090000	2.24454500	0.28174100
C	-1.79090000	1.55626700	0.91005400
H	1.34789300	-0.65174400	0.02165000
H	-0.57987700	-0.90106200	1.45573400
H	-0.95330500	-1.68315800	-0.07115600
H	-2.32308700	0.29313600	-0.76560400
H	-2.87755100	-0.31964600	0.78234400
H	1.50287800	1.85562400	-0.21638500
H	-0.35777400	3.19575300	0.77615900
H	-0.77784300	2.47525600	-0.76826900
H	-1.63420400	1.44360400	1.98875100
H	-2.67188700	2.19268400	0.78571100
C	2.24586400	0.18689400	-2.60326600
C	2.67467800	1.36929200	-3.21340900
C	3.16954700	-0.82613100	-2.32392300
C	4.02186600	1.53723400	-3.53940500
H	1.96224100	2.15622200	-3.42979000
C	4.51636700	-0.64640800	-2.63720500
H	2.84012200	-1.75303600	-1.86914100
C	4.94426300	0.53342500	-3.24806300
H	4.34771000	2.45601100	-4.01399700
H	5.22812100	-1.43340200	-2.41436300
H	5.99072600	0.66746200	-3.49710400
O	1.12440200	1.20643100	1.71364400
Se	0.35876600	-0.06133100	-2.21153700
C	2.00478200	2.08841700	2.22088400
C	2.35452300	1.74839600	3.64545500
H	1.44871500	1.71569700	4.25446200
H	2.81499700	0.75865200	3.68628700
H	3.04238000	2.49095300	4.04421500
O	2.45401100	3.02829800	1.59832600

7

E = -346.989474

ZPVE = 0.145469

Symbol	X	Y	Z
C	-0.85887600	1.59052300	0.10523000
H	-0.44627900	0.57863300	0.16686300

H	-1.94490000	1.50128000	0.20798500
C	-0.31889700	2.41644200	1.25907800
H	-0.73883800	3.42511900	1.26497400
H	0.77010500	2.49731400	1.22317500
C	-0.51024700	2.21714100	-1.24866600
H	0.57254900	2.29358300	-1.38511400
H	-0.90699300	1.61164000	-2.06665700
H	-0.93204100	3.22219300	-1.34277800
O	-0.69301600	1.75170000	2.49672700
C	-0.30618900	2.32450900	3.64859600
C	-0.76028000	1.52541100	4.84051500
H	-1.84841900	1.43160900	4.83301200
H	-0.34251200	0.51732100	4.79257500
H	-0.43851600	2.01432700	5.75747800
O	0.33011900	3.35718900	3.69819400

11

E = -501.727971

ZPVE = 0.213009

Symbol	X	Y	Z
C	-1.46318500	1.05247400	0.43073500
C	-0.01045500	1.45331500	0.50815200
C	-1.07009100	2.50280100	0.27691900
H	-1.80891800	0.52824400	-0.45181400
H	-1.95310300	0.75459600	1.35033500
H	0.63879800	1.19985500	-0.32106500
H	0.46805500	1.42513400	1.48054400
H	-1.13157200	2.91132300	-0.72726400
C	-1.41385600	3.48696000	1.36518100
H	-1.36949300	3.00536000	2.34317000
C	-2.74784100	4.16200400	1.17262100
C	-3.98837900	3.55016900	1.77949300
C	-3.43406300	4.83950200	2.33401400
H	-2.87155200	4.63076500	0.20100300
H	-3.87087000	2.65371600	2.37706000
H	-4.90304600	3.58666000	1.20046300
H	-3.97199600	5.75857400	2.13565000
H	-2.94479600	4.80201100	3.30047000
O	-0.37539600	4.53672900	1.34541100
C	0.33294400	4.78936900	2.45749800
C	1.32340600	5.90118900	2.22705900
H	1.95422500	5.67074600	1.36639500
H	0.78785000	6.82732900	2.00478300
H	1.93852100	6.03929300	3.11377100
O	0.18796300	4.19977600	3.50972600

<u>For Table 5, DMSO (ROC(O)OH): B3LYP/6-311++G(d,p)</u>

1

E = -535.585474

ZPVE = 0.165262

Symbol	X	Y	Z
C	-0.60304900	-0.95162800	-0.09054000
C	0.92465200	-0.81955500	-0.06048200
C	1.37265000	0.61897500	0.16094400
C	-0.71180300	1.18418700	1.21485700
C	-1.20744900	-0.25327500	1.13402800
H	2.44008100	0.69837400	0.35429600
H	1.33087400	-1.40401400	0.77133400
H	1.38447900	-1.19610600	-0.97689000
H	-0.99848000	-0.49882000	-1.00579800
H	-0.88227800	-2.00796500	-0.11121500
H	-1.01688300	1.67095500	2.14082500
H	-1.09051900	1.77393200	0.37305700
H	-0.92387500	-0.78713300	2.04792400
H	-2.30042200	-0.24880100	1.08497400
O	0.73602100	1.25774800	1.22209000
O	1.09791200	1.34061900	-1.09209300
C	1.83646000	2.41949700	-1.34668400
O	2.75605300	2.84564100	-0.68781600
O	1.39456900	2.96938100	-2.48959700
H	1.94132400	3.74678700	-2.67418400

6

E = -3132.217229

ZPVE = 0.269254

Symbol	X	Y	Z
C	-2.04343700	0.17324500	0.28603900
C	-0.79443400	-0.71305000	0.39512400
C	0.45935800	-0.05615700	-0.19584200
C	0.67905500	1.36888700	0.32225000
C	-0.57561100	2.24134100	0.28913500
C	-1.79707600	1.55204000	0.91347000
H	1.34200600	-0.65535500	0.02509700
H	-0.58955100	-0.90880900	1.45442000
H	-0.96030100	-1.68522900	-0.07568100
H	-2.32772600	0.29393100	-0.76661100
H	-2.88483500	-0.32215900	0.77902000
H	1.50111900	1.85002700	-0.20475000
H	-0.36103500	3.19097200	0.78629700
H	-0.77926800	2.47633100	-0.76035700
H	-1.64252100	1.43662500	1.99211200
H	-2.67657300	2.19017800	0.78903200
C	2.24752400	0.19132800	-2.59250100
C	2.68116800	1.37955900	-3.18760900
C	3.16694100	-0.82814000	-2.32288400

C	4.02969500	1.54694100	-3.50828700
H	1.97165800	2.17107800	-3.39668100
C	4.51499700	-0.64904000	-2.63098100
H	2.83330200	-1.75918500	-1.87982800
C	4.94800400	0.53665200	-3.22671800
H	4.35965100	2.47013700	-3.97127800
H	5.22371800	-1.44088100	-2.41589800
H	5.99546100	0.67018800	-3.47178100
O	1.11301800	1.19544200	1.72355800
Se	0.35866800	-0.05594800	-2.20836800
C	1.97781100	2.07563000	2.21188300
O	2.46513000	3.02010400	1.63242000
O	2.24139900	1.74497100	3.48830900
H	2.87300100	2.39140000	3.83512500

7

E = -382.946750

ZPVE = 0.123427

Symbol	X	Y	Z
C	-0.85867800	1.58734500	0.12045500
H	-0.44334100	0.57679200	0.18167900
H	-1.94430800	1.49764600	0.22458800
C	-0.31810600	2.41525200	1.27100900
H	-0.74174300	3.42163000	1.28089700
H	0.77067900	2.49158100	1.23981200
C	-0.51143400	2.21672500	-1.23264200
H	0.57099100	2.29528100	-1.36969300
H	-0.90766900	1.60996900	-2.04967800
H	-0.93612500	3.22047900	-1.32591500
O	-0.69534300	1.74686200	2.51087400
C	-0.30524700	2.32557700	3.63894000
O	0.33037500	3.35038600	3.74273000
O	-0.73592500	1.58065600	4.67045600
H	-0.44644000	2.01091500	5.48773300

11

E = -537.685800

ZPVE = 0.191003

Symbol	X	Y	Z
C	-1.46248700	1.04807000	0.41820800
C	-0.00831500	1.44352300	0.48059700
C	-1.06641600	2.49800000	0.26500900
H	-1.82122500	0.53083500	-0.46311600
H	-1.94332500	0.74794200	1.34178900
H	0.63072100	1.19324700	-0.35731600

H	0.48140100	1.40942000	1.44717700
H	-1.13944100	2.91135300	-0.73615200
C	-1.39800900	3.47486500	1.36089600
H	-1.34554500	2.99139500	2.33738300
C	-2.72418000	4.16529300	1.18221900
C	-3.96412700	3.56434800	1.80178100
C	-3.39491300	4.84909000	2.34970400
H	-2.85242100	4.63313100	0.21099100
H	-3.84864900	2.66764800	2.39928300
H	-4.88214200	3.60679300	1.22874000
H	-3.92532800	5.77274100	2.15296500
H	-2.89861200	4.80880200	3.31222800
O	-0.34154600	4.51694000	1.33633800
C	0.29445200	4.79948100	2.46236500
O	0.13300500	4.28957800	3.54966400
O	1.18798900	5.77465300	2.21012300
H	1.64946700	5.96923400	3.03834600

For Table 5, DMSO (ROCOCHCl$_2$): B3LYP/6-311++G(d,p)

1

E = -1418.872731

ZPVE = 0.169751

Symbol	X	Y	Z
C	-0.62146200	-0.94574800	-0.09034900
C	0.90581300	-0.80779500	-0.08759800
C	1.35246100	0.62087500	0.18579400
C	-0.71431700	1.13813800	1.29682900
C	-1.20185700	-0.29858800	1.17322300
H	2.42387100	0.70017400	0.35535000
H	1.33334200	-1.42421800	0.70983500
H	1.34803400	-1.14289800	-1.02833900
H	-1.03810300	-0.45964700	-0.97858300
H	-0.89636800	-2.00181000	-0.14627900
H	-0.99866100	1.58754300	2.24773100
H	-1.11521600	1.75714400	0.48738300
H	-0.89471100	-0.86444700	2.05974300
H	-2.29557900	-0.29934400	1.14879400
O	0.73446600	1.22302300	1.27255000
O	1.05176100	1.39400800	-1.04618900
C	1.77164200	2.47926600	-1.29036400
C	1.33857400	3.18971300	-2.57799500
O	2.68128100	2.91178800	-0.62528500
Cl	1.56557200	2.12148300	-4.00640500
Cl	-0.35915000	3.76735900	-2.44458300
H	1.96446100	4.06135500	-2.72515400

6

E = -4015.505267

ZPVE = 0.273763

Symbol	X	Y	Z
C	-2.04321900	0.16661900	0.27656200
C	-0.79575100	-0.72124400	0.38989000
C	0.45879300	-0.07085700	-0.20652700
C	0.67954400	1.35722800	0.29936600
C	-0.57227300	2.23285600	0.26799900
C	-1.79449000	1.54844500	0.89625500
H	1.34071300	-0.66956300	0.01824500
H	-0.59030400	-0.91136000	1.45000000
H	-0.96356600	-1.69589200	-0.07497200
H	-2.32839900	0.28173800	-0.77636300
H	-2.88475100	-0.32449900	0.77342900
H	1.50412400	1.83463500	-0.22688200
H	-0.35504500	3.18412000	0.76073100
H	-0.77564400	2.46366600	-0.78241800
H	-1.64067200	1.43935000	1.97549200
H	-2.67246100	2.18767500	0.76748100
C	2.24283900	0.18708100	-2.60463700
C	2.66021800	1.37651900	-3.20886200
C	3.17582200	-0.81759700	-2.32647000
C	4.00646700	1.55986800	-3.53022000
H	1.93995600	2.15648900	-3.42449200
C	4.52147700	-0.62220900	-2.63515700
H	2.85485800	-1.74969300	-1.87634000
C	4.93838300	0.56458900	-3.24006100
H	4.32398400	2.48379400	-4.00037000
H	5.24095200	-1.40239600	-2.41338600
H	5.98406000	0.71065900	-3.48556600
O	1.11499200	1.19343400	1.70852400
Se	0.35726500	-0.08214100	-2.21890300
C	2.00704000	2.03720300	2.19534500
C	2.37274700	1.72503600	3.65105300
O	2.51661100	2.96950500	1.61935200
Cl	0.94749300	1.96876500	4.72241300
Cl	3.04660700	0.06708100	3.81394400
H	3.13943400	2.41787000	3.97549600

7

E = -1266.234492

ZPVE = 0.128013

Symbol	X	Y	Z
C	-0.85784000	1.59417700	0.08637600
H	-0.44742000	0.58159600	0.14430200
H	-1.94357100	1.50970800	0.19217200
C	-0.31208000	2.41551500	1.23825400

H	-0.73040000	3.42380100	1.25868400
H	0.77714200	2.48654800	1.21331000
C	-0.50903800	2.22669700	-1.26484400
H	0.57353500	2.29997900	-1.40323100
H	-0.90974300	1.62447300	-2.08298800
H	-0.92884600	3.23281300	-1.35414200
O	-0.69232600	1.74323900	2.48084200
C	-0.31810700	2.30544100	3.61553900
C	-0.77257200	1.51225300	4.84452100
O	0.31342000	3.32874700	3.73514000
Cl	-2.56645400	1.41021100	4.91537300
Cl	-0.01434700	-0.11872000	4.86684300
H	-0.44457300	2.03103900	5.73692200

11

E = -1420.973845

ZPVE = 0.195543

Symbol	X	Y	Z
C	-1.47266000	1.03540100	0.40911700
C	-0.02119200	1.43908300	0.46482400
C	-1.08602300	2.48839300	0.25564700
H	-1.83362700	0.51897200	-0.47168400
H	-1.94754300	0.73124700	1.33439700
H	0.61514200	1.19519500	-0.37691200
H	0.47356300	1.40642200	1.42882500
H	-1.16697900	2.90358900	-0.74394100
C	-1.42063600	3.45845600	1.35471400
H	-1.35751900	2.97667900	2.33123000
C	-2.74630600	4.14944000	1.18546500
C	-3.98203000	3.54226500	1.80854200
C	-3.41428800	4.82576200	2.35919500
H	-2.87942900	4.62030200	0.21657300
H	-3.86151700	2.64322000	2.40137200
H	-4.90153700	3.58426600	1.23800100
H	-3.94709300	5.74908000	2.16790000
H	-2.91403000	4.78260100	3.31950100
O	-0.36187400	4.51025400	1.32292700
C	0.26948300	4.82892400	2.43460900
C	1.32054900	5.92501700	2.21476800
O	0.10178700	4.35785900	3.53630600
Cl	0.54975900	7.44685700	1.64442400
Cl	2.60125700	5.36855600	1.08085600
H	1.80199100	6.14393200	3.15993300

<u>For Table 5, DMSO (ROCOCF$_3$): B3LYP/6-311++G(d,p)</u>

1

E = -797.455013

ZPVE = 0.164276

Symbol	X	Y	Z
C	-0.61508200	-0.93153100	-0.11037200
C	0.91279900	-0.80433000	-0.08771700
C	1.36658900	0.61661300	0.20632400
C	-0.71423700	1.14616500	1.28453300
C	-1.20615100	-0.28750400	1.14973200
H	2.43665100	0.69001000	0.38623100
H	1.32665100	-1.42967200	0.70999600
H	1.36588700	-1.13397500	-1.02503100
H	-1.01779700	-0.43807500	-1.00104800
H	-0.89564700	-1.98539100	-0.17546900
H	-1.00417500	1.59349400	2.23440700
H	-1.10280100	1.77105800	0.47364400
H	-0.91157600	-0.85847100	2.03709200
H	-2.29938200	-0.28244200	1.11317900
O	0.73680200	1.22580100	1.27459000
O	1.09330400	1.40338800	-1.04156400
C	1.80883800	2.49048600	-1.25270400
C	1.33881000	3.16701300	-2.57308500
O	2.69796800	2.94831200	-0.58738700
F	1.46479600	2.32834400	-3.61910000
F	2.06268000	4.26147900	-2.82916600
F	0.04457100	3.53171800	-2.49012600

6

E = -3394.087532

ZPVE = 0.268299

Symbol	X	Y	Z
C	-2.02781700	0.16870100	0.29792900
C	-0.77204700	-0.70742900	0.41049700
C	0.47301300	-0.05133300	-0.19953100
C	0.68267900	1.38287500	0.29014800
C	-0.57562100	2.24781100	0.26393800
C	-1.78751600	1.55739600	0.90534100
H	1.36214200	-0.63972100	0.02392900
H	-0.55848500	-0.88829900	1.47074100
H	-0.93370900	-1.68677600	-0.04623200
H	-2.32046800	0.27298000	-0.75404200
H	-2.86187400	-0.32561400	0.80389600
H	1.50355300	1.86311500	-0.23924300
H	-0.36327400	3.20525000	0.74643400
H	-0.78693700	2.46805000	-0.78711500
H	-1.62661200	1.45854000	1.98463000
H	-2.67126200	2.18838300	0.77677900
C	2.24627000	0.17933100	-2.60709200
C	2.67012300	1.36729300	-3.20968300
C	3.17181500	-0.83460100	-2.33790100

C	4.01608100	1.54009200	-3.53801500
H	1.95532300	2.15402100	-3.41873500
C	4.51722500	-0.64988600	-2.65404600
H	2.84514200	-1.76531200	-1.88904000
C	4.94082600	0.53553500	-3.25699100
H	4.33895700	2.46284500	-4.00677200
H	5.23114900	-1.43714300	-2.43950500
H	5.98626600	0.67332400	-3.50818000
O	1.13074000	1.23377600	1.70624000
Se	0.36083700	-0.07591000	-2.21103800
C	1.99059900	2.10639800	2.18587500
C	2.33139900	1.73462300	3.65748800
O	2.48139600	3.05875600	1.64014000
F	2.86192400	0.49915500	3.73448700
F	3.21366700	2.59770300	4.17139100
F	1.22682200	1.75740400	4.42825400

7

E = -644.816746

ZPVE = 0.122535

Symbol	X	Y	Z
C	-0.85530300	1.59194400	0.10722000
H	-0.43693300	0.58362300	0.17787200
H	-1.93964200	1.50273400	0.22127700
C	-0.30664500	2.43597300	1.24012600
H	-0.73298200	3.44057500	1.25149100
H	0.78171700	2.51085300	1.21111800
C	-0.51871500	2.20722000	-1.25530700
H	0.56239300	2.28543700	-1.40144600
H	-0.92055900	1.58965600	-2.06120700
H	-0.94623400	3.20880200	-1.35685400
O	-0.67553700	1.78056600	2.50204700
C	-0.28501500	2.35555100	3.61899000
C	-0.76938300	1.51423300	4.83306500
O	0.34792700	3.36867300	3.75284400
F	-2.11165200	1.40510800	4.84127400
F	-0.39211800	2.08391600	5.98207300
F	-0.25496200	0.27015900	4.79426000

11

E = -799.556552

ZPVE = 0.190054

Symbol	X	Y	Z
C	-1.46204000	1.03826800	0.39508000
C	-0.01227500	1.44367800	0.46374600
C	-1.07716100	2.49418000	0.25986600
H	-1.81810200	0.53309400	-0.49409700

H	-1.94204900	0.72290200	1.31389900
H	0.62934400	1.21197100	-0.37734200
H	0.47715300	1.40062600	1.43006700
H	-1.15400700	2.92092900	-0.73497900
C	-1.42228000	3.44763100	1.36789400
H	-1.36973300	2.95509400	2.33942300
C	-2.73633200	4.15589100	1.19393200
C	-3.98325700	3.55562400	1.80250600
C	-3.40811000	4.82862700	2.36792300
H	-2.85665000	4.63483500	0.22751900
H	-3.87651100	2.65069600	2.38890300
H	-4.89628600	3.61054000	1.22290700
H	-3.92914200	5.75893800	2.17844500
H	-2.91740100	4.77295900	3.33246000
O	-0.34635000	4.49713600	1.36449600
C	0.24938100	4.81007100	2.49140500
C	1.31839600	5.90732200	2.21750400
O	0.06768200	4.36876900	3.59644200
F	0.75600800	7.01073000	1.68735000
F	2.25302000	5.46604900	1.35293600
F	1.93675200	6.26134000	3.34934900

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