

Linear Free-Energy Relationships for the Alkyl Radical Affinities of Nitroxides: A Theoretical Study

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SUPPORTING INFORMATION

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Table S.1 Values of electronic descriptors for alkyl groups

Radical	σ_U	μ (D)	EA (eV)	IP (eV)	ω
1	-0.01	0.00	-0.08	9.88	1.21
2	-0.01	0.25	-0.40	8.63	0.94
3	-0.01	0.23	-0.01	8.49	1.06
4	-0.01	0.31	0.02	8.21	1.03
5	0.01	0.20	-0.52	7.80	0.80
6	-0.01	0.19	-0.35	7.22	0.78
7	-	1.55	-0.79	8.21	0.76
8	-	1.25	-0.37	9.61	1.07
9	0.15	3.35	1.55	10.31	2.01
10	0.20	3.89	1.27	9.36	1.74
11	0.17	4.13	1.08	8.64	1.56
12	0.14	0.13	0.88	7.39	1.31
13	0.03	0.38	0.82	7.03	1.24
14	0.07	0.65	0.77	6.73	1.18
15	0.05	1.75	1.47	9.91	1.92
16	0.15	1.65	1.24	8.92	1.68
17	0.09	1.97	1.12	8.27	1.54
18	-	1.85	-0.12	7.65	0.91
19	-	1.65	0.00	8.27	1.03
20	0.09	1.64	1.28	9.20	1.74
21	0.09	1.64	1.47	9.05	1.83
22	0.07	1.98	1.25	8.50	1.64
23	-	3.49	1.00	8.79	1.54
24	0.09	3.29	1.50	9.65	1.91
25	0.02	0.08	0.40	8.27	1.19
26	0.03	0.47	0.25	7.64	1.05
27	0.12	0.91	0.49	7.99	1.20
28	0.07	0.41	0.42	6.95	1.04
29	0.00	0.16	-0.05	7.53	0.92
R	1	0.77	0.76	0.29	0.69
R^2	1	0.60	0.58	0.08	0.48

Table S.2 Values of steric descriptors for alkyl groups

Radical	v	E'_s	$V(\text{\AA}^3)$	$V^a(\text{\AA}^3)$	$CV(\text{\AA}^3)$	$E_R(\text{kcal mol}^{-1})$	$\theta(^{\circ})$	$\Omega(^{\circ 2})$	$order$
1	0.52	0	32.2	32.2	31.8	17	1.85	-	0
2	0.56	-	-	-	-	-	2.05	-	1
3	0.68	-	-	-	-	-	2.04	-	1
4	0.73	-	124.4	68.2	519.2	-	2.05	2.69	1
5	0.76	-	-	-	-	-	2.26	-	2
6	1.24	1.43	86.9	86.9	172.9	59	2.47	-	3
7	0.53	-	-	-	-	-	1.98		1
8	0.62	-	-	-	-	-	1.98		1
9	0.58	0.89	51.6	51.6	90.7	24	2.04	-	1
10	0.79	-	69.9	69.9	133.6	-	2.25	-	2
11	1.20	-	88.1	88.1	180.1	-	2.46	-	3
12	0.70	0.39	115.9	79.8	361.9	42	2.06	-	1
13	0.86	0.9	134	97.8	412.7	66	2.37	-	2
14	1.28	-	151.7	115.5	622.4	-	2.67	-	3
15	0.80	-	75.6	50.7	291.7	-	2.13	-	1
16	1.00	-	93.8	68.9	261.4	-	2.34	-	2
17	1.43	-	112	87.1	310.3	-	2.58	-	3
18	-	-	-	-	-	-	2.11		2
19	0.70	-	-	-	-	-	2.26		2
20	0.83	-	72.1	87.1	154.5	-	2.29	2.63	2
21	1.02	-	90.7	86.5	261.4	-	2.55	2.85	2
22	1.24	-	90.4	68.9	185.8	-	2.55	3.28	3
23	-	-	-	-	-	-	2.60	-	2
24	0.82	-	104.4	85.2	403.2	-	2.56	3.44	2
25	0.69	0.31	64.6	63.7	120.3	33	2.04	2.27	1
26	0.86	-	82.9	82	170.8	-	2.27	2.81	2
27	0.72	-	79.1	60.3	204.9	-	2.08	1.96	1
28	0.72	-	102.1	98.5	233.2	-	2.24	2.7	2
29	0.87	0.69	110.8	99	265.4	59	2.25	3.13	2
<i>R</i>	1	0.81	0.47	0.55	0.29	0.81	0.88	0.60	0.89
<i>R</i> ²	1	0.66	0.22	0.30	0.09	0.65	0.77	0.36	0.79

Table S.3 Values of radical stabilization descriptors for alkyl groups

Radical	σ_{RS}	ρ	$\rho\%$	RSE (kJmol ⁻¹)
1	0.00	1.16	1.00	0.0
2	0.07	1.09	-	14.1
3	0.07	1.09	-	12.6
4	0.07	1.09	0.87	10.3
5	0.10	1.02	-	24.0
6	0.12	0.96	0.65	29.7
7	-	0.93	-	31.5
8	-	0.99	-	12.4
9	0.16	0.89	0.59	31.9
10	0.19	0.84	0.53	47.3
11	0.22	0.80	0.47	59.0
12	0.31	0.79	0.40	59.0
13	0.34	0.77	0.37	68.0
14	0.36	0.75	0.35	69.9
15	0.15	0.97	0.77	21.5
16	0.18	0.89	0.68	41.2
17	0.20	0.83	0.6	54.9
18	-	0.98	-	24.4
19	-	0.96	-	27.0
20	0.18	0.89	0.69	41.2
21	0.18	0.89	0.69	39.7
22	0.21	0.83	0.6	55.8
23	-	0.91	-	41.0
24	0.28	0.83	0.6	43.4
25	0.43	0.7	0.46	72.0
26	0.46	0.66	0.43	84.6
27	0.25	0.81	0.48	51.4
28	0.54	0.58	0.28	116.2
29	0.1	1.02	0.76	20.2
<i>R</i>	1	-0.96	-0.88	0.96
<i>R</i> ²	1	0.91	0.78	0.92

Table S.4 Tolman's cone angle for alkyl groups, calculated using various ligands

Radical	R-TEMPO	R-Br	R-Cl	R-dithiocarbamate
1	2.16	1.74	1.85	1.83
4	2.39	1.94	2.05	2.03
6	2.83	2.33	2.47	2.45
9	2.38	1.92	2.04	2.02
10	2.60	2.13	2.25	2.23
11	2.81	2.34	2.46	2.43
12	2.55	1.95	2.06	2.06
13	2.78	2.23	2.37	2.33
14	3.11	2.50	2.67	2.60
15	2.54	2.03	2.13	2.22
16	2.67	2.25	2.34	2.33
17	3.00	2.48	2.58	2.62
20	2.71	2.18	2.29	2.30
21	2.84	2.43	2.55	2.28
22	2.81	2.41	2.55	2.62
24	2.91	2.34	2.56	2.45
25	2.39	1.93	2.04	2.03
26	2.62	2.15	2.27	2.25
27	2.38	1.99	2.08	2.09
28	2.61	2.11	2.24	2.24
29	2.60	2.14	2.25	2.24
<i>R</i>	1	0.97	0.97	0.94
<i>R</i> ²	1	0.93	0.95	0.88

Table S.5 Calculated $\log(K_{calc})$ values (298 K) ^a, fitting parameters μ , θ , and ρ (0 K) and $\log(K_{eq})$ values calculated through the fitting of a new equation for the combination of different alkyl radicals with TEMPO (training set I)

Species	$\log(K_{calc})$	μ (D)	θ (°)	ρ^c	$\log(K_{eq})^d$
B1	28.0	0.00	1.85	1.16	30.3
B2	28.6	0.25	2.05	1.09	28.1
B3	29.2	0.23	2.04	1.09	28.1
B5	27.0	0.20	2.26	1.02	25.9
B6	24.6	0.19	2.47	0.96	24.0
B7	30.9	1.55	1.98	0.93	23.9
B8	34.7	1.25	1.98	0.99	25.5
B9	22.4	3.35	2.04	0.89	22.1
B10	21.6	3.89	2.25	0.84	20.2
B11	17.7 ^b	4.13	2.46	0.80	18.7
B12	20.7 ^b	0.13	2.06	0.79	20.8
B13	19.8 ^b	0.38	2.37	0.77	19.5
B14	17.6 ^b	0.65	2.67	0.75	18.2
B15	24.0	1.75	2.13	0.97	24.4
B16	22.1 ^b	1.65	2.34	0.89	22.0
B17	18.9 ^b	1.97	2.58	0.83	19.9
B18	31.1 ^b	1.85	2.11	0.98	24.7
B19	28.7	1.65	2.26	0.96	23.9

^aG3(MP2)-RAD//B3-LYP/6-31G(d) values except where noted. ^bONIOM approximation with the full system calculated at the RMP2/6-311+G(3df,2p) level. ^cSpin density on the radical center. ^dFound from Equation (10).

Table S.6 Calculated $\log(K_{calc})$ values (298 K) ^a, fitting parameters IP and RSE (0 K) and $\log(K_{eq})$ values calculated through the fitting of a new equation for the combination of different alkyl radicals with TEMPO (training set I)

Species	$\log(K_{calc})$	IP (eV) ^c	RSE (kJmol ⁻¹)	$\log(K_{eq})$ ^d
B1	28.0	9.88	0.0	29.0
B2	28.6	8.63	14.1	27.6
B3	29.2	8.49	12.6	28.0
B5	27.0	7.80	24.0	26.5
B6	24.6	7.22	29.7	26.0
B7	30.9	8.21	31.5	24.6
B8	34.7	9.61	12.4	26.9
B9	22.4	10.31	31.9	22.2
B10	21.6	9.36	47.3	20.2
B11	17.7 ^b	8.64	59.0	18.6
B12	20.7 ^b	7.39	59.0	20.0
B13	19.8 ^b	7.03	68.0	18.6
B14	17.6 ^b	6.73	69.9	18.6
B15	24.0	9.91	21.5	24.7
B16	22.1 ^b	8.92	41.2	21.9
B17	18.9 ^b	8.27	54.9	19.9
B18	31.1 ^b	7.65	24.4	26.6
B19	28.7	8.27	27.0	25.4

^aG3(MP2)-RAD//B3-LYP/6-31G(d) values except where noted. ^bONIOM approximation with the full system calculated at the RMP2/6-311+G(3df,2p) level. ^cVertical ionization potential ^dFound from Equation (13).

Table S.7 Calculated $\log(K_{calc})$ values (298 K) ^a, fitting parameters (0 K) and $\log(K_{eq})$ values calculated through the fitting of a new equation for the combination of methyl radical with different nitroxides (training set II)

Species	$\log(K_{calc})$	RSE_{nxd} (kJmol ⁻¹)	$\log(K_{eq})^c$
A1	26.7	0.0	27.3
B1	28.0	-4.3	28.0
C1	28.5	-5.6	28.2
D1	28.3	-6.5	28.3
E1	28.6	-8.2	28.6
F1	28.9 ^b	-10.4	29.0
G1	29.5 ^b	-13.3	29.4
H1	25.6 ^b	3.3	26.8
I1	25.8	9.9	25.7
J1	26.3	7.8	26.1
K1	26.9	5.0	26.5
L1	26.8	7.7	26.1
M1	26.2	6.9	26.2
N1	26.7 ^b	3.8	26.7
O1	24.5 ^b	15.6	24.8
P1	26.3	7.2	26.2
Q1	26.5 ^b	4.9	26.5
R1	26.9 ^b	2.4	26.9
S1	28.3	-3.3	27.8
T1	27.6	0.3	27.3
U1	28.8 ^b	-11.4	29.1
V1	25.9 ^b	5.8	26.4

^aG3(MP2)-RAD//B3-LYP/6-31G(d) values except where noted. ^bONIOM approximation with the full system calculated at the RMP2/6-311+G(3df,2p) level. ^cFound from Equation (15).

Table S.8 Calculated $\log(K_{calc})$ values (298 K) ^a, fitting parameters (0 K) and $\log(K_{eq})$ values calculated through the fitting of a new equation for combinations in training sets I and II

Species	$\log(K_{calc})$	IP (eV) ^c	RSE (kJmol ⁻¹)	RSE_{nxd} (kJmol ⁻¹)	$\log(K_{eq})^d$
Training set I					
B1	28.0	9.88	0.0	-4.3	28.2
B2	28.6	8.63	14.1	-4.3	27.0
B3	29.2	8.49	12.6	-4.3	27.5
B5	27.0	7.80	24.0	-4.3	26.2
B6	24.6	7.22	29.7	-4.3	25.8
B7	30.9	8.21	31.5	-4.3	24.3
B8	34.7	9.61	12.4	-4.3	26.2
B9	22.4	10.31	31.9	-4.3	21.8
B10	21.6	9.36	47.3	-4.3	20.1
B11	17.7 ^b	8.64	59.0	-4.3	18.8
B12	20.7 ^b	7.39	59.0	-4.3	20.2
B13	19.8 ^b	7.03	68.0	-4.3	19.0
B14	17.6 ^b	6.73	69.9	-4.3	19.0
B15	24.0	9.91	21.5	-4.3	24.2
B16	22.1 ^b	8.92	41.2	-4.3	21.7
B17	18.9 ^b	8.27	54.9	-4.3	19.9
B18	31.1 ^b	7.65	24.4	-4.3	26.3
B19	28.7	8.27	27.0	-4.3	25.1
Training set II					
A1	26.7	9.88	0.0	0.0	27.4
C1	28.5	9.88	0.0	-5.6	28.4
D1	28.3	9.88	0.0	-6.5	28.6
E1	28.6	9.88	0.0	-8.2	28.8
F1	28.9 ^b	9.88	0.0	-10.4	29.2
G1	29.5 ^b	9.88	0.0	-13.3	29.7
H1	25.6 ^b	9.88	0.0	3.3	26.9
I1	25.8	9.88	0.0	9.9	25.7
J1	26.3	9.88	0.0	7.8	26.1
K1	26.9	9.88	0.0	5.0	26.6
L1	26.8	9.88	0.0	7.7	26.1
M1	26.2	9.88	0.0	6.9	26.3

N1	26.7 ^b	9.88	0.0	3.8	26.8
O1	24.5 ^b	9.88	0.0	15.6	24.8
P1	26.3	9.88	0.0	7.2	26.2
Q1	26.5 ^b	9.88	0.0	4.9	26.6
R1	26.9 ^b	9.88	0.0	2.4	27.0
S1	28.3	9.88	0.0	-3.3	28.0
T1	27.6	9.88	0.0	0.3	27.4
U1	28.8 ^b	9.88	0.0	-11.4	29.4
V1	25.9 ^b	9.88	0.0	5.8	26.4
Test set					
A13	17.2 ^b	7.03	68.0	0.0	18.2
A16	20.2 ^b	8.92	41.2	0.0	21.0
A17	17.2 ^b	8.27	54.9	0.0	19.2
A20	19.5 ^b	8.50	41.2	0.0	21.5
A23	21.7 ^b	8.79	41.0	0.0	21.2
B20	21.5 ^b	8.50	41.2	-4.3	22.2
B23	24.3 ^b	8.79	41.0	-4.3	21.9
I13	18.3 ^b	7.03	68.0	9.9	16.5
I16	20.8 ^b	8.92	41.2	9.9	19.3
I17	17.5 ^b	8.27	54.9	9.9	17.5
I20	20.4 ^b	8.50	41.2	9.9	19.8
I23	22.5 ^b	8.79	41.0	9.9	19.5
P13	18.9 ^b	7.03	68.0	7.2	17.0
P16	20.8 ^b	8.92	41.2	7.2	19.7
P17	18.3 ^b	8.27	54.9	7.2	18.0
P20	20.4 ^b	8.50	41.2	7.2	20.2
P23	22.6 ^b	8.79	41.0	7.2	19.9

^aG3(MP2)-RAD//B3-LYP/6-31G(d) values except where noted. ^bONIOM approximation with the full system calculated at the RMP2/6-311+G(3df,2p) level. ^cVertical ionization potential. ^dFound from Equation (16).

Table S.9 Calculated $\log (K_{calc})$ values (298 K) ^a, fitting parameters (0 K) and $\log (K_{eq})$ values calculated from Equation (16) for combinations in the test set

Species	$\log (K_{calc})$	IP (eV) ^c	RSE (kJmol ⁻¹)	RSE_{nxd} (kJmol ⁻¹)	$\log (K_{eq})$ ^d
A13	17.2 ^b	7.03	68.0	0.0	18.2
A16	20.2 ^b	8.92	41.2	0.0	21.0
A17	17.2 ^b	8.27	54.9	0.0	19.2
A20	19.5 ^b	8.50	41.2	0.0	21.5
A23	21.7 ^b	8.79	41.0	0.0	21.2
B20	21.5 ^b	8.50	41.2	-4.3	22.2
B23	24.3 ^b	8.79	41.0	-4.3	21.9
I13	18.3 ^b	7.03	68.0	9.9	16.5
I16	20.8 ^b	8.92	41.2	9.9	19.3
I17	17.5 ^b	8.27	54.9	9.9	17.5
I20	20.4 ^b	8.50	41.2	9.9	19.8
I23	22.5 ^b	8.79	41.0	9.9	19.5
P13	18.9 ^b	7.03	68.0	7.2	17.0
P16	20.8 ^b	8.92	41.2	7.2	19.7
P17	18.3 ^b	8.27	54.9	7.2	18.0
P20	20.4 ^b	8.50	41.2	7.2	20.2
P23	22.6 ^b	8.79	41.0	7.2	19.9

^aG3(MP2)-RAD//B3-LYP/6-31G(d) values except where noted. ^bONIOM approximation with the full system calculated at the RMP2/6-311+G(3df,2p) level. ^cVertical ionization potential. ^dFound from Equation (16).

Table S.10 Calculated $\log(K_{calc})$ values (298 K)^a, fitting parameters (0 K) and $\log(K_{eq})$ values calculated from Equation (17) for combinations in the training and test sets

Species	$\log(K_{calc})$	IP (eV) ^c	RSE (kJmol ⁻¹)	RSE_{nxd} (kJmol ⁻¹)	$\log(K_{eq})$ ^d
Training set I					
B1	28.0	9.88	0.0	-4.3	28.0
B2	28.6	8.63	14.1	-4.3	26.9
B3	29.2	8.49	12.6	-4.3	27.3
B5	27.0	7.80	24.0	-4.3	26.0
B6	24.6	7.22	29.7	-4.3	25.7
B7	30.9	8.21	31.5	-4.3	24.3
B8	34.7	9.61	12.4	-4.3	26.1
B9	22.4	10.31	31.9	-4.3	21.9
B10	21.6	9.36	47.3	-4.3	20.2
B11	17.7 ^b	8.64	59.0	-4.3	18.9
B12	20.7 ^b	7.39	59.0	-4.3	20.3
B13	19.8 ^b	7.03	68.0	-4.3	19.1
B14	17.6 ^b	6.73	69.9	-4.3	19.1
B15	24.0	9.91	21.5	-4.3	24.2
B16	22.1 ^b	8.92	41.2	-4.3	21.8
B17	18.9 ^b	8.27	54.9	-4.3	20.0
B18	31.1 ^b	7.65	24.4	-4.3	26.1
B19	28.7	8.27	27.0	-4.3	25.0
Training set II					
A1	26.7	9.88	0.0	0.0	27.4
C1	28.5	9.88	0.0	-5.6	28.2
D1	28.3	9.88	0.0	-6.5	28.3
E1	28.6	9.88	0.0	-8.2	28.5
F1	28.9 ^b	9.88	0.0	-10.4	28.8
G1	29.5 ^b	9.88	0.0	-13.3	29.2
H1	25.6 ^b	9.88	0.0	3.3	27.0
I1	25.8	9.88	0.0	9.9	26.1
J1	26.3	9.88	0.0	7.8	26.4
K1	26.9	9.88	0.0	5.0	26.8
L1	26.8	9.88	0.0	7.7	26.4
M1	26.2	9.88	0.0	6.9	26.5

N1	26.7 ^b	9.88	0.0	3.8	26.9
O1	24.5 ^b	9.88	0.0	15.6	25.4
P1	26.3	9.88	0.0	7.2	26.5
Q1	26.5 ^b	9.88	0.0	4.9	26.8
R1	26.9 ^b	9.88	0.0	2.4	27.1
S1	28.3	9.88	0.0	-3.3	27.9
T1	27.6	9.88	0.0	0.3	27.4
U1	28.8 ^b	9.88	0.0	-11.4	28.9
V1	25.9 ^b	9.88	0.0	5.8	26.7
Test set					
A13	17.2 ^b	7.03	68.0	0.0	18.5
A16	20.2 ^b	8.92	41.2	0.0	21.2
A17	17.2 ^b	8.27	54.9	0.0	19.5
A20	19.5 ^b	8.50	41.2	0.0	21.7
A23	21.7 ^b	8.79	41.0	0.0	21.4
B20	21.5 ^b	8.50	41.2	-4.3	22.2
B23	24.3 ^b	8.79	41.0	-4.3	21.9
I13	18.3 ^b	7.03	68.0	9.9	17.2
I16	20.8 ^b	8.92	41.2	9.9	19.9
I17	17.5 ^b	8.27	54.9	9.9	18.2
I20	20.4 ^b	8.50	41.2	9.9	20.4
I23	22.5 ^b	8.79	41.0	9.9	20.1
P13	18.9 ^b	7.03	68.0	7.2	17.6
P16	20.8 ^b	8.92	41.2	7.2	20.3
P17	18.3 ^b	8.27	54.9	7.2	18.5
P20	20.4 ^b	8.50	41.2	7.2	20.7
P23	22.6 ^b	8.79	41.0	7.2	20.4

^aG3(MP2)-RAD//B3-LYP/6-31G(d) values except where noted. ^bONIOM approximation with the full system calculated at the RMP2/6-311+G(3df,2p) level. ^cVertical ionization potential. ^dFound from Equation (17).

Table S.11 Experimental^a rate constants k_c (at 298 K in tBB), fitting parameters (0 K) and $\log (k_{c,eq})$ values calculated from Equation (18) for combination reactions of alkyl radicals with nitroxides

Species	$\log (k_c)$	IP (eV) ^b	RSE (kJmol ⁻¹)	RSE_{nxd} (kJmol ⁻¹)	$\log (k_{c,eq})$ ^c
A12	8.3	7.39	59.0	0.0	8.0
B12	8.4	7.39	59.0	-4.3	8.4
B13	8.3	7.03	68.0	-4.3	8.0
B14	7.7	6.73	69.9	-4.3	8.0
B15	9.4	9.91	21.5	-4.3	9.6
B17	8.8	8.27	54.9	-4.3	8.3
P13	8.2	7.03	68.0	7.2	6.8
P14	8.1	6.73	69.9	7.2	6.8
V12	7.0	7.39	59.0	5.8	7.4
V13	6.5	7.03	68.0	5.8	7.0
V14	5.3	6.73	69.9	5.8	7.0
V15	8.9	9.91	21.5	5.8	8.6
V17	6.4	8.27	54.9	5.8	7.3

^bAs reported by Fischer, Marque and coworkers. ^bVertical ionization potential. ^cFound from Equation (18).

Table S.12 Experimental^a rate constants k_d (at 393 K in tBB), fitting parameters (0 K) and $\log (k_{d,eq})$ values calculated from Equation (19) for combination reactions of alkyl radicals with nitroxides

Species	$\log (k_d)$	IP (eV) ^b	RSE (kJmol ⁻¹)	RSE_{nxd} (kJmol ⁻¹)	$\log (k_{d,eq})$ ^c
A12	-3.7	7.39	59.0	0.0	-3.2
A13	-1.9	7.03	68.0	0.0	-2.5
B1	-11.2	9.88	0.0	-4.3	-8.3
B6	-5.0	7.22	29.7	-4.3	-6.8
B10	-3.5	9.36	47.3	-4.3	-3.8
B11	-0.9	8.64	59.0	-4.3	-3.0
B12	-5.0	7.39	59.0	-4.3	-3.7
B13	-3.3	7.03	68.0	-4.3	-3.0
B14	-1.1	6.73	69.9	-4.3	-3.0
B15	-7.1	9.91	21.5	-4.3	-6.1
B16	-4.5	8.92	41.2	-4.3	-4.7
B17	-1.7	8.27	54.9	-4.3	-3.7
B25	-4.1	8.27	72.0	-4.3	-1.9
B26	-3.4	7.64	84.6	-4.3	-1.0
B28	3.8	6.95	116.2	-4.3	1.8
B29	-7.6	7.53	20.2	-4.3	-7.6
I13	-3.8	7.03	68.0	9.9	-1.4
P13	-4.2	7.03	68.0	7.2	-1.7
P14	-2.4	6.73	69.9	7.2	-1.7
V4	-8.1	8.21	10.3	5.8	-7.1
V6	-4.2	7.22	29.7	5.8	-5.6
V9	-3.7	10.31	31.9	5.8	-3.7
V10	-2.6	9.36	47.3	5.8	-2.7
V11	0.1	8.64	59.0	5.8	-1.9
V12	-3.5	7.39	59.0	5.8	-2.6
V13	-2.3	7.03	68.0	5.8	-1.9
V14	0.2	6.73	69.9	5.8	-1.9
V15	-5.4	9.91	21.5	5.8	-5.0
V16	-2.5	8.92	41.2	5.8	-3.5
V17	-0.1	8.27	54.9	5.8	-2.5
V20	-3.0	9.2	41.2	5.8	-3.4
V21	-2.7	9.05	39.7	5.8	-3.6
V22	-0.6	8.5	55.8	5.8	-2.3

V24	-2.4	9.65	43.4	5.8	-2.9
V25	-3.1	8.27	72.0	5.8	-0.8
V27	-2.9	7.99	51.4	5.8	-3.0
V29	-7.2	7.53	20.2	5.8	-6.4

^bAs reported by Fischer, Marque and coworkers. ^bVertical ionization potential. ^cFound from Equation (19).

Table S.13 Experimental^a rate constants k_c (at 298 K in tBB), fitting parameters (0 K) and $\log (k_{c,eq})$ values calculated from Equation (20) for combination reactions of alkyl radicals with nitroxides

Species	$\log (k_c)$	IP (eV) ^b	θ (°)	RSE (kJmol ⁻¹)	RSE_{nxd} (kJmol ⁻¹)	$\log (k_{c,eq})$ ^c
A12	8.3	7.39	2.06	59.0	0.0	8.1
B12	8.4	7.39	2.06	59.0	-4.3	8.5
B13	8.3	7.03	2.37	68.0	-4.3	8.1
B14	7.7	6.73	2.67	69.9	-4.3	7.8
B15	9.4	9.91	2.13	21.5	-4.3	9.5
B17	8.8	8.27	2.58	54.9	-4.3	8.2
P13	8.2	7.03	2.37	68.0	7.2	6.9
P14	8.1	6.73	2.67	69.9	7.2	6.6
V12	7.0	7.39	2.06	59.0	5.8	7.5
V13	6.5	7.03	2.37	68.0	5.8	7.0
V14	5.3	6.73	2.67	69.9	5.8	6.8
V15	8.9	9.91	2.13	21.5	5.8	8.5
V17	6.4	8.27	2.58	54.9	5.8	7.2

^bAs reported by Fischer, Marque and coworkers. ^bVertical ionization potential. ^cFound from Equation (20).

Table S.14 Experimental^a rate constants k_d (at 393 K in tBB), fitting parameters (0 K) and $\log (k_{d,eq})$ values calculated from Equation (21) for combination reactions of alkyl radicals with nitroxides

Species	$\log (k_d)$	IP (eV) ^b	θ (°)	RSE (kJmol ⁻¹)	RSE_{nxd} (kJmol ⁻¹)	$\log (k_{d,eq})$ ^c
A12	-3.7	7.39	2.06	59.0	0.0	-5.0
A13	-1.9	7.03	2.37	68.0	0.0	-2.7
B1	-11.2	9.88	1.85	0.0	-4.3	-9.7
B6	-5.0	7.22	2.47	29.7	-4.3	-5.7
B10	-3.5	9.36	2.25	47.3	-4.3	-3.7
B11	-0.9	8.64	2.46	59.0	-4.3	-2.1
B12	-5.0	7.39	2.06	59.0	-4.3	-5.3
B13	-3.3	7.03	2.37	68.0	-4.3	-3.1
B14	-1.1	6.73	2.67	69.9	-4.3	-1.4
B15	-7.1	9.91	2.13	21.5	-4.3	-6.2
B16	-4.5	8.92	2.34	41.2	-4.3	-4.1
B17	-1.7	8.27	2.58	54.9	-4.3	-2.0
B25	-4.1	8.27	2.27	72.0	-4.3	-2.3
B26	-3.4	7.64	2.04	84.6	-4.3	-3.0
B28	3.8	6.95	2.24	116.2	-4.3	0.3
B29	-7.6	7.53	2.25	20.2	-4.3	-7.5
I13	-3.8	7.03	2.37	68.0	9.9	-1.9
P13	-4.2	7.03	2.37	68.0	7.2	-2.1
P14	-2.4	6.73	2.67	69.9	7.2	-0.5
V4	-8.1	8.21	2.05	10.3	5.8	-8.2
V6	-4.2	7.22	2.47	29.7	5.8	-4.9
V9	-3.7	10.31	2.04	31.9	5.8	-4.7
V10	-2.6	9.36	2.25	47.3	5.8	-2.9
V11	0.1	8.64	2.46	59.0	5.8	-1.2
V12	-3.5	7.39	2.06	59.0	5.8	-4.5
V13	-2.3	7.03	2.37	68.0	5.8	-2.2
V14	0.2	6.73	2.67	69.9	5.8	-0.6
V15	-5.4	9.91	2.13	21.5	5.8	-5.4
V16	-2.5	8.92	2.34	41.2	5.8	-3.3
V17	-0.1	8.27	2.58	54.9	5.8	-1.2
V20	-3.0	9.2	2.29	41.2	5.8	-3.3
V21	-2.7	9.05	2.55	39.7	5.8	-2.1
V22	-0.6	8.5	2.55	55.8	5.8	-1.1

V24	-2.4	9.65	2.56	43.4	5.8	-1.2
V25	-3.1	8.27	2.04	72.0	5.8	-2.8
V27	-2.9	7.99	2.08	51.4	5.8	-4.6
V29	-7.2	7.53	2.25	20.2	5.8	-6.7

^bAs reported by Fischer, Marque and coworkers. ^bVertical ionization potential. ^cFound from Equation (21).

APPENDIX S1: Geometries of the species in this study

NOTE: All species had zero imaginary frequencies, as determined from frequency calculations at the B3-LYP/6-31G(d) level

DBN• (A)

```
1\1\GINC-AC27\FOpt\UB3LYP\6-31G(d)\C8H18N1O1(2)\JOH501\13-Oct-2006\0\
# UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\dbn_3\0,2\N,0.086
676393,-0.0289569824,-0.2101692723\O,1.274667638,-0.0911022481,-0.7035
929955\C,-0.3620070154,1.3925564994,0.0618667796\C,-0.4443604176,-1.30
97344046,0.401084604\C,-1.9045160561,-1.5693512106,-0.0228288026\C,0.4
193109189,-2.4592743379,-0.1487459585\C,-0.3080527061,-1.2802033621,1.
9374802489\C,-1.8274124185,1.5272440584,0.4996489237\C,0.5674020513,1.
9916398436,1.1380605006\C,-0.1819272335,2.158708748,-1.2637190109\H,0.
0330344105,-3.4043915051,0.2486247153\H,0.378269924,-2.4963617895,-1.2
407199587\H,1.4644838447,-2.3519364626,0.1430830661\H,-0.6115015138,-2
.2484948044,2.3524792362\H,0.7325158484,-1.0984501561,2.2251155619\H,-
0.9348993843,-0.513457395,2.4013852659\H,-2.175999689,-2.5961353611,0.
2463819683\H,-2.6219763047,-0.9077145572,0.4636789761\H,-2.0142282526,
-1.4666553212,-1.1076606017\H,-0.4537587934,3.2106275479,-1.1228525904
\H,0.8525242997,2.0986038843,-1.6039435408\H,-0.827157554,1.7376825983
,-2.042888488\H,0.378602061,3.0660332106,1.2441109575\H,0.4077119255,1
.5234929233,2.1148860617\H,1.6105078889,1.8454674368,0.8463928685\H,-2
.0329500287,2.5918357933,0.6566754969\H,-2.5195232337,1.1700910365,-0.
2679548001\H,-2.0463066024,1.0167763242,1.4409707871\Version=IA64L-G0
3RevD.01\State=2-A\HF=-445.599719\S2=0.753796\S2-1=0.\S2A=0.75001\RMSD
=5.976e-09\RMSF=9.462e-06\Thermal=0.\Dipole=-0.9066189,0.0568884,0.568
8285\PG=C01 [X(C8H18N1O1)]\@
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TEMPO• (B)

```
1\1\GINC-LC22\FOpt\UB3LYP\6-31G(d)\C9H18N1O1(2)\JOH501\23-Feb-2006\0\
# UB3LYP/6-31G* OPT FREQ=NORAMAN MAXDISK=78643200\tempo_1s\0,2\N,0.,
-0.7434209403,-0.2055568746\O,0.,-2.0200229887,-0.0536930208\C,0.,2.12
91122715,0.0202793419\H,0.,3.1640205144,-0.3430045373\H,0.,2.188129084
3,1.1160257969\C,1.2471385297,1.4014636869,-0.4850966271\C,-1.24713852
97,1.4014636869,-0.4850966271\C,1.3316319116,-0.0694129504,-0.02866995
47\C,-1.3316319116,-0.0694129504,-0.0286699547\C,2.3409037477,-0.82546
55447,-0.9084597306\C,-2.3409037477,-0.8254655447,-0.9084597306\C,1.76
16105348,-0.1821678854,1.4497256469\C,-1.7616105348,-0.1821678854,1.44
97256469\H,2.1613559084,1.9128572411,-0.159270535\H,-2.1613559084,1.91
28572411,-0.159270535\H,1.2461755503,1.4303666274,-1.5834226174\H,-1.2
461755503,1.4303666274,-1.5834226174\H,2.0267037652,-0.8094181301,-1.9
575486217\H,-2.0267037652,-0.8094181301,-1.9575486217\H,3.3238440946,-
0.3468698717,-0.8343424769\H,-3.3238440946,-0.3468698717,-0.8343424769
\H,2.4264203456,-1.8666991071,-0.5927537894\H,-2.4264203456,-1.8666991
071,-0.5927537894\H,2.801008229,0.1459162404,1.5646144668\H,-2.8010082
29,0.1459162404,1.5646144668\H,1.1414032892,0.4302012714,2.1114446532\
H,-1.1414032892,0.4302012714,2.1114446532\H,1.6868923818,-1.2242044777
,1.7731554021\H,-1.6868923818,-1.2242044777,1.7731554021\Version=IA32
L-G03RevC.02\State=2-A'\HF=-483.7197701\S2=0.753695\S2-1=0.\S2A=0.7500
09\RMSD=3.459e-09\RMSF=7.184e-06\Dipole=0.,1.1367503,0.065858\PG=CS [S
G(C1H2N1O1),X(C8H16)]\@
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4-amino-TEMPO• (C)

```
1\1\GINC-LC95\FOpt\UB3LYP\6-31G(d)\C9H19N2O1(2)\JOH501\24-Feb-2006\0\
# UB3LYP/6-31G* OPT FREQ=NORAMAN MAXDISK=78643200\ntempo_1\0,2\N,1.0
25731725,-0.2936895048,-0.0052493203\O,2.3111388737,-0.3068730089,-0.0
123838237\C,-1.8151823173,0.2953301141,0.0017965305\N,-3.2622869159,0.
0528195581,-0.0694742084\H,-1.6893573865,1.3856417523,-0.0050383438\C,
-1.1314423866,-0.2924895128,1.2458898079\C,-1.1460418993,-0.2974449382
,-1.2390515774\C,0.3866610098,-0.033772605,1.3281094562\C,0.3695684162
```

, -0.0348680397, -1.3315746\C, 1.023891024, -1.0092716788, 2.3317910178\C, 0.9981868004, -1.0081475972, -2.3428874266\C, 0.6947975591, 1.4150026581, 1.7645605643\C, 0.6702388437, 1.414532831, -1.7706342334\H, -1.3104336846, -1.3780080303, 1.2450257141\H, -1.3189190915, -1.3842821366, -1.2320533568\H, -1.596007368, 0.101243257, 2.1598842823\H, -1.6300918946, 0.0922778699, -2.1412095538\H, 0.86649674, -2.0459665898, 2.0154964182\H, 0.852274109, -2.0453481745, -2.0228324442\H, 0.5667214393, -0.8745100071, 3.3183928048\H, 0.5243678446, -0.8777632279, -3.3220737465\H, 2.0985783354, -0.8345999169, 2.4094451188\H, 2.0703202313, -0.8269014259, -2.4378930452\H, 0.1786808876, 2.156043899, 1.1467040145\H, 0.1557895429, 2.1544480024, -1.1500069789\H, 0.3828494761, 1.5681795661, 2.804043021\H, 0.3485065648, 1.5657318075, -2.8071406818\H, 1.7709887901, 1.5955754844, 1.6929123535\H, 1.7465312496, 1.5979142728, -1.7076731316\H, -3.4378079378, -0.9520895216, -0.0244577722\H, -3.7167748018, 0.450259427, 0.7526133825\Version=IA32L-G03RevC.02\State=2-A\HF=-539.0627624\S2=0.753691\S2-1=0.\S2A=0.750009\RMSD=8.174e-09\RMSF=8.534e-06\Dipole=-0.9353891, 0.0124369, 0.4430936\PG=C01 [X(C9H19N2O1)]\@

4-hydroxy-TEMPO• (D)

1\1\GINC-LC151\FOpt\UB3LYP\6-31G(d)\C9H18N1O2(2)\JOH501\27-Feb-2006\0\ \# UB3LYP/6-31G* OPT FREQ=NORAMAN MAXDISK=104857600\ohtempo_1s\0,2\N, 1.0254691088, 0., -0.2529401447\O, 2.3102405844, 0., -0.2183358214\C, -1.8249937794, 0., 0.2211166731\O, -3.2232762137, 0., -0.0587455764\H, -1.7747618716, 0., 1.315027019\H, -3.3251891239, 0., -1.0247426078\C, -1.1360419068, 1.2447195679, -0.338331613\C, -1.1360419068, -1.2447195679, -0.338331613\C, 0.3694892873, 1.3310321062, -0.0166536613\C, 0.3694892873, -1.3310321062, -0.0166536613\C, 1.0414114204, 2.3395563969, -0.9632262732\C, 1.0414114204, -2.3395563969, -0.9632262732\C, 0.6143161204, 1.7662705834, 1.4443798454\C, 0.6143161204, -1.7662705834, 1.4443798454\H, -1.2673452647, 1.2393822518, -1.431271053\H, -1.2673452647, -1.2393822518, -1.431271053\H, -1.6332436663, 2.1462157954, 0.037304709\H, -1.6332436663, -2.1462157954, 0.037304709\H, 0.932337534, 2.0227844944, -2.0059434455\H, 0.932337534, -2.0227844944, -2.0059434455\H, 0.5711507667, 3.3223189568, -0.8480968702\H, 0.5711507667, -3.3223189568, -0.8480968702\H, 2.1066346595, 2.4249919232, -0.741180947\H, 2.1066346595, -2.4249919232, -0.741180947\H, 0.2912137596, 2.8038489574, 1.5849999169\H, 0.2912137596, -2.8038489574, 1.5849999169\H, 0.069772793, 1.1463596346, 2.1629892268\H, 0.069772793, -1.1463596346, 2.1629892268\H, 1.6823873621, 1.6989828613, 1.6693125482\H, 1.6823873621, -1.6989828613, 1.6693125482\Version=IA32L-G03RevC.02\State=2-A\HF=-558.9281808\S2=0.753684\S2-1=0.\S2A=0.750009\RMSD=3.244e-09\RMSF=4.161e-06\Dipole=-0.5867701, 0., -0.2403593\PG=CS [SG(C1H2N1O2), X(C8H16)]\@

3-carboxy-TEMPO• (E)

1\1\GINC-LC49\FOpt\UB3LYP\6-31G(d)\C10H18N1O3(2)\JOH501\01-Mar-2006\0\ \# UB3LYP/6-31G* OPT FREQ=NORAMAN MAXDISK=134217728\sidectempo_4\0,2\N, 1.1793804017, -0.355626939, -0.6184197005\O, 2.4636606365, -0.3723579723, -0.6443450747\C, -1.6305287098, 0.2233271874, -0.5776713552\H, -2.7025568267, -0.0044490778, -0.5526628345\H, -1.5526209217, 1.3151099229, -0.5822144728\C, -0.9974485729, -0.3957515352, -1.821638789\C, -0.9591647172, -0.3474122312, 0.6791249202\C, 0.5122256567, -0.1213684095, -1.9438281534\C, 0.5765001284, -0.0512343331, 0.7309567654\C, 1.1374341375, -1.107650591, -2.9438062143\C, 1.260911224, -0.9949516104, 1.7353856224\C, 0.793606799, 1.3235074539, -2.4075077024\C, 0.8955950116, 1.4126923232, 1.100104591\H, -1.4893897223, -0.0243070568, -2.7286301047\C, -1.6671109937, 0.1709878078, 1.9209136082\H, -1.1614106008, -1.4819360952, -1.7997497777\H, -1.0717931877, -1.4382239304, 0.6713719214\H, 1.0099573039, -2.1395032972, -2.5997150656\H, 1.1006541669, -2.0408740824, 1.4530187965\H, 0.644342004, -1.0040536916, -3.9168478388\H, 0.8495936562, -0.8428928359, 2.7367817908\H, 2.2051411354, -0.9162757089, -3.0638109104\H, 2.3351477124, -0.8068823325, 1.753878408\H, 0.4664572928, 1.4521930219, -3.4454417276\H, 0.6731804263, 1.6026643089, 2.154496986\H, 0.2729409802, 2.0670806038, -1.7967919202\H, 0.3220667761, 2.1315096271, 0.5092968209\H, 1.8677246571, 1.5215877197, -2.3534505101\H, 1.9615085113, 1.5873753564, 0.9317643147\O, -2.1361533069, 1.2810387643, 2.050

2525508\O,-1.7418631284,-0.762386602,2.9036677182\H,-2.2038795671,-0.3
319637703,3.6488422821\\Version=IA32L-G03RevC.02\State=2-A\HF=-672.281
9762\S2=0.753705\S2-1=0.\S2A=0.750009\RMSD=4.159e-09\RMSF=3.491e-06\Di
pole=-0.8422461,-0.2459218,-0.0151603\PG=C01 [X(C10H18N1O3)]\\@

3,4-dicarboxy-TEMPO• (F)

1\1\GINC-LC44\FOpt\UB3LYP\6-31G(d)\C11H18N1O5(2)\JOH501\09-Mar-2006\0\
\# UB3LYP/6-31G* OPT FREQ=NORAMAN MAXDISK=402653184\\sidecctempo_2\\0,
2\N,1.801515265,-0.3007463064,-0.4949441636\O,3.0856077618,-0.28500780
51,-0.5083746423\C,-1.0287684224,0.2091695771,-0.4652987918\C,-2.50750
45078,-0.1408722584,-0.4861511313\H,-0.9610126698,1.3010479657,-0.4706
46697\C,-0.3542652362,-0.3711059116,-1.7202738054\C,-0.3568107446,-0.3
62858093,0.7908895711\C,1.1427711581,-0.0356280065,-1.8149525886\C,1.1
765964333,-0.0532335894,0.8562235232\C,1.8042304513,-0.9633826226,-2.8
47803043\C,1.8656734563,-1.0250711191,1.8307797368\C,1.3788676731,1.43
35601101,-2.2226242661\C,1.4740472818,1.4010012833,1.2816437374\H,-0.8
537064953,0.0020377058,-2.6203297993\C,-1.0762951909,0.1622926566,2.02
81291773\H,-0.4793988069,-1.4619410317,-1.7104308568\H,-0.4794143495,-
1.450589631,0.7808833323\H,1.7087900575,-2.0110624546,-2.5441763169\H,
1.7175374455,-2.0613319196,1.5092265583\H,1.3154273499,-0.8373335787,-
3.8201024389\H,1.4484611969,-0.91271283,2.8338130609\H,2.8656875374,-0
.7320396736,-2.9499987998\H,2.9375770425,-0.8249723175,1.8578754091\H,
1.0433420625,1.5952392466,-3.2530935976\H,1.2439963835,1.5473928998,2.
3415560591\H,0.8426849786,2.1383756234,-1.580436635\H,0.8941317966,2.1
340355043,0.7146266077\H,2.4473055121,1.6589204668,-2.1640124839\H,2.5
381843733,1.5973830574,1.1277262041\O,-1.6352034193,1.2361092908,2.098
6768773\O,-1.0191799365,-0.6955732059,3.0712271585\H,-1.5093858147,-0.
268385385,3.7998419708\O,-3.0419774642,-0.9980425339,0.1835415762\O,-3
.1809590787,0.6011297411,-1.3962653321\H,-4.1083714717,0.2990044417,-1
.361530251\\Version=IA32L-G03RevC.02\State=2-A\HF=-860.8474055\S2=0.75
3691\S2-1=0.\S2A=0.750009\RMSD=7.058e-09\RMSF=2.955e-06\Dipole=-0.5941
715,0.1119977,-0.343216\PG=C01 [X(C11H18N1O5)]\\@

3,5-dicarboxy-TEMPO• (G)

1\1\GINC-LC83\FOpt\UB3LYP\6-31G(d)\C11H18N1O5(2)\JOH501\15-Mar-2006\0\
\# UB3LYP/6-31G* OPT FREQ=NORAMAN MAXDISK=268435456\\oppcctempo_2s\\0,
2\N,1.5174257229,-0.3403220046,0.\O,2.8012107438,-0.3404748815,0.\C,-1
.2987356854,0.1554326902,0.\H,-1.2625264472,1.2470884118,0.\H,-2.36227
24555,-0.1085248937,0.\O,-1.8882754998,1.1477115899,2.6292477624\O,-1.
8882754998,1.1477115899,-2.6292477624\C,-1.3848865103,0.0547487588,2.4
898462145\C,-1.3848865103,0.0547487588,-2.4898462145\O,-1.4522966033,-
0.9012858142,3.4504581973\O,-1.4522966033,-0.9012858142,-3.4504581973\
H,-1.9439380158,-0.5019249432,4.1940056849\H,-1.9439380158,-0.50192494
32,-4.1940056849\C,-0.6316657863,-0.4178394937,1.2552101991\C,-0.63166
57863,-0.4178394937,-1.2552101991\H,-0.7043018192,-1.5116489359,1.2287
687486\H,-0.7043018192,-1.5116489359,-1.2287687486\C,0.8873690552,-0.0
650635656,1.3419236281\C,0.8873690552,-0.0650635656,-1.3419236281\C,1.
1460021395,1.4063077139,1.7284799555\C,1.1460021395,1.4063077139,-1.72
84799555\C,1.5876309733,-0.9917462993,2.3507844277\C,1.5876309733,-0.9
917462993,-2.3507844277\H,0.5532490107,2.1087022792,1.1377759446\H,0.5
532490107,2.1087022792,-1.1377759446\H,0.9032176377,1.5759046475,2.781
6849354\H,0.9032176377,1.5759046475,-2.7816849354\H,2.2067042871,1.623
5263334,1.5771166893\H,2.2067042871,1.6235263334,-1.5771166893\H,1.145
0143113,-0.8676567601,3.34255214\H,1.1450143113,-0.8676567601,-3.34255
214\H,1.4787337312,-2.0401821085,2.0542466155\H,1.4787337312,-2.040182
1085,-2.0542466155\H,2.6519719551,-0.7591226901,2.3995129957\H,2.65197
19551,-0.7591226901,-2.3995129957\\Version=IA32L-G03RevC.02\State=2-A'
\HF=-860.8430788\S2=0.753705\S2-1=0.\S2A=0.750009\RMSD=7.659e-09\RMSF=
2.318e-06\Dipole=-0.5701541,-0.6840996,0.\PG=CS [SG(C1H2N1O1),X(C10H16
O4)]\\@

4-carboxy-2,2,6,6-tetraethylpiperidin-1-yloxy• (H)

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1\1\GINC-AC36\FOpt\UB3LYP\6-31G(d)\C14H26N1O3(2)\JOH501\04-Apr-2006\0\
\# UB3LYP/6-31G* OPT FREQ=noraman maxdisk=671088640\ctempoeth_26\0,2
\N,1.506184311,0.0014075229,-0.2616849882\O,2.7905109397,0.0332607735,
-0.3379958667\C,-1.3091226194,-0.0945091781,0.3012163167\C,-2.80064878
56,-0.1483868913,0.0244630273\H,-1.1962804136,-0.0052261299,1.38820954
04\C,-0.6979710851,1.1481331496,-0.3748365676\C,-0.6077479758,-1.34386
23496,-0.2306527541\C,0.8110812384,1.3232980736,-0.0938119714\C,0.9140
079356,-1.3528382794,0.015374919\C,1.4234105998,2.2717865205,-1.158535
3539\C,1.597037116,-2.3654219748,-0.9434581149\C,1.0133120188,1.867134
5593,1.3526360913\C,1.2603520264,-1.7146831603,1.4921102483\H,-1.22466
79012,2.0504256763,-0.0508427808\H,-1.0402928711,-2.2450164916,0.21577
87366\H,-0.8525934526,1.0550316625,-1.4580837678\H,-0.8175344986,-1.41
14775014,-1.3025907655\H,1.2571240775,1.8095078963,-2.140052444\C,1.62
38255078,-1.9832018099,-2.4273142221\C,0.8697412849,3.7012820511,-1.17
06923122\H,1.0742215615,-3.3223676669,-0.8246140291\H,2.5055916187,2.2
921278403,-1.0157065183\H,2.625520444,-2.5186774285,-0.6027667241\H,0.
4267295975,2.7916225812,1.4326918257\C,0.9884535392,-3.1617452515,1.92
36840846\H,0.5540607258,1.1672024578,2.0602094392\H,0.7134240903,-1.04
10957534,2.1634892475\C,2.4530639131,2.1465486468,1.7973040871\H,2.324
4238348,-1.490972669,1.625891461\O,-3.3599396774,-0.9022266634,-0.7411
713951\O,-3.4732667815,0.7922649342,0.7376572987\H,-4.4107177236,0.706
9628728,0.479961938\H,2.4568206683,2.4938376959,2.8372274402\H,3.07809
68443,1.2535578035,1.7268872486\H,2.9234186026,2.9253767436,1.18786415
\H,1.345763096,4.2734542576,-1.97473374\H,-0.2114563324,3.7319075063,-
1.3474767037\H,1.0710225225,4.2314316287,-0.2333685536\H,2.0825723084,
-2.7909586917,-3.0087657942\H,0.6215041167,-1.8181792228,-2.838624387\
H,2.2154310716,-1.0777491005,-2.5848189648\H,1.2273602491,-3.280657611
4,2.9866230158\H,-0.0617845732,-3.4480819307,1.7944151903\H,1.60205883
1,-3.8778170983,1.3687934124\Version=IA64L-G03RevD.01\State=2-A\HF=-8
29.5286031\S2=0.754061\S2-1=0.\S2A=0.750011\RMSD=7.399e-09\RMSF=1.875e
-06\Thermal=0.\Dipole=-0.7081192,0.3858622,0.5318177\PG=C01 [X(C14H26N
1O3)]\@
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PROXYL• (I)

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1\1\GINC-AC24\FOpt\UB3LYP\6-31G(d)\C8H16N1O1(2)\JOH501\08-Feb-2007\0\
\# UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\proxyl_1c2v\0,2\N
,0.,0.,-0.0015115311\O,0.,0.,1.2744073363\C,1.2599403567,0.0001224556,
-0.7968992085\C,-1.2599403567,-0.0001224556,-0.7968992085\C,0.72038645
29,-0.2760312376,-2.2164817156\C,-0.7203864529,0.2760312376,-2.2164817
156\H,1.3431566966,0.1855603524,-2.989328976\H,-1.3431566966,-0.185560
3524,-2.989328976\H,0.7124168473,-1.3560796869,-2.4049191929\H,-0.7124
168473,1.3560796869,-2.4049191929\C,1.9248445118,1.3838144722,-0.67090
3006\C,-1.9248445118,-1.3838144722,-0.670903006\C,2.1967095165,-1.0911
653876,-0.2686669487\C,-2.1967095165,1.0911653876,-0.2686669487\H,1.29
88224567,2.171099688,-1.1052610945\H,-1.2988224567,-2.171099688,-1.105
2610945\H,2.8939705963,1.3942338745,-1.1826742603\H,-2.8939705963,-1.3
942338745,-1.1826742603\H,2.0837389957,1.6191744517,0.3860982878\H,-2.
0837389957,-1.6191744517,0.3860982878\H,1.7308083454,-2.0791274147,-0.
3495400638\H,-1.7308083454,2.0791274147,-0.3495400638\H,3.1323786875,-
1.1009334462,-0.8388186756\H,-3.1323786875,1.1009334462,-0.8388186756\
H,2.4269928996,-0.9090076418,0.784862575\H,-2.4269928996,0.9090076418,
0.784862575\Version=IA64L-G03RevD.01\State=2-B\HF=-444.4105462\S2=0.7
53779\S2-1=0.\S2A=0.75001\RMSD=7.253e-09\RMSF=2.947e-05\Thermal=0.\Dip
ole=0.,0.,-1.2008263\PG=C02 [C2(N1O1),X(C8H16)]\@
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3-amino-PROXYL• (J)

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1\1\GINC-LC108\FOpt\UB3LYP\6-31G(d)\C8H17N2O1(2)\JOH501\27-Feb-2006\0\
\# UB3LYP/6-31G* OPT FREQ=NORAMAN MAXDISK=104857600\proxyl_2\0,2\N,
-0.3495353695,-0.8589101749,-0.0700828306\C,1.1389013038,-0.8179943903
,-0.158823541\C,1.402910719,0.7003991655,-0.168022312\C,-1.0142699442,
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0.4535670019,0.1310149654\C,0.2014522042,1.337968071,0.5554325684\H,0.3357463554,1.2018465311,1.6366004123\N,0.1386399402,2.7755360462,0.32589098\C,-1.6585898649,0.8939211439,-1.1962771225\C,1.5944600428,-1.5326124106,-1.4369497989\C,-2.0804237842,0.3291083517,1.2230058956\C,1.7261743439,-1.5171780602,1.0813331799\H,2.6875612766,-1.5233791344,-1.5102979345\H,1.2495924369,-2.5704019131,-1.4283456647\H,1.1838764862,-1.0437903865,-2.327091886\O,-1.007214035,-1.9435681922,-0.2131072667\H,2.8180953359,-1.5749643044,1.0093281763\H,1.4711281166,-0.9812775598,2.0022142234\H,1.3245786125,-2.5325578731,1.1545543107\H,-2.3458675632,0.1126689087,-1.534942101\H,-2.224939166,1.8238932889,-1.0730917448\H,-0.9114446188,1.0469488521,-1.9837337012\H,-2.8424780775,-0.3979790436,0.9287394667\H,-1.6361818517,-0.0074762617,2.165983868\H,-2.5673293932,1.2965641627,1.3946794636\H,1.4452711927,1.0697867438,-1.2012309093\H,2.3481862616,0.9692455793,0.3116458177\H,-0.0301130769,2.9721234259,-0.6593437621\H,-0.6353921634,3.1878401857,0.8442500436\\Version=IA32L-G03RevC.02\State=2-A\HF=-499.7528128\S2=0.753773\S2-1=0.\S2A=0.75001\RMSD=7.698e-09\RMSF=1.309e-05\Dipole=0.1652956,0.867629,-0.0375614\PG=C01 [X(C8H17N2O1)]\@

3-methoxy-PROXYL• (K)

1\1\GINC-LC32\FOpt\UB3LYP\6-31G(d)\C9H18N1O2(2)\JOH501\27-Feb-2006\0\\# UB3LYP/6-31G* OPT FREQ=NORAMAN MAXDISK=104857600\\meoproxyl_4\\0,2\N,-0.6483395965,-0.9504459557,0.1199905662\C,0.8377463004,-0.8812272523,0.0856085387\C,1.0840291588,0.6467862371,0.1136756076\C,-1.3420220581,0.3240091367,0.4547771485\C,-0.1502420238,1.2218555475,0.8493912846\H,0.0141692931,1.1766611439,1.9322501079\H,-0.3194734387,2.271464067,0.5909227023\C,-2.0834706014,0.8277432402,-0.7975136933\C,1.3608694607,-1.5961145286,-1.1632017683\C,-2.3291909663,0.0823942529,1.6027191181\C,1.3926372308,-1.5551783413,1.3570378207\H,2.4554777163,-1.5728536376,-1.1857127256\H,1.0272618761,-2.6372497405,-1.1416711314\H,0.9862467849,-1.1234181546,-2.0721705259\O,-1.278611543,-2.0487370521,-0.0338541505\H,2.4867223133,-1.6057284008,1.3238904972\H,1.1003397991,-1.0167886843,2.2654891537\H,0.9957917265,-2.5726101769,1.4235961425\H,-2.7831506601,0.0594116756,-1.1417577005\H,-2.6495921364,1.7383014892,-0.5680322878\H,-1.3771607088,1.0469438199,-1.6027095752\H,-3.0639840957,-0.6724669188,1.3093833349\H,-1.8113718494,-0.2766617316,2.4988850656\H,-2.8556150928,1.0097980924,1.8542644681\O,1.1885237056,1.1374753288,-1.2182932587\H,2.015680041,0.8756388696,0.6527100018\C,1.7709785577,2.4213566501,-1.3158853238\H,1.8425081212,2.6559430127,-2.3809217929\H,1.1664141569,3.198638143,-0.8247340512\H,2.7808056753,2.4384429543,-0.8760887702\\Version=IA32L-G03RevC.02\State=2-A\HF=-558.9253695\S2=0.753778\S2-1=0.\S2A=0.75001\RMSD=4.778e-09\RMSF=1.904e-06\Dipole=0.781984,1.3284181,0.4398636\PG=C01 [X(C9H18N1O2)]\@

3-hydroxy-PROXYL• (L)

1\1\GINC-AC35\FOpt\UB3LYP\6-31G(d)\C8H16N1O2(2)\JOH501\01-May-2006\0\\# UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\\ohproxyl_9\\0,2\N,-0.0118882577,-0.0143080881,-0.016699883\C,1.4742699315,-0.0048632165,-0.0351381308\C,1.7808301338,1.5185326032,-0.0282803196\C,-0.6574890755,1.2936095353,0.2883535476\C,0.5675532503,2.1495944094,0.6765147349\H,0.7188278674,2.1196983365,1.7612197574\H,0.4620571161,3.1964738466,0.3797267404\C,-1.3722643753,1.8018402903,-0.9772511376\C,1.972046383,-0.7528725438,-1.2753606916\C,-1.6600839917,1.1110065469,1.4341198925\C,1.9973268972,-0.6864222453,1.244394419\H,3.0682673706,-0.7879123207,-1.2975231878\H,1.5942245561,-1.7782597205,-1.2522113045\H,1.6065426732,-0.2814236703,-2.1916994047\O,-0.6836365695,-1.0857092288,-0.1863382215\H,3.0895161499,-0.7755024461,1.2208416378\H,1.7195813954,-0.1260601503,2.1438732519\H,1.5652508056,-1.6887095278,1.3214484539\H,-2.095136261,1.0517278424,-1.3139639751\H,-1.9088745213,2.733787873,-0.7644791099\H,-0.653484259,1.9890403181,-1.7789555574\H,-2.427505052,0.3866818638,1.1470346\H,-1.1637189259,0.7417416985,2.3383655603\H,-2.1454917199,2.0643751527,1.6705567971\O,1.8566517546,2.0994914462,-1.328522882\H,2.7115486951,1.7159770765,0.5233237029\H,2.6024280291,1.6937543189,-1.7

969792902\\Version=IA64L-G03RevD.01\\State=2-A\\HF=-519.6186544\\S2=0.753784\\S2-1=0.\\S2A=0.75001\\RMSD=7.337e-09\\RMSF=5.527e-06\\Thermal=0.\\Dipole=1.0089545,0.5786473,0.3019848\\PG=C01 [X(C8H16N1O2)]\\@

3-carboxy-PROXYL• (M)

1\\1\\GINC-LC45\\FOpt\\UB3LYP\\6-31G(d)\\C9H16N1O3(2)\\JOH501\\24-Feb-2006\\0\\
UB3LYP/6-31G* OPT FREQ=NORAMAN MAXDISK=134217728\\cproxyl_1\\0,2\\N,-
0.9386281158,-0.7922993282,-0.6499716908\\C,0.3818744661,-0.9189196302,
0.0258225899\\C,0.8393884235,0.5747315301,0.0321812775\\C,-1.4773656507,
0.5904186514,-0.7775393784\\C,-0.4654722188,1.3934514186,0.0625540515\\H
, -0.8062947697,1.4893900322,1.0975924319\\H,-0.3172805527,2.4054351206,
-0.3265682978\\C,-1.4681646273,0.9866878746,-2.265740366\\C,1.2956542074
, -1.828799074,-0.8008424269\\C,-2.9051509541,0.6366405061,-0.2212885597
\\C,0.1624665074,-1.509441505,1.4317835962\\H,2.2775833561,-1.9138401819
, -0.3256098783\\H,0.84793899,-2.8228965029,-0.8837312867\\H,1.4315906585
, -1.4308919172,-1.8121757308\\O,-1.593566478,-1.8167833363,-1.033762672
2\\H,1.1197974374,-1.7218062761,1.9200829593\\H,-0.4085390663,-0.8322989
023,2.0744475847\\H,-0.3939782702,-2.4461220569,1.3333292499\\H,-2.03628
20151,0.2524807607,-2.8452260146\\H,-1.9247653892,1.9731743461,-2.40432
24998\\H,-0.4483932238,1.0213948112,-2.6653733894\\H,-3.5430327448,-0.06
16474711,-0.7704436889\\H,-2.9217941474,0.3562098939,0.8371510971\\H,-3.
3194431685,1.6461338655,-0.3184254153\\C,1.7711440209,0.9124690316,1.17
68369876\\O,1.4658158149,1.4775593766,2.2036699333\\H,1.385572139,0.7572
303,-0.89998134\\O,3.0356787459,0.4813859246,0.9339595089\\H,3.558047869
3,0.7134209369,1.7255152645\\Version=IA32L-G03RevC.02\\State=2-A\\HF=-63
2.9754585\\S2=0.753776\\S2-1=0.\\S2A=0.75001\\RMSD=8.928e-09\\RMSF=4.993e-0
6\\Dipole=0.7485791,0.6098897,-0.0282996\\PG=C01 [X(C9H16N1O3)]\\@

3,4-dicarboxy-PROXYL• (N)

1\\1\\GINC-LC107\\FOpt\\UB3LYP\\6-31G(d)\\C10H16N1O5(2)\\JOH501\\02-Mar-2006\\0
\\# UB3LYP/6-31G* OPT FREQ=NORAMAN MAXDISK=134217728\\ccproxyl_2\\0,2\\
N,-0.9088773745,-1.4624081311,-0.231795359\\C,0.5791462747,-1.453166108
7,-0.2637137309\\C,0.8557624594,0.0798859925,-0.2827131429\\C,-1.5787174
27,-0.1551647484,0.0081790645\\C,-0.356554164,0.7232701034,0.4106033826
\\H,-0.2251757167,0.6692727354,1.4957892957\\C,-0.4976840898,2.188351191
6,0.0515887794\\C,-2.2660036744,0.2922538626,-1.2958193119\\C,1.07140299
07,-2.1667676444,-1.5271536747\\C,-2.6073133648,-0.3029269606,1.1342257
531\\C,1.1025179219,-2.1657862656,0.9977170639\\H,2.1639815353,-2.139429
5071,-1.5739512936\\H,0.7362484617,-3.2074320671,-1.5178489403\\H,0.6721
016542,-1.6866605213,-2.4267786775\\O,-1.5755800723,-2.5349240599,-0.40
27913305\\H,2.1922990237,-2.2680761135,0.9621978886\\H,0.8359486667,-1.6
247582163,1.9114554645\\H,0.6593394753,-3.1646236233,1.0459525585\\H,-2.
9381346937,-0.5036651524,-1.6292265278\\H,-2.8543747927,1.2014051601,-1
.1326854982\\H,-1.5406787714,0.4885031521,-2.0921002939\\H,-3.3707924184
, -1.0297262029,0.843939946\\H,-2.1301398248,-0.6567850883,2.0542008267\\
H,-3.0842262938,0.6602671475,1.3378859724\\C,2.1596531162,0.485796514,0
.373351659\\O,2.2696820995,1.0401732477,1.4448559756\\H,0.9004579896,0.4
176382789,-1.3228042254\\O,3.2287601829,0.140730117,-0.3834592174\\H,4.0
190080349,0.4292015193,0.1120324506\\O,0.0888072369,2.7570530439,-0.842
9252778\\O,-1.3894955833,2.8161532305,0.8549027231\\H,-1.4243718744,3.74
37651646,0.5522505303\\Version=IA32L-G03RevC.02\\State=2-A\\HF=-821.5407
522\\S2=0.753778\\S2-1=0.\\S2A=0.75001\\RMSD=6.918e-09\\RMSF=1.015e-05\\Dipo
le=0.2974317,0.4773418,0.0762367\\PG=C01 [X(C10H16N1O5)]\\@

3-carboxy-2,2,5,5-tetraethylpyrrolidin-1-yloxy• (O)

1\\1\\GINC-LC105\\FOpt\\UB3LYP\\6-31G(d)\\C13H24N1O3(2)\\JOH501\\25-Mar-2006\\0
\\# UB3LYP/6-31G* OPT FREQ=NORAMAN MAXDISK=671088640\\cproxyleth_29\\0
,2\\N,0.7968701922,0.6111372606,0.0823382428\\C,-0.6719303426,0.85696871
43,0.1178342852\\C,-1.1842003679,-0.5048293723,-0.4544977914\\C,1.221707
7969,-0.8132888456,-0.0628584756\\C,-0.1388712856,-1.5409772589,-0.0009

381109\H,-0.3667246361,-1.8642237033,1.019008139\H,-0.160579662,-2.433
0310695,-0.633675459\C,1.8887171932,-1.027714489,-1.4498466567\C,-1.02
81214136,2.0900044714,-0.7393279193\C,2.1535801762,-1.1681717868,1.115
5910312\C,-1.15005946,1.055203895,1.5876233244\H,-2.1164019619,2.21592
01958,-0.6946651348\H,-0.5822940727,2.9631788003,-0.2543611212\C,-0.56
51323168,2.0688367508,-2.199237982\O,1.635879773,1.5644086318,0.235096
2852\H,-2.2338800789,1.2328273007,1.556708489\H,-1.0136089843,0.112106
3948,2.1298925359\C,-0.4784449351,2.1836850948,2.3790974063\C,3.217223
2788,-0.3026848494,-1.6921570549\H,2.0319983026,-2.1081611255,-1.58120
97457\H,1.1673836047,-0.7248793619,-2.2201597238\H,2.9889663792,-0.460
6739646,1.1160989069\H,1.5981214101,-0.9846504284,2.0444937279\C,2.675
9817392,-2.6090939343,1.1141823373\C,-2.5911495579,-0.8705175058,-0.03
15123151\O,-2.8976040711,-1.6968989669,0.7992646096\H,-1.1895719562,-0
.4315469067,-1.5460740195\O,-3.5195563447,-0.1438624712,-0.7070876324\
H,-4.3881516542,-0.4287658117,-0.364221763\H,-0.8560352187,2.181946240
7,3.408076362\H,0.6071336735,2.0629070768,2.4084043438\H,-0.6905389748
3,1.695729127,1.9537159178\H,-0.8292576886,3.0156764741,-2.6831056702\
H,0.5210675275,1.9549110027,-2.2655613933\H,-1.0364646114,1.2702868171
, -2.7834238215\H,3.5587334205,-0.481567291,-2.7182896793\H,3.116317497
5,0.7745554822,-1.5406483537\H,4.003158261,-0.6598086669,-1.0175539424
\H,3.2735889242,-2.7952718958,2.0133371906\H,1.8583073538,-3.339849686
3,1.1065665581\H,3.3150839121,-2.8131224646,0.2483813859\\Version=IA32
L-G03RevC.02\State=2-A\HF=-790.2211675\S2=0.754168\S2-1=0.\S2A=0.75001
2\RMSD=8.408e-09\RMSE=2.849e-06\Dipole=-0.5971661,-0.361735,-0.4130486
\PG=C01 [X(C13H24N1O3)]\@

TMIO• (P)

1\1\GINC-AC35\FOpt\UB3LYP\6-31G(d)\C12H16N1O1(2)\JOH501\28-Feb-2006\O\
\# UB3LYP/6-31G* OPT FREQ=NORAMAN MAXDISK=134217728\\tmio_1c2v_2\\O,2\
O,0.,0.,-2.7800581119\N,0.,0.,-1.5057552508\C,1.2625040228,0.,-0.71307
32792\C,-1.2625040228,0.,-0.7130732792\C,0.7000380857,0.,0.6928829269\
C,-0.7000380857,0.,0.6928829269\C,1.4056709073,0.,1.8948649635\C,-1.40
56709073,0.,1.8948649635\H,2.492899722,0.,1.8992572854\H,-2.492899722,
0.,1.8992572854\C,0.6990894526,0.,3.1001372598\C,-0.6990894526,0.,3.10
01372598\H,1.2399009592,0.,4.0426547966\H,-1.2399009592,0.,4.042654796
6\C,-2.0733777389,-1.2649410868,-1.048711587\C,-2.0733777389,1.2649410
868,-1.048711587\C,2.0733777389,1.2649410868,-1.048711587\C,2.07337773
89,-1.2649410868,-1.048711587\H,-2.2816000136,-1.2877418305,-2.1227719
232\H,-2.2816000136,1.2877418305,-2.1227719232\H,2.2816000136,1.287741
8305,-2.1227719232\H,2.2816000136,-1.2877418305,-2.1227719232\H,-3.023
8476994,-1.2687194109,-0.5041274401\H,-3.0238476994,1.2687194109,-0.50
41274401\H,3.0238476994,1.2687194109,-0.5041274401\H,3.0238476994,-1.2
687194109,-0.5041274401\H,-1.517448926,-2.168884498,-0.7810348559\H,-1
.517448926,2.168884498,-0.7810348559\H,1.517448926,2.168884498,-0.7810
348559\H,1.517448926,-2.168884498,-0.7810348559\\Version=IA64L-G03RevC
.02\State=2-B1\HF=-596.8384326\S2=0.753786\S2-1=0.\S2A=0.750011\RMSD=7
.719e-09\RMSE=2.533e-05\Dipole=0.,0.,1.1308772\PG=C02V [C2(N1O1),SGV(C
8H4),X(C4H12)]\@

5-carboxy-TMIO• (Q)

1\1\GINC-LC56\FOpt\UB3LYP\6-31G(d)\C13H16N1O3(2)\JOH501\27-Feb-2006\O\
\# UB3LYP/6-31G* OPT FREQ=NORAMAN MAXDISK=134217728\\ctmio_2s\\O,2\O,3
.5900321109,0.6674141869,0.\N,2.3596694848,0.3378055878,0.\C,1.9235466
458,-1.0876967636,0.\C,1.2660515236,1.3517449981,0.\C,0.420797207,-0.9
118670152,0.\C,0.0557764666,0.4417539608,0.\C,-0.554699225,-1.90800140
53,0.\C,-1.2840939033,0.8075207817,0.\H,-0.2755335333,-2.9583137019,0.
\H,-1.5973305032,1.8469802159,0.\C,-1.901224334,-1.5459238372,0.\C,-2.
2687451835,-0.1914879337,0.\H,-2.6722702593,-2.3080371105,0.\C,-3.6906
06606,0.241153948,0.\O,-4.0665005426,1.396800117,0.\O,-4.5648584779,-0
.7986986914,0.\H,-5.4522138468,-0.3946079754,0.\C,1.3767478747,2.22135
68571,-1.2653399541\C,1.3767478747,2.2213568571,1.2653399541\C,2.45646
78292,-1.7842609218,-1.2656556718\C,2.4564678292,-1.7842609218,1.26565
56718\H,3.5472704102,-1.7023533411,-1.2887829709\H,3.5472704102,-1.702

3533411,1.2887829709\H,2.0520963069,-1.3187022603,-2.1698338616\H,2.0520963069,-1.3187022603,2.1698338616\H,2.1809192738,-2.8443363009,-1.2677612742\H,2.1809192738,-2.8443363009,1.2677612742\H,2.3581189554,2.7046980352,-1.2870383179\H,2.3581189554,2.7046980352,1.2870383179\H,0.6009948696,2.9944373621,-1.2694534236\H,0.6009948696,2.9944373621,1.2694534236\H,1.2660367004,1.6146979705,-2.1695826133\H,1.2660367004,1.6146979705,2.1695826133\\Version=IA32L-G03RevC.02\State=2-A"\HF=-785.4116562\S2=0.753783\S2-1=0.\S2A=0.750011\RMSD=9.949e-09\RMSF=7.999e-06\Dipole=-0.6150363,-0.8933109,0.\PG=CS [SG(C9H4N1O3),X(C4H12)]\\@

5,6-dicarboxy-TMIO• (R)

1\1\GINC-LC98\FOpt\UB3LYP\6-31G(d)\C14H16N1O5(2)\JOH501\02-Mar-2006\0\ \# UB3LYP/6-31G* OPT FREQ=NORAMAN MAXDISK=134217728\\23cctmio_2\0,2\O,-4.2119810438,0.0056010636,0.0239083059\N,-2.9386598425,0.0069217773,0.0170227933\C,-2.1477152902,1.2706843577,0.0601648437\C,-2.1459812049,-1.2557674745,-0.0219667066\C,-0.7436773756,0.7080652758,0.0317669926\C,-0.7423201417,-0.690040303,-0.0124015981\C,0.4574046912,1.4108351695,0.0430245087\C,0.4594373955,-1.390290388,-0.0257501656\C,1.6714255347,0.7184558204,0.0018508827\C,1.6751780586,-0.6927749349,-0.0091523353\C,2.9084290901,1.5631901316,-0.0695048226\C,-2.4823101213,-2.0303321743,-1.3091971983\C,-2.4726517011,-2.1027754414,1.2214396613\C,-2.4876466464,2.128205821,-1.1723886015\C,-2.4708241938,2.0337941902,1.3578005226\H,-3.5622768666,2.3331760606,-1.1812399399\H,-3.5441358297,2.2428525803,1.3936251979\H,-2.2239411205,1.608172966,-2.0986337876\H,-2.2000691397,1.443696957,2.2387746738\H,-1.9463400012,3.0797646603,-1.1413296968\H,-1.9236273995,2.9816724423,1.3938263827\H,-3.5559909191,-2.2392079827,-1.3330000861\H,-3.5465631642,-2.3107234508,1.2424340654\H,-1.936241456,-2.9791653364,-1.3419526911\H,-1.929048942,-3.0532644214,1.1943612953\H,-2.2200276561,-1.4481587297,-2.198042173\H,-2.201505959,-1.5736690091,2.1403159816\H,0.4740196869,-2.4749041961,-0.0281162069\O,3.0993152093,2.5439525262,0.6158948003\O,3.7409943011,1.1810261984,-1.0626876426\H,4.5173977726,1.7696375745,-1.0058234034\C,2.9511812574,-1.4508950095,0.1424661583\O,3.9514414176,-1.0337359536,0.6857833055\O,2.8684394943,-2.7114511698,-0.3554414229\H,3.7268119053,-3.1295578556,-0.1551628114\H,0.4769068437,2.4959537387,0.0722320261\\Version=IA32L-G03RevC.02\State=2-A'\HF=-973.97042\S2=0.75378\S2-1=0.\S2A=0.750011\RMSD=7.030e-09\RMSF=1.624e-05\Dipole=0.2392904,-0.7063043,-0.5764904\PG=C01[X(C14H16N1O5)]\\@

TMAO• (S)

1\1\GINC-AC21\FOpt\UB3LYP\6-31G(d)\C16H18N1O1(2)\JOH501\15-May-2006\0\ \# UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\\sb_1s\0,2\N,0.,0.,0.\O,-1.28471,0.,0.\C,2.84232,0.05404,0.\C,4.28001,-0.02859,0.\C,4.98026,-0.06307,1.23256\C,4.98026,-0.06307,-1.23256\H,6.06538,-0.12765,1.21559\H,6.06538,-0.12765,-1.21559\C,4.29669,-0.00822,2.42279\C,4.29669,-0.00822,-2.42279\H,4.83192,-0.02874,3.36811\H,4.83192,-0.02874,-3.36811\C,2.88815,0.07447,2.42451\C,2.88815,0.07447,-2.42451\H,2.37477,0.1211,3.37977\H,2.37477,0.1211,-3.37977\C,2.15598,0.09855,1.25082\C,2.15598,0.09855,-1.25082\C,0.63808,0.21062,1.33335\C,0.63808,0.21062,-1.33335\C,0.22928,1.61328,1.84735\C,0.22928,1.61328,-1.84735\C,0.05263,-0.87948,2.2592\C,0.05263,-0.87948,-2.2592\H,0.3764,-1.87299,1.93365\H,0.3764,-1.87299,-1.93365\H,0.37893,-0.72949,3.29167\H,0.37893,-0.72949,-3.29167\H,-1.03708,-0.83473,2.22308\H,-1.03708,-0.83473,-2.22308\H,0.66665,2.4034,1.22867\H,0.66665,2.4034,-1.22867\H,-0.85996,1.70352,1.82116\H,-0.85996,1.70352,-1.82116\H,0.57665,1.75848,2.875\H,0.57665,1.75848,-2.875\\Version=IA64L-G03RevD.01\State=2-A'\HF=-750.4707755\S2=0.753764\S2-1=0.\S2A=0.75001\RMSD=5.032e-09\RMSF=1.800e-05\Thermal=0.\Dipole=-0.2387135,0.9807209,0.\PG=CS [SG(C2N1O1),X(C14H18)]\\@

2,2-dimethylindolin-1-yloxy• (T)

1\1\GINC-AC30\FOpt\UB3LYP\6-31G(d)\C10H12N1O1(2)\JOH501\08-Jul-2009\0\ \# UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\\dmino_1s\\0,2\C,0 .,-0.0397867926,2.6942608641\C,0.,0.0915380279,4.0914231368\C,0.,-1.0522307662,4.8770979228\C,0.,-2.3087432416,4.2570341005\C,0.,-2.467917757,2.869055257\C,0.,-1.3074389915,2.0957702428\C,0.,-1.2218769931,6.382984531\C,0.,-2.7651765354,6.6173286416\N,0.,-3.3159588851,5.215617293\H,-0.8802063916,-0.7548763892,6.8412443959\H,0.8802063916,-0.7548763892,6.8412443959\H,0.,-3.4617196746,2.4353440879\H,0.,1.0779681388,4.5490266825\H,0.,-1.3883132122,1.0121331807\H,0.,0.8498792911,2.0711036854\O,0.,-4.5656887959,4.9767973608\C,-1.2653875816,-3.2653257781,7.3244711399\C,1.2653875816,-3.2653257781,7.3244711399\H,-1.280490845,-2.9226534862,8.3649290541\H,1.280490845,-2.9226534862,8.3649290541\H,-2.1658127776,-2.8924134555,6.8240273971\H,2.1658127776,-2.8924134555,6.8240273971\H,-1.2922525523,-4.3588482952,7.3118040197\H,1.2922525523,-4.3588482952,7.3118040197\\Version=IA64L-G03RevE.01\State=2-A\HF=-518.2136034\S2=0.764663\S2-1=0.\S2A=0.750154\RMSD=7.454e-09\RMSF=6.813e-05\Thermal=0.\Dipole=0.,1.0903476,0.4940349\PG=CS [SG(C8H4N1O1),X(C2H8)]\@

2,2-diphenylindolin-1-yloxy• (U)

1\1\GINC-AC10\FOpt\UB3LYP\6-31G(d)\C20H16N1O1(2)\JOH501\13-Jul-2009\0\ \# UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\\dpino_1\\0,2\C,2.361881909,1.9970304832,-0.7809070497\C,1.136481367,1.356708484,-0.5420929002\C,-0.0454281116,2.0393846724,-0.8584221323\C,-0.0054225108,3.3382944643,-1.3697350672\C,1.2178590303,3.9714031345,-1.585285883\C,2.402218151,3.2920824317,-1.2942568116\C,1.1391676351,-0.1007260394,-0.0525630655\N,1.3276236654,-0.9592454225,-1.2896928251\C,0.1378393044,-1.584564574,-1.6606280808\C,-0.8416187057,-1.3857719196,-0.6803155857\C,-0.2444651482,-0.6141497807,0.4749571608\C,-2.106938609,-1.9248327837,-0.8651916696\C,-2.3706922881,-2.6559277759,-2.0335968645\C,-1.3732442932,-2.8453096344,-2.9996967912\C,-0.0962185863,-2.3101970138,-2.8297039813\O,2.3805938781,-0.924952452,-2.0008443361\C,2.2311441981,-0.36517004,0.9862826128\C,2.257588215,0.4309595565,2.1418382936\C,3.1756442943,0.181775845,3.1600908588\C,4.0900098813,-0.8669485037,3.0379813629\C,4.0740716778,-1.6586790499,1.8909286114\C,3.1506901002,-1.4136182207,0.870857763\H,0.6931919349,-2.4322849073,-3.5628599883\H,-1.5984755663,-3.4136996365,-3.8979261717\H,-3.3587115076,-3.0791235165,-2.1902507344\H,-2.8843368525,-1.7853763015,-0.1179759461\H,1.5578777334,1.2568204336,2.2402132307\H,3.178794524,0.8101391827,4.0469050394\H,4.8099684407,-1.0606081197,3.8286163091\H,4.7849878212,-2.4733964017,1.7809433777\H,3.1637467179,-2.0278535311,-0.0213291285\H,-1.0115127879,1.5633878284,-0.725896998\H,-0.9352171915,3.8509512882,-1.6018050308\H,1.2487660256,4.9830169215,-1.9811396639\H,3.3626893064,3.7699973132,-1.4678424088\H,3.287160155,1.474299761,-0.5654055977\H,-0.0791266425,-1.279229346,1.329858075\H,-0.874871165,0.2042411703,0.8323330166\\Version=IA64L-G03RevE.01\State=2-A\HF=-901.6734016\S2=0.76389\S2-1=0.\S2A=0.75014\RMSD=4.317e-09\RMSF=1.486e-05\Thermal=0.\Dipole=-0.8300138,0.116961,0.643874\PG=C01 [X(C20H16N1O1)]\@

SG1• (V)

1\1\GINC-AC59\FOpt\UB3LYP\6-31G(d)\C13H29N1O4P1(2)\JOH501\16-Jan-2007\0\ \# UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\\sglprop_16\\0,2\N,-0.3466716311,0.0082163205,-0.0688688755\O,0.8877470763,0.3496159987,-0.1714992813\C,-1.3333276103,1.1356479246,0.1202698191\C,-0.6454209496,-1.4242034462,0.0559787683\P,-0.1631934522,-2.0495242933,1.765062384\O,0.7857052683,-0.9484880527,2.4728390465\O,-1.5661932676,-1.7440392081,2.5241363482\C,-0.1263945182,-2.2849136113,-1.1573010102\C,2.2332899905,-1.0372111712,2.3916379922\C,2.8117899145,-0.1267236326,3.4583108108\C,-1.6958100473,-2.0991119206,3.9250860203\C,-3.1479730538,-1.914730403,4.3234512895\O,0.3407695072,-3.4474568485,1.8554299795\C,-2.7821438726,0.6315618339,0.1366428648\C,-0.9988444696,1.8361585196,1.4510

691729\C,-1.1292839836,2.1052650556,-1.0577679494\H,-1.7314114054,-1.5249677889,0.0589884849\C,-0.8553979053,-3.6460986413,-1.1199317899\C,-0.5123845044,-1.5582836653,-2.4620026575\C,1.3968093412,-2.5215049219,-1.1465126465\H,2.5320616712,-2.0788005123,2.5448578099\H,2.5314382095,-0.7166727411,1.3900621701\H,3.9065648704,-0.1585708941,3.4190344512\H,2.4909348624,0.9075787056,3.2992181736\H,2.4923465174,-0.4414469191,4.457270959\H,-1.3734255956,-3.1373829254,4.0550683669\H,-1.0337832951,-1.4510988609,4.5094753462\H,-3.279742943,-2.1717740163,5.3804433779\H,-3.4631633301,-0.8760153359,4.1797036855\H,-3.7988143923,-2.5613706278,3.726487934\H,-1.648771121,2.7077907464,1.5877676042\H,-1.1417425295,1.1572814401,2.2965958436\H,0.0420501315,2.1690745932,1.4468499862\H,-3.446578811,1.4963351993,0.2369214833\H,-3.0494272701,0.1213043517,-0.7956072158\H,-2.9785410606,-0.0356116412,0.9811189983\H,-1.7536012334,2.9946191688,-0.9195984601\H,-0.0832846365,2.4127438516,-1.1179411023\H,-1.4085029306,1.6333405183,-2.0062120353\H,-0.2387051445,-2.1808176768,-3.3217018149\H,-1.5930087263,-1.3740400896,-2.5198813703\H,0.0082587144,-0.6015244821,-2.5590560776\H,-0.5510565503,-4.2477225195,-1.9842734498\H,-0.6142740273,-4.2060804638,-0.2132857073\H,-1.9446348737,-3.5178077052,-1.174659474\H,1.6749821869,-3.1238613733,-2.019992092\H,1.9421289917,-1.5764549809,-1.190383202\H,1.7044018887,-3.0724328575,-0.2530929591\\Version=IA64L-G03RevD.01\State=2-A\HF=-1209.8553603\S2=0.754003\S2-1=0.\S2A=0.750012\RMSD=7.020e-09\RMSF=4.294e-05\Thermal=0.\Dipole=-0.857121,0.7157603,0.3984884\PG=C01 [X(C13H29N104P1)]\\@

•CH₃ (1)

1\1\GINC-LC122\FOpt\UB3LYP\6-31G(d)\C1H3(2)\JOH501\11-Apr-2005\0\\# UB3LYP/6-31G* OPT FREQ MAXDISK=65536000\\ch3_6dub3 rad\\0,2\C,0.,0.,0.\H,0.,1.082622,0.\H,-0.9375781547,-0.541311,0.\H,0.9375781547,-0.541311,0.\\Version=IA32L-G03RevC.02\State=2-A2"\HF=-39.8382922\S2=0.753763\S2-1=0.\S2A=0.750007\RMSD=4.899e-09\RMSF=4.641e-05\Dipole=0.,0.,0.\PG=D03H [O(C1),3C2(H1)]\\@

•CH₂CH₃ (2)

1\1\GINC-LC141\FOpt\UB3LYP\6-31G(d)\C2H5(2)\JOH501\01-Mar-2005\0\\# UB3LYP/6-31G* OPT FREQ MAXDISK=65536000\\eth_2sym2_6dub3 opt freq\\0,2\C,0.,0.,0.\C,0.,1.48959,0.\H,-1.02386,-0.41629,0.\H,0.49917,-0.40758,0.8877\H,0.49917,-0.40758,-0.8877\H,-0.08019,2.0476,0.92757\H,-0.08019,2.0476,-0.92757\\Version=x86-Linux-G03RevB.03\State=2-A'\HF=-79.1578672\S2=0.753925\S2-1=0.\S2A=0.75001\RMSD=6.578e-09\RMSF=3.593e-05\Dipole=0.0850963,0.0505436,0.\PG=CS [SG(C2H1),X(H4)]\\@

•CH₂CH₂CH₃ (3)

1\1\GINC-AC45\FOpt\UB3LYP\6-31G(d)\C3H7(2)\JOH501\08-May-2007\0\\# UB3LYP/6-31G* OPT FREQ=noraman maxdisk=134217728\\ch2ch2ch3_1\\0,2\C,0.00615,0.00178,-0.00216\C,1.49813,-0.00764,0.01039\C,-0.59908,1.41317,0.0014\H,-1.69402,1.3762,0.02192\H,2.0521,0.78072,0.51282\H,2.05655,-0.87417,-0.33031\H,-0.38351,-0.54891,0.87554\H,-0.36213,-0.56007,-0.87284\H,-0.29535,1.9723,-0.89192\H,-0.26592,1.9805,0.8777\\Version=IA64L-G03RevD.01\State=2-A\HF=-118.4713715\S2=0.753881\S2-1=0.\S2A=0.75001\RMSD=3.444e-09\RMSF=2.554e-06\Thermal=0.\Dipole=0.0489268,0.0715637,0.0475383\PG=C01 [X(C3H7)]\\@

•CH₂(CH₂)₄CH₃ (4)

1\1\GINC-AC21\FOpt\UB3LYP\Gen\C6H13(2)\CYL509\22-Jul-2008\0\\#B3LYP/GEN 6D INT (GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\\r.nhexyl.diff.freq\\0,2\C,0.7247952821,1.2553812536,1.4444161827\C,0.7332546199,1.270032318,2.9369621215\H,1.5020710524,0.7450321823,3.4974430227\H,-0.1058167162,1.6733467239,3.4974436099\H,1.7561439912,1.2771916359,1.

0627596738\H,0.2280091189,2.1594607829,1.0627602168\C,0.0102542967,0.0
177604356,0.8374009971\H,0.4993549354,-0.8945598773,1.2073749246\C,0.0
103877567,0.0179925333,-0.6974031097\H,-1.0243883926,-0.0148261851,1.2
07375468\H,1.0487002344,0.0570981626,-1.0611192157\H,-0.4749021329,0.9
367504802,-1.0611186722\C,-0.6934244387,-1.2010454475,-1.310022564\H,-
0.2085066969,-2.1190733887,-0.9472466357\C,-0.6896722013,-1.1945454188
, -2.8436436633\H,-1.7309186301,-1.2401083716,-0.9472460771\H,0.3348126
978,-1.191065106,-3.2378320466\H,-1.1989007975,-0.3055751438,-3.237831
4785\H,-1.1992305163,-2.0771259644,-3.2490225758\\Version=IA64L-G03Rev
C.02\State=2-A\HF=-236.4215506\S2=0.753873\S2-1=0.\S2A=0.75001\RMSD=5.
119e-09\RMSF=9.579e-06\Dipole=0.0264906,0.0458825,0.1524451\PG=C01 [X(
C6H13)]\\@

•CH(CH₃)₂ (5)

1\1\GINC-AC40\FOpt\UB3LYP\6-31G(d)\C3H7(2)\JOH501\27-Feb-2007\0\\# UB3
LYP/6-31G* OPT FREQ=noraman maxdisk=134217728\\chme2_2s\\0,2\C,0.,0.,0
.\H,1.08778,0.,0.\C,-0.7109,1.30115,0.17283\C,-0.7109,-1.30115,0.17283
\H,-0.12833,2.14167,-0.22129\H,-0.12833,-2.14167,-0.22129\H,-1.68733,1.
.29786,-0.33234\H,-1.68733,-1.29786,-0.33234\H,-0.91747,1.52734,1.2356
5\H,-0.91747,-1.52734,1.23565\\Version=IA64L-G03RevD.01\State=2-A'\HF=
-118.4781544\S2=0.754002\S2-1=0.\S2A=0.750011\RMSD=6.966e-09\RMSF=1.51
6e-05\Thermal=0.\Dipole=0.0681339,-0.0420556,0.\PG=CS [SG(C1H1),X(C2H6
)]\\@

•C(CH₃)₃ (6)

1\1\GINC-AC40\FOpt\UB3LYP\6-31G(d)\C3H7(2)\JOH501\27-Feb-2007\0\\# UB3
LYP/6-31G* OPT FREQ=noraman maxdisk=134217728\\chme2_2s\\0,2\C,0.,0.,0
.\H,1.08778,0.,0.\C,-0.7109,1.30115,0.17283\C,-0.7109,-1.30115,0.17283
\H,-0.12833,2.14167,-0.22129\H,-0.12833,-2.14167,-0.22129\H,-1.68733,1.
.29786,-0.33234\H,-1.68733,-1.29786,-0.33234\H,-0.91747,1.52734,1.2356
5\H,-0.91747,-1.52734,1.23565\\Version=IA64L-G03RevD.01\State=2-A'\HF=
-118.4781544\S2=0.754002\S2-1=0.\S2A=0.750011\RMSD=6.966e-09\RMSF=1.51
6e-05\Thermal=0.\Dipole=0.0681339,-0.0420556,0.\PG=CS [SG(C1H1),X(C2H6
)]\\@

•CH₂OH (7)

1\1\GINC-AC43\FOpt\UB3LYP\6-31G(d)\C1H3O1(2)\JOH501\19-Feb-2007\0\\# U
B3LYP/6-31G* OPT FREQ=noraman maxdisk=134217728\\ch2oh_1\\0,2\H,0.0539
098849,0.0051141709,0.0341784915\O,1.0099238576,0.1134739506,-0.081337
8927\C,1.3384431149,1.4237021764,0.1475501815\H,2.3873859182,1.6279061
624,-0.0333764464\H,0.5955772244,2.1904235397,-0.0670260986\\Version=I
A64L-G03RevD.01\State=2-A\HF=-115.0520326\S2=0.752927\S2-1=0.\S2A=0.75
0006\RMSD=5.600e-09\RMSF=2.167e-05\Thermal=0.\Dipole=-0.5715567,0.1981
962,-0.0613129\PG=C01 [X(C1H3O1)]\\@

•CH₂F (8)

1\1\GINC-AC18\FOpt\UB3LYP\6-31G(d)\C1H2F1(2)\JOH501\19-Feb-2007\0\\# U
B3LYP/6-31G* OPT FREQ=noraman maxdisk=134217728\\ch2f_2\\0,2\F,0.00580
4342,0.0021311747,0.0229855352\C,1.3438931985,-0.0078245133,-0.0885212
018\H,1.8197457765,0.959969899,0.0336036425\H,1.819466683,-0.939826926
1,0.1998820561\\Version=IA64L-G03RevD.01\State=2-A\HF=-139.0642659\S2=
0.753038\S2-1=0.\S2A=0.750006\RMSD=8.367e-09\RMSF=1.637e-05\Thermal=0.
\Dipole=0.4749973,0.0104757,0.1204848\PG=C01 [X(C1H2F1)]\\@

•CH₂C≡N (9)

1\1\GINC-AC36\FOpt\UB3LYP\6-31G(d)\C2H2N1(2)\JOH501\19-Feb-2007\0\#\ U
B3LYP/6-31G* OPT FREQ=noraman maxdisk=134217728\ch2cn_1s\0,2\C,0.,0.
,0.\C,0.,0.,1.38251\N,0.,0.,-1.17677\H,0.,0.9358236303,1.9297030341\H,
0.,-0.9358236303,1.9297030341\Version=IA64L-G03RevD.01\State=2-B1\HF=
-132.0946681\S2=0.768747\S2-1=0.\S2A=0.750144\RMSD=3.682e-09\RMSF=4.65
4e-05\Thermal=0.\Dipole=0.,0.,-1.3178343\PG=C02V [C2(C1C1N1),SGV(H2)]\@
\@

•CH(CH₃)C≡N (10)

1\1\GINC-AC35\FOpt\UB3LYP\6-31G(d)\C3H4N1(2)\JOH501\05-Mar-2007\0\#\ U
B3LYP/6-31G* OPT FREQ=noraman maxdisk=134217728\an_1\0,2\C,0.0572853
608,0.0034909758,0.\C,1.4443410841,0.0128593863,0.\C,-0.7711955167,1.2
49689711,0.\H,-0.1519040957,2.1495862977,0.\H,-1.4277517503,1.27878853
16,-0.8809902152\H,-1.4277517503,1.2787885316,0.8809902152\H,-0.437002
0692,-0.9645245719,0.\N,2.6209687382,0.0282511381,0.\Version=IA64L-G0
3RevD.01\State=2-A\HF=-171.4162801\S2=0.76697\S2-1=0.\S2A=0.750126\RM
SD=6.120e-09\RMSF=7.117e-05\Thermal=0.\Dipole=-1.5251874,0.1359253,0.\
PG=CS [SG(C3H2N1),X(H2)]\@

•C(CH₃)₂C≡N (11)

1\1\GINC-AC33\FOpt\UB3LYP\6-31G(d)\C4H6N1(2)\JOH501\05-Mar-2007\0\#\ U
B3LYP/6-31G* OPT FREQ=noraman maxdisk=134217728\man_3s\0,2\C,0.,0.,0
.\C,0.,0.,1.39173\N,0.,0.,-1.17667\C,0.,-1.2971871308,2.1479693065\C,0
.,1.2971871308,2.1479693065\H,0.,-2.1626497139,1.4813362209\H,0.,2.162
6497139,1.4813362209\H,0.8813830084,-1.3640848503,2.8023092374\H,-0.88
13830084,-1.3640848503,2.8023092374\H,-0.8813830084,1.3640848503,2.802
3092374\H,0.8813830084,1.3640848503,2.8023092374\Version=IA64L-G03Rev
D.01\State=2-B1\HF=-210.7373225\S2=0.76567\S2-1=0.\S2A=0.750113\RMSD=4
.322e-09\RMSF=8.663e-06\Thermal=0.\Dipole=0.,0.,-1.6235847\PG=C02V [C2
(C1C1N1),SGV(C2H2),X(H4)]\@

•CH₂Ph (12)

1\1\GINC-AC17\FOpt\UB3LYP\6-31G(d)\C7H7(2)\JOH501\19-Feb-2007\0\#\ UB3
LYP/6-31G* OPT FREQ=noraman maxdisk=134217728\ch2ph_1s\0,2\C,0.00000
00117,0.,0.\C,0.0000000117,0.,1.40687\C,0.0000000117,0.,-2.83492\H,0.0
000000117,0.,-3.92119\H,0.0000000117,-0.9280274624,1.9694437125\H,0.00
00000117,0.9280274624,1.9694437125\C,0.0000000117,-1.2180774854,-0.742
9400194\C,0.0000000117,1.2180774854,-0.7429400194\C,0.0000000117,-1.21
20641953,-2.1288369739\C,0.0000000117,1.2120641953,-2.1288369739\H,0.0
000000117,-2.1606878954,-0.2009325066\H,0.0000000117,2.1606878954,-0.2
009325066\H,0.0000000117,-2.1540130532,-2.6714927354\H,0.0000000117,2.
1540130532,-2.6714927354\Version=IA64L-G03RevD.01\State=2-A\HF=-270.
9151433\S2=0.783658\S2-1=0.\S2A=0.750768\RMSD=7.458e-09\RMSF=7.911e-05
\Thermal=0.\Dipole=0.,-0.0525407,0.\PG=C02V [C2(H1C1C1C1),SGV(C4H6)]\@
\@

•CH(CH₃)Ph (13)

1\1\GINC-AC58\FOpt\UB3LYP\6-31G(d)\C8H9(2)\JOH501\05-Mar-2007\0\#\ UB3
LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\sty_3s\0,2\C,1.8331677
936,-0.6472350012,0.\C,0.4616353856,-0.2965455013,0.\C,2.9650047627,0.
3328443342,0.\H,2.9414225683,0.9925192956,0.8806781786\H,3.9309520566,
-0.1802371212,0.\H,2.9414225683,0.9925192956,-0.8806781786\H,2.0768360
969,-1.7071091271,0.\C,0.0160532685,1.0571390391,0.\C,-1.3370625099,1.
3658132803,0.\C,-2.3017340819,0.3498973754,0.\C,-0.5413194958,-1.30989
3688,0.\C,-1.8898129499,-0.990644949,0.\H,0.748755732,1.858782883,0.\H

, -1.6493966141, 2.4072611861, 0.\H, -3.3592755858, 0.5983744564, 0.\H, -0.2291028867, -2.3518602452, 0.\H, -2.6315401083, -1.7854585128, 0.\Version=IA64L-G03RevD.01\State=2-A"\HF=-310.2333536\S2=0.779924\S2-1=0.\S2A=0.750613\RMSD=6.913e-09\RMSF=9.329e-06\Thermal=0.\Dipole=0.1484964, 0.0260667, 0.\PG=CS [SG(C8H7), X(H2)]\@

•C(CH₃)₂Ph (14)

1\1\GINC-AC17\FOpt\UB3LYP\6-31G(d)\C9H11(2)\JOH501\23-Nov-2007\0\# UB3LYP/6-31G* OPT FREQ=noraman maxdisk=134217728\ch2c2\0,2\C,-2.660569, 0., 0.\H, -3.746949, 0., 0.\C, -1.950988, -1.206978, 0.\C, -1.950988, 1.206978, 0.\H, -2.489033, -2.151859, 0.\H, -2.489033, 2.151859, 0.\C, -0.563018, -1.212138, 0.\C, -0.563018, 1.212138, 0.\H, -0.040307, -2.163035, 0.\H, -0.040307, 2.163035, 0.\C, 0.186295, 0., 0.\C, 1.616479, 0., 0.\C, 2.382511, -1.29574, 0.\C, 2.382511, 1.29574, 0.\H, 3.461754, -1.118645, 0.\H, 3.461754, 1.118645, 0.\H, 2.151712, -1.914902, 0.879954\H, 2.151712, 1.914902, 0.879954\H, 2.151712, -1.914902, -0.879954\H, 2.151712, 1.914902, -0.879954\Version=IA64L-G03RevD.01\State=2-B1\HF=-349.5492998\S2=0.775869\S2-1=0.\S2A=0.750465\RMSD=5.106e-09\RMSF=2.697e-05\Thermal=0.\Dipole=0., 0., -0.2540136\PG=C02V[C2(C1C1C1H1), SGV(C6H6), X(H4)]\@

•CH₂C(=O)OCH₃ (15)

1\1\GINC-AC17\FOpt\UB3LYP\6-31G(d)\C3H5O2(2)\JOH501\21-Nov-2007\0\# UB3LYP/6-31G* OPT FREQ=noraman maxdisk=134217728\ch2coome_1\0,2\C, 1.1076136189, 0.0116386504, 0.\C, 1.7704940396, 1.2980305068, 0.\O, 1.1963244266, 2.378049686, 0.\O, 3.1254620108, 1.1708181946, 0.\H, 0.0253384185, -0.0078334929, 0.\C, 3.848655264, 2.407769486, 0.\H, 1.6724991425, -0.9127712282, 0.\H, 3.6064646705, 2.9980541152, -0.8887255661\H, 3.6064646705, 2.9980541152, 0.8887255661\H, 4.9037737381, 2.1318999669, 0.\Version=IA64L-G03RevD.01\State=2-A"\HF=-267.7237414\S2=0.757602\S2-1=0.\S2A=0.750034\RMSD=4.842e-09\RMSF=1.047e-04\Thermal=0.\Dipole=0.4559382, -0.5149408, 0.\PG=CS [SG(C3H3O2), X(H2)]\@

•CH(CH₃)C(=O)OCH₃ (16)

1\1\GINC-AC42\FOpt\UB3LYP\6-31G(d)\C4H7O2(2)\JOH501\05-Mar-2007\0\# UB3LYP/6-31G* OPT FREQ=noraman maxdisk=134217728\ma_2\0,2\C, -0.0010917438, -0.0093539643, 0.\C, 1.4482911137, 0.0190152313, 0.\O, 2.1361265985, 1.0323318263, 0.\O, 1.9752600859, -1.2375951058, 0.\C, 3.4064540785, -1.2937565772, 0.\H, 3.6590107748, -2.3548901754, 0.\C, -0.7990383756, 1.2425509347, 0.\H, 3.8143828721, -0.8030386962, -0.8887074416\H, 3.8143828721, -0.8030386962, 0.8887074416\H, -0.142151845, 2.1155043342, 0.\H, -1.4589129605, 1.2933743594, -0.8789122629\H, -1.4589129605, 1.2933743594, 0.8789122629\H, -0.4905705103, -0.9785778302, 0.\Version=IA64L-G03RevD.01\State=2-A"\HF=-307.0484402\S2=0.756691\S2-1=0.\S2A=0.750029\RMSD=6.285e-09\RMSF=5.807e-05\Thermal=0.\Dipole=-0.3948313, -0.5132152, 0.\PG=CS [SG(C4H3O2), X(H4)]\@

•C(CH₃)₂C(=O)OCH₃ (17)

1\1\GINC-SC78\FOpt\UB3LYP\6-31G(d)\C5H9O2(2)\MLC501\29-Oct-2004\0\# B3LYP/6-31G* OPT FREQ MAXDISK=402653184\MMAuni_rad-c1-6dub3\0,2\C, 2.3430964191, -0.2764647032, 0.\C, 0.8937249479, -0.6357066727, 0.\C, -0.080125223, 0.4463895884, 0.\O, 0.2032150793, 1.6395157023, 0.\O, -1.3715884573, 0.0049437522, 0.\C, -2.3621656303, 1.0386224055, 0.\H, -3.3239638805, 0.5236159558, 0.\H, 2.479217262, 0.8062055674, 0.\C, 0.4999529855, -2.0773620628, 0.\H, 2.852086413, -0.6996174129, 0.879246416\H, 2.852086413, -0.6996174129, -0.879246416\H, -2.2655262185, 1.6695355674, 0.8884336076\H, -2.2655262185, 1.6695355674, -0.8884336076\H, -0.5820140911, -2.2116107304, 0.\H, 0.9168631747, -2.5932970344, -0.878419892\H, 0.9168631747, -2.5932970344, 0.878419892\Version=DEC-AXP-OSF/1-G03RevB.03\State=2-A"\HF=-346.3696451\S2=0.756

647\S2-1=0.\S2A=0.750029\RMSD=8.233e-09\RMSF=4.233e-05\Dipole=-0.1566944,-0.7582412,0.\PG=CS [SG(C5H3O2),X(H6)]\@

•CH(CH₃)OC(=O)CH₃ (18)

1\1\GINC-AC24\FOpt\UB3LYP\6-31G(d)\C4H7O2(2)\JOH501\07-Mar-2007\0\# UB3LYP/6-31G* OPT FREQ=noraman maxdisk=134217728\\vac_5\\0,2\C,0.0525637755,0.1021307886,-0.3327505698\O,1.1955174838,-0.0949075831,0.4147971158\C,-0.6941236708,1.3427568098,-0.0132385301\H,-0.0318866156,2.2179974273,-0.0086203595\H,-1.4793379265,1.5087530836,-0.7575174805\H,-1.1787725577,1.3025566782,0.9779732807\H,-0.3784662916,-0.7853170655,-0.7785556761\C,1.8170239344,-1.3156329178,0.3532523188\O,1.3974472586,-2.2442733592,-0.2967348038\C,3.0700643292,-1.3061414477,1.1919644034\H,3.5071192535,-2.3051431246,1.1989587886\H,3.7917537496,-0.5926087498,0.7789276871\H,2.8450672775,-0.9872305398,2.2147138253\\Version=IA64L-G03RevD.01\State=2-A\HF=-307.0439986\S2=0.753621\S2-1=0.\S2A=0.750009\RMSD=4.137e-09\RMSF=2.127e-06\Thermal=0.\Dipole=0.1151027,0.638564,0.4561504\PG=C01 [X(C4H7O2)]\@

•CH(CH₃)Cl (19)

1\1\GINC-AC11\FOpt\UB3LYP\6-31G(d)\C2H4Cl1(2)\JOH501\06-Mar-2007\0\# UB3LYP/6-31G* OPT FREQ=noraman maxdisk=134217728\\vcl_3\\0,2\C,-0.0673472792,0.0192193207,-0.2424224296\Cl,1.5978066316,-0.0398155931,0.2463251331\C,-0.8419927248,1.2691524082,-0.0306703444\H,-0.309582796,2.1432103849,-0.4247301772\H,-1.8096361607,1.1937414041,-0.5392674643\H,-1.0397119451,1.4648048539,1.0365562687\H,-0.5271157259,-0.9559027787,-0.3504009863\\Version=IA64L-G03RevD.01\State=2-A\HF=-538.7611966\S2=0.753945\S2-1=0.\S2A=0.750011\RMSD=6.162e-09\RMSF=1.212e-05\Thermal=0.\Dipole=-0.6398134,0.1145761,-0.0270263\PG=C01 [X(C2H4Cl1)]\@

•CH(CH₃)C(=O)OH (20)

1\1\GINC-AC27\FOpt\UB3LYP\6-31G(d)\C3H5O2(2)\JOH501\06-Feb-2009\0\# UB3LYP/6-31G* OPT FREQ=noraman maxdisk=134217728\\aa_1\\0,2\C,1.9432509995,-0.5168824129,0.\C,0.4915585712,-0.824902101,0.\C,-0.5035281534,0.2276446379,0.\O,-0.2661052747,1.4287996166,0.\O,-1.7790735587,-0.259055305,0.\H,2.1078394922,0.5630079356,0.\H,0.1437643638,-1.85355786,0.\H,2.4404163495,-0.9535423143,0.8789206777\H,2.4404163495,-0.9535423143,-0.8789206777\H,-2.3586943912,0.5245193168,0.\\Version=IA64L-G03RevE.01\State=2-A\HF=-267.7416405\S2=0.756997\S2-1=0.\S2A=0.75003\RMSD=4.599e-09\RMSF=6.399e-05\Thermal=0.\Dipole=-0.5338796,-0.3592299,0.\PG=CS [SG(C3H3O2),X(H2)]\@

•CH(CH₂CH₃)C(=O)OH (21)

1\1\GINC-AC12\FOpt\UB3LYP\Gen\C4H7O2(2)\CYL509\13-Dec-2008\0\#B3LYP/gen 6D INT(grid=ultrafine) OPT Freq=noraman maxdisk=1342177280\\r.CHET-COOH.freq\\0,2\C,0.2883184168,-1.735564068,0.0638966437\C,-0.3108256447,-0.4162116386,0.3991074507\C,-0.3703889658,0.672544436,-0.5527437123\O,0.0594348801,0.6432048585,-1.7014284943\O,-0.9738358862,1.7878395504,-0.0386203836\C,1.3762021463,-2.1735146797,1.0675524187\H,-0.7262855798,-0.2430297917,1.3889193901\H,-0.5103712537,-2.4969048148,0.0665201008\H,-0.9666438885,2.4600251489,-0.7446734841\H,1.7567111438,-3.1669982922,0.8047694603\H,0.981363553,-2.2221973793,2.0894798332\H,2.2193874057,-1.4740142969,1.0627975644\H,0.6917486731,-1.7028380324,-0.9531717874\\Version=IA64L-G03RevE.01\State=2-A\HF=-307.0714305\S2=0.756668\S2-1=0.\S2A=0.750028\RMSD=9.066e-09\RMSF=1.891e-06\Thermal=0.\Dipole=-0.105142,-0.3237175,0.6775058\PG=C01 [X(C4H7O2)]\@

• **C(CH₃)₂C(=O)OH (22)**

1\1\GINC-X17\FOpt\UB3LYP\Gen\C4H7O2(2)\CYL509\05-Feb-2009\0\#\B3LYP/gen
6D INT(grid=ultrafine) OPT Freq=noraman maxdisk=1342177280\|r.PCOOH.
nodiff.freq\|0,2\C,0.001270184,0.0039754053,0.\C,1.4945325063,-0.00258
5646,0.\C,-0.6860426374,1.283303058,0.\O,-0.1353483055,2.3816388926,0.
\O,-2.0530317264,1.1822411517,0.\H,-2.3906392338,2.0961282468,0.\H,1.9
009604588,1.0106501205,0.\C,-0.7313695074,-1.2989786774,0.\H,-1.814652
2967,-1.1712014145,0.\H,1.8808550349,-0.5398332631,0.8797706977\H,1.88
08550349,-0.5398332631,-0.8797706977\H,-0.449744756,-1.8993073053,0.87
90086739\H,-0.449744756,-1.8993073053,-0.8790086739\|Version=EM64L-G03
RevE.01\State=2-A\HF=-307.0791308\S2=0.756605\S2-1=0.\S2A=0.750028\RM
SD=8.517e-09\RMSF=2.898e-05\Thermal=0.\Dipole=-0.1022551,-0.9020686,0.
\PG=CS [SG(C4H3O2),X(H4)]\|@

• **CH(CH₃)C(=O)NH₂ (23)**

1\1\GINC-AC12\FOpt\UB3LYP\6-31G(d)\C3H6N1O1(2)\JOH501\06-Feb-2009\0\#\
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=134217728\|am_1\|0,2\H,-0.1279
891283,0.3368605091,0.0973698725\H,0.0308437372,-0.1260264115,1.742606
5868\N,0.4747908246,0.0277519996,0.8481767296\C,1.7814733286,0.4830165
93,0.7898917789\O,2.2346125674,1.0066287003,-0.2307940992\C,2.58592397
97,0.2610371552,1.9887868203\C,4.0083035399,0.6822184464,2.0463057747\
H,4.6719286162,-0.1760089688,2.2309326707\H,4.2956291442,1.1553337897,
1.1044254335\H,4.1854875825,1.3884334803,2.871341353\H,2.1373328081,-0
.2341632935,2.848258079\|Version=IA64L-G03RevE.01\State=2-A\HF=-247.87
1389\S2=0.756499\S2-1=0.\S2A=0.750028\RMSD=9.358e-09\RMSF=4.956e-05\Th
ermal=0.\Dipole=-0.6305433,-0.3060399,1.1795752\PG=C01 [X(C3H6N1O1)]\|@

• **CH(CH₃)C(=O)CH₂CH₃ (24)**

1\1\GINC-AC15\FOpt\UB3LYP\Gen\C5H9O1(2)\CYL509\22-Jul-2008\0\#\B3LYP/G
EN 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|r.penta
none.diff.freq\|0,2\C,-0.6298908874,1.3670134714,0.2280695663\C,0.3424
313554,0.3006579536,0.2266353276\H,-0.2807631021,2.2990198714,0.669193
624\C,-2.022872244,1.316948963,-0.3001158076\H,-2.2895960483,0.3452193
353,-0.7236512886\H,-2.1708530349,2.0807884245,-1.0789232683\H,-2.7481
442457,1.5540039997,0.4933821118\C,-0.0195604505,-1.0628354268,-0.3642
23897\O,1.4706973763,0.506207178,0.7096530553\C,1.1192381657,-2.080062
7594,-0.2876854588\H,-0.3338762149,-0.9188433634,-1.4086891158\H,-0.90
92404335,-1.445055694,0.1580816351\H,2.0023022571,-1.7247833364,-0.828
1196266\H,0.8057783512,-3.0353985528,-0.7239110889\H,1.4227378254,-2.2
549413195,0.7493341925\|Version=IA64L-G03RevC.02\State=2-A\HF=-271.143
6192\S2=0.763587\S2-1=0.\S2A=0.750068\RMSD=9.369e-09\RMSF=2.814e-06\Di
pole=-1.3600809,-0.0257207,-0.5078473\PG=C01 [X(C5H9O1)]\|@

• **CH₂CH=CH₂ (25)**

1\1\GINC-AC9\FOpt\UB3LYP\Gen\C3H5(2)\CYL509\25-Apr-2008\0\#\B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\|r_All.freq
\|0,2\H,-0.6819645175,-0.2799343141,-2.065003995\C,-0.7433109904,-0.17
68375808,-0.9862631131\C,0.3909506536,0.0191948756,-0.2095954224\H,1.3
515075498,0.0659767918,-0.7243714733\H,-1.7311742966,-0.2333280958,-0.
5350582964\C,0.3970214298,0.1598914436,1.1719186915\H,1.3199569653,0.3
109802596,1.7228103394\H,-0.5262922589,0.1228129275,1.7452624892\|Vers
ion=IA64L-G03RevC.02\State=2-A\HF=-117.267918\S2=0.779608\S2-1=0.\S2A=
0.750171\RMSD=8.094e-09\RMSF=2.307e-05\Dipole=0.0234678,0.0010209,-0.0

125914\PG=C01 [X(C3H5)]\@

•CH(CH₃)CH=CH₂ (26)

1\1\GINC-AC30\FOpt\UB3LYP\Gen\C4H7(2)\CYL509\22-Jul-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|r.allme.d
iff.freq\0,2\C,-0.4095100832,0.7602054517,0.2272520412\C,0.2790148956
, -0.2357061258,0.9197710564\C,-0.6623406351,0.8048347903,-1.2482517064
\H,-0.8061676517,1.5915003352,0.8082973217\C,0.8662142164,-1.377987420
7,0.3937104438\H,-1.7408962336,0.8341030394,-1.4623266518\H,-0.2338514
111,1.714649394,-1.6939041248\H,-0.241323196,-0.0549379958,-1.77726080
28\H,0.3627418414,-0.0959653463,1.9982512531\H,1.3785109724,-2.0851125
408,1.0383171128\H,0.8407153165,-1.612317059,-0.6662651177\|Version=IA
64L-G03RevC.02\State=2-A\HF=-156.5871691\S2=0.778021\S2-1=0.\S2A=0.750
163\RMSD=8.045e-09\RMSF=4.926e-06\Dipole=-0.0981107,0.1407222,-0.10306
05\PG=C01 [X(C4H7)]\@

•CH₂C=CCH₃ (27)

1\1\GINC-AC5\FOpt\UB3LYP\Gen\C4H5(2)\CYL509\23-Jul-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=2684354560\|r.butyne.d
iff.freq\0,2\C,-1.7851874254,0.0008716175,1.0800524854\H,-1.783567773
5,0.0005740267,2.1664289371\C,-0.6113891956,0.0034241676,0.368628851\H
, -2.7475142157,0.0013091103,0.5758984142\C,0.4424883107,0.0041648975,-
0.270397613\C,1.6919228233,-0.0042968969,-1.0223599226\H,2.1186076963,
-1.01566234,-1.0732363825\H,2.4439819493,0.6438290566,-0.5533228767\H,
1.541485266,0.3449674325,-2.0513108967\|Version=IA64L-G03RevC.02\State
=2-A\HF=-155.3367699\S2=0.769778\S2-1=0.\S2A=0.750166\RMSD=8.960e-09\R
MSF=1.120e-04\Dipole=0.3347972,-0.0061251,-0.1984121\PG=C01 [X(C4H5)]\@

cyclohexa-1,4-diene-3-yl radical (28)

1\1\GINC-AC2\FOpt\UB3LYP\Gen\C6H7(2)\CYL509\22-Jul-2008\0\#B3LYP/GEN
6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|r.chexadie
ne.diff.freq\0,2\C,1.1245278672,0.0141292024,-0.9286191674\C,0.252462
2686,0.4790729214,1.2956510404\C,-1.2172363892,-0.4915782064,-0.498770
0297\C,-1.1196784425,-0.0137520399,0.9244612209\C,-0.1449161412,-0.466
8009014,-1.3492322502\C,1.2904708068,0.4811804647,0.403266244\H,-1.868
7891831,0.7810549817,1.1081176208\H,2.2660595063,0.8474810651,0.716890
3572\H,1.9616541569,0.0245329839,-1.6200653989\H,0.4015355283,0.840930
6484,2.310723296\H,-2.180166314,-0.8641883728,-0.8414915363\H,-1.43127
76157,-0.8206125124,1.6161546668\H,-0.2627958973,-0.8227074382,-2.3708
713538\|Version=IA64L-G03RevC.02\State=2-A\HF=-232.8035752\S2=0.788257
\S2-1=0.\S2A=0.750824\RMSD=9.338e-09\RMSF=2.995e-05\Dipole=-0.1597101,
-0.0018941,0.1318422\PG=C01 [X(C6H7)]\@

cyclohexayl radical (29)

1\1\GINC-AC29\FOpt\UB3LYP\Gen\C6H11(2)\CYL509\22-Jul-2008\0\#B3LYP/GE
N 6D INT(GRID=ULTRAFINE) OPT FREQ=NORAMAN MAXDISK=1342177280\|r.chexan
e.diff.freq\0,2\C,0.9424814186,0.4764428439,-1.0291762068\C,0.4817416
662,-0.0477573368,1.3944826935\C,-1.0434437996,-0.9549414873,-0.422191
1734\C,-0.9674025773,-0.3709072275,0.997400584\C,-0.4100446553,-0.0013
180253,-1.459503783\C,1.1403350451,0.920867818,0.387195297\H,1.0625451
04,-0.980915682,1.4265155054\H,-0.5087475371,-1.9155249935,-0.44507154
4\H,-1.5724253761,0.5482262868,1.0463667916\H,-1.0907873453,0.86580908
25,-1.5844011426\H,0.6858927228,1.9225999619,0.5318715543\H,1.69127414
95,0.720501268,-1.7796944753\H,0.5156997561,0.3831787264,2.4039527856\H,
-2.0862408675,-1.1644590343,-0.6952580241\H,-1.4079890526,-1.0730025
443,1.7178891442\H,-0.358831334,-0.4836458331,-2.4441779453\H,2.207607
1939,1.0429132509,0.6127628822\|Version=IA64L-G03RevC.02\State=2-A\HF=

-235.2214868\S2=0.754007\S2-1=0.\S2A=0.750012\RMSD=4.720e-09\RMSF=5.38
4e-06\Dipole=-0.0731711,0.0487927,0.0370634\PG=C01 [X(C6H11)]\@

DBN-H (A-H)

1\1\GINC-AC29\FOpt\UB3LYP\6-31G(d)\C8H19N1O1\JOH501\23-Apr-2009\0\#\ U
B3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\dbnh_1\0,1\C,1.61508
4366,0.0190295264,1.4796959282\C,0.0848929319,-0.0086450466,1.33567688
54\C,-0.4329289932,-1.4287073784,1.6596199745\N,-0.3616495652,0.532457
5162,0.0026595841\C,0.1401848796,0.0519638578,-1.3325794146\C,0.024009
314,-1.4675748402,-1.5691842081\O,-1.8045704907,0.3275164317,-0.003232
5603\C,-0.4949286602,0.9762017318,2.376878184\C,1.5938511029,0.5218120
086,-1.550707685\C,-0.7144313792,0.7825450657,-2.395190968\H,2.0323440
032,0.9883733532,1.1910928644\H,1.702863531,1.576125124,-1.2761372254\
H,2.1074002927,-0.7661001013,0.9000557784\H,2.3279841568,-0.0606049538
,-0.9932780165\H,1.8663947893,-0.1550672575,2.5317768477\H,1.843679301
4,0.4200912463,-2.6126205089\H,-0.1448907986,1.9941970342,2.1733347701
\H,-0.6999909497,1.8649475906,-2.2202131852\H,-0.175510191,0.694927761
8,3.3865631465\H,-0.2992685398,0.5955769864,-3.3912691361\H,-1.5874992
144,0.9718310003,2.354198608\H,-1.7503011696,0.4389991336,-2.387441320
3\H,-0.2355800518,-1.6584764048,2.7133855005\H,0.2239465576,-1.6998474
527,-2.6222173963\H,0.0599787867,-2.1974235223,1.0590332881\H,0.743751
3719,-2.0334681275,-0.9694921094\H,-1.5103471422,-1.4938388786,1.49267
61988\H,-0.9841191786,-1.8193116432,-1.3306972535\H,-2.1399160608,1.23
5396238,-0.063245571\Version=IA64L-G03RevE.01\State=1-A\HF=-446.20469
7\S2=0.\S2-1=0.\S2A=0.\RMSD=2.674e-09\RMSF=4.103e-06\Thermal=0.\Dipole
=0.1555515,0.2057923,-0.056473\PG=C01 [X(C8H19N1O1)]\@

TEMPO-H (B-H)

1\1\GINC-AC23\FOpt\UB3LYP\6-31G(d)\C9H19N1O1\JOH501\03-Oct-2006\0\#\ U
B3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\tempoh_2s\0,1\N,-0.0
003220003,-0.0007655112,0.\O,1.4496238328,-0.0016222242,0.\C,-2.541542
982,1.3326452354,0.\H,-3.6381553958,1.2937175504,0.\H,-2.2744583444,2.
396828887,0.\C,-1.9957124197,0.6406551416,-1.2516781843\C,-1.995712419
7,0.6406551416,1.2516781843\C,-0.4513160206,0.5856544738,-1.2946215752
\C,-0.4513160206,0.5856544738,1.2946215752\C,-0.0258787387,-0.40780809
53,-2.3936919975\C,-0.0258787387,-0.4078080953,2.3936919975\C,0.151474
0028,1.9683930461,-1.6342697269\C,0.1514740028,1.9683930461,1.63426972
69\H,-2.350759883,1.1392322372,-2.1624192058\H,-2.350759883,1.13923223
72,2.1624192058\H,-2.3798422229,-0.3879605488,-1.2805655897\H,-2.37984
22229,-0.3879605488,1.2805655897\H,-0.3773105053,-1.4169181284,-2.1517
480324\H,-0.3773105053,-1.4169181284,2.1517480324\H,-0.4541494736,-0.1
138445584,-3.358836355\H,-0.4541494736,-0.1138445584,3.358836355\H,1.0
626210609,-0.4328743251,-2.4999851923\H,1.0626210609,-0.4328743251,2.4
999851923\H,-0.0304576372,2.2000013685,-2.6904203501\H,-0.0304576372,2
.2000013685,2.6904203501\H,-0.2803627658,2.780063278,-1.0439710141\H,-
0.2803627658,2.780063278,1.0439710141\H,1.2320657072,1.9594470418,-1.4
69662847\H,1.2320657072,1.9594470418,1.469662847\H,1.6559626815,-0.949
1357996,0.\Version=IA64L-G03RevD.01\State=1-A\HF=-484.3260143\S2=0.\
S2-1=0.\S2A=0.\RMSD=2.702e-09\RMSF=8.901e-06\Thermal=0.\Dipole=-0.2408
723,-0.1847723,0.\PG=CS [SG(C1H3N1O1),X(C8H16)]\@

4-amino-TEMPO-H (C-H)

1\1\GINC-AC37\FOpt\UB3LYP\6-31G(d)\C9H20N2O1\JOH501\03-Oct-2006\0\#\ U
B3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\ntempoh_1\0,1\N,-0.0
803183,-0.2632346747,0.0042970439\O,1.3393754466,0.0246591165,0.012038
6433\C,-2.8564351655,0.5350290952,0.0001708248\N,-4.2979839635,0.25754
65904,-0.0856471603\H,-2.761405151,1.6280493521,0.0112714593\C,-2.1676
409549,-0.0475605999,1.2447734838\C,-2.1627274778,-0.0144166704,-1.248
088329\C,-0.6441297312,0.2028080237,1.3026880808\C,-0.6399305762,0.23
86943456,-1.2835969217\C,-0.0371617491,-0.704231042,2.3914779458\C,-0.
0253034093,-0.6367085719,-2.3938457673\C,-0.3261346984,1.6716188965,1.
668414882\C,-0.3205932129,1.717113337,-1.606045066\H,-2.3461005226,-1.

1328620043,1.2518718466\H,-2.3373356891,-1.0999966176,-1.2862687371\H,-2.623386243,0.3572277778,2.158766426\H,-2.6218389053,0.4147420608,-2.1456815886\H,-0.1763304716,-1.7588907132,2.129841171\H,-0.1624957008,-1.6985124222,-2.1616486747\H,-0.5224682475,-0.5192258062,3.3565766078\H,-0.5077689283,-0.4269503955,-3.3550869605\H,1.0335442353,-0.511940201,2.5087665135\H,1.0452000887,-0.4380734176,-2.5014245777\H,-0.9009644609,2.3938178173,1.0842523168\H,-0.8982894113,2.4225540636,-1.0044461263\H,-0.5579359334,1.8470752901,2.7255279895\H,-0.550042226,1.9221014268,-2.6581202073\H,0.7371409307,1.8744970679,1.5158058933\H,0.7422095592,1.9161005605,-1.4447607087\H,-4.4459848456,-0.7522638096,-0.049807464\H,-4.7661946136,0.6334944562,0.7391286066\H,1.7313203284,-0.8622223321,-0.0032609416\\Version=IA64L-G03RevD.01\State=1-A\HF=-539.6691055\ S2=0.\S2-1=0.\S2A=0.\RMSD=2.758e-09\RMSF=5.839e-06\Thermal=0.\Dipole=0.0073127,-0.4255866,0.4310105\PG=C01 [X(C9H20N2O1)]\\@

4-hydroxy-TEMPO-H (D-H)

1\1\GINC-AC5\FOpt\UB3LYP\6-31G(d)\C9H19N1O2\JOH501\03-Oct-2006\0\\# UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\\ohtempoh_4s\0,1\N,-0.0000435853,-0.0000797081,0.\O,1.4477774823,0.0000070148,0.\C,-2.5524999887,-1.3273572659,0.\O,-3.9801460843,-1.3508871433,0.\H,-2.2743354801,-2.3861244913,0.\H,-4.2815649075,-0.4275682012,0.\C,-1.9966209414,-0.6403630136,1.2483904497\C,-1.9966209414,-0.6403630136,-1.2483904497\C,-0.4535157642,-0.5862605179,1.2944414639\C,-0.4535157642,-0.5862605179,-1.2944414639\C,-0.030256922,0.4076770597,2.3939906136\C,-0.030256922,0.4076770597,-2.3939906136\C,0.1491913576,-1.9686444135,1.6375414689\C,0.1491913576,-1.9686444135,-1.6375414689\H,-2.3836306162,0.3896687913,1.2676055362\H,-2.3836306162,0.3896687913,-1.2676055362\H,-2.3695992027,-1.1425243465,2.1485466663\H,-2.3695992027,-1.1425243465,-2.1485466663\H,-0.3738771593,1.41823408,2.147327846\H,-0.3738771593,1.41823408,-2.147327846\H,-0.4655993943,0.1185731519,3.3571180434\H,-0.4655993943,0.1185731519,-3.3571180434\H,1.0578719403,0.4262457004,2.5058261555\H,1.0578719403,0.4262457004,-2.5058261555\H,-0.0403976198,-2.2017098103,2.6916814325\H,-0.0403976198,-2.2017098103,-2.6916814325\H,-0.2737275679,-2.7821025183,1.0437042038\H,-0.2737275679,-2.7821025183,-1.0437042038\H,1.2310934456,-1.9549034233,1.4816541927\H,1.2310934456,-1.9549034233,-1.4816541927\H,1.6562994523,0.9471383149,0.\\Version=IA64L-G03RevD.01\State=1-A\HF=-559.5348601\S2=0.\S2-1=0.\S2A=0.\RMSD=1.856e-09\RMSF=4.371e-06\Thermal=0.\Dipole=0.2170245,0.7009944,0.\PG=CS [SG(C1H3N1O2),X(C8H16)]\\@

3-carboxy-TEMPO-H (E-H)

1\1\GINC-AC57\FOpt\UB3LYP\6-31G(d)\C10H19N1O3\JOH501\03-Oct-2006\0\\# UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\\ctempoh_3\0,1\N,-0.0831449408,-0.2664830554,-0.0066349018\O,1.3382948185,0.0104325739,-0.0124731895\C,-2.8328201432,0.5669085617,-0.0010195517\C,-4.3204829253,0.271473324,-0.0160551164\H,-2.7322582073,1.65839622,-0.0314376386\C,-2.1655976224,-0.0279749959,-1.2585705398\C,-2.1630469425,-0.0087839065,1.2486937852\C,-0.6410170282,0.2157196063,-1.3012037637\C,-0.6379803342,0.2308676827,1.2846581968\C,-0.0431758229,-0.6882960841,-2.3979237581\C,-0.036070267,-0.6606230891,2.3887207422\C,-0.3132327615,1.6845973561,-1.6545526472\C,-0.3028417892,1.7028408362,1.6188794474\H,-2.6153233291,0.3895194208,-2.1657544677\H,-2.6083137582,0.4176132111,2.1548882237\H,-2.3498791247,-1.1100496952,-1.2675600349\H,-2.3628551775,-1.0856449933,1.2802261952\H,-0.1952270668,-1.7435282601,-2.1465004898\H,-0.1920545914,-1.7183801552,2.1512060439\H,-0.5236193377,-0.487487863,-3.3621445651\H,-0.5125029375,-0.4477616489,3.3522342971\H,1.0295722323,-0.5064369684,-2.5096543877\H,1.0376220728,-0.4794775493,2.4942707944\H,-0.5336791662,1.8682383915,-2.7125311615\H,-0.5430671577,1.9059917877,2.6690192024\H,-0.8899717981,2.4072694879,-1.0722970032\H,-0.8605605295,2.4207628662,1.01276017\H,0.749243532,1.8806251987,-1.4894319882\H,0.7644631129,1.8879207523,1.4729490972\O,-4.9003756529,-0.5332698261,0.6797253705\O,-4.9677266104,1.0191271827,-0.9491675474\H,-5.9035693762,0.7453717275,-0.9093084951\H,1.72368863,-0.8794880968,-0.0003703186\

\Version=IA64L-G03RevD.01\State=1-A\HF=-672.8921598\S2=0.\S2-1=0.\S2A=0.\RMSD=5.490e-09\RMSF=5.576e-06\Thermal=0.\Dipole=0.1579385,0.1103075,-0.3874744\PG=C01 [X(C10H19N1O3)]\@

3,4-dicarboxy-TEMPO-H (F-H)

1\1\GINC-AC27\FOpt\UB3LYP\6-31G(d)\C11H19N1O5\JOH501\15-May-2009\0\#\UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\sidecctempoh_1\0,1\C,-0.6775220268,1.2838877138,-0.0212014383\N,-1.7710715407,0.3851432767,-0.5077163545\C,-1.858590522,-1.028947956,-0.0532625074\C,-0.5026041057,-1.6805998121,-0.3858609399\C,0.695172738,-0.8900791166,0.1707535709\C,0.6685873572,0.5527389728,-0.3582396964\O,-3.0280344514,1.0215776435,-0.1784589769\C,1.9880142473,-1.582589182,-0.2232660617\O,2.160048343,-2.7416056124,0.4573218372\C,1.8723904119,1.3062142682,0.1912149798\O,2.3284078663,2.2585495072,-0.6549900414\C,-2.9399379602,-1.7034246726,-0.9205060962\C,-2.2349028356,-1.225689432,1.432510388\C,-0.7868683579,2.5640016534,-0.8752446652\C,-0.7763600635,1.6801988503,1.469963169\O,2.7761736637,-1.1968556253,-1.0597994078\O,2.3846266505,1.1029526701,1.2719298439\H,0.66361778,-0.8876963594,1.2643021581\H,-0.4912936489,-2.7017523838,0.0089945187\H,-0.4016190161,-1.74930088,-1.4766769145\H,0.7645766183,0.5255417312,-1.4478310613\H,-2.7476336117,-1.519219203,-1.9830326745\H,-0.7874322837,2.3113350188,-1.9410325883\H,-2.941069644,-2.7859574206,-0.7505204926\H,0.0512234345,3.2374584952,-0.6827452729\H,-3.9337787601,-1.3202768939,-0.6730084203\H,-1.7138737937,3.0932053313,-0.6394167943\H,-2.5031145313,-2.2736645407,1.6091512673\H,-0.1392355662,2.5471875509,1.6728282583\H,-1.4218584623,-0.9765730714,2.1181713033\H,-0.4634271736,0.8874541194,2.1519502792\H,-3.0993489406,-0.6064012919,1.6854511136\H,-1.8075527795,1.9567795083,1.7020309806\H,3.0965329781,2.6657740706,-0.210373873\H,2.9961349888,-3.1249006751,0.1311201968\H,-3.3858720021,1.2417327472,-1.0527505872\Version=IA64L-G03RevE.01\State=1-A\HF=-861.4551018\S2=0.\S2-1=0.\S2A=0.\RMSD=6.931e-09\RMSF=7.459e-06\Thermal=0.\Dipole=-0.4966782,-0.1603982,-0.3225463\PG=C01 [X(C11H19N1O5)]\@

3,5-dicarboxy-TEMPO-H (G-H)

1\1\GINC-AC27\FOpt\UB3LYP\6-31G(d)\C11H19N1O5\JOH501\27-Apr-2009\0\#\UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\oppcctempoh_1s\0,1\C,-1.305005,0.867077,0.01593\N,0.,1.468768,-0.400074\C,1.305005,0.867077,0.01593\C,1.259727,-0.610041,-0.501925\C,0.,-1.349821,-0.035004\C,-1.259727,-0.610041,-0.501925\O,0.,2.838025,0.067814\C,2.490065,-1.396864,-0.080462\O,3.464932,-1.379409,-1.026554\C,-2.490065,-1.396864,-0.080462\O,-3.464932,-1.379409,-1.026554\C,1.616339,0.959702,1.525694\C,2.389727,1.643645,-0.758053\C,-1.616339,0.959702,1.525694\C,-2.389727,1.643645,-0.758053\O,2.621211,-1.996109,0.964542\O,-2.621211,-1.996109,0.964542\H,0.,-1.467585,1.050662\H,0.,-2.365993,-0.446772\H,4.202167,-1.903929,-0.658679\H,-4.202167,-1.903929,-0.658679\H,1.259627,-0.557974,-1.596502\H,-1.259627,-0.557974,-1.596502\H,1.05428,0.243065,2.12626\H,-1.05428,0.243065,2.12626\H,2.678361,0.76411,1.704131\H,-2.678361,0.76411,1.704131\H,1.392919,1.969296,1.878894\H,-1.392919,1.969296,1.878894\H,3.36979,1.176399,-0.63008\H,-3.36979,1.176399,-0.63008\H,2.156568,1.662643,-1.828249\H,-2.156568,1.662643,-1.828249\H,2.451537,2.672197,-0.394023\H,-2.451537,2.672197,-0.394023\H,0.,3.341484,-0.761372\Version=IA64L-G03RevE.01\State=1-A\HF=-861.4510055\S2=0.\S2-1=0.\S2A=0.\RMSD=3.800e-09\RMSF=3.475e-06\Thermal=0.\Dipole=-0.4817351,-1.0754792,0.\PG=CS [SG(C1H3N1O1),X(C10H16O4)]\@

4-carboxy-1-methoxy-2,2,6,6-tetraethylpiperidine (H-H)

1\1\GINC-AC23\FOpt\UB3LYP\6-31G(d)\C14H27N1O3\JOH501\01-Jun-2009\0\#\UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\ctempoethH_1\0,1\C,1.0480393551,0.1413344237,-0.1190646907\N,2.3299519801,0.3901848028,0.5992256609\C,2.4267986096,0.418604418,2.0851032556\C,1.3202419126,1.3707489638,2.5941580082\C,-0.0700342997,1.0474292699,2.0085704537\C,-0.0

052987708,1.0992124079,0.4803867339\O,3.3175939704,-0.5372637757,0.1007908187\H,3.9399380347,0.0428396681,-0.3676461968\C,-1.0901946862,2.0325434387,2.5469836741\O,-1.3989529742,1.772072859,3.8453057816\C,3.8193726262,1.0186832897,2.4421671077\C,4.237599509,2.2938580324,1.7016496342\C,2.309927929,-0.9912902435,2.7441933259\C,2.7008825693,-1.0953751479,4.2268403725\C,1.283028155,0.5100732199,-1.6137955689\C,1.9964613095,1.8363265115,-1.8982688431\C,0.5716854682,-1.3438047803,-0.0451895328\C,-0.5522631343,-1.7559966938,-1.0091255435\O,-1.5779680897,2.9637522725,1.9441118608\H,-0.3808216099,0.0557010805,2.356722794\H,1.290403286,1.3313756028,3.6875559574\H,-0.9848470823,0.8650322219,0.049979676\H,1.5706685787,2.4002222119,2.314192998\H,0.2172725581,2.1301888209,0.1901349305\H,3.830488881,1.220223683,3.5198483229\H,0.3048627973,0.5264508695,-2.1086273344\H,4.5765236046,0.2443809144,2.2699298085\H,1.8477767371,-0.3045293853,-2.0830766864\H,1.2833797751,-1.3559865734,2.6446872309\H,0.2347899956,-1.5679015993,0.9711207326\H,2.9368706807,-1.6739955427,2.1615363549\H,1.4465366555,-1.976297074,-0.2269630933\H,-2.0290105422,2.4668984947,4.1148830188\H,2.0443597679,2.0078990854,-2.9800415203\H,1.4796173915,2.6929956225,-1.4535266856\H,3.0209340154,1.8421816332,-1.5135336388\H,5.2281382626,2.6147473607,2.0448232605\H,4.2890441877,2.141118811,0.619680227\H,3.5470136986,3.1256590372,1.8764998371\H,-0.8575116284,-2.7880004716,-0.8001794726\H,-1.4453173334,-1.128225293,-0.9032462653\H,-0.2401885162,-1.7165985881,-2.0574021167\H,2.4908286696,-2.106900655,4.593378115\H,3.7659556874,-0.9056277855,4.3925811693\H,2.1346490082,-0.4004631038,4.858529068\\Version=IA64L-G03RevE.01\State=1-A\HF=-830.1320533\S2=0.\S2-1=0.\S2A=0.\RMSD=5.864e-09\RMSF=1.907e-05\Thermal=0.\Dipole=0.2712249,-0.1747888,0.2956501\PG=C01 [X(C14H27N1O3)]\\@

PROXYL (I-H)

1\1\GINC-AC57\FOpt\UB3LYP\6-31G(d)\C8H17N1O1\JOH501\03-Oct-2006\0\\# U B3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\\proxylh_1\0,1\N,0.0151425741,-0.0633454312,0.0347180027\C,1.4991536153,-0.0497269663,-0.0128015469\C,1.7256925049,1.4735402232,-0.013773043\C,-0.5077924615,1.0107240442,0.9407752014\C,0.6847291212,2.011296721,0.9899389986\H,1.1070693237,2.0390686842,2.0003016933\H,0.3697595753,3.0317493972,0.7489436929\C,-1.7432588992,1.6220865944,0.2585164466\C,1.9505114701,-0.7255706239,-1.3129027245\C,-0.8963257744,0.5152002914,2.344591435\C,2.1854312991,-0.7329381031,1.1883496471\H,3.0352332501,-0.6393419894,-1.4458780663\H,1.6980995172,-1.7922070657,-1.2970205352\H,1.4543728949,-0.2671443376,-2.1749208714\O,-0.4813475496,-1.3596520593,0.4029907807\H,3.2676606126,-0.7861384548,1.0216404635\H,2.0214798493,-0.1924756286,2.1254839512\H,1.8055751294,-1.7509199472,1.3112839157\H,-2.5145277273,0.8567740989,0.1104546416\H,-2.1765489111,2.4256404708,0.8667208807\H,-1.4800480694,2.030281296,-0.7231486669\H,-1.7176325063,-0.2043921798,2.2948184931\H,-0.0594294563,0.0311070086,2.8557906243\H,-1.2200581451,1.3675114898,2.9538895313\H,1.53314316,1.8705879026,-1.0171418519\H,2.7530414905,1.738140895,0.2574546052\H,-0.9836058875,-1.6232863304,-0.3834756987\\Version=IA64L-G03RevD.01\State=1-A\HF=-445.0116674\S2=0.\S2-1=0.\S2A=0.\RMSD=6.125e-09\RMSF=1.591e-05\Thermal=0.\Dipole=0.0271714,0.1867588,-0.195595\PG=C01 [X(C8H17N1O1)]\\@

3-amino-PROXYL-H (J-H)

1\1\GINC-AC41\FOpt\UB3LYP\6-31G(d)\C8H18N2O1\JOH501\04-Jan-2007\0\\# U B3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\\nproxylh_1\0,1\N,0.0022465965,-0.0212976238,0.4799745191\C,1.4556825081,-0.005741083,0.1098230797\C,1.7918550266,1.5097309509,0.1747663359\C,-0.6264215067,1.2945546923,0.2366585414\C,0.5375576759,2.2034535966,0.7382582552\H,0.5526072877,2.1284201139,1.8328078594\N,0.5121769153,3.6253783906,0.415832856\C,-0.9986635554,1.5664511371,-1.2350720444\C,1.7589829575,-0.6022453517,-1.2760181367\C,-1.8811654343,1.4111123922,1.1090416312\C,2.2090035765,-0.8095699974,1.1832685296\H,2.8312929043,-0.5087375116,-1.4851944465\H,1.491061895,-1.6611875674,-1.3157978549\H,1.212881166,-0.0899600122,-2.0731688597\O,-0.7095968638,-1.0761804119,-0.1865643253\H,3.28

59667907,-0.8337277576,0.9775896138\H,2.0529942444,-0.3719571519,2.174
9927598\H,1.8458937365,-1.8439489311,1.2083605999\H,-1.616438784,0.748
7763589,-1.6158536131\H,-1.5742926109,2.4952121604,-1.3218641378\H,-0.
1225814566,1.6557789776,-1.8854982949\H,-2.6535468757,0.7107142083,0.7
715246662\H,-1.6442067154,1.1847052634,2.1542405378\H,-2.3048596133,2.
421832115,1.0567436123\H,1.9999813285,1.8964103837,-0.8307265975\H,2.6
756806107,1.7206549154,0.7839660672\H,0.4280658721,3.7578441348,-0.591
1355707\H,-0.3009052448,4.0715846646,0.8379665254\H,-1.0091924314,-1.6
277410561,0.5527078915\\Version=IA64L-G03RevD.01\State=1-A\HF=-500.354
5929\S2=0.\S2-1=0.\S2A=0.\RMSD=3.470e-09\RMSF=6.084e-06\Thermal=0.\Dip
ole=-0.3633324,-0.0673963,0.0630833\PG=C01 [X(C8H18N2O1)]\@

3-methoxy-PROXYL-H (K-H)

1\1\GINC-AC35\FOpt\UB3LYP\6-31G(d)\C9H19N1O2\JOH501\04-Jan-2007\0\#\ U
B3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\\meoproxylh_3\\0,1\N,0
.0313048225,0.1150799998,-0.4679674461\C,1.4501568934,0.0016348063,-0.
0572638589\C,1.821443596,1.4991923283,-0.1195485258\C,-0.625969544,1.3
000635213,0.1707139885\C,0.5928662102,2.2169784051,0.4822055313\H,0.74
0996944,2.3099942724,1.5636676896\H,0.4554177126,3.2258379041,0.080308
9137\C,-1.5636746159,1.9239498359,-0.8771044935\C,2.2070766279,-0.8280
129959,-1.0999951535\C,-1.4345639921,0.9708395739,1.4384160265\C,1.680
7097431,-0.5965605241,1.3441439944\H,3.2850106259,-0.784986157,-0.9111
942323\H,1.8938699924,-1.8773114522,-1.0583385312\H,2.0096909157,-0.44
915152,-2.1088636502\O,-0.6864229562,-1.0980903936,-0.2027922328\H,2.7
519440441,-0.7253084689,1.5224586713\H,1.2926245087,0.0409670283,2.142
4346926\H,1.1902080941,-1.5716234123,1.410412681\H,-2.3321169783,1.201
3254395,-1.1761591158\H,-2.0710911507,2.8107276224,-0.478137929\H,-1.0
056877026,2.2146565955,-1.7736093018\H,-2.2677513339,0.30210499,1.2073
880184\H,-0.8216302607,0.4893164652,2.2047270113\H,-1.8417151001,1.897
0795555,1.8609887372\O,3.0394379876,1.7264919239,0.5645959472\H,-0.948
4397662,-1.3865917617,-1.0908584727\C,3.58345906,3.0135639058,0.355255
8009\H,4.5500086636,3.0372721067,0.8657510143\H,3.7403905144,3.2175740
67,-0.7163576581\H,2.9464036876,3.8092666712,0.7699386734\H,1.94036275
7,1.7868696676,-1.1768967899\\Version=IA64L-G03RevD.01\State=1-A\HF=-5
59.5271623\S2=0.\S2-1=0.\S2A=0.\RMSD=4.102e-09\RMSF=1.641e-05\Thermal=
0.\Dipole=-0.0523648,0.4968759,-0.3996695\PG=C01 [X(C9H19N1O2)]\@

3-hydroxy-PROXYL-H (L-H)

1\1\GINC-AC29\FOpt\UB3LYP\6-31G(d)\C8H17N1O2\JOH501\04-Jan-2007\0\#\ U
B3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\\ohproxylh_4\\0,1\N,0.
0384255605,0.1344207496,-0.4540504872\C,1.4579086331,0.0292548754,-0.0
562684503\C,1.8222758944,1.5362318103,-0.1014047532\C,-0.6231939946,1.
3214172395,0.1815344481\C,0.5934574162,2.2287779078,0.519504809\H,0.72
81814005,2.2912242868,1.6072448306\H,0.4715240143,3.2530373014,0.15427
85805\C,-1.5385268362,1.957606603,-0.8782635152\C,2.2223586798,-0.7839
014688,-1.1050421103\C,-1.4538067816,0.985290123,1.4328441301\C,1.6993
236347,-0.5802706305,1.3402601052\H,3.3010489878,-0.7175380492,-0.9260
950125\H,1.93186512,-1.8400273018,-1.0670820575\H,2.0106243738,-0.4037
574186,-2.1101716645\O,-0.6731185511,-1.0822808359,-0.1852535866\H,2.7
733388262,-0.708345619,1.5157839412\H,1.293149161,0.0332253095,2.15193
28705\H,1.2247006645,-1.5631202779,1.401086383\H,-2.3036801045,1.24042
96437,-1.1979503092\H,-2.0491842031,2.843177611,-0.481160437\H,-0.9619
687595,2.2533095291,-1.7610574579\H,-2.2868903007,0.3232461101,1.18369
59763\H,-0.8558960659,0.4920549464,2.2044331576\H,-1.8619387879,1.9098
138623,1.8581823018\O,3.0629606084,1.875274986,0.4936230365\H,-0.93900
13127,-1.3720445441,-1.0718166336\H,2.994143611,1.6883890294,1.4434530
614\H,1.9290191116,1.8320342216,-1.1498611568\\Version=IA64L-G03RevD.0
1\State=1-A\HF=-520.2199912\S2=0.\S2-1=0.\S2A=0.\RMSD=2.579e-09\RMSF=9
.546e-06\Thermal=0.\Dipole=-0.4098225,-0.0925361,0.1145179\PG=C01 [X(C
8H17N1O2)]\@

3-carboxy-PROXYL-H (M-H)

1\1\GINC-AC48\FOpt\UB3LYP\6-31G(d)\C9H17N1O3\JOH501\04-Jan-2007\0\#\ U
B3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\ccproxylh_3\0,1\N,0.0
419630101,0.163191204,-0.4936693836\C,1.4723281479,0.0768649464,-0.102
4672057\C,1.7853391083,1.6066242632,-0.1002647342\C,-0.6515762541,1.29
30940781,0.1999505511\C,0.5323504596,2.2435134166,0.5323915468\H,0.677
5223658,2.3266813237,1.6127750573\H,0.3642694873,3.2552991302,0.150292
4201\C,-1.6281309972,1.9198897891,-0.8093741258\C,2.2258153891,-0.6862
417854,-1.1975752369\C,-1.4255826758,0.8790414904,1.4640199608\C,1.727
7374471,-0.5872226019,1.2660942558\H,3.305940499,-0.6628480465,-1.0238
1426\H,1.9032241074,-1.733334933,-1.2120766793\H,2.0193451012,-0.24800
7692,-2.1797008315\O,-0.6255481275,-1.0866621672,-0.272103491\H,2.7993
574554,-0.7666652894,1.4082230491\H,1.3854438681,0.0253421341,2.103798
1525\H,1.2121859561,-1.5502862438,1.3036353723\H,-2.3730752366,1.18095
26311,-1.1272990657\H,-2.1623662373,2.7697298833,-0.3678069888\H,-1.09
40489907,2.2678829792,-1.700028177\H,-2.2356718197,0.1882072005,1.2168
040364\H,-0.7812320317,0.3911893564,2.1999384903\H,-1.8607177407,1.769
77393,1.9321299938\C,3.062671023,1.9630197803,0.6281403578\O,3.1516950
813,2.355998742,1.7712420507\H,1.8968290693,1.918120937,-1.1439961256\
O,4.1576980785,1.7740342917,-0.1545419804\H,4.9268195896,1.9996636994,
0.402830273\H,-0.8773051327,-1.3534064475,-1.1699472824\Version=IA64L
-G03RevD.01\State=1-A\HF=-633.5779209\S2=0.\S2-1=0.\S2A=0.\RMSD=8.736e
-09\RMSF=3.780e-06\Thermal=0.\Dipole=0.0677963,-0.1090856,-0.670472\PG
=C01 [X(C9H17N1O3)]\@

3,4-dicarboxy-PROXYL-H (N-H)

1\1\GINC-AC25\FOpt\UB3LYP\6-31G(d)\C10H17N1O5\JOH501\27-Apr-2009\0\#\
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\ccproxylh_1_2\0,1\C
, -0.7244672773, -0.5067697897, -0.3887391431\C, 0.6965851767, -0.497824933
8, 0.1958992501\C, 1.2385599434, 0.9651627002, -0.01075072\N, 0.0239266016,
1.6569796531, -0.5444826713\C, -1.2306458962, 0.951016457, -0.1857504442\O
, -0.0194946634, 3.027581992, -0.1296339928\C, 1.7735590644, 1.5381018114, 1
.3125764124\C, 2.3275218595, 1.0824700127, -1.0914672367\C, 1.561386453, -1
.5868257184, -0.4037861174\O, 2.6665346661, -1.8151709493, 0.3482342382\C,
-1.7327166273, 1.214350917, 1.2494101551\C, -2.3121385062, 1.3556982316, -1
.1942857668\C, -1.5922809616, -1.5701348219, 0.2498188856\O, -2.7516468905
, -1.7525911303, -0.428818339\O, -1.322443666, -2.200660071, 1.2494901114\O
, 1.3342130723, -2.1988464197, -1.4249217387\H, -0.6803083711, -0.714221641
3, -1.4621488319\H, 2.6111915304, 0.9220167761, 1.6575509853\H, 2.126199744
9, 2.5633701529, 1.1766711056\H, 1.0099001384, 1.5458461533, 2.0949130094\H
, 3.2647267065, 0.6169325093, -0.7690483189\H, 2.0043793871, 0.6188650192, -
2.0285118554\H, 2.5252818537, 2.1422575274, -1.2864990603\H, -1.8100503919
, 2.2915052005, 1.4174216362\H, -2.7265129969, 0.7744520902, 1.3892310972\H
, -1.0750493587, 0.7925146443, 2.0142774245\H, -2.5570720665, 2.4164387913,
-1.069561492\H, -1.9558821158, 1.2007808348, -2.2178813704\H, -3.225711452
5, 0.7724438102, -1.0485843496\H, 0.6429389115, -0.7030463416, 1.2681095694
\H, 3.1680316883, -2.5148428481, -0.1120864143\H, -3.2415324556, -2.4443235
212, 0.0555650189\H, 0.0155048996, 3.5053059022, -0.9732370368\Version=IA
64L-G03RevE.01\State=1-A\HF=-822.1432531\S2=0.\S2-1=0.\S2A=0.\RMSD=4.5
93e-09\RMSF=3.214e-06\Thermal=0.\Dipole=-0.0273601, 0.4772915, -0.189410
4\PG=C01 [X(C10H17N1O5)]\@

3-carboxy-1-methoxy-2,2,5,5-tetraethylpyrrolidine (O-H)

1\1\GINC-AC28\FOpt\UB3LYP\6-31G(d)\C13H25N1O3\JOH501\01-Jun-2009\0\#\
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\ccproxylethH_1\0,1\C
, -0.7595706152, 0.7542657122, -0.1615098689\C, 0.7625411296, 0.5722170437,
-0.3246312923\C, 1.1337190457, -0.5188420509, 0.7341990431\N, -0.053397844
2, -1.3917061709, 0.5260002345\C, -1.3152459578, -0.6079984992, 0.337190042
6\O, -0.169092037, -2.3729204843, 1.5630665801\H, -0.0304718297, -3.2061719
855, 1.0856739349\C, 2.4134626743, -1.3199333101, 0.3990997319\C, 2.4334018
591, -2.0804462899, -0.9306036156\C, 1.2224116779, 0.0472730932, 2.18568834

6\C,2.5801269579,0.5969701881,2.6538379859\C,1.5212453225,1.8726816492
, -0.1878771961\O,2.7392585787,1.8090508813, -0.789773758\C, -2.179870590
8, -1.3409548659, -0.7213270031\C, -1.5211259465, -1.5950782101, -2.0802897
295\C, -2.1331250912, -0.4536638411, 1.6479689027\C, -3.4006770091, 0.40568
02723, 1.5388365741\O, 1.1381936457, 2.8741597772, 0.3778746863\H, -0.94744
03613, 1.5437801838, 0.5703261704\H, -1.2209269474, 1.0772538516, -1.099539
3381\H, 3.2673288063, -0.6353134758, 0.4270967124\H, 2.566722662, -2.035746
5816, 1.2179044984\H, 0.4768793524, 0.839168087, 2.3090302059\H, 0.93072339
83, -0.7680328488, 2.8556631116\H, -2.487758612, -2.3023986748, -0.28631031
15\H, -3.1023952041, -0.7690607296, -0.8785748217\H, -2.3998693908, -1.4532
430568, 2.0061015117\H, -1.4848413073, -0.0223405325, 2.4171301517\H, 0.991
12193, 0.164309523, -1.3123599543\H, 3.1586329421, 2.6776620348, -0.6388172
459\H, 2.4710280014, 1.0252388583, 3.6568095008\H, 3.3441206056, -0.1843782
645, 2.7150767449\H, 2.9640640028, 1.391019746, 2.0058274247\H, 3.367895967
1, -2.6462849291, -1.0206159705\H, 1.6007499437, -2.7859326746, -1.00722584
27\H, 2.3810197635, -1.4085751339, -1.7942071444\H, -2.2138329575, -2.12268
65382, -2.7461384777\H, -1.2410031018, -0.6605302222, -2.5814734961\H, -0.6
179074388, -2.2025047896, -1.9778316784\H, -3.8489606739, 0.5365758669, 2.5
303720407\H, -3.1886735969, 1.4062643845, 1.1436344517\H, -4.1616537534, -0
.0516999929, 0.8983311576\Version=IA64L-G03RevE.01\State=1-A\HF=-790.8
1982\S2=0.\S2-1=0.\S2A=0.\RMSD=9.115e-09\RMSF=2.232e-06\Thermal=0.\Dip
ole=0.2759603, -0.4717553, -0.3782783\PG=C01 [X(C13H25N1O3)]\@

TMIO-H (P-H)

1\1\GINC-AC40\FOpt\UB3LYP\6-31G(d)\C12H17N1O1\JOH501\06-Jan-2007\0\#\n
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\ctmioh_3s\0,1\N, -0.0
000128892, -0.00005004, 0.\O, -1.4329252708, -0.0003923171, 0.\H, -1.6429797
396, 0.9463900676, 0.\C, 4.1232108531, -2.0004282253, -0.6989841736\C, 4.123
2108531, -2.0004282253, 0.6989841736\H, 5.0027231665, -2.3403804311, -1.239
4910906\H, 5.0027231665, -2.3403804311, 1.2394910906\C, 2.9999323175, -1.56
22768504, -1.4066183303\C, 2.9999323175, -1.5622768504, 1.4066183303\H, 3.0
062888385, -1.5607630559, -2.4939625442\H, 3.0062888385, -1.5607630559, 2.4
939625442\C, 1.8806538845, -1.1290356323, -0.6991811767\C, 1.8806538845, -1
.1290356323, 0.6991811767\C, 0.5492974939, -0.6380983324, -1.2365056043\C,
0.5492974939, -0.6380983324, 1.2365056043\C, 0.6894615418, 0.4518791827, -2
.3117688045\C, 0.6894615418, 0.4518791827, 2.3117688045\C, -0.2993227751, -
1.8035988059, -1.790675969\C, -0.2993227751, -1.8035988059, 1.790675969\H,
1.3079760589, 1.275596246, -1.9437739279\H, 1.3079760589, 1.275596246, 1.94
37739279\H, 1.1406235023, 0.0534729055, -3.2279262965\H, 1.1406235023, 0.05
34729055, 3.2279262965\H, -0.2993879258, 0.8477069048, -2.5713165347\H, -0.
2993879258, 0.8477069048, 2.5713165347\H, 0.1670329915, -2.1991322744, -2.7
000957658\H, 0.1670329915, -2.1991322744, 2.7000957658\H, -0.3844642467, -2
.6249402685, -1.0747357021\H, -0.3844642467, -2.6249402685, 1.0747357021\H
, -1.3063367493, -1.4567302171, -2.0374720001\H, -1.3063367493, -1.45673021
71, -2.0374720001\Version=IA64L-G03RevD.01\State=1-A'\HF=-597.4401638\S
2=0.\S2-1=0.\S2A=0.\RMSD=3.927e-09\RMSF=5.126e-06\Thermal=0.\Dipole=0.
0993048, 0.1771814, 0.\PG=CS [SG(H1N1O1),X(C12H16)]\@

5-carboxy-TMIO-H (Q-H)

1\1\GINC-AC36\FOpt\UB3LYP\6-31G(d)\C13H17N1O3\JOH501\06-Jan-2007\0\#\n
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\ctmioh_3\0,1\O, 0.00
4407574, 0.027633583, -0.0584209808\N, 1.4318899246, -0.0174069011, 0.03881
71264\C, 2.0264588463, 1.3543313362, 0.00762718\C, 2.0282650093, -0.8990854
966, -1.012836078\C, 3.3922707351, 1.0258595095, -0.5626401313\C, 3.3931174
274, -0.2494220095, -1.140923753\C, 4.5418830096, 1.8137905317, -0.57984740
25\C, 4.541040801, -0.7493292322, -1.7404099607\H, 4.5470107694, 2.80225743
89, -0.1280702669\H, 4.5745027524, -1.7357198244, -2.1926687223\C, 5.697921
7957, 1.3189380484, -1.1836835082\C, 5.701165076, 0.0406738326, -1.76343678
45\H, 6.6020151685, 1.916989246, -1.2059545175\C, 6.9098398499, -0.52760438
3, -2.4125028002\O, 6.9740541037, -1.6263613946, -2.928884737\O, 7.97931017
83, 0.3114006393, -2.3817103669\H, 8.6985845163, -0.1687158747, -2.83184745
18\C, 1.2734977584, -0.8952346247, -2.3602566693\C, 2.0865081434, -2.331956
9539, -0.4592624229\C, 1.2748332862, 2.364530452, -0.8885958164\C, 2.078042

8489,1.8859854092,1.4494274879\H,0.2401420412,2.4680301403,-0.55154393
19\H,1.059603837,1.990174959,1.8410176973\H,1.2658645239,2.0573168161,
-1.9373871458\H,2.6290003836,1.1953441855,2.0942615887\H,1.7627277882,
3.3437160569,-0.8296022507\H,2.5559284609,2.8713344602,1.4955311843\H,
0.2429668879,-1.2305376373,-2.2167901477\H,1.0706837725,-2.703234147,-
0.28046538\H,1.7692138762,-1.5751919295,-3.0618152157\H,2.5714788738,-
3.0131984455,-1.1676193104\H,1.2508639807,0.0979262089,-2.8158889805\H
,2.6364710499,-2.3561692432,0.4859410025\H,-0.2772350498,-0.3638347568
,0.7831414657\Version=IA64L-G03RevD.01\State=1-A\HF=-786.0141065\S2=0
.\S2-1=0.\S2A=0.\RMSD=4.973e-09\RMSF=2.665e-05\Thermal=0.\Dipole=-0.24
74292,0.5361145,0.5482475\PG=C01 [X(C13H17N1O3)]\@

5,6-dicarboxy-TMIO-H (R-H)

1\1\GINC-AC27\FOpt\UB3LYP\6-31G(d)\C14H17N1O5\JOH501\27-Apr-2009\0\#\n
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\23cctmioh_2_2\0,1\C
,1.6730233489,0.6942055011,-0.0715413154\C,0.4562711364,1.3918893441,-
0.0833173177\C,-0.7430148463,0.6885042124,-0.0949781583\C,-0.742900101
5,-0.7083751778,-0.1124771439\C,0.4570034667,-1.4122081317,-0.09877862
75\C,1.6702416228,-0.7171080467,-0.0560312032\C,-2.1604640532,1.227276
4083,-0.0871001478\N,-2.8959045353,-0.0049830671,-0.5112622982\C,-2.15
93876905,-1.247887759,-0.1203574717\O,-4.2372901371,-0.0119182544,-0.0
137770002\C,-2.5470896155,-1.8205617408,1.261041704\C,-2.3997718178,-2
.3092104071,-1.2061067196\C,-2.5471152046,1.7610223405,1.3099019603\C,
-2.4053686374,2.3174358865,-1.1427878351\C,2.9068358953,-1.5578347643,
0.0463156562\O,3.726776278,-1.1567763782,1.0436546305\C,2.9495272324,1
.4493499101,-0.224562407\O,2.8609945069,2.7216708631,0.2439848602\O,3.
1102295647,-2.551438886,-0.6172359593\O,3.958517077,1.0230935531,-0.74
5148999\H,-3.6123458281,-2.0645017502,1.2806093164\H,-3.4633799645,-2.
5719294444,-1.2360002055\H,-2.3412063674,-1.1166197933,2.07134253\H,-2
.1084058308,-1.9267877527,-2.1884375962\H,-1.9752723861,-2.7345976419,
1.4558356838\H,-1.8344020389,-3.2254593068,-1.0018556923\H,-3.61239694
85,2.0040924323,1.338243655\H,-3.4699703107,2.5766783603,-1.1654909791
\H,-1.9747150853,2.6689690661,1.5301222639\H,-1.8443462448,3.230372133
6,-0.9124336648\H,-2.3394340699,1.0343960321,2.0993390702\H,-2.1130357
219,1.9636366555,-2.1356199483\H,0.470747431,2.4762157404,-0.105813481
3\H,4.5041431202,-1.7453668336,1.0050550422\H,3.7222389467,3.133435926
2,0.0435628012\H,0.4783516764,-2.497641455,-0.1102677886\H,-4.76528586
73,-0.0046797746,-0.8274902142\Version=IA64L-G03RevE.01\State=1-A\HF=
-974.5732909\S2=0.\S2-1=0.\S2A=0.\RMSD=9.118e-09\RMSF=6.726e-06\Therma
l=0.\Dipole=-0.9294696,0.7143922,0.3563956\PG=C01 [X(C14H17N1O5)]\@

TMAO-H (S-H)

1\1\GINC-AC52\FOpt\UB3LYP\6-31G(d)\C16H19N1O1\JOH501\06-Jan-2007\0\#\n
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\sbh_2s\0,1\N,0.0000
069383,0.000120372,0.\O,1.4466110793,-0.000304981,0.\C,-2.6542292708,-
0.8031009913,0.\C,-4.0813800185,-0.983566756,0.\H,1.6534236567,0.94724
71278,0.\C,-4.774847435,-1.07969035,1.2334714711\C,-4.774847435,-1.079
69035,-1.2334714711\H,-5.853811601,-1.2133624066,1.2182573266\H,-5.853
811601,-1.2133624066,-1.2182573266\C,-4.089895183,-1.0151622647,2.4222
597235\C,-4.089895183,-1.0151622647,-2.4222597235\H,-4.6186359658,-1.0
96672555,3.3681844457\H,-4.6186359658,-1.096672555,-3.3681844457\C,-2.
6887972057,-0.8406168446,2.4239902823\C,-2.6887972057,-0.8406168446,-2
.4239902823\H,-2.1769586255,-0.8005158828,3.3798724016\H,-2.1769586255
, -0.8005158828,-3.3798724016\C,-1.9667477632,-0.724791108,1.2503058105
\C,-1.9667477632,-0.724791108,-1.2503058105\C,-0.4452780644,-0.5802713
566,1.2950226755\C,-0.4452780644,-0.5802713566,-1.2950226755\C,-0.0244
176557,0.4563684496,2.3625551167\C,-0.0244176557,0.4563684496,-2.36255
51167\C,0.1977070703,-1.9469910377,1.6504984577\C,0.1977070703,-1.9469
910377,-1.6504984577\H,-0.4895487423,1.424943018,2.1551379329\H,-0.489
5487423,1.424943018,-2.1551379329\H,-0.3093554089,0.1398850488,3.36924
86431\H,-0.3093554089,0.1398850488,-3.3692486431\H,1.0624180414,0.5733
203626,2.3512132297\H,1.0624180414,0.5733203626,-2.3512132297\H,-0.196
0718803,-2.7597413217,1.0364398119\H,-0.1960718803,-2.7597413217,-1.03

64398119\H,-0.0169801786,-2.1943253456,2.6956339411\H,-0.0169801786,-2.1943253456,-2.6956339411\H,1.2822894051,-1.8975137913,1.5220607633\H,1.2822894051,-1.8975137913,-1.5220607633\\Version=IA64L-G03RevD.01\State=1-A'\HF=-751.0760599\S2=0.\S2-1=0.\S2A=0.\RMSD=9.713e-09\RMSF=4.659e-06\Thermal=0.\Dipole=-0.0169425,0.1756819,0.\PG=CS [SG(C2H1N1O1),X(C14H18)]\\@

2,2-dimethyl-1-methoxy-indoline (T-H)

1\1\GINC-AC25\FOpt\UB3LYP\6-31G(d)\C10H13N1O1\JOH501\09-Jul-2009\0\\#UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\\dminoh_2\\0,1\C,-2.2740755099,1.8645092649,-0.5960399545\C,-0.990162854,1.474738283,-0.2410297863\C,0.0963976224,2.3152518529,-0.5163513967\C,-0.0640993585,3.5360401994,-1.1638879805\C,-1.3625489152,3.9140904247,-1.5247448521\C,-2.4591677589,3.0948207558,-1.2434906844\C,-0.4656818599,0.2398749837,0.4581643954\C,1.0538619664,0.265954334,0.1115739434\N,1.2795293344,1.7485375956,0.0051656041\O,2.4394706427,2.0801851238,-0.7632715606\C,1.3148096121,-0.4387736284,-1.2305388885\C,1.9437487655,-0.3061869559,1.2146283619\H,0.7946226743,4.1575714241,-1.394073166\H,-1.5161182447,4.8596892061,-2.0384696968\H,-3.4579099446,3.407122608,-1.5353568094\H,-3.1248864063,1.2188287869,-0.3902486383\H,-0.6033242413,0.3199127025,1.5458908983\H,-0.9423571431,-0.6914641547,0.133791667\H,1.1197794941,-1.5126407168,-1.1318567726\H,2.3518482458,-0.3010403851,-1.5462529155\H,0.6624509496,-0.0419739246,-2.0154606978\H,1.7504523563,-1.3755948001,1.3564504066\H,3.0017153511,-0.1901631129,0.9522515016\H,1.7650581267,0.2090116807,2.1643053458\H,3.0209900953,2.4894004521,-0.1026323241\\Version=IA64L-G03RevE.01\State=1-A'\HF=-518.8171576\S2=0.\S2-1=0.\S2A=0.\RMSD=5.091e-09\RMSF=1.894e-05\Thermal=0.\Dipole=0.2546263,-0.2657784,0.3873461\PG=C01 [X(C10H13N1O1)]\\@

2,2-diphenyl-1-methoxy-indoline (U-H)

1\1\GINC-AC28\FOpt\UB3LYP\6-31G(d)\C20H17N1O1\JOH501\13-Jul-2009\0\\#UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\\dpinoh_1\\0,1\C,-3.1515260044,-0.4230975235,1.2628568603\C,-1.7678610381,-0.5282456807,1.0870181141\C,-1.0115785876,-1.1888593822,2.0670454331\C,-1.6228364373,-1.7247286376,3.1993146913\C,-3.0054095599,-1.6171377875,3.3666457226\C,-3.7649109185,-0.9676072113,2.3940725694\C,-1.0540640437,0.1079857483,-0.1057766961\N,-2.0401693498,0.7170396456,-1.0701030966\C,-1.4288928809,1.8304102979,-1.6803998448\C,-0.387743958,2.3051293648,-0.873171082\C,-0.283179624,1.4007318947,0.33416535\C,0.3120862433,3.4435995056,-1.2453385958\C,-0.027771765,4.0907189399,-2.4438014123\C,-1.0600896117,3.5956706683,-3.2436889765\C,-1.781788118,2.4540332436,-2.8724193402\C,-0.1637892254,-0.9101174373,-0.8461817455\C,-0.6504953468,-2.2096010936,-1.0758580936\C,0.0931201876,-3.1415398025,-1.8005320536\C,1.344023608,-2.7958822432,-2.3138704353\C,1.8371785037,-1.5088694155,-2.1021695697\C,1.0896276643,-0.5745937039,-1.3819703726\O,-2.6851467347,-0.1739828903,-1.947325678\H,-2.5872038679,2.0620486579,-3.4842511068\H,-1.3102211634,4.1018868745,-4.1724076059\H,0.5189640496,4.9773415214,-2.7518976196\H,1.1223616438,3.8233087383,-0.6270520117\H,0.0634195635,-1.2901916388,1.9396227423\H,-1.0191026401,-2.2295687401,3.9491199634\H,-3.4846058348,-2.0386437708,4.2463661824\H,-4.8421770935,-0.8818232981,2.5114744204\H,-3.7430353767,0.0863282768,0.5108740068\H,1.494370109,0.422311307,-1.2492240451\H,2.808233175,-1.2241103816,-2.498622733\H,1.9279121051,-3.5222062445,-2.872819007\H,-0.3056912157,-4.1402664428,-1.9577072997\H,-1.6154568995,-2.4937007968,-0.6685148231\H,-1.9810492232,-0.5819433528,-2.4967682581\H,-0.8077234656,1.8404777571,1.1909236213\H,0.7385061318,1.1826880334,0.6581048253\\Version=IA64L-G03RevE.01\State=1-A'\HF=-902.2797768\S2=0.\S2-1=0.\S2A=0.\RMSD=8.948e-09\RMSF=7.628e-06\Thermal=0.\Dipole=0.8253559,-0.3203178,-0.0682162\PG=C01 [X(C20H17N1O1)]\\@

SG1-H (V-H)

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1\1\GINC-AC24\FOpt\UB3LYP\6-31G(d)\C13H30N1O4P1\JOH501\27-Feb-2008\0\
# UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\sglhp1\0,1\N,
-0.1477312063,0.0685781021,0.3025707504\O,1.2926869687,0.2061994615,0.
3502441651\C,-0.7635268519,1.3994292245,0.6114491088\C,-0.5054519252,-
1.126056882,1.0863005096\P,0.7347491952,-1.588360204,2.4254576556\O,1.
305759822,-0.2663527723,3.1691016836\O,-0.3489939307,-2.0835322652,3.5
353493693\C,-0.8030496924,-2.3474516379,0.1247069112\C,2.6887673058,0.
143125929,3.0337634006\C,3.1367595616,0.7410463765,4.3560279573\C,0.13
18773488,-2.6962943145,4.7533372132\C,-1.0730580181,-3.1236749394,5.57
14009093\O,1.7943027844,-2.5758704205,2.0715779418\C,-2.2912206942,1.2
776046664,0.4580155159\C,-0.4348273769,1.9587028286,2.008147183\C,-0.2
503321255,2.3731504337,-0.4667818312\H,-1.4263226506,-0.9217606008,1.6
408965294\C,-1.1340358032,-3.6254105024,0.9253136463\C,-2.0336991525,-
1.9948231013,-0.7339026343\C,0.3858414367,-2.62793165,-0.8163564294\H,
3.2917818363,-0.726218283,2.75828545\H,2.7416491322,0.8730801787,2.221
4935114\H,4.1699242197,1.0981041626,4.272048473\H,2.5020812186,1.58768
96896,4.6380257056\H,3.0942793774,-0.0035108084,5.1580028084\H,0.76597
51112,-3.5512066624,4.4947973203\H,0.7413858272,-1.9657573297,5.298226
3733\H,-0.7446641814,-3.5905632667,6.5068887483\H,-1.7013442707,-2.261
3061633,5.816603158\H,-1.6797120158,-3.8475875865,5.0179420008\H,-0.91
45666344,2.9370244146,2.1311470801\H,-0.7945836766,1.3044890615,2.8072
838786\H,0.6414369489,2.0894671443,2.1375141427\H,-2.7378485572,2.2695
070939,0.5845263175\H,-2.5662807153,0.9042978682,-0.5321971402\H,-2.74
21876989,0.6239040006,1.2115452118\H,-0.7440465821,3.3449329498,-0.358
5794928\H,0.8278581245,2.5269364373,-0.3794021979\H,-0.467542589,1.986
309522,-1.4686886449\H,-2.2573773823,-2.8212077278,-1.4190671297\H,-2.
9242991993,-1.8266418948,-0.1155733065\H,-1.8531407977,-1.0983428359,-
1.3328619334\H,-1.4738872874,-4.4058298152,0.2340791527\H,-0.261592096
1,-4.010850194,1.4586274563\H,-1.9348316375,-3.4499674622,1.6525247969
\H,0.1564617653,-3.4911289304,-1.4527885976\H,0.5637167866,-1.77756288
72,-1.4861545169\H,1.2969120637,-2.8486531253,-0.2545253839\H,1.570877
9144,-0.1013852821,-0.5275127975\Version=IA64L-G03RevE.01\State=1-A\H
F=-1210.4589209\S2=0.\S2-1=0.\S2A=0.\RMSD=6.798e-09\RMSF=5.519e-06\Th
ermal=0.\Dipole=-0.3669182,0.6912109,0.1358294\PG=C01 [X(C13H30N1O4P1)]
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DBN-CH₃ (A1)

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1\1\GINC-AC56\FOpt\UB3LYP\6-31G(d)\C9H21N1O1\JOH501\15-Oct-2006\0\# U
B3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\medbn_6\0,1\N,-0.083
9556638,-0.0092172279,-0.3248034649\O,1.3171701502,0.0852808514,0.0544
86268\C,-0.6302772168,1.37995979,-0.0819545596\C,-0.6527350796,-1.2364
412767,0.3507137889\C,-1.9688606692,-1.638901296,-0.3521581604\C,0.328
2056189,-2.4040542338,0.1055233951\C,-0.8699376946,-1.1168895198,1.873
8184322\C,-2.1530212693,1.4356590836,-0.2938680248\C,-0.2868518216,1.9
808618511,1.3023369437\C,0.0089061699,2.2845907152,-1.1604975017\H,-0.
1057340285,-3.3226086493,0.5144742652\H,0.4914546195,-2.5623130697,-0.
9654200973\H,1.290989924,-2.2372879104,0.5916729906\H,-1.1394478466,-2.
0957121957,2.2884309754\H,0.044921107,-0.7809701672,2.3712943847\H,-1.
6795848883,-0.4260132649,2.1260138209\H,-2.2257269828,-2.6655834219,-
0.0678678012\H,-2.8187722326,-1.0116875178,-0.0839738424\H,-1.84253991
87,-1.607705172,-1.4391446741\H,-0.4370979504,3.2847566587,-1.11945447
41\H,1.0843945638,2.396731411,-1.002375421\H,-0.1601371595,1.872133307
3,-2.1605987202\H,-0.5084333341,3.054690614,1.2954600776\H,-0.86723690
14,1.5343713512,2.1125601199\H,0.7752837138,1.8547533496,1.5225441733\
H,-2.4607513471,2.4871663807,-0.3005965707\H,-2.4462673668,0.995178269
6,-1.2515893261\H,-2.7111783636,0.9459974265,0.5081285178\C,2.16633212
46,-0.1360076482,-1.0646745324\H,3.1779295567,0.0700073009,-0.69789357
15\H,2.1195172808,-1.1694208139,-1.4253033738\H,1.935252906,0.53895502
43,-1.8946940373\Version=IA64L-G03RevD.01\State=1-A\HF=-485.5095526\S
2=0.\S2-1=0.\S2A=0.\RMSD=4.118e-09\RMSF=3.081e-06\Thermal=0.\Dipole=-0
.1084762,-0.04633,-0.1207215\PG=C01 [X(C9H21N1O1)]\@
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TEMPO-CH₃ (B1)

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1\1\GINC-AC46\FOpt\UB3LYP\6-31G(d)\C10H21N1O1\JOH501\27-Apr-2006\0\#\n
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\\mectempo_1sc_2\\0,1\N,0.0002988286,0.0002439874,0.\O,1.2737059142,0.6883183539,0.\C,2.3506
876745,-0.2411398131,0.\C,-2.8852271085,-0.0017544587,0.\H,-3.83338298
96,-0.5541032208,0.\H,-3.1525735473,1.0627004942,0.\H,3.2570855991,0.3
738897387,0.\H,2.3451131472,-0.8780068873,-0.8913880676\H,2.3451131472
,-0.8780068873,0.8913880676\C,-0.8020811717,1.8269541872,-1.6192712668
\C,-0.8020811717,1.8269541872,1.6192712668\C,-0.6850577871,0.319741142
9,-1.2916421285\C,-0.6850577871,0.3197411429,1.2916421285\C,0.12994426
37,-0.3436453112,-2.4192770086\C,0.1299442637,-0.3436453112,2.41927700
86\C,-2.075688509,-0.3545016231,-1.24880994\C,-2.075688509,-0.35450162
31,1.24880994\H,-1.9330723624,-1.443302447,-1.2797272846\H,-1.93307236
24,-1.443302447,1.2797272846\H,-2.6196523776,-0.0788674,-2.1611714295\
H,-2.6196523776,-0.0788674,2.1611714295\H,-0.4243351909,-0.2839997465,
-3.3631944188\H,-0.4243351909,-0.2839997465,3.3631944188\H,0.313614339
6,-1.3990122926,-2.1929785899\H,0.3136143396,-1.3990122926,2.192978589
9\H,1.0911307072,0.1578999551,-2.5653486667\H,1.0911307072,0.157899955
1,2.5653486667\H,-1.0670442347,1.9535642908,-2.6756148675\H,-1.0670442
347,1.9535642908,2.6756148675\H,-1.5667249108,2.3373165777,-1.0297144256\
H,-1.5667249108,2.3373165777,1.0297144256\H,0.1558469011,2.32426701
31,-1.4474030607\H,0.1558469011,2.3242670131,1.4474030607\\Version=IA6
4L-G03RevD.01\State=1-A'\HF=-523.6320317\S2=0.\S2-1=0.\S2A=0.\RMSD=7.8
56e-09\RMSF=4.716e-06\Thermal=0.\Dipole=-0.127016,-0.1853998,0.\PG=CS
[SG(C2H3N1O1),X(C8H18)]\\@
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4-amino-TEMPO-CH₃ (C1)

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1\1\GINC-AC31\FOpt\UB3LYP\6-31G(d)\C10H22N2O1\JOH501\26-Apr-2006\0\#\n
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\\mentempo_1\\0,1\N,-0
.0882266789,-0.3080656736,0.0422564771\O,1.3312971369,-0.0283277328,0.
0615882518\C,-2.8621883289,0.54189856,-0.000475032\N,-4.3056634453,0.2
791117017,-0.0995236531\H,-2.7552318193,1.6338389841,-0.0003663126\C,-
2.1917196187,-0.0334575666,1.2556804999\C,-2.1602952953,-0.0286466232,
-1.2328629309\C,-0.6650440075,0.1991182811,1.3257017627\C,-0.633447572
1,0.2046327607,-1.2540352183\C,-0.0995302537,-0.6766141935,2.461425736
6\C,-0.0371479558,-0.6658424706,-2.3781067248\C,-0.3350114131,1.673037
1306,1.6622386427\C,-0.2944494864,1.679798446,-1.5748040033\H,-2.38290
31771,-1.1163620762,1.2765338007\H,-2.3475067785,-1.1122900731,-1.2636
247212\H,-2.6494226362,0.3894219825,2.1605507154\H,-2.6019721265,0.397
7091764,-2.1405616846\H,-0.2366824123,-1.7389230666,2.2350023758\H,-0.
1792880859,-1.729269821,-2.1600302007\H,-0.6206129655,-0.4528646923,3.
3995364989\H,-0.5347156631,-0.4385282113,-3.3278312096\H,0.9658208127,
-0.4838211182,2.618461949\H,1.031602869,-0.4713269932,-2.5067342866\H,
-0.8974534399,2.3903925445,1.0610187523\H,-0.8774723397,2.3943135324,-
0.9899683447\H,-0.5739868531,1.8709354073,2.7137718765\H,-0.5019364567
,1.880687457,-2.6321938041\H,0.7315779869,1.8602278815,1.5147805769\H,
0.7667890907,1.8681525871,-1.3938340418\H,-4.4650719382,-0.7288002712,
-0.0575501962\H,-4.7787405805,0.6665363419,0.7171396252\C,2.0836676165
,-1.2356619048,0.0675026786\H,3.1317093448,-0.9177043446,0.082579223\H
,1.8770894804,-1.8449390451,0.9542801889\H,1.9008069905,-1.8388068969,
-0.8285072674\\Version=IA64L-G03RevD.01\State=1-A'\HF=-578.9751527\S2=0
.\S2-1=0.\S2A=0.\RMSD=2.269e-09\RMSF=8.217e-06\Thermal=0.\Dipole=0.026
6285,-0.3348963,0.436248\PG=C01 [X(C10H22N2O1)]\\@
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4-hydroxy-TEMPO-CH₃ (D1)

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1\1\GINC-AC48\FOpt\UB3LYP\6-31G(d)\C10H21N1O2\JOH501\27-Apr-2006\0\#\n
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\\meohtempo_1s\\0,1\N,
0.0002769133,-0.0008074844,0.\O,-1.2739435205,-0.684830841,0.\C,-2.349
2331909,0.2470608004,0.\C,2.8903820097,-0.0011405906,0.\O,4.1639237054
,0.6446594491,0.\H,3.9991799845,1.6019071979,0.\H,3.1386097688,-1.0674
276472,0.\H,-3.2563457869,-0.3666567792,0.\H,-2.3422562699,0.883503699
```

7,0.8915958698\H,-2.3422562699,0.8835036997,-0.8915958698\C,2.0771344078,0.3468777489,1.246175224\C,2.0771344078,0.3468777489,-1.246175224\C,0.6856531848,-0.3230568236,1.2915932697\C,0.6856531848,-0.3230568236,-1.2915932697\C,0.7986911535,-1.8305136108,1.6211784331\C,0.7986911535,-1.8305136108,-1.6211784331\C,-0.1264390479,0.3420279842,2.4203767553\C,-0.1264390479,0.3420279842,-2.4203767553\H,-0.1649421219,-2.3213774177,1.4629752606\H,-0.1649421219,-2.3213774177,-1.4629752606\H,1.0762679386,-1.9556007701,2.6742544026\H,1.0762679386,-1.9556007701,-2.6742544026\H,1.5519415706,-2.3489099894,1.0245655747\H,1.5519415706,-2.3489099894,-1.0245655747\H,-0.3072962538,1.398135377,2.1958102673\H,-0.3072962538,1.398135377,-2.1958102673\H,0.4271967909,0.2789622011,3.3641780017\H,0.4271967909,0.2789622011,-3.3641780017\H,-1.0887206028,-0.1580808608,2.5639286451\H,-1.0887206028,-0.1580808608,-2.5639286451\H,2.6383529715,0.0735317078,2.147272581\H,2.6383529715,0.0735317078,-2.147272581\H,1.9401763369,1.4386687012,1.2684436573\H,1.9401763369,1.4386687012,-1.2684436573\\Version=IA64L-G03RevD.01\State=1-A'\HF=-598.8408598\S2=0.\S2-1=0.\S2A=0.\RMSD=9.050e-09\RMSF=5.649e-06\Thermal=0.\Dipole=-0.5263791,0.4274046,0.\PG=CS [SG(C2H3N1O2),X(C8H18)]\\@

3-carboxy-TEMPO-CH₃ (E1)

1\1\GINC-AC40\FOpt\UB3LYP\6-31G(d)\C11H21N1O3\JOH501\27-Apr-2006\0\\#UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\\mesidectempo_1\\0,1\N,-0.0908038312,-0.3031589889,-0.0436352553\O,1.3294006037,-0.0284565513,-0.0574219055\C,-2.843003274,0.5103866504,0.0009865991\H,-3.9084578582,0.249282467,0.0045404352\H,-2.7991081402,1.602801824,0.0501943682\C,-2.1816747066,-0.0234659492,-1.2668037294\C,-2.164416038,-0.0926142083,1.2398688945\C,-0.6611784039,0.2334943254,-1.319866987\C,-0.6209660703,0.1897214976,1.2725021537\C,-0.0768082589,-0.6060675998,-2.4725729273\C,0.0202886774,-0.6900721678,2.3645733171\C,-0.3496118265,1.7191658687,-1.6132104252\C,-0.2935869035,1.6650779421,1.5966980591\H,-2.6416395303,0.4249232868,-2.1560503974\C,-2.8595311401,0.4108479053,2.4932693812\H,-2.3537577651,-1.106244651,-1.330991757\H,-2.279920173,-1.1820434531,1.2110079017\H,-0.2014656028,-1.6758345808,-2.2755395616\H,-0.1177254945,-1.752215607,2.1387342153\H,-0.5979042593,-0.3650650697,-3.4063676922\H,-0.4343752595,-0.4865526308,3.3382042332\H,0.9861537398,-0.3952388593,-2.6205188626\H,1.090122826,-0.4812928104,2.4446623619\H,-0.5776583959,1.9391463157,-2.6627519412\H,-0.4214145104,1.8532130728,2.6673629058\H,-0.9329737169,2.4117359681,-1.0029076191\H,-0.9331051393,2.3761697652,1.0727305171\H,0.7115394458,1.9223951475,-1.4479356052\H,0.7482638354,1.8670180506,1.3375587824\O,-3.2554657215,1.5423205518,2.6757757317\O,-3.0258166029,-0.564695897,3.4246261254\H,-3.4776093854,-0.138101293,4.1782196846\C,2.0809648892,-1.236694729,-0.0966910173\H,3.1281489182,-0.9169991175,-0.1214910595\H,1.9116417984,-1.855835508,0.7907013331\H,1.8605632742,-1.8281609674,-0.9914302571\\Version=IA64L-G03RevD.01\State=1-A'\HF=-712.1948372\S2=0.\S2-1=0.\S2A=0.\RMSD=7.584e-09\RMSF=9.767e-06\Thermal=0.\Dipole=0.0875496,-0.6119207,-0.0899902\PG=C01 [X(C11H21N1O3)]\\@

3,4-dicarboxy-TEMPO-CH₃ (F1)

1\1\GINC-AC21\FOpt\UB3LYP\6-31G(d)\C12H21N1O5\JOH501\27-Apr-2006\0\\#UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\\mesidecctempo_1\\0,1\N,-0.09165763,-0.2993925537,-0.0437275948\O,1.3283024672,-0.0295340014,-0.0548749207\C,-2.8422030491,0.5265710264,-0.000895403\C,-4.325630577,0.201977619,-0.0214346809\H,-2.7636874043,1.6177310025,0.0180810687\C,-2.1733505413,-0.0222077491,-1.2720868223\C,-2.1707389465,-0.0690038054,1.2459307485\C,-0.6559439459,0.2420545069,-1.3162720484\C,-0.6233028193,0.1931995543,1.2725495686\C,-0.0733210025,-0.5910660886,-2.4750705011\C,0.0125506243,-0.6986842507,2.3582576839\C,-0.3473416203,1.7296761995,-1.6042292039\C,-0.2815070215,1.664904331,1.6054598848\H,-2.6369009577,0.4224294123,-2.1586383403\C,-2.8582824755,0.4822235129,2.4880772261\H,-2.3436589247,-1.1055083805,-1.3208531901\H,-2.3201610648,-1.1528074834,1.2380101607\H,-0.1939072588,-1.6618933392,-2.282837006\H,-0.1408106647,-1.7574631793,2.127114715\H,-0.5965081671,-0.3461704226,

-3.4064276446\H,-0.4318134975,-0.4942215502,3.3350090062\H,0.988447429
8,-0.3749857079,-2.6226081489\H,1.0853243686,-0.5022559623,2.427266737
2\H,-0.5848591752,1.9569778917,-2.6497972203\H,-0.4104991438,1.8465787
216,2.6773412713\H,-0.921957415,2.419217458,-0.9827210175\H,-0.9096689
71,2.3890197102,1.084442027\H,0.7157088053,1.9283951131,-1.4463064535\H,
0.7636575935,1.8579650827,1.3534056435\O,-3.32737148,1.5969663988,2.
5844463136\O,-2.8947659771,-0.4053409444,3.5086936853\H,-3.3634073633,
0.0451152789,4.2373683739\O,-4.8875683465,-0.608919229,0.6830877351\O,
-4.9790143906,0.917472278,-0.9688850987\H,-5.9125714509,0.6367670618,-
0.9236952464\C,2.077289936,-1.2401289165,-0.1045012683\H,3.1252379337,
-0.9226451388,-0.1141972504\H,1.8968470356,-1.8714912704,0.7716981965\H,
1.8643750877,-1.8173421864,-1.0102209857\Version=IA64L-G03RevD.01\State=1-A\HF=-900.7607499\S2=0.\S2-1=0.\S2A=0.\RMSD=5.987e-09\RMSF=4.22
2e-06\Thermal=0.\Dipole=0.3782816,-0.267709,-0.417076\PG=C01 [X(C12H21
N1O5)]\@

3,5-dicarboxy-TEMPO-CH₃ (G1)

1\1\GINC-AC48\FOpt\UB3LYP\6-31G(d)\C12H21N1O5\JOH501\28-Apr-2006\0\#\#
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\meoppcctempo_1\0,1\N,
-0.0808169955,-0.2853236373,0.\O,1.3339569573,0.0119382566,0.\C,-2.8
427193626,0.4487002702,0.\H,-2.8350112866,1.5407968517,0.\H,-3.8996175
451,0.1560852735,0.\O,-3.3284915881,1.5355976538,2.6298869642\O,-3.328
4915881,1.5355976538,-2.6298869642\C,-2.8907007087,0.4146008376,2.4875
434597\C,-2.8907007087,0.4146008376,-2.4875434597\O,-3.0290718167,-0.5
385119483,3.4457183642\O,-3.0290718167,-0.5385119483,-3.4457183642\H,-
3.5041774199,-0.1083523534,4.1827844139\H,-3.5041774199,-0.1083523534,
-4.1827844139\C,-2.1618928278,-0.1024201856,1.2577190429\C,-2.16189282
78,-0.1024201856,-1.2577190429\H,-2.2449301793,-1.1950143362,1.2593516
634\H,-2.2449301793,-1.1950143362,-1.2593516634\C,-0.6311310181,0.2272
238258,1.3005046697\C,-0.6311310181,0.2272238258,-1.3005046697\C,-0.35
00464679,1.7188778236,1.5915209565\C,-0.3500464679,1.7188778236,-1.591
5209565\C,0.0238876908,-0.6071487928,2.4193153622\C,0.0238876908,-0.60
71487928,-2.4193153622\H,-0.9965102078,2.399424354,1.0366971345\H,-0.9
965102078,2.399424354,-1.0366971345\H,-0.5045496789,1.9283999507,2.654
5011814\H,-0.5045496789,1.9283999507,-2.6545011814\H,0.6913002443,1.94
30194439,1.3493607181\H,0.6913002443,1.9430194439,-1.3493607181\H,-0.4
470148368,-0.390514222,3.3821360538\H,-0.4470148368,-0.390514222,-3.38
21360538\H,-0.0837939175,-1.6782021273,2.2208150303\H,-0.0837939175,-1
.6782021273,-2.2208150303\H,1.0864483908,-0.3667471048,2.5048789855\H,
1.0864483908,-0.3667471048,-2.5048789855\C,2.1098403237,-1.1827990662,
0.\H,3.1501337116,-0.8410591623,0.\H,1.9274614402,-1.7914672116,0.8915
729832\H,1.9274614402,-1.7914672116,-0.8915729832\Version=IA64L-G03Re
vD.01\State=1-A\HF=-900.756519\S2=0.\S2-1=0.\S2A=0.\RMSD=2.587e-09\RM
SF=9.335e-06\Thermal=0.\Dipole=0.364202,-1.0618957,0.\PG=CS [SG(C2H3N1
O1),X(C10H18O4)]\@

4-carboxy-1-methoxy-2,2,6,6-tetraethylpiperidine (H1)

1\1\GINC-AC20\FOpt\UB3LYP\6-31G(d)\C15H29N1O3\JOH501\10-May-2006\0\#\#
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=671088640\mectempoeth_13\0,1\N,
1.243307146,0.0046753215,-0.3071234665\O,2.5851955655,0.1006611359,0.
.2253925137\C,-1.6046397988,-0.0788342857,0.2297705549\C,-3.0599524678
, -0.1483835338,-0.1909425893\H,-1.5998491972,0.0271436376,1.3202553348
\C,-0.936987752,1.1552575626,-0.4057144462\C,-0.8391978591,-1.32371431
62,-0.216021596\C,0.5517680066,1.3102851491,-0.0208955664\C,0.65666349
45,-1.2996932582,0.1675520959\C,1.1918051041,2.3919522315,-0.939344874
4\C,1.3842954927,-2.4442281886,-0.5967069918\C,0.7002165342,1.76797120
16,1.4661212452\C,0.8415186444,-1.5281389073,1.7032510936\H,-1.4694010
111,2.0697798647,-0.1255143401\H,-1.2935728582,-2.2281496036,0.2028690
334\H,-1.0245062303,1.0520798783,-1.4926076267\H,-0.9483514271,-1.4037
20354,-1.3009216995\C,1.151965631,2.1377905487,-2.4522122011\C,1.33776
91934,-2.4019049228,-2.1299828887\H,0.6861618197,3.3425741855,-0.73814
18222\H,0.945722563,-3.3933254556,-0.269578877\H,2.2294688052,2.532475
0973,-0.6147835752\H,2.4268988939,-2.4664653137,-0.2572507283\C,0.2951

498442,3.2131012802,1.7987285596\C,0.5756250351,-2.9456635304,2.23509946\H,0.1121303324,1.1057579902,2.10698337\H,0.1864453074,-0.8440875952,2.2501918126\H,1.74552516,1.6188418449,1.7506977032\H,1.8654229795,-1.2414169206,1.9586599677\O,-3.5353383806,-0.8991734596,-1.0148783193\O,-3.8124899896,0.7776797115,0.4611063399\H,-4.7177789141,0.6821225092,0.1093554282\C,3.5801373827,0.0598603816,-0.7904589512\H,4.5294164977,0.151841518,-0.2522294668\H,3.572080692,-0.8847364333,-1.343664288\H,3.4876937926,0.8899197644,-1.4984861328\H,2.0173100566,-3.1550325556,-2.5461919323\H,0.3378292261,-2.6250877328,-2.5169739257\H,1.6322926969,-1.4235836452,-2.5184963087\H,1.7990249184,2.8550376523,-2.9707213441\H,1.4903909789,1.1286986162,-2.7010880863\H,0.1448599715,2.261856843,-2.8647740128\H,0.6132254313,-2.9381884599,3.330776412\H,-0.4130054809,-3.3250834174,1.9496406589\H,1.3219485675,-3.668915347,1.8923062035\H,0.3294951037,3.3609478277,2.884467428\H,0.9683341759,3.9513666976,1.3519905126\H,-0.725263678,3.4511187853,1.4747403297\\Version=IA64L-G03RevD.01\State=1-A\HF=-869.4345616\S2=0.\S2-1=0.\S2A=0.\RMSD=7.981e-09\RMSE=1.002e-05\Thermal=0.\Dipole=0.2474826,0.4021018,0.2368626\PG=C01 [X(C15H29N1O3)]\@

PROXYL-CH₃ (I1)

1\1\GINC-AC26\FOpt\UB3LYP\6-31G(d)\C9H19N1O1\JOH501\27-Apr-2006\0\#\ U B3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\\meproxy1_1\\0,1\N,0.0548064615,-0.047966193,0.5625852888\C,1.4960925515,0.0162997496,0.1302536561\C,1.7865132428,1.5459459014,0.1397215899\C,-0.6133702249,1.2673302213,0.3664283919\C,0.5432915884,2.1982943853,0.7722717519\H,0.6317089861,2.2166536469,1.8648911899\H,0.3823060275,3.2272880581,0.434036918\C,-1.0799174963,1.5350871877,-1.0800706416\C,1.7613592581,-0.6054532466,-1.2505088016\C,-1.8139080331,1.3664621012,1.3156328302\C,2.3378964458,-0.7159286532,1.1906381866\H,2.8162607006,-0.4635295594,-1.5144469338\H,1.5493996582,-1.6778874101,-1.2512739697\H,1.1498603392,-0.1443709945,-2.0309654972\O,-0.6646303425,-1.0816784814,-0.1197848336\H,3.4068963896,-0.6586518546,0.9499467653\H,2.1796062963,-0.275521927,2.1807812161\H,2.0619319562,-1.77500566,1.2449594545\H,-1.7423477119,0.7343620651,-1.4187119323\H,-1.6306502819,2.4819693713,-1.1251587303\H,-0.2440562017,1.6031414736,-1.7828561624\H,-2.5951253092,0.6535983184,1.0286121119\H,-1.5083094289,1.1483601246,2.3441165899\H,-2.2519413115,2.3713007314,1.2854463838\H,1.9275570786,1.9077055763,-0.8847320745\H,2.7037094614,1.7817067849,0.6892261751\C,-1.0675662238,-2.0831953852,0.8054086673\H,-1.650189664,-2.8020409789,0.2197828177\H,-0.2080372814,-2.595368254,1.2562355161\H,-1.6918869309,-1.668497099,1.6057140759\\Version=IA64L-G03RevD.01\State=1-A\HF=-484.3195144\S2=0.\S2-1=0.\S2A=0.\RMSE=5.172e-09\RMSF=4.642e-06\Thermal=0.\Dipole=0.0912537,0.1088516,0.1375361\PG=C01 [X(C9H19N1O1)]\@

3-amino-PROXYL-CH₃ (J1)

1\1\GINC-AC18\FOpt\UB3LYP\6-31G(d)\C9H20N2O1\JOH501\27-Apr-2006\0\#\ U B3LYP/6-31G* OPT FREQ=noraman maxdisk=6710886400\\menproxyl_3\\0,1\N,0.0152708432,-0.0066318005,0.5317041034\C,1.4698424428,0.0120294052,0.1394266699\C,1.7932301491,1.5311821078,0.1282530437\C,-0.616204919,1.3088401051,0.2724696141\C,0.5591449557,2.2309974448,0.7201566343\H,0.6102023481,2.1738526515,1.8149150215\N,0.5176667354,3.6468543217,0.3754752951\C,-1.0208646441,1.5450010594,-1.1964732074\C,1.7598125317,-0.6439905569,-1.2210727323\C,-1.8487123319,1.4676116942,1.1702109149\C,2.2631949754,-0.7194789441,1.2369185778\H,2.8256629858,-0.5356527151,-1.4548161478\H,1.5183802007,-1.7100520843,-1.2075622401\H,1.1861827749,-0.1829740559,-2.0299663662\O,-0.7053386648,-1.0560270695,-0.1260062677\H,3.3396433886,-0.6887692991,1.0274497411\H,2.0856100154,-0.2587428762,2.2142634183\H,1.9628213226,-1.7714122844,1.2999722708\H,-1.6841351952,0.7433948302,-1.5309986067\H,-1.5570636217,2.4956467712,-1.298556914\H,-0.160985355,1.572061188,-1.8731278389\H,-2.6496715411,0.7860586354,0.8627498153\H,-1.5941907539,1.2533074928,2.2135176574\H,-2.2447528838,2.4893858518,1.1089124434\H,1.9515344877,1.8805670354,-0.8998957958\H,2.7016774295,1.7728476335,0.6878443981\H,0.4113607665,3.7637270111,-0.

631233318\H,-0.2868115722,4.0972132111,0.8093800588\C,-1.1592057439,-2
.0064830899,0.8295190396\H,-1.739736811,-2.7381817775,0.2579043531\H,-
0.3257428824,-2.5157704512,1.3294115964\H,-1.7985614333,-1.5430814457,
1.5902447679\Version=IA64L-G03RevD.01\State=1-A\HF=-539.662353\S2=0.\
S2-1=0.\S2A=0.\RMSD=7.228e-09\RMSF=7.500e-06\Thermal=0.\Dipole=-0.3450
258,-0.0720162,-0.0210981\PG=C01 [X(C9H20N2O1)]\@

3-methoxy-PROXYL-CH₃ (K1)

1\1\GINC-AC48\FOpt\UB3LYP\6-31G(d)\C10H21N1O2\JOH501\27-Apr-2006\0\#\#
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\memeoproxyl_5\0,1\N
,0.0194054423,-0.0130669275,0.5206055043\C,1.4749924333,-0.001425352,0
.1411384516\C,1.8091793504,1.5182708995,0.1517578344\C,-0.6096303525,1
.3036201345,0.2449823577\C,0.5491919459,2.213524408,0.705288556\H,0.57
65317438,2.2154593912,1.8073821757\O,0.3431786867,3.535139147,0.242238
8296\C,-0.9850015311,1.5491104275,-1.2298714599\C,1.7751096486,-0.6417
32702,-1.2250586045\C,-1.8542971347,1.4742772018,1.1230382587\C,2.2535
265074,-0.7531350535,1.235688027\H,2.8443197634,-0.5399520913,-1.44623
94248\H,1.524657054,-1.7057602989,-1.2251746653\H,1.2134252101,-0.1665
819547,-2.033379708\O,-0.6950492323,-1.0627623586,-0.1379281899\H,3.33
24539356,-0.7246166283,1.0387813715\H,2.066118855,-0.3077250087,2.2184
094089\H,1.9477688246,-1.8045590513,1.2772594876\H,-1.6450405541,0.749
883471,-1.577062553\H,-1.5047567541,2.5064571885,-1.325873316\H,-0.112
2683699,1.5845423678,-1.8871653967\H,-2.6615109356,0.8134950237,0.7880
828951\H,-1.6242540644,1.2375989435,2.1673211817\H,-2.2151151801,2.507
0614843,1.0662129742\H,1.9879254543,1.8837018441,-0.8653913472\H,2.705
9984574,1.7330296975,0.7416912278\C,1.2208817293,4.4846752641,0.812176
1229\H,0.9149547918,5.4654133846,0.438172429\H,1.1571342339,4.48596726
22,1.9123913508\H,2.2687256772,4.3092669188,0.5257567079\C,-1.18208870
15,-1.9942164745,0.8202574519\H,-1.7352722953,-2.741549496,0.241970832
\H,-0.3662500997,-2.4862509914,1.3643227536\H,-1.8544545396,-1.5183500
71,1.5437984754\Version=IA64L-G03RevD.01\State=1-A\HF=-598.835066\S2=0.
\S2-1=0.\S2A=0.\RMSD=2.642e-09\RMSF=1.981e-06\Thermal=0.\Dipole=0.40
60909,0.0613323,0.4056866\PG=C01 [X(C10H21N1O2)]\@

3-hydroxy-PROXYL-CH₃ (L1)

1\1\GINC-AC42\FOpt\UB3LYP\6-31G(d)\C9H19N1O2\JOH501\28-Apr-2006\0\#\# U
B3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\meohproxyl_10\0,1\N,
0.0727466546,0.2195664756,-0.5639814426\C,1.4875410257,0.078955571,-0.
1136389476\C,1.847560716,1.5847511988,-0.083518028\C,-0.6046397621,1.3
384377727,0.179979547\C,0.6107454466,2.224190936,0.586455908\H,0.72624
26976,2.2383075943,1.6754090567\H,0.5033968823,3.2607723822,0.25483092
3\C,-1.5377512247,2.0735398067,-0.7989950972\C,2.2808710137,-0.7264297
47,-1.1484828233\C,-1.4272175427,0.8788989378,1.3967755336\C,1.6709488
847,-0.5770618942,1.2710097826\H,3.3471861004,-0.7236837557,-0.8970030
977\H,1.9386634643,-1.7669736505,-1.1580618452\H,2.1705500794,-0.31249
7638,-2.1530709429\O,-0.6340943129,-1.015552802,-0.4308830555\H,2.7346
002714,-0.7667479821,1.4542716562\H,1.3019060891,0.043296073,2.0916739
103\H,1.1429650205,-1.5343706326,1.3018647329\H,-2.3348242626,1.410396
1599,-1.1536854507\H,-2.010592277,2.93436952,-0.3109838384\H,-0.983993
7379,2.4390434074,-1.6702879897\H,-2.2580453549,0.2383199002,1.0892144
242\H,-0.8268556046,0.321416721,2.1197065614\H,-1.8410373833,1.7576901
63,1.9053494877\O,2.0800032521,2.1148007502,-1.3854596466\H,2.76775036
18,1.7720918044,0.4772659965\C,-1.1135590286,-1.4457245517,-1.69982243
55\H,1.3446332025,1.7988815442,-1.9375941272\H,-1.6105952726,-2.402655
4702,-1.5114728261\H,-1.8358930682,-0.7380943993,-2.1250526559\H,-0.29
49623305,-1.592054195,-2.4144432701\Version=IA64L-G03RevD.01\State=1-A
\HF=-559.5289718\S2=0.\S2-1=0.\S2A=0.\RMSD=3.352e-09\RMSF=6.959e-06\T
hermal=0.\Dipole=-0.4739338,-0.2702428,0.1077061\PG=C01 [X(C9H19N1O2)]
\@

3-carboxy-PROXYL-CH₃ (M1)

```
1\1\GINC-AC30\FOpt\UB3LYP\6-31G(d)\C10H19N1O3\JOH501\27-Apr-2006\0\#\#
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\\mecproxyl_2\\0,1\N,0
.0554430045,0.1593208817,-0.5222505586\C,1.4797986392,0.0390373087,-0.
1073352905\C,1.8336957843,1.5596242489,-0.0901360562\C,-0.6136472836,1
.3134052974,0.1667428027\C,0.5927578308,2.2213487608,0.5355119588\H,0.
723887321,2.2791651585,1.6193144939\H,0.4601916172,3.2453338429,0.1721
507866\C,-1.5422964156,1.9994496792,-0.8505380187\C,2.2480194889,-0.73
45226727,-1.1853356198\C,-1.4280269329,0.9189307107,1.4112542483\C,1.6
944347745,-0.6360498781,1.2635771725\H,3.3246368578,-0.7110246531,-0.9
900716632\H,1.9271645377,-1.7817957713,-1.1990373316\H,2.0620763553,-0
.3018120953,-2.1735849753\O,-0.6343470158,-1.0725592642,-0.2909785672\
H,2.7610855376,-0.8211584094,1.4328775257\H,1.3316462316,-0.0297918193
,2.0971525866\H,1.1740618348,-1.5967986775,1.2792525756\H,-2.346881874
7,1.3240450289,-1.1619958475\H,-2.0049638936,2.8932742243,-0.414372862
6\H,-0.9840746698,2.2964126656,-1.7445861759\H,-2.2565197658,0.2567814
527,1.1468032176\H,-0.815746634,0.4076552137,2.158615435\H,-1.84263243
29,1.8225335788,1.8734712558\C,3.1114183603,1.8771889795,0.655506137\O
,3.197128587,2.2470774083,1.8065899027\H,1.9639328747,1.876377752,-1.1
301846233\O,4.2100558383,1.6826611389,-0.1206431259\H,4.9778192367,1.8
84272456,0.4477685484\C,-1.1574585023,-1.5753189161,-1.5154860865\H,-1
.6329964083,-2.5268982065,-1.2568347245\H,-1.906059088,-0.9001481056,-
1.9475203495\H,-0.3662837949,-1.7481273184,-2.2542367702\\Version=IA64
L-G03RevD.01\State=1-A\HF=-672.8855756\S2=0.\S2-1=0.\S2A=0.\RMSD=7.126
e-09\RMSF=4.017e-06\Thermal=0.\Dipole=0.0383159,-0.1217548,-0.5915562\
PG=C01 [X(C10H19N1O3)]\\@
```

3,4-dicarboxy-PROXYL-CH₃ (N1)

```
1\1\GINC-AC43\FOpt\UB3LYP\6-31G(d)\C11H19N1O5\JOH501\27-Apr-2006\0\#\#
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\\meccproxyl_3\\0,1\N,
0.0280615616,-0.0264987902,0.564485775\C,1.4653920433,-0.0020053485,0.
1261728548\C,1.7705821405,1.541243839,0.1155122879\C,-0.6375615303,1.2
87393498,0.352135475\C,0.5486600875,2.2093434628,0.7580871271\H,0.6464
409232,2.1931643081,1.8478512378\C,0.4036782526,3.6537588921,0.3285950
257\C,-1.1128257628,1.5380685818,-1.0946541097\C,1.7168918651,-0.61238
26943,-1.2623101045\C,-1.8290981884,1.3980963248,1.3109424916\C,2.2814
493017,-0.7738843814,1.1790575798\H,2.7691616585,-0.4687997887,-1.5312
973448\H,1.5002585822,-1.6836080867,-1.2649220542\H,1.098592218,-0.144
0867954,-2.0328320697\O,-0.7014716347,-1.0657995844,-0.0917106423\H,3.
3472869451,-0.7800719971,0.9260916878\H,2.1559781068,-0.3357828044,2.1
737400487\H,1.9411030978,-1.8134567493,1.2201394188\H,-1.7589634162,0.
7168038264,-1.4133551494\H,-1.6891156844,2.4684184298,-1.1468790449\H,
-0.2865553031,1.6203524056,-1.8060829108\H,-2.6112792154,0.6877006558,
1.0220662968\H,-1.5170045634,1.1732427246,2.3356029752\H,-2.2565776784
,2.4046887297,1.2873995242\C,3.0608396694,1.9438595775,0.7982319437\O,
3.1595353121,2.4520741588,1.8940001389\H,1.8543432451,1.8750218965,-0.
921851611\O,4.1417618858,1.663321294,0.0285402003\H,4.9218078838,1.94
30329668,0.544546652\O,0.9994111564,4.184554773,-0.5841976026\H,-0.497
7900454,4.3224184247,1.088834881\H,-0.5252526524,5.2323174792,0.736037
8323\C,-1.1420470406,-2.0307173553,0.858994889\H,-1.7251914152,-2.7559
010949,0.2826153681\H,-0.3007642913,-2.5417971736,1.342229275\H,-1.774
7775146,-1.5789736047,1.6312416574\\Version=IA64L-G03RevD.01\State=1-A
\HF=-861.4507393\S2=0.\S2-1=0.\S2A=0.\RMSD=5.745e-09\RMSF=3.691e-06\Th
ermal=0.\Dipole=-0.2905146,-0.4497889,0.0442702\PG=C01 [X(C11H19N1O5)]
\\@
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3-carboxy-1-methoxy-2,2,5,5-tetraethylpyrrolidine (O1)

```
1\1\GINC-AC41\FOpt\UB3LYP\6-31G(d)\C14H27N1O3\JOH501\04-May-2006\0\#\#
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\\mecproxyleth_21\\0,1
\N,0.0446500949,0.0323515714,0.0091920601\C,1.5394223786,0.0956434171,
0.0094110459\C,1.6786414595,1.653574039,0.0158176523\C,-0.5552348804,1
```

.0802107862,0.9090512427\C,0.5934144288,2.1210392154,1.0010422105\H,1.0141621231,2.1510295526,2.0090446269\H,0.2568488312,3.1361677887,0.7696320343\C,-1.8243143178,1.6542464287,0.2258224659\C,2.0821375272,-0.5816022544,-1.2703878288\C,-0.9380860011,0.523600865,2.3074572574\C,2.1649473246,-0.5697008359,1.2768725308\H,3.1742194028,-0.511472941,-1.2622717793\H,1.8463253581,-1.6511384247,-1.1878927737\C,1.5763002272,-0.0506107991,-2.6161304223\O,-0.404425651,-1.283393062,0.346365872\H,2.0175513665,0.09151799,2.1365582641\H,1.5830165916,-1.4749559123,1.4745648691\C,3.652968938,-0.9534339201,1.2224788158\C,-1.6431986861,2.2247011406,-1.1837465909\H,-2.5820185036,0.8590608604,0.1964953683\H,-2.2357649732,2.438472686,0.8731717386\H,-1.6951703664,-0.2562685456,2.1760000769\H,-0.0651609495,0.0222871738,2.7362570252\C,-1.4523376305,1.5630985273,3.314202722\C,3.0541725387,2.1673673173,0.3751655816\O,3.4184249789,2.5475192948,1.4671718063\H,1.4517881151,2.0085721726,-0.9925178454\O,3.8884249759,2.1622706556,-0.6990644442\H,4.747346047,2.4931282999,-0.3737505666\H,3.9665466712,-1.3246778073,2.2049293759\H,3.8481769866,-1.749052292,0.4965684631\H,4.3029107841,-0.1077525585,0.9766835339\H,1.9307162405,-0.696967089,-3.4275088639\H,0.4841606741,-0.0218960942,-2.6574887136\H,1.9523178024,0.9569909933,-2.8238211588\H,-2.5993115471,2.5984856693,-1.5680169417\H,-0.9388684707,3.0654725216,-1.1986212848\H,-1.2719020782,1.4635370031,-1.8747001434\H,-1.614911756,1.0880582269,4.2884832908\H,-0.7382003986,2.38084678,3.4673799271\H,-2.405646544,2.0060968808,3.0077802504\C,-1.1885425079,-1.8289864287,-0.707935084\H,-1.4897452972,-2.8212360977,-0.3569272626\H,-2.0836171775,-1.2267257507,-0.9047783893\H,-0.6133941295,-1.9295170442,-1.6355800149\Version=IA64L-G03RevD.01\State=1-A\HF=-830.126686\S2=0.\S2-1=0.\S2A=0.\RMSD=4.083e-09\RMSF=4.505e-06\Thermal=0.\Dipole=-0.1519889,-0.1771936,-0.5457637\PG=C01 [X(C14H27N1O3)]\@

TMIO-CH₃ (P1)

1\1\GINC-AC20\FOpt\UB3LYP\6-31G(d)\C13H19N1O1\JOH501\28-Apr-2006\0\#\UB3LYP/6-31G* OPT FREQ=noraman maxdisk=671088640\metmio_1\0,1\O,-0.0005938313,0.,-0.0674746013\N,1.339741182,0.,-0.5638293033\C,2.0761221287,1.2375524485,-0.1424968741\C,2.0761221287,-1.2375524485,-0.1424968741\C,3.4937667998,0.6985674021,-0.1042546684\C,3.4937667998,-0.6985674021,-0.1042546684\C,4.6930309185,1.4061933658,-0.0526030778\C,4.6930309185,-1.4061933658,-0.0526030778\H,4.6990375567,2.4934886778,-0.0564691366\H,4.6990375567,-2.4934886778,-0.0564691366\C,5.8974959357,0.699006124,0.00290582\C,5.8974959357,-0.6990006124,0.00290582\H,6.8394335113,1.2397358282,0.042811833\H,6.8394335113,-1.2397358282,0.042811833\C,1.877197957,-2.3184002834,-1.2187672747\C,1.6536501819,-1.7973854632,1.2337623224\C,1.6536501819,1.7973854632,1.2337623224\C,1.877197957,2.3184002834,-1.2187672747\H,0.8292560665,-2.6370678991,-1.2503753316\H,0.5926504706,-2.060521591,1.2296784141\H,0.5926504706,2.060521591,1.2296784141\H,0.8292560665,2.6370678991,-1.2503753316\H,2.4861772449,-3.2044479731,-1.0036146785\H,2.2367236402,-2.6976565158,1.4582009323\H,2.2367236402,2.6976565158,1.4582009323\H,2.4861772449,3.2044479731,-1.0036146785\H,2.1539853507,-1.9322744794,-2.2038385641\H,1.8258994337,-1.0781859329,2.0384650711\H,1.8258994337,1.0781859329,2.0384650711\H,2.1539853507,1.9322744794,-2.2038385641\C,-0.9194550236,0.,-1.1542917338\H,-1.9123631542,0.,-0.692955462\H,-0.8073867865,0.8917116357,-1.7825292504\H,-0.8073867865,-0.8917116357,-1.7825292504\Version=IA64L-G03RevD.01\State=1-A\HF=-636.7478904\S2=0.\S2-1=0.\S2A=0.\RMSD=8.165e-10\RMSF=2.499e-05\Thermal=0.\Dipole=0.0242068,0.,-0.1160721\PG=CS [SG(C1H1N1O1),X(C12H18)]\@

5-carboxy-TMIO-CH₃ (Q1)

1\1\GINC-AC25\FOpt\UB3LYP\6-31G(d)\C14H19N1O3\JOH501\28-Apr-2006\0\#\UB3LYP/6-31G* OPT FREQ=noraman maxdisk=671088640\metmio_2\0,1\N,-0.0049008205,0.0758018128,0.5587906558\C,1.4379065257,0.0272815005,0.152047245\C,1.7501927729,1.5101639867,0.1208432792\C,0.5719711318,2.2644440113,0.1058939007\C,0.6242508327,3.6510809762,0.0591302598\C,1.8743081358,4.2883572178,0.0237724996\C,2.9949070181,2.1370606227,0.088124683

1\C,3.0551732195,3.5296112089,0.038117942\C,-0.6470760967,1.3618319544
,0.1272224172\H,-0.2720565834,4.263516305,0.0507068406\C,1.8904596231,
5.7724511521,-0.0241861931\H,3.912833272,1.5554285259,0.1035077378\H,4
.0141623132,4.0348600984,0.0134225335\O,-0.7199301956,-1.0559645797,0.
0619976913\C,-1.3254589336,1.307206913,-1.2590578722\C,-1.6796577758,1
.7789323709,1.1879094154\C,2.2299974931,-0.7284596357,1.2327721044\C,1
.6976145957,-0.6226626363,-1.2255401179\H,-2.0961204318,2.7677905455,0
.9636822188\H,-2.5112655266,1.0659324664,1.2082993896\H,-1.2205383284,
1.8072909298,2.1800900874\H,-1.7672041969,2.2829901437,-1.4897148233\H
, -0.6163977362,1.0639049698,-2.0542273112\H,-2.1178859931,0.5543977515
, -1.2648116508\H,3.3058477613,-0.703382382,1.0234466344\H,2.0516194253
, -0.2879170443,2.2176701279\H,1.9225956461,-1.7796477415,1.2601323956\H
,2.7737083508,-0.6292920098,-1.4318635039\H,1.3339094095,-1.653229352
8,-1.2307518585\H,1.2042556858,-0.0805780313,-2.0360478031\O,0.9029654
858,6.481480566,-0.038076222\O,3.1456403197,6.2942004245,-0.052605514\H
,3.0240126645,7.2610630264,-0.0824546912\C,-1.2349648879,-1.819536347
5,1.148189371\H,-1.7544209088,-2.6646824681,0.6853698356\H,-0.43480130
09,-2.1919820898,1.7987026534\H,-1.9429619663,-1.2406751615,1.75300564
18\\Version=IA64L-G03RevD.01\State=1-A\HF=-825.3217837\S2=0.\S2-1=0.\S
2A=0.\RMSD=4.161e-09\RMSF=2.807e-06\Thermal=0.\Dipole=0.4215695,-0.663
7837,0.1352335\PG=C01 [X(C14H19N1O3)]\@

5,6-dicarboxy-TMIO-CH₃ (R1)

1\1\GINC-AC46\FOpt\UB3LYP\6-31G(d)\C15H19N1O5\JOH501\01-May-2006\0\#\n
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=671088640\me23cctmio_3\0,1\O,
-0.0021622705,0.0014368009,-0.0523235658\N,1.3320208815,-0.0015938167,
-0.5581870398\C,2.0713287065,1.2386237604,-0.1488836254\C,2.0705278301
, -1.2382802131,-0.1369633136\C,3.4870078775,0.6982076599,-0.1210858176
\C,3.4869433073,-0.6975940345,-0.1134195339\C,4.6866501833,1.402220108
7,-0.0856186812\C,4.6849385398,-1.4010019032,-0.0509920224\C,5.8998304
747,0.7072511764,-0.0470622816\C,5.900891258,-0.7036288555,-0.00626972
46\C,7.1404986825,1.5465596962,-0.0991569552\C,1.8669323576,-2.3246220
437,-1.2066904085\C,1.6628539965,-1.7910927022,1.2465886087\C,1.865170
0063,2.3162096086,-1.2268644358\C,1.6685605825,1.8032696507,1.23149430
31\H,0.816321927,2.6313325989,-1.2501604118\H,0.607311625,2.0641741922
,1.2375990498\H,2.1339343018,1.9285049773,-2.213514043\H,1.8506448248,
1.0875942804,2.0370002681\H,2.4732227199,3.2039883275,-1.0177272864\H,
2.2526371451,2.7052000278,1.4448638453\H,0.8188506793,-2.6425474797,-1
.2290219428\H,0.6013356872,-2.0508430676,1.252176704\H,2.4772088805,-3
.209367856,-0.990637037\H,2.2446381645,-2.6926686459,1.4684319315\H,2.
1364052644,-1.9438474589,-2.1957691949\H,1.8433102904,-1.0694726359,2.
0472251028\H,4.6981824715,-2.4850513751,-0.0155882959\O,7.3077662113,2
.5530155409,0.5551528565\O,8.0137261906,1.1265453811,-1.0418169576\H,8
.7879485991,1.716459751,-0.9723904154\C,7.1666306717,-1.4559381081,0.2
276432316\O,8.1457614396,-1.0210284568,0.7959754881\O,7.1031165561,-2.
735733552,-0.224212653\H,7.9519816867,-3.143787311,0.0295266614\H,4.7
084044577,2.4875429662,-0.0998206444\C,-0.9318587109,-0.0034975383,-1.
131492969\H,-1.9196649448,-0.0013053101,-0.6601105707\H,-0.8250735644,
0.8855146616,-1.764026786\H,-0.8251249878,-0.8982687993,-1.7559414373\
\Version=IA64L-G03RevD.01\State=1-A\HF=-1013.8810185\S2=0.\S2-1=0.\S2A
=0.\RMSD=4.802e-09\RMSF=7.412e-06\Thermal=0.\Dipole=-0.9251136,-0.7218
753,-0.6979008\PG=C01 [X(C15H19N1O5)]\@

TMAO-CH₃ (S1)

1\1\GINC-AC51\FOpt\UB3LYP\6-31G(d)\C17H21N1O1\JOH501\12-Oct-2006\0\#\n
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=671088640\mesb_1s\0,1\O,1.327
2652878,-0.168401902,0.\C,2.0329168906,-1.40632918,0.\H,3.0913980857,-
1.1254395786,0.\N,-0.1021549719,-0.3872455634,0.\C,-2.851185128,0.0071
262457,0.\C,-4.2887787119,-0.0470400428,0.\H,-6.0755167852,-0.10856806
77,-1.2174899171\H,-6.0755167852,-0.1085680677,1.2174899171\C,-4.98921
93296,-0.0641243141,-1.2329256296\C,-4.9892193296,-0.0641243141,1.2329
256296\C,-4.302738625,-0.0134401403,-2.4210975425\C,-4.302738625,-0.01
34401403,2.4210975425\H,-4.8370803787,-0.0173537799,-3.367383589\H,-4.

8370803787,-0.0173537799,3.367383589\C,-2.8918775468,0.0426576416,-2.4
225642433\C,-2.8918775468,0.0426576416,2.4225642433\H,-2.3840902797,0.
0896672074,-3.3797729658\H,-2.3840902797,0.0896672074,3.3797729658\C,-
2.1591017166,0.0422421733,-1.2495091491\C,-2.1591017166,0.0422421733,1.
2495091491\C,-0.6323707611,0.1483391487,-1.2898364464\C,-0.6323707611
,0.1483391487,1.2898364464\H,-0.3102010954,-1.8073013885,-2.211422364\
H,-0.3102010954,-1.8073013885,2.211422364\C,-0.0531527606,-0.760427386
7,-2.3972848762\C,-0.0531527606,-0.7604273867,2.3972848762\H,-0.433420
6341,-0.4776855887,-3.3818517589\H,-0.4334206341,-0.4776855887,3.38185
17589\H,1.0337118393,-0.6567519219,-2.4323833558\H,1.0337118393,-0.656
7519219,2.4323833558\C,-0.2233220102,1.6113928386,-1.6137179483\C,-0.2
233220102,1.6113928386,1.6137179483\H,-0.7675625864,2.3402062219,-1.01
05401277\H,-0.7675625864,2.3402062219,1.0105401277\H,-0.4471602489,1.8
278999484,-2.6638209026\H,-0.4471602489,1.8278999484,2.6638209026\H,0.
8498418256,1.7457097848,-1.4539866891\H,0.8498418256,1.7457097848,1.45
39866891\H,1.8151153669,-2.0045023665,-0.8904814724\H,1.8151153669,-2.
0045023665,0.8904814724\\Version=IA64L-G03RevD.01\State=1-A\HF=-790.3
809925\S2=0.\S2-1=0.\S2A=0.\RMSD=6.263e-09\RMSF=5.049e-05\Thermal=0.\D
ipole=0.0598834,-0.0918384,0.\PG=CS [SG(C3H1N1O1),X(C14H20)]\\@

2,2-dimethy-1-methoxy-lindoline (T1)

1\1\GINC-AC28\FOpt\UB3LYP\6-31G(d)\C11H15N1O1\JOH501\08-Jul-2009\0\#\n
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\\dminome_1\\0,1\O,2.3
20716376,1.9548988815,-1.0862840341\N,1.0721847943,1.2792735248,-1.220
2545163\C,-0.035693156,2.1223597478,-0.976972093\C,-1.0893318591,1.373
3699443,-0.4370760119\C,-0.610075923,-0.0492935483,-0.25509661\C,0.941
2641354,0.0998931358,-0.2954447703\C,-0.1653068379,3.4813492782,-1.246
9269457\C,-1.4004274072,4.082900692,-0.9788751624\C,-2.4667100389,3.34
55973488,-0.4573703746\C,-2.3117346373,1.9792666216,-0.1820196213\H,0.
6712850149,4.0545051943,-1.6322418231\H,-1.5264034161,5.1446910119,-1.
1748553913\H,-3.4155687472,3.8340958111,-0.254379625\H,-3.134572239,1.
4075117469,0.2412693317\H,-0.9502042303,-0.5184280802,0.6745179606\H,-
0.9460054024,-0.6838274351,-1.0875903803\C,1.6482363127,-1.1169798719,
-0.8923855893\H,1.4746927666,-2.0043603586,-0.2726535148\H,2.730456047
1,-0.9524710143,-0.9416203561\H,1.2823575593,-1.3216709618,-1.90378417
87\C,1.4899603527,0.4225144424,1.1051374376\H,1.3594374883,-0.44284213
11,1.7648962952\H,2.5541445924,0.6662698678,1.0578712955\H,0.962836717
1,1.2743014277,1.5474303914\C,3.0166572862,1.9149727631,-2.3295443783\
H,3.94886362,2.4600691969,-2.153387039\H,3.2432434011,0.8867888236,-2.
6356830628\H,2.4455034302,2.407969941,-3.1253312339\\Version=IA64L-G03
RevE.01\State=1-A\HF=-558.1254369\S2=0.\S2-1=0.\S2A=0.\RMSD=3.147e-09\
RMSF=8.133e-06\Thermal=0.\Dipole=0.2237889,-0.394965,-0.1224454\PG=C01
[X(C11H15N1O1)]\\@

2,2-dipheny-1-methoxy-lindoline (U1)

1\1\GINC-AC27\FOpt\UB3LYP\6-31G(d)\C21H19N1O1\JOH501\13-Jul-2009\0\#\n
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\\dpinome_2\\0,1\C,-3.
0704685302,-0.0966160998,1.4621823219\C,-1.789326854,-0.518870249,1.08
17188744\C,-1.1162385744,-1.4257518734,1.9135701055\C,-1.7148373908,-1.
.9130660684,3.0762618184\C,-2.9994931429,-1.501546756,3.4330602387\C,-
3.6731500425,-0.588500137,2.6212603878\C,-1.0779927598,0.0985358578,-0.
1302353127\N,-2.0725509367,0.711497334,-1.0996861666\C,-1.4523774405,
1.8410952651,-1.6845375263\C,-0.4284714974,2.3157113584,-0.8589279222\
C,-0.3187235784,1.3940667343,0.3311503299\C,0.2627751384,3.470410261,-
1.2006997904\C,-0.0674983499,4.1339792333,-2.3908556582\C,-1.079069559
6,3.6354987673,-3.2159421823\C,-1.7891370084,2.4788680928,-2.874294223
8\C,-0.1724365542,-0.9055994217,-0.864919013\C,-0.6338284661,-2.209014
4073,-1.1119833513\C,0.1386548098,-3.127195277,-1.8195777587\C,1.39584
94658,-2.7618275889,-2.3051517304\C,1.8646601793,-1.4698584947,-2.0774
999384\C,1.0876089223,-0.5516368963,-1.3667301471\O,-2.5528886683,-0.1
949128053,-2.0861232827\H,-2.5616080238,2.0772483865,-3.5209232283\H,-
1.3173855494,4.1488763644,-4.1438849968\H,0.4721201019,5.0324406663,-2.
.6766162807\H,1.0606507517,3.8465740045,-0.5644044498\H,-0.1183893034,

-1.7601508948,1.647235658\H,-1.1736848885,-2.6181853047,3.7019769395\H
,-3.4683452211,-1.8853437272,4.3352585337\H,-4.6712761699,-0.252087710
6,2.8905025325\H,-3.5901012769,0.6273409075,0.8442129236\H,1.475677374
6,0.450237224,-1.222307683\H,2.8390448143,-1.1673893389,-2.4522908836\H,
2.0013592316,-3.4773485472,-2.8553041548\H,-0.2435942757,-4.12994971
48,-1.9926453479\H,-1.6068064956,-2.5093675561,-0.7381388591\C,-3.9575
701241,-0.3936200472,-1.9377943606\H,-0.8429271443,1.8162425169,1.1966
978501\H,0.7037329641,1.1744211955,0.6518771059\H,-4.2414565572,-1.025
2342827,-2.7846057044\H,-4.2005756813,-0.9057173381,-1.0003225125\H,-4
.5042676885,0.5557983677,-1.9869791546\\Version=IA64L-G03RevE.01\State
=1-A\HF=-941.5851239\S2=0.\S2-1=0.\S2A=0.\RMSD=3.063e-09\RMSF=1.745e-0
6\Thermal=0.\Dipole=-0.1912922,-0.1760114,0.246535\PG=C01 [X(C21H19N10
1)]\@

SG1-CH₃ (V1)

1\1\GINC-AC51\FOpt\UB3LYP\6-31G(d)\C14H32N1O4P1\JOH501\15-Jan-2007\0\\
UB3LYP/6-31G* OPT FREQ=norman maxdisk=402653184\\mesglprop_21\\0,1\N,
0.0800968042,0.293940635,-0.7759134665\O,0.6619777498,-0.0456075729,
0.5076261319\C,-0.674768114,1.5850440253,-0.5697619194\C,-0.6890643888
, -0.8831338948,-1.254137438\P,-1.0519856539,-2.1483920844,0.0895465519
\O,-1.5811343788,-1.4404673758,1.4504967031\O,-2.4836501885,-2.6577505
643,-0.4953402733\C,-0.0299209837,-1.5467406162,-2.5361803381\C,-0.803
0022293,-1.4504267764,2.66944448\C,-1.7504701583,-1.6579655916,3.83882
79118\C,-3.1602945288,-3.7503123128,0.1653330514\C,-4.378206913,-4.118
8708326,-0.6625281678\O,-0.0259359467,-3.2050783327,0.3198649573\C,-1.
257596196,2.0526589949,-1.9158587484\C,-1.808257131,1.4964083802,0.470
1285686\C,0.3523235743,2.63847261,-0.1143110606\H,-1.6863134587,-0.549
9320934,-1.5594963982\C,-0.8558081215,-2.7594280138,-3.0187080907\C,-0
.0165825007,-0.5087747826,-3.6763524402\C,1.4209861578,-2.0008175401,-
2.2929919629\H,-0.0561789067,-2.2469119653,2.6105238413\H,-0.283927893
9,-0.4904658728,2.7397230969\H,-1.1927720883,-1.6183503124,4.781946962
\H,-2.5198231289,-0.8789728802,3.8612109234\H,-2.2473208418,-2.6317367
903,3.7742589784\H,-2.4688299056,-4.5950663143,0.2580991778\H,-3.44908
14597,-3.4263359654,1.1720308294\H,-4.9244232587,-4.93810974,-0.181370
6778\H,-5.053781172,-3.2628811888,-0.7602051042\H,-4.0822078119,-4.442
2752004,-1.6655029582\H,-2.2831456196,2.4789290611,0.575896451\H,-2.58
39028538,0.7830681328,0.1760313964\H,-1.4259698953,1.1948112,1.4466725
45\H,-1.7391161861,3.0253119659,-1.7683370687\H,-0.4771126484,2.172474
6387,-2.671446465\H,-2.0191737934,1.3733135028,-2.3099190221\H,-0.1314
9485,3.6188357303,-0.043946069\H,0.7654646204,2.3950556931,0.867261501
4\H,1.1747288814,2.7149262503,-0.8338733569\H,0.4404047977,-0.95273266
83,-4.5687427145\H,-1.0281148158,-0.1854667604,-3.9498291327\H,0.56940
93306,0.3722899282,-3.4028613609\H,-0.4680643628,-3.0903621149,-3.9894
410318\H,-0.7842369788,-3.6041076038,-2.3290593103\H,-1.9147463454,-2.
5098738331,-3.1456457326\H,1.8031092076,-2.492144017,-3.1962721774\H,2
.0682290296,-1.1434379547,-2.0891942775\H,1.4865970345,-2.7097313798,-
1.4637084661\C,2.0860157012,-0.1200137729,0.4645907996\H,2.4271811646,
-1.0838220084,0.077065171\H,2.5044829672,0.6934001298,-0.1350612435\H,
2.4110886875,-0.0148741507,1.504856444\\Version=IA64L-G03RevD.01\State
=1-A\HF=-1249.7616562\S2=0.\S2-1=0.\S2A=0.\RMSD=5.585e-09\RMSF=1.080e-
05\Thermal=0.\Dipole=-0.3991965,0.7229453,0.2295435\PG=C01 [X(C14H32N1
O4P1)]\@

TEMPO-CH₂CH₃ (B2)

1\1\GINC-AC53\FOpt\UB3LYP\6-31G(d)\C11H23N1O1\JOH501\21-Feb-2007\0\\#
UB3LYP/6-31G* OPT FREQ=norman maxdisk=402653184\\tempoch2ch3_1\\0,1\N
, -0.3035380896,0.1490692731,0.\O,0.3772395411,1.4251685459,0.\C,-0.550
4257654,2.5139041788,0.\C,-0.2872605697,-2.7371915564,0.\H,-0.83359103
31,-3.6888570995,0.\H,0.778592516,-2.9975612752,0.\C,0.2766148847,3.79
11174212,0.\H,-1.1957570655,2.4653456963,0.8852053866\H,-1.1957570655,
2.4653456963,-0.8852053866\C,1.5284998828,-0.6438813227,1.6188259773\C
,1.5284998828,-0.6438813227,-1.6188259773\C,0.0204387358,-0.53499788,1

.2913446734\C,0.0204387358,-0.53499788,-1.2913446734\C,-0.6467586562,0.2749456251,2.4203217661\C,-0.6467586562,0.2749456251,-2.4203217661\C,-0.6454470765,-1.9299465463,1.248593889\C,-0.6454470765,-1.9299465463,-1.248593889\H,-1.7349291507,-1.7931936066,1.2788095899\H,-1.7349291507,-1.7931936066,-1.2788095899\H,-0.3669706849,-2.4725012364,2.1609325799\H,-0.3669706849,-2.4725012364,-2.1609325799\H,-0.5812814069,-0.279205587,3.3639631251\H,-0.5812814069,-0.279205587,-3.3639631251\H,-1.7037238105,0.4516787005,2.1964585051\H,-1.7037238105,0.4516787005,-2.1964585051\H,-0.1513321044,1.2394226031,2.565804201\H,-0.1513321044,1.2394226031,-2.565804201\H,1.6559509961,-0.9084823264,2.6752086048\H,1.6559509961,-0.9084823264,-2.6752086048\H,2.0438467328,-1.4054751347,1.0296677123\H,2.0438467328,-1.4054751347,-1.0296677123\H,2.0208337504,0.3166566434,1.4474324704\H,2.0208337504,0.3166566434,-1.4474324704\H,-0.3810496213,4.6674354937,0.\H,0.9174989265,3.8396368799,0.886746559\H,0.9174989265,3.8396368799,-0.886746559\Version=IA64L-G03RevD.01\State=1-A'\HF=-562.9511382\S2=0.\S2-1=0.\S2A=0.\RMSD=8.619e-09\RMSF=3.717e-06\Thermal=0.\Dipole=-0.1597581,-0.0948486,0.\PG=CS [SG(C3H3N1O1),X(C8H2O)]\@

TEMPO-CH₂CH₂CH₃ (B3)

1\1\GINC-AC57\FOpt\UB3LYP\6-31G(d)\C12H25N1O1\JOH501\22-Feb-2007\0\#\UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\tempoch2ch2ch3_1s\0,1\N,-0.3237823115,0.1291034527,0.\O,0.3211099002,1.4235631913,0.\C,-0.6365594363,2.4852675753,0.\C,-0.2352947925,-2.7558091677,0.\H,-0.7576414401,-3.7208390353,0.\H,0.8370353478,-2.9896132685,0.\C,0.1460221773,3.7942019323,0.\H,-1.2815722586,2.4199402748,0.885414702\H,-1.2815722586,2.4199402748,-0.885414702\C,1.5268920051,-0.6160871323,1.619242158\C,1.5268920051,-0.6160871323,-1.619242158\C,0.0167236,-0.5464082453,1.2914464467\C,0.0167236,-0.5464082453,-1.2914464467\C,-0.6723039173,0.2459875969,2.4196983704\C,-0.6723039173,0.2459875969,-2.4196983704\C,-0.613297031,-1.9576705725,1.2486746051\C,-0.613297031,-1.9576705725,-1.2486746051\H,-1.7060430439,-1.8493253459,1.2794747761\H,-1.7060430439,-1.8493253459,-1.2794747761\H,-0.3207600593,-2.4927245342,2.1610550718\H,-0.3207600593,-2.4927245342,-2.1610550718\H,-0.5952287632,-0.3071964312,3.3630336296\H,-0.5952287632,-0.3071964312,-3.3630336296\H,-1.7327701185,0.3966404451,2.1932045499\H,-1.7327701185,0.3966404451,-2.1932045499\H,-0.201669742,1.2225303808,2.5671610493\H,-0.201669742,1.2225303808,-2.5671610493\H,1.6621052485,-0.8766012573,2.6756480471\H,1.6621052485,-0.8766012573,-2.6756480471\H,2.0609864537,-1.3644691033,1.0298030141\H,2.0609864537,-1.3644691033,-1.0298030141\H,1.993490683,0.3570134862,1.4466255363\H,1.993490683,0.3570134862,-1.4466255363\C,-0.7743785791,5.0193479296,0.\H,0.8022948785,3.8142816192,0.8793670451\H,0.8022948785,3.8142816192,-0.8793670451\H,-0.193019596,5.9475854325,0.\H,-1.4221335706,5.0330247922,-0.884992893\H,-1.4221335706,5.0330247922,0.\H,0.884992893\Version=IA64L-G03RevD.01\State=1-A'\HF=-602.2645707\S2=0.\S2-1=0.\S2A=0.\RMSD=7.067e-09\RMSF=3.077e-06\Thermal=0.\Dipole=-0.1419137,-0.0790552,0.\PG=CS [SG(C4H3N1O1),X(C8H22)]\@

TEMPO-CH(CH₃)₂ (B5)

1\1\GINC-AC58\FOpt\UB3LYP\6-31G(d)\C12H25N1O1\JOH501\27-Feb-2007\0\#\UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\tempochme2_1\0,1\N,-0.1555658805,0.022616255,-0.0821555297\O,0.9714361085,-0.1176331712,0.8160751398\C,2.2495924666,-0.3471097207,0.1793273532\C,-3.0235312743,0.174506503,-0.5299601871\H,-3.8669966236,0.3117588595,-1.2183740656\H,-3.4623018792,0.0164643035,0.4631331923\C,3.2400935884,-0.3234685005,1.3409680051\C,2.6151004401,0.6454177299,-0.9208268219\C,-1.2293517673,1.3446271629,1.8480593746\C,-1.3046826552,-1.8185027146,1.3095756715\C,-0.8701823092,1.2760453596,0.343519138\C,-0.9344192923,-1.2649828029,-0.0863003665\C,0.0420088939,2.4771286414,0.0349221827\C,-0.086060603,-2.3392755575,-0.7979375708\C,-2.133455108,1.4163566022,-0.5361497843\C,-2.1955146701,-1.0372258113,-0.9535477159\H,-1.8158341701,1.6164040247,-1.5686092466\H,-1.8758150614,-0.8993028918,-1.9955082033\H,-2.6889137724,2.3001371332,-0.1976611774\H,-2.7970284694,-1.9546009903,-0.92

47717026\H,-0.5096297264,3.4081241227,0.2095545654\H,-0.7212373322,-3.1962635279,-1.0515631235\H,0.3686939898,2.4640132415,-1.0086144314\H,0.3463450698,-1.9461393823,-1.7235814447\H,0.9241943545,2.4820723305,0.6794689767\H,0.7201685675,-2.7117817516,-0.159784608\H,-1.5039570313,2.373247055,2.1097172893\H,-1.5838054182,-2.8752355425,1.2225682468\H,-2.0712511254,0.7061791378,2.1225775908\H,-2.1462904011,-1.2993716292,1.7722473884\H,-0.3672499062,1.0588775343,2.4553201093\H,-0.4443037161,-1.748431262,1.9798535639\H,3.5483945924,0.3234556202,-1.3981396853\H,1.832804991,0.6812977714,-1.6826435412\H,2.7671089681,1.6542517994,-0.5240365637\H,4.2477519002,-0.5671656465,0.9868844722\H,3.2656106124,0.6700044182,1.8026057935\H,2.9563027768,-1.0509940402,2.1081924926\H,2.2484108728,-1.3513406627,-0.2605147764\Version=IA64L-G03RevD.01\State=1-A\HF=-602.2633236\S2=0.\S2-1=0.\S2A=0.\RMSD=5.854e-09\RMSF=6.690e-06\Thermal=0.\Dipole=-0.0802075,-0.0836857,-0.179901\PG=C01 [X(C12H25N1O1)]\@

TEMPO-C(CH₃)₃ (B6)

1\1\GINC-AC57\FOpt\UB3LYP\6-31G(d)\C13H27N1O1\JOH501\21-Feb-2007\0\#\UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\tempocme3_1\0,1\N,-0.1152876631,0.0504953763,-0.0515137461\O,1.3172108254,0.1238374127,0.1532555182\C,2.0003099074,1.426121202,0.0724909067\C,-2.5201362032,-1.6209690022,-0.1851453552\H,-3.6026130274,-1.7207797256,-0.3356743058\H,-2.1435023347,-2.6319932947,0.0136491739\C,3.1586166629,1.2087766863,-0.9164247669\C,2.6075422596,1.7124526898,1.4585049794\C,1.1104992694,2.5878178386,-0.3687791558\C,-0.0532176399,-1.6901762601,1.8484565677\C,0.435915162,-2.1163958035,-1.3304769157\C,-0.729146799,-0.4399394389,1.2376397453\C,-0.3474843635,-0.7832766002,-1.2895897239\C,-0.6412715032,0.6898342486,2.2794792965\C,0.0678907144,0.042739517,-2.5204340496\C,-2.2356807661,-0.6933703234,0.9911506707\C,-1.8688330758,-1.0319900152,-1.4314851791\H,-2.7233483432,0.2731403719,0.8030808684\H,-2.3556778291,-0.074039431,-1.6604211244\H,-2.6656432395,-1.0890258561,1.9199420606\H,-2.0227566907,-1.6806410776,-2.303097413\H,-1.2780906549,0.444604057,3.1375132196\H,-0.2390287193,-0.4835154425,-3.4318191994\H,-0.9885073181,1.6387275873,1.8589716652\H,-0.4192910539,1.0221180656,-2.5145631499\H,0.3751271302,0.8165029583,2.6531485582\H,1.1484674107,0.1837336462,-2.5719254139\H,-0.3717998737,-1.804709293,2.8913746597\H,0.4202841266,-2.5192740559,-2.3500297966\H,-0.3074628858,-2.6164813695,1.3293174338\H,0.0176753948,-2.8819200794,-0.6737796435\H,1.0328546615,-1.5748973759,1.8348826472\H,1.4771035933,-1.9506509719,-1.0452894974\H,1.7036516413,3.5094746355,-0.3410254168\H,0.7384406829,2.4562819025,-1.3860804346\H,0.2521029483,2.7127698709,0.2939896936\H,3.3599674988,2.5062939037,1.3867013265\H,1.8535408239,2.0375893111,2.178739754\H,3.0971980653,0.8136266961,1.8477363406\H,3.8199080476,2.0825174858,-0.9316143421\H,3.7507924353,0.3374149865,-0.6166994206\H,2.7977407226,1.0427349671,-1.9342166078\Version=IA64L-G03RevD.01\State=1-A\HF=-641.5703441\S2=0.\S2-1=0.\S2A=0.\RMSD=5.153e-09\RMSF=3.684e-06\Thermal=0.\Dipole=-0.1483104,0.0981592,-0.0378225\PG=C01 [X(C13H27N1O1)]\@

TEMPO-CH₂OH (B7)

1\1\GINC-AC28\FOpt\UB3LYP\6-31G(d)\C10H21N1O2\JOH501\21-Feb-2007\0\#\UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\tempoch2oh_5\0,1\N,0.0315319237,0.0258900943,0.0192178627\O,1.4846158414,-0.0074713401,0.0315101516\C,2.0568453042,1.2873734748,-0.0628518368\C,-2.5062927872,-1.3810400645,-0.0520794577\H,-3.6032740323,-1.3614856643,-0.0670595428\H,-2.2192317273,-2.4396677007,-0.0739107553\O,2.191221766,1.9729501212,1.1523398533\H,1.4934688073,1.8826051679,-0.7884347885\H,3.0740325113,1.1037176854,-0.4184005461\C,0.1789421715,-1.9946088485,1.6049006614\C,0.2157269359,-1.936831386,-1.6350623862\C,-0.4470264818,-0.6152697196,1.2928678491\C,-0.4092969933,-0.5648015822,-1.292752637\C,-0.0974129265,0.3296723918,2.4570650797\C,-0.0098012773,0.4206293457,-2.4089735291\C,-1.9894749039,-0.7050384813,1.2168905572\C,-1.9529028595,-0.644791241,-1.2712415346\H,-2.3978148612,0.3139758152,1.2608849634\H,-2.3538801065,0.3780708163,-1.2774270693\H,-2.3436697082,-1.2269310351,2.114

5507505\H,-2.2824572536,-1.120578996,-2.2033668328\H,-0.5454688474,-0.0451442558,3.38422305\H,-0.467510187,0.1086164028,-3.3547356531\H,-0.5065427865,1.3312021937,2.272353412\H,-0.3575776717,1.4330473165,-2.1786430323\H,0.9818944482,0.4061502782,2.6026810547\H,1.0734865042,0.443838104,-2.5602475414\H,-0.0255786585,-2.2590879728,2.648761837\H,0.047818816,-2.1599479503,-2.6952017005\H,-0.2195106752,-2.7992353907,0.9833558861\H,-0.2109643172,-2.7598931666,-1.0588507511\H,1.2624609126,-1.9577029591,1.4703379536\H,1.2940283144,-1.9162637041,-1.4594746106\H,1.3080848053,2.2782322511,1.4123032829\Version=IA64L-G03RevD.01\State=1-A\HF=-598.8500349\S2=0.\S2-1=0.\S2A=0.\RMSD=9.741e-09\RMSF=2.844e-06\Thermal=0.\Dipole=-0.7976459,-0.0728131,-0.3098766\PG=C01 [X(C10H21N1O2)]\@

TEMPO-CH₂F (B8)

1\1\GINC-AC10\FOpt\UB3LYP\6-31G(d)\C10H20F1N1O1\JOH501\19-Feb-2007\0\#\UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\tempoch2f_2\0,1\N,-0.0046247068,0.0090319011,0.0156028624\O,1.4530033004,0.0022522183,-0.018769646\C,1.9877564704,1.279156331,-0.055108122\C,-2.5350336291,-1.3774068789,0.0131293887\H,-3.6318667862,-1.3502779433,0.0212937497\H,-2.2559900333,-2.4383512705,-0.0033726405\F,2.2455272921,1.7827385402,1.2130844029\H,1.3133896211,1.9776526627,-0.5545253397\H,2.9523105498,1.1881327306,-0.5661500464\C,0.1802847476,-1.9975336837,1.6132142383\C,0.1518207157,-1.9612253962,-1.6316661708\C,-0.4418986247,-0.6153974033,1.3082987729\C,-0.4621020376,-0.5855909955,-1.2836051059\C,-0.0514941513,0.3432995934,2.4480606935\C,-0.0764216723,0.4013950825,-2.4031708347\C,-1.9865127421,-0.6928410549,1.2652019327\C,-2.0056333915,-0.6598589299,-1.2286778074\H,-2.3841103027,0.3299845224,1.3107954056\H,-2.4024034931,0.364244999,-1.2397634299\H,-2.3248119392,-1.2054244529,2.1741665914\H,-2.3562716695,-1.1472928363,-2.1469599708\H,-0.5345105143,0.0180158442,3.3767339991\H,-0.5360691225,0.087475876,-3.3471784636\H,-0.3785569005,1.3631033165,2.2231652571\H,-0.4299879564,1.4111983311,-2.170009686\H,1.0270453859,0.3623421608,2.6083401788\H,1.0064031813,0.4325717224,-2.5597042558\H,0.0065183143,-2.2476325315,2.6661483763\H,-0.0409298091,-2.1907677022,-2.6861476386\H,-0.2435058543,-2.8063097625,1.0136472682\H,-0.2649097473,-2.7781374817,-1.0396135048\H,1.2602951051,-1.9734953727,1.4473251594\H,1.2343804003,-1.9459321362,-1.481925614\Version=IA64L-G03RevD.01\State=1-A\HF=-622.8725255\S2=0.\S2-1=0.\S2A=0.\RMSD=2.753e-09\RMSF=7.789e-06\Thermal=0.\Dipole=-0.4745377,-0.2646008,-0.5713065\PG=C01 [X(C10H20F1N1O1)]\@

TEMPO-CH₂C≡N (B9)

1\1\GINC-AC7\FOpt\UB3LYP\6-31G(d)\C11H20N2O1\JOH501\21-Feb-2007\0\#\UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\tempoch2cn_1s\0,1\N,-0.0006082585,0.0001209881,0.\O,1.4524385644,-0.0000661756,\C,1.9262806309,1.3414927706,0.\C,-2.5358379333,-1.365021696,0.\H,-3.6321094172,-1.324590487,0.\H,-2.2700569342,-2.4293116296,0.\C,3.3964774394,1.2879030353,0.\H,1.5879616986,1.8903920127,0.8864827822\H,1.5879616986,1.8903920127,-0.8864827822\C,0.1655488195,-1.9924712478,1.6172827684\C,0.1655488195,-1.9924712478,-1.6172827684\C,-0.445511538,-0.6094345156,1.2950140096\C,-0.445511538,-0.6094345156,-1.2950140096\C,-0.0388416368,0.3591193497,2.4229085765\C,-0.0388416368,0.3591193497,-2.4229085765\C,-1.9902797049,-0.6717713804,1.2496046663\C,-1.9902797049,-0.6717713804,-1.2496046663\H,-2.3788590712,0.3550723062,1.2813337866\H,-2.3788590712,0.3550723062,-1.2813337866\H,-2.3388189441,-1.17257491,2.1613751625\H,-2.3388189441,-1.17257491,-2.1613751625\H,-0.4911995585,0.0377441606,3.3677730894\H,-0.4911995585,0.0377441606,-3.3677730894\H,-0.3859457804,1.3751778672,2.2069332287\H,-0.3859457804,1.3751778672,-2.2069332287\H,1.0459590343,0.3747409537,2.5669895254\H,1.0459590343,0.3747409537,-2.5669895254\H,-0.0121068817,-2.2308072641,2.6722959909\H,-0.0121068817,-2.2308072641,-2.6722959909\H,-0.2647294175,-2.802571803,1.0254350428\H,-0.2647294175,-2.802571803,-1.0254350428\H,1.2458944683,-1.980245423,1.4518664422\H,1.2458944683,-1.980245423,-1.4518664422\N,4.5562229331,1.2721329821,0.\Version=IA64L-G03RevD.01\State=1-A\HF=-615.86

66239\S2=0.\S2-1=0.\S2A=0.\RMSD=2.717e-09\RMSF=2.934e-05\Thermal=0.\Dipole=-1.8211693,-0.0825748,0.\PG=CS [SG(C3H2N2O1),X(C8H18)]\@

TEMPO-CH(CH₃)C≡N (B10)

1\1\GINC-AC53\FOpt\UB3LYP\6-31G(d)\C12H22N2O1\JOH501\05-Mar-2007\0\#\UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\tempoan_1\0,1\N,-0.0816853495,0.0184041994,0.0377511396\O,1.3441802645,0.1793512702,0.2899100227\C,1.7576072602,1.5454029626,0.3168739367\C,-2.4449687332,-1.6511429783,-0.0939827647\H,-3.5197522747,-1.7581104733,-0.2865869795\H,-2.0833489308,-2.6494983585,0.1820304003\C,2.1819533179,2.0515427683,-1.0128383326\C,2.9374145272,1.6408391435,1.2911126259\C,-0.0630463092,-1.5794816172,2.0578612946\C,0.557880206,-2.2229333798,-1.0552708051\C,-0.7230173005,-0.3815775695,1.337616575\C,-0.223190619,-0.8914850101,-1.1510212822\C,-0.6638646588,0.8301956167,2.2896169131\C,0.2877736592,-0.1327996491,-2.3878343787\C,-2.2165230347,-0.6576913625,1.0441620026\C,-1.7361477772,-1.1454665115,-1.3493944214\H,-2.6989647368,0.2935499516,0.7816764976\H,-2.2051523755,-0.204297132,-1.6663931921\H,-2.6849786068,-1.0056133888,1.9733657639\H,-1.8520805058,-1.8531341649,-2.1793946862\H,-1.2839459344,0.6329332472,3.1713224096\H,-0.0021492382,-0.6769138824,-3.2941816141\H,-1.0480605119,1.7313748671,1.8002282793\H,-0.1436007849,0.8713290082,-2.4363474453\H,0.3525313014,1.0219168423,2.6458156349\H,1.3757059247,-0.0409313781,-2.3902114284\H,-0.4308007552,-1.6329612916,3.0891990527\H,0.6044920741,-2.685240212,-2.0479175871\H,-0.2823092956,-2.5384124053,1.5850801164\H,0.0984905516,-2.9492104986,-0.3811758297\H,1.0221682413,-1.4542547725,2.0920798635\H,1.5827052419,-2.0414932666,-0.7216999834\H,3.3257784656,2.663142728,1.3258349768\H,2.6117063953,1.3465813848,2.2923477897\H,3.7418678466,0.9719498954,0.9726073981\H,0.926345397,2.1725850376,0.6494624817\N,2.5543470581,2.4868003793,-2.0224444444\Version=IA64L-G03RevD.01\State=1-A\HF=-655.1836032\S2=0.\S2-1=0.\S2A=0.\RMSD=7.853e-09\RMSF=7.567e-06\Thermal=0.\Dipole=-0.745638,-0.5919885,1.2725652\PG=C01 [X(C12H22N2O1)]\@

TEMPO-C(CH₃)₂C≡N (B11)

1\1\GINC-AC37\FOpt\UB3LYP\6-31G(d)\C13H24N2O1\JOH501\05-Mar-2007\0\#\UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\tempoman_1\0,1\N,-0.0473037927,0.0179551187,-0.0579057048\O,1.3699318077,0.1314668536,0.2460230889\C,2.0374049521,1.3805589067,-0.0626264817\C,-2.4434233599,-1.6431176678,-0.1068844111\H,-3.5174611988,-1.7588983341,-0.2983757926\H,-2.0839866254,-2.623054767,0.2301254466\C,2.9459532271,1.141665079,-1.2212569064\C,2.9420193524,1.670528614,1.1511057246\C,-0.0858079143,-1.481281035,2.0378681966\C,0.5656116599,-2.2797773734,-1.0483171812\C,-0.7189004822,-0.3072661252,1.2538268615\C,-0.2112728764,-0.9528997578,-1.2027704179\C,-0.6548266319,0.94392266,2.1483408683\C,0.2733943926,-0.2671777188,-2.493981844\C,-2.2129395632,-0.5816914039,0.9656701087\C,-1.7272604372,-1.2116262753,-1.3834770902\H,-2.6827156542,0.3561794366,0.639353904\H,-2.194765078,-0.288552597,-1.752667669\H,-2.6917660093,-0.8637456637,1.9116192815\H,-1.8432096924,-1.9620827555,-2.1749962009\H,-1.2511447218,0.7776915628,3.0525880342\H,-0.0269375398,-0.8724224917,-3.3570826329\H,-1.0635841053,1.816333147,1.6296389965\H,-0.1819793344,0.7221767797,-2.6062860241\H,0.367812616,1.1623865979,2.4644183213\H,1.3590167793,-0.1657975334,-2.5338469856\H,-0.4753851613,-1.4849449885,3.0624494751\H,0.5994799186,-2.7940874408,-2.0155255283\H,-0.3086086987,-2.4574553737,1.6030193386\H,0.1094368387,-2.9663280048,-0.3317109001\H,0.9993556522,-1.3679086566,2.0874820125\H,1.5936450292,-2.0852417177,-0.7342666362\H,3.6227449289,2.4997593213,0.9349754611\H,2.3267667538,1.9347226979,2.0151839935\H,3.5353459073,0.7851809833,1.3948469118\C,1.1240408524,2.5698835712,-0.3789114967\N,3.6979402452,0.9741601906,-2.0901149925\H,1.7470589828,3.4327718845,-0.6351112532\H,0.458351126,2.3531364032,-1.213546166\H,0.5200678548,2.8214378735,0.4938362902\Version=IA64L-G03RevD.01\State=1-A\HF=-694.4938971\S2=0.\S2-1=0.\S2A=0.\RMSD=4.913e-09\RMSF=4.340e-06\Thermal=0.\Dipole=-1.2109459,0.1798127,1.0157915\PG=C01 [X(C13H24N2O1)]\@

TEMPO-CH₂Ph (B12)

1\1\GINC-AC4\FOpt\UB3LYP\6-31G(d)\C16H25N1O1\JOH501\19-Feb-2007\0\#\ U
B3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\tempoch2ph_4\0,1\N,-
0.2610848723,0.0166244196,0.2310293306\O,1.0961278276,0.1169939508,0.7
240665326\C,1.5422697182,1.4812915609,0.7288869009\C,-2.6110654669,-1.
5157595134,-0.4463182468\H,-3.6432944691,-1.5561195211,-0.8163807029\H
, -2.3252915595,-2.5518573069,-0.2257179343\C,2.8926244877,1.517620441,
1.4041165223\H,0.8266090112,2.1149123141,1.2622159403\H,1.6100980898,1
.8529006678,-0.3019221937\C,-0.6017962921,-1.7752147112,2.0420569615\C
,0.4961317465,-2.1162318346,-0.9879966968\C,-1.1066258395,-0.480355583
,1.36323481\C,-0.2305406983,-0.7522341895,-1.0527366006\C,-1.137876942
1,0.6282867498,2.4335344492\C,0.497992899,0.1195328163,-2.0945579101\C
, -2.5420780158,-0.6561697465,0.8168626861\C,-1.6961456168,-0.919760185
9,-1.517145474\H,-2.9489874626,0.3381339041,0.5877719371\H,-2.08308044
9,0.0686010665,-1.8000808999\H,-3.1646914579,-1.0790744109,1.615356437
4\H,-1.7003291032,-1.5352093193,-2.4257320818\H,-1.8721443234,0.376459
2585,3.2074313863\H,0.3853992672,-0.3214500764,-3.0918469997\H,-1.4230
578285,1.587490837,1.9887670655\H,0.0773153756,1.1300386364,-2.1143425
608\H,-0.1645515323,0.7386816751,2.9204504295\H,1.5690166465,0.1883892
233,-1.882116059\H,-1.121360229,-1.9139153874,2.9975041049\H,0.6946785
19,-2.4746735672,-2.0049464576\H,-0.7788430023,-2.6716506492,1.4438240
021\H,-0.0831853579,-2.889249625,-0.4789260514\H,0.4692646562,-1.70064
56234,2.246210297\H,1.4540335202,-2.0099612698,-0.4723454145\C,3.94793
30917,0.7274578326,0.9268884807\C,5.1980924619,0.76630005,1.5417815514
\C,5.4144586645,1.6028083455,2.6403234969\C,3.1175135816,2.3454227236,
2.5089755535\C,4.3716897148,2.3939601097,3.1219078007\H,3.7810026097,0
.0735494566,0.0753549333\H,6.0063610092,0.1458949281,1.1631435653\H,6.
3903909305,1.6355232987,3.1175732251\H,2.3048958819,2.9584139958,2.892
4433461\H,4.530310808,3.0449942589,3.9777105378\Version=IA64L-G03RevD
.01\State=1-A\HF=-754.6843944\S2=0.\S2-1=0.\S2A=0.\RMSD=4.183e-09\RMSF
=3.660e-06\Thermal=0.\Dipole=-0.1835205,0.0230823,-0.0857975\PG=C01 [X
(C16H25N1O1)]\@

TEMPO-CH(CH₃)Ph (B13)

1\1\GINC-AC58\FOpt\UB3LYP\6-31G(d)\C17H27N1O1\JOH501\05-Mar-2007\0\#\ U
B3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\temposty_5\0,1\N,-0
.1259116989,-0.0181174435,0.0838352392\O,1.2529054758,0.096103667,-0.3
594302327\C,1.7687722461,1.4467942487,-0.3094896804\C,-2.3824771418,-1
.6998857511,0.8266518606\H,-3.4213772151,-1.8097101551,1.1626372536\H,
-1.9889358607,-2.7172313672,0.7090065849\C,1.701971226,2.170151852,-1.
646112411\C,3.2232045057,1.3294359793,0.1614349391\C,0.7324241971,-1.9
562340899,1.5437249217\C,-0.2710910495,-1.977078021,-1.5729667006\C,-0
.1097573987,-0.6641650055,1.4430709323\C,-0.9033575683,-0.679359223,-1
.0195149788\C,0.4658652466,0.3562945021,2.4460029369\C,-1.0229252711,0
.3237314001,-2.1805877474\C,-1.5758640351,-0.9227777791,1.8633585172\C
, -2.336153684,-0.9420511901,-0.497872789\H,-2.0642471321,0.0468259764,
2.0315739721\H,-2.8386243199,0.026006278,-0.3661106507\H,-1.5636665759
, -1.4437795982,2.8289946655\H,-2.8854281069,-1.4795916252,-1.280884524
9\H,0.3218820605,-0.0128991973,3.4681950599\H,-1.7659502109,-0.0385621
908,-2.9013113976\H,-0.0467178611,1.3195161663,2.3552964313\H,-1.34460
69789,1.3030329633,-1.8132714352\H,1.537779858,0.5121127901,2.30385295
17\H,-0.0770438444,0.4502372706,-2.7085152761\H,0.8912008403,-2.210145
5847,2.5985669114\H,-0.7589446277,-2.2463531344,-2.5171902706\H,0.2560
602044,-2.8176230607,1.0706572511\H,-0.3756793136,-2.830155406,-0.8987
330176\H,1.7096741297,-1.8063600631,1.0787523394\H,0.792225193,-1.8241
743241,-1.7722520837\H,3.6878805923,2.3198901906,0.2105990707\H,3.2820
148478,0.8628959407,1.1492249845\H,3.8039888662,0.7187932808,-0.537902
5537\H,1.1808581005,2.0072298579,0.4217640364\C,2.2804586486,1.6140415
896,-2.7962946339\C,2.2583900392,2.3016831786,-4.0085803745\C,1.662625
4923,3.5636400845,-4.0894411584\C,1.1081173149,3.4327165621,-1.7393469
769\C,1.0881005338,4.1281405598,-2.9509790417\H,2.7361980364,0.6286808
07,-2.7414348698\H,2.7065097675,1.8540991206,-4.8921255651\H,1.6465934
072,4.1006288378,-5.034192507\H,0.6545845222,3.8760305176,-0.855308038
1\H,0.6201045429,5.1078305887,-3.0042819439\Version=IA64L-G03RevD.01\

State=1-A\HF=-793.9974364\S2=0.\S2-1=0.\S2A=0.\RMSD=3.868e-09\RMSF=8.6
94e-06\Thermal=0.\Dipole=-0.1015575,0.0869709,0.1207916\PG=C01 [X(C17H
27N1O1)]\@

TEMPO-C(CH₃)₂Ph (B14)

1\1\GINC-AC29\FOpt\UB3LYP\6-31G(d)\C18H29N1O1\JOH501\22-Nov-2007\0\#\n
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\tempocme2ph_1_2\0,1
\N,-0.0805445815,0.111699624,0.1402057715\O,1.3567065849,0.2905960185,
0.1941906628\C,1.9099782349,1.6440913949,0.0330083714\C,-2.361573366,-
1.7168664752,0.154287436\H,-3.4454017278,-1.8884304474,0.1423891122\H,
-1.8941714771,-2.7088523076,0.1847053166\C,2.7546865151,1.6501391871,-
1.2548829816\C,2.8834913228,1.815288362,1.2185697957\C,0.3705942054,-1
.7854141098,1.8245119736\C,0.4145436608,-1.8663132762,-1.4368546348\C,
-0.4691406337,-0.5423123434,1.4431781851\C,-0.4290727099,-0.6056842539
, -1.1405223878\C,-0.3036759068,0.4938157439,2.5699275949\C,-0.23929925
58,0.3752145083,-2.3122010404\C,-1.9739102666,-0.8944517391,1.37962143
01\C,-1.9371454687,-0.9523147882,-1.0959061969\H,-2.5490923255,0.04159
32293,1.3692476119\H,-2.5088180386,-0.0154234339,-1.1429352718\H,-2.23
66556234,-1.4173921886,2.3078071722\H,-2.1782166031,-1.5157957457,-2.0
058744646\H,-0.7093967569,0.0873664568,3.5036428663\H,-0.6182572115,-0
.0821982809,-3.233803547\H,-0.8487620254,1.4138437716,2.337711996\H,-0
.8010903272,1.2985738477,-2.1396486532\H,0.7462577701,0.7368051903,2.7
434748634\H,0.8100531105,0.6253454074,-2.4742339665\H,0.2065721169,-2.
0259250355,2.881469388\H,0.228432797,-2.1939913951,-2.4663766744\H,0.1
114304948,-2.6753521124,1.2472255464\H,0.1795275048,-2.7062251639,-0.7
801950074\H,1.434021958,-1.5806127442,1.6830576718\H,1.4791508767,-1.6
432615595,-1.3423263579\H,3.4952828012,2.7132604843,1.0802671606\H,2.3
407367565,1.910068137,2.1635640332\H,3.5557351506,0.9548132281,1.28731
03764\C,0.8566900726,2.7506759848,0.0728182342\C,3.5690545559,0.541917
9987,-1.5407688293\C,4.3929270421,0.522897068,-2.6644831777\C,4.429266
7135,1.6195133402,-3.5289989776\C,2.8056027972,2.7444520896,-2.1276677
243\C,3.6328067431,2.729561417,-3.254376835\H,3.5433673834,-0.31689851
3,-0.8778634792\H,5.0089232714,-0.3501363989,-2.8652030763\H,5.0713925
908,1.6071460019,-4.4057124329\H,2.1938930543,3.6211912528,-1.94239312
95\H,3.6486862937,3.5906905744,-3.9177517042\H,1.3575789786,3.72428099
33,0.0896504679\H,0.183830534,2.7200485032,-0.7849443152\H,0.256632413
8,2.6686424974,0.9787818272\Version=IA64L-G03RevD.01\State=1-A\HF=-83
3.3038485\S2=0.\S2-1=0.\S2A=0.\RMSD=3.237e-09\RMSF=3.792e-06\Thermal=0
.\Dipole=-0.1821098,0.06072,0.0199705\PG=C01 [X(C18H29N1O1)]\@

TEMPO-CH₂C(=O)OCH₃ (B15)

1\1\GINC-AC26\FOpt\UB3LYP\6-31G(d)\C12H23N1O3\JOH501\21-Nov-2007\0\#\n
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\tempoch2coome_1\0,1
\N,-0.3533728376,0.033145682,-0.0439144509\O,1.0375487401,0.3527447676
, -0.2910900179\C,1.2282428018,1.7345354975,-0.5064574935\C,-2.43932390
91,-1.861995416,0.5522793014\H,-3.4970131678,-2.0873786053,0.738045103
4\H,-1.9050187386,-2.8171354378,0.6276992091\C,2.2079429321,1.94843321
62,-1.6541402823\H,1.6243584905,2.2317071184,0.3899113529\C,0.51860783
51,-1.5907458806,1.7468829183\C,0.0773363823,-2.0729184289,-1.44744377
19\C,-0.4553447083,-0.4505066452,1.3689970083\C,-0.8167314178,-0.84419
88803,-1.1673777931\C,-0.1512128782,0.7552664311,2.2793529302\C,-0.839
2322832,0.0227416817,-2.4416345083\C,-1.9245615824,-0.8723708222,1.599
0710086\C,-2.2704739269,-1.2601228381,-0.8435475921\H,-2.5529992654,0.
0282360657,1.5731410171\H,-2.9110543141,-0.3711736355,-0.9228510254\H,
-2.00766127,-1.289494252,2.6105969031\H,-2.6043257935,-1.9620812767,-1
.6177566921\H,-0.393872725,0.509021978,3.319452872\H,-1.3256520827,-0.
528639611,-3.2547688113\H,-0.7475718813,1.623958435,1.9811495522\H,-1.
4056385705,0.9448779989,-2.2695891558\H,0.9082548568,1.0264703704,2.24
12568088\H,0.1725307951,0.2769699571,-2.7673947137\H,0.5611982383,-1.6
886915555,2.838091423\H,-0.209288633,-2.5196388272,-2.4067542014\H,0.2
197764627,-2.5612141548,1.3447761721\H,-0.0095478217,-2.8522082836,-0.
6868469999\H,1.5247628395,-1.3635396644,1.3860006046\H,1.1237073069,-1
.7659511752,-1.5170623071\O,2.5532331842,1.1256605381,-2.469726244\O,2

.6298997291,3.2328839395,-1.6475571473\C,3.5217756069,3.5934403227,-2.7158457611\H,3.7496841468,4.6486936359,-2.5633282978\H,4.4338416003,2.9924996336,-2.6721149559\H,3.0415057928,3.4396884659,-3.6859533625\H,0.2784800658,-2.2200496551,-0.7572585996\\Version=IA64L-G03RevD.01\State=1-A\HF=-751.5035121\S2=0.\S2-1=0.\S2A=0.\RMSD=9.305e-09\RMSF=2.734e-06\Thermal=0.\Dipole=-0.2360302,0.5719564,0.2410152\PG=C01 [X(C12H23N1O3)]\@

TEMPO-CH(CH₃)C(=O)OCH₃ (B16)

1\1\GINC-AC57\FOpt\UB3LYP\6-31G(d)\C13H25N1O3\JOH501\05-Mar-2007\0\#\UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\\tempoma_2\0,1\N,0.2430153038,-0.0974272162,0.3196882292\O,1.4928467647,-0.2620818006,1.0426696228\C,2.1978461328,0.9710826789,1.2316959175\C,-2.2658798757,-1.170521897,-0.6569311312\H,-3.2087235987,-1.0375557184,-1.2021996693\H,-2.2576949893,-2.2103134631,-0.3071762242\C,3.2355137249,1.2077771592,0.1271469348\C,2.9398802367,0.8538237616,2.563045366\C,-0.7958223974,-1.5570243906,2.1644619278\C,0.6720018465,-2.4678797416,-0.5852550715\C,-0.8731027953,-0.2709336297,1.3098452169\C,0.2933313951,-0.997592505,-0.8805017725\C,-0.8475382521,0.9369850001,2.2673956699\C,1.3477223666,-0.4274642907,-1.8473720589\C,-2.2032290349,-0.2026206697,0.5234656123\C,-1.0811951968,-0.903242854,-1.5837814066\H,-2.3297013394,0.8210787575,0.1458157023\H,-1.1846355511,0.1056823306,-2.006176051\H,-3.0239020256,-0.3852079903,1.2285764591\H,-1.0763376351,-1.6024586719,-2.4292482597\H,-1.7524453939,0.9333782504,2.8859743732\H,1.2349257319,-0.8969188738,-2.8316457639\H,-0.8208554391,1.8770394348,1.7067543984\H,1.2145712016,0.6532956481,-1.9638239067\H,0.0104919993,0.9035534104,2.944282485\H,2.3629927646,-0.62673799,-1.4988838274\H,-1.4782895632,-1.4726977171,3.0183731979\H,0.934415952,-2.9692841982,-1.5242025147\H,-1.0774183164,-2.4546325107,1.6105280822\H,-0.1360630487,-3.0422106859,-0.1262177107\H,0.2170523556,-1.6952117514,2.5506675874\H,1.5435365843,-2.5069350245,0.072729833\H,3.5113798944,1.7658316225,2.7692322153\H,2.2315919855,0.6911581324,3.3801055964\H,3.6359225518,0.0114318068,2.5197365683\O,4.1465395657,0.4555138038,-0.1416089525\O,3.0373176423,2.3956525861,-0.4847116144\C,3.9964399367,2.7307201602,-1.5028198133\H,3.7098053906,3.7197283537,-1.8612851979\H,5.0071624518,2.7477950158,-1.0866392921\H,3.9594052351,2.0009481986,-2.3158216292\H,1.4912454384,1.8015274788,1.2311508718\\Version=IA64L-G03RevD.01\State=1-A\HF=-790.8184338\S2=0.\S2-1=0.\S2A=0.\RMSD=4.718e-09\RMSF=3.483e-06\Thermal=0.\Dipole=-0.5199074,0.6094741,-0.0996684\PG=C01 [X(C13H25N1O3)]\@

TEMPO-C(CH₃)₂C(=O)OCH₃ (B17)

1\1\GINC-AC52\FOpt\UB3LYP\6-31G(d)\C14H27N1O3\JOH501\03-Mar-2007\0\#\UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\\tempomma_1\0,1\N,0.0578612229,-0.248460883,-0.3668814342\O,1.2844978106,-0.4807004414,0.3712373302\C,2.4674454081,-0.8755499611,-0.3731449516\C,-2.733241296,0.5940242933,-0.3327119396\H,-3.6851354305,0.7564759951,-0.8539913508\H,-2.9001776172,0.8904878647,0.7102134426\C,3.4615599372,0.3090150013,-0.4337205684\C,2.2209326173,-1.4007189351,-1.784562247\C,3.1393920923,-1.9443207869,0.5118040031\C,-0.1354119178,1.8933111496,1.046869032\C,-1.0650200918,-1.1386662202,1.7734508686\C,-0.2357116185,1.2296632516,-0.3453934231\C,-0.962688567,-1.1839606284,0.2298809963\C,0.7703978806,1.9345922519,-1.2751978465\C,-0.5864531844,-2.6215096124,-0.1729235689\C,-1.6360804229,1.4424817495,-0.9690261889\C,-2.3309350402,-0.8756327756,-0.4214661976\H,-1.5791401478,1.1983482241,-2.0387218924\H,-2.2849980777,-1.1644978646,-1.4804352067\H,-1.8741531199,2.5113648674,-0.9010380517\H,-3.0825596091,-1.5206608007,0.0506716974\H,0.4437102619,2.9666678736,-1.4481786593\H,-1.3814262421,-3.308554,0.1391996186\H,0.8320752062,1.4319160712,-2.2448340495\H,-0.4721767324,-2.7036780394,-1.2576540201\H,1.7679839722,1.9844050075,-0.8371644807\H,0.33955417,-2.946792459,0.3072197085\H,-0.1253329582,2.9836030091,0.9297181624\H,-1.6314333152,-2.0085568448,2.1259781346\H,-0.9715759228,1.6455997009,1.704016911\H,-1.5755821907,-0.2479140036,2.1448867971\H,0.7934150113,1.5936448977,1.5374449262\H,-0.069518709,-1.1757018629,2.2210950992\H,3.1854

62721,-1.5968704438,-2.2585044948\H,1.6458971797,-2.3269240862,-1.7512
990664\H,1.6791192311,-0.6781214278,-2.3948317408\H,4.1354345079,-2.19
29211874,0.1285696585\H,3.2386270879,-1.5740253087,1.5355266647\H,2.53
53946667,-2.856039083,0.5220269463\O,4.1737049492,0.5699798067,-1.3797
339701\O,3.512719435,0.9824690002,0.7360756573\C,4.469550763,2.0532327
655,0.784848063\H,4.3958837459,2.4643229353,1.7920307674\H,5.478107215
4,1.6773891883,0.5930149113\H,4.2294879512,2.8173327515,0.040385953\Version=IA64L-G03RevD.01\State=1-A\HF=-830.1275044\S2=0.\S2-1=0.\S2A=0.
\RMSD=7.032e-09\RMSF=5.939e-06\Thermal=0.\Dipole=-0.3554103,0.0969234,
0.4609248\PG=C01 [X(C14H27N1O3)]\@

TEMPO-CH(CH₃)OC(=O)CH₃ (B18)

1\1\GINC-AC52\FOpt\UB3LYP\6-31G(d)\C13H25N1O3\JOH501\07-Mar-2007\0\#\n
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\tempovac_9\0,1\N,0.
0393559678,0.0521560145,-0.0202626413\O,1.496290553,0.0817553053,-0.08
49565937\C,2.029466628,1.3702010575,0.0113542782\C,-2.4290441278,-1.45
26461686,0.1795762333\H,-3.5247212754,-1.477972349,0.232547133\H,-2.09
66342522,-2.4973779148,0.2219604284\O,2.1375824787,1.9312816661,-1.330
2502164\C,3.4266979089,1.2586132958,0.5959117956\C,0.3646866023,-1.844
2052219,1.692688238\C,0.2202908679,-2.0057877007,-1.5525551257\C,-0.32
83071046,-0.5122791239,1.3248046628\C,-0.449775923,-0.6437029674,-1.25
86952123\C,0.0571250889,0.531028851,2.392895964\C,-0.1818990264,0.2829
206351,-2.4585072849\C,-1.8675641555,-0.6568229441,1.3564840013\C,-1.9
839323759,-0.7936184009,-1.1245512655\H,-2.309783731,0.3484974628,1.34
48335755\H,-2.4345002482,0.2063011645,-1.1841108907\H,-2.1455634269,-1
.1156068032,2.3135579397\H,-2.3446013682,-1.3565052911,-1.9943816479\H
, -0.3624426134,0.2350491332,3.3611361434\H,-0.6914447062,-0.1135408164
, -3.3447112727\H,-0.3393728849,1.5182611023,2.1351026044\H,-0.56564258
04,1.2883578563,-2.2576861094\H,1.1411992599,0.6069223965,2.5180234999
\H,0.8842608916,0.3592181044,-2.6764282595\H,0.2376636167,-2.036912108
2,2.7643975163\H,-0.0133906376,-2.309832421,-2.579351736\H,-0.0430432
002,-2.7042980641,1.1580332607\H,-0.1190012537,-2.8066043052,-0.892046
1199\H,1.4359167019,-1.786815397,1.4842416446\H,1.3062087744,-1.922435
5152,-1.4639606832\H,3.8851067895,2.2501583489,0.6426664805\H,3.385721
7588,0.8406100688,1.6059884165\H,4.0415099418,0.6054009087,-0.03080324
23\H,1.3788859125,2.0275054013,0.5846867711\C,2.0517695059,3.276826328
1,-1.4443120695\O,1.9459242292,4.0338240575,-0.5024740811\C,2.11031208
32,3.695888956,-2.8954677638\H,2.1058895935,4.7845552952,-2.9596850728
\H,3.0120432739,3.2952639567,-3.369513287\H,1.2492864634,3.2890169672,
-3.4364800115\Version=IA64L-G03RevD.01\State=1-A\HF=-790.8371549\S2=0
.\S2-1=0.\S2A=0.\RMSD=3.011e-09\RMSF=3.563e-06\Thermal=0.\Dipole=-0.22
85731,-0.6475953,-0.2353891\PG=C01 [X(C13H25N1O3)]\@

TEMPO-CH(CH₃)Cl (B19)

1\1\GINC-AC3\FOpt\UB3LYP\6-31G(d)\C11H22Cl1N1O1\JOH501\06-Mar-2007\0\#\n
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\tempovcl_1\0,1\N,
-0.1957971342,0.0806466301,-0.0208804114\O,1.2400201239,0.3140437577,0
.1379894307\C,1.5880691996,1.6490140696,0.2494773774\C,-2.4562506619,-
1.7349844466,-0.0126193158\H,-3.5330703354,-1.9055403157,-0.1351448927\H
, -2.0178472677,-2.7110966251,0.2294881954\C1,2.0257168219,2.448974705
4,-1.3959037959\C,2.8213622834,1.753095262,1.128390561\C,0.0531175305,
-1.5324619109,1.9770720129\C,0.5058493254,-2.1143813142,-1.1737022619\C
, -0.7227020996,-0.3706683537,1.3158985742\C,-0.359443189,-0.832684711
4,-1.2067664456\C,-0.6821051907,0.8317002538,2.2815017422\C,0.01793449
6,-0.040472126,-2.4696118425\C,-2.21297724,-0.7354166128,1.1163944742\C
, -1.8639277659,-1.1790369993,-1.3059203194\H,-2.7675116683,0.18643341
09,0.8950345473\H,-2.409686048,-0.267142065,-1.5826348962\H,-2.5968203
98,-1.1155420054,2.0713220183\H,-1.9891310021,-1.887528838,-2.13377633
54\H,-1.2456215157,0.5865693382,3.1888397511\H,-0.2914398736,-0.606058
8139,-3.3565000847\H,-1.1401129931,1.7154078766,1.8255773128\H,-0.4828
425745,0.9316211777,-2.4827528807\H,0.3368114125,1.0784841591,2.592916
2452\H,1.0936439991,0.1309156162,-2.5331966879\H,-0.2474626914,-1.6179
930045,3.0277843617\H,0.5134248829,-2.5665133765,-2.1720085171\H,-0.13

55255292,-2.4982991641,1.5056267891\H,0.1369924085,-2.871784808,-0.478
5770172\H,1.1290305904,-1.3422603811,1.9483281993\H,1.5380333307,-1.87
3724356,-0.907740636\H,3.1553898884,2.7904793973,1.2000159747\H,2.5900
736222,1.3787672094,2.1316761253\H,3.6307515322,1.1490779874,0.7094153
272\H,0.7470737306,2.2517093966,0.5817073202\\Version=IA64L-G03RevD.01
\State=1-A\HF=-1022.5502512\S2=0.\S2=1=0.\S2A=0.\RMSD=6.620e-09\RMSF=1
.056e-05\Thermal=0.\Dipole=-0.5919315,-0.6119132,0.9158416\PG=C01 [X(C
11H22Cl1N1O1)]\@

DBN-CH(CH₃)Ph (A13)

1\1\GINC-AC58\FOpt\UB3LYP\6-31G(d)\C16H27N1O1\JOH501\26-Jun-2007\0\#\#
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\dbnphet_8\0,1\N,-0.
1721924339,-0.5917551173,0.8632665839\O,0.9338550981,-0.6194911882,-0.
0847455183\C,-1.3789855271,-0.0916382067,0.0852287421\C,0.3313777955,0
.1341664602,2.0944970072\C,-0.6104025896,-0.1584549635,3.2871515616\C,
1.6886982384,-0.482652182,2.4865929288\C,0.5405253726,1.6536007028,1.9
244036031\C,-2.55464189,0.2754273205,1.0102489203\C,-1.0932758577,1.10
5357715,-0.8496829604\C,-1.8689145179,-1.2753190618,-0.7796801208\H,2.
0141644177,-0.0464419356,3.4370796929\H,1.5950721686,-1.5639114084,2.6
279365101\H,2.4579213282,-0.2873877367,1.7401110671\H,1.0325652731,2.0
6170869,2.8154927732\H,1.1819633698,1.8601250863,1.0621945524\H,-0.400
1621885,2.1965628113,1.7978733296\H,-0.0839479482,0.0744013889,4.21930
68252\H,-1.5264490102,0.4307255406,3.285323653\H,-0.8782966319,-1.2198
162599,3.3063068604\H,-2.8102082037,-1.0068728352,-1.2730800032\H,-1.1
576315665,-1.5368632085,-1.5642642502\H,-2.0485821002,-2.1575554983,-0
.1558542488\H,-1.9801139527,1.2971156218,-1.4652318851\H,-0.8708835403
,2.0226804885,-0.3001792973\H,-0.2584134215,0.8887622997,-1.5173192596
\H,-3.4314076415,0.4602582086,0.3803414856\H,-2.8064337655,-0.53874020
83,1.6956409135\H,-2.3796648493,1.1865995007,1.5868999809\C,1.25992632
5,-1.9432985161,-0.5686619128\H,0.486979093,-2.6300218449,-0.212783295
7\C,1.2827361358,-1.9269175517,-2.0920502866\C,2.629988151,-2.40753982
45,-0.0507437591\H,2.9097987355,-3.3469207115,-0.5402969924\H,3.398371
1901,-1.6641151198,-0.2899962851\H,2.6230779171,-2.5718852088,1.028335
4042\C,1.7815008221,-0.8195606884,-2.7911235124\C,1.858967566,-0.83435
60844,-4.1841670535\C,1.4465012578,-1.9599305125,-4.9004061223\C,0.872
9982698,-3.0512749548,-2.8194761471\C,0.9535983978,-3.0700728607,-4.21
31319259\H,2.1003514557,0.0575919426,-2.236356528\H,2.2435339721,0.035
127847,-4.7113481968\H,1.506696307,-1.9706581479,-5.9854706452\H,0.482
1128207,-3.9186206053,-2.2909587769\H,0.6252961582,-3.9497491829,-4.76
08734111\\Version=IA64L-G03RevD.01\State=1-A\HF=-755.8731457\S2=0.\S2=
1=0.\S2A=0.\RMSD=9.890e-09\RMSF=4.344e-06\Thermal=0.\Dipole=-0.0978809
, -0.0615473,0.0782945\PG=C01 [X(C16H27N1O1)]\@

DBN-CH(CH₃)C(=O)OCH₃ (A16)

1\1\GINC-AC25\FOpt\UB3LYP\6-31G(d)\C12H25N1O3\JOH501\08-Feb-2009\0\#\#
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\dbnma_4\0,1\C,0.948
1694763,-0.3941505691,-0.3182174219\C,-0.5024916607,-0.6766487815,-0.7
751008992\C,-1.2610330284,0.6421157441,-1.0308856028\N,-1.1576103121,-
1.6241202539,0.2087386729\C,-1.6599614997,-1.1523700079,1.561314609\C,
-1.8667232293,-2.4222915793,2.4184326411\O,-2.3313454072,-2.1896926795
, -0.449380238\C,-2.299637515,-3.6219827544,-0.5323413573\H,-1.60757067
04,-4.0112199389,0.2150311111\C,-0.6112100542,-0.3011941886,2.29889115
67\C,-2.9946309602,-0.3721395828,1.516974361\C,-0.3796169123,-1.415915
2539,-2.1218339783\C,-3.7297852357,-4.1206135488,-0.314449407\C,-1.852
9955127,-4.111011742,-1.9181686288\O,-0.7656618789,-4.9096968241,-1.83
07406917\C,-0.3109810984,-5.4656389129,-3.0771342085\O,-2.423228452,-3
.8644795121,-2.9579086417\H,0.2171936628,-0.8060605855,-2.8083870809\H
,0.1367563896,-2.3724297224,-1.9896509343\H,-1.3503977758,-1.595231703
4,-2.5822469627\H,-0.7880048204,1.1838841046,-1.8585679962\H,-2.299479
2791,0.4419417701,-1.3113885016\H,-1.2538099316,1.3084992203,-0.163508
084\H,1.5069697597,0.0292141244,-1.1600881306\H,1.0245758344,0.3177218
928,0.502910856\H,1.4394758557,-1.3258000607,-0.0193306053\H,-2.120974
0076,-2.1391267742,3.4460539614\H,-2.6832152538,-3.0425187724,2.044086

3784\H,-0.9517836065,-3.0233016854,2.443408393\H,-3.3680307274,-0.2382
247398,2.539083165\H,-2.8836068587,0.6208706307,1.0760943544\H,-3.7472
55769,-0.919835762,0.9470397288\H,-0.9659006372,-0.1398745524,3.322667
6555\H,0.3568526325,-0.8066753074,2.3585823612\H,-0.4721632899,0.68483
44767,1.8504991516\H,-3.7719317587,-5.213602889,-0.3845448815\H,-4.100
6327029,-3.8188322843,0.6685116739\H,-4.3818060646,-3.7013652942,-1.08
58381815\H,0.539961291,-6.0980605695,-2.8227743588\H,-1.1040919315,-6.
0538216046,-3.5461992286\H,-0.0080520601,-4.6688445268,-3.7615222096\\
Version=IA64L-G03RevE.01\State=1-A\HF=-752.6945905\S2=0.\S2-1=0.\S2A=0
.\RMSD=2.603e-09\RMSF=2.498e-06\Thermal=0.\Dipole=0.5409011,-0.2615336
,0.4616348\PG=C01 [X(C12H25N1O3)]\@

DBN-C(CH₃)₂C(=O)OCH₃ (A17)

1\1\GINC-AC30\FOpt\UB3LYP\6-31G(d)\C13H27N1O3\JOH501\09-Nov-2007\0\#\#
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\dbnmma_2\0,1\N,-0.1
300336869,0.0531678348,-0.0367224621\O,1.3232437685,0.05303412,-0.0802
538782\C,-0.5460177136,1.5143561759,0.0579328837\C,-0.5184272728,-0.93
98715335,1.0466878571\C,-1.9971483363,-1.3496941939,0.8489688261\C,0.3
016402585,-2.2314322759,0.8455328955\C,-0.2655272866,-0.4720592759,2.4
96694158\C,-2.0217382145,1.6781288131,0.4710646365\C,0.3342913716,2.36
41908496,1.0027862486\C,-0.4532042674,2.1034753045,-1.3667602537\H,-0.
0683602683,-2.9928001686,1.5404376533\H,0.1869367057,-2.6255178938,-0.
1683679721\H,1.3604127891,-2.0750244037,1.0490990311\H,-0.460695578,-1.
2999019786,3.1889192798\H,0.7768172071,-0.1654367421,2.6263754263\H,-
0.9114818428,0.3570378068,2.7962163634\H,-2.1928317019,-2.2649133823,1.
4186673369\H,-2.7131372188,-0.6041539699,1.1916145422\H,-2.1922664726
, -1.5591494226,-0.2077949215\H,-0.7865445676,3.1476149103,-1.355384865
8\H,0.5592962527,2.0964146515,-1.7703191887\H,-1.0992089926,1.54951031
79,-2.0553092215\H,0.0469088326,3.4181349876,0.9076422077\H,0.20904340
3,2.0838722469,2.0508015248\H,1.3894087908,2.2677663228,0.7440495188\H
, -2.2810427175,2.7376111165,0.3707027609\H,-2.6937617119,1.1129966553,
-0.1808995338\H,-2.2155542941,1.4003488903,1.5090070544\C,1.965036227,
-0.287970522,-1.341498549\C,1.0539370519,-0.8782278401,-2.4143030545\C
, 2.657256744,0.9794059153,-1.8978503346\C,3.1038680373,-1.2644983649,-
0.982569025\H,3.7866672925,-1.3837490899,-1.831623312\H,3.6706798408,-
0.8801682206,-0.1304601783\H,2.6980692537,-2.2467187579,-0.729174976\H
, 1.6562296078,-1.0968196311,-3.2999556554\H,0.5952888803,-1.8030459322
, -2.0614212722\H,0.2625516979,-0.1886105475,-2.7045819018\O,2.68356213
4,1.3024609041,-3.0670118678\O,3.3063602636,1.6613799377,-0.9306885582
\C,4.0268747643,2.8223258501,-1.37585834\H,4.5008786554,3.231178866,-0.
.483150381\H,4.7780941237,2.5466556519,-2.1207546481\H,3.3433881903,3.
553236018,-1.8163858537\\Version=IA64L-G03RevD.01\State=1-A\HF=-792.00
36053\S2=0.\S2-1=0.\S2A=0.\RMSD=4.711e-09\RMSF=2.490e-06\Thermal=0.\Di
pole=0.0314046,0.0340805,0.5744539\PG=C01 [X(C13H27N1O3)]\@

DBN-CH(CH₃)C(=O)OH (A20)

1\1\GINC-AC29\FOpt\UB3LYP\6-31G(d)\C11H23N1O3\JOH501\10-Feb-2009\0\#\#
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\dbnaa_3\0,1\C,0.991
1639165,-0.1296358005,-0.0306605636\C,-0.3545100166,-0.5789477729,-0.6
473520947\C,-1.2085515925,0.6439501416,-1.0418299411\N,-1.0214670193,-
1.564205257,0.2908186143\C,-1.7444132968,-1.1082377606,1.5455653331\C,
-1.9338357586,-2.365349381,2.4253547632\O,-2.0307155611,-2.2857127049,
-0.4798648314\C,-1.8313634475,-3.7052667544,-0.481180939\H,-1.21993986
8,-3.9858636331,0.3768702189\C,-0.8914950162,-0.1313099125,2.374354190
1\C,-3.1340579515,-0.4760414293,1.2969089122\C,0.0101018881,-1.3340204
286,-1.9402185399\C,-3.215137653,-4.3569224834,-0.4459539452\C,-1.1326
433079,-4.1904358582,-1.7587926721\O,0.0187185475,-4.8537607117,-1.484
5169879\O,-1.5581796757,-4.0581600389,-2.883723175\H,0.6101589049,-0.6
753788768,-2.577110855\H,0.6145547799,-2.2184212642,-1.7141735266\H,-0.
.872254365,-1.6388133403,-2.5017767136\H,-0.6945441788,1.2129516478,-1.
.8255074264\H,-2.178295885,0.3284856201,-1.4384414878\H,-1.377744508,1.
.3275602763,-0.2049895883\H,1.6011040187,0.3334100788,-0.814106335\H,0.
.8906535822,0.604027815,0.7683973675\H,1.5368381243,-0.9957042111,0.35

74461756\H,-2.3429416997,-2.0764733236,3.3999742386\H,-2.6327311567,-3.0777713215,1.9827346761\H,-0.9755019969,-2.8684370174,2.5910912481\H,-3.6594016045,-0.3731940543,2.253705088\H,-3.0679539985,0.5189045423,0.851421419\H,-3.7370751884,-1.1076898853,0.6419777193\H,-1.3921269226,0.0224631252,3.3364362366\H,0.1050963289,-0.5331926866,2.5782906394\H,-0.7914373649,0.8505166188,1.9069619797\H,-3.1288936387,-5.4492985069,-0.4647710564\H,-3.7565825493,-4.0639795547,0.4571949408\H,-3.7868242471,-4.0414436267,-1.3231607763\H,0.3683873778,-5.1550682693,-2.3456583051\\Version=IA64L-G03RevE.01\\State=1-A\\HF=-713.3875204\\S2=0.\\S2-1=0.\\S2A=0.\\RMSD=8.164e-09\\RMSF=3.705e-06\\Thermal=0.\\Dipole=0.3258008,-0.0492513,0.6033256\\PG=C01 [X(C11H23N1O3)]\\@

DBN-CH(CH₃)C(=O)NH₂ (A23)

1\\1\\GINC-AC25\\FOpt\\UB3LYP\\6-31G(d)\\C11H24N2O2\\JOH501\\08-Feb-2009\\0\\#
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\\dbnam_3\\0,1\\C,1.0992943359,-0.1266703898,0.5521789976\\C,-0.0464797968,-0.599998232,-0.3745490629\\C,-0.7569369075,0.6108497116,-1.0161266736\\N,-0.9406762479,-1.5538133579,0.4032856389\\C,-1.9614434142,-1.0348885839,1.4008578822\\C,-2.4054762582,-2.241929197,2.2520261997\\O,-1.7347660762,-2.322149597,-0.5517000206\\C,-1.2530847218,-3.6628407166,-0.7777288694\\H,-0.1741738143,-3.6883190727,-0.6186882251\\C,-1.3396927633,-0.0184547665,2.3756250271\\C,-3.2302093282,-0.4128607068,0.7689827025\\C,0.6496567447,-1.3816757273,-1.5102362574\\C,-1.9065113921,-4.7328312292,0.1012165004\\C,-1.496869643,-4.0298212326,-2.2556374358\\N,-2.2497337144,-3.1459859364,-2.9637569597\\O,-1.0617091684,-5.0760091632,-2.7169355772\\H,1.3449999894,-0.7058354235,-2.0184643748\\H,1.2364834003,-2.2192665544,-1.121171504\\H,-0.0523601704,-1.7534133209,-2.2573928115\\H,-0.0505967078,1.1576516659,-1.6516831067\\H,-1.5911063307,0.2888937645,-1.6478131762\\H,-1.1367050202,1.3173526916,-0.2737972585\\H,1.9037923861,0.2910898226,-0.0629294241\\H,0.8060960227,0.6475169847,1.2598510711\\H,1.5060068378,-0.9747452229,1.1120606575\\H,-3.0291915253,-1.8975090639,3.0844613501\\H,-2.9948985094,-2.9492207553,1.6682891569\\H,-1.5359492097,-2.7627873694,2.6655785303\\H,-3.9703105654,-0.2355848331,1.5579922316\\H,-3.0386376179,0.544941573,0.2813232502\\H,-3.6746209864,-1.0933509774,0.0399013358\\H,-2.070886197,0.1831486413,3.1655899777\\H,-0.4367760847,-0.4113229945,2.851717729\\H,-1.1072092033,0.9398807524,1.90660646\\H,-1.5923118497,-5.7143871306,-0.2646413173\\H,-1.599234232,-4.6314459663,1.1434574995\\H,-2.9988860542,-4.6740202943,0.0423138807\\H,-2.4293266902,-3.3327664786,-3.9397271307\\H,-2.534455516,-2.2743973133,-2.5425688933\\Version=IA64L-G03RevE.01\\State=1-A\\HF=-693.5228355\\S2=0.\\S2-1=0.\\S2A=0.\\RMSD=3.720e-09\\RMSF=2.270e-06\\Thermal=0.\\Dipole=-0.3443664,1.4085006,0.3836023\\PG=C01 [X(C11H24N2O2)]\\@

TEMPO-CH(CH₃)C(=O)OH (B20)

1\\1\\GINC-AC30\\FOpt\\UB3LYP\\6-31G(d)\\C12H23N1O3\\JOH501\\07-Feb-2009\\0\\#
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\\tempoaa_1\\0,1\\C,-0.6836837969,0.0589152655,-0.1654759858\\C,0.3163605981,0.7396074294,0.767282278\\C,1.5339511131,1.1799647135,-0.0423633346\\C,2.2130777701,0.0257421406,-0.8174110909\\N,1.1490795237,-0.6556776838,-1.6323169719\\C,-0.0918402943,-1.1415317701,-0.9402492859\\O,1.766726975,-1.8039707612,-2.275851396\\C,1.9592334396,-1.6200154231,-3.6825172613\\C,3.2221024762,-2.393279604,-4.0622675703\\C,3.0004349027,-0.9001781468,0.1386393176\\C,3.2196975486,0.6651761686,-1.7943448266\\C,0.1086996284,-2.3622142116,-0.0126074898\\C,-1.1088731659,-1.5399167024,-2.0255622793\\C,0.791013266,-2.1934759771,-4.4931816717\\O,0.2383705329,-1.2636853602,-5.310138444\\O,0.4137398553,-3.3431738929,-4.459348794\\H,-0.1485987676,1.6089816743,1.2489380447\\H,0.6132052807,0.0625142232,1.5777688258\\H,1.2179155636,1.9438311437,-0.765702124\\H,-1.0457569044,0.7965071958,-0.8946144009\\H,2.2900737431,1.6461269543,0.6018387509\\H,-1.5607887339,-0.2964721067,0.3894235359\\H,3.9029727381,1.3190545247,-1.2402079187\\H,-2.1003188677,-1.6579556488,-1.5727802573\\H,2.7021678726,1.270990013,-2.5453383757\\H,-1.1726431651,-0.7647414941,-2.7963130305\\H,3.830247795,-0.0856391823,-2.3036611816\\H,-0.8441053106,-2.4894307435,-2.4948830959\\H,3.909906

408,-0.3898813372,0.4767992528\H,-0.8691446703,-2.7863714126,0.2439237
132\H,2.433702334,-1.1776927103,1.0299412384\H,0.6122145441,-2.1165272
237,0.9248136824\H,3.296950002,-1.8155657677,-0.3793001292\H,0.6868655
609,-3.1350096188,-0.5251125073\H,3.4223390016,-2.3047198709,-5.135897
0462\H,4.0830299136,-2.0059394025,-3.5106619369\H,3.0884793307,-3.4514
011397,-3.8205651558\H,2.0502607716,-0.5565363979,-3.9053671973\H,-0.4
678058127,-1.7231628567,-5.8047598803\\Version=IA64L-G03RevE.01\State=
1-A\HF=-751.5112862\S2=0.\S2-1=0.\S2A=0.\RMSD=5.909e-09\RMSF=5.139e-06
\Thermal=0.\Dipole=0.0961794,0.727132,0.005603\PG=C01 [X(C12H23N1O3)]\
\@

TEMPO-CH(CH₃)C(=O)NH₂ (B23)

1\1\GINC-AC30\FOpt\UB3LYP\6-31G(d)\C12H24N2O2\JOH501\07-Feb-2009\0\#\
UB3LYP/6-31G* OPT FREQ=norman maxdisk=268435456\\tempoam_2\0,1\C,-0.
6040536146,0.2432595063,-0.2551671707\C,0.4115963098,0.7407441921,0.77
18935432\C,1.7298090389,1.0465197271,0.0632597309\C,2.2999397517,-0.14
78741601,-0.7376566689\N,1.2113185523,-0.6353422536,-1.6490675249\C,-0.
1223335275,-0.9908425434,-1.0552631173\O,1.7325038487,-1.7921950639,-
2.3577919068\C,1.6155959238,-1.6804896705,-3.7926690585\C,2.9580356493
, -1.4030699268,-4.476839868\C,2.8973001789,-1.2185901498,0.2058969618\
C,3.4447860983,0.3928678637,-1.6129577198\C,-0.1476998158,-2.257644191
6,-0.1682608354\C,-1.1208246033,-1.2047452171,-2.2103090119\C,1.035867
9271,-2.9831165993,-4.3749586887\N,1.0050956126,-4.0412638689,-3.52113
52828\O,0.6848982996,-3.0414640137,-5.545591351\H,0.0332207261,1.64379
11463,1.2669192632\H,0.5595238959,-0.0028622254,1.5650452067\H,1.57010
84378,1.881421009,-0.6321668162\H,-0.813624266,1.0538493692,-0.9658068
955\H,2.4957110373,1.3709622111,0.7786707133\H,-1.5568404456,-0.013745
3977,0.2240893482\H,4.1501239911,0.9528972584,-0.9881938908\H,-2.13659
95569,-1.2733086861,-1.804189491\H,3.0558090893,1.0676513802,-2.382304
3055\H,-1.0918956323,-0.3655463058,-2.9122965242\H,3.9959468574,-0.415
7117451,-2.0972067222\H,-0.9263878695,-2.1307214117,-2.757293877\H,3.8
378634285,-0.8467896967,0.6286619905\H,-1.1875013364,-2.5513502915,0.0
154911787\H,2.244061453,-1.4715151771,1.0436268397\H,0.3270030077,-2.1
137534342,0.803767645\H,3.1181858001,-2.1334995038,-0.3500439921\H,0.3
482468477,-3.0939371366,-0.6673040602\H,2.8294296057,-1.5011795736,-5.
5585159927\H,3.3154474261,-0.395982642,-4.2551970991\H,3.7119922885,-2
.1267378666,-4.1475144736\H,0.9109067016,-0.8804510024,-4.0254666453\H
,0.6389654014,-4.9231636728,-3.849270382\H,1.2692174817,-3.9203512359,
-2.5551430492\\Version=IA64L-G03RevE.01\State=1-A\HF=-731.6468528\S2=0
.\S2-1=0.\S2A=0.\RMSD=5.951e-09\RMSF=5.808e-06\Thermal=0.\Dipole=0.119
9968,0.0926385,1.5212099\PG=C01 [X(C12H24N2O2)]\@

PROXYL-CH(CH₃)Ph (I13)

1\1\GINC-AC2\FOpt\UB3LYP\6-31G(d)\C16H25N1O1\JOH501\23-Jun-2007\0\#\ U
B3LYP/6-31G* OPT FREQ=norman maxdisk=402653184\\proxylphet_7\0,1\N,0
.1174978842,0.2003582174,0.0471065593\C,1.6211539696,0.3225002868,0.10
49170738\C,1.8640198243,1.7956295828,-0.3342073373\C,-0.4680297129,1.3
055251266,-0.7652067097\C,0.4740133339,2.4513450066,-0.3551314871\H,0.
2008930771,2.8101667909,0.644362276\H,0.4106651904,3.301530899,-1.0424
815162\C,-0.4332297012,1.0604751384,-2.2879713738\C,2.3675134196,-0.66
26384668,-0.8082172103\C,-1.9143586012,1.5540143259,-0.3199215817\C,2.
0534617526,0.1036232842,1.5648741938\H,3.438722907,-0.4277275566,-0.78
87428727\H,2.2408318011,-1.6941123794,-0.4716688101\H,2.023842022,-0.5
982629627,-1.8447127795\O,-0.3173699133,-1.0672157821,-0.4601285152\H,
3.1417958994,0.2006224276,1.6664692312\H,1.578093917,0.8404953706,2.22
18644924\H,1.7654091042,-0.8934510962,1.9114116093\H,-0.9451459899,0.1
269557421,-2.534702685\H,-0.9394983422,1.880799616,-2.8103632553\H,0.5
87747362,0.9989588837,-2.6768041388\H,-2.5597110632,0.7101224596,-0.58
8344413\H,-1.9628144139,1.6948211986,0.7648661155\H,-2.3203902534,2.44
89203746,-0.8065643921\H,2.310706478,1.8205999575,-1.3344323375\H,2.55
84173187,2.3091855862,0.3385906347\C,-1.0919770405,-1.8017524775,0.512
4835802\C,-2.2300952271,-2.4755085226,-0.2595276278\C,-0.2517471595,-2
.8209800787,1.2663092886\H,-1.4992317084,-1.0779569234,1.2250204867\C,

-0.3256912246,-2.9132278703,2.6603806145\C,0.4084125776,-3.8785131118,
3.3543356391\C,1.231647062,-4.7636772713,2.6582868011\C,0.5761846686,-
3.7183481551,0.576465354\C,1.3147053789,-4.6794039517,1.2657469177\H,-
0.961212596,-2.2209135808,3.2086306805\H,0.34028706,-3.9336379821,4.43
78110876\H,1.807022476,-5.5129697246,3.1955589217\H,0.6455436935,-3.65
27771793,-0.5059573439\H,1.9553295419,-5.3647704959,0.7165434124\H,-2.
8532911425,-3.0686985884,0.41811281\H,-2.8573159252,-1.7247308583,-0.7
509248992\H,-1.8308677049,-3.1469652592,-1.0273464939\Version=IA64L-G
03RevD.01\State=1-A\HF=-754.6894032\S2=0.\S2-1=0.\S2A=0.\RMSD=3.582e-0
9\RMSF=3.124e-06\Thermal=0.\Dipole=-0.0215974,0.1017176,0.0799793\PG=C
01 [X(C16H25N1O1)]\@

PROXYL-CH(CH₃)C(=O)OCH₃ (I16)

1\1\GINC-AC26\FOpt\UB3LYP\6-31G(d)\C12H23N1O3\JOH501\07-Feb-2009\0\#\#
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\proxylma_4\0,1\C,0.
7266814226,0.090380667,1.0698452822\C,0.752854411,-1.2392608534,0.3025
534861\C,2.1997434136,-1.3615048283,-0.2544743119\N,2.9446552166,-0.27
06731939,0.4906471531\C,2.1427905376,0.197339426,1.6619461797\O,4.2398
782788,-0.7116656707,0.9379138847\C,5.2721134585,0.1366296389,0.460940
0663\H,4.9379608964,1.1779819015,0.4649440407\C,2.7821502614,-2.765134
4167,-0.0357114255\C,2.2265053169,-1.0144658703,-1.7538646415\C,2.2917
189899,-0.6802931383,2.9224191285\C,2.5239260467,1.6444042609,1.999869
3677\C,6.4657926572,-0.0505043779,1.4035029487\C,5.7031671586,-0.21759
17473,-0.9656369342\O,6.2694102676,0.8573932864,-1.5579920203\C,6.7925
512032,0.6325203851,-2.8781315512\O,5.6151504989,-1.305086385,-1.49119
1488\H,0.5503619088,0.9283479709,0.3845829859\H,-0.0455007861,0.126772
3362,1.8454917988\H,2.1538477463,-3.4968771735,-0.5579842032\H,3.79843
02362,-2.8321702602,-0.4291208985\H,2.8051829441,-3.0342326969,1.02486
9173\H,1.6404502579,-1.7454031719,-2.3250948328\H,1.7994364833,-0.0203
672261,-1.928493219\H,3.2487814936,-1.0270154244,-2.1394926257\H,3.336
8150236,-0.7257945392,3.2378678149\H,1.7020317941,-0.2533891045,3.7421
759167\H,1.9463224785,-1.7055630521,2.7605299168\H,3.5407891738,1.7031
524995,2.4052097404\H,2.4706199485,2.2745366797,1.1060649997\H,1.84475
38587,2.0544827595,2.7569703054\H,0.5354388437,-2.0738646146,0.9780916
745\H,0.0076217643,-1.274815309,-0.4985624144\H,7.3111564359,0.5635432
746,1.0783488517\H,6.1851122187,0.241616862,2.4196892122\H,6.773590629
3,-1.1007978316,1.4148540573\H,7.2245452422,1.5843344076,-3.1883365689
\H,7.5554670346,-0.1504052695,-2.8615707242\H,5.9920792348,0.333722799
4,-3.5600381256\Version=IA64L-G03RevE.01\State=1-A\HF=-751.5105676\S2
=0.\S2-1=0.\S2A=0.\RMSD=5.282e-09\RMSF=2.816e-06\Thermal=0.\Dipole=0.1
410169,0.6885862,0.0084616\PG=C01 [X(C12H23N1O3)]\@

PROXYL-C(CH₃)₂C(=O)OCH₃ (I17)

1\1\GINC-AC25\FOpt\UB3LYP\6-31G(d)\C13H25N1O3\JOH501\08-Nov-2007\0\#\#
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\proxylmma_1\0,1\N,-
0.073553956,0.0498795926,0.0465687727\C,1.4188415937,-0.136903423,-0.1
319816939\C,1.9491024159,1.3256079992,-0.1693261512\C,-0.4653832961,1.
4420448049,-0.3318536995\C,0.7512809391,2.2060966415,0.2183009397\H,0.
668631043,2.2883555514,1.3085307811\H,0.8157419284,3.2209063908,-0.188
0701834\C,-0.6326123648,1.6632305815,-1.8506050389\C,1.806434249,-0.89
95520679,-1.4087908877\C,-1.7627681311,1.840270057,0.3793940371\C,1.95
51150045,-0.8760257344,1.1067217183\H,2.8998244728,-0.933217915,-1.486
5573353\H,1.430598116,-1.9244823217,-1.4020217235\H,1.4168960263,-0.41
29870799,-2.3073186169\O,-0.8433283477,-0.8816739707,-0.7242542246\H,3
.0421006413,-1.0077554446,1.0351175689\H,1.7387811062,-0.3047840963,2.
01633300399\H,1.4995751086,-1.864381683,1.2168197521\H,-1.3760828449,0.
9733654568,-2.2575150015\H,-0.9728586596,2.6880682958,-2.040141872\H,0
.3010495944,1.516600348,-2.4015462452\H,-2.6155080103,1.2710769927,-0.
0065780628\H,-1.6846625324,1.6641952421,1.4566187547\H,-1.9732497779,2
.9037963649,0.215287511\H,2.2944893904,1.5757448094,-1.1784782406\H,2.
8020161775,1.463166124,0.5029399909\C,-1.5539922136,-1.9052981043,0.02
93621335\C,-2.7996527264,-2.1790496274,-0.8251604519\C,-0.6761021108,-
3.178291544,0.0759582632\C,-1.9286321343,-1.5057795571,1.4523706457\H,

-3.3590970647,-3.0368025072,-0.4352657331\H,-3.4519145197,-1.300412846
4,-0.8076556155\H,-2.5141030139,-2.3890891642,-1.8581810342\H,-2.46457
14074,-2.3338280387,1.9257994245\H,-1.0466581616,-1.2809676236,2.05093
85074\H,-2.5795086424,-0.629171429,1.4370317998\O,-0.2605039284,-3.706
965672,1.0860128432\O,-0.4225281435,-3.6582297695,-1.1604733267\C,0.38
59480306,-4.8457414268,-1.2071767322\H,0.4692428971,-5.1003148378,-2.2
640582101\H,1.373558852,-4.6550059125,-0.7789418282\H,-0.0913355992,-5
.6564934553,-0.6505015747\\Version=IA64L-G03RevD.01\State=1-A\HF=-790.
8205391\S2=0.\S2-1=0.\S2A=0.\RMSD=9.793e-09\RMSF=5.328e-06\Thermal=0.\
Dipole=0.0311495,0.1304361,-0.5295599\PG=C01 [X(C13H25N1O3)]\\@

PROXYL-CH(CH₃)C(=O)OH (I20)

1\1\GINC-AC25\FOpt\UB3LYP\6-31G(d)\C11H21N1O3\JOH501\07-Feb-2009\0\\#
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\\proxylaa_2\\0,1\C,0.
9970440768,0.0355265138,0.2079868802\C,0.9553546819,-1.497833267,0.281
1988131\C,2.4420749725,-1.9508455718,0.227882127\N,3.1993968799,-0.654
246277,0.4401760762\C,2.2833377709,0.4015052469,0.9692699072\O,4.31368
31726,-0.820858188,1.3364652796\C,5.5304116667,-0.4062483024,0.7394457
211\H,5.3519799415,0.4380687228,0.0670533464\C,2.7517177291,-3.0251846
982,1.2800708488\C,2.7939292419,-2.4777791687,-1.174479893\C,2.0662933
53,0.3460302497,2.4956073238\C,2.8178441415,1.7854516568,0.5788748421\
C,6.4719961285,0.0020620422,1.8784860279\C,6.1849984552,-1.5238586271,
-0.075049935\O,7.0945361208,-1.0094982276,-0.9414968226\O,5.989716072,
-2.7125924988,0.0355573247\H,1.0771533691,0.3710066251,-0.8330885219\H
,0.1133431107,0.5130070249,0.6440508797\H,2.1208540472,-3.9021865251,1
.0906009402\H,3.798710739,-3.3302498717,1.2308904286\H,2.5441263414,-2
.6714388158,2.2946441829\H,2.2222731513,-3.3880160382,-1.3948859015\H,
2.557739143,-1.7294808642,-1.9395131371\H,3.856780894,-2.7221443545,-1
.2438771564\H,3.016457577,0.4518532522,3.0245989987\H,1.4066864086,1.1
652691852,2.8051680346\H,1.6070344968,-0.5932000484,2.8175640941\H,3.7
477135141,2.0161978473,1.1117813112\H,3.0143331633,1.832027035,-0.4973
01723\H,2.0910835488,2.5656693219,0.8349117809\H,0.4951494308,-1.82117
55554,1.2214938984\H,0.3691094216,-1.9398900004,-0.530739682\H,7.44460
14535,0.3095119796,1.483416325\H,6.0334190982,0.8350539894,2.435385565
7\H,6.6168734069,-0.8375979822,2.5655623369\H,7.50777228,-1.7734528104
, -1.3870385225\\Version=IA64L-G03RevE.01\State=1-A\HF=-712.2035823\S2=
0.\S2-1=0.\S2A=0.\RMSD=6.470e-09\RMSF=3.581e-06\Thermal=0.\Dipole=0.10
43343,0.5729877,-0.1550052\PG=C01 [X(C11H21N1O3)]\\@

PROXYL-CH(CH₃)C(=O)NH₂ (I23)

1\1\GINC-AC30\FOpt\UB3LYP\6-31G(d)\C11H22N2O2\JOH501\07-Feb-2009\0\\#
UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\\proxylam_1\\0,1\C,1.
0730571149,0.191427778,0.4646473488\C,0.9963913145,-1.301284318,0.1101
176529\C,2.4735543208,-1.7610966133,-0.0483864841\N,3.2585266642,-0.57
59847268,0.4802238892\C,2.370535531,0.3162934736,1.2833288099\O,4.3843
588172,-0.9820529548,1.2744162185\C,5.6243315018,-0.868595668,0.553286
5958\H,5.4850222997,-1.2706777567,-0.4569652768\C,2.7364968233,-3.0746
885544,0.7032186919\C,2.8293416546,-1.9374098568,-1.5359766971\C,2.162
5397789,-0.1461228923,2.7415336988\C,2.9183904145,1.7471016351,1.27928
50003\C,6.1420674585,0.5627745122,0.4571125132\C,6.6642922811,-1.77597
80471,1.236070654\N,6.1837265246,-2.5854281453,2.2168690984\O,7.832722
9665,-1.7658319115,0.8731872698\H,1.1548375967,0.8000145761,-0.4436638
242\H,0.2008507569,0.5448262707,1.0240920979\H,2.0819260057,-3.8552744
663,0.2978261362\H,3.7706260452,-3.411653321,0.5887374007\H,2.52404763
39,-2.982515241,1.7728573578\H,2.2254196137,-2.7351586126,-1.985646162
\H,2.6457773213,-1.0098052191,-2.0879838753\H,3.883803889,-2.203456939
8,-1.6666146428\H,3.1193531986,-0.2013019375,3.2671862987\H,1.52482542
47,0.5720567546,3.269668674\H,1.681365211,-1.1267520426,2.8055487311\H
,3.8556241823,1.8131409827,1.8404324131\H,3.1038038492,2.0863419115,0.
2551379372\H,2.1990577363,2.4302007645,1.7465518042\H,0.5117812191,-1.
8611230372,0.9175754317\H,0.4148184868,-1.4853159751,-0.7989434774\H,7
.1180620059,0.5588883853,-0.0345622995\H,5.4468956881,1.1764119635,-0.
1202755424\H,6.2584154068,0.9984752021,1.4553819934\H,6.8371550211,-3.

1614911906,2.7277919767\H,5.2285242415,-2.490317782,2.5276565874\\Version=IA64L-G03RevE.01\State=1-A\HF=-692.3377228\S2=0.\S2-1=0.\S2A=0.\RMSD=4.834e-09\RMSF=1.477e-06\Thermal=0.\Dipole=-1.5500907,-0.1419773,0.4585712\PG=C01 [X(C11H22N2O2)]\@

TMIO-CH(CH₃)Ph (P13)

1\1\GINC-AC55\FOpt\UB3LYP\6-31G(d)\C20H25N1O1\JOH501\22-Jun-2007\0\#\UB3LYP/6-31G* OPT FREQ=noraman maxdisk=402653184\|tmiofet_1\|0,1\O,0.3876345992,0.0597909759,-0.3834767746\N,1.7703413367,-0.0166921497,-0.0344579921\C,2.4559894961,1.3192826311,-0.1088107713\C,1.9344304939,-0.6350048832,1.3249338049\C,3.50846148,1.1379975851,0.9689235843\C,3.2203551657,0.032095892,1.7705812018\C,4.6380093559,1.9159886365,1.2172713294\C,4.0565903352,-0.311983753,2.8311320655\H,4.8701851266,2.7754873856,0.5931029832\H,3.8377674397,-1.1746504047,3.4559481388\C,5.4769178211,1.5762301538,2.2821543395\C,5.1882521271,0.4679849848,3.0843865832\H,6.3608450205,2.1751336496,2.4852978411\H,5.8487387502,0.2097389703,3.9079945231\C,2.0799399937,-2.1565719714,1.1577671265\C,0.7866288785,-0.3279468904,2.3119989886\C,1.5441060231,2.5261358281,0.1978043771\C,3.0782386682,1.4821511735,-1.5061835497\H,1.1546766215,-2.5887053403,0.7600151655\H,-0.1624113815,-0.7170927675,1.9348628685\H,0.7491392568,2.6058291902,-0.5477634766\H,2.2990389147,1.5289402638,-2.272742984\H,2.2837966098,-2.6401765881,2.1204854858\H,0.9995180939,-0.8003366434,3.2776650013\H,2.1381454613,3.4465374728,0.1697590527\H,3.6640948934,2.4072920087,-1.5652138598\H,2.8967308882,-2.3894013147,0.4685578197\H,0.6741859585,0.7459873728,2.4821779491\H,1.0859131779,2.4524687983,1.1875742479\H,3.7368126753,0.637681453,-1.7298120349\C,0.0818615379,-0.7012515375,-1.5745008522\C,-1.1709836755,-1.5281096321,-1.2694898402\C,-0.1324866227,0.2063391575,-2.7750706958\H,0.9320074812,-1.3623316364,-1.7669356265\H,-1.4690181424,-2.1110703883,-2.1475799681\H,-0.9857658254,-2.2144911085,-0.4366419036\H,-2.0061975366,-0.8730012928,-0.9990031463\C,0.4211989494,-0.1158898345,-4.0190808391\C,0.1869311365,0.6890932716,-5.1364294408\C,-0.6035109734,1.8327636783,-5.0202879432\C,-0.9279623678,1.3562308919,-2.6697622424\C,-1.1588249764,2.1652575352,-3.7818189105\H,1.0447744017,-1.0024874239,-4.1140902906\H,0.6275759233,0.4249803155,-6.0943578125\H,-0.7841725608,2.4629417487,-5.8870885609\H,-1.3573807128,1.618742688,-1.7068161468\H,-1.7737693176,3.0562118477,-3.6829988153\\Version=IA64L-G03RevD.01\State=1-A\HF=-907.1176061\S2=0.\S2-1=0.\S2A=0.\RMSD=5.171e-09\RMSF=2.563e-06\Thermal=0.\Dipole=0.0051309,-0.0591661,-0.0858508\PG=C01 [X(C20H25N1O1)]\@

TMIO-CH(CH₃)C(=O)OCH₃ (P16)

1\1\GINC-AC26\FOpt\UB3LYP\6-31G(d)\C15H22N2O2\JOH501\07-Feb-2009\0\#\UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\|tmioam_2\|0,1\C,0.8394209496,0.7220857035,0.4451347304\C,-0.2219167749,0.2700518111,-0.3434303744\C,-0.7856772053,-0.9754329266,-0.0713953501\C,-0.2996724691,-1.7594088785,0.9753364569\C,0.7562775683,-1.3100723699,1.7665592579\C,1.3260112077,-0.0635529549,1.494467302\C,-1.9146302498,-1.6795281209,-0.7989656688\N,-2.2485149865,-2.7542540436,0.201408057\C,-1.0519751324,-3.0732750303,1.0633860991\O,-2.7383918446,-3.9219141805,-0.468624397\C,-3.9607320882,-4.4137807174,0.1123607742\H,-3.8910338581,-4.3374929253,1.2025514532\C,-0.1825812089,-4.2427754204,0.553988093\C,-1.5295320705,-3.3760444623,2.4948095704\C,-3.1382719424,-0.7713005595,-0.9973370282\C,-1.4397858401,-2.2080161851,-2.1710954187\C,-5.200998112,-3.6643456324,-0.3659838797\C,-4.0799705487,-5.9140183499,-0.2130287509\N,-3.0171445431,-6.4627718224,-0.8605194593\O,-5.0715075783,-6.5455246907,0.1254220252\H,1.1356865972,-1.9152654047,2.5862905838\H,-0.5986200723,0.887602089,-1.1550580868\H,2.1494995985,0.2982605516,2.1043225945\H,1.2865753822,1.6918026536,0.2434001192\H,-3.9459176717,-1.3146207744,-1.4969261674\H,-2.2253787438,-2.7980537933,-2.6501912204\H,-0.742326506,-5.1822088897,0.5688512098\H,-2.0818345507,-4.3212338752,2.5318782416\H,-2.8818615113,0.0914648299,-1.623047635\H,-1.1969722148,-1.3605607033,-2.8216488617\H,0.688846521,-4.3558870672,1.2082514278\H,-0.6761796573,-3.4697854583,3.1767048559\H,-3.5043219956,-0.4063604505,-0.03339

29479\H,-0.5430968791,-2.8275509152,-2.0844775523\H,0.1842549545,-4.06
88702005,-0.4611303361\H,-2.1803534014,-2.5756577686,2.8575687321\H,-6
.0924699889,-4.1582006877,0.0290815959\H,-5.1775355482,-2.6299587391,-
0.015280862\H,-5.2558960048,-3.669732206,-1.4603629872\H,-3.0817621282
, -7.4267748482,-1.1549416023\H,-2.2741254518,-5.8712435862,-1.20138459
36\Version=IA64L-G03RevE.01\State=1-A\HF=-844.7660674\S2=0.\S2-1=0.\S
2A=0.\RMSD=6.271e-09\RMSF=2.916e-06\Thermal=0.\Dipole=1.3064493,0.6645
663,-0.4171453\PG=C01 [X(C15H22N2O2)]\@

TMIO-C(CH₃)₂C(=O)OCH₃ (P17)

1\1\GINC-AC13\FOpt\UB3LYP\6-31G(d)\C17H25N1O3\JOH501\08-Nov-2007\0\#\n
UB3LYP/6-31G* OPT FREQ=norman maxdisk=402653184\|tmionma_2\|0,1\O,0.1
749354764,-0.0866594541,-0.1326189121\N,1.5993638268,-0.016819967,-0.0
394699914\C,2.0920670547,1.4061839267,0.074215253\C,2.0698044011,-0.83
42513955,1.1356276314\C,3.3402337582,1.1862054653,0.9065974345\C,3.328
8166248,-0.0745522849,1.5040753585\C,4.3994445767,2.0642685457,1.13061
37676\C,4.3741362515,-0.4761937628,2.3339755148\H,4.4151481893,3.04710
00181,0.6660442974\H,4.3708316161,-1.4588970715,2.7994529764\C,5.44784
85662,1.6668479195,1.9647963326\C,5.4356051679,0.4033446258,2.56338403
25\H,6.278758047,2.3433858154,2.1470926269\H,6.2568411756,0.1020131929
,3.208395691\C,2.3685391315,-2.269998937,0.6750735321\C,1.0859666887,-
0.8764066884,2.3265856018\C,1.1155045956,2.3698118966,0.7818838063\C,2
.4194246776,1.9392756652,-1.3307720291\H,1.4457008493,-2.7821580581,0.
3809714955\H,0.1446895641,-1.3494311629,2.0356217843\H,0.1756975899,2.
425056202,0.2304415237\H,1.5058514781,2.0489559287,-1.9209447985\H,2.8
197715916,-2.8511344131,1.4877959396\H,1.5304199384,-1.4574599709,3.14
25272603\H,1.5629620296,3.3698904458,0.8218167542\H,2.8908129843,2.927
0529053,-1.2663090574\H,3.0570544855,-2.268432862,-0.1747686726\H,0.86
37197926,0.1225740273,2.7083705464\H,0.9090167735,2.058588635,1.809384
4351\H,3.1071467748,1.2629105675,-1.8480390507\C,-0.3682949426,-0.5798
499941,-1.3733816693\C,-1.4917840837,-1.5440490152,-0.9491692549\C,-1.
0052706198,0.6145925667,-2.1228861762\C,0.6393949322,-1.2763637233,-2.
2959644177\H,-2.067762459,-1.8838094388,-1.8134328818\H,-1.0519544036,
-2.4121444507,-0.4481958371\H,-2.1680303817,-1.0480485666,-0.245371866
2\O,-0.9760650171,1.7770370157,-1.786306555\O,-1.6401918512,0.19274758
66,-3.2419892072\C,-2.2812885384,1.2228952759,-4.0135858339\H,-2.73765
0661,0.711208318,-4.8613946799\H,-3.0414455572,1.7327960871,-3.4160989
757\H,-1.5479130987,1.9574247147,-4.3565551618\H,0.1144296407,-1.62870
73706,-3.1875880562\H,1.4431754962,-0.6028721847,-2.5981936601\H,1.088
5378675,-2.1323265751,-1.7890268509\Version=IA64L-G03RevD.01\State=1-
A\HF=-943.2488783\S2=0.\S2-1=0.\S2A=0.\RMSD=4.074e-09\RMSF=7.257e-06\T
hermal=0.\Dipole=-0.2293945,-0.4683939,-0.5535712\PG=C01 [X(C17H25N1O3

TMIO-CH(CH₃)C(=O)OH (P20)

1\1\GINC-AC26\FOpt\UB3LYP\6-31G(d)\C15H21N1O3\JOH501\08-Feb-2009\0\#\n
UB3LYP/6-31G* OPT FREQ=norman maxdisk=268435456\|tmioaa_1\|0,1\C,0.85
93672749,0.6287682956,0.7104725852\C,-0.2808254546,0.3162505274,-0.034
5156642\C,-0.8248387638,-0.9630914306,0.0649110209\C,-0.2444212664,-1.
9201657218,0.8984619397\C,0.8916598721,-1.6101710228,1.6444824288\C,-1.
4431296858,-0.3300699358,1.5441486437\C,-2.0192545511,-1.5411079332,-0.
.6669803539\N,-2.2679579275,-2.7752490939,0.1566751612\C,-1.0033824946
, -3.2324134154,0.8399150693\O,-2.8346223308,-3.8034611291,-0.665517150
5\C,-4.1437549433,-4.160159875,-0.2458014768\H,-4.5524809615,-3.363857
3571,0.3838121435\C,-0.2216614029,-4.3127264224,0.0646423635\C,-1.3537
066931,-3.7533041625,2.2448871591\C,-3.2638371151,-0.6416392139,-0.588
0382426\C,-1.6690783657,-1.8157592205,-2.1462047479\C,-5.0086093178,-4
.3607272327,-1.4967917744\C,-4.1238980067,-5.4486797489,0.5800230774\O
, -5.3320707278,-5.6564639223,1.1635733454\O,-3.1992794344,-6.218446404
7,0.7031166654\H,1.3465018123,-2.3499272554,2.2986421391\H,-0.73228370
21,1.0652825969,-0.680715096\H,2.3289348281,-0.0774888258,2.1210353488
\H,1.2931629,1.6229493331,0.6426145101\H,-4.1211494925,-1.130287953,-1.
.0656312987\H,-2.4944711194,-2.3190261204,-2.6560660887\H,-0.8336505047

, -5.2103873932, -0.0477275962\H, -1.9211085924, -4.6850543053, 2.1779766501\H, -3.0948006107, 0.3089833825, -1.1072661048\H, -1.4736736328, -0.8646867498, -2.6541913671\H, 0.6866139058, -4.571747097, 0.6207540417\H, -0.4411119461, -3.9607579545, 2.8162866151\H, -3.5192193806, -0.4309989203, 0.4544066198\H, -0.7757764481, -2.4378666513, -2.2432944415\H, 0.0807289534, -3.9652836816, -0.9271305547\H, -1.9432963688, -3.0106165134, 2.7909404767\H, -6.0173712943, -4.6819358669, -1.2230006878\H, -5.0722918666, -3.4215822812, -2.0539481436\H, -4.5600622681, -5.1185264706, -2.1473366454\H, -5.2593081736, -6.502109853, 1.6456134303\Version=IA64L-G03RevE.01\State=1-A\HF=-864.6313871\S2=0.\S2-1=0.\S2A=0.\RMSD=9.395e-09\RMSF=2.776e-06\Thermal=0.\Dipole=-0.5299761, 0.2599876, 0.0160279\PG=C01 [X(C15H21N1O3)]\@

TMIO-CH(CH₃)C(=O)NH₂ (P23)

1\1\GINC-AC26\FOpt\UB3LYP\6-31G(d)\C15H22N2O2\JOH501\07-Feb-2009\0\#\UB3LYP/6-31G* OPT FREQ=noraman maxdisk=268435456\tmioam_2\0,1\C, 0.8394209496, 0.7220857035, 0.4451347304\C, -0.2219167749, 0.2700518111, -0.3434303744\C, -0.7856772053, -0.9754329266, -0.0713953501\C, -0.2996724691, -1.7594088785, 0.9753364569\C, 0.7562775683, -1.3100723699, 1.7665592579\C, 1.3260112077, -0.0635529549, 1.494467302\C, -1.9146302498, -1.6795281209, -0.7989656688\N, -2.2485149865, -2.7542540436, 0.201408057\C, -1.0519751324, -3.0732750303, 1.0633860991\O, -2.7383918446, -3.9219141805, -0.468624397\C, -3.9607320882, -4.4137807174, 0.1123607742\H, -3.8910338581, -4.3374929253, 1.2025514532\C, -0.1825812089, -4.2427754204, 0.553988093\C, -1.5295320705, -3.3760444623, 2.4948095704\C, -3.1382719424, -0.7713005595, -0.9973370282\C, -1.4397858401, -2.2080161851, -2.1710954187\C, -5.200998112, -3.6643456324, -0.3659838797\C, -4.0799705487, -5.9140183499, -0.2130287509\N, -3.0171445431, -6.4627718224, -0.8605194593\O, -5.0715075783, -6.5455246907, 0.1254220252\H, 1.1356865972, -1.9152654047, 2.5862905838\H, -0.5986200723, 0.887602089, -1.1550580868\H, 2.1494995985, 0.2982605516, 2.1043225945\H, 1.2865753822, 1.6918026536, 0.2434001192\H, -3.9459176717, -1.3146207744, -1.4969261674\H, -2.2253787438, -2.7980537933, -2.6501912204\H, -0.742326506, -5.1822088897, 0.5688512098\H, -2.0818345507, -4.3212338752, 2.5318782416\H, -2.8818615113, 0.0914648299, -1.623047635\H, -1.1969722148, -1.3605607033, -2.8216488617\H, 0.688846521, -4.3558870672, 1.2082514278\H, -0.6761796573, -3.4697854583, 3.1767048559\H, -3.5043219956, -0.4063604505, -0.0333929479\H, -0.5430968791, -2.8275509152, -2.0844775523\H, 0.1842549545, -4.0688702005, -0.4611303361\H, -2.1803534014, -2.5756577686, 2.8575687321\H, -6.0924699889, -4.1582006877, 0.0290815959\H, -5.1775355482, -2.6299587391, -0.015280862\H, -5.2558960048, -3.669732206, -1.4603629872\H, -3.0817621282, -7.4267748482, -1.1549416023\H, -2.2741254518, -5.8712435862, -1.2013845936\Version=IA64L-G03RevE.01\State=1-A\HF=-844.7660674\S2=0.\S2-1=0.\S2A=0.\RMSD=6.271e-09\RMSF=2.916e-06\Thermal=0.\Dipole=1.3064493, 0.6645663, -0.4171453\PG=C01 [X(C15H22N2O2)]\@