SUPPLEMENTARY MATERIALS

A quantitative scale for the extent of conjugation of carbonyl groups. "Carbonylicity" percentage as a chemical driving force

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TABLE OF CONTENT:

1. Table S1 for Method independence study (see section 2.3)

Table S1A. The computed ΔH_{H2} values (kJ mol^{-1}) and calculated carbonylicity % at differing levels of theory for 19 selected compounds.

			Method[a]								Average	MAX – MIN	S.Dev.
			A	**B**	**C**	**D**	**E**	**F**	**G**	**H**			
3	**F**	ΔH_{H2}	–39.95	–14.98	2.20	–8.14	–20.89	16.90	–2.90	–19.46	–10.90	56.85	17.11
		%	**28.97**	**27.38**	**35.05**	**34.81**	**33.46**	**34.54**	**30.98**	**32.42**	**32.20**	**7.67**	**2.86**
4	**OH**	ΔH_{H2}	–14.35	16.27	29.97	20.01	7.43	42.48	23.12	4.97	16.24	56.83	17.23
		%	**39.83**	**41.04**	**48.46**	**48.41**	**47.84**	**46.30**	**43.04**	**44.85**	**44.97**	**8.63**	**3.37**
5	**NH_2**	ΔH_{H2}	–17.65	24.89	38.98	29.62	18.89	48.59	29.50	11.37	23.02	66.24	20.02
		%	**38.43**	**44.80**	**52.81**	**53.05**	**53.66**	**49.11**	**45.99**	**48.12**	**48.25**	**15.23**	**5.17**
6	**CH_3**	ΔH_{H2}	–85.16	–53.60	–44.03	–53.71	–59.31	–36.90	–49.25	–62.77	–55.59	48.26	14.49
		%	**9.77**	**10.51**	**12.74**	**12.80**	**13.95**	**9.79**	**9.49**	**10.36**	**11.18**	**4.46**	**1.72**
13	**NH_3^+**	ΔH_{H2}	–156.00	–128.44	–106.87	–116.40	–120.60	–95.03	–112.67	–120.56	–119.57	60.97	17.84
		%	**–20.31**	**–22.18**	**–17.59**	**–17.48**	**–17.18**	**–16.95**	**–19.92**	**–19.08**	**–18.84**	**5.23**	**1.86**
2	**O^-**	ΔH_{H2}	127.35	151.25	136.75	126.81	110.13	159.22	145.99	113.25	133.84	49.09	17.65
		%	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**
11	**NH^-**	ΔH_{H2}	148.31	172.65	159.37	149.39	118.76	180.07	168.55	122.07	152.40	61.31	22.56
		%	**108.90**	**109.35**	**110.92**	**110.90**	**104.39**	**109.59**	**110.46**	**104.49**	**108.63**	**6.53**	**2.68**
12	**CH_2^-**	ΔH_{H2}	115.50	141.18	140.24	130.61	99.09	152.99	141.27	149.34	133.78	53.90	18.17
		%	**94.97**	**95.60**	**101.68**	**101.83**	**94.40**	**97.13**	**97.81**	**118.38**	**100.23**	**23.98**	**7.86**

[a]**A**: HF/3-21G; **B**: HF/6-31G(d); **C**: B3LYP/6-31G(d); **D**: B3LYP/6-31G(d,p); **E**: B3LYP/6-311++G(2d,2p); **F**: MP2(fc)/6-31G(d); **G**: CCSD/6-31G(d); **H**: G3MP2B3

Table S1B. The computed ΔH_{H2} values (kJ mol^{-1}) and calculated carbonylicity % at differing levels of theory for 19 selected compounds.

			Method[a]								Average	MAX – MIN	S.Dev.
			A	**B**	**C**	**D**	**E**	**F**	**G**	**H**			
7	**Cl**	ΔH_{H2}	–74.72	–43.37	–18.22	–28.08	–33.25	–9.25	–29.88	–38.22	–34.37	65.47	19.55
		%	**14.20**	**14.98**	**25.20**	**25.18**	**27.18**	**22.51**	**18.46**	**22.86**	**21.32**	**12.98**	**4.89**
8	**SH**	ΔH_{H2}	–70.64	–35.58	–12.37	–22.55	–28.85	–5.83	–25.37	–36.03	–29.65	64.81	19.61
		%	**15.93**	**18.39**	**28.02**	**27.85**	**29.42**	**24.08**	**20.56**	**23.97**	**23.53**	**13.49**	**4.88**
9	**PH_2**	ΔH_{H2}	–98.27	–60.35	–42.07	–52.12	–58.49	–37.20	–52.39	–64.76	–58.21	61.07	18.61
		%	**4.20**	**7.57**	**13.68**	**13.57**	**14.37**	**9.65**	**8.03**	**9.34**	**10.05**	**10.17**	**3.57**
10	**SiH_3**	ΔH_{H2}	–118.21	–80.11	–67.69	–78.19	–86.28	–61.77	–74.09	–89.33	–81.96	56.44	17.23
		%	**–4.27**	**–1.07**	**1.32**	**0.98**	**0.25**	**–1.65**	**–2.03**	**–3.17**	**–1.21**	**5.59**	**1.98**
14	**S^-**	ΔH_{H2}	19.64	52.59	71.83	61.81	51.31	81.24	61.06	44.82	55.54	61.60	18.62
		%	**54.27**	**56.90**	**68.66**	**68.60**	**70.13**	**64.13**	**60.63**	**65.15**	**63.56**	**15.86**	**5.81**
17	**PH_3^+**	ΔH_{H2}	–192.85	–144.30	–119.54	–129.54	–133.05	–114.52	–129.93	–143.75	–138.44	78.33	24.30
		%	**–35.96**	**–29.11**	**–23.71**	**–23.83**	**–23.50**	**–25.91**	**–27.92**	**–30.89**	**–27.60**	**12.46**	**4.34**
15	**PH^-**	ΔH_{H2}	19.94	51.35	73.80	63.46	47.20	80.26	59.62	39.41	54.38	60.32	19.38
		%	**54.40**	**56.36**	**69.61**	**69.40**	**68.04**	**63.68**	**59.96**	**62.39**	**62.98**	**15.21**	**5.83**
24	**NO_2**	ΔH_{H2}	–103.08	–80.83	–60.68	–70.70	–77.48	–42.56	–67.41	–75.15	–72.24	60.52	17.32
		%	**2.16**	**–1.38**	**4.70**	**4.59**	**4.72**	**7.19**	**1.07**	**4.05**	**3.39**	**8.57**	**2.66**

[a]**A**: HF/3-21G; **B**: HF/6-31G(d); **C**: B3LYP/6-31G(d); **D**: B3LYP/6-31G(d,p); **E**: B3LYP/6-311++G(2d,2p); **F**: MP2(fc)/6-31G(d); **G**: CCSD/6-31G(d); **H**: G3MP2B3

2. Correlation between carbonylicity and computed NBO charges, C=O bond distance and carbonyl IR frequency.

The associated IR frequency and bond distances for a carbonyl group are very characteristic and predetermine its chemical properties; the correlation between their computed values and the calculated carbonylicity values of all model compounds (**1**–**25**, **38**–**49**) therefore reported herein. When the IR frequencies of model compounds (**1**–**25**, **38**–**49**) are considered, the linear fit exhibits a relatively poor R^2 value (R^2 = 0.237 in **Figure 5A**), but the trend is significant. An IR frequency consists of the reduced mass of the different atoms involved in the vibration and the force constant of the relevant chemical bonds. As the carbonyl groups are connected to various functional groups, including atoms with differing atomic masses, exact correlation is not expected between the carbonyl IR frequency and the carbonylicity value.

The bond distance between the C and O atoms of the carbonyl group is also considered as a indicator of the conjugation between the carbonyl and the linked functional groups [–C(=O)–X]. A moderate correlation between the carbonylicity value and the C=O bond distance is observed (R^2 = 0.602; **Figure 4B**). Stronger conjugation (higher carbonylicity value) increases, while weaker conjugation (lower carbonylicity value) decreases the C=O bond distance.

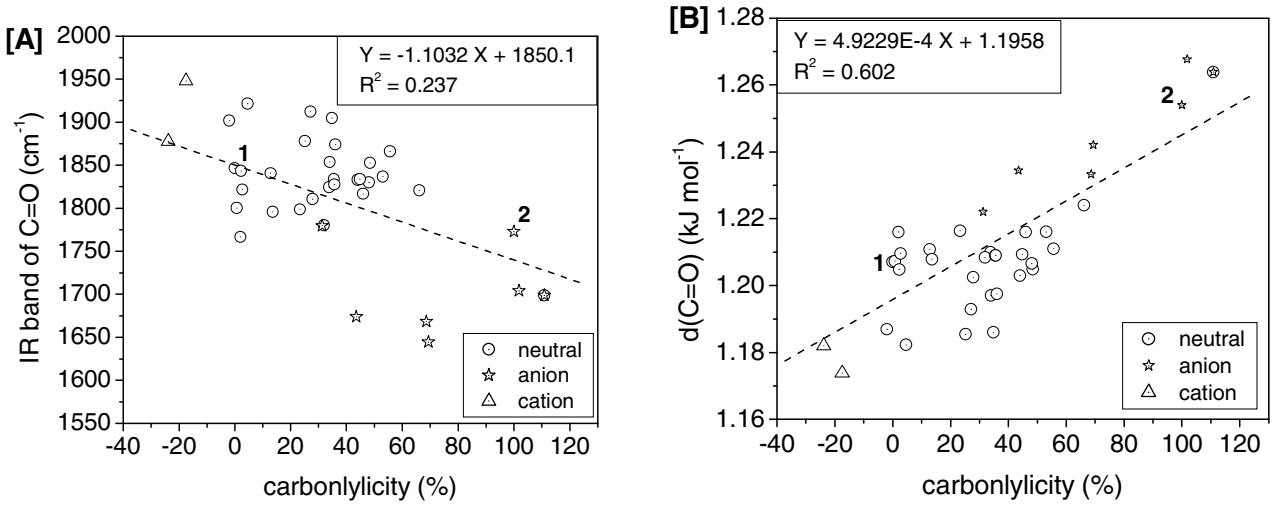

Figure S1. Correlation between calculated Carbonylicity percentage and the carbonyl IR frequencies ($\nu_{C=O}$) **[A]** as well as C=O distances [*d*(C=O)] **[B]** of the carbonyl group for model compounds **1**–**25**, **38**–**49**.

It may be presumed that the NBO charge of the carbonyl-C atom correlates with the strength of the carbonyl group, namely the carbonylicilty value (**Figure 5**). However, in contrast to expectations, no correlation was identified (R^2 = 0.055), attributed to the strong effect the X group significantly disturbing the overall NBO charge of the C atom.

The correlation may be improved significantly (ten-fold increase in R^2 value) if the compounds are separated into three clusters, specifically those that have negative, neutral or positive X substituents (Figure 6).

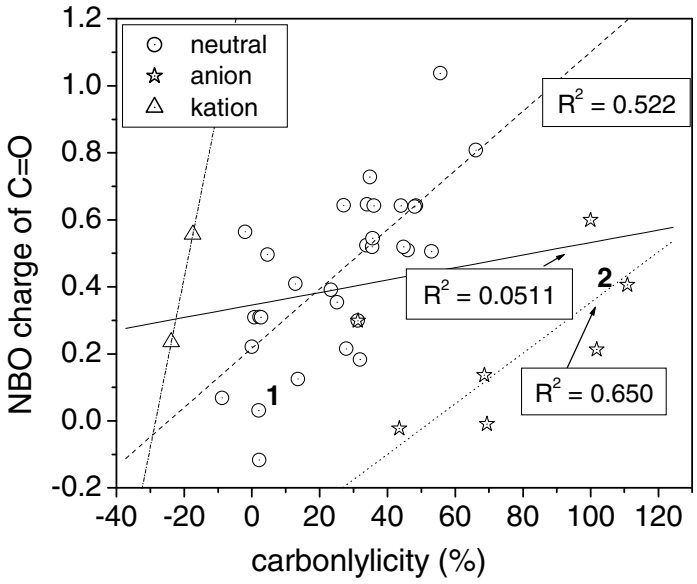

Figure S2. Correlation between calculated Carbonylicity percentage and the NBO charges of the carbonyl group for model compounds **1**–**25**, **38**–**49**. Solid line all points are included in the correlation. Broken lines represent correlations for three clusters.

Table S2. Computed NBO charges, *d*(C=O) bond distances in Å, and $\nu_{C=O}$ in cm^{-1} for the compounds examined (**1**–**25**, **38**–**49**), obtained at the B3LYP/6-31G(d,p) level of theory.

	NBO	d(CO)	$\nu_{C=O}$		NBO	d(CO)	$\nu_{C=O}$
1	0.221	1.2070	1846.5	**2**	0.599	1.2540	1772.8
3	0.728	1.1860	1904.6	**4**	0.642	1.2049	1852.6
5	0.505	1.2161	1836.6	**6**	0.409	1.2108	1840.5
7	0.354	1.1854	1877.8	**8**	0.215	1.2025	1810.5
9	0.125	1.2079	1795.9	**10**	0.031	1.2160	1766.6
11	0.406	1.2639	1698.9	**12**	0.213	1.2677	1704.1
13	0.556	1.1738	1948.0	**14**	0.136	1.2333	1668.3
15	–0.010	1.2421	1644.6	**16**	–0.023	1.2344	1674.0
17	0.235	1.1820	1877.6	**18**	0.639	1.2066	1830.1
19	0.183	1.2084	1780.1	**20**	0.309	1.2073	1800.2
21	0.309	1.2096	1821.6	**22**	0.310	1.2048	1843.2
23	0.299	1.2220	1779.6	**24**	0.496	1.1823	1921.4
25	0.391	1.2164	1798.7	**–**	**–**	**–**	**–**
38	0.519	1.2093	1833.7	**39**	0.642	1.1975	1873.9
40	0.509	1.2160	1816.7	**41**	0.642	1.2030	1832.8
42	0.519	1.2090	1833.8	**43**	0.646	1.1970	1853.5
44	0.524	1.2100	1824.5	**45**	0.643	1.1929	1912.0
46	0.808	1.2240	1820.6	**47**	1.037	1.2110	1866.1
48	0.564	1.1869	1901.7	**49**	0.545	1.2090	1827.7

3. Raw data

Table S3. Total energies (E), zero point corrected energies (E_{ZPE}), internal energies (U), enthalpies (H) and Gibbs free energies (G) in hartree and entropies (S) in cal mol^{-1} K^{-1} for the compounds examined, computed at the B3LYP/6-31G(d,p) level of theory.

Compound	E	E_{ZPE}	U	H	G	S
H2	-1.17853933	-1.168363	-1.166003	-1.165058	-1.179850	31.132
1	-114.50319920	-114.476478	-114.473612	-114.472667	-114.498142	53.616
2	-189.17881477	-189.158615	-189.155647	-189.154703	-189.182419	58.332
3	-213.76432940	-213.743281	-213.740259	-213.739315	-213.767321	58.944
4	-189.76222082	-189.728222	-189.725064	-189.724119	-189.752304	59.320
5	-169.89702718	-169.851634	-169.847771	-169.846827	-169.876393	62.227
6	-153.83572943	-153.780138	-153.776233	-153.775289	-153.805112	62.767
7	-574.11840897	-574.099221	-574.095967	-574.095023	-574.124455	61.945
8	-512.71309144	-512.681450	-512.681450	-512.680506	-512.710533	63.198
9	-456.45593419	-456.420205	-456.416014	-456.415070	-456.446350	65.833
10	-405.19578624	-405.153591	-405.148707	-405.147763	-405.181636	71.291
11	-169.28620611	-169.253791	-169.250696	-169.249752	-169.277758	58.943
12	-153.21225087	-153.170414	-153.166908	-153.165964	-153.194653	60.381
13	-170.20432995	-170.145937	-170.141888	-170.140944	-170.171202	63.683
14	-512.16091826	-512.142525	-512.139343	-512.138399	-512.167586	61.429
15	-455.88993680	-455.863992	-455.860412	-455.859468	-455.889421	63.041
16	-404.61008746	-404.578411	-404.574140	-404.573196	-404.604451	65.782
17	-456.76135311	-456.715960	-456.711063	-456.710119	-456.743478	70.211
18	-229.06833302	-229.006109	-229.001553	-229.000608	-229.033000	68.174
19	-552.03363466	-551.976028	-551.971618	-551.970674	-552.003482	69.051
20	-206.73640584	-206.709831	-206.705829	-206.704885	-206.735641	64.731
21	-227.82135419	-227.784292	-227.780089	-227.779144	-227.810569	66.138
22	-303.07344192	-303.030149	-303.025313	-303.024369	-303.058206	71.217
23	-302.51356910	-302.483955	-302.479170	-302.478226	-302.512225	71.556
24	-319.00220187	-318.971644	-318.967000	-318.966056	-318.999604	70.609
25	-345.58268482	-345.472652	-345.466360	-345.465416	-345.503171	79.462
26	-247.29471625	-247.213993	-247.209270	-247.208326	-247.241611	70.054
27	-286.64172544	-286.530521	-286.525106	-286.524162	-286.559353	74.066
28	-325.96050510	-325.819903	-325.813518	-325.812574	-325.850237	79.268
29	-365.26794792	-365.098306	-365.090761	-365.089817	-365.130410	85.435
30	-267.15907956	-267.090261	-267.085973	-267.085029	-267.117383	68.094
31	-306.50084396	-306.402139	-306.396984	-306.396040	-306.430775	73.106
32	-345.81454313	-345.686815	-345.680574	-345.679629	-345.717131	78.929
33	-385.12964510	-384.972772	-384.965555	-384.964611	-385.004299	83.532
34	-323.52760425	-323.433826	-323.428551	-323.427607	-323.462755	73.976
35	-343.37279423	-343.292352	-343.287113	-343.286169	-343.321350	74.044
36	-246.03110160	-245.974748	-245.970544	-245.969600	-246.001530	67.203
37	-265.89780772	-265.854364	-265.850096	-265.849152	-265.881192	67.436
38	-400.95519710	-400.827359	-400.820002	-400.819058	-400.859637	85.407
39	-420.80650733	-420.692105	-420.684753	-420.683809	-420.724613	85.880
40	-247.29615040	-247.216554	-247.211233	-247.210289	-247.244738	72.503
41	-267.15048802	-267.083713	-267.078533	-267.077589	-267.111980	72.383
42	-451.79548908	-451.712465	-451.704944	-451.704000	-451.745317	86.959
43	-471.64488508	-471.574921	-471.567475	-471.566531	-471.607969	87.213
44	-283.22751224	-283.171417	-283.166433	-283.165489	-283.199278	71.117
45	-303.07602527	-303.033292	-303.028226	-303.027282	-303.061907	72.874
46	-303.89379991	-303.773733	-303.766058	-303.765113	-303.805583	85.175
47	-265.00493638	-264.965056	-264.961353	-264.960409	-264.990949	64.278
48	-361.97783966	-361.866510	-361.860216	-361.859272	-361.897042	79.492
49	-323.50758683	-323.415275	-323.409664	-323.408720	-323.444681	75.688

Table S3cont.

Compound		E	E_{ZPE}	U	H	G	S
50trans		-248.53528410	-248.433064	-248.426502	-248.425558	-248.463523	79.904
50cis		-248.53119159	-248.429233	-248.423541	-248.422597	-248.458129	74.784
51trans		-268.39676321	-268.306851	-268.300667	-268.299723	-268.336661	77.742
51cis		-268.38436472	-268.294586	-268.288551	-268.287607	-268.323940	76.468
52		-229.09148008	-229.029519	-229.024943	-229.023999	-229.056769	68.970
53		-480.77463802	-480.562113	-480.554296	-480.553352	-480.594629	86.877
54		-229.09148008	-229.029519	-229.024943	-229.023999	-229.056769	68.970
55		-727.99052792	-727.909102	-727.902347	-727.901402	-727.940905	83.140
56	**2**	-496.27938556	-496.146740	-496.136490	-496.135546	-496.184181	102.362
56	**4**	-496.27938556	-496.146740	-496.136490	-496.135546	-496.184181	102.362
58		-287.84250942	-287.712143	-287.704385	-287.703441	-287.744102	85.579
59		-245.14357950	-245.092124	-245.087822	-245.086877	-245.118430	66.408
61		-460.13777872	-459.995561	-459.986537	-459.985592	-460.031135	95.853
63		-664.63774197	-664.492937	-664.481394	-664.480450	-664.532877	110.342
67a		-973.40338160	-973.097980	-973.078372	-973.077428	-973.145281	142.810
67b		-535.53315076	-535.306443	-535.292629	-535.291685	-535.346598	115.575
68		-623.69464030	-623.547957	-623.537282	-623.536338	-623.585910	104.335
70		-847.28419698	-846.881536	-846.862137	-846.861193	-846.931891	148.798
71		-694.65728864	-694.291209	-694.275321	-694.274377	-694.335724	129.116
72		-1892.23510436	-1891.636411	-1891.602213	-1891.601269	-1891.706382	221.228
74		-1197.56856186	-1197.337896	-1197.320659	-1197.319715	-1197.384207	135.735
75		-1197.56856186	-1197.337896	-1197.320659	-1197.319715	-1197.384207	135.735
77		-1198.11873463	-1197.874786	-1197.857256	-1197.856312	-1197.921621	137.455

Table S4. Total energies (*E*), zero point corrected energies (E_{ZPE}), internal energies (*U*), enthalpies (*H*) and Gibbs free energies (*G*) in hartree and entropies (*S*) in cal mol^{-1} K^{-1} for the hydrogenate compounds examined, computed at the B3LYP/6-31G(d,p) level of theory.

Compound	E	E_{ZPE}	U	H	G	S
1	-115.72396333	-115.672552	-115.669250	-115.668306	-115.695279	56.770
2	-190.31652243	-190.276247	-190.272359	-190.271415	-190.301311	62.921
3	-214.95549718	-214.911569	-214.908422	-214.907478	-214.936141	60.325
4	-190.94309813	-190.886699	-190.882492	-190.881548	-190.912199	64.510
5	-171.07489477	-171.005819	-171.001536	-171.000592	-171.031188	64.395
6	-155.04620936	-154.966050	-154.961768	-154.960824	-154.991430	64.416
7	-575.31733929	-575.275095	-575.271730	-575.270786	-575.300797	63.164
8	-513.91066474	-513.859629	-513.855107	-513.854162	-513.886234	67.501
9	-457.66521926	-457.605785	-457.600941	-457.599997	-457.632834	69.113
10	-406.41505713	-406.348767	-406.343575	-406.342631	-406.375987	70.203
11	-170.41505999	-170.363003	-170.358802	-170.357858	-170.388255	63.977
12	-154.34900924	-154.286718	-154.282173	-154.281229	-154.312229	65.244
13	-171.43953486	-171.355968	-171.351323	-171.350379	-171.382340	67.269
14	-513.32559059	-513.284763	-513.280838	-513.279894	-513.310804	65.057
15	-457.05386823	-457.005730	-457.001275	-457.000331	-457.032167	67.004
16	-405.79515456	-405.740398	-405.735400	-405.734455	-405.767453	69.449
17	-457.99971465	-457.929980	-457.925508	-457.924564	-457.956605	67.437
18	-230.24942251	-230.164919	-230.159254	-230.158310	-230.194289	75.724
19	-553.22928169	-553.147913	-553.142047	-553.141103	-553.177311	76.205
20	-207.95584030	-207.905474	-207.900896	-207.899952	-207.932083	67.627
21	-229.03898030	-228.978576	-228.973609	-228.972665	-229.006119	70.411
22	-304.29151714	-304.224706	-304.219178	-304.218233	-304.253585	74.403
23	-303.70867974	-303.655392	-303.650114	-303.649170	-303.684033	73.376
24	-320.21798985	-320.163684	-320.159013	-320.158069	-320.191898	71.200
25	-346.78387319	-346.650699	-346.643550	-346.642606	-346.682708	84.403
26	-248.46993437	-248.365931	-248.360744	-248.359800	-248.393912	71.796
27	-287.81420771	-287.680482	-287.674431	-287.673486	-287.710001	76.852
28	-327.13829442	-326.974793	-326.968029	-326.967085	-327.005079	79.965
29	-366.44834840	-366.255632	-366.247578	-366.246634	-366.287840	86.725
30	-268.33605965	-268.244808	-268.239573	-268.238629	-268.273383	73.146
31	-307.68250772	-307.561106	-307.555170	-307.554226	-307.590650	76.661
32	83.85900000	-346.850935	-346.843898	-346.842953	-346.882798	83.859
33	-386.31489025	-386.135412	-386.127407	-386.126463	-386.167652	86.690
34	-324.69541009	-324.579115	-324.573001	-324.572057	-324.608852	77.442
35	-344.55107784	-344.447434	-344.441558	-344.440613	-344.477050	76.687
36	-247.22172459	-247.142153	-247.137260	-247.136316	-247.169703	70.269
37	-267.08649974	-267.019841	-267.015664	-267.014720	-267.046747	67.407
38	-402.13898637	-401.988587	-401.980294	-401.979350	-402.021939	89.635
39	-421.99776903	-421.860089	-421.851912	-421.850968	-421.893658	89.848
40	-248.47909405	-248.376699	-248.370529	-248.369585	-248.406029	76.703
41	-268.33494868	-268.245834	-268.239387	-268.238443	-268.278211	83.699
42	-452.98709969	-452.880953	-452.872542	-452.871597	-452.915052	91.458
43	-472.83670796	-472.744010	-472.736281	-472.735337	-472.777581	88.910
44	-284.42050297	-284.341108	-284.335349	-284.334404	-284.370200	75.339
45	-304.27458996	-304.208349	-304.202484	-304.201540	-304.238094	76.936
46	-305.06056202	-304.917231	-304.909476	-304.908531	-304.948521	84.166
47	-266.17954967	-266.117779	-266.113076	-266.112132	-266.144607	68.351
48	-363.19670780	-363.061994	-363.055455	-363.054511	-363.093390	81.828
49	-324.69906445	-324.583716	-324.577141	-324.576196	-324.614647	80.926

Table S4. continued

Compound		E	E_{ZPE}	U	H	G	S
50trans		-249.70988603	-249.584444	-249.577768	-249.576824	-249.613944	78.127
50cis		78.67600000	-249.583064	-249.576361	-249.575417	-249.612799	78.676
51trans		-269.57195283	-269.459349	-269.452504	-269.451560	-269.489699	80.271
51cis		-269.57195283	-269.459349	-269.452504	-269.451560	-269.489699	80.271
52		-230.26957861	-230.185031	-230.179792	-230.178847	-230.212310	70.427
53		-481.98083364	-481.744463	-481.736365	-481.735421	-481.776564	86.594
54		-230.26957861	-230.185031	-230.179792	-230.178847	-230.212310	70.427
55		-729.17864797	-729.074269	-729.066810	-729.065865	-729.106651	85.840
56	**2**	-497.45342655	-497.297845	-497.287130	-497.286186	-497.334836	102.392
56	**4**	-497.47476161	-497.318686	-497.308587	-497.307643	-497.355541	100.810
58		-289.01749112	-288.863986	-288.856147	-288.855203	-288.895134	84.041
59		-246.31391520	-246.239445	-246.234587	-246.233643	-246.266376	68.892
61		-461.32370737	-461.157565	-461.148421	-461.147476	-461.192175	94.075
63		-665.82234404	-665.654073	-665.642084	-665.641140	-665.693156	109.477
67a		-974.60322782	-974.273673	-974.253857	-974.252913	-974.320961	143.219
67b		-536.73060705	-536.480290	-536.465936	-536.464992	-536.520675	117.193
68		-624.88448409	-624.714670	-624.704213	-624.703269	-624.751599	101.719
70		-848.47237973	-848.046242	-848.026520	-848.025576	-848.095652	147.487
71		-695.81892387	-695.429989	-695.413648	-695.412704	-695.475169	131.469
72		-1893.42675983	-1892.804154	-1892.769435	-1892.768490	-1892.874167	222.415
74		-1198.73986724	-1198.486911	-1198.469011	-1198.468067	-1198.533795	138.336
75		-1198.73986724	-1198.486911	-1198.469011	-1198.468067	-1198.533795	138.336
77		-1199.30181379	-1199.035253	-1199.017041	-1199.016097	-1199.083407	141.665