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Supplementary Information

Theoretical Study of Thermochemical Properties using Composite Methods Adapted to ONIOM

Gabriel Heerdt* and Nelson H. Morgon

Instituto de Química, Universidade Estadual de Campinas, CP 6154, 13083-970 Campinas-SP, Brazil

Table S1 presents the experimental data and results for the proton affinities of all molecules calculated, considering only the results obtained with the B3LYP functional, and G3(MP2) and G3(B3) theories.

Table S1. Experimental and calculated proton affinities (kJ mol^{-1}) for all the molecules considered

Aliphatic alcohols	Experimental	Equation 6 (B3LYP)	G3(MP2)	G3(B3)
ethanol	1582 ± 8.4	1584.480	1589.436	1582.586
1,1-dimethyl-ethanol	1566 ± 8.4	1569.523	1573.049	1566.200
2-butanol	1565 ± 8.4	1565.044	1570.715	1562.942
2-methyl-1-propanol	1567 ± 8.4	1568.260	1577.050	1569.758
1-pentanol	1568 ± 8.4	1577.555	1583.081	1586.177
2-pentanol	1562 ± 8.4	1562.163	1567.816	1559.663
3-pentanol	1560 ± 8.4	1555.244	1563.654	1555.496
2-methyl-1-butanol	1564 ± 8.4	1566.022	1564.568	1566.888
3-methyl-1-butanol	1566 ± 8.4	1576.614	1576.365	1574.801
2-methyl-2-butanol	1561 ± 8.4	1559.882	1567.474	1560.104
3-methyl-2-butanol	1559 ± 8.4	1563.031	1570.632	1562.603
2,2-dimethyl-2-propanol	1559 ± 8.4	1557.752	1568.313	1560.729
1-hexanol	1565 ± 8.4	1577.112	1582.397	1575.082
2-hexanol	1560 ± 8.4	1560.891	1566.292	1557.993
3-hexanol	1556 ± 8.4	1552.486	1560.909	1552.569
2-ethyl-1-butanol	1561 ± 8.4	1561.491	1571.723	1562.845
2-methyl-1-pentanol	1561 ± 8.4	1564.881	1562.235	1565.932
3-methyl-1-pentanol	1563 ± 8.4	1576.094	1580.604	1573.591
4-methyl-1-pentanol	1564 ± 8.4	1575.721	1580.383	1588.264
2-methyl-2-pentanol	1558 ± 8.4	1556.951	1564.643	1557.355
3-methyl-2-pentanol	1557 ± 8.4	1555.613	1563.473	1555.349
4-methyl-2-pentanol	1557 ± 8.4	1556.517	1563.705	1554.435
2-methyl-3-pentanol	1555 ± 8.4	1549.374	1559.821	1551.994
3-methyl-3-pentanol	1556 ± 8.4	1550.486	1561.867	1544.538
2,3-dimethyl-1-butanol	1560 ± 8.4	1563.250	1572.523	1564.840
2,3-dimethyl-2-butanol	1556 ± 8.4	1550.476	1560.627	1553.028
3,3-dimethyl-2-butanol	1554 ± 8.4	1549.374	1560.322	1542.251
1-heptanol	1564 ± 8.4	1576.859	1581.987	1574.691
2-heptanol	1558 ± 8.4	1560.170	1565.374	1579.578

*e-mail: gabheerdt@iqm.unicamp.br

Table S1. continuation

Aliphatic alcohols	Experimental	Equation 6 (B3LYP)	G3(MP2)	G3(B3)
1-octanol	1563 ± 813	1576.700	1581.651	1579.589
1-nonanol	1561 ± 13	1563.488	1562.659	1571.245
1-decanol	1560 ± 8.4	1576.586	1571.396	1584.358
Cyclic alcohols				
cyclopentanol	1563 ± 19	1568.190	1570.486	1559.046
1-methyl-cyclopentanol	1559 ± 8.4	1559.997	1559.497	1559.479
t-2-methyl-cyclopentanol	1558 ± 8.4	1560.718	1557.284	1561.663
Aliphatic ketones				
propanone	1543 ± 8.4	1543.035	1540.013	1538.009
3-pentanone	1542 ± 9.6	1535.151	1536.897	1536.351
3-methyl-2-butanone	1545 ± 11	1540.647	1538.222	1544.506
Cyclic ketones				
cyclopentanone	1540 ± 18	1536.850	1532.954	1534.397
cyclohexanone	1533 ± 8.4	1543.095	1537.748	1521.792
Radicals				
ethyl	616 ± 2	623.350	629.896	638.587
isopropyl	671.4 ± 2	667.986	659.093	654.889
n-propyl	668 ± 2	678.480	677.590	674.251
tert-butyl	698.6 ± 4	702.558	704.445	701.473
2-butyl	690 ± 4	699.469	701.147	700.023
isobutyl	678.5 ± 4	689.145	689.008	694.227
Alkenes				
propylene	1698 ± 8.4	1702.059	1693.642	1714.597
1-butene	1724 ± 8.4	1728.598	1728.406	1729.335
2-butene	1701 ± 8.4	1689.364	1689.502	1687.355
2-methyl-1-butene	1687 ± 8.4	1678.599	1669.977	1677.878

Table S2 presents the experimental and calculated electron affinities, considering only the B3LYP functional and the G3(MP2) and G3(B3) theories.

Table S2. Experimental and calculated electron affinities (eV) for all the molecules considered

Aliphatic alcohols	Experimental	Equation 6 (B3LYP)	G3(MP2)	G3(B3)
ethanol	1712 ± 0.10	1.613	1.738	1.688
1,1-dimethyl-ethanol	1.910 ± 0.10	1.901	1.979	1.964
2-butanol	1.950 ± 0.10	1.898	1.976	1.960
2-methyl-1-propanol	1.870 ± 0.11	1.811	1.862	1.846
1-pentanol	1.890 ± 0.13	1.685	1.800	1.748
2-pentanol	1.920 ± 0.12	1.928	2.008	1.994
3-pentanol	1.950 ± 0.15	2.057	2.038	2.023
2-methyl-1-butanol	1.900 ± 0.12	1.833	1.881	1.870
3-methyl-1-butanol	1.910 ± 0.15	1.741	1.818	1.797
2-methyl-2-butanol	1.930 ± 0.15	1.993	2.062	2.016
3-methyl-2-butanol	1.930 ± 0.15	1.930	2.275	1.967

Table S2. continuation

Aliphatic alcohols	Experimental	Equation 6 (B3LYP)	G3(MP2)	G3(B3)
2,2-dimethyl-2-propanol	1.930 ± 0.13	1.899	1.941	1.916
1-hexanol	2.000 ± 0.13	1.688	1.806	1.755
2-hexanol	1.940 ± 0.13	1.941	1.994	2.011
3-hexanol	1.980 ± 0.13	2.022	2.067	2.056
2-ethyl-1-butanol	1.910 ± 0.12	1.873	1.911	1.910
2-methyl-1-pentanol	1.930 ± 0.12	1.843	1.895	1.879
3-methyl-1-pentanol	1.890 ± 0.12	1.746	1.833	1.810
4-methyl-1-pentanol	1.930 ± 0.14	1.738	1.831	1.915
2-methyl-2-pentanol	1.970 ± 0.15	2.045	2.050	2.041
3-methyl-2-pentanol	1.940 ± 0.12	1.992	2.286	2.032
4-methyl-2-pentanol	1.970 ± 0.12	1.990	2.054	2.050
2-methyl-3-pentanol	1.990 ± 0.15	2.051	2.010	2.058
3-methyl-3-pentanol	1.980 ± 0.15	2.014	2.087	2.006
2,3-dimethyl-1-butanol	1.930 ± 0.12	1.850	1.896	1.877
2,3-dimethyl-2-butanol	1.980 ± 0.12	2.08	2.034	2.016
3,3-dimethyl-2-butanol	1.980 ± 0.04	2.027	2.002	2.044
1-heptanol	1.970 ± 0.13	1.688	1.911	1.894
2-heptanol	1.960 ± 0.12	1.948	2.033	2.024
1-octanol	2.073 ± 0.13	1.686	2.009	2.001
1-nonanol	1.930 ± 0.16	1.693	1.880	1.881
1-decanol	1.860 ± 0.12	1.690	1.768	1.771
Cyclic alcohols				
cyclopentanol	1.500 ± 0.10	1.768	1.674	1.645
1-methyl-cyclopentanol	1.950 ± 0.12	1.997	1.993	1.967
t-2-methyl-cyclopentanol	1.960 ± 0.12	1.919	1.979	1.904
Aliphatic ketones				
propanone	1.760 ± 0.02	1.734	1.752	1.759
3-pentanone	1.430 ± 0.13	1.525	1.560	1.581
3-methyl-2-butanone	1.270 ± 0.18	1.467	1.448	1.343
Cyclic ketones				
cyclopentanone	1.620 ± 0.01	1.741	1.704	1.645
cyclohexanone	1.530 ± 0.20	1.628	1.599	1.585
Radicals				
ethyl	0.950 ± 0.12	1.012	0.984	0.954
isopropyl	0.690 ± 0.12	0.796	0.805	0.779
n-propyl	-0.070 ± 0.12	0.040	0.024	0.011
tert-butyl	0.650 ± 0.12	0.956	0.883	0.814
2-butyl	-0.120 ± 0.09	0.029	0.014	0.009
isobutyl	0.050 ± 0.12	0.011	0.089	0.098
Alkenes				
propylene	0.560 ± 0.19	0.678	0.548	0.653
1-butene	0.600 ± 0.10	0.377	0.603	0.607
2-butene	0.570 ± 0.10	0.699	0.789	0.673
2-methyl-1-butene	0.660 ± 0.15	0.693	0.595	0.685