

**Correlation of Hydrogen-Atom Abstraction
Reaction Efficiencies for Aryl Radicals with
their Vertical Electron Affinities and the
Vertical Ionization Energies of the Hydrogen
Atom Donors**

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radical a
UB3LYP/6-31+G(d)

7	-2.794373	-0.000067	0.000263
6	-3.469274	1.097290	0.435854
6	-4.853902	1.124362	0.433487
6	-5.561957	0.000241	-0.000636
6	-4.853875	-1.124005	-0.434352
6	-3.469237	-1.097198	-0.435935
6	-1.339871	-0.000160	0.000553
6	-0.653640	1.040793	-0.629664
6	0.738590	1.030521	-0.627715
6	1.465932	-0.000296	0.000355
6	0.738580	-1.031081	0.628478
6	-0.653702	-1.041274	0.630530
1	-2.859025	1.916536	0.795586
1	-5.363998	2.014148	0.786504
1	-6.647645	0.000327	-0.000929
1	-5.363956	-2.013665	-0.787699
1	-2.858929	-1.916484	-0.795456
1	-1.192486	1.825439	-1.154048
1	1.268806	1.817045	-1.155161
1	1.268786	-1.817808	1.155622
1	-1.192541	-1.826003	1.154794
6	2.948384	-0.000014	0.000539
6	3.660437	-1.207855	-0.133936
6	5.062139	-1.218559	-0.139625
6	5.690709	0.000289	-0.001027
6	5.062010	1.218988	0.138555
6	3.660252	1.208022	0.134489
1	3.124800	-2.144570	-0.269151
1	5.611394	-2.148393	-0.258452
1	5.611368	2.148848	0.256711
1	3.124585	2.144653	0.270132

E = -710.1052788 au
ZPE = 0.250755 au
(H298 - E0) = 0.014515 au

radical b
UB3LYP/6-31+G(d)

6	-2.123966	0.038835	-1.226350
6	-1.487403	0.247085	0.000397
6	-2.120776	0.028159	1.226967
6	-3.450891	-0.420198	1.230536
6	-4.041360	-0.614765	-0.000037
6	-3.454183	-0.409395	-1.230376
1	-1.597483	0.220433	-2.159986
1	-1.591860	0.201781	2.160746
1	-3.975179	-0.597444	2.165174
1	-3.980840	-0.578559	-2.165176
6	1.852300	-2.395082	-0.003143
6	0.755002	-1.554403	-0.002243
6	0.959313	-0.158552	-0.000345
6	2.288230	0.376333	0.000298
6	3.387374	-0.525140	-0.000580
6	3.173361	-1.885023	-0.002241
1	1.695200	-3.469602	-0.004491
1	-0.248951	-1.960835	-0.003026
7	-0.108163	0.735521	0.000727
6	2.462662	1.778793	0.001815
1	4.394896	-0.119121	-0.000067
1	4.014336	-2.571305	-0.003015
6	1.366264	2.622402	0.002579
6	0.086844	2.065362	0.002041
1	3.469862	2.187186	0.002260
1	1.472659	3.701214	0.003758
1	-0.812129	2.671121	0.002822

E = -632.6913495 au
ZPE = 0.216580 au
(H298 - E0) = 0.012518 au

E(+ electron) = -632.8400407 au

radical c
UB3LYP/6-31+G(d)

7	0.664761	0.000000	0.000000
6	1.336746	1.017100	-0.601771
6	2.721949	1.042785	-0.606409
6	3.428803	0.000000	-0.000003
6	2.721950	-1.042784	0.606407
6	1.336748	-1.017099	0.601774
6	-0.794296	0.000000	0.000002
6	-1.464823	1.085030	0.575222
6	-2.867794	1.087985	0.575390
6	-3.489432	0.000000	-0.000003
6	-2.867792	-1.087986	-0.575393
6	-1.464821	-1.085030	-0.575220
1	0.724902	1.773104	-1.078857
1	3.232880	1.865988	-1.094046
1	4.514557	-0.000001	-0.000006
1	3.232884	-1.865986	1.094043
1	0.724906	-1.773101	1.078865
1	-0.912372	1.899619	1.036772
1	-3.421072	1.909151	1.021671
1	-3.421067	-1.909152	-1.021678
1	-0.912368	-1.899619	-1.036769

E = -479.0363028 au
ZPE = 0.169873 au
(H298 - E0) = 0.009829 au

E(+ electron) = -479.1972253 au

E(+ electron) = -710.2267659 au

radical d
UB3LYP/6-31+G(d)

6	-2.293325	-2.351960	-0.249602
6	-1.187304	-1.543491	-0.082611
6	-1.335574	-0.133868	0.011763
6	-2.662881	0.428216	-0.083751
6	-3.777909	-0.436149	-0.252626
6	-3.594793	-1.799353	-0.331295
1	-2.164111	-3.427882	-0.322914
1	-0.200782	-1.996348	-0.031961
6	-0.262950	0.793613	0.177813
6	-2.753192	1.824596	-0.010498
1	-4.769044	0.001170	-0.321178
1	-4.449005	-2.456691	-0.461636
6	-1.734878	2.713310	0.136565
6	-0.428025	2.162480	0.235116
1	-1.886610	3.787344	0.185843
1	0.429851	2.817018	0.369142
7	1.101500	0.270553	0.293754
6	1.510129	-0.281179	1.463700
6	2.803928	-0.765405	1.597679
6	3.693119	-0.679794	0.524885
6	3.233446	-0.106600	-0.657802
6	1.933314	0.363397	-0.771581
1	0.775161	-0.304556	2.258907
1	3.111729	-1.199115	2.542927
1	4.714210	-1.042729	0.592310
1	1.541352	0.801757	-1.681248
9	4.036457	-0.000079	-1.714778

E = -731.9148605 au
ZPE = 0.208271 au
(H298 - E0) = 0.013359 au

radical e
UB3LYP/6-31+G(d)

6	-2.252441	-2.421506	-0.246862
6	-1.168015	-1.582859	-0.080248
6	-1.338513	-0.172910	0.008406
6	-2.668605	0.383002	-0.089873
6	-3.701934	-0.549661	-0.253272
6	-3.575803	-1.899435	-0.334753
1	-2.100558	-3.495399	-0.315458
1	-0.173385	-2.015870	-0.024925
6	-0.284386	0.770236	0.173706
6	-2.867099	1.788769	-0.029302
1	-4.426391	-2.562650	-0.464019
6	-1.799419	2.647313	0.121172
6	-0.486413	2.132537	0.224964
1	-1.955218	3.720208	0.167118
1	0.355371	2.806977	0.357634
7	1.091176	0.276126	0.294535
6	1.511350	-0.252706	1.470792
6	2.813844	-0.712117	1.608334
6	3.698805	-0.626323	0.532091
6	3.226743	-0.077285	-0.657229
6	1.918539	0.368847	-0.774177
1	0.778195	-0.279204	2.267556
1	3.131183	-1.127655	2.558578
1	4.726027	-0.971070	0.601850
1	1.517202	0.788941	-1.688418
9	4.025437	0.028251	-1.717562
1	-3.879505	2.173165	-0.106107

E = -731.9151154 au
ZPE = 0.208332 au
(H298 - E0) = 0.013360 au

radical f
UB3LYP/6-31+G(d)

7	0.335009	0.248066	-0.080852
6	1.148168	-0.775664	0.282472
6	2.522373	-0.605403	0.221349
6	3.085561	0.601506	-0.186092
6	2.218300	1.634380	-0.543361
6	0.845563	1.437045	-0.493170
6	-1.111888	0.059721	-0.027342
6	-1.676933	-0.993158	-0.755028
6	-3.066409	-1.176459	-0.704967
6	-3.780653	-0.288329	0.070752
6	-3.263387	0.760216	0.801288
6	-1.873338	0.939468	0.749311
1	0.686196	-1.690661	0.631876
1	4.164700	0.716061	-0.218394
1	2.601392	2.592671	-0.877009
1	0.124383	2.187731	-0.790794
1	-1.058306	-1.641536	-1.370479
1	-3.540989	-1.976522	-1.265572
1	-3.885295	1.416704	1.402843
1	-1.398333	1.729457	1.325450
9	3.297450	-1.625591	0.581865

E = -578.2656500 au
ZPE = 0.161441 au
(H298 - E0) = 0.010658 au

E(+ electron) = -578.4375882 au

E(+ electron) = -732.0838293 au

radical g
UB3LYP/6-31+G(d)

7	0.688426	-0.011224	-0.003996
6	1.375786	-1.048766	0.542878
6	2.760721	-1.047924	0.556800
6	3.451057	0.040747	0.016223
6	2.728217	1.102749	-0.534923
6	1.344212	1.051167	-0.541980
6	-0.769942	-0.043861	-0.021633
6	-1.416054	-1.119334	-0.651942
6	-2.791156	-1.074364	-0.622617
6	-3.565455	-0.089423	-0.049323
6	-2.879098	0.970660	0.566829
6	-1.481009	0.995557	0.584300
1	0.775583	-1.843091	0.970029
1	3.284251	-1.888040	1.000218
1	4.536599	0.061070	0.023918
1	3.226259	1.961958	-0.971071
1	0.720857	1.821600	-0.979445
1	-0.863531	-1.910991	-1.151675
1	-4.651072	-0.120879	-0.063810
1	-3.436153	1.771618	1.044759
1	-0.955439	1.802072	1.087373

E = -479.036568 au
ZPE = 0.169905
(H298 - E0) = 0.009841 au

E(+ electron) = -479.2153706 au

radical j
UB3LYP/6-31+G(d)

6	-2.496045	0.615383	0.000000
6	-1.322373	1.337596	0.000001
6	-0.067743	0.663884	-0.000002

E(+ electron) = -732.0862421 au

radical h
UB3LYP/6-31+G(d)

6	2.514229	-0.605876	-0.000012
6	1.337276	-1.340067	0.000000
6	0.106112	-0.650400	0.000000
6	0.036129	0.779953	0.000001
6	1.261505	1.514787	0.000012
6	2.409079	0.787417	0.000001
1	-1.042558	-2.358329	0.000007
1	3.479135	-1.105127	0.000001
1	1.361251	-2.427270	-0.000009
7	-1.087642	-1.341365	0.000008
6	-1.239074	1.394099	-0.000006
1	1.247488	2.601594	0.000006
6	-2.398081	0.633227	-0.000006
6	-2.293399	-0.758664	0.000000
1	-1.301226	2.479174	0.000007
1	-3.380101	1.092175	-0.000023
1	-3.153149	-1.419528	0.000014

E = -401.6284718 au
ZPE = 0.136521 au
(H298 - E0) = 0.007771 au

E(+ electron) = -401.8083163 au

radical k
UB3LYP/6-31+G(d)

7	-0.998879	0.070220	-0.028321
6	-1.754285	0.862948	0.777324
6	-3.128563	0.701099	0.836835

radical i
UB3LYP/6-31+G(d)

7	0.356506	0.237541	-0.078534
6	1.178872	-0.792041	0.246085
6	2.551235	-0.602333	0.205138
6	3.102565	0.627998	-0.144416
6	2.225768	1.665144	-0.464344
6	0.855327	1.449752	-0.434937
6	-1.088001	0.026057	-0.054204
6	-1.632934	-1.012184	-0.826855
6	-3.000222	-1.143068	-0.746379
6	-3.854963	-0.362382	0.000775
6	-3.268059	0.667581	0.755481
6	-1.883758	0.863950	0.731790
1	0.725056	-1.727462	0.549311
1	4.180463	0.756656	-0.162440
1	2.599989	2.641587	-0.752390
1	0.127027	2.203773	-0.705535
1	-1.018086	-1.642284	-1.464646
1	-4.928537	-0.526568	0.016638
1	-3.890266	1.308880	1.373363
1	-1.432073	1.640940	1.341641
9	3.336212	-1.627684	0.527220

E = -578.2658766 au
ZPE = 0.161440 au
(H298 - E0) = 0.010666 au

E(+ electron) = -578.4514271 au

radical l
UB3LYP/6-31+G(d)

7	-1.373583	0.110740	-0.037273
6	-2.193673	0.749098	0.839426
6	-3.534015	0.410765	0.923453

6	-0.018914	-0.783172	0.000000
6	-1.256895	-1.426601	-0.000001
6	-2.472466	-0.813525	-0.000002
1	1.211329	2.439524	0.000003
1	-3.453919	1.127340	0.000004
1	-1.344433	2.423512	0.000001
6	1.151624	1.355978	-0.000001
6	1.247412	-1.431202	0.000002
1	-3.402866	-1.375510	0.000005
6	2.394600	-0.687355	-0.000001
7	2.308560	0.685610	0.000000
1	1.305841	-2.514019	0.000003
1	3.393692	-1.104408	-0.000001
1	3.175237	1.218379	0.000002

E = -401.6277515 au
ZPE = 0.136753 au
(H298 - E0) = 0.007782 au

E(+ electron) = -401.8138432 au

radical m
UB3LYP/6-31+G(d)

6	2.462318	0.614180	0.000000
6	1.280237	1.333539	0.000000
6	0.052669	0.642479	-0.000001
6	0.006118	-0.792960	0.000000
6	1.255721	-1.429041	0.000000
6	2.465871	-0.812867	0.000000
1	-1.133377	2.326715	-0.000001
1	3.411319	1.143234	0.000001
1	1.297407	2.420062	0.000001
7	-1.154465	1.308716	0.000000

6	-3.734789	-0.298867	0.070932
6	-2.941634	-1.110059	-0.745964
6	-1.573034	-0.901947	-0.785847
6	0.445346	0.266793	-0.081552
6	0.940709	1.511873	-0.476822
6	2.333319	1.695801	-0.526976
6	3.125031	0.626855	-0.182002
6	2.652132	-0.607451	0.207241
6	1.271716	-0.807207	0.266007
1	-1.214177	1.595855	1.364493
1	-3.707898	1.346055	1.488694
1	-4.810096	-0.444199	0.110185
1	-3.374380	-1.891959	-1.360685
1	-0.901455	-1.472273	-1.416254
1	0.269315	2.314961	-0.766975
1	2.755307	2.646869	-0.839587
9	3.475898	-1.607055	0.540310
1	0.876770	-1.762379	0.600522

E = -578.2680206 au
ZPE = 0.161784 au
(H298 - E0) = 0.010673 au

E(+ electron) = -578.4547972 au

radical n
UB3LYP/6-31+G(d)

7	1.606133	0.142394	-0.042718
6	2.443465	0.708215	0.867795
6	3.766481	0.308223	0.949905
6	4.233707	-0.695343	0.095603
6	3.357179	-1.269919	-0.829673
6	2.045480	-0.829837	-0.886555
6	0.218818	0.585843	-0.115642
6	-0.057455	1.938562	-0.378479
6	-1.392034	2.271492	-0.426131
6	-2.459319	1.419741	-0.251008

6	-4.036718	-0.606465	0.106843
6	-3.177391	-1.256507	-0.783799
6	-1.847468	-0.875119	-0.844843
6	0.031027	0.497235	-0.118009
6	0.353688	1.823141	-0.442831
6	1.703404	2.089286	-0.495183
6	2.733732	1.206475	-0.272413
6	2.356348	-0.110436	0.044857
6	1.005804	-0.471915	0.126825
1	-1.729128	1.506305	1.459570
1	-4.166864	0.934127	1.632052
1	-5.083704	-0.888539	0.163614
1	-3.530505	-2.045573	-1.438952
1	-1.131814	-1.313977	-1.529643
1	-0.405434	2.567856	-0.665431
1	3.780231	1.489735	-0.331215
17	3.575364	-1.310203	0.356599
1	0.732693	-1.485016	0.402794

E = -938.6260884 au
ZPE = 0.160112 au
(H298 - E0) = 0.011073 au

E(+ electron) = -938.8137898 au

radical o
UB3LYP/6-31+G(d)

7	0.790401	-0.000228	-0.000755
6	1.455181	1.032523	-0.587085
6	2.845237	1.069928	-0.595187
6	3.477372	-0.000104	0.000727
6	2.844693	-1.070153	0.595999
6	1.454640	-1.032779	0.586515
6	-0.671012	0.000018	-0.000854
6	-1.345814	1.075574	0.579818
6	-2.742225	1.067955	0.575470
6	-3.438251	0.000252	0.000762

6 -1.251607 -1.440179 0.000000
 1 3.403413 -1.361439 0.000002
 6 -2.423791 -0.698198 0.000000
 6 -2.346545 0.695439 0.000000
 1 -1.285094 -2.525831 -0.000001
 1 -3.397256 -1.174781 0.000002
 1 -3.221099 1.336677 0.000001

E = -401.6283466 au
ZPE = 0.136658 au
(H298 - E0) = 0.007765 au

E(+ electron) = -401.8197893 au

6 -2.117526 0.086843 0.000225
 6 -0.795551 -0.350894 0.075231
 1 2.006315 1.458036 1.516372
 1 4.413302 0.773141 1.686152
 1 5.266754 -1.025198 0.150603
 1 3.682655 -2.046604 -1.513350
 1 1.319266 -1.211701 -1.594206
 1 0.732939 2.663232 -0.556505
 1 -3.498628 1.729433 -0.297843
 1 -0.590412 -1.391706 0.299538
 7 -3.200352 -0.912520 0.207457
 8 -2.851821 -2.072434 0.413287
 8 -4.352194 -0.501980 0.155267

E = -683.5304958 au
ZPE = 0.172013 au
(H298 - E0) = 0.012435 au

E(+ electron) = -683.7290400 au

6 -2.742996 -1.067543 -0.574756
 6 -1.346577 -1.075447 -0.580854
 1 0.837309 1.793663 -1.049628
 1 3.370666 1.896007 -1.064412
 1 3.369655 -1.896221 1.065754
 1 0.836334 -1.793804 1.048648
 1 -0.798266 1.888292 1.049206
 1 -3.282304 1.892345 1.030835
 1 -4.524060 0.000260 0.001470
 1 -3.283891 -1.891831 -1.029339
 1 -0.799747 -1.888447 -1.050574

E = -479.0338684 au
ZPE = 0.169795 au
(H298 - E0) = 0.009830 au

E(+ electron) = -479.2393437 au

radical p

UB3LYP/6-31+G(d)

6 2.382646 0.743305 0.000000
 6 1.168005 1.404193 0.000000
 6 -0.013637 0.641238 0.000000
 6 0.038397 -0.794600 -0.000001
 6 1.306632 -1.435821 0.000000
 6 2.454131 -0.673149 0.000000
 1 -1.292517 2.252971 -0.000003
 1 3.301482 1.321928 0.000001
 1 1.124123 2.490382 0.000000
 7 -1.260818 1.235766 0.000000
 6 -1.203678 -1.427137 -0.000001
 1 1.346099 -2.520105 0.000000
 1 3.426112 -1.156201 0.000001
 6 -2.436200 -0.831909 0.000001
 6 -2.425544 0.568902 0.000000

radical q

UB3LYP/6-31+G(d)

7 -0.761584 -0.040980 -0.022376
 6 -1.410711 -1.074153 -0.641434
 6 -2.777921 -1.067115 -0.621324
 6 -3.557548 -0.088025 -0.046120
 6 -2.855935 0.963026 0.567443
 6 -1.467595 0.956168 0.573612
 6 0.696165 -0.011992 -0.007533
 6 1.387747 -1.113132 0.502566
 6 2.783299 -1.078655 0.512352
 6 3.463258 0.039044 0.018768
 6 2.752058 1.130739 -0.488691
 6 1.356219 1.113277 -0.507053
 1 -0.794325 -1.821249 -1.127745
 1 -4.643772 -0.116366 -0.056768
 1 -3.381901 1.777312 1.056021

radical r

UB3LYP/6-31+G(d)

7 0.000007 1.236420 0.000000
 6 1.197844 0.601206 -0.000010
 6 1.231397 -0.788604 0.000008
 6 -0.000020 -1.411974 0.000000
 6 -1.231413 -0.788591 -0.000008
 6 -1.197815 0.601241 0.000008
 1 0.000028 2.255084 0.000002
 1 2.083991 1.227020 -0.000005
 1 2.177052 -1.321917 0.000012
 1 -2.177104 -1.321840 -0.000008
 1 -2.083974 1.227041 0.000011

E = -247.9670767 au
ZPE = 0.089691 au
(H298 - E0) = 0.005306 au

1 -3.373931 -1.377770 0.000002
1 -3.330152 1.168305 0.000001

E = -401.6286226 au
ZPE = 0.136551 au
(H298 - E0) = 0.007773 au

E(+ electron) = -401.8376208 au

radical s
UB3LYP/6-31+G(d)

7 1.185068 0.506758 -0.000001
6 1.128284 -0.852825 -0.000011
6 -0.123602 -1.405481 0.000007
6 -1.301194 -0.688027 -0.000003
6 -1.180858 0.713803 -0.000003
6 0.081722 1.291345 -0.000001
1 2.101185 0.954957 0.000017
1 2.064805 -1.400125 0.000024
1 -2.276481 -1.168428 0.000011
1 -2.059509 1.350995 0.000009
1 0.248410 2.362409 0.000013

E = -247.9634691 au
ZPE = 0.089702 au
(H298 - E0) = 0.005317 au

E(+ electron) = -248.1879596 au

1 -0.879282 1.722168 1.063732
1 0.852940 -1.966208 0.910923
1 3.335516 -1.921908 0.915554
1 4.548821 0.059065 0.029026
1 3.280542 1.993690 -0.881946
1 0.798335 1.945265 -0.927685

E = -479.0314631 au
ZPE = 0.169814 au
(H298 - E0) = 0.009836 au

E(+ electron) = -479.2439007 au

radical t
UB3LYP/6-31+G(d)

7 1.274749 -0.000955 -0.000357
6 1.942352 0.465471 -1.090878
6 3.325722 0.479717 -1.108615
6 4.029704 -0.000110 0.000389
6 3.325423 -0.480386 1.108998
6 1.942051 -0.466912 1.090553
6 -0.171353 -0.000425 -0.000328
6 -0.864174 1.212829 0.095228
6 -2.263501 1.221083 0.094819
6 -2.889338 0.001048 0.000312
6 -2.264792 -1.219669 -0.094649
6 -0.865425 -1.212995 -0.095450
1 1.329810 0.809686 -1.915618
1 3.838301 0.858036 -1.986410
1 5.115610 0.000243 0.000677
1 3.837747 -0.858451 1.987045
1 1.329287 -0.811331 1.915044
9 -0.176300 2.357071 0.191867
9 -2.924010 2.371227 0.189532
9 -2.926665 -2.369051 -0.188978
9 -0.179027 -2.358069 -0.192479

E(+ electron) = -248.1833653 au

radical u
UB3LYP/6-31+G(d)

7 0.194918 -1.126245 -0.000008
6 -0.456409 0.065289 -0.000008
6 0.272720 1.254722 0.000000
6 1.673648 1.200254 -0.000007
6 2.253396 -0.054318 0.000007
6 1.556033 -1.227043 0.000004
1 -0.365168 -1.979883 -0.000009
17 -2.163773 0.019925 0.000004
1 -0.256237 2.201949 0.000006
1 2.262646 2.114153 0.000014
1 1.982150 -2.224649 0.000014

E = -707.5486253 au
ZPE = 0.079740 au
(H298 - E0) = 0.006401 au

E(+ electron) = -707.7794424 au

E = -875.9498144 au
ZPE = 0.137264 au
(H298 - E0) = 0.013557 au

E(+ electron) = -876.1767597 au

radical v

UB3LYP/6-31+G(d)

7	-0.130453	1.088163	-0.000099
6	0.540586	-0.098344	-0.000336
6	-0.233736	-1.231585	-0.000067
6	-1.607183	-1.241771	0.000042
6	-2.252057	0.013355	0.000057
6	-1.486590	1.166310	0.000054
1	0.416602	1.950652	0.000002
17	2.244025	-0.076541	0.000100
1	-2.177688	-2.167493	0.000134
1	-3.334466	0.087164	0.000182
1	-1.905819	2.165929	0.000181

E = -707.5487847 au
ZPE = 0.079875 au
(H298 - E0) = 0.006410 au

E(+ electron) = -707.7861607 au

radical w

UB3LYP/6-31+G(d)

7	1.139284	-0.731656	0.000004
6	-0.027291	-1.370246	-0.000003
6	-1.252133	-0.754868	-0.000003
6	-1.221144	0.650555	0.000003
6	0.001679	1.340285	0.000000
6	1.190012	0.633949	-0.000004
1	2.007890	-1.268576	0.000007
1	-2.178482	-1.319513	0.000002
1	-2.157610	1.202578	0.000008
1	0.030209	2.424592	-0.000003
1	2.176262	1.084461	0.000001

E = -247.9620326 au
ZPE = 0.089444 au
(H298 - E0) = 0.005317 au

E(+ electron) = -248.2079811 au

a

UB3LYP/6-31+G(d)

7	-2.853814	-0.000074	0.000151
6	-3.528965	1.094825	0.441725
6	-4.913558	1.122017	0.439329
6	-5.621786	0.000307	-0.000530
6	-4.913656	-1.121570	-0.440088
6	-3.529051	-1.094716	-0.441912
6	-1.399802	-0.000212	0.000374
6	-0.713093	1.048350	-0.617019
6	0.678887	1.038178	-0.614852

b

UB3LYP/6-31+G(d)

6	1.870981	-2.409315	-0.005333
6	0.785415	-1.553772	-0.003938
6	1.008793	-0.160671	-0.000606
6	2.344733	0.355995	0.000878
6	3.431435	-0.560395	-0.000549
6	3.198901	-1.917239	-0.003553
1	1.699303	-3.481606	-0.007950
1	-0.224320	-1.945697	-0.005315
7	-0.046521	0.747118	0.000652

c

UB3LYP/6-31+G(d)

6	-0.732337	0.000000	0.000000
6	-1.408675	1.085857	0.560045
6	-2.804930	1.078100	0.555085
6	-3.500846	0.000000	0.000000
6	-2.804929	-1.078101	-0.555085
6	-1.408675	-1.085857	-0.560045
7	0.726567	0.000000	0.000000
6	1.398933	1.031484	-0.575495
6	2.783800	1.057481	-0.579174

6 1.406757 -0.000305 0.000414
 6 0.678792 -1.038779 0.615595
 6 -0.713225 -1.048920 0.617641
 1 -2.918781 1.912023 0.806010
 1 -5.423466 2.009928 0.797250
 1 -6.707451 0.000421 -0.000742
 1 -5.423648 -2.009332 -0.798252
 1 -2.918905 -1.911989 -0.806070
 1 -1.251895 1.839321 -1.131904
 1 1.209170 1.831358 -1.132040
 1 1.209019 -1.832130 1.132568
 1 -1.252079 -1.839965 1.132354
 6 2.888281 -0.000010 0.000808
 6 3.606814 -1.203329 -0.123799
 6 5.001517 -1.202030 -0.128219
 6 5.703182 0.000273 -0.001121
 6 5.001403 1.202406 0.127259
 6 3.606672 1.203522 0.124761
 1 3.075129 -2.142676 -0.251497
 1 5.539989 -2.139085 -0.238860
 1 6.789491 0.000376 -0.002043
 1 5.540117 2.139421 0.237037
 1 3.075002 2.142810 0.252934

E = -710.7943247 au
ZPE = 0.263939 au
(H298 - E0) = 0.014537 au

d
UB3LYP/6-31+G(d)
 6 2.215868 -2.406969 -0.266389
 6 1.125838 -1.579320 -0.094882
 6 1.301049 -0.172460 0.010641
 6 2.626981 0.375549 -0.077708
 6 3.723441 -0.512543 -0.250992
 6 3.525290 -1.872660 -0.341041
 1 2.068994 -3.480006 -0.348601

6 2.537969 1.756127 0.003122
 1 4.444422 -0.168171 0.000580
 1 4.030530 -2.614845 -0.004742
 6 1.452984 2.614023 0.003981
 6 0.166034 2.073737 0.002878
 1 3.550531 2.151008 0.004126
 1 1.573518 3.691333 0.005602
 1 -0.725008 2.691115 0.004126
 6 -1.432720 0.276784 0.000511
 6 -2.072689 0.060759 1.221366
 6 -3.402427 -0.368331 1.213254
 6 -4.066991 -0.574247 0.000351
 6 -3.407825 -0.351112 -1.212443
 6 -2.078096 0.078003 -1.220465
 1 -1.545106 0.223437 2.157158
 1 -3.915972 -0.537945 2.154820
 1 -5.100830 -0.906591 0.000342
 1 -3.925816 -0.507568 -2.153846
 1 -1.554577 0.253631 -2.156184

E = -633.3817344 au
ZPE = 0.229790 au
(H298 - E0) = 0.012539 au

e
UB3LYP/6-31+G(d)
 6 2.215868 -2.406969 -0.266389
 6 1.125838 -1.579320 -0.094882
 6 1.301049 -0.172460 0.010641
 6 2.626981 0.375549 -0.077708
 6 3.723441 -0.512543 -0.250992
 6 3.525290 -1.872660 -0.341041
 1 2.068994 -3.480006 -0.348601

6 3.490755 0.000000 0.000000
 6 2.783799 -1.057481 0.579174
 6 1.398933 -1.031484 0.575495
 1 -0.861731 1.907053 1.014987
 1 -3.345336 1.910603 0.995066
 1 -4.586657 -0.000001 0.000000
 1 -3.345336 -1.910603 -0.995067
 1 -0.861731 -1.907052 -1.014987
 1 0.787247 1.799002 -1.033863
 1 3.294425 1.892887 -1.045922
 1 4.576513 -0.000001 0.000000
 1 3.294424 -1.892887 1.045922
 1 0.787246 -1.799001 1.033864

E = -479.7272300 au
ZPE = 0.183138 au
(H298 - E0) = 0.009851 au

f
UB3LYP/6-31+G(d)
 7 0.395783 0.252834 -0.078160
 6 1.203776 -0.778800 0.273657
 6 2.578745 -0.614978 0.215289
 6 3.148758 0.593316 -0.177745
 6 2.286814 1.634548 -0.523417
 6 0.913144 1.443667 -0.476242
 6 -1.051887 0.071021 -0.028532

1	0.131024	-2.013720	-0.049525
6	0.241620	0.764043	0.182788
6	2.814068	1.782594	0.000036
1	4.725276	-0.096382	-0.315268
1	4.371126	-2.540227	-0.474757
6	1.748297	2.642637	0.155144
6	0.435559	2.126591	0.248946
1	3.824625	2.176440	-0.068285
1	1.904868	3.714922	0.212908
1	-0.408450	2.797123	0.387025
7	-1.131937	0.262961	0.295067
6	-1.546621	-0.300210	1.457188
6	-2.848558	-0.762990	1.587979
6	-3.739494	-0.643984	0.519790
6	-3.273283	-0.059920	-0.654822
6	-1.965204	0.388320	-0.765400
1	-0.809399	-0.350032	2.249052
1	-3.161165	-1.206605	2.527019
1	-4.766639	-0.989819	0.584791
1	-1.568057	0.834260	-1.669110
9	-4.077529	0.077916	-1.707598

E = -732.6049584 au
ZPE = 0.221462 au
(H298 - E0) = 0.013366 au

g
UB3LYP/6-31+G(d)

6	-0.732337	0.000000	0.000000
6	-1.408675	1.085857	0.560045
6	-2.804930	1.078100	0.555085
6	-3.500846	0.000000	0.000000
6	-2.804929	-1.078101	-0.555085
6	-1.408675	-1.085857	-0.560045
7	0.726567	0.000000	0.000000
6	1.398933	1.031484	-0.575495
6	2.783800	1.057481	-0.579174

1	0.131024	-2.013720	-0.049525
6	0.241620	0.764043	0.182788
6	2.814068	1.782594	0.000036
1	4.725276	-0.096382	-0.315268
1	4.371126	-2.540227	-0.474757
6	1.748297	2.642637	0.155144
6	0.435559	2.126591	0.248946
1	3.824625	2.176440	-0.068285
1	1.904868	3.714922	0.212908
1	-0.408450	2.797123	0.387025
7	-1.131937	0.262961	0.295067
6	-1.546621	-0.300210	1.457188
6	-2.848558	-0.762990	1.587979
6	-3.739494	-0.643984	0.519790
6	-3.273283	-0.059920	-0.654822
6	-1.965204	0.388320	-0.765400
1	-0.809399	-0.350032	2.249052
1	-3.161165	-1.206605	2.527019
1	-4.766639	-0.989819	0.584791
1	-1.568057	0.834260	-1.669110
9	-4.077529	0.077916	-1.707598

E = -732.6049584 au
ZPE = 0.221462 au
(H298 - E0) = 0.013366 au

h
UB3LYP/6-31+G(d)

6	-2.417940	-0.720690	-0.000001
6	-1.221685	-1.412392	0.000000
6	-0.019790	-0.679666	0.000000
6	-0.020680	0.749655	0.000000
6	-1.273937	1.420686	0.000001
6	-2.446248	0.697473	0.000000
1	1.206422	-2.332867	0.000001
1	-3.352969	-1.272638	-0.000002
1	-1.205280	-2.499138	-0.000001

6	-1.622793	-0.992479	-0.731117
6	-3.007873	-1.159236	-0.678857
6	-3.795793	-0.274641	0.063867
6	-3.203853	0.783594	0.760203
6	-1.820216	0.965795	0.719301
1	0.737032	-1.695155	0.612770
1	4.228451	0.702626	-0.208083
1	2.674896	2.594591	-0.846026
1	0.196166	2.201222	-0.766219
1	-1.008313	-1.659012	-1.330032
1	-3.468534	-1.974581	-1.228015
1	-4.872466	-0.410180	0.100267
1	-3.814789	1.463505	1.345920
1	-1.351528	1.767970	1.282462
9	3.348408	-1.643518	0.565071

E = -578.9567321 au
ZPE = 0.174614 au
(H298 - E0) = 0.010685 au

i
UB3LYP/6-31+G(d)

7	0.395783	0.252834	-0.078160
6	1.203776	-0.778800	0.273657
6	2.578745	-0.614978	0.215289
6	3.148758	0.593316	-0.177745
6	2.286814	1.634548	-0.523417
6	0.913144	1.443667	-0.476242
6	-1.051887	0.071021	-0.028532
6	-1.622793	-0.992479	-0.731117
6	-3.007873	-1.159236	-0.678857

6	3.490755	0.000000	0.000000
6	2.783799	-1.057481	0.579174
6	1.398933	-1.031484	0.575495
1	-0.861731	1.907053	1.014987
1	-3.345336	1.910603	0.995066
1	-4.586657	-0.000001	0.000000
1	-3.345336	-1.910603	-0.995067
1	-0.861731	-1.907052	-1.014987
1	0.787247	1.799002	-1.033863
1	3.294425	1.892887	-1.045922
1	4.576513	-0.000001	0.000000
1	3.294424	-1.892887	1.045922
1	0.787246	-1.799001	1.033864

E = -479.727230 au
ZPE = 0.183138 au
(H298 - E0) = 0.009851 au

j			
UB3LYP/6-31+G(d)			
6	2.451097	-0.720666	-0.000001
6	1.263790	-1.416530	-0.000001
6	0.033406	-0.701249	0.000000
6	0.033731	0.739479	0.000001
6	1.274136	1.418922	0.000001
6	2.453531	0.699473	0.000000
1	-1.286612	-2.445546	0.000004
1	3.395612	-1.255750	0.000001
1	1.253658	-2.502856	-0.000002
6	-1.201491	-1.363879	0.000002
6	-1.219133	1.414555	0.000001
1	1.288472	2.504877	-0.000002
1	3.403436	1.226119	0.000000
6	-2.389252	0.707364	-0.000003
7	-2.342866	-0.666875	0.000000
1	-1.255340	2.499190	0.000004
1	-3.375364	1.154359	-0.000005

7	1.204096	-1.314917	0.000001
6	1.222960	1.423860	0.000000
1	-1.288961	2.506678	0.000002
1	-3.402503	1.210972	-0.000001
6	2.418658	0.720313	-0.000001
6	2.380831	-0.674509	0.000000
1	1.232818	2.510718	0.000001
1	3.377463	1.225591	-0.000001
1	3.271317	-1.293281	0.000002

E = -402.3205867 au
ZPE = 0.149844 au
(H298 - E0) = 0.007770 au

k			
UB3LYP/6-31+G(d)			
7	-1.049699	0.069205	-0.028093
6	-1.626513	-0.924068	-0.755382
6	-2.996832	-1.120743	-0.717851
6	-3.789425	-0.276266	0.065002
6	-3.180473	0.744852	0.800064
6	-1.804641	0.894385	0.744429
6	0.396167	0.253135	-0.077754
6	1.216036	-0.822793	0.267133
6	2.591357	-0.618344	0.208250
6	3.151725	0.597845	-0.172559
6	2.299734	1.650709	-0.510010
6	0.911221	1.490337	-0.467218
1	-0.955347	-1.520140	-1.361844
1	-3.431297	-1.919972	-1.308595
1	-4.866029	-0.412188	0.101799
1	-3.758996	1.415958	1.425695
1	-1.262867	1.642391	1.310475

6	-3.795793	-0.274641	0.063867
6	-3.203853	0.783594	0.760203
6	-1.820216	0.965795	0.719301
1	0.737032	-1.695155	0.612770
1	4.228451	0.702626	-0.208083
1	2.674896	2.594591	-0.846026
1	0.196166	2.201222	-0.766219
1	-1.008313	-1.659012	-1.330032
1	-3.468534	-1.974581	-1.228015
1	-4.872466	-0.410180	0.100267
1	-3.814789	1.463505	1.345920
1	-1.351528	1.767970	1.282462
9	3.348408	-1.643518	0.565071

E = -578.9567321 au
ZPE = 0.174614 au
(H298 - E0) = 0.010685 au

l			
UB3LYP/6-31+G(d)			
7	-1.390245	0.095793	-0.034759
6	-1.871132	-0.883476	-0.845698
6	-3.205506	-1.250725	-0.792789
6	-4.062901	-0.592460	0.093426
6	-3.553329	0.417814	0.914112
6	-2.208440	0.740248	0.838805
6	0.020734	0.460241	-0.101608
6	0.974919	-0.532594	0.123675
6	2.324365	-0.176499	0.055753
6	2.704786	1.139467	-0.226530
6	1.724925	2.109342	-0.445508
6	0.368325	1.781113	-0.386535
1	-1.156974	-1.328593	-1.527932
1	-3.563288	-2.034894	-1.451251
1	-5.113185	-0.863178	0.144006
1	-4.183934	0.946994	1.620361
1	-1.738611	1.489259	1.464645

1 -3.222688 -1.177076 0.000000

E = -402.3197234 au
ZPE = 0.149967 au
(H298 - E0) = 0.007779 au

1 0.821994 -1.777582 0.600064
1 4.231045 0.705715 -0.200571
1 2.718790 2.602857 -0.819673
1 0.251739 2.302037 -0.758900
9 3.398746 -1.637533 0.544842

E = -578.9630551 au
ZPE = 0.174805 au
(H298 - E0) = 0.010682 au

1 0.688042 -1.549171 0.372920
17 3.536139 -1.391829 0.340744
1 3.757509 1.397470 -0.274210
1 2.020354 3.128482 -0.674784
1 -0.393032 2.529344 -0.585710

E = -939.3169138 au
ZPE = 0.173310 au
(H298 - E0) = 0.011082 au

m
UB3LYP/6-31+G(d)
6 -2.417940 -0.720690 -0.000001
6 -1.221685 -1.412392 0.000000
6 -0.019790 -0.679666 0.000000
6 -0.020680 0.749655 0.000000
6 -1.273937 1.420686 0.000001
6 -2.446248 0.697473 0.000000
1 1.206422 -2.332867 0.000001
1 -3.352969 -1.272638 -0.000002
1 -1.205280 -2.499138 -0.000001
7 1.204096 -1.314917 0.000001
6 1.222960 1.423860 0.000000
1 -1.288961 2.506678 0.000002
1 -3.402503 1.210972 -0.000001
6 2.418658 0.720313 -0.000001
6 2.380831 -0.674509 0.000000
1 1.232818 2.510718 0.000001
1 3.377463 1.225591 -0.000001
1 3.271317 -1.293281 0.000002

E = -402.3205867 au
ZPE = 0.149844 au
(H298 - E0) = 0.007770 au

n
UB3LYP/6-31+G(d)
7 -1.617100 0.124975 -0.039466
6 -2.452942 0.693580 0.870160
6 -3.780290 0.306400 0.945197
6 -4.253789 -0.689028 0.085059
6 -3.378759 -1.267839 -0.838720
6 -2.062752 -0.839448 -0.888310
6 -0.223497 0.550155 -0.101346
6 0.072633 1.896695 -0.334896
6 1.409830 2.294594 -0.388641
6 2.434635 1.360493 -0.214986
6 2.094760 0.029473 0.011485
6 0.773599 -0.405255 0.075522
1 -2.011109 1.435111 1.524852
1 -4.425333 0.774077 1.681222
1 -5.290011 -1.009557 0.134725
1 -3.708464 -2.038548 -1.527073
1 -1.337646 -1.224978 -1.595018
1 -0.722849 2.619039 -0.494588
1 1.653765 3.335123 -0.577076
1 3.478857 1.649130 -0.254431
1 0.558227 -1.448370 0.279691
7 3.169531 -0.976749 0.201939
8 2.816600 -2.139083 0.389920
8 4.325522 -0.574359 0.155984

o
UB3LYP/6-31+G(d)
6 -0.732337 0.000000 0.000000
6 -1.408675 1.085857 0.560045
6 -2.804930 1.078100 0.555085
6 -3.500846 0.000000 0.000000
6 -2.804929 -1.078101 -0.555085
6 -1.408675 -1.085857 -0.560045
7 0.726567 0.000000 0.000000
6 1.398933 1.031484 -0.575495
6 2.783800 1.057481 -0.579174
6 3.490755 0.000000 0.000000
6 2.783799 -1.057481 0.579174
6 1.398933 -1.031484 0.575495
1 -0.861731 1.907053 1.014987
1 -3.345336 1.910603 0.995066
1 -4.586657 -0.000001 0.000000
1 -3.345336 -1.910603 -0.995067
1 -0.861731 -1.907052 -1.014987
1 0.787247 1.799002 -1.033863
1 3.294425 1.892887 -1.045922
1 4.576513 -0.000001 0.000000
1 3.294424 -1.892887 1.045922
1 0.787246 -1.799001 1.033864

E = -479.727230 au
ZPE = 0.183138 au

E = -684.2225295 au
ZPE = 0.185274 au
(H298 - E0) = 0.012441 au

(H298 - E0) = 0.009851 au

p
UB3LYP/6-31+G(d)
6 -2.417940 -0.720690 -0.000001
6 -1.221685 -1.412392 0.000000
6 -0.019790 -0.679666 0.000000
6 -0.020680 0.749655 0.000000
6 -1.273937 1.420686 0.000001
6 -2.446248 0.697473 0.000000
1 1.206422 -2.332867 0.000001
1 -3.352969 -1.272638 -0.000002
1 -1.205280 -2.499138 -0.000001
7 1.204096 -1.314917 0.000001
6 1.222960 1.423860 0.000000
1 -1.288961 2.506678 0.000002
1 -3.402503 1.210972 -0.000001
6 2.418658 0.720313 -0.000001
6 2.380831 -0.674509 0.000000
1 1.232818 2.510718 0.000001
1 3.377463 1.225591 -0.000001
1 3.271317 -1.293281 0.000002

E = -402.3205867 au
ZPE = 0.149844 au
(H298 - E0) = 0.007770 au

q
UB3LYP/6-31+G(d)
6 -0.732337 0.000000 0.000000
6 -1.408675 1.085857 0.560045
6 -2.804930 1.078100 0.555085
6 -3.500846 0.000000 0.000000
6 -2.804929 -1.078101 -0.555085
6 -1.408675 -1.085857 -0.560045
7 0.726567 0.000000 0.000000
6 1.398933 1.031484 -0.575495
6 2.783800 1.057481 -0.579174
6 3.490755 0.000000 0.000000
6 2.783799 -1.057481 0.579174
6 1.398933 -1.031484 0.575495
1 -0.861731 1.907053 1.014987
1 -3.345336 1.910603 0.995066
1 -4.586657 -0.000001 0.000000
1 -3.345336 -1.910603 -0.995067
1 -0.861731 -1.907052 -1.014987
1 0.787247 1.799002 -1.033863
1 3.294425 1.892887 -1.045922
1 4.576513 -0.000001 0.000000
1 3.294424 -1.892887 1.045922
1 0.787246 -1.799001 1.033864

E = -479.727230 au
ZPE = 0.183138 au
(H298 - E0) = 0.009851 au

s
UB3LYP/6-31+G(d)
7 1.310308 -0.000169 0.000000
6 0.667587 1.191102 -0.000005

t
UB3LYP/6-31+G(d)
1 -5.157452 0.000000 0.000000
6 -4.071567 0.000000 0.000000

r
UB3LYP/6-31+G(d)
7 1.310308 -0.000169 0.000000
6 0.667587 1.191102 -0.000005
6 -0.717291 1.212801 0.000003
6 -1.416896 0.000166 0.000000
6 -0.717609 -1.212622 -0.000003
6 0.667302 -1.191249 0.000004
1 2.328819 -0.000286 0.000005
1 1.287491 2.080316 -0.000003
1 -1.235282 2.165590 0.000008
1 -2.502900 0.000329 0.000000
1 -1.235788 -2.165308 -0.000005
1 1.286949 -2.080643 0.000002

E = -248.6608206 au
ZPE = 0.103073 au
(H298 - E0) = 0.005326 au

u
UB3LYP/6-31+G(d)
7 0.143520 -1.112150 -0.000001
6 -0.522144 0.070331 -0.000010

6	-0.717291	1.212801	0.000003
6	-1.416896	0.000166	0.000000
6	-0.717609	-1.212622	-0.000003
6	0.667302	-1.191249	0.000004
1	2.328819	-0.000286	0.000005
1	1.287491	2.080316	-0.000003
1	-1.235282	2.165590	0.000008
1	-2.502900	0.000329	0.000000
1	-1.235788	-2.165308	-0.000005
1	1.286949	-2.080643	0.000002

E = -248.6608206 au
ZPE = 0.103073 au
(H298 - E0) = 0.005326 au

6	-3.367241	0.572502	-1.063720
6	-3.367241	-0.572502	1.063720
6	-1.983916	-0.556699	1.047201
6	-1.983916	0.556699	-1.047201
1	-3.879479	1.023818	-1.906503
1	-3.879479	-1.023818	1.906503
7	-1.316039	0.000000	0.000000
1	-1.371800	-0.968574	1.840437
1	-1.371800	0.968574	-1.840437
6	0.129228	0.000000	0.000000
6	0.829985	1.204779	0.109849
6	0.829985	-1.204779	-0.109849
6	2.224244	-1.195025	-0.108096
6	2.224244	1.195025	0.108096
9	0.153487	2.355359	0.221735
9	0.153487	-2.355359	-0.221735
6	2.927792	0.000000	0.000000
9	2.874821	-2.354286	-0.217888
9	2.874821	2.354286	0.217888
1	4.013152	0.000000	0.000000

E = -876.6491229 au
ZPE = 0.149947 au
(H298 - E0) = 0.013526 au

6	0.203770	1.256766	-0.000002
6	1.597862	1.192336	0.000001
6	2.255571	-0.046700	0.000001
6	1.498137	-1.201165	0.000000
1	-0.407206	-1.970417	-0.000002
1	-0.325019	2.203186	0.000000
1	2.173708	2.113238	0.000009
1	3.337539	-0.115003	0.000004
1	1.912021	-2.203062	0.000006
17	-2.229109	0.007512	0.000003

E = -708.246883 au
ZPE = 0.093068 au
(H298 - E0) = 0.006413 au

v

UB3LYP/6-31+G(d)

7	0.143520	-1.112150	-0.000001
6	-0.522144	0.070331	-0.000010
6	0.203770	1.256766	-0.000002
6	1.597862	1.192336	0.000001
6	2.255571	-0.046700	0.000001
6	1.498137	-1.201165	0.000000
1	-0.407206	-1.970417	-0.000002
1	-0.325019	2.203186	0.000000
1	2.173708	2.113238	0.000009
1	3.337539	-0.115003	0.000004

w

UB3LYP/6-31+G(d)

7	1.310308	-0.000169	0.000000
6	0.667587	1.191102	-0.000005
6	-0.717291	1.212801	0.000003
6	-1.416896	0.000166	0.000000
6	-0.717609	-1.212622	-0.000003
6	0.667302	-1.191249	0.000004
1	2.328819	-0.000286	0.000005
1	1.287491	2.080316	-0.000003
1	-1.235282	2.165590	0.000008
1	-2.502900	0.000329	0.000000

1 1.912021 -2.203062 0.000006
17 -2.229109 0.007512 0.000003

E = -708.246883 au
ZPE = 0.093068 au
(H298 - E0) = 0.006413 au

cyclohexane
UB3LYP/6-31+G(d)

6 -1.464751 0.117960 -0.226507
6 -0.834478 -1.209311 0.226757
6 0.630130 -1.327224 -0.227016
6 1.464615 -0.118111 0.226960
6 0.834697 1.209203 -0.226620
6 -0.630140 1.327404 0.226432
1 1.071792 -2.257373 0.155607
1 -0.877967 -1.272806 1.325323
1 -1.419175 -2.056741 -0.156157
1 -1.542555 0.124070 -1.324955
1 -2.490662 0.200391 0.157416
1 1.541281 -0.124493 1.325487
1 2.490879 -0.200545 -0.155998
1 1.419288 2.056582 0.156572
1 0.878775 1.272675 -1.325164
1 -0.663447 1.397864 1.324904
1 -1.071599 2.257126 -0.157480
1 0.662949 -1.396281 -1.325594

E = -235.8864021 au
ZPE = 0.170612 au
(H298 - E0) = 0.006649 au

E(- electron) = -235.5114109 au

isopropanol
UB3LYP/6-31+G(d)

6 1.327481 -0.560092 -0.089353

1 -1.235788 -2.165308 -0.000005
1 1.286949 -2.080643 0.000002

E = -248.6608206 au
ZPE = 0.103073 au
(H298 - E0) = 0.005326 au

cyclohexyl radical
UB3LYP/6-31+G(d)

6 -1.290182 0.779435 0.159779
6 -0.000001 1.464862 -0.168421
6 1.290180 0.779437 0.159778
6 1.270080 -0.712513 -0.241577
6 0.000001 -1.413712 0.265716
6 -1.270079 -0.712515 -0.241578
1 2.137145 1.293128 -0.313034
1 -0.000002 2.524383 -0.415107
1 -1.476193 0.835282 1.252115
1 -2.137147 1.293125 -0.313033
1 1.309945 -0.789087 -1.337793
1 2.166216 -1.215466 0.145519
1 0.000002 -2.466263 -0.047844
1 0.000001 -1.415785 1.367164
1 -1.309943 -0.789088 -1.337794
1 -2.166214 -1.215470 0.145517
1 1.476191 0.835285 1.252115

E = -235.2215018 au
ZPE = 0.155817 au
(H298 - E0) = 0.006996 au

isopropanol radical
UB3LYP/6-31+G(d)

6 -1.361268 -0.547647 0.026614

isopropanol

MPW1K/6-31+G(d,p)

6 1.317175 -0.545370 -0.088406

6 0.001614 0.038162 0.364436
 1 1.364181 -0.619770 -1.183595
 1 2.162749 0.062478 0.248070
 1 1.456685 -1.568636 0.320235
 1 -0.006418 0.090592 1.465788
 8 -0.037879 1.374388 -0.164243
 1 -0.874311 1.790315 0.097342
 6 -1.205464 -0.777245 -0.103317
 1 -1.173168 -1.794062 0.307527
 1 -2.147233 -0.317735 0.225730
 1 -1.221238 -0.843235 -1.197754

E = -194.365579 au
ZPE = 0.108098 au
(H298 - E0) = 0.006391 au

E(- electron) = -193.9891069 au

valine

UB3LYP/6-31+G(d)

7 -0.654520 1.883500 -0.397468
 1 -1.669407 1.906787 -0.333173
 6 -0.168784 0.522808 -0.629257
 1 -0.132383 0.259305 -1.702105
 6 1.283486 0.383296 -0.072085
 6 -1.177084 -0.449259 -0.026963
 1 1.773672 1.307313 -0.412363
 6 1.317039 0.385652 1.462282
 6 2.066286 -0.795361 -0.668771
 8 -2.240202 -0.135101 0.467638
 1 0.913356 -0.549737 1.871568
 1 2.348111 0.482356 1.822894
 1 0.734332 1.222028 1.861514
 1 2.043192 -0.778789 -1.766454
 1 3.116765 -0.741198 -0.358156
 1 1.666262 -1.759052 -0.339818
 8 -0.793408 -1.744861 -0.137236

6 -0.008443 0.026120 -0.233220
 1 -2.143225 0.090425 -0.400356
 1 -1.450051 -1.547413 -0.412441
 1 -1.570218 -0.639756 1.109656
 8 0.040572 1.381455 0.060653
 1 0.944750 1.710018 -0.065729
 6 1.234228 -0.765332 0.033937
 1 1.438450 -0.866239 1.118125
 1 1.147199 -1.776549 -0.378201
 1 2.121425 -0.300971 -0.420262

E = -193.7103783 au
ZPE = 0.094371 au
(H298 - E0) = 0.006571 au

6 0.001655 0.044529 0.361173
 1 1.350276 -0.602633 -1.175171
 1 2.144062 0.077085 0.244689
 1 1.450013 -1.546456 0.317112
 1 -0.005120 0.092492 1.455929
 8 -0.049653 1.355345 -0.162775
 1 -0.874548 1.763374 0.088594
 6 -1.185619 -0.777123 -0.101183
 1 -1.141567 -1.787035 0.303686
 1 -2.125714 -0.332211 0.226085
 1 -1.199442 -0.839592 -1.188224

E = -194.3221307 au
ZPE = 0.111226 au
(H298 - E0) = 0.006305 au

1 -1.511135 -2.284350 0.246073
1 -0.357902 2.507715 -1.142160

E = -402.3830168 au
ZPE = 0.164596 au
(H298 - E0) = 0.010449 au

E(- electron) = -402.0415306 au

	radical g		
	MPW1K/6-31+G(d,p)		
6	-0.759651	-0.045151	-0.023669
6	-1.399131	-1.108783	-0.652180
6	-2.766018	-1.064151	-0.621626
6	-3.531798	-0.085113	-0.046579
6	-2.849618	0.962067	0.567834
6	-1.461677	0.984459	0.583527
7	0.682555	-0.012845	-0.006431
6	1.358953	-1.037449	0.540566
6	2.733304	-1.037430	0.559099
6	3.416680	0.041884	0.018044
6	2.700447	1.093045	-0.535750
6	1.327068	1.037822	-0.542379
1	-0.852024	-1.895346	-1.151637
1	-4.610500	-0.116751	-0.062421
1	-3.400412	1.757642	1.046446
1	-0.935914	1.782986	1.085701
1	0.760180	-1.826144	0.965826
1	3.253736	-1.869670	1.004527
1	4.495761	0.063407	0.027518
1	3.195119	1.945362	-0.972486
1	0.704825	1.801217	-0.979776

E = -478.906097 au
ZPE = 0.175138 au
(H298 - E0) = 0.009603 au

	radical I		
	MPW1K/6-31+G(d,p)		
7	-1.359886	0.112295	-0.038331
6	-1.824474	-0.861778	-0.840018
6	-3.143264	-1.244113	-0.781475
6	-3.994454	-0.602201	0.106391
6	-3.497158	0.405775	0.919917
6	-2.167449	0.742146	0.832513
6	0.028905	0.494326	-0.117780
6	0.993094	-0.469115	0.127391
6	2.334680	-0.113948	0.046454
6	2.710484	1.190662	-0.268829
6	1.689911	2.072337	-0.490971
6	0.348219	1.808116	-0.440065
1	-1.111085	-1.294676	-1.522062
1	-3.493931	-2.026745	-1.434506
1	-5.034739	-0.884311	0.163679
1	-4.125627	0.922923	1.626670
1	-1.703891	1.494856	1.449023
1	0.718987	-1.475940	0.402246
#	3.532497	-1.298617	0.353649
1	3.750794	1.471054	-0.328713
1	-0.404716	2.550018	-0.661205

E = -938.5004522 au
ZPE = 0.165243 au
(H298 - E0) = 0.010780 au

	radical n		
	MPW1K/6-31+G(d,p)		
7	-1.588808	0.143337	-0.043360
6	-2.018855	-0.821206	-0.876440
6	-3.319587	-1.260832	-0.821795
6	-4.189012	-0.688437	0.095577
6	-3.727637	0.310179	0.941691
6	-2.414798	0.706416	0.856613
6	-0.217013	0.580199	-0.115149
6	0.786509	-0.351476	0.076731
6	2.098439	0.081910	0.000811
6	2.442365	1.401089	-0.249362
6	1.384246	2.251464	-0.425322
6	0.058013	1.920193	-0.377901
1	-1.294558	-1.201720	-1.578093
1	-3.642076	-2.034787	-1.499307
1	-5.215584	-1.017374	0.151148
1	-4.370863	0.773405	1.672239
1	-1.979387	1.454609	1.498748
1	0.583886	-1.387115	0.301565
1	3.477027	1.704656	-0.296678
1	-0.725876	2.642203	-0.556177
7	3.161801	-0.905757	0.207257
8	2.813836	-2.044150	0.405962
8	4.293722	-0.502590	0.159858

E = -683.3087118 au
ZPE = 0.178031 au

(H298 - E0) = 0.012097 au

radical g + isopropanol TS

MPW1K/6-31+G(d,p)

6	0.884529	0.852699	0.081553
6	0.999821	2.221256	0.270970
6	-0.153710	2.989609	0.327244
6	-1.404214	2.391495	0.202897
6	-1.461925	1.028118	0.015578
6	-0.347233	0.226273	-0.052769
7	2.083266	0.051740	0.026043
6	3.047407	0.357189	-0.858698
6	4.197911	-0.391775	-0.927594
6	4.347007	-1.481896	-0.082707
6	3.336481	-1.787462	0.816567
6	2.212626	-0.996735	0.856159
1	1.968849	2.679878	0.402690
1	-0.074904	4.054994	0.483931
1	-2.300682	2.991498	0.255787
1	-2.786211	0.118569	-0.084873
1	-0.441653	-0.837817	-0.229715
1	2.847548	1.197500	-1.502769
1	4.956382	-0.126309	-1.645956
1	5.240036	-2.086437	-0.125595
1	3.416354	-2.622238	1.493709
1	1.400102	-1.155853	1.545634
6	-3.480397	-0.840454	-0.132706
6	-4.682116	-0.486948	-0.971970
1	-5.352046	-1.343559	-1.049563
1	-4.392003	-0.182453	-1.977462
6	-3.795104	-1.208268	1.292313
1	-2.884723	-1.446565	1.837210
1	-4.442771	-2.083653	1.317313
8	-2.699451	-1.855072	-0.694528
1	-2.813900	-1.863629	-1.642754
1	-5.235814	0.334646	-0.524357
1	-4.298319	-0.388775	1.799672

radical l + isopropanol TS

MPW1K/6-31+G(d,p)

6	0.882760	0.279397	-0.003402
6	1.007014	1.656472	0.082647
6	-0.148192	2.426431	0.077377
6	-1.404546	1.831706	-0.002806
6	-1.455426	0.460761	-0.084525
6	-0.348047	-0.354236	-0.090413
7	2.083314	-0.520819	-0.001354
6	3.038589	-0.288740	-0.917876
6	4.188366	-1.041386	-0.935806
6	4.346118	-2.057617	-0.004609
6	3.344943	-2.287511	0.927234
6	2.220573	-1.496875	0.912013
1	1.971754	2.129816	0.181520
1	-2.293854	2.443782	0.001807
1	-2.800648	-0.463340	-0.123845
1	-0.449490	-1.427613	-0.185682
1	2.833057	0.496428	-1.626703
1	4.939956	-0.836275	-1.680708
1	5.239167	-2.663708	-0.005775
1	3.432358	-3.063076	1.670635
1	1.413971	-1.599235	1.619110
6	-3.480355	-1.424868	-0.097575
6	-4.663638	-1.166739	-0.995894
1	-5.323513	-2.034502	-1.007236
1	-4.350948	-0.956072	-2.018457
6	-3.828652	-1.660634	1.347877
1	-2.930892	-1.836082	1.935811
1	-4.468466	-2.537359	1.438328
8	-2.675808	-2.478987	-0.543027
1	-2.789277	-2.597750	-1.483951
1	-5.236690	-0.313020	-0.642787
1	-4.352892	-0.803181	1.762802
#	-0.012198	4.134226	0.190198

radical n + isopropanol TS

MPW1K/6-31+G(d,p)

6	0.877954	0.081416	-0.016608
6	1.029346	1.453375	0.060455
6	-0.117392	2.226468	0.045469
6	-1.38944	1.682609	-0.032728
6	-1.467777	0.310981	-0.107172
6	-0.373228	-0.519247	-0.104255
7	2.058417	-0.746411	-0.006153
6	3.029548	-0.527954	-0.910217
6	4.164299	-1.302837	-0.9182
6	4.291045	-2.326288	0.009842
6	3.274434	-2.541492	0.928817
6	2.165773	-1.729788	0.904345
1	1.991356	1.932484	0.154895
1	-2.253185	2.329735	-0.033541
1	-2.842035	-0.622154	-0.138709
1	-0.501083	-1.591511	-0.189236
1	2.850646	0.265574	-1.617074
1	4.929043	-1.107867	-1.652405
1	5.17245	-2.949218	0.01673
1	3.338405	-3.321746	1.669735
1	1.350286	-1.820846	1.60286
6	-3.498626	-1.589428	-0.089901
6	-4.664133	-1.394033	-1.026446
1	-5.305641	-2.275529	-1.017532
1	-4.330475	-1.21763	-2.048761
6	-3.879161	-1.775426	1.355298
1	-2.994106	-1.912904	1.971974
1	-4.506527	-2.658916	1.463797
8	-2.659157	-2.642326	-0.476451
1	-2.797727	-2.845516	-1.399412
1	-5.264049	-0.540037	-0.722325

E = -673.2288315 au
ZPE = 0.283220 au
(H298 - E0) = 0.016113 au

E = -1132.824318 au
ZPE = 0.273679 au
(H298 - E0) = 0.017296 au

1	-4.427833	-0.912037	1.723816
7	0.036761	3.680288	0.130085
8	1.16485	4.108408	0.180124
8	-0.972146	4.336523	0.140762

E = -877.6345392 au
ZPE = 0.286910 au
(H298 - E0) = 0.018572 au

⁴⁷Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, J., J. A.;; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Baboul, A. G.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Gonzalez, C.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Andres, J. L.; Gonzalez, C.; Head-Gordon, M.; Replogle, E. S.; Pople, J. A., Gaussian 98, Revision A. 7, Inc.: Pittsburgh PA, 1998.