Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information File

Reactivity of Germanone: Far Apart from Ketones

Available Information:

1. Complete Gaussian09 reference
2. E=O anharmonicity corrected stretching frequencies (in cm^{-})[1] of formaldehyde, acetone, 2,4-Dimethyl-3-pentanone, diphenyl ketone and their heavier analogs at B3LYP/6-311++G(d,p) level.
3. Cartesian Coordinates for Optimized Structures, their Energies in Hartrees and their low frequencies in cm^{-1}.

Gaussian 09 reference:

*Gaussian 09, Revision **A.1***, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

Table S1. *E=O anharmonicity corrected stretching frequencies (in cm^{-})[1] of formaldehyde, acetone, 2,4-Dimethyl-3-pentanone, diphenyl ketone and their heavier analogs at B3LYP/6-311++G(d,p) level.*

Molecule	E=O Anharmonic Stretching frequency[I]
X_2CO[a]	1789.86
X_2SiO[a]	1194.44
X_2GeO[a]	939.29
X_2CO[b]	1766.82
X_2SiO[b]	1199.08
X_2GeO[b]	930.37
X_2CO[c]	1728.75
X_2SiO[c]	1179.93
X_2GeO[c]	915.32
X_2CO[d]	1682.36
X_2SiO[d]	1187.72
X_2GeO[d]	918.20

B3LYP/6-311++G(d,p)

Reactants

Formaldehye (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	0.290159
1	0.000000	0.939368	0.878232
1	0.000000	-0.939368	0.878232
8	0.000000	0.000000	-0.911410

B3LYP/6-311++G(d,p) = - -114.5418487 Hartrees
Low frequencies = 1202.5126 1259.3304 1531.4415 1815.8108 2884.4272 2941.5043

Formaldehye (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	0.002396	0.000044	0.001712
1	-0.006436	-0.000014	1.484471
1	1.380822	-0.000014	-0.544717
8	-1.260715	0.000144	-0.861810

B3LYP/6-311++G(d,p) = - 365.9532032 Hartrees
Low frequencies = 678.2478 704.3408 1018.6271 1209.6771 2222.7807 2241.0098

Formaldehye (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	-0.006578	0.000000	-0.004253
1	0.002406	0.000000	1.536787
1	1.402341	0.000000	-0.628619
8	-1.390605	0.000000	-0.899026

B3LYP/6-311++G(d,p) = -2153.4141775 Hartrees
Low frequencies = 565.4442 575.5551 872.9614 947.5039 2085.8565 2095.4288

Acetone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.184907	-0.000002
8	0.000009	1.396505	0.000000
6	1.290569	-0.612857	-0.002025
1	1.287483	-1.353941	-0.807135
1	2.143188	0.055486	-0.114214
1	1.383880	-1.165200	0.939128
6	-1.290576	-0.612845	0.002024
1	-1.383874	-1.165236	-0.939103
1	-1.287515	-1.353890	0.807172
1	-2.143190	0.055511	0.114167

B3LYP/6-311++G(d,p) = - 193.2182695 Hartrees
Low frequencies = 66.4768 131.9917 379.9920 489.8314 535.7046 782.4750 883.7555 888.8748 1083.1023 1115.8168

Acetone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-0.000002	0.192460	-0.000011
8	-0.000201	1.727343	0.000006
6	1.555576	-0.843969	-0.001194
1	1.629946	-1.425118	0.924065
1	1.549303	-1.559487	-0.829642
1	2.436722	-0.206866	-0.086016
6	-1.555402	-0.844250	0.001194

1	-1.629645	-1.425599	-0.923944
1	-1.549114	-1.559574	0.829810
1	-2.436622	-0.207221	0.085836

B3LYP/6-311++G(d,p) = -444.6455586 Hartrees
Low frequencies = 27.8221 73.1413 216.8720 256.3873 288.4365
618.8668 688.8291 689.5490 801.4726 808.3430

Acetone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	0.000002	0.124319	-0.000008
8	0.000314	1.778569	0.000012
6	-1.648037	-0.942932	0.000010
1	-1.674843	-1.583575	0.884948
1	-2.509904	-0.276969	0.000271
1	-1.675102	-1.583192	-0.885198
6	1.647763	-0.943369	0.000000
1	1.674788	-1.583427	0.885358
1	1.674366	-1.584222	-0.884789
1	2.509761	-0.277574	-0.000478

B3LYP/6-311++G(d,p) = - -2232.0973343 Hartrees
Low frequencies =

4-Dimethyl-3-pentanone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.345223	1.799543	0.014036
6	-1.411010	0.249662	-0.374628
1	-1.802732	1.054182	-1.007074
6	1.164554	-0.438576	-0.194498
1	0.916620	-1.165241	-0.975049
6	-2.148836	0.343887	0.977518
1	-1.967329	1.310732	1.450197
1	-3.226035	0.233272	0.825210
1	-1.828461	-0.443017	1.666523
6	-1.676516	-1.089323	-1.073397
1	-2.750996	-1.214270	-1.234632
1	-1.191279	-1.143809	-2.051624
1	-1.336523	-1.941004	-0.477698
6	1.168309	-1.187105	1.157199
1	0.215183	-1.677689	1.365611
1	1.944741	-1.956618	1.152355
1	1.382341	-0.496310	1.977486
6	2.538257	0.168071	-0.493977
1	3.299807	-0.616572	-0.513058
1	2.546799	0.677044	-1.460655

1	2.813709	0.902301	0.265342
6	0.068969	0.633494	-0.180754

B3LYP/6-311++G(d,p) = - 350.5101511 Hartrees
Low frequencies = 49.7229 63.6146 195.1813 206.6607 216.6895
226.3402 255.1572 258.0791 292.4126 318.1167

4-Dimethyl-3-pentanone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	0.059552	0.728687	-0.130593
8	0.372879	2.212961	0.126295
6	-1.724685	0.119549	-0.341020
1	-2.192557	0.918556	-0.929880
6	1.405354	-0.602174	-0.208009
1	1.149453	-1.257692	-1.051201
6	-2.449920	0.072465	1.023666
1	-2.390431	1.029544	1.546934
1	-3.509259	-0.164630	0.878319
1	-2.032064	-0.698597	1.679005
6	-1.866668	-1.206410	-1.108582
1	-2.924751	-1.456203	-1.241039
1	-1.416048	-1.161514	-2.104315
1	-1.403044	-2.039268	-0.571357
6	1.382930	-1.466959	1.075667
1	0.414300	-1.945905	1.246961
1	2.131566	-2.262751	1.004114
1	1.624446	-0.870407	1.960467
6	2.797139	0.005119	-0.452270
1	3.554741	-0.785501	-0.486668
1	2.843119	0.557250	-1.393812
1	3.068860	0.702273	0.343698

B3LYP/6-311++G(d,p) = - 601.9284527 Hartrees
Low frequencies = 31.6166 43.4748 113.8060 128.0054 185.8409
201.9959 217.5156 226.3672 247.8580

4-Dimethyl-3-pentanone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	-0.000080	-0.468934	0.000250
8	0.000324	-2.127715	0.001458
6	1.677217	0.585766	-0.260911
1	1.508929	1.146120	-1.189385
6	-1.677818	0.585222	0.260829
1	-1.511163	1.142581	1.191420
6	-2.882268	-0.345957	0.440191
1	-2.736978	-1.047984	1.263420

1	-3.785409	0.240152	0.645138
1	-3.063938	-0.938685	-0.460068
6	-1.879240	1.599559	-0.878448
1	-2.767892	2.210548	-0.685411
1	-1.031874	2.282425	-0.987696
1	-2.034078	1.099029	-1.839333
6	1.880743	1.596473	0.881280
1	2.769219	2.207857	0.688682
1	1.033722	2.279203	0.994089
1	2.037057	1.092876	1.840321
6	2.881259	-0.344952	-0.445189
1	2.734917	-1.043785	-1.270953
1	3.784273	0.241761	-0.648976
1	3.063815	-0.941164	0.452575

B3LYP/6-311++G(d,p) = - 2389.3845372 Hartrees
Low frequencies = 24.1347 47.1167 80.6404 102.3130 161.8948
204.4796 214.6728 218.7219 245.3274

Diphenyl ketone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.000000	2.318493	0.000002
6	1.299790	0.348285	0.025968
6	1.442109	-0.891116	0.663125
6	2.426383	0.957151	-0.544331
6	2.688669	-1.510929	0.725075
1	0.585809	-1.359776	1.132600
6	3.664046	0.326331	-0.502434
1	2.311256	1.926742	-1.013482
6	3.798048	-0.908807	0.134663
1	2.793013	-2.461762	1.235363
1	4.527062	0.797889	-0.958815
1	4.765599	-1.396680	0.174823
1	-2.311270	1.926746	1.013471
6	-2.426389	0.957152	0.544325
6	-1.299791	0.348285	-0.025960
6	-3.664052	0.326330	0.502418
6	-1.442103	-0.891122	-0.663112
6	-3.798047	-0.908810	-0.134673
1	-4.527072	0.797890	0.958791
6	-2.688662	-1.510936	-0.725071
1	-0.585797	-1.359782	-1.132575
1	-4.765597	-1.396685	-0.174842
1	-2.793002	-2.461771	-1.235355
6	-0.000001	1.098062	0.000008

B3LYP/6-311++G(d,p) = - 576.7821673 Hartrees

Diphenyl ketone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.000000	2.711050	0.000028
6	1.587790	0.207461	0.023635
6	1.699868	-1.123030	0.464020
6	2.756464	0.885844	-0.370465
6	2.938632	-1.759164	0.496760
1	0.823409	-1.663426	0.803047
6	3.991454	0.244993	-0.347991
1	2.687797	1.921274	-0.685457
6	4.083039	-1.078161	0.084091
1	3.011750	-2.782795	0.846712
1	4.882693	0.777769	-0.659964
1	5.046367	-1.575644	0.106394
1	-2.687814	1.921286	0.685400
6	-2.756474	0.885850	0.370429
6	-1.587793	0.207461	-0.023636
6	-3.991463	0.244996	0.347945
6	-1.699859	-1.123041	-0.463992
6	-4.083037	-1.078168	-0.084107
1	-4.882709	0.777777	0.659889
6	-2.938621	-1.759179	-0.496739
1	-0.823392	-1.663442	-0.802991
1	-5.046363	-1.575655	-0.106416
1	-3.011729	-2.782818	-0.846668
14	0.000000	1.173008	0.000010

B3LYP/6-311++G(d,p) = - 828.2052664 Hartrees
Low frequencies = 36.5900 37.2310 79.9948 104.2893 144.9124 156.0694 238.3283 263.0446 325.8771

Diphenyl ketone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-0.000003	-2.643897	0.000024
6	-1.680153	-0.006441	0.021423
6	-1.795693	1.342258	0.387595
6	-2.836646	-0.729366	-0.309929
6	-3.045068	1.959475	0.410660
1	-0.920053	1.913414	0.674023
6	-4.082130	-0.107211	-0.292880
1	-2.753771	-1.778889	-0.570739
6	-4.186428	1.236944	0.065353
1	-3.127897	3.000863	0.701036
1	-4.970909	-0.670841	-0.553500
1	-5.157318	1.719538	0.081724
1	2.753786	-1.778898	0.570698

6	2.836654	-0.729371	0.309902
6	1.680157	-0.006444	-0.021424
6	4.082136	-0.107212	0.292848
6	1.795688	1.342262	-0.387577
6	4.186427	1.236950	-0.065363
1	4.970920	-0.670844	0.553448
6	3.045059	1.959483	-0.410645
1	0.920042	1.913418	-0.673985
1	5.157314	1.719548	-0.081738
1	3.127883	3.000876	-0.701004
32	0.000001	-0.986406	0.000002

B3LYP/6-311++G(d,p) = - 2615.6561727 Hartrees
Low frequencies = 31.8332 38.0163 71.7856 98.2584 132.6120
150.1076 225.7065 231.1238 244.7206

Transition State: Addition of Acetone

Formaldehye (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.669687	-0.556435	-0.106072
1	2.012322	-0.410285	-1.138656
1	1.895747	-1.540390	0.308656
8	1.696694	0.435796	0.711773
1	0.204229	1.578128	-1.257746
6	-0.402490	1.354978	-0.381226
6	-0.812766	0.015915	-0.223577
1	0.713986	1.159064	0.370355
1	-1.099267	2.136246	-0.101812
8	-0.004329	-0.948031	-0.485947
6	-2.114180	-0.372314	0.422575
1	-1.916920	-0.868699	1.377245
1	-2.626331	-1.096805	-0.216573
1	-2.764201	0.487756	0.581727

B3LYP/6-311++G(d,p) = -307.711664 Hartrees
Low frequencies = -1414.3685 71.6372 113.8698 178.3690 336.0582
432.7869 492.1224 539.9136 572.1801 644.8715

Formaldehye (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.849611	-0.681941	-0.073162
1	2.263863	-0.507093	-1.076656
1	2.163865	-1.643757	0.340078
8	1.880241	0.315586	0.775723
1	0.453556	1.991741	-1.161247

6	-0.080138	1.708097	-0.252693
1	1.002758	1.192619	0.405922
1	-0.653672	2.535891	0.158059
8	0.314904	-1.080970	-0.480149
6	-2.407729	-0.480475	0.430397
1	-2.306016	-0.697836	1.498739
1	-2.720859	-1.403181	-0.063741
1	-3.177922	0.281685	0.298836
14	-0.768372	0.078494	-0.242274

B3LYP/6-311++G(d,p) = -559.1475674 Hartrees
Low frequencies = -1384.7776 56.1723 92.1583 161.9911
205.6543 265.3137 286.5529 428.2901 501.0205 553.5471

Formaldehye (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	2.035286	-0.744213	-0.077672
1	2.456185	-0.541519	-1.076243
1	2.397082	-1.703585	0.309411
8	2.107045	0.238419	0.801406
1	0.675631	2.024143	-1.097210
6	0.227577	1.772234	-0.133509
1	1.264667	1.200979	0.460649
1	-0.338681	2.603608	0.281304
8	0.554866	-1.159662	-0.433562
6	-2.303159	-0.586429	0.515341
1	-2.224850	-0.648893	1.603858
1	-2.462720	-1.587622	0.114872
1	-3.131381	0.069851	0.248638
32	-0.615295	0.103232	-0.175406

B3LYP/6-311++G(d,p) = -2346.6077363 Hartrees
Low frequencies = -1328.9708 56.9604 88.0793 142.5801 166.2000
193.9699 235.3710 456.3129 512.8564 538.3947

Acetone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-0.773469	-0.550046	1.247677
6	-1.673021	1.455082	0.332787
1	-1.739973	1.952756	-0.634202
6	-1.953006	-0.818445	-0.838205
1	-2.008919	-0.314052	-1.802395
1	0.860425	-2.144895	-0.325861
6	1.428117	-1.389950	0.209891
6	1.414076	-0.080440	-0.289623

1	0.253245	-1.069439	1.012205
1	2.308894	-1.747613	0.729685
8	0.366445	0.396423	-0.852172
6	2.545792	0.885098	-0.025194
1	2.182012	1.737812	0.554578
1	2.903800	1.275724	-0.982217
1	3.379298	0.413907	0.496790
6	-1.227310	0.023793	0.182730
1	-2.970884	-0.992365	-0.469394
1	-1.468556	-1.786765	-0.958998
1	-0.986134	1.996279	0.982208
1	-2.664902	1.456807	0.799246

B3LYP/6-311++G(d,p) = - 386.3788217Hartrees
Low frequencies = -1210.0266 75.9090 79.2707 113.9447 198.2672 235.7831 239.6726 252.4361 334.5357 387.3231

Acetone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.612804	-0.911973	-1.385238
6	1.842087	1.635267	-0.506773
1	1.914799	2.248228	0.396227
6	1.961099	-0.889353	1.280318
1	2.057383	-0.231016	2.148928
1	-1.298567	-2.072578	0.311494
6	-1.738601	-1.295472	-0.315119
6	-1.647391	0.021553	0.234472
1	-0.770153	-1.223002	-1.103862
1	-2.714271	-1.573678	-0.703095
8	-0.519552	0.486838	0.623799
6	-2.812951	0.959856	0.274591
1	-2.481619	1.992527	0.376032
1	-3.444547	0.702768	1.132509
1	-3.428155	0.839537	-0.620233
1	2.968114	-1.191236	0.975069
1	1.429151	-1.793459	1.588494
1	1.246597	2.172741	-1.248470
1	2.849996	1.512530	-0.914690
14	1.092843	-0.040956	-0.146559

B3LYP/6-311++G(d,p) = -637.8836768 Hartrees
Low frequencies = -881.1921 62.1181 72.1192 98.7897 126.5288 143.9446 187.4111 201.0177 225.5492 307.4724

Acetone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z

8	0.332700	-0.877323	-1.480540
6	1.579045	1.805124	-0.406247
1	1.581537	2.357038	0.535322
6	1.851349	-0.994202	1.309217
1	1.846839	-0.407414	2.229917
1	-1.536173	-2.092841	0.291168
6	-1.978756	-1.298812	-0.311036
6	-1.922625	-0.003316	0.294334
1	-1.010362	-1.175292	-1.107605
1	-2.937670	-1.578689	-0.738436
8	-0.835477	0.442382	0.790186
6	-3.096976	0.932628	0.265551
1	-2.778977	1.962436	0.424863
1	-3.795421	0.650321	1.061157
1	-3.635879	0.840875	-0.680500
1	2.886602	-1.184673	1.016299
1	1.358083	-1.951017	1.484216
1	0.936319	2.310476	-1.127341
1	2.596254	1.773505	-0.803155
32	0.934964	-0.021054	-0.124187

B3LYP/6-311++G(d,p) = -2425.3279786 Hartrees
Low frequencies = -887.7570 57.5770 65.4714 91.2083 91.9246
104.1567 155.6690 163.4520 176.1707 233.1638

4-Dimethyl-3-pentanone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-0.158390	-0.087295	1.346842
6	-0.762689	1.496585	-0.379798
1	-0.522887	1.483380	-1.446597
6	-1.432367	-1.044176	-0.486251
1	-1.748632	-0.690095	-1.473212
6	0.152076	2.499187	0.330291
1	1.203268	2.227896	0.243386
1	0.024104	3.491184	-0.111419
1	-0.090936	2.564551	1.393232
6	-2.230320	1.955185	-0.240051
1	-2.311562	2.986798	-0.593013
1	-2.918291	1.352435	-0.834840
1	-2.559311	1.935374	0.802546
6	-2.679853	-1.236895	0.407607
1	-3.251987	-0.322762	0.558651
1	-3.343228	-1.975347	-0.050550
1	-2.379079	-1.609743	1.389245
6	-0.757535	-2.411296	-0.666942
1	-1.477135	-3.110512	-1.102517
1	0.110063	-2.351088	-1.320897
1	-0.449522	-2.825328	0.297059

1	1.529374	-2.146937	0.885840
6	2.116352	-1.237722	0.941669
6	2.127867	-0.375805	-0.160259
1	0.885121	-0.553657	1.422300
1	2.988182	-1.276358	1.584053
8	1.090562	-0.215564	-0.897955
6	3.331602	0.492301	-0.457959
1	3.029763	1.463769	-0.850926
1	3.929318	-0.005530	-1.229129
1	3.966264	0.621522	0.420633
6	-0.543509	0.056522	0.115871

B3LYP/6-311++G(d,p) = -543.6637638 Hartrees
Low frequencies = -1067.0303 46.6875 66.6622 81.8167 93.8897
129.3896 183.0720 192.8056 202.4850 217.1124

4-Dimethyl-3-pentanone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.015089	-0.075673	1.688422
6	-0.972335	1.746270	-0.455848
1	-0.898454	1.704620	-1.551706
6	-1.461648	-1.378682	-0.579265
1	-1.797999	-1.038117	-1.568807
6	-0.033919	2.856016	0.050431
1	1.000501	2.694876	-0.265843
1	-0.346679	3.832666	-0.336346
1	-0.043022	2.908255	1.142474
6	-2.436284	2.065992	-0.091385
1	-2.715499	3.058062	-0.463896
1	-3.138756	1.348165	-0.523341
1	-2.584389	2.070314	0.992911
6	-2.710455	-1.660927	0.284024
1	-3.357033	-0.785814	0.388032
1	-3.311282	-2.462192	-0.160728
1	-2.423688	-1.976640	1.291050
6	-0.650327	-2.673465	-0.774483
1	-1.275535	-3.457199	-1.216928
1	0.209793	-2.527220	-1.432966
1	-0.285666	-3.057224	0.184122
1	1.900529	-2.028554	0.989091
6	2.357884	-1.041301	1.066254
6	2.303654	-0.278479	-0.141197
1	1.385082	-0.514251	1.654540
1	3.325339	-1.064959	1.559705
8	1.188742	-0.093036	-0.745270
6	3.499029	0.431356	-0.697895
1	3.203195	1.213905	-1.395317
1	4.127770	-0.295517	-1.224520
1	4.104871	0.846908	0.110988

14	-0.434523	0.034207	0.165603

B3LYP/6-311++G(d,p) = - 795.1650189 Hartrees
Low frequencies = -911.7760 34.0572 40.0561 60.4071 69.0693
80.6397 114.8978 126.3983 171.0518 192.4074

4-Dimethyl-3-pentanone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.173823	-0.117491	1.752737
6	-0.842287	1.879143	-0.489458
1	-0.732758	1.830092	-1.579082
6	-1.530792	-1.424221	-0.613746
1	-1.830814	-1.079042	-1.610458
6	0.149765	2.904073	0.072719
1	1.176829	2.685878	-0.230209
1	-0.095265	3.909703	-0.288822
1	0.121793	2.922331	1.165290
6	-2.295975	2.255111	-0.156275
1	-2.526169	3.255018	-0.541649
1	-3.017806	1.562764	-0.598672
1	-2.466685	2.275227	0.924415
6	-2.790033	-1.623029	0.248108
1	-3.403576	-0.719928	0.310303
1	-3.417741	-2.416937	-0.172881
1	-2.525920	-1.913849	1.268729
6	-0.742211	-2.732065	-0.759039
1	-1.377125	-3.512625	-1.194346
1	0.131001	-2.615009	-1.404925
1	-0.401202	-3.097105	0.214733
1	1.934655	-2.157201	0.833280
6	2.430851	-1.194818	0.959812
6	2.427014	-0.377840	-0.215149
1	1.488253	-0.637830	1.582649
1	3.384782	-1.275426	1.473996
8	1.353240	-0.179852	-0.873866
6	3.651862	0.374868	-0.653339
1	3.392898	1.173759	-1.347233
1	4.338253	-0.319310	-1.150433
1	4.180906	0.779742	0.213228
32	-0.416249	0.042536	0.148104

B3LYP/6-311++G(d,p) = - 2582.6131301 Hartrees
Low frequencies = -899.5588 32.5424 40.0140 56.9843 67.3038
78.5705 91.4430 96.9137 146.1892 167.7683

Diphenyl ketone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z

8	0.090801	1.067498	1.590490
1	0.224210	3.543198	0.674626
6	-0.793853	3.253794	0.439237
6	-1.020786	2.375511	-0.619951
1	-0.520851	1.926185	1.324915
1	-1.581484	3.917484	0.776109
8	-0.118751	1.547817	-0.999499
6	-2.389439	2.273994	-1.265822
1	-2.771206	1.253027	-1.192026
1	-2.285210	2.503248	-2.330622
1	-3.110004	2.967335	-0.828896
6	-0.968034	-0.666991	0.332581
6	-1.919500	-0.869296	1.340784
6	-1.140253	-1.301171	-0.907762
6	-3.017151	-1.698880	1.118396
1	-1.783884	-0.385018	2.299785
6	-2.237525	-2.124259	-1.126565
1	-0.435196	-1.105322	-1.704841
6	-3.177817	-2.328432	-0.113182
1	-3.743105	-1.854079	1.908465
1	-2.369407	-2.599312	-2.092139
1	-4.032572	-2.972423	-0.287469
6	1.576370	-0.184609	0.245587
6	2.595424	0.779649	0.267420
6	1.904668	-1.512540	-0.056441
6	3.904636	0.426590	-0.026135
1	2.340659	1.804951	0.497543
6	3.222773	-1.866366	-0.339528
1	1.138504	-2.276437	-0.046420
6	4.223363	-0.898948	-0.331865
1	4.680699	1.183513	-0.020431
1	3.464828	-2.899353	-0.562090
1	5.247518	-1.173514	-0.558633
6	0.197139	0.215954	0.612279

B3LYP/6-311++G(d,p) = -769.9353024 Hartrees
Low frequencies = -558.6515 33.4279 49.7452 64.6382 71.7332
92.6631 97.5322 126.5494 144.4375 198.5812

Diphenyl ketone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	0.035965	0.364833	0.549795
8	0.149087	1.243037	1.868791
1	1.967790	2.862185	0.508801
6	0.973067	3.310211	0.507505
6	0.137570	2.877580	-0.564946
1	0.513534	2.545185	1.398230
1	0.990434	4.380464	0.688997

8	-0.027916	1.625459	-0.796091
6	-0.674062	3.818642	-1.397663
1	-1.593503	3.342617	-1.738670
1	-0.083580	4.096349	-2.279012
1	-0.891959	4.736481	-0.849700
6	-1.593919	-0.508095	0.242554
6	-2.357193	-0.922541	1.346120
6	-2.083216	-0.788175	-1.043807
6	-3.560893	-1.603555	1.170311
1	-2.009973	-0.698796	2.349301
6	-3.287356	-1.467083	-1.222388
1	-1.530612	-0.459301	-1.918165
6	-4.026651	-1.879034	-0.114190
1	-4.136750	-1.914772	2.035176
1	-3.651025	-1.670601	-2.223955
1	-4.963545	-2.407818	-0.251942
6	1.535214	-0.674989	0.113073
6	2.710693	-0.499647	0.862236
6	1.545955	-1.626181	-0.920137
6	3.860345	-1.235876	0.579358
1	2.712298	0.208790	1.684210
6	2.694168	-2.361194	-1.208398
1	0.648012	-1.806802	-1.501905
6	3.854444	-2.164849	-0.459803
1	4.756767	-1.089951	1.172476
1	2.683102	-3.090924	-2.010858
1	4.747124	-2.740020	-0.680664

B3LYP/6-311++G(d,p) = -1021.437926 Hartrees
Low frequencies = -952.3191 19.9186 24.6357 38.7173 47.7346
68.0679 74.2892 82.4396 136.6372 151.9954

Diphenyl ketone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.136601	1.329390	-1.857844
1	-1.599784	3.040189	-0.409738
6	-0.562871	3.376726	-0.376689
6	0.187803	2.855859	0.722471
1	-0.147882	2.589332	-1.278536
1	-0.455927	4.442098	-0.559596
8	0.167822	1.609789	1.002114
6	1.119676	3.714859	1.527671
1	1.911008	3.114683	1.976184
1	0.547546	4.194017	2.330430
1	1.542182	4.511870	0.912439
6	1.591202	-0.817879	-0.158241
6	2.799372	-0.460225	-0.770754
6	1.550107	-1.951134	0.662369
6	3.950206	-1.214663	-0.551237

1	2.829088	0.401389	-1.429149
6	2.702512	-2.705600	0.881391
1	0.619285	-2.258174	1.127600
6	3.903161	-2.335692	0.277443
1	4.881289	-0.932460	-1.030602
1	2.661765	-3.582266	1.518597
1	4.798547	-2.923962	0.446007
6	-1.716536	-0.544544	-0.108434
6	-2.606502	-0.807402	-1.158012
6	-2.093109	-0.873632	1.200760
6	-3.844970	-1.396441	-0.904345
1	-2.335959	-0.541240	-2.174575
6	-3.333005	-1.458790	1.453942
1	-1.428397	-0.658798	2.031125
6	-4.208101	-1.724020	0.400922
1	-4.526532	-1.594820	-1.724290
1	-3.617087	-1.704978	2.471360
1	-5.171909	-2.180206	0.598481
32	0.013241	0.269542	-0.517357

B3LYP/6-311++G(d,p) = -2808.8820985 Hartrees
Low frequencies = -951.2988 18.2126 25.0261 32.3677 42.2826
57.5110 71.9221 82.6562 125.7850 140.5755

Products: Addition of Acetone

Formaldehye (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.444951	-0.384809	-0.474757
1	1.434554	0.330785	-1.305622
1	1.992967	-1.281365	-0.754628
8	2.081788	0.135063	0.657713
1	0.209313	1.919072	-0.493077
6	-0.721195	1.439647	-0.217833
6	-0.869965	0.116304	-0.071771
1	1.654770	0.961476	0.909818
1	-1.577957	2.085573	-0.088741
8	0.116717	-0.822665	-0.218869
6	-2.161737	-0.554880	0.282107
1	-2.432639	-1.279339	-0.491336
1	-2.966391	0.172644	0.385337
1	-2.054978	-1.105604	1.221019

B3LYP/6-311++G(d,p) = -307.7561688 Hartrees
Low frequencies = 88.9853 136.9756 181.0762 300.3072 370.4282
418.0434 474.9857 517.1169 624.5443 725.7426

Formaldehye (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.276833	0.172250	-0.021852
8	0.204245	-0.668207	-0.224939
6	2.574956	-0.560632	-0.165782
1	2.637010	-1.023102	-1.155532
6	1.151434	1.473551	0.250217
1	-2.372813	0.721452	-1.343216
1	2.641457	-1.365796	0.572395
1	2.034141	2.079131	0.403943
1	3.423048	0.111788	-0.035267
1	0.187108	1.961797	0.313857
1	-1.405685	-0.242107	1.745341
14	-1.374256	-0.529820	0.299283
1	-1.966158	-1.829991	-0.075986
8	-2.198978	0.729868	-0.398934

B3LYP/6-311++G(d,p) = -559.250617 Hartrees
Low frequencies = 51.6204 91.5115 150.8282 200.4172 256.2969
320.9630 388.4091 499.1188 512.2543 640.1209

Formaldehye (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.661211	0.135081	-0.032273
8	-0.594489	-0.695222	0.159976
6	-2.939272	-0.536094	0.377118
1	-3.085422	-1.450550	-0.205276
6	-1.589755	1.381760	-0.516659
1	-0.657570	1.844113	-0.820032
1	-3.796732	0.120781	0.229844
1	-2.487920	1.970158	-0.640917
1	-2.888196	-0.826627	1.430486
1	1.299145	1.773817	0.888524
32	1.136129	-0.305760	-0.217767
1	1.221027	0.191924	-1.667082
1	1.884128	-1.585155	0.121604
8	1.756594	0.927894	0.922808

B3LYP/6-311++G(d,p) = -2346.6956596 Hartrees
Low frequencies = 38.8433 76.5234 147.2578 190.0073 203.0341
257.4377 327.3446 467.0113 508.6901 551.1282

Acetone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z

6	-1.427306	0.026261	0.051956
8	-0.248022	-0.641337	0.199934
6	-1.618619	1.343706	-0.119614
1	0.430807	1.233819	-1.371115
6	-2.559110	-0.959942	0.104896
1	-2.460314	-1.691209	-0.702317
1	-0.836887	2.089362	-0.110563
1	-3.522628	-0.458342	0.017521
1	-2.627899	1.711640	-0.240516
1	-2.530097	-1.511191	1.049217
1	1.714172	-1.893346	-0.890771
6	2.008593	-1.229527	-0.077475
6	1.058716	-0.042072	-0.028272
1	1.975639	-1.779228	0.864132
1	3.026438	-0.878628	-0.254906
8	1.120248	0.563206	-1.298228
6	1.419494	0.919085	1.108995
1	0.751135	1.777172	1.161773
1	2.436742	1.284145	0.954694
1	1.374479	0.395790	2.066287

B3LYP/6-311++G(d,p) = -386.4112169 Hartrees
Low frequencies = 68.9887 128.5148 174.9562 183.2843 191.5734
242.7982 311.2752 327.2661 345.0916 381.1254

Acetone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-1.339728	-1.139069	-1.162837
6	-1.260755	-0.843820	1.632031
6	-2.090788	1.533523	-0.235739
1	-1.907540	1.996681	-1.209688
1	-3.152277	1.276758	-0.176908
1	-1.878807	2.283788	0.531031
1	-0.570654	-1.683653	1.740112
1	-1.092521	-0.155867	2.465199
1	-2.279458	-1.233159	1.712979
14	-1.024099	0.019279	-0.002318
1	-1.251477	-0.907294	-2.090420
6	1.961196	-1.307111	-0.271159
6	1.766727	0.002188	-0.084561
1	1.149983	-1.984080	-0.505698
1	2.959837	-1.716522	-0.201792
8	0.541486	0.615479	-0.156494
6	2.853518	0.993557	0.206342
1	2.864615	1.773952	-0.560732
1	3.831037	0.511433	0.235266
1	2.671205	1.486768	1.166267

B3LYP/6-311++G(d,p) = -637.9371494 Hartrees

Low frequencies = 46.0144 74.1804 108.6997 127.4822 144.7421
187.5625 196.8782 212.0665 239.8239 268.1567

Acetone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.008173	0.024310	-0.103991
8	-0.825959	0.709519	-0.161588
6	-2.143772	-1.286675	-0.339640
1	1.020944	-0.836550	-2.175495
6	-3.147095	0.943318	0.233920
1	-3.205413	1.752141	-0.500901
1	-3.119983	-1.747959	-0.275005
1	-2.984616	1.407029	1.211986
1	-1.305536	-1.911786	-0.620599
1	-4.097438	0.408700	0.247545
1	0.214440	-1.737800	1.729960
6	1.013054	-0.998189	1.675845
1	1.976016	-1.511599	1.692563
1	0.945385	-0.333189	2.538376
32	0.854425	0.022287	0.026061
8	1.161467	-1.177778	-1.286700
6	1.958153	1.614284	-0.195465
1	1.733516	2.085959	-1.153564
1	1.748176	2.329305	0.601896
1	3.015840	1.346336	-0.168430

B3LYP/6-311++G(d,p) = -2425.3765969 Hartrees
Low frequencies = 48.3294 67.8217 70.9947 100.2158 108.9462
158.3988 183.8881 186.4193 196.1800 205.5416

4-Dimethyl-3-pentanone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.453566	0.032505	1.453543
6	1.360927	-1.159045	-0.486630
1	1.177538	-1.187626	-1.566287
6	0.781249	1.371778	-0.531467
1	1.369224	1.163741	-1.432385
6	0.998785	-2.539498	0.084920
1	-0.055341	-2.776282	-0.062353
1	1.591367	-3.312877	-0.410497
1	1.231908	-2.611982	1.154406
6	2.850698	-0.874800	-0.250482
1	3.447274	-1.708278	-0.631220
1	3.193836	0.028103	-0.757873
1	3.068416	-0.770147	0.815923

6	1.657134	2.203040	0.421739
1	2.536544	1.662052	0.770016
1	1.996038	3.106508	-0.093505
1	1.089386	2.508109	1.302905
6	-0.419082	2.213934	-0.991017
1	-0.048221	3.120449	-1.478333
1	-1.042198	1.679509	-1.709010
1	-1.049195	2.518687	-0.154156
1	-1.651873	0.974550	1.821626
6	-2.395254	0.472019	1.225068
6	-2.107357	-0.241036	0.129884
1	0.263514	-0.841803	1.812730
1	-3.431571	0.549545	1.526502
8	-0.880227	-0.480766	-0.438132
6	-3.151894	-0.935965	-0.699288
1	-2.949477	-2.010124	-0.749935
1	-3.138327	-0.555757	-1.725366
1	-4.146336	-0.783437	-0.279830
6	0.418257	-0.038234	0.051167

B3LYP/6-311++G(d,p) = - 543.6936525Hartrees
Low frequencies = 29.7938 59.7955 85.4136 109.3888 170.1864
192.1352 197.0170 217.6232 240.8273 250.7024

4-Dimethyl-3-pentanone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	0.397270	-0.019524	0.112265
8	0.488355	0.142182	1.774216
6	1.540452	-1.381457	-0.533121
1	1.296337	-1.467544	-1.601101
6	0.749690	1.696387	-0.603692
1	1.153045	1.501435	-1.608386
6	1.238181	-2.743124	0.122455
1	0.187751	-3.023684	0.013560
1	1.844411	-3.534888	-0.331117
1	1.479196	-2.733635	1.191731
6	3.036450	-1.034385	-0.413557
1	3.652972	-1.841316	-0.824567
1	3.294081	-0.119979	-0.954717
1	3.333686	-0.897421	0.631111
6	1.825390	2.459843	0.197120
1	2.762831	1.904115	0.279218
1	2.050024	3.417317	-0.285720
1	1.479961	2.667859	1.212749
6	-0.512811	2.563717	-0.777414
1	-0.257120	3.510610	-1.265746
1	-1.273643	2.068765	-1.384999
1	-0.967766	2.804739	0.187143
1	-2.047444	0.755346	1.801086

6	-2.773120	0.296562	1.143217
6	-2.415245	-0.380945	0.047721
1	0.311126	-0.621989	2.328133
1	-3.821152	0.398242	1.390222
8	-1.121119	-0.578575	-0.354682
6	-3.378179	-1.040416	-0.895131
1	-3.168365	-2.112457	-0.960871
1	-3.265355	-0.627361	-1.902461
1	-4.409073	-0.900761	-0.568844

B3LYP/6-311++G(d,p) = -795.2164974 Hartrees
Low frequencies = 28.9723 37.1736 47.9311 68.9998 99.0191
115.3193 157.8895 166.2402 184.1203 201.6231

4-Dimethyl-3-pentanone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.455132	0.085631	2.004078
6	1.965521	-0.892386	-0.561833
1	1.780904	-0.905523	-1.642182
6	0.198927	1.983135	-0.324450
1	1.213090	2.390294	-0.225303
6	2.004715	-2.344086	-0.061572
1	1.066443	-2.866057	-0.260706
1	2.811135	-2.897265	-0.556042
1	2.199777	-2.390244	1.015370
6	3.286846	-0.156816	-0.290334
1	4.125491	-0.698953	-0.741108
1	3.292834	0.855261	-0.705017
1	3.487380	-0.078164	0.782625
6	-0.725659	2.768098	0.617375
1	-0.418771	2.670205	1.660442
1	-0.709370	3.832302	0.355272
1	-1.758821	2.421762	0.537771
6	-0.230325	2.104666	-1.795178
1	-0.264118	3.158176	-2.093704
1	0.457537	1.593549	-2.475524
1	-1.227365	1.684789	-1.953686
1	-2.163010	0.158696	1.769830
6	-2.785534	-0.367148	1.057864
6	-2.280554	-0.958962	-0.031963
1	0.472357	-0.792362	2.397656
1	-3.847294	-0.422851	1.256804
8	-0.962086	-0.965909	-0.386205
6	-3.102882	-1.737241	-1.020412
1	-2.735288	-2.765986	-1.085462
1	-3.012907	-1.298934	-2.019238
1	-4.154914	-1.755420	-0.733800
32	0.420444	0.086043	0.194876

B3LYP/6-311++G(d,p) = -2582.6611508 Hartrees
Low frequencies = 18.1815 30.1096 44.4232 60.9472 77.9689
96.5084 116.2505 154.4133 170.3298 194.6702

Diphenyl ketone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.107859	0.502127	1.995373
1	2.456697	1.122594	1.587866
6	2.509288	1.951137	0.900700
6	1.510852	2.293338	0.085286
1	-0.573167	1.104176	2.318076
1	3.419140	2.536109	0.877470
8	0.284157	1.666686	-0.033648
6	1.546588	3.462088	-0.855241
1	0.724853	4.151839	-0.639140
1	1.428614	3.127974	-1.890893
1	2.489455	4.001422	-0.765005
6	-0.021753	0.415881	0.592738
6	-1.481637	0.117285	0.214748
6	-2.149163	-0.911417	0.890030
6	-2.156842	0.821925	-0.784240
6	-3.468858	-1.223420	0.577555
1	-1.631907	-1.469374	1.661578
6	-3.479213	0.505744	-1.097497
1	-1.651211	1.621512	-1.307382
6	-4.139462	-0.515446	-0.419680
1	-3.972638	-2.021873	1.110895
1	-3.992610	1.063828	-1.872780
1	-5.167078	-0.759109	-0.664975
6	0.902403	-0.701665	0.098876
6	1.449340	-1.637696	0.977487
6	1.157693	-0.820115	-1.270151
6	2.250415	-2.672049	0.492971
1	1.256912	-1.549560	2.038603
6	1.959085	-1.850158	-1.751852
1	0.730726	-0.100837	-1.959112
6	2.508794	-2.781462	-0.870662
1	2.674679	-3.390212	1.186029
1	2.153835	-1.927562	-2.815735
1	3.132381	-3.585249	-1.245705

B3LYP/6-311++G(d,p) = -769.9679389 Hartrees
Low frequencies = 31.8770 45.9542 53.1342 61.0905 79.1355
106.5964 172.9680 189.8472 210.9774 247.0387

Diphenyl ketone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z

14	-0.054277	0.344811	0.634854
8	0.147752	0.422161	2.287611
1	2.093610	2.169429	1.651378
6	2.058733	2.838740	0.802037
6	1.098565	2.766519	-0.122677
1	-0.535717	0.844023	2.814023
1	2.833167	3.588631	0.714329
8	0.074216	1.848248	-0.091331
6	0.977493	3.675513	-1.308257
1	0.012248	4.191294	-1.292368
1	1.022139	3.097987	-2.236947
1	1.774303	4.419596	-1.316231
6	-1.789842	-0.194042	0.183727
6	-2.249669	-1.464794	0.570267
6	-2.668451	0.638975	-0.527277
6	-3.540682	-1.886923	0.261373
1	-1.593202	-2.136602	1.115191
6	-3.960917	0.218684	-0.838877
1	-2.332831	1.621542	-0.838492
6	-4.398849	-1.044239	-0.444716
1	-3.876493	-2.871566	0.567869
1	-4.625111	0.876111	-1.389467
1	-5.403581	-1.372390	-0.687925
6	1.296412	-0.809238	0.057462
6	2.170182	-1.428708	0.964612
6	1.453891	-1.086126	-1.310676
6	3.169099	-2.293415	0.518962
1	2.065488	-1.229076	2.024975
6	2.451758	-1.948201	-1.758733
1	0.790180	-0.627429	-2.037532
6	3.311697	-2.553497	-0.842611
1	3.836135	-2.762697	1.234017
1	2.558450	-2.149122	-2.819147
1	4.088817	-3.225862	-1.189570

B3LYP/6-311++G(d,p) = -1021.4911101 Hartrees
Low frequencies = 15.1679 24.7880 33.3991 42.1018 49.2555
65.5168 111.5160 141.9889 154.0805 197.0696

Diphenyl ketone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.171953	0.391301	2.317000
1	2.007239	2.137157	1.546603
6	1.995450	2.821159	0.707973
6	1.039824	2.788638	-0.226618
1	-0.543124	0.847988	2.771163
1	2.785106	3.557506	0.643781

8	-0.005108	1.901093	-0.244101
6	0.955550	3.740194	-1.385167
1	-0.000109	4.273411	-1.365762
1	1.002810	3.192927	-2.331947
1	1.765994	4.469300	-1.356601
32	-0.067561	0.260084	0.535510
6	-1.880985	-0.301994	0.095405
6	-2.329115	-1.572829	0.481194
6	-2.753206	0.546971	-0.598105
6	-3.626110	-1.985998	0.182185
1	-1.668536	-2.247443	1.016773
6	-4.050325	0.131360	-0.897474
1	-2.412727	1.529710	-0.901976
6	-4.487396	-1.133680	-0.508031
1	-3.963243	-2.971027	0.485555
1	-4.718746	0.795092	-1.434966
1	-5.496108	-1.455809	-0.742127
6	1.406439	-0.870696	-0.035871
6	2.315159	-1.378072	0.901043
6	1.563503	-1.197957	-1.388688
6	3.365119	-2.197621	0.488380
1	2.200103	-1.129282	1.949626
6	2.615096	-2.014805	-1.799407
1	0.867661	-0.817128	-2.129588
6	3.516204	-2.515483	-0.860324
1	4.065446	-2.585825	1.219790
1	2.730270	-2.261292	-2.849139
1	4.333910	-3.152244	-1.179681

B3LYP/6-311++G(d,p) = -2808.9297463 Hartrees
Low frequencies = 19.6153 25.2904 32.4791 40.9759 45.4227
62.9019 102.0378 132.8018 152.8123 181.2340

Transition State: Addition of Water

Formaldehye (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	1.140698	-0.161907	-0.110665
1	0.219105	-0.909638	-0.040029
1	1.657560	-0.113297	0.707339
8	-1.021943	-0.493813	0.026629
6	-0.365074	0.633315	0.000550
1	-0.353873	1.233632	-0.917444
1	-0.282388	1.235182	0.919123

B3LYP/6-311++G(d,p) = -190.9428732 Hartrees
Low frequencies = -1778.6941 417.3698 513.7036 718.7125
762.4836 1003.9138 1195.7172 1275.1944 1305.0642
1354.9291

Formaldehye (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-1.348785	0.109045	-0.110196
1	-0.687711	0.998007	-0.026024
1	-1.986797	0.012743	0.609520
8	0.796295	1.017527	0.023364
1	0.612812	-1.367163	-1.193763
1	0.450750	-1.354407	1.233519
14	0.430776	-0.521554	0.005100

B3LYP/6-311++G(d,p) = -442.430122 Hartrees
Low frequencies = -994.4548 439.8173 468.1667 519.0098 651.0093
727.5324 795.2839 886.5656 1004.9064 1104.1075

Formaldehye (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-1.577160	-0.386544	-0.110411
1	-1.310938	0.702376	-0.030425
1	-2.093623	-0.709172	0.639679
8	-0.067739	1.426598	0.021060
1	0.979261	-0.885288	-1.271110
1	0.869538	-0.940246	1.292144
32	0.459842	-0.202753	0.002641

B3LYP/6-311++G(d,p) = -2229.8850181 Hartrees
Low frequencies = -1050.2529 343.1457 434.7899 475.8157
559.0546 685.9737 737.2186 775.1631 841.3455 894.0229

Acetone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	1.380423	-0.165504	-0.720673
1	1.420283	-0.157570	0.512034
1	1.696397	0.651716	-1.129212
6	-0.765798	1.357064	-0.208832
8	0.470135	-0.084569	1.295471
6	-0.970491	-1.205725	-0.294533
1	-1.867709	-1.282907	0.329815
1	-1.275400	-1.129908	-1.338952
1	-0.371898	-2.102970	-0.143272
1	-1.664756	1.513974	0.397504

1	-0.059438	2.149016	0.043212
1	-1.050052	1.414321	-1.260999
6	-0.202360	0.006146	0.168612

B3LYP/6-311++G(d,p) = -269.6139819 Hartrees
Low frequencies = -1791.5201 193.2673 231.8859 242.5125 297.4726 372.9349 411.1956 478.0984 515.4952 670.1109

Acetone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	1.326048	-0.224913	-1.053965
1	1.742048	-0.297866	-0.035359
1	1.682321	0.519725	-1.555364
6	-0.811534	1.711805	-0.086260
8	1.034038	-0.246966	1.271462
6	-1.344625	-1.340674	-0.216451
1	-2.130914	-1.381051	0.544317
1	-1.824758	-1.166559	-1.183468
1	-0.850994	-2.314440	-0.237173
1	-1.586198	1.924558	0.657979
1	-0.038269	2.475886	0.024660
1	-1.273217	1.809460	-1.073433
14	-0.118840	-0.001534	0.209581

B3LYP/6-311++G(d,p) = -521.119577 Hartrees
Low frequencies = -871.0936 113.4887 137.7348 165.6409 207.0914 241.9048 275.7085 404.9083 470.7701 621.6149

Acetone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-1.524202	-0.131165	1.108651
1	-1.851095	-0.132396	0.039357
1	-1.849364	0.640077	1.589594
6	1.003782	1.720717	0.198523
8	-1.197614	-0.111698	-1.240358
6	1.215296	-1.569041	0.279676
32	0.136612	-0.000438	-0.164679
1	1.989519	-1.699398	-0.480528
1	1.694336	-1.446301	1.252633
1	0.576154	-2.451584	0.288520
1	1.823727	1.859380	-0.510933
1	0.289462	2.533549	0.066070
1	1.415746	1.743540	1.209476

B3LYP/6-311++G(d,p) = -2308.5669008 Hartrees

Low frequencies = -940.0396 77.7522 101.3911 129.3794
166.2023 180.9594 209.5664 315.7051 480.5039
553.0562

4-Dimethyl-3-pentanone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-0.443738	-1.076719	1.585697
1	-0.567624	-1.895126	0.663223
1	-1.291476	-0.752984	1.917320
6	-1.035699	0.583867	-0.518982
1	-0.746926	0.779554	-1.562792
8	-0.346252	-1.736637	-0.530452
6	1.464365	-0.257311	-0.010875
1	1.851637	-1.240024	0.272541
6	2.013012	0.057578	-1.417609
1	3.105900	0.055535	-1.393072
1	1.689545	-0.689392	-2.145510
1	1.694244	1.045507	-1.764427
6	1.963120	0.749839	1.033574
1	1.467641	0.597233	1.993036
1	3.036464	0.599322	1.181901
1	1.826922	1.787869	0.726225
6	-2.484499	0.074530	-0.550815
1	-3.120497	0.804687	-1.057360
1	-2.558093	-0.878869	-1.071587
1	-2.887334	-0.054288	0.459949
6	-0.940655	1.907773	0.251857
1	-1.054990	1.751183	1.328369
1	0.001291	2.428862	0.088161
1	-1.743326	2.575154	-0.072568
6	-0.043554	-0.517506	-0.121380

B3LYP/6-311++G(d,p) = -426.9021915 Hartrees
Low frequencies = -1769.1995 23.6594 83.5567 177.1296 192.5766
198.0386 210.6124 222.8783 254.9685 284.7198

4-Dimethyl-3-pentanone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-0.504684	-1.506242	1.375156
1	-0.720336	-2.169240	0.523438
1	-1.300648	-1.284425	1.875691
6	-1.246787	0.913385	-0.391319
1	-1.051492	1.300057	-1.403285
8	-0.511825	-1.940190	-0.934276
6	1.776118	-0.171262	-0.123550

1	2.237196	-1.159031	-0.249291
6	2.246075	0.714416	-1.297292
1	3.334607	0.833034	-1.273887
1	1.986308	0.283398	-2.268760
1	1.811010	1.718022	-1.248678
6	2.236531	0.394269	1.232990
1	1.945716	-0.255000	2.062230
1	3.327978	0.488364	1.251448
1	1.824669	1.388894	1.424914
6	-2.718016	0.455514	-0.359660
1	-3.385673	1.285527	-0.613868
1	-2.901477	-0.362574	-1.058484
1	-3.010106	0.111448	0.639940
6	-0.994043	2.063957	0.600970
1	-1.124512	1.741230	1.639765
1	0.011074	2.481545	0.509998
1	-1.703774	2.880122	0.427682
14	-0.067695	-0.566542	-0.267052

B3LYP/6-311++G(d,p) = -678.40089589 Hartrees
Low frequencies = -838.8517 34.0856 53.5386 116.9161 136.3673
138.3023 186.6593 218.7950 226.4005 231.3388

4-Dimethyl-3-pentanone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-0.511200	-1.562158	1.466825
1	-0.701326	-2.151300	0.538118
1	-1.327094	-1.404381	1.957954
6	-1.333947	1.092426	-0.362627
1	-1.174638	1.467512	-1.382624
8	-0.550249	-1.956040	-0.877917
6	1.897141	-0.062480	-0.068442
1	2.330902	-1.058794	-0.199290
6	2.395770	0.845716	-1.204520
1	3.483084	0.966056	-1.141339
1	2.171488	0.434212	-2.192892
1	1.957645	1.847611	-1.148555
6	2.284783	0.470418	1.317814
1	1.942547	-0.191711	2.115971
1	3.375121	0.552757	1.395041
1	1.872195	1.466441	1.503159
6	-2.777467	0.580409	-0.264322
1	-3.483537	1.381719	-0.508537
1	-2.956989	-0.256507	-0.941836
1	-3.012998	0.244533	0.751371
6	-1.046480	2.233762	0.623302
1	-1.145127	1.905247	1.662730
1	-0.043935	2.650676	0.499469
1	-1.760886	3.051170	0.473675

32	-0.048552	-0.428787	-0.260653

B3LYP/6-311++G(d,p) = -2465.8524445 Hartrees
Low frequencies = -910.7730 36.0233 43.0651 92.5301 107.2419
108.1124 162.3087 221.5637 226.4615 231.4198

Diphenyl ketone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-0.042269	1.981674	1.453157
1	0.048726	2.547559	0.284154
1	0.769981	1.933177	1.974182
8	-0.066477	2.077867	-0.771542
6	1.283871	0.207000	-0.068425
6	1.567467	-0.741253	0.925189
6	2.263760	0.522130	-1.015622
6	2.810328	-1.363519	0.964833
1	0.822810	-0.967285	1.679745
6	3.502317	-0.115984	-0.983024
1	2.038098	1.265930	-1.769189
6	3.778275	-1.057562	0.005764
1	3.027658	-2.084113	1.745152
1	4.252582	0.127395	-1.726770
1	4.744903	-1.547762	0.035697
6	-1.303383	0.130620	-0.113795
6	-2.514001	0.833545	-0.010919
6	-1.335103	-1.262559	-0.253812
6	-3.723549	0.153851	-0.017602
1	-2.487452	1.910794	0.082993
6	-2.552812	-1.940941	-0.276978
1	-0.414676	-1.818237	-0.373352
6	-3.746755	-1.236861	-0.151160
1	-4.652101	0.705286	0.076467
1	-2.565322	-3.018044	-0.398790
1	-4.693418	-1.765531	-0.164108
6	-0.034050	0.910617	-0.154300

B3LYP/6-311++G(d,p) = -653.1728775 Hartrees
Low frequencies = -1660.3623 33.0657 59.8991 89.6981 114.5383
139.3942 218.4888 233.5962 243.9240 291.2403

Diphenyl ketone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-0.075174	2.232488	1.320759
1	0.046418	2.856439	0.415960
1	0.683720	2.275840	1.917259
8	0.065726	2.447826	-1.000836

6	1.549489	0.050636	-0.048848
6	1.647547	-1.084785	0.773807
6	2.692130	0.464778	-0.755135
6	2.848576	-1.781657	0.889314
1	0.781658	-1.429785	1.329951
6	3.891390	-0.236919	-0.647260
1	2.630282	1.341457	-1.391439
6	3.970502	-1.359153	0.176161
1	2.909677	-2.653874	1.530905
1	4.762415	0.091190	-1.203723
1	4.903917	-1.904640	0.262289
6	-1.572412	0.054685	-0.120132
6	-2.768785	0.632427	0.339235
6	-1.609278	-1.272647	-0.577334
6	-3.955085	-0.095393	0.351807
1	-2.771708	1.658089	0.691426
6	-2.798785	-2.000133	-0.574494
1	-0.705389	-1.746239	-0.946009
6	-3.971957	-1.413186	-0.106064
1	-4.867476	0.364938	0.714621
1	-2.808407	-3.022186	-0.936813
1	-4.897556	-1.978265	-0.100083
14	-0.009426	1.068043	-0.217862

B3LYP/6-311++G(d,p) = -904.6759713 Hartrees
Low frequencies = -909.6634 25.0982 44.7769 64.0285
85.7066 110.9121 139.5284 192.3615 238.5503 245.9635

Diphenyl ketone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z

8	0.102623	-2.165978	1.475001
1	-0.019004	-2.753025	0.526029
1	-0.668051	-2.239594	2.051926
8	-0.065817	-2.458738	-0.864394
32	0.009048	-0.881651	-0.185194
6	-1.648129	0.135718	-0.035802
6	-1.754389	1.317903	0.710137
6	-2.782080	-0.366456	-0.690082
6	-2.974635	1.985639	0.800773
1	-0.890651	1.718172	1.230502
6	-3.999279	0.307167	-0.603985
1	-2.704756	-1.285192	-1.262111
6	-4.095581	1.481806	0.141229
1	-3.050995	2.896605	1.384064
1	-4.871108	-0.084592	-1.116089
1	-5.043497	2.004035	0.209724
6	1.664498	0.138047	-0.107789
6	2.858054	-0.513455	0.233101

6	1.698556	1.498239	-0.441507
6	4.060128	0.188777	0.252159
1	2.847530	-1.567999	0.484152
6	2.905337	2.197534	-0.429631
1	0.788592	2.018013	-0.721734
6	4.084757	1.543914	-0.079160
1	4.978395	-0.321230	0.521183
1	2.923257	3.248739	-0.695033
1	5.022894	2.087629	-0.067904

B3LYP/6-311++G(d,p) = -2692.1229408 Hartrees
Low frequencies = -987.4818 18.6018 38.9245 59.2712 74.5523
94.3013 127.3309 172.6046 216.1976 228.8359

Products: Addition of Water

Formaldehye (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	1.182440	-0.226130	-0.139991
1	1.350561	-0.821784	0.597372
1	-1.350688	-0.821556	0.597492
8	-1.182475	-0.226116	-0.140018
6	0.000058	0.505021	0.094588
1	0.000087	1.312648	-0.634666
1	-0.000030	0.918534	1.112348

B3LYP/6-311++G(d,p) = -191.0149366 Hartrees
Low frequencies = 185.7712 391.1678 536.7422 994.5335
1040.0445 1053.0622 1154.4089 1370.9250 1393.6065
1442.0381

Formaldehye (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	1.392298	-0.433858	-0.128375
1	1.732946	-0.965676	0.593242
1	-1.733033	-0.965562	0.593274
8	-1.392283	-0.433874	-0.128390
1	0.000014	1.406117	-1.079539
1	-0.000022	1.096706	1.381484
14	-0.000002	0.455019	0.040404

B3LYP/6-311++G(d,p) = -442.5123251 Hartrees
Low frequencies = 117.4933 280.9082 336.9574 607.8206 712.9798
796.9986 830.0984 878.3152 901.4919 957.2518

Formaldehye (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-1.483117	0.668409	-0.130331
1	-1.725438	1.153705	0.663782
1	1.725553	1.153544	0.663832
8	1.483115	0.668418	-0.130350
1	-0.000024	-1.228562	-1.212365
1	0.000021	-1.029328	1.392197
32	-0.000003	-0.335749	0.018063

B3LYP/6-311++G(d,p) = -2229.9571147 Hartrees
Low frequencies = 41.2864 222.0951 264.4509 527.7760 663.0761 664.5544 672.5802 805.7305 846.2669 884.7349

Acetone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-0.198025	-0.830016	1.155022
1	-0.469651	-0.266149	1.886784
1	-0.685282	-1.533803	-0.991527
1	-2.095636	0.439173	-0.215465
6	-1.143131	0.974227	-0.173722
6	0.011892	-0.020491	-0.013312
1	-1.021848	1.542945	-1.097548
1	-1.178441	1.680880	0.661589
8	0.055101	-0.923802	-1.093616
6	1.374786	0.661532	0.038792
1	1.568838	1.198071	-0.892449
1	2.146992	-0.095478	0.179695
1	1.417133	1.373298	0.867131

B3LYP/6-311++G(d,p) = -269.6773394 Hartrees
Low frequencies = 184.0345 221.8546 265.2524 284.2397 347.9070 366.1369 443.0283 503.6702 528.2501 769.2415

Acetone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-0.270760	-1.030801	1.309391
1	-0.823496	-0.730350	2.032996
1	-0.318388	-1.828314	-1.366602
1	-2.392059	0.537303	-0.368289
6	-1.465645	1.106692	-0.245872
1	-1.333541	1.721164	-1.141381
1	-1.598880	1.786906	0.601995
8	0.228089	-1.041708	-1.304144

6	1.606157	0.917920	0.179102
1	1.836001	1.477381	-0.732299
1	2.434718	0.231409	0.371031
1	1.555569	1.630392	1.007925
14	0.009884	-0.028107	-0.003338

B3LYP/6-311++G(d,p) = -521.1990874 Hartrees
Low frequencies = 118.4969 136.4316 153.9343 181.1853 203.2099 234.9577 256.2197 311.3153 338.7419 623.6760

Acetone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.299772	-1.048256	1.430956
1	-0.420138	-1.657898	1.620503
1	0.419976	-1.659416	-1.619099
1	-2.506464	0.332450	0.209942
6	-1.662450	1.023050	0.169114
1	-1.791421	1.676988	-0.695391
1	-1.649865	1.628584	1.076934
8	-0.299874	-1.049563	-1.430034
6	1.662587	1.022741	-0.169888
1	1.650569	1.626660	-1.078803
1	2.506603	0.332054	-0.209027
1	1.790949	1.678327	0.693453
32	-0.000007	0.017189	-0.000039

B3LYP/6-311++G(d,p) = -2308.63946082 Hartrees
Low frequencies = 96.6477 103.1494 155.7904 181.0417 191.4530 219.0553 226.8134 231.9460 343.0783 569.8560

4-Dimethyl-3-pentanone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.068785	-0.428069	1.510452
1	-0.172779	0.440300	1.847550
1	-0.567260	-2.240441	0.295482
6	-1.276192	0.297085	-0.438214
1	-1.052619	0.621332	-1.460993
8	0.033952	-1.775105	-0.297153
6	1.340402	0.155200	-0.535007
1	1.264773	-0.073694	-1.605035
6	-1.689100	1.536303	0.379097
1	-0.879308	2.250528	0.533876
1	-2.491782	2.069184	-0.137486
1	-2.087443	1.246908	1.357819

6	-2.474526	-0.663002	-0.511172
1	-3.362044	-0.125580	-0.856602
1	-2.294027	-1.488482	-1.200167
1	-2.711723	-1.077364	0.474978
6	2.571546	-0.573996	0.022574
1	2.484433	-1.652393	-0.105485
1	3.472215	-0.234927	-0.497349
1	2.696608	-0.367634	1.088628
6	1.519112	1.673010	-0.390903
1	2.480662	1.966672	-0.820144
1	0.746945	2.245177	-0.908798
1	1.533250	1.980736	0.660316
6	0.028457	-0.413754	0.078129

B3LYP/6-311++G(d,p) = -426.9632436 Hartrees
Low frequencies = 70.4397 88.3431 193.4792 195.0313
223.6821 226.5894 260.1716 275.4298 296.6122
304.2655

4-Dimethyl-3-pentanone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.027967	-0.512423	1.768868
1	-0.370021	0.197836	2.275934
1	-0.436821	-2.671683	0.066078
6	-1.561479	0.429821	-0.506621
1	-1.342137	0.769373	-1.528606
8	0.074138	-2.021113	-0.420902
6	1.616494	0.323816	-0.585470
1	1.549738	0.198301	-1.675705
6	-1.941038	1.671010	0.326866
1	-1.130804	2.401882	0.394781
1	-2.805152	2.182548	-0.110709
1	-2.227197	1.391955	1.347682
6	-2.754125	-0.544150	-0.587482
1	-3.645688	-0.034628	-0.969889
1	-2.545702	-1.389502	-1.247268
1	-3.011232	-0.944587	0.399630
6	2.855727	-0.452727	-0.098268
1	2.789402	-1.513271	-0.349794
1	3.766413	-0.051505	-0.557049
1	2.969950	-0.373571	0.987220
6	1.758438	1.829357	-0.292080
1	2.693124	2.216542	-0.712191
1	0.942552	2.418087	-0.720852
1	1.786013	2.026006	0.785233
14	0.025473	-0.435589	0.092150

B3LYP/6-311++G(d,p) = -678.4805304 Hartrees
Low frequencies = 38.4193 42.7832 109.4131 143.0274

165.5372 168.9240 195.2656 203.0524 230.2490
232.5794

4-Dimethyl-3-pentanone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.125650	-0.370643	1.833678
1	-0.570948	-0.879913	2.259150
1	0.628389	-2.596428	-0.244000
6	-1.740061	0.408918	-0.591701
1	-1.723716	0.253303	-1.677020
8	-0.102344	-2.046954	-0.543232
6	1.685855	0.541781	-0.533028
1	1.528221	0.847828	-1.574294
32	-0.007597	-0.325868	0.023169
6	-1.878546	1.911919	-0.307967
1	-1.094015	2.499793	-0.792465
1	-2.840517	2.282899	-0.679265
1	-1.839683	2.122751	0.765154
6	-2.911307	-0.395382	-0.007278
1	-3.861381	-0.044925	-0.426364
1	-2.818218	-1.461275	-0.225562
1	-2.976582	-0.272961	1.079293
6	2.853483	-0.456619	-0.491705
1	2.682065	-1.317262	-1.143836
1	3.779335	0.026604	-0.823615
1	3.024353	-0.825102	0.524478
6	1.981374	1.789877	0.314887
1	2.915364	2.258900	-0.014795
1	1.191075	2.541223	0.238163
1	2.088113	1.530149	1.370767

B3LYP/6-311++G(d,p) = -2465.9246572 Hartrees
Low frequencies = 25.5005 42.3211 91.2352 117.7749
141.9544 172.1915 203.9551 214.5293 231.7733
237.7375

Diphenyl ketone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.078335	1.972080	-1.159875
1	-0.758755	2.445718	-1.234034
1	0.758718	2.445796	1.233670
8	-0.078400	1.972189	1.159524
6	0.000000	1.156162	-0.000139
6	1.269835	0.300045	0.033333
6	2.155284	0.252798	-1.045173
6	1.547225	-0.456275	1.177997

6	3.303952	-0.536885	-0.977122
1	1.946972	0.839713	-1.929495
6	2.692965	-1.243024	1.243553
1	0.862832	-0.426140	2.017869
6	3.576228	-1.286109	0.164264
1	3.986339	-0.562759	-1.819584
1	2.896022	-1.824250	2.136161
1	4.468512	-1.900072	0.214684
6	-1.269800	0.299968	-0.033400
6	-2.155294	0.253041	1.045086
6	-1.547157	-0.456641	-1.177864
6	-3.303982	-0.536617	0.977181
1	-1.947014	0.840106	1.929317
6	-2.692936	-1.243373	-1.243280
1	-0.862703	-0.426772	-2.017695
6	-3.576243	-1.286137	-0.164041
1	-3.986401	-0.562274	1.819622
1	-2.895936	-1.824848	-2.135739
1	-4.468536	-1.900096	-0.214336

B3LYP/6-311++G(d,p) = -653.237994 Hartrees
Low frequencies = 31.2952 34.8095 61.4536 155.8801
210.3552 219.7174 273.8905 313.1863 324.7252 351.5631

Diphenyl ketone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-0.053754	1.842526	1.663695
1	0.749986	2.229411	2.018550
1	0.731684	2.718325	-1.331591
8	-0.061299	2.226676	-1.106111
6	-1.596469	0.160162	0.021360
6	-2.177030	-0.425428	1.157896
6	-2.221426	-0.037178	-1.220344
6	-3.339173	-1.187473	1.056712
1	-1.725894	-0.270103	2.131954
6	-3.383830	-0.798845	-1.323843
1	-1.804171	0.421845	-2.109966
6	-3.943146	-1.377108	-0.185373
1	-3.776470	-1.627711	1.946293
1	-3.855907	-0.936367	-2.290609
1	-4.848517	-1.969026	-0.264970
6	1.579993	0.143145	0.016530
6	2.205578	-0.064269	-1.224652
6	2.170405	-0.439485	1.151261
6	3.374179	-0.816844	-1.328760
1	1.773065	0.361903	-2.124554
6	3.338448	-1.193285	1.052701
1	1.710769	-0.308090	2.125954
6	3.943626	-1.381989	-0.188839

1	3.839142	-0.963367	-2.297657
1	3.775430	-1.633406	1.942512
1	4.852280	-1.968601	-0.267898
14	-0.014850	1.135939	0.153816

B3LYP/6-311++G(d,p) = -904.7536838 Hartrees
Low frequencies = 31.3673 36.4627 42.9800 113.2379 130.9576 141.0856 196.9595 214.7862 246.2041 251.3847

Diphenyl ketone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-0.084802	1.953397	1.461863
1	0.755669	2.356987	1.699240
1	0.757014	2.395948	-1.709942
8	-0.051324	1.903263	-1.537514
6	-1.688678	-0.048724	-0.017021
6	-2.375531	-0.265644	1.183857
6	-2.223409	-0.547554	-1.211505
6	-3.574755	-0.976886	1.189555
1	-1.982757	0.136567	2.110892
6	-3.422028	-1.258805	-1.203291
1	-1.714534	-0.367211	-2.152022
6	-4.096958	-1.475915	-0.002644
1	-4.103195	-1.136096	2.123110
1	-3.831333	-1.637895	-2.133236
1	-5.030201	-2.028324	0.002870
6	1.683046	-0.056142	0.013753
6	2.368246	-0.343066	-1.174537
6	2.228665	-0.492462	1.229108
6	3.571389	-1.047718	-1.148697
1	1.961465	-0.019002	-2.126830
6	3.430681	-1.198254	1.255628
1	1.714337	-0.284748	2.161923
6	4.103818	-1.475355	0.066467
1	4.091252	-1.263354	-2.075766
1	3.841016	-1.531447	2.202610
1	5.038647	-2.024447	0.086796
32	-0.013603	0.927153	-0.020890

B3LYP/6-311++G(d,p) = -2692.1906086 Hartrees
Low frequencies = 22.0995 29.6572 37.1017 84.6148 121.1503 123.6429 177.4247 198.3724 215.2235 222.5055

Transition State: Addition of Carbon dioxide

Formaldehye (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.675944	-1.026513	-0.000001
8	0.032322	1.153766	-0.000001
6	-0.696064	0.145480	-0.000001
8	-1.753905	-0.323121	0.000001
1	1.932668	0.331620	0.926451
1	1.932675	0.331622	-0.926445
6	1.446026	0.005136	0.000001

B3LYP/6-311++G(d,p) = - 303.11476732 Hartrees
Low frequencies = -803.9041 148.9052 337.0545 543.7176 598.2908
686.5198 772.6265 1132.0379 1201.3423

Formaldehye (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-0.494532	1.236869	-0.000016
8	0.356817	-1.144693	-0.000015
6	1.149945	-0.226484	-0.000002
8	2.140669	0.350089	0.000011
1	-1.983342	-0.617685	1.220540
1	-1.983400	-0.617708	-1.220486
14	-1.354040	-0.067416	0.000009

B3LYP/6-311++G(d,p) = -554.5948083 Hartrees
Low frequencies =-334.9700 122.4124 259.2291 334.2598 508.2733
616.9622 641.2189 689.4470 828.6796 1011.4029

Formaldehye (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.063680	1.252997	-0.000007
8	0.802884	-1.178617	0.000000
6	1.564005	-0.231126	-0.000012
8	2.577419	0.317603	-0.000024
1	-1.702083	-0.549741	1.286440
1	-1.702105	-0.549756	-1.286405
32	-1.047866	-0.020300	0.000009

B3LYP/6-311++G(d,p) = -2342.0519364 Hartrees
Low frequencies = -366.2952 110.0662 236.6786 292.6874 379.1176
569.2435 613.7642 659.3954 706.2694 869.9224

Acetone (C)

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
8	1.052023	-0.240056	0.000000
6	0.042544	1.532328	1.286237
1	0.892769	2.216140	1.408784
1	-0.872914	2.123603	1.271792
1	0.041985	0.840167	2.126558
6	0.042544	1.532328	-1.286237
1	0.041985	0.840167	-2.126558
1	-0.872914	2.123603	-1.271792
1	0.892769	2.216140	-1.408784
8	-1.188174	-0.508336	0.000000
6	-0.242988	-1.320827	0.000000
8	0.042544	-2.455746	0.000000
6	0.262095	0.801718	0.000000

B3LYP/6-311++G(d,p) = -381.7931236 Hartrees
Low frequencies = -729.5633 86.6659 153.1034 198.1897 215.7295
268.1555 336.6497 461.6793 498.9580 542.3616

Acetone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-0.006223	0.815241	0.000000
8	1.404603	0.135925	0.000000
6	-0.781239	1.491050	1.553586
1	-0.478070	2.535691	1.683770
1	-1.873411	1.466483	1.511186
1	-0.442960	0.935352	2.430135
6	-0.781239	1.491050	-1.553586
1	-0.442960	0.935352	-2.430135
1	-1.873411	1.466483	-1.511186
1	-0.478070	2.535691	-1.683770
8	-0.781239	-1.151291	0.000000
6	0.280512	-1.728702	0.000000
8	1.047610	-2.585737	0.000000

B3LYP/6-311++G(d,p) = - 633.2865802Hartrees
Low frequencies = -324.5875 72.5335 91.7366 113.6591 147.9996
168.2845 212.3006 275.8995 302.1543 327.4553

Acetone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	1.225475	-0.764263	0.000000
6	-0.169484	1.582653	1.651119
1	0.512230	2.429426	1.767471
1	-1.192035	1.962240	1.610456

1	-0.051801	0.910961	2.500708
6	-0.169484	1.582653	-1.651119
1	-0.051801	0.910961	-2.500708
1	-1.192035	1.962240	-1.610456
1	0.512230	2.429426	-1.767471
8	-1.310539	-1.007621	0.000000
6	-0.518292	-1.922794	0.000000
8	-0.169484	-3.025455	0.000000
32	0.270099	0.634950	0.000000

B3LYP/6-311++G(d,p) = -2420.7366789 Hartrees
Low frequencies = -336.2891 64.6295 69.2402 86.9719 108.8574
142.0713 172.6036 230.4277 230.8974 292.7010

4-Dimethyl-3-pentanone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	0.792746	-0.212790	-1.035935
6	-1.092672	-1.162059	0.117951
1	-0.459091	-2.049866	0.193030
1	-0.827341	1.342559	1.346886
6	-1.958874	-1.365164	-1.150127
1	-1.337489	-1.410530	-2.045513
1	-2.494249	-2.312970	-1.056805
1	-2.701265	-0.575424	-1.276958
6	-1.933378	-1.054552	1.392646
1	-2.517856	-1.968683	1.523115
1	-1.299577	-0.935019	2.274027
1	-2.638974	-0.219981	1.354175
6	-1.492156	1.974212	-0.604268
1	-2.442513	1.445412	-0.530681
1	-1.667236	3.015776	-0.326253
1	-1.158832	1.952616	-1.644489
6	0.828017	2.299747	0.347862
1	0.531101	3.309541	0.641250
1	1.576087	1.946944	1.057886
1	1.284873	2.353096	-0.642252
6	1.972719	-0.683253	0.023001
8	1.364306	-0.589247	1.109083
8	3.007368	-0.965401	-0.455442
6	-0.111148	-0.025398	-0.101559
6	-0.406342	1.390805	0.339649

B3LYP/6-311++G(d,p) = -539.0858091 Hartrees
Low frequencies = -689.8250 55.4721 72.4675 78.5044 167.8710
181.7904 201.0913 203.8627 223.3269 241.7629

4-Dimethyl-3-pentanone (Si)

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
14	-0.053638	-0.053121	-0.265385
8	1.013660	-0.285664	-1.392883
6	-1.309602	-1.402318	0.144431
1	-0.696250	-2.308216	0.233491
6	-0.471740	1.678945	0.355515
1	-0.824894	1.571567	1.389040
6	-2.277862	-1.623913	-1.039859
1	-1.741001	-1.804927	-1.974136
1	-2.916102	-2.492287	-0.846092
1	-2.939026	-0.764779	-1.191485
6	-2.064017	-1.193849	1.469171
1	-2.719321	-2.047304	1.672886
1	-1.385128	-1.092206	2.320642
1	-2.696541	-0.301319	1.437639
6	-1.633077	2.263419	-0.483828
1	-2.535191	1.646041	-0.443862
1	-1.902372	3.257034	-0.111204
1	-1.348645	2.375227	-1.534464
6	0.745526	2.620325	0.343223
1	0.453932	3.622027	0.676715
1	1.539468	2.271168	1.008173
1	1.166195	2.709250	-0.661584
6	2.358133	-0.776416	0.236162
8	1.513078	-0.590036	1.079298
8	3.374717	-1.036143	-0.237572

B3LYP/6-311++G(d,p) = -790.5694428 Hartrees
Low frequencies = -323.1234 29.4404 38.1523 56.3106 96.6919
110.1782 124.2570 191.4898 194.5529 209.5853

4-Dimethyl-3-pentanone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	1.172539	-0.322518	-1.319337
6	-1.385177	-1.478633	0.199804
1	-0.740546	-2.353863	0.330307
6	-0.495972	1.815825	0.395366
1	-0.861882	1.710669	1.422412
6	-2.303411	-1.729795	-1.009753
1	-1.733737	-1.930093	-1.920415
1	-2.942127	-2.599049	-0.818585
1	-2.965759	-0.879948	-1.203553
6	-2.169541	-1.227195	1.493349
1	-2.826686	-2.077487	1.707016
1	-1.512074	-1.097269	2.357212
1	-2.805878	-0.339856	1.417441
6	-1.625947	2.402076	-0.473306
1	-2.539243	1.800715	-0.440504

1	-1.885080	3.405492	-0.118663
1	-1.320632	2.496646	-1.519664
6	0.757515	2.698340	0.382878
1	0.502433	3.715344	0.701275
1	1.527828	2.322021	1.059542
1	1.192436	2.757794	-0.617925
6	2.448650	-0.796406	0.272561
8	1.660100	-0.621761	1.171967
8	3.465018	-1.063128	-0.213027
32	-0.088344	-0.030535	-0.219941

B3LYP/6-311++G(d,p) = -2578.0234196 Hartrees
Low frequencies = -331.7345 16.3636 28.8347 46.3110 74.6034
84.9023 88.8461 170.4590 176.1284 202.2998

Diphenyl ketone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-0.028944	1.633732	-0.874617
6	0.182533	2.532810	0.383945
8	0.099712	1.720048	1.339058
8	0.336408	3.694303	0.202352
6	-1.329849	-0.238852	-0.161263
6	-1.429932	-1.641275	-0.135060
6	-2.509951	0.529736	-0.162577
6	-2.676622	-2.255637	-0.091333
1	-0.537284	-2.249342	-0.185535
6	-3.749175	-0.088093	-0.106710
1	-2.439002	1.608389	-0.197935
6	-3.835589	-1.482247	-0.068246
1	-2.743437	-3.337187	-0.084327
1	-4.650924	0.512584	-0.094874
1	-4.806571	-1.963205	-0.030292
6	1.247504	-0.254117	-0.122167
6	2.253676	0.021433	-1.059935
6	1.500146	-1.164571	0.916890
6	3.478230	-0.634863	-0.982054
1	2.058276	0.740574	-1.845012
6	2.731853	-1.799130	1.000958
1	0.751587	-1.325934	1.682523
6	3.719062	-1.544233	0.045754
1	4.246592	-0.428344	-1.717860
1	2.931217	-2.481855	1.818721
1	4.678354	-2.044832	0.113074
6	-0.039588	0.449787	-0.257009

B3LYP/6-311++G(d,p) = -765.3559665 Hartrees
Low frequencies = -558.8806 34.8862 60.7336 63.4409 88.9029
98.0776 145.9019 222.7011 238.2286 287.1840

Diphenyl ketone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-0.021521	0.583800	-0.407538
8	-0.036512	1.941873	-1.194367
6	-0.002605	2.879300	0.718870
8	-0.036806	1.828327	1.316338
8	0.030202	4.018825	0.547359
6	-1.583133	-0.398697	-0.193976
6	-1.600312	-1.784663	0.036109
6	-2.811917	0.272233	-0.333083
6	-2.806171	-2.474812	0.141928
1	-0.670208	-2.335049	0.119403
6	-4.016029	-0.416054	-0.222780
1	-2.819501	1.335945	-0.545133
6	-4.013742	-1.790227	0.018180
1	-2.803306	-3.544946	0.316276
1	-4.954909	0.115176	-0.331514
1	-4.952141	-2.327433	0.100806
6	1.573841	-0.335809	-0.153848
6	2.626168	-0.069615	-1.046902
6	1.793329	-1.254834	0.886653
6	3.852273	-0.718414	-0.915785
1	2.480905	0.654302	-1.841707
6	3.023081	-1.893101	1.024948
1	1.010009	-1.462161	1.608061
6	4.050933	-1.630434	0.119143
1	4.652727	-0.507300	-1.615969
1	3.181421	-2.591985	1.838731
1	5.006947	-2.131189	0.225208

B3LYP/6-311++G(d,p) = -1016.8424596 Hartrees
Low frequencies = -335.7177 23.2993 37.8307 45.4778 62.0294 75.3124 106.5420 152.9451 176.8253 186.5619

Diphenyl ketone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	-0.000909	1.984798	-1.077031
6	0.048800	2.889821	0.761378
8	-0.001838	1.892800	1.444832
8	0.103227	4.031675	0.563612
6	-1.687596	-0.504370	-0.146563
6	-1.756844	-1.893246	0.032224
6	-2.874703	0.237635	-0.238327
6	-2.993788	-2.526718	0.135103
1	-0.852385	-2.488728	0.077328
6	-4.108355	-0.397992	-0.130555

1	-2.829380	1.308127	-0.405400
6	-4.167793	-1.778830	0.059351
1	-3.040984	-3.601326	0.270688
1	-5.022199	0.181091	-0.199695
1	-5.129527	-2.272959	0.140835
6	1.664392	-0.495653	-0.110200
6	2.764176	-0.042764	-0.853679
6	1.827450	-1.569690	0.776401
6	4.002816	-0.667085	-0.723366
1	2.647437	0.800921	-1.525500
6	3.070209	-2.184280	0.911159
1	0.997310	-1.918143	1.380645
6	4.155309	-1.736936	0.157469
1	4.848406	-0.314920	-1.303258
1	3.193155	-3.008238	1.605022
1	5.121059	-2.218671	0.262282
32	-0.012537	0.446229	-0.360520

B3LYP/6-311++G(d,p) = -2804.2929635 Hartrees
Low frequencies = -337.7021 20.6750 30.5972 39.9033 53.5967
68.6168 88.2162 141.3601 159.0976 168.2284

Products: Addition of Carbon dioxide

Formaldehye (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.581260	0.000001	-0.000049
8	-1.757631	-0.000001	-0.000083
8	0.343488	1.018488	0.000023
6	1.358317	0.000000	0.000067
8	0.343491	-1.018488	0.000023
1	1.951395	0.000002	0.913653
1	1.951479	0.000002	-0.913464

B3LYP/6-311++G(d,p) = -303.159721 Hartrees
Low frequencies = 267.5988 532.8376 761.2266 825.0727 871.8506
1033.4596 1080.4359 1091.6029 1105.9169 1147.4873

Formaldehye (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.887709	0.000001	-0.000018
8	-2.067043	0.000001	-0.000050
8	-0.026142	1.085633	0.000206
8	-0.026150	-1.085630	-0.000189
14	1.292859	-0.000001	0.000022
1	2.090435	-0.000229	1.235488

1	2.090469	0.000212	-1.235421

B3LYP/6-311++G(d,p) = -554.636638 Hartrees
Low frequencies = 185.5915 511.4502 553.4071 618.0281 657.1564
689.1205 790.2277 800.2684 892.8391 949.1278

Formaldehye (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.310433	0.000000	0.000015
8	2.495287	0.000000	0.000656
8	0.479987	-1.100077	-0.000805
8	0.479987	1.100077	-0.000806
1	-1.774389	0.000002	1.311503
1	-1.775373	-0.000002	-1.310511
32	-0.998591	0.000000	0.000205

B3LYP/6-311++G(d,p) = -2342.0939783 Hartrees
Low frequencies = 170.6399 443.6763 469.6260 488.0771 579.6388
609.4445 706.9200 790.5192 825.2931 863.9287

Acetone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.502125	-1.280389	0.000254
1	-0.834680	-2.142752	-0.000226
6	-1.501472	1.281037	0.000256
1	-0.833539	2.143015	-0.000199
1	-2.138059	-1.321823	-0.886672
1	-2.136460	1.323088	0.887839
1	-2.137105	-1.322080	0.887856
1	-2.137374	1.322854	-0.886682
6	1.254220	-0.000074	-0.000188
8	2.435053	0.000263	-0.000383
8	0.342142	-0.000533	1.019252
6	-0.706445	0.000108	0.000059
8	0.341824	-0.000529	-1.019394

B3LYP/6-311++G(d,p) = -381.8317874 Hartrees
Low frequencies = 140.1324 185.8499 227.3237 335.6322
340.2355 360.1015 504.7515 576.7587 664.4039 774.0347

Acetone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	0.688185	-0.000001	-0.000078

8	-0.650390	0.000018	1.083419
6	1.669632	1.570485	0.000175
1	2.312149	1.625855	0.883926
1	2.313531	1.625524	-0.882578
1	1.008445	2.439429	-0.000472
6	1.669670	-1.570463	0.000185
1	1.008501	-2.439420	-0.000333
1	2.313473	-1.625548	-0.882636
1	2.312287	-1.625760	0.883868
8	-0.650293	0.000002	-1.083562
6	-1.504734	-0.000091	-0.000058
8	-2.688116	0.000022	-0.000169

B3LYP/6-311++G(d,p) = -633.3321868 Hartrees
Low frequencies = 108.4340 109.2376 131.2816 188.5156 200.6683
217.2258 316.6948 504.5779 517.5972 680.6151

Acetone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.727480	-0.000138	-0.000100
8	2.916493	0.000026	-0.000114
8	0.903083	-0.000141	-1.098905
1	-0.841776	2.506897	-0.003662
6	-1.557412	1.685149	0.000289
32	-0.594150	0.000010	-0.000099
1	-2.185836	1.752659	0.890510
1	-2.192501	1.749722	-0.885389
8	0.903088	-0.000150	1.098699
6	-1.557853	-1.684874	0.000283
1	-2.186194	-1.752254	0.890572
1	-2.193054	-1.749207	-0.885330
1	-0.842455	-2.506829	-0.003794

B3LYP/6-311++G(d,p) = -2420.7811314 Hartrees
Low frequencies = 77.4955 91.0959 98.3069 157.8960 162.0131
164.9902 252.7697 430.7962 441.8438 586.1838

4-Dimethyl-3-pentanone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.000053	-0.137898	0.000023
8	-0.197612	0.914883	-1.000078
6	1.285736	-0.934094	-0.249267
6	-1.286339	-0.933275	0.249281
6	1.590545	-1.879604	0.925364
1	0.819622	-2.639596	1.067222

1	2.533608	-2.399671	0.742282
6	2.493537	-0.032116	-0.545907
1	3.357291	-0.654407	-0.791445
6	-1.591714	-1.878595	-0.925350
1	-0.821313	-2.639131	-1.067120
1	-2.535157	-2.397992	-0.742330
6	-2.493552	-0.030487	0.545837
1	-3.357753	-0.652201	0.791268
1	2.308979	0.630222	-1.392720
1	-2.308628	0.631702	1.392688
1	-1.695939	-1.317684	-1.858370
1	1.695244	-1.318741	1.858360
1	2.758174	0.576758	0.321795
1	-2.757686	0.578598	-0.321872
1	-1.093574	-1.535815	1.143169
1	1.092548	-1.536526	-1.143135
8	0.198032	0.914762	1.000135
6	0.000622	1.824075	-0.000003
8	0.001066	3.006160	-0.000013

B3LYP/6-311++G(d,p) = -539.1243472 Hartrees
Low frequencies = 60.5088 63.0274 112.0071 185.2485 188.4650
214.1943 223.8973 238.4665 259.6355 282.0943

4-Dimethyl-3-pentanone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-0.009425	-0.091587	0.116191
8	1.142925	-0.522545	-1.097151
6	-1.498653	-1.234277	0.142435
1	-1.051207	-2.223550	0.305309
6	-0.260323	1.757565	0.317580
1	-0.790524	1.874557	1.273666
6	-2.251873	-1.278513	-1.203969
1	-1.585441	-1.513056	-2.037721
1	-3.027301	-2.050342	-1.172106
1	-2.748639	-0.329617	-1.425003
6	-2.446650	-0.939552	1.322337
1	-3.245233	-1.687024	1.361183
1	-1.929883	-0.964952	2.286187
1	-2.924391	0.039942	1.222138
6	-1.151624	2.354735	-0.793411
1	-2.145238	1.900507	-0.824324
1	-1.288614	3.427585	-0.626549
1	-0.694982	2.234469	-1.780332
6	1.084765	2.504249	0.422614
1	0.908543	3.569955	0.599166
1	1.700683	2.125650	1.240945
1	1.661558	2.413501	-0.501861

6	2.008150	-0.937125	-0.106226
8	1.310993	-0.696299	1.056435
8	3.094814	-1.393393	-0.228725

B3LYP/6-311++G(d,p) = -790.6151688 Hartrees
Low frequencies = 31.6773 38.7259 81.9360 99.8143 113.9718
142.9947 203.3878 217.0237 230.0683 236.5551

4-Dimethyl-3-pentanone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	0.000048	-0.159672	0.000021
8	0.186504	1.349922	-1.082584
6	-1.706077	-1.108638	-0.291524
1	-1.547817	-1.682333	-1.212734
6	1.706430	-1.108177	0.291612
1	1.548820	-1.680528	1.213769
6	2.854557	-0.113087	0.509430
1	2.656415	0.562954	1.343563
1	3.779671	-0.656491	0.728312
1	3.027759	0.495097	-0.381964
6	1.986562	-2.091665	-0.858162
1	2.908402	-2.646712	-0.656697
1	1.186094	-2.825842	-0.987769
1	2.123689	-1.568235	-1.808942
6	-1.986953	-2.090497	0.859481
1	-2.908707	-2.645763	0.658229
1	-1.186626	-2.824562	0.990613
1	-2.124614	-1.565713	1.809434
6	-2.854114	-0.113924	-0.511503
1	-2.655442	0.561008	-1.346403
1	-3.779043	-0.657692	-0.730264
1	-3.027979	0.495452	0.378951
8	-0.000183	3.360954	0.000276
6	-0.000438	2.169973	0.000137
8	-0.186566	1.349743	1.082857

B3LYP/6-311++G(d,p) = -2578.0699199 Hartrees
Low frequencies = 31.2681 35.8488 72.7625 77.1881 84.9983
146.0287 202.5655 222.8005 227.5078 228.1675

Diphenyl ketone (C)

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.000059	0.622377	0.000020
8	0.020535	1.680082	-1.019505
8	-0.021620	1.680173	1.019367

6	-0.000048	2.589884	-0.000115
8	-0.001645	3.770560	-0.000189
6	-1.279699	-0.172985	-0.037601
6	-2.333913	0.107982	0.833893
6	-1.420519	-1.187244	-0.991339
6	-3.519828	-0.621080	0.750473
1	-2.224059	0.887699	1.576423
6	-2.610398	-1.902269	-1.079972
1	-0.601939	-1.414463	-1.664680
6	-3.662061	-1.622265	-0.206783
1	-4.331656	-0.402529	1.434741
1	-2.715635	-2.680665	-1.826994
1	-4.586478	-2.184894	-0.272263
6	1.279948	-0.172409	0.037706
6	1.421736	-1.185601	0.992435
6	2.333477	0.107975	-0.834792
6	2.611900	-1.900152	1.081021
1	0.603694	-1.412343	1.666595
6	3.519686	-0.620625	-0.751398
1	2.222880	0.886900	-1.578042
6	3.662882	-1.620751	0.206815
1	2.717898	-2.677704	1.828816
1	4.330989	-0.402525	-1.436432
1	4.587524	-2.183014	0.272271

B3LYP/6-311++G(d,p) = -765.3839939 Hartrees
Low frequencies = 3.0187 30.5963 66.1957 80.6716 117.0464
199.7682 222.0921 285.5814 307.5207 337.9281

Diphenyl ketone (Si)

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-0.000027	0.628591	0.000026
8	-0.125655	1.974414	1.074565
6	-0.000029	2.827371	0.000068
8	0.125593	1.974450	-1.074465
8	0.000000	4.012034	0.000090
6	1.570628	-0.347191	0.043354
6	2.727193	0.154706	-0.579495
6	1.650659	-1.574465	0.724195
6	3.925879	-0.551187	-0.522108
1	2.685428	1.096498	-1.115271
6	2.852272	-2.275505	0.786450
1	0.773525	-1.985905	1.212758
6	3.989324	-1.764491	0.161965
1	4.809092	-0.155156	-1.010248
1	2.901687	-3.218145	1.319616
1	4.924174	-2.311995	0.207856
6	-1.570639	-0.347249	-0.043345
6	-1.650445	-1.574794	-0.723724

6	-2.727393	0.154862	0.578982
6	-2.852023	-2.275890	-0.786040
1	-0.773158	-1.986403	-1.211867
6	-3.926046	-0.551077	0.521527
1	-2.685802	1.096857	1.114417
6	-3.989266	-1.764655	-0.162086
1	-2.901262	-3.218745	-1.318841
1	-4.809408	-0.154876	1.009258
1	-4.924089	-2.312199	-0.208027

B3LYP/6-311++G(d,p) = -1016.8867655 Hartrees
Low frequencies = 22.9685 41.3699 51.4048 63.0122 78.5887
122.0245 170.0559 206.1821 243.9949 262.5219

Diphenyl ketone (Ge)

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	0.000015	0.490664	0.000026
8	0.133682	1.995096	-1.088679
8	-0.000460	4.008194	-0.000032
6	-0.000275	2.817877	-0.000009
8	-0.133988	1.995097	1.088692
6	1.672255	-0.472037	0.048732
6	1.760430	-1.733850	0.652880
6	2.816507	0.108502	-0.516188
6	2.981428	-2.403647	0.696997
1	0.884283	-2.195525	1.095881
6	4.033120	-0.567973	-0.473006
1	2.754538	1.081472	-0.990336
6	4.115758	-1.821094	0.133456
1	3.046880	-3.376741	1.170186
1	4.915705	-0.116780	-0.911706
1	5.064956	-2.343974	0.166871
6	-1.672132	-0.472212	-0.048698
6	-2.816456	0.108245	0.516159
6	-1.760183	-1.734042	-0.652828
6	-4.033015	-0.568325	0.472929
1	-2.754585	1.081226	0.990297
6	-2.981127	-2.403936	-0.696994
1	-0.883980	-2.195657	-1.095782
6	-4.115528	-1.821461	-0.133518
1	-4.915656	-0.117193	0.911579
1	-3.046480	-3.377042	-1.170171
1	-5.064686	-2.344414	-0.166972

B3LYP/6-311++G(d,p) = -2804.3357985 Hartrees
Low frequencies = 25.4377 40.9297 45.0402 54.7054 63.8601
113.2400 163.8871 189.4618 229.6228 231.3122