Proton-Coupled Electron Transfer in the Reduction of Carbonyls using SmI_2–H_2O: Implications for the Reductive Coupling of Acyl-Type Ketyl Radicals with SmI_2–H_2O

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Electronic Supplementary Information

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Computational Details

Computational Methods. All calculations were performed using Gaussian 09 suite of programs [A1] according to the procedure described by Knowles et al. (Tarantino, K. T.; Liu, P.; Knowles, R. R. *J. Am. Chem. Soc.* **2013**, *135*, 10022). All of the geometry optimizations were performed at the CBS-QB3 level (Montgomery, J. A., Jr.; Frisch, M. J.; Ochterski, J. W.; Petersson, G. A. *J. Chem. Phys.* **1999**, *110*, 2822; Montgomery, J. A., Jr.; Frisch, M. J.; Ochterski, J. W.; Petersson, G. A. *J. Chem. Phys.* **2000**, *112*, 6532). All reported energies correspond to those calculated using the CBS-QB3 method. An excellent correlation between the CBS-QB3 and the B3LYP/6-311++G(d,p) level was found for BDFE determination. All of the optimized geometries were verified as minima (no imaginary frequencies). Calculation of the solution phase electrochemical redox potential was performed according to Nicewicz et al. (Roth, H. G.; Romero, N. A.; Nicewicz, D. A. *Synlett* **2016**, *27*, 714) at the B3LYP/6-311++G(d,p) level of theory. In general, an excellent agreement with the published data for available compounds has been found, all values are given vs. SCE: e.g., **15**, the published $-E_{1/2}$ of 1.98 V (Dahlén, A.; Nilsson, A.; Hilmersson, G. *J. Org. Chem.* **2006**, *71*, 1576) vs. $-E_{1/2}$ of 1.92 V at the B3LYP/6-311++G(d,p) level; **1**, the published $-E_{1/2}$ of 2.79 V (Bard, A. J. *Encyclopedia of Electrochemistry of the Elements*, Marcel Dekker, 1978) vs. $-E_{1/2}$ of 2.74 V at the B3LYP/6-311++G(d,p) level; **8**, the published $-E_{1/2}$ of 2.84 V (Vanysek, P. *CRC Handbook of Chemistry and Physics*, CRC Press, 2000) vs. $-E_{1/2}$ of 2.80 V at the B3LYP/6-311++G(d,p) level; **14**, the published $-E_{1/2}$ of 1.67 V (Vanysek, P. *CRC Handbook of Chemistry and Physics*, CRC Press, 2000) vs. $-E_{1/2}$ of 1.74 V at the B3LYP/6-311++G(d,p) level; **12**, the published $-E_{1/2}$ of 1.39 V (Hartmann, K. H.; Troll, T. *Tetrahedron* **1995**, *51*, 4655) vs. $-E_{1/2}$ of 1.30 V at the B3LYP/6-311++G(d,p) level. Calculation of solution phase electrochemical potentials was also performed at the CBS-QB3 level. An

excellent agreement with the B3LYP/6-311++G(d,p) level of theory was found for determination of electrochemical redox potentials for **1**-**15** ($Y = 0.994X + 0.134$, $R^2 = 0.994$). Note that the established accuracy in experimentally measured redox potentials due to solvent effects is ±0.1 V (Bard, A. J. *Encyclopedia of Electrochemistry of the Elements*, Marcel Dekker, 1978; Bard, A. J.; Faulkner, L. R. *Electrochemical Methods: Fundamentals and Applications*, Wiley, 2000). Studies on the determination of the redox potential of Sm(II) reductants have been published (Szostak, M.; Spain, M.; Procter, D. J. *J. Org. Chem.* **2014**, *79*, 2522, and references cited therein).

Table SI-1. *Bond Dissociation Free Energy (BDFE) for the O–H Bond in Ketyl for Compounds* ***1-15*** *Calculated at the B3LYP/6-311++G(d,p) Level.*[a]

Compound	No.	$\Delta G°_{(ketyl)}$ [au]	$\Delta G°_{(carbonyl)}$ [au]	$\Delta G°_{(hydrogen)}$ [au]	BDFE [kcal/mol]
Cyclohexanone	**1**	-310.403316	-309.861422	-0.512911	18.19
Glutarimide	**2**	-400.542796	-400.015352	-0.512911	9.12
Tetrahydro-2*H*-pyran-2-one	**3**	-346.341255	-345.809949	-0.512911	11.54
2-Piperidinone	**4**	-326.457629	-325.935941	-0.512911	5.51
Methyl acetate	**5**	-268.932367	-268.415681	-0.512911	2.37
Acetamide	**6**	-209.762238	-209.244020	-0.512911	3.33
N-Acetylacetamide	**7**	-362.437646	-361.907803	-0.512911	10.62
Acetone	**8**	-193.702898	-193.163763	-0.512911	16.46
Acetaldehyde	**9**	-154.396456	-153.852036	-0.512911	19.77
Methyl benzoate	**10**	-460.679780	-460.149905	-0.512911	10.64
Benzamide	**11**	-401.514165	-400.975793	-0.512911	15.98
Phthalimide	**12**	-513.702778	-513.154848	-0.512911	21.97
Acetophenone	**13**	-385.452897	-384.897514	-0.512911	26.65
Benzaldehyde	**14**	-346.149109	-345.590442	-0.512911	28.71
Anthracene	**15**	-540.070998	-539.502022	-0.512911	35.18

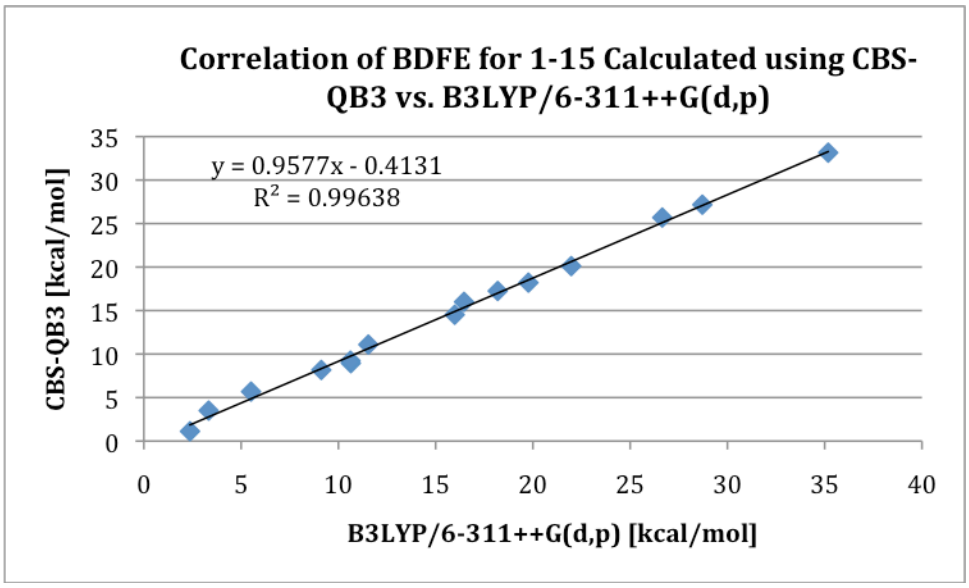
[a] $BDFE_{O–H} = –[G°(ketyl) – (G°(carbonyl) + G°(hydrogen))]$. See Tarantino, K. T.; Liu, P.; Knowles, R. R. *J. Am. Chem. Soc.* **2013**, *135*, 10022 for details.

Table SI-2. *Redox Potentials of Compounds **1-15** vs. SCE in CH_3CN Calculated at the B3LYP/6-311++G(d,p) Level.*[a]

Compound	No.	G° (neutral)	G° (ketyl radical)	$\Delta G°_{1/2}$ [kcal/mol]	$E°_{1/2}$ [V]
Cyclohexanone	**1**	-309.868758	-309.930463	-38.73	-2.74
Glutarimide	**2**	-400.028889	-400.093506	-40.56	-2.66
Tetrahydro-2*H*-pyran-2-one	**3**	-345.821935	-345.879419	-36.08	-2.86
2-Piperidinone	**4**	-325.947362	-325.989734	-26.60	-3.27
Methyl acetate	**5**	-268.422544	-268.472615	-31.43	-3.06
Acetamide	**6**	-209.254941	-209.293717	-24.34	-3.37
N-Acetylacetamide	**7**	-361.919047	-361.986873	-42.58	-2.58
Acetone	**8**	-193.169706	-193.229377	-37.46	-2.80
Acetaldehyde	**9**	-153.858517	-153.925210	-41.86	-2.61
Methyl benzoate	**10**	-460.156902	-460.241337	-53.00	-2.12
Benzamide	**11**	-400.987776	-401.067143	-49.82	-2.26
Phthalimide	**12**	-513.166510	-513.281161	-71.97	-1.30
Acetophenone	**13**	-384.905288	-384.996967	-57.55	-1.93
Benzaldehyde	**14**	-345.597605	-345.695653	-61.55	-1.75
Anthracene	**15**	-539.507274	-539.599087	-57.63	-1.92

[a] $\Delta G°_{1/2}$ = G°(ketyl radical) – G°(neutral). See Roth, H. G.; Romero, N. A.; Nicewicz, D. A. *Synlett* **2016**, *27*, 714 for details. The accuracy is approximately ± 0.1 V due to solvent effects.

Figure SI-1. *Correlation of BDFE for the O–H Bond in Ketyl for Compounds **1-15** Calculated at using CBS-QB3 vs. B3LYP/6-311++G(d,p).*



Appendix 1 - Full Reference for Gaussian 09

Gaussian 09, Revision D.01, 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, J. A., Jr.; 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, M. J.; 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.

Cyclohexanone

CBS-QB3 Energy: -309.306938 au

CBS-QB3 Free Energy: -309.343951 au

Geometry:

C	1.16070200	0.00000000	0.06755400
C	0.39314300	1.28528200	0.34732600
C	-1.01496600	1.26545800	-0.28208900
C	-1.79022000	0.00000000	0.10565300
C	-1.01496600	-1.26545800	-0.28208900
H	-1.56454500	2.16215500	0.01878600
H	0.99181900	2.12643100	-0.00624300
H	-2.77226100	0.00000000	-0.37712600
O	2.29723300	0.00000000	-0.34825100
H	-1.97373000	0.00000000	1.18790300
H	-0.91910100	1.31011900	-1.37349900
H	0.29537800	1.37894200	1.43752900
H	-1.56454500	-2.16215500	0.01878600
H	-0.91910100	-1.31011900	-1.37349900
H	0.99181900	-2.12643100	-0.00624300
H	0.29537800	-1.37894100	1.43752900
C	0.39314300	-1.28528200	0.34732600

Cyclohexanone radical

CBS-QB3 Energy: -309.843739 au

CBS-QB3 Free Energy: -309.881919 au

Geometry:

C	1.02990000	-0.02601300	-0.16525400

C	0.37281100	1.27605900	0.17460900
C	-1.10914800	1.28393200	-0.24055400
C	-1.83529900	0.02552000	0.25526600
C	-1.15066600	-1.25274900	-0.24834900
H	-1.59750000	2.18435500	0.14416500
H	0.90343400	2.11021900	-0.30469000
H	-2.88064600	0.04593100	-0.06898000
O	2.40020800	-0.11149700	-0.03396200
H	-1.84816000	0.02256700	1.35318300
H	-1.17317700	1.32792300	-1.33382700
H	0.44353800	1.45761800	1.26508400
H	-1.67155200	-2.13753000	0.12998200
H	-1.21704800	-1.28804600	-1.34199400
H	0.84572700	-2.13963700	-0.30881800
H	0.39226400	-1.48553700	1.25823700
C	0.32914900	-1.30105100	0.16877200
H	2.78096900	0.75992800	-0.18758000

Glutarimide

CBS-QB3 Energy: -399.354224 au

CBS-QB3 Free Energy: -399.392473 au

Geometry:

C	1.26083400	-0.45171800	0.02542400
C	1.25809300	1.05501800	0.20667600
C	-0.00000100	1.72240100	-0.35589100
C	-1.25809200	1.05501800	0.20667900
C	-1.26083400	-0.45171800	0.02542400

N	0.00000000	-1.04947800	-0.04337900
H	0.00000000	2.78800700	-0.11615900
H	2.17370700	1.43227500	-0.24995100
H	-2.17370800	1.43227500	-0.24994400
O	2.26440600	-1.12243400	-0.04346000
O	-2.26440600	-1.12243300	-0.04346100
H	-1.33902800	1.24627400	1.28416900
H	-0.00000200	1.64389100	-1.44797400
H	1.33903200	1.24627600	1.28416500
H	0.00000000	-2.05772900	-0.15516100

Glutarimide radical

CBS-QB3 Energy: -399.875944 au

CBS-QB3 Free Energy: -399.915958 au

Geometry:

C	1.20521800	-0.29381100	-0.23992900
C	1.14977400	1.15015600	0.15545100
C	-0.17545900	1.77047300	-0.30342400
C	-1.36117100	0.97657900	0.25859700
C	-1.26383900	-0.52496500	0.02283400
N	0.01612000	-1.01883700	-0.13357000
H	-0.23571300	2.81391300	0.01480100
H	2.00161900	1.68849200	-0.27356000
H	-2.31208500	1.30079700	-0.16671800
O	2.27859300	-1.06531300	0.17140400
O	-2.23400900	-1.25896500	-0.01479700
H	-1.43554200	1.12393900	1.34276100

H	-0.21506900	1.76664700	-1.39754000
H	1.24343500	1.23471100	1.25225800
H	0.07223800	-2.01741500	-0.29252600
H	3.08446800	-0.65559000	-0.15851500

Tetrahydro-*2H*-pyran-2-one

CBS-QB3 Energy: -345.231281 au

CBS-QB3 Free Energy: -345.267955 au

Geometry:

C	-1.14060600	-0.01519200	-0.01260500
C	-0.35028500	1.28462400	-0.11397700
C	1.12495700	1.19917600	0.28821000
C	1.73483100	-0.06412700	-0.31760500
C	0.96496400	-1.27717900	0.17641300
H	1.65698200	2.09601900	-0.03907100
H	-0.90002100	2.03228800	0.45940500
H	2.78627800	-0.17729200	-0.03689000
O	-2.34008200	-0.03642400	0.01891700
H	1.69279700	-0.01573300	-1.41156500
H	1.21459900	1.15848800	1.37986600
H	-0.43057300	1.58512400	-1.16586000
H	1.27242400	-2.19238400	-0.33006000
H	1.12053000	-1.41466300	1.25249800
O	-0.46194100	-1.19303300	-0.04778400

Tetrahydro-*2H*-pyran-2-one radical

CBS-QB3 Energy: -345.758543 au

CBS-QB3 Free Energy: -345.796100 au

Geometry:

C	-0.99828000	0.05032800	0.23576300
C	-0.26639200	1.30550900	-0.13916400
C	1.21985200	1.18672900	0.23373700
C	1.78943400	-0.14439000	-0.27537000
C	0.93066400	-1.30997300	0.20830300
H	1.78203500	2.02922600	-0.17759400
H	-0.73622800	2.15937000	0.35405800
H	2.81886400	-0.28809700	0.06855300
O	-2.33882900	0.08109800	-0.02559900
H	1.80697700	-0.14705400	-1.37098100
H	1.32343500	1.23134400	1.32375800
H	-0.36827800	1.46444100	-1.22670800
H	1.24611800	-2.25745600	-0.22963100
H	0.97838600	-1.39377000	1.30187500
O	-0.44051200	-1.14442200	-0.18632400
H	-2.66825700	-0.82063100	0.07244200

2-Piperidinone

CBS-QB3 Energy: -325.369377 au

CBS-QB3 Free Energy: -325.406189 au

Geometry:

C	-1.14982200	-0.01126200	-0.01923300
C	-0.37408100	1.29860400	-0.12265200
C	1.09425400	1.21291400	0.30902900
C	1.75402700	-0.01825900	-0.31634600

C	1.03925800	-1.28595000	0.14552800
N	-0.40865200	-1.16372100	-0.02227700
H	1.62445200	2.12578800	0.02371300
H	-0.93231000	2.03991500	0.45163600
H	2.81042600	-0.08431400	-0.04159700
O	-2.36809200	-0.03558600	0.00995200
H	1.70535600	0.05282900	-1.40887000
H	1.15742200	1.14201000	1.40151800
H	-0.44014000	1.60783500	-1.17262400
H	-0.96965000	-1.99912600	0.07514400
H	1.38307400	-2.15030000	-0.43001700
H	1.28485500	-1.48018500	1.19946700

2-Piperidinone radical

CBS-QB3 Energy: -325.886859 au

CBS-QB3 Free Energy: -325.925890 au

Geometry:

C	1.02248000	0.01635500	-0.23571900
C	0.31405100	1.29343000	0.10354300
C	-1.18135900	1.22307000	-0.24424700
C	-1.80635900	-0.05999700	0.31838400
C	-1.04998500	-1.29183800	-0.18291800
N	0.37346600	-1.16896900	0.14498100
H	-1.70166400	2.10518400	0.13942800
H	0.80385300	2.12248300	-0.41344200
H	-2.85897500	-0.13790000	0.03004200
O	2.38891300	-0.02209900	-0.05095900

H	-1.76751400	-0.03981600	1.41355300
H	-1.29571300	1.23192900	-1.33426300
H	0.42440000	1.49127900	1.18884900
H	0.92160900	-1.98360200	-0.10494400
H	-1.43267700	-2.19833200	0.29280200
H	-1.20398000	-1.39370500	-1.26916100
H	2.59212400	0.07593900	0.89567900

Methyl acetate

CBS-QB3 Energy: -267.970811 au

CBS-QB3 Free Energy: -268.007073 au

Geometry:

O	0.29004600	1.37123700	-0.00000200
C	0.46227600	0.17907100	0.00000700
O	-0.54859700	-0.71935800	0.00000200
C	-1.87493900	-0.16151500	-0.00000200
H	-2.54991900	-1.01454000	-0.00000200
H	-2.03246100	0.45297900	0.88779700
H	-2.03245700	0.45297700	-0.88780400
C	1.79915500	-0.51905900	-0.00000100
H	1.88479200	-1.16010400	0.88019000
H	1.88477500	-1.16012100	-0.88018100
H	2.59471700	0.22280000	-0.00001600

Methyl acetate radical

CBS-QB3 Energy: -268.482123 au

CBS-QB3 Free Energy: -268.519333 au

Geometry:

O	0.35114400	1.36509700	-0.13587300
C	0.44040500	0.03139700	0.25290000
O	-0.62300900	-0.69449900	-0.18503800
C	-1.91567200	-0.14133100	0.07300300
H	-2.63422800	-0.88817000	-0.26196500
H	-2.04777200	0.04430800	1.14438400
H	-2.06385000	0.79001000	-0.47665500
C	1.74658900	-0.66263600	0.00962900
H	1.71075800	-1.67753500	0.40729400
H	1.96496000	-0.71915800	-1.06782100
H	2.56908800	-0.13073200	0.49485800
H	1.04803800	1.85191300	0.31400500

Acetamide

CBS-QB3 Energy: -208.884432 au

CBS-QB3 Free Energy: -208.915439 au

Geometry:

C	0.07725800	0.14793500	-0.00000200
O	0.35310100	1.33168200	0.00000100
N	1.03581800	-0.82647100	-0.00000100
H	0.81641500	-1.80681300	0.00000600
H	2.00239300	-0.54155900	0.00000600
C	-1.36122500	-0.34752000	0.00000000
H	-1.86576600	0.05637600	-0.87975600
H	-1.86575000	0.05633300	0.87978600
H	-1.45902200	-1.43499400	-0.00002500

Acetamide radical

CBS-QB3 Energy: -209.398077 au

CBS-QB3 Free Energy: -209.431496 au

Geometry:

C	0.03647400	0.01620400	-0.26731500
O	0.48764400	1.27935700	0.13137300
N	0.97853000	-0.99031100	-0.05937000
H	0.84820800	-1.53684600	0.79316300
H	1.92479900	-0.63320300	-0.09955100
C	-1.38950600	-0.32232700	0.02936700
H	-2.06984200	0.45887600	-0.32120800
H	-1.56008600	-0.43842700	1.11536400
H	-1.66837500	-1.25763200	-0.45924600
H	-0.10737700	1.94129700	-0.23622700

N-Acetylacetamide

CBS-QB3 Energy: -361.306191 au

CBS-QB3 Free Energy: -361.347445 au

Geometry:

C	1.19334000	0.15587700	-0.00001000
O	1.16886700	1.36590800	-0.00000300
N	0.04695400	-0.63824400	-0.00000700
H	0.16805400	-1.64321800	-0.00000600
C	2.48107300	-0.64858300	0.00000400
H	3.32213300	0.04102200	-0.00003600
H	2.53692100	-1.29010500	-0.88403700
H	2.53694300	-1.29002400	0.88410300

C	-1.31681600	-0.27987800	0.00000000
O	-2.13617500	-1.17129700	0.00000700
C	-1.67279000	1.18316900	0.00000300
H	-2.75872000	1.25714400	0.00001400
H	-1.25220400	1.68624800	-0.87208700
H	-1.25218600	1.68625000	0.87208300

N-Acetylacetamide radical

CBS-QB3 Energy: -361.829345au

CBS-QB3 Free Energy: -361.872641 au

Geometry:

C	1.25517500	0.13116700	-0.04488000
O	1.30027800	1.33423700	-0.24124300
N	0.08103200	-0.58590800	0.01823400
H	0.14653900	-1.59118300	0.09123700
C	2.51385900	-0.69773600	0.14838500
H	3.12016800	-0.62754200	-0.75798000
H	2.32552000	-1.75038900	0.36956100
H	3.09579300	-0.26231700	0.96299400
C	-1.21817800	-0.12058500	-0.22024700
O	-2.09050700	-1.18219300	-0.04681500
C	-1.65709600	1.23233100	0.23708100
H	-2.61335500	1.49526600	-0.22641900
H	-0.91374500	1.97903300	-0.03280400
H	-1.79446100	1.25703800	1.33101300
H	-2.97440800	-0.88596500	-0.28282100

Acetone

CBS-QB3 Energy: -192.814097 au

CBS-QB3 Free Energy: -192.847077 au

Geometry:

C	0.00000000	0.00000000	0.18625200
O	0.00000000	0.00000000	1.39537600
C	0.00000000	1.29149000	-0.61333300
H	-0.92991100	1.37695400	-1.18530400
H	0.08894200	2.14128600	0.06193200
H	0.82086900	1.30192000	-1.33688800
C	0.00000000	-1.29149000	-0.61333300
H	-0.82086900	-1.30192000	-1.33688800
H	0.92991100	-1.37695400	-1.18530400
H	-0.08894200	-2.14128600	0.06193200

Acetone radical

CBS-QB3 Energy: -193.348953 au

CBS-QB3 Free Energy: -193.383046 au

Geometry:

C	0.00883800	0.02697700	-0.22671600
O	-0.04198300	1.37937800	0.05942300
C	1.36055100	-0.54660400	0.02575600
H	1.45028200	-1.54302500	-0.41302200
H	2.13496900	0.09412300	-0.40375800
H	1.57540600	-0.63712900	1.10488600
C	-1.23218900	-0.76463200	0.03304800
H	-1.14434500	-1.77558300	-0.37112000

H	-1.44775400	-0.85688000	1.11292100
H	-2.11146400	-0.30070400	-0.43084500
H	-0.94442600	1.68972800	-0.06697400

Acetaldehyde

CBS-QB3 Energy: -153.578557 au

CBS-QB3 Free Energy: -153.607405 au

Geometry:

C	0.23559800	0.39726700	-0.00000600
O	1.23303900	-0.27660100	-0.00000800
C	-1.16866000	-0.14776700	0.00000900
H	-1.70789300	0.22225600	-0.87888000
H	-1.15523800	-1.23752500	0.00000200
H	-1.70787200	0.22224600	0.87891500
H	0.30506900	1.50883300	0.00001100

Acetaldehyde radical

CBS-QB3 Energy: -154.116458 au

CBS-QB3 Free Energy: -154.146890 au

Geometry:

C	-0.09177400	0.50735800	-0.10102900
O	-1.16819800	-0.34132300	0.02227800
C	1.22780500	-0.16340000	0.01118900
H	1.41321500	-0.56118400	1.02248300
H	1.29164500	-1.00948700	-0.68084900
H	2.03366600	0.53541400	-0.22472100
H	-0.23047100	1.52685500	0.25408000

H	-1.97865600	0.17523500	-0.01017700

Methyl benzoate

CBS-QB3 Energy: -459.359019 au

CBS-QB3 Free Energy: -459.402403 au

Geometry:

C	1.23359400	0.39528600	-0.00002000
O	1.72483400	1.49987500	0.00000400
C	-0.23176100	0.12129400	-0.00001000
C	-0.75108800	-1.17783100	-0.00001400
C	-1.10076000	1.21727600	0.00000500
C	-2.12841400	-1.37446700	-0.00000500
H	-0.07377300	-2.02130900	-0.00002500
C	-2.47606000	1.01643200	0.00001400
H	-0.67778700	2.21411700	0.00000800
C	-2.99144900	-0.27956500	0.00000900
H	-2.52915600	-2.38169800	-0.00000900
H	-3.14675800	1.86803200	0.00002500
H	-4.06447200	-0.43591300	0.00001600
O	1.96992400	-0.73760200	-0.00000400
C	3.39530300	-0.55032700	0.00001100
H	3.70859900	0.00072400	0.88805000
H	3.82048900	-1.55158200	-0.00005900
H	3.70860300	0.00085500	-0.88794400

Methyl benzoate radical

CBS-QB3 Energy: -459.881469 au

CBS-QB3 Free Energy: -459.927141 au

Geometry:

C	1.17034700	0.30014800	-0.10268700
O	1.78151300	1.51514100	-0.01281100
C	-0.21909300	0.10758200	-0.06352000
C	-0.77770400	-1.20599800	-0.03252400
C	-1.12607200	1.21041300	-0.04540700
C	-2.14398700	-1.38708100	0.04510400
H	-0.10933000	-2.05634400	-0.06479100
C	-2.49151900	1.00241700	0.03687200
H	-0.75562800	2.22658800	-0.13841800
C	-3.01971700	-0.29189400	0.08917800
H	-2.54371400	-2.39527300	0.07232600
H	-3.15849900	1.85796000	0.04608900
H	-4.09016500	-0.44575700	0.15112600
O	2.00586400	-0.72543500	-0.33662100
C	3.31377300	-0.66913600	0.25387600
H	3.24357200	-0.57952900	1.34232500
H	3.79045200	-1.61137600	-0.00921400
H	3.89025600	0.16580900	-0.14573200
H	1.19787400	2.12158300	0.45640100

Benzamide

CBS-QB3 Energy: -400.270800 au

CBS-QB3 Free Energy: -400.310682 au

Geometry:

C	1.71928800	-0.13828900	-0.03472400

O	2.28194500	-1.18994600	-0.28291800
C	0.21958800	-0.02278400	-0.01216600
C	-0.45940300	1.19378400	-0.14372400
C	-0.51582600	-1.20519300	0.11540000
C	-1.85141800	1.22740700	-0.12746500
H	0.09117500	2.11538000	-0.29580600
C	-1.90523600	-1.17014500	0.14035800
H	0.02631900	-2.13958000	0.19018100
C	-2.57602400	0.04680800	0.02139400
H	-2.36944800	2.17305000	-0.24013400
H	-2.46675000	-2.09121400	0.24812800
H	-3.65982300	0.07414700	0.03596000
N	2.41854700	1.01634900	0.21921000
H	1.98979400	1.77303100	0.72576700
H	3.41753400	0.91078400	0.31033900

Benzamide radical

CBS-QB3 Energy: -400.802840 au

CBS-QB3 Free Energy: -400.844300 au

Geometry:

C	1.61266300	-0.01058800	-0.00598300
O	2.35212900	-1.15584000	-0.13028100
C	0.20772000	-0.00028600	-0.00202400
C	-0.52504900	1.22291800	-0.09959700
C	-0.54822200	-1.20826400	0.10481700
C	-1.90677800	1.22195400	-0.09712800
H	0.01375300	2.15526100	-0.22025400

C	-1.93063300	-1.18350200	0.10098700
H	-0.03806200	-2.15652500	0.23975000
C	-2.63044700	0.02543800	0.00036600
H	-2.43697200	2.16463600	-0.18423400
H	-2.47738800	-2.11620100	0.19200500
H	-3.71356500	0.03560300	0.00013600
N	2.39886100	1.12420500	0.10094700
H	2.13655800	1.76734000	0.83734000
H	3.38818800	0.91982200	0.09937500
H	1.84290700	-1.79866500	-0.63711900

Phtalimide

CBS-QB3 Energy: -512.292781 au

CBS-QB3 Free Energy: -512.333558 au

Geometry:

C	-1.24242100	-1.17294800	-0.00010700
C	-1.24242100	1.17294800	-0.00010500
N	-2.00982500	0.00000000	0.00003400
O	-1.66984800	-2.30024900	0.00005600
O	-1.66984800	2.30024900	0.00005600
H	-3.01922900	0.00000000	0.00018200
C	0.17550800	0.69709700	-0.00005000
C	1.35631700	1.42059600	-0.00000200
C	2.55382800	0.69913000	0.00003600
C	2.55382800	-0.69913000	0.00003600
C	1.35631700	-1.42059600	-0.00000200
H	1.34467900	2.50388700	0.00000000

H	3.49871600	1.23018500	0.00007000
H	3.49871600	-1.23018400	0.00007000
H	1.34468000	-2.50388700	-0.00000100
C	0.17550800	-0.69709700	-0.00005000

Phtalimide radical

CBS-QB3 Energy: -512.833476 au

CBS-QB3 Free Energy: -512.876076 au

Geometry:

C	-1.23409800	-1.00927600	-0.00000100
C	-1.12823100	1.29479700	0.00000100
N	-1.96369100	0.14398000	-0.00000200
O	-1.88726600	-2.18536200	-0.00000100
O	-1.53734600	2.44299300	0.00000200
H	-2.97107300	0.19032700	0.00000300
C	0.22497500	0.73480100	-0.00000100
C	1.46063700	1.37323700	0.00000100
C	2.61270500	0.59604500	0.00000300
C	2.53243800	-0.81507000	0.00000100
C	1.31560200	-1.47059900	-0.00000200
H	1.50968100	2.45611700	0.00000200
H	3.58615100	1.07175000	0.00000500
H	3.44837300	-1.39513800	0.00000100
H	1.28287000	-2.55564200	-0.00000600
C	0.13823400	-0.69245400	-0.00000300
H	-1.24682600	-2.90520500	0.00001300

Acetophenone

CBS-QB3 Energy: -384.202640 au

CBS-QB3 Free Energy: -384.243270 au

Geometry:

C	-1.69815100	-0.20467300	-0.00000100
O	-2.20915600	-1.30709400	0.00000300
C	-2.56027700	1.04522400	0.00000200
H	-2.35898100	1.66021900	-0.88194800
H	-3.60613200	0.74339500	0.00000100
H	-2.35898100	1.66021300	0.88195600
C	-0.20404900	-0.05389600	-0.00000100
C	0.43292700	1.19327900	-0.00000100
C	0.57729200	-1.21710200	-0.00000100
C	1.82302000	1.27482400	-0.00000100
H	-0.14999200	2.10637000	0.00000000
C	1.96330100	-1.13581200	-0.00000100
H	0.06877200	-2.17322300	-0.00000100
C	2.58938100	0.11162300	-0.00000100
H	2.30723900	2.24472800	-0.00000100
H	2.55886000	-2.04173000	-0.00000100
H	3.67180100	0.17598100	-0.00000100

Acetophenone radical

CBS-QB3 Energy: -384.751308 au

CBS-QB3 Free Energy: -384.794687 au

Geometry:

C	1.59565700	-0.04784500	-0.01487400

O	2.16385000	-1.29714000	0.02935400
C	2.54051800	1.10596800	-0.00684700
H	3.06130800	1.19620400	0.95742700
H	3.31140800	0.98153700	-0.78018000
H	2.04058200	2.05284500	-0.20150600
C	0.18258000	0.00035500	-0.00655100
C	-0.54066300	1.22697900	0.00489800
C	-0.58105600	-1.20379800	-0.00875900
C	-1.92464300	1.23992800	0.00729500
H	-0.00953100	2.17070900	0.01838000
C	-1.96377600	-1.17025200	-0.00600800
H	-0.05888100	-2.15097100	-0.01493000
C	-2.65424300	0.04669200	0.00110300
H	-2.44616500	2.19116500	0.01644900
H	-2.51723700	-2.10343000	-0.00917300
H	-3.73765600	0.06521300	0.00350800
H	3.11912600	-1.21431900	-0.04635100

Benzaldehyde

CBS-QB3 Energy: -344.968450 au

CBS-QB3 Free Energy: -345.005358 au

Geometry:

C	1.99246200	0.46543700	-0.00001000
O	2.84277900	-0.39428200	0.00001200
C	0.53290000	0.21258700	-0.00000500
C	-0.35953200	1.28883000	-0.00000100
C	0.04300300	-1.09959700	-0.00000600

C	-1.73234700	1.05946800	0.00000300
H	0.02625700	2.30377800	-0.00000100
C	-1.32594500	-1.32765300	-0.00000200
H	0.75432800	-1.91705700	-0.00000900
C	-2.21385900	-0.24841800	0.00000200
H	-2.42441800	1.89362700	0.00000600
H	-1.70785400	-2.34217900	-0.00000200
H	-3.28296100	-0.42953200	0.00000500
H	2.27232900	1.54170300	0.00001700

Benzaldehyde radical

CBS-QB3 Energy: -345.519892 au

CBS-QB3 Free Energy: -345.559121 au

Geometry:

C	1.87369300	0.58128200	-0.00012000
O	2.89549100	-0.31022000	0.00017800
C	0.50581600	0.25855700	-0.00009700
C	-0.46222000	1.30521800	-0.00002600
C	0.01738400	-1.07960800	-0.00014900
C	-1.81458700	1.02640200	0.00007600
H	-0.12002100	2.33480900	-0.00001200
C	-1.34238900	-1.34145400	-0.00003900
H	0.70475300	-1.92108800	-0.00039000
C	-2.27312000	-0.29841500	0.00010600
H	-2.52803900	1.84330500	0.00015600
H	-1.68607600	-2.37022200	-0.00009500
H	-3.33515700	-0.51176600	0.00021400

H	2.22578100	1.60362900	-0.00043700
H	2.54737000	-1.20879100	0.00062900

Anthracene

CBS-QB3 Energy: -538.497883 au

CBS-QB3 Free Energy: -538.542296 au

Geometry:

C	-3.65429500	0.71220000	0.00000200
C	-2.47628300	1.40483400	-0.00000200
C	-1.22168000	0.72140500	-0.00000200
C	-1.22168000	-0.72140500	-0.00000200
C	-2.47628300	-1.40483400	0.00000000
C	-3.65429500	-0.71219900	0.00000400
C	0.00000000	1.40166600	-0.00000100
C	0.00000000	-1.40166600	-0.00000200
C	1.22168000	-0.72140500	-0.00000200
C	1.22168000	0.72140500	-0.00000100
C	2.47628300	1.40483400	0.00000100
H	2.47548900	2.48986200	0.00000200
C	3.65429500	0.71220000	0.00000400
C	3.65429500	-0.71219900	0.00000100
C	2.47628300	-1.40483400	-0.00000200
H	0.00000000	2.48750500	-0.00000300
H	-4.59894100	1.24425700	0.00000500
H	-2.47548800	2.48986200	-0.00000500
H	-2.47548900	-2.48986200	0.00000000
H	-4.59894100	-1.24425700	0.00000900

H	0.00000000	-2.48750500	-0.00000400
H	4.59894100	1.24425700	0.00000700
H	4.59894100	-1.24425700	0.00000300
H	2.47548900	-2.48986200	-0.00000400

Anthracene radical

CBS-QB3 Energy: -539.057824 au

CBS-QB3 Free Energy: -539.105603 au

Geometry:

C	-3.71001900	-0.64462100	-0.05715000
C	-2.51262000	-1.35779200	-0.02447100
C	-1.28276500	-0.70768800	0.02225000
C	-1.24772000	0.71254100	0.02971000
C	-2.47383500	1.42096700	-0.00052600
C	-3.68458900	0.75413600	-0.04237700
C	0.00000000	-1.50750700	0.09047000
C	0.00000000	1.39559500	0.05368200
C	1.24772000	0.71254100	0.02971000
C	1.28276500	-0.70768800	0.02225000
C	2.51262000	-1.35779200	-0.02447100
H	2.53735800	-2.44363000	-0.03323000
C	3.71001900	-0.64462100	-0.05715000
C	3.68458900	0.75413600	-0.04237700
C	2.47383500	1.42096700	-0.00052600
H	0.00000000	-2.25962900	-0.70862200
H	-4.65549600	-1.17340600	-0.09348900
H	-2.53735800	-2.44363000	-0.03323000

H	-2.44861000	2.50574900	0.00630500
H	-4.61238200	1.31476400	-0.06611400
H	0.00000000	2.48043700	0.06219600
H	4.65549600	-1.17340600	-0.09348900
H	4.61238200	1.31476400	-0.06611400
H	2.44861000	2.50574900	0.00630500
H	0.00000000	-2.08681800	1.02532400