Supporting Information

For

Synthesis of Unsymmetric HetAr–X–HetAr' Compounds by Rhodium-catalyzed Heteroaryl Exchange Reactions

Mieko Arisawa*, Saori Tanii, Takeru Tazawa, and Masahiko Yamaguchi*

Department of Organic Chemistry, Graduate School of Pharmaceutical Sciences, Tohoku University, Sendai, 980-8578, Japan

Contents

	Structure of compounds for computational studies
Page S2-S3	1. Method
Page S3	References
Page S4-S6	2. Structure of compounds
Page S6-S19	3. Cartesian coordinates for compounds and total free energies at 298.15 K of compounds including vibrational frequencies

Computational Studies

1. Method: Energy-optimization of all compounds were implemented using MacroModel version 9.3 program[1] in the MMFFs[2] force field. Then, the energies of all compounds for DFT calculations were implemented by Jaguar 9.0.[3]

The optimization protocol was carried out as follows: Energy minimization was conducted using Polak-Ribiere Conjugate Gradient (PRCG) method until a final gradient below 0.05 kJ/Å·mol was reached. Then, conformational searching was carried out using the Monte Carlo multiple minimum (MCMM) method, followed by energy minimization with PRCG method. To the lowest energy-minimum conformer was minimized again using the PRCG method until a final gradient below 0.05 kJ/Å.

Parameters used in the conformational search are as follows: Solvent (None), maximum number of steps (10,000), maximum number of iterations (500), gradient (0.005), energy window for saving structure (21.0 kJ/mol), and maximum distance between atoms in equal (0.5 Å). Parameters used in the multiple-minimization are as follows: Solvent (None), maximum number of iterations (10,000), and maximum distance between atoms in equal (0.5 Å). The other settings were used as default.

Then, the energies of all compounds for DFT calculations were implemented by Jaguar 9.0,[3)] which used B3LYP_6-31G** for optimization and B3LYP_6-311G** for calculation of single point energy at 298.15 K. The property is vibrational frequencies, solvation is none, and the other settings were used as default.

Total Free Energies (at 298.15 K) of compounds including vibrational frequencies

Diphenyl ether, E = -538.496873 a.u.

Diphenyl sulfide, E = -861.479903 a.u.

S-Phenyl thiobenzate, E = -974.841529 a.u.

Phenyl benzoate, E = -651.873551 a.u.

S-Pheny methansulfonic acid, E = -1218.386188 a.u.

Methansulfonic acid phenyl ester, E = -895.404972 a.u.

Thioanisole, E = -669.748303 a.u.

Anisole, E = -346.760172 a.u.

N-(Phenylthio)succinimide, E = -989.932671 a.u.

N-(Phenoxy)succinimide, E = -666.905728 a.u.

1,2-Diphenylethanone, E = -615.917356 a.u.

Diphenylmethane, E = -502.566358 a.u.

Benzyl phenyl ether, E = -577.792982 a.u.

Benzophenone, E = -576.620318 a.u.

Toluene, E = -271.538254 a.u.

Phenol, E = -307.476246 a.u.

N-(Benzyl)succinimide, E = -631.029188 a.u.

Benzyl cholide, E = -731.169926 a.u.

Phenyl hypochloride, E = -767.034653 a.u.

Hydrogen fluoride, E = -100.476901 a.u.

Benzoyl fluoride, E = -444.880072 a.u.

Fluorobenzene, E = -331.508593 a.u.

Hexafluorobenzene, E = -827.819294 a.u.

1,2,3,4,5-pentafluoro-6-phenoxybenzene, E = -1034.817000 a.u.

2-Fluorobenzothiazole, E = -821.996240 a.u.

Di(2-benzothiazolyl) ether, E = -1519.474007 a.u.

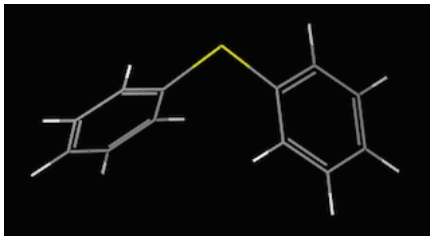
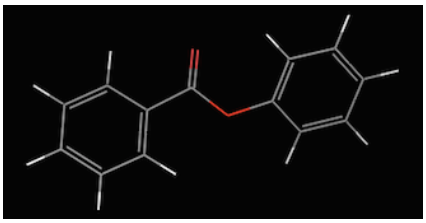
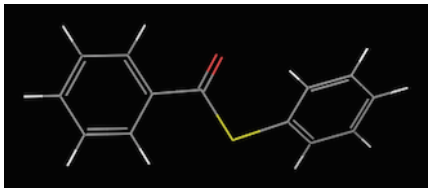
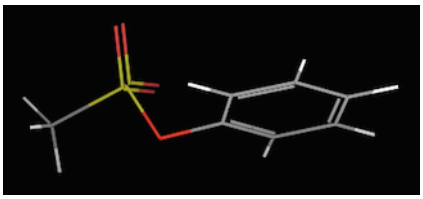
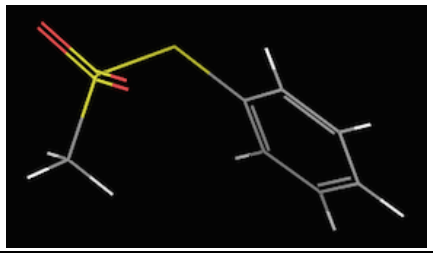
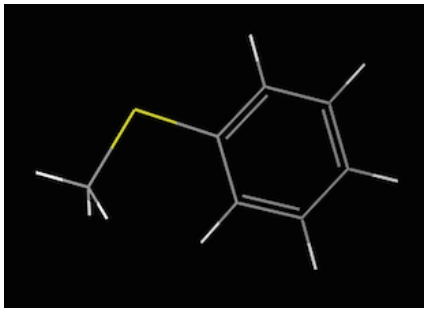
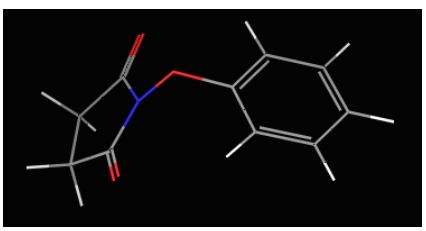
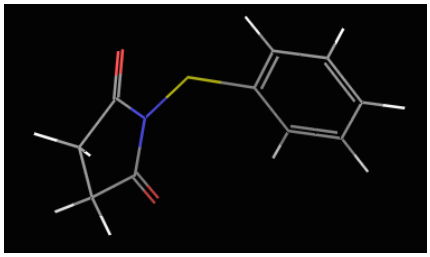
[2,3'(2H')-bibenzothiazol]-2'-one, E = -1519.509650 a.u.

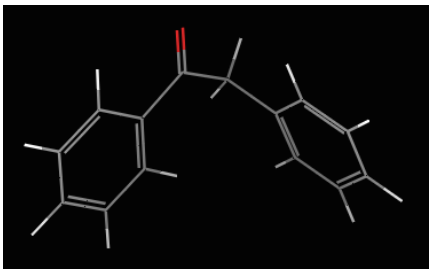
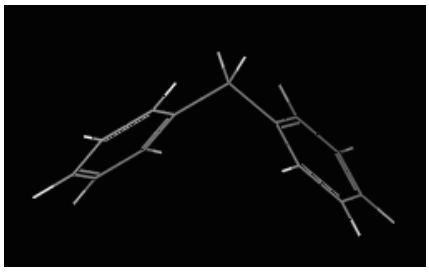
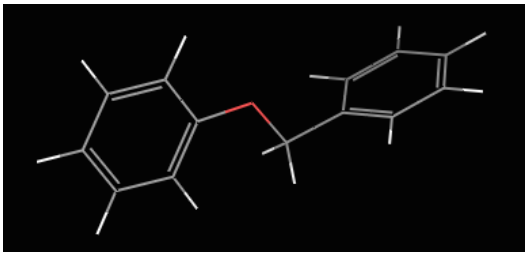
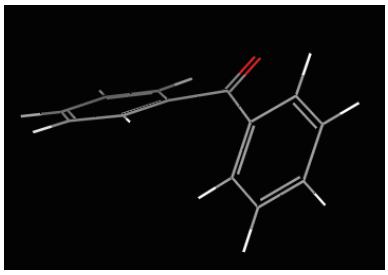
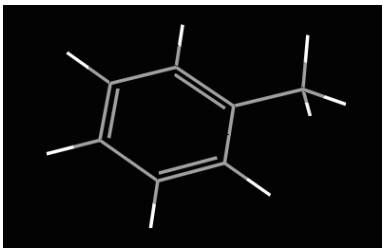
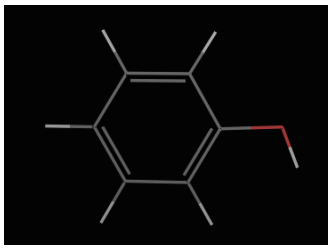
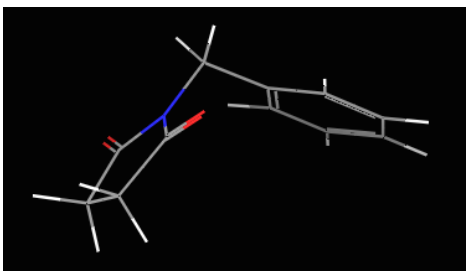
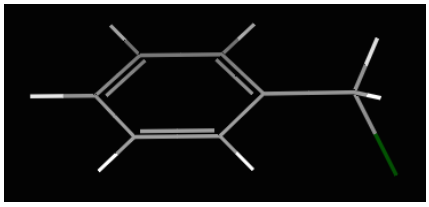
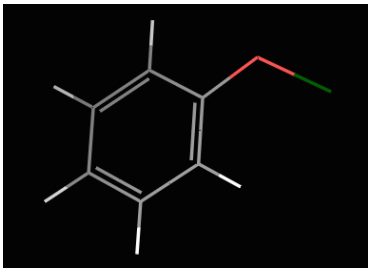
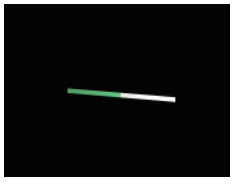
References

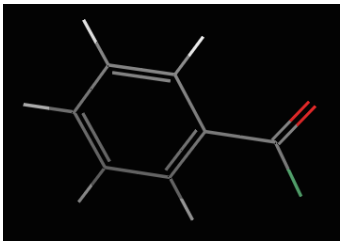
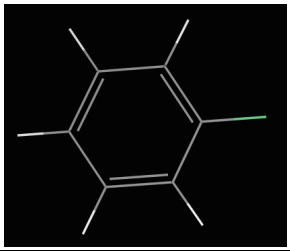
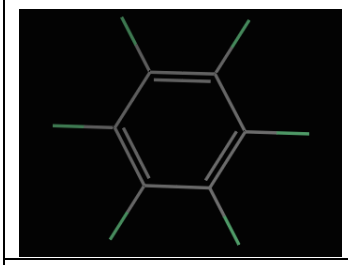
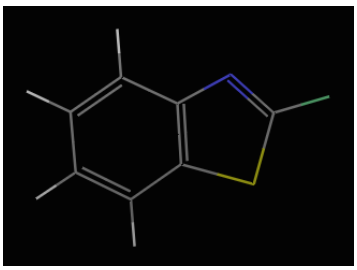
1. F. Mahamadi, N. G. J. Richards, W. C. Guida, R. Liskamp, M. Lipton, C. Caufield, G. Chang, T. Hendrickson, and W. C. Still, *J. Comput. Chem.* 1990, **11**, 440.
2. a) T. A. Halgren, *J. Comput. Chem.* 1996, **17**, 490; b) T. A. Halgren, *J. Comput. Chem.* 1996, **17**, 520; c) T. A. Halgren, *J. Comput. Chem.* 1996, **17**, 553; d) T. A. Halgren, R. B. Nachbar, *J. Comput. Chem.* 1996, **17**, 587; e) T. A. Halgren, *J. Comput. Chem.* 1996, **17**, 616.
3. A. D. Bochevarov, E. Harder, T. F. Hughes, J. R. Greenwood, D. A. Braden, D. M. Philipp, D. Rinaldo, M. D. Halls, J. Zhang, and R. A. Friesner, *Int. J. Quant. Chem.* 2013, **113**, 2110.

2. Structure of compounds

Figure S1. Structure of compounds

Diphenyl ether 	**Diphenyl sulfide** 
Phenyl benzoate 	***S*-Phenyl thiobenzate** 
Methansulfonic acid phenyl ester 	***S*-Pheny methansulfonic acid** 
Anisole 	**Thioanisole** 
***N*-(Phenoxy)succinimide** 	***N*-(Phenylthio)succinimide** 

1,2-Diphenylethanone 	**Diphenylmethane** 
Benzyl phenyl ether 	**Benzophenone** 
Toluene 	**Phenol** 
***N*-(Benzyl)succinimide** 	**Benzyl chloride** 
Phenol hypochlorite 	**Hydrogen fluoride** 

Benzoyl fluoride 	**Fluorobenzene** 
Hexafluorobenzene 	**1,2,3,4,5-Pentafluoro-6-phenoxybenzene** 
2-Fluorobenzothiazole 	**Di(2-benzothiazolyl) ether** 
[2,3'(2H')-bibenzothiazol]-2'-one 	

3. Cartesian coordinates for compounds and total free energies at 298.15 K of compounds including vibrational frequencies

Diphenyl ether

Total Free Energy = -538.496873 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
O	-0.23440	2.81940	2.18380
C	-3.94670	1.62140	0.71780
C	-3.10240	0.67150	1.29470
C	-1.84650	1.03630	1.77770
C	-1.43450	2.36740	1.66900

C	-2.27030	3.32680	1.09650
C	-3.52680	2.94920	0.62580
H	-4.92370	1.32910	0.34520
H	-3.42370	-0.36280	1.37820
H	-1.19200	0.30170	2.23410
H	-1.92320	4.35260	1.03170
H	-4.17660	3.69650	0.17960
C	3.31610	0.65170	1.93550
C	2.42490	0.62580	0.86180
C	1.22010	1.32500	0.92050
C	0.90690	2.04780	2.07500
C	1.79080	2.08350	3.15410
C	2.99550	1.38670	3.07780
H	4.25270	0.10540	1.88090
H	2.66920	0.06320	-0.03480
H	0.52980	1.31340	0.08410
H	1.52070	2.65810	4.03390
H	3.68270	1.41440	3.91850

Diphenyl sulfide

Total Free Energy = -861.479903 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
S	-1.96870	3.44650	1.55180
C	1.84640	1.88920	3.57730
C	1.82180	2.16460	2.21080
C	0.64420	2.60050	1.60170
C	-0.51300	2.78530	2.36670
C	-0.48470	2.52290	3.74310
C	0.68860	2.06570	4.33850
H	2.76030	1.53920	4.04780
H	2.71570	2.02540	1.60970
H	0.61820	2.79230	0.53350
H	-1.37820	2.67300	4.33990
H	0.70120	1.85700	5.40450
C	-5.48130	0.92070	3.08930
C	-5.58050	2.30860	3.00380
C	-4.49150	3.06680	2.57130
C	-3.30060	2.43290	2.19890
C	-3.20550	1.03660	2.27060
C	-4.28940	0.28940	2.72570
H	-6.32560	0.33290	3.43690
H	-6.50140	2.80880	3.28940
H	-4.56010	4.14930	2.52710
H	-2.28610	0.54220	1.97510
H	-4.20600	-0.79200	2.78590

***S*-Phenyl thiobenzoate**

Total Free Energy = -974.841529 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z

C	-3.49150	-0.84670	2.77060
O	-3.58910	-2.05310	2.81050
C	-2.83920	1.18170	-0.94980
C	-2.88730	-0.21260	-0.88610
C	-3.10360	-0.84560	0.33320
C	-3.27150	-0.08880	1.50270
C	-3.22610	1.31010	1.43250
C	-3.00960	1.94030	0.20940
H	-2.67070	1.67670	-1.90190
H	-2.75660	-0.80440	-1.78720
H	-3.14470	-1.92680	0.40730
H	-3.36310	1.91100	2.32560
H	-2.97600	3.02440	0.16060
S	-3.56860	0.17920	4.28340
C	-4.32450	-2.93110	7.55860
C	-5.26040	-1.92800	7.30760
C	-5.03790	-1.00140	6.28840
C	-3.86610	-1.07130	5.52830
C	-2.92200	-2.07220	5.78420
C	-3.15890	-3.00310	6.79350
H	-4.50190	-3.65550	8.34820
H	-6.17010	-1.86930	7.89790
H	-5.76960	-0.22760	6.07980
H	-2.01430	-2.12190	5.19390
H	-2.42850	-3.78360	6.98530

Phenyl benzoate

Total Free Energy = -651.873551 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	-0.05310	1.26820	2.65300
O	-0.06560	2.42130	3.02260
C	-3.61140	-0.90520	1.69480
C	-2.37600	-1.54690	1.58720
C	-1.20260	-0.86140	1.89230
C	-1.26450	0.47530	2.30850
C	-2.50610	1.11610	2.41550
C	-3.67540	0.42710	2.10920
H	-4.52420	-1.44340	1.45600
H	-2.32740	-2.58270	1.26510
H	-0.24050	-1.35340	1.81140
H	-2.52980	2.15090	2.73990
H	-4.63590	0.92650	2.19320
O	1.08770	0.52640	2.49530
C	4.92720	1.96220	3.25820
C	3.91750	2.19390	4.19370
C	2.61580	1.75110	3.96130
C	2.34050	1.07580	2.77260
C	3.33570	0.83440	1.82950
C	4.63330	1.27990	2.07750
H	5.93750	2.31070	3.44970
H	4.14100	2.72330	5.11520

H	1.82810	1.93350	4.68080
H	3.08370	0.30130	0.91880
H	5.41270	1.09370	1.34470

_S_-Phenyl methansulfonic acid

Total Free Energy = -1218.386188 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
S	-0.38450	1.91580	2.51020
O	-0.61700	2.85900	1.41230
O	-1.14270	1.98910	3.76470
C	-0.57330	0.23480	1.87370
H	0.00420	0.14360	0.95450
H	-0.23060	-0.46590	2.63550
H	-1.63980	0.09940	1.68120
S	1.72900	2.09810	2.92440
C	2.27790	-0.42380	6.70510
C	2.82330	-0.84680	5.49200
C	2.62710	-0.09090	4.33710
C	1.89710	1.10420	4.40260
C	1.35920	1.53620	5.62290
C	1.54330	0.76220	6.76710
H	2.42670	-1.01700	7.60240
H	3.39670	-1.76750	5.44200
H	3.04190	-0.41530	3.38810
H	0.79190	2.45860	5.66310
H	1.11820	1.09080	7.71060

Methansulfonic acid phenyl ester

Total Free Energy = -895.404972 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
S	-0.65360	1.20410	2.79370
O	-2.10670	1.33680	2.82850
O	0.18530	2.36040	2.49110
C	-0.18390	-0.17590	1.75020
H	0.88930	-0.33700	1.84850
H	-0.74850	-1.05480	2.05960
H	-0.43960	0.10910	0.72870
O	-0.13540	0.51050	4.22090
C	-0.92110	2.55870	7.77220
C	0.17960	2.91840	6.99280
C	0.44140	2.25420	5.79460
C	-0.41640	1.23180	5.39650
C	-1.52310	0.86270	6.15530
C	-1.76950	1.53240	7.35340
H	-1.11860	3.07860	8.70480
H	0.83770	3.71930	7.31580
H	1.28650	2.51880	5.16970
H	-2.17150	0.06820	5.80330
H	-2.62790	1.25360	7.95690

Thioanisole

Total Free Energy = -669.748303 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	-0.11220	1.88930	1.34410
C	-0.66260	3.04160	1.92930
C	-1.96900	2.99330	2.43010
C	-2.70760	1.81050	2.34530
C	-2.15960	0.66870	1.76570
C	-0.85590	0.71620	1.26560
H	0.90070	1.91550	0.95180
H	-2.42160	3.86620	2.88600
H	-3.72030	1.78930	2.73830
H	-2.73850	-0.24770	1.70340
H	-0.41390	-0.16620	0.81160
S	0.38430	4.48730	1.97550
C	-0.65740	5.74500	2.78210
H	-0.04500	6.64760	2.82880
H	-1.55550	5.95680	2.19730
H	-0.92960	5.45000	3.79810

Anisole

Total Free Energy = -346.760172 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	0.62170	1.64740	2.41880
C	-0.30740	2.66340	2.66860
C	-1.67160	2.43500	2.43870
C	-2.09830	1.20120	1.96340
C	-1.17770	0.17900	1.71050
C	0.17510	0.41170	1.94080
H	1.68010	1.80400	2.59010
H	-2.37210	3.23890	2.64020
H	-3.15760	1.03510	1.78860
H	-1.51420	-0.78400	1.33920
H	0.90230	-0.37260	1.74900
O	0.01030	3.90790	3.13540
C	1.37500	4.19970	3.38740
H	1.40160	5.22920	3.74760
H	1.79660	3.53810	4.15520
H	1.98200	4.12070	2.47620

***N*-(Phenylthio)succinicmide**

Total Free Energy = -989.932671 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	2.20070	2.04040	1.76790
O	2.98990	2.84830	1.34030
C	1.02770	0.74570	3.35880

O	0.70170	0.32460	4.44280
N	2.09060	1.64170	3.11720
C	1.14350	1.27320	0.97810
C	0.38180	0.43030	2.01210
S	3.14400	2.22360	4.36760
C	0.95160	5.96930	5.82790
C	1.88300	6.06770	4.79240
C	2.54240	4.92730	4.33390
C	2.26120	3.68540	4.91710
C	1.32760	3.58390	5.95610
C	0.67310	4.72980	6.40730
H	0.44180	6.85990	6.18410
H	2.09680	7.03220	4.34140
H	3.26070	4.98490	3.52310
H	1.11500	2.61180	6.38810
H	-0.05280	4.65480	7.21160
H	1.64880	0.67520	0.21440
H	0.51250	1.99540	0.45270
H	-0.68300	0.67090	2.07400
H	0.45650	-0.64670	1.83700

***N*-(Phenoxy)succinicmide**

Total Free Energy = -666.905728 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	0.82970	-0.33960	2.84030
C	-0.38370	-0.34450	1.88700
C	-0.52320	1.08880	1.38320
C	1.34460	1.09650	2.85140
H	0.57500	-0.62390	3.86490
H	1.63900	-0.99930	2.51600
H	-1.31750	-0.63110	2.37840
H	-0.25720	-1.00750	1.02680
O	2.27200	1.56060	3.47250
O	-1.34800	1.54580	0.62680
N	0.52770	1.80410	1.96480
O	0.60740	3.18170	1.85620
C	3.04260	4.55740	-1.24270
C	1.68800	4.31380	-1.47810
C	0.87300	3.82870	-0.45470
C	1.44300	3.59600	0.79280
C	2.78900	3.83260	1.05280
C	3.59080	4.31740	0.01890
H	3.67180	4.93470	-2.04350
H	1.26340	4.50150	-2.45980
H	-0.18090	3.62000	-0.60150
H	3.18040	3.62680	2.04300
H	4.64440	4.50800	0.20010

1,2-Diphenylethanone

Total Free Energy = -615.917356 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	-2.45970	-0.01910	2.31030
C	-3.25040	0.64140	1.35920
C	-3.62290	-0.03960	0.18920
C	-3.21050	-1.34920	-0.02760
C	-2.42180	-1.99910	0.92560
C	-2.04960	-1.33370	2.09380
H	-2.17640	0.47950	3.23040
H	-4.23820	0.48570	-0.53340
H	-3.50260	-1.86730	-0.93640
H	-2.10020	-3.02330	0.75840
H	-1.44200	-1.83980	2.83800
C	-3.72980	2.05060	1.52680
O	-4.46110	2.56320	0.69080
C	-3.33300	2.84960	2.77070
C	-5.76790	1.80660	6.19870
C	-4.37780	1.81270	6.30570
C	-3.59240	2.14650	5.20160
C	-4.18280	2.48040	3.97780
C	-5.58100	2.47510	3.88140
C	-6.36650	2.14060	4.98290
H	-6.38100	1.54260	7.05560
H	-3.90190	1.55660	7.24810
H	-2.50870	2.15210	5.29420
H	-6.05080	2.73240	2.93620
H	-7.44890	2.13850	4.89060
H	-2.27270	2.71000	3.00270
H	-3.48320	3.90160	2.50930

Diphenylmethne

Total Free Energy = -502.566358 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	-2.25850	1.92750	0.51980
C	-1.77920	2.38370	1.75590
C	-1.71220	1.47810	2.81930
C	-2.11420	0.15020	2.65760
C	-2.59100	-0.29020	1.42480
C	-2.66260	0.60510	0.35500
H	-2.30400	2.61510	-0.32090
H	-1.34210	1.81430	3.78500
H	-2.05180	-0.53810	3.49590
H	-2.90250	-1.32270	1.29510
H	-3.03110	0.26980	-0.61060
C	-1.33630	3.82830	1.92590
H	-1.03180	3.98450	2.96810
H	-2.18950	4.49610	1.75450
C	1.90270	4.96950	-0.71870
C	0.68720	5.64860	-0.76870
C	-0.35570	5.28190	0.08510
C	-0.20180	4.23440	0.99870

C	1.02540	3.55740	1.03750
C	2.06850	3.92140	0.18970
H	2.71500	5.25090	-1.38280
H	0.54620	6.46380	-1.47300
H	-1.30100	5.81750	0.04050
H	1.15690	2.73170	1.73200
H	3.01220	3.38470	0.23410

Benzyl phenyl ether

Total Free Energy = -577.792982 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	-4.41900	1.88160	1.76930
C	-3.46470	1.59970	0.78610
C	-3.87460	0.98380	-0.40100
C	-5.21470	0.65660	-0.60410
C	-6.15950	0.94250	0.38200
C	-5.75980	1.55580	1.57000
H	-4.10720	2.35540	2.69670
H	-3.13800	0.75680	-1.16760
H	-5.52120	0.17860	-1.53000
H	-7.20390	0.68820	0.22530
H	-6.49180	1.77940	2.34060
C	-2.01160	1.91940	1.02000
O	-1.41040	0.79130	1.66440
C	2.61410	0.78280	2.73500
C	2.08820	1.90820	2.10770
C	0.74330	1.95890	1.72870
C	-0.08400	0.85970	1.98570
C	0.44050	-0.27740	2.61740
C	1.77900	-0.31060	2.98700
H	3.65970	0.75400	3.02530
H	2.72430	2.76550	1.90510
H	0.35840	2.84680	1.24170
H	-0.22230	-1.11590	2.80500
H	2.17460	-1.19660	3.47580
H	-1.90790	2.80900	1.65630
H	-1.50030	2.12110	0.06890

Benzophenone

Total Free Energy = -576.620318 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	-2.46180	1.06910	0.68730
C	-3.09610	2.18960	1.24380
C	-4.00290	2.00720	2.29950
C	-4.29420	0.73060	2.76710
C	-3.66300	-0.38110	2.20260
C	-2.74060	-0.20900	1.17070
H	-1.73160	1.19740	-0.10470

H	-4.46480	2.88480	2.73950
H	-5.00810	0.59880	3.57490
H	-3.88540	-1.37820	2.57190
H	-2.23490	-1.06980	0.74320
C	-2.79030	3.59790	0.82500
O	-2.90740	4.51140	1.63490
C	-1.53880	4.64440	-3.15430
C	-2.33620	3.51470	-2.97020
C	-2.73170	3.13840	-1.68670
C	-2.34200	3.89970	-0.57490
C	-1.56170	5.04910	-0.77380
C	-1.15230	5.41200	-2.05210
H	-1.22470	4.93110	-4.15380
H	-2.65400	2.92690	-3.82630
H	-3.36520	2.26790	-1.55230
H	-1.29160	5.64440	0.09210
H	-0.53690	6.29570	-2.19330

Toluene

Total Free Energy = -271.538254 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	-0.00940	0.23170	1.20200
C	-0.06280	0.94890	0.00000
C	-0.00940	0.23170	-1.20200
C	0.08910	-1.15960	-1.20470
C	0.13780	-1.86140	0.00000
C	0.08910	-1.15960	1.20470
H	-0.04350	0.77030	2.14620
H	-0.04350	0.77030	-2.14620
H	0.13020	-1.69570	-2.14890
H	0.21570	-2.94480	0.00000
H	0.13020	-1.69570	2.14890
C	-0.20450	2.45310	0.00000
H	0.25840	2.89900	-0.88550
H	-1.26050	2.75180	0.00000
H	0.25840	2.89900	0.88550

Phenol

Total Free Energy = -307.476246 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	-1.16280	0.40740	0.00000
C	-0.45490	-0.79860	0.00000
C	0.94340	-0.79060	0.00000
C	1.62330	0.42420	0.00000
C	0.92550	1.63430	0.00000
C	-0.46890	1.61730	0.00000
H	-2.25120	0.39810	0.00000
H	1.47380	-1.73700	0.00000
H	2.70950	0.42430	0.00000

H	1.46220	2.57790	0.00000
H	-1.02570	2.55000	0.00000
O	-1.07580	-2.01800	0.00000
H	-2.03200	-1.88220	0.00000

***N*-(Benzyl)succinimide**

Total Free Energy = -631.029188 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	-3.05030	-0.70860	0.86820
C	-3.55890	-1.79820	1.76400
C	-2.94770	-3.06860	1.20510
C	-2.13470	-2.61160	0.03090
H	-3.23370	-1.61570	2.79230
H	-4.65180	-1.82850	1.72780
H	-2.29930	-3.55750	1.93800
H	-3.71670	-3.77200	0.87280
O	-1.46480	-3.35560	-0.67000
O	-3.30850	0.47670	1.01610
N	-2.26540	-1.26160	-0.09850
C	-1.63330	-0.49490	-1.15000
C	-4.21650	-0.22230	-4.59610
C	-4.28600	0.74460	-3.59470
C	-3.44710	0.66070	-2.48260
C	-2.52430	-0.38880	-2.36590
C	-2.47200	-1.36280	-3.37360
C	-3.31210	-1.27670	-4.48470
H	-4.87110	-0.15670	-5.46130
H	-4.99660	1.56300	-3.67720
H	-3.52130	1.41680	-1.70220
H	-1.77890	-2.19920	-3.29440
H	-3.26270	-2.03540	-5.26160
H	-1.39690	0.50900	-0.77760
H	-0.68500	-0.97020	-1.42820

Benzyl chloride

Total Free Energy = -731.169926 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	0.00440	0.10730	1.85720
C	-0.80550	1.24900	1.81710
C	-2.19640	1.09780	1.87760
C	-2.76720	-0.17040	1.96810
C	-1.95220	-1.30270	2.00190
C	-0.56490	-1.16150	1.94770
H	1.08530	0.21570	1.81890
H	-2.83250	1.97890	1.85500
H	-3.84730	-0.27540	2.01090
H	-2.39660	-2.29140	2.07050
H	0.07330	-2.03990	1.97460
C	-0.19280	2.61240	1.71080

H	-0.85380	3.32050	1.21120
H	0.76860	2.59020	1.19790
Cl	0.15710	3.35980	3.35410

Phenol hypochlorite

Total Free Energy = -767.034653 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	0.44150	-0.57620	1.86220
C	-0.34930	0.57460	1.86610
C	-1.73910	0.47050	1.93110
C	-2.34240	-0.78740	1.95790
C	-1.55470	-1.93860	1.93370
C	-0.16400	-1.83360	1.88920
H	1.52530	-0.50470	1.84760
H	-2.35280	1.36690	1.95520
H	-3.42540	-0.87020	2.00010
H	-2.02470	-2.91880	1.95560
H	0.44870	-2.73150	1.88110
O	0.18630	1.83650	1.87750
Cl	1.31770	2.13050	0.65980

Hydrogen fluoride

Total Free Energy = -100.476901 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
H	0.00000	0.00000	0.87870
F	0.00000	0.00000	-0.04660

Benzoyl fluoride

Total Free Energy = -444.880072 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	-0.84000	0.97270	0.00000
C	-0.00770	-0.15100	0.00000
C	1.38310	-0.00170	0.00000
C	1.94100	1.27720	0.00000
C	1.11190	2.40000	0.00000
C	-0.27590	2.24930	0.00000
H	-1.92220	0.86420	0.00000
H	2.03180	-0.87550	0.00000
H	3.02170	1.39880	0.00000
H	1.54920	3.39600	0.00000
H	-0.91670	3.12810	0.00000
C	-0.60410	-1.50050	0.00000
O	0.03690	-2.53840	0.00000
F	-1.94130	-1.59620	0.00000

Fluorobenzene

Total Free Energy = -331.508593 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	0.00000	1.21060	-0.18620
C	0.00000	0.00000	-0.87070
C	0.00000	-1.21060	-0.18620
C	0.00000	-1.21090	1.20840
C	0.00000	0.00000	1.90470
C	0.00000	1.21090	1.20840
H	0.00000	2.14230	-0.74230
H	0.00000	-2.14230	-0.74230
H	0.00000	-2.15190	1.75250
H	0.00000	0.00000	2.99230
H	0.00000	2.15190	1.75250
F	0.00000	0.00000	-2.21030

Hexafluorobenzene

Total Free Energy = -827.819294 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	-1.38970	0.00000	0.00000
C	-0.69490	-1.20350	0.00000
C	0.69490	-1.20350	0.00000
C	1.38970	0.00000	0.00000
C	0.69490	1.20350	0.00000
C	-0.69490	1.20350	0.00000
F	-1.36490	-2.36400	0.00000
F	-2.72970	0.00000	0.00000
F	-1.36490	2.36400	0.00000
F	1.36490	2.36400	0.00000
F	2.72970	0.00000	0.00000
F	1.36490	-2.36400	0.00000

1,2,3,4,5-Pentafluoro-6-phenoxybenzene

Total Free Energy = -1034.817000 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	-1.47850	1.12860	2.02310
C	-0.49880	0.22110	2.43410
C	-0.77880	-1.14760	2.35420
C	-1.99990	-1.60050	1.86370
C	-2.96910	-0.68300	1.46290
C	-2.70950	0.68240	1.54560
O	0.66070	0.68610	2.98560
C	4.37080	0.13970	1.15770
C	4.26420	0.50510	2.50140

C	3.01420	0.67010	3.09210
C	1.86790	0.46810	2.32510
C	1.95300	0.11140	0.98080
C	3.21390	-0.05440	0.40520
H	5.34720	0.00850	0.70200
H	5.15890	0.65940	3.09700
H	2.90830	0.94990	4.13470
H	1.05570	-0.03100	0.38870
H	3.28460	-0.33410	-0.64180
F	0.14300	-2.03460	2.74330
F	-2.25000	-2.91180	1.78680
F	-4.14550	-1.11410	0.99840
F	-3.63750	1.56250	1.15590
F	-1.23880	2.44110	2.08580

2-Fluorobenzothiazole

Total Free Energy = -821.996240 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	-0.23780	2.12080	0.00000
C	1.02160	2.72860	0.00000
C	2.18370	1.96350	0.00000
C	2.11270	0.56650	0.00000
H	3.15570	2.45170	0.00000
H	3.01770	-0.03330	0.00000
C	-0.64880	-1.67210	0.00000
C	0.85590	-0.07240	0.00000
C	-0.29770	0.71720	0.00000
H	1.09200	3.81460	0.00000
H	-1.14350	2.71990	0.00000
S	-1.67810	-0.31390	0.00000
F	-1.12460	-2.89770	0.00000
N	0.64080	-1.43970	0.00000

Di(2-benzothiazolyl) ether

Total Free Energy = -1519.474007 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	5.07890	8.81000	-0.28790
C	4.63920	9.01400	-1.59960
C	3.64610	8.21160	-2.15250
C	3.06800	7.18230	-1.40220
H	3.31450	8.38280	-3.17400
H	2.29240	6.55360	-1.82860
C	3.60040	6.07470	1.94300
C	3.49160	6.95670	-0.07680
C	4.48990	7.77450	0.45680
H	5.85460	9.43660	0.14180
H	5.08060	9.81120	-2.19440
S	4.81430	7.27530	2.07210

O	3.36830	5.24140	2.95630
C	2.12670	4.80160	3.15670
N	3.01180	5.97530	0.77210
C	0.15990	3.52120	3.77400
C	-0.07400	4.82010	3.31780
C	-1.40420	5.27870	3.23230
C	-2.45690	4.43400	3.59930
C	-2.19990	3.14330	4.05080
C	-0.88940	2.66460	4.14700
H	-1.59920	6.28650	2.87890
H	-3.48150	4.79190	3.52970
H	-0.69050	1.65740	4.50030
N	1.05720	5.54800	2.99420
S	1.85690	3.23200	3.78540
H	-3.02820	2.49660	4.33320

[2,3'(2H')-bibenzothiazol]-2'-one

Total Free Energy = -1519.509650 a.u.

Atom	Coodinates (Angstroms)		
	X	Y	Z
C	1.85130	4.17890	3.19560
C	1.25150	5.34720	3.67580
C	0.00030	5.74710	3.21660
C	-0.68110	4.98360	2.26280
H	-0.45290	6.65840	3.59990
H	-1.65710	5.29250	1.90240
C	0.14440	1.93280	0.56730
C	-0.09550	3.80230	1.76480
C	1.15610	3.42210	2.23840
C	0.75230	-0.16430	-0.57380
C	-1.39510	-0.26350	-1.92580
C	-1.33220	0.85350	-1.08740
C	-2.40600	1.74190	-1.09080
C	-3.50900	1.50040	-1.92200
C	-3.54680	0.37620	-2.75060
C	-2.48050	-0.51790	-2.75570
H	-2.43470	2.63040	-0.47090
H	-4.34450	2.19780	-1.92020
H	-4.40860	0.20110	-3.39020
H	-2.50090	-1.39450	-3.39640
O	1.84850	-0.42000	-0.10330
H	1.77150	5.94980	4.41790
H	2.82780	3.86670	3.55380
N	-0.64930	2.95200	0.82490
S	1.61220	1.96310	1.46420
N	-0.12110	0.89890	-0.33250
S	0.04830	-1.26410	-1.78240