

Influence of Lewis Acid Strength on Hydride Transfer to Unsaturated Substrates

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1) Plots of Hydride Acceptor Ability versus ΔG_{H^-} of Lewis Acid-Substrate Adducts

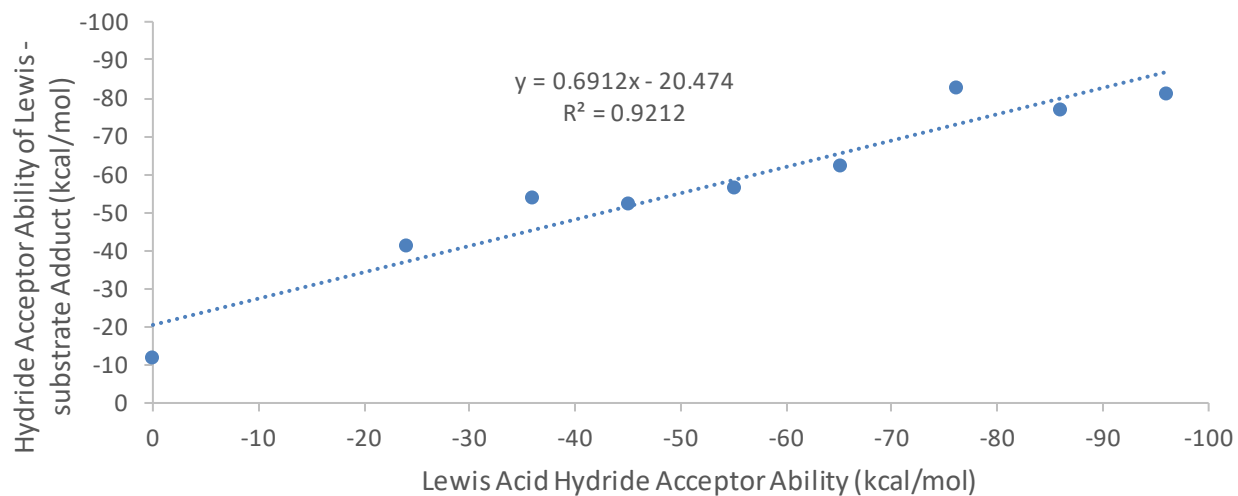


Figure S1. Plot showing the effect of Lewis acid strength on the resulting ΔG_{H^-} of the acetone-Lewis acid adduct.

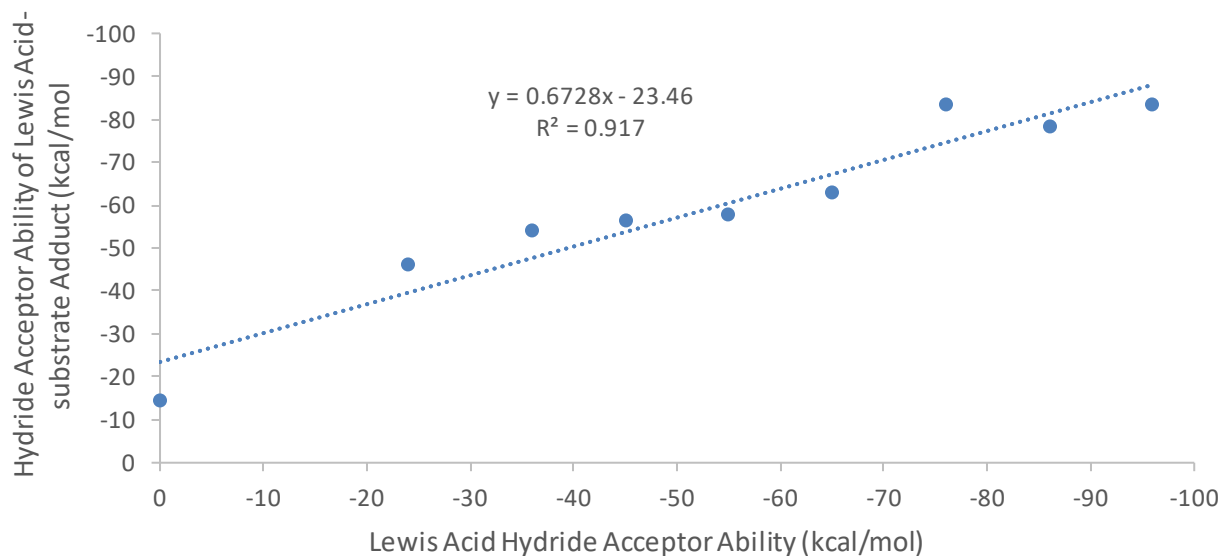


Figure S2. Plot showing the effect of Lewis acid strength on the resulting ΔG_{H^-} of the cyclohexanone-Lewis acid adduct.

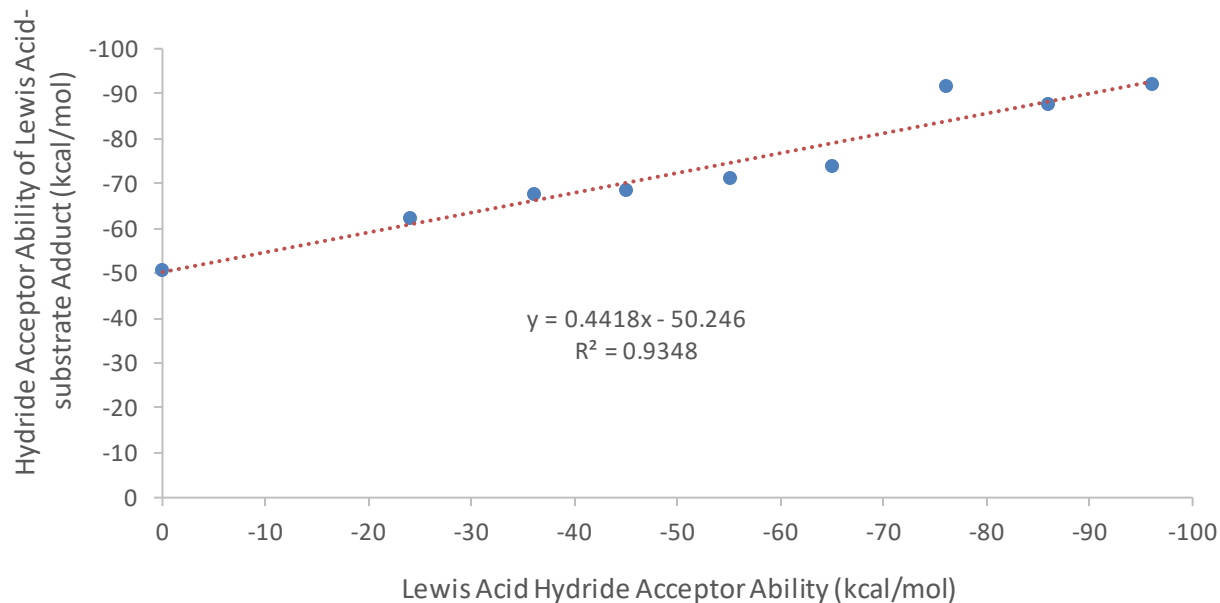


Figure S3. Plot showing the effect of Lewis acid strength on the resulting ΔG_{H^-} of the cyclohexathione-Lewis acid adduct.

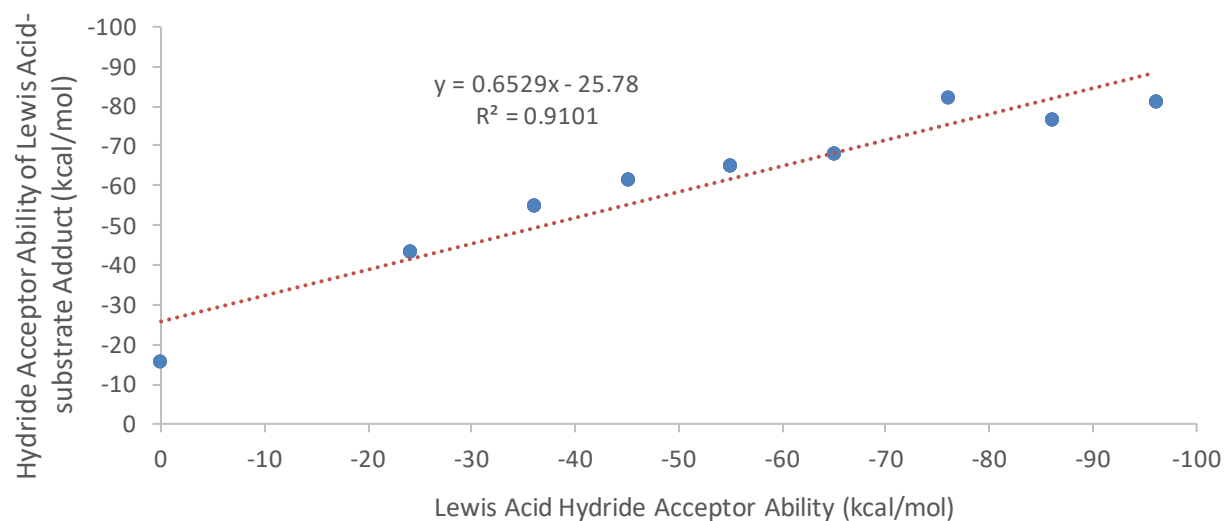


Figure S4. Plot showing the effect of Lewis acid strength on the resulting ΔG_{H^-} of the acetophenone-Lewis acid adduct.

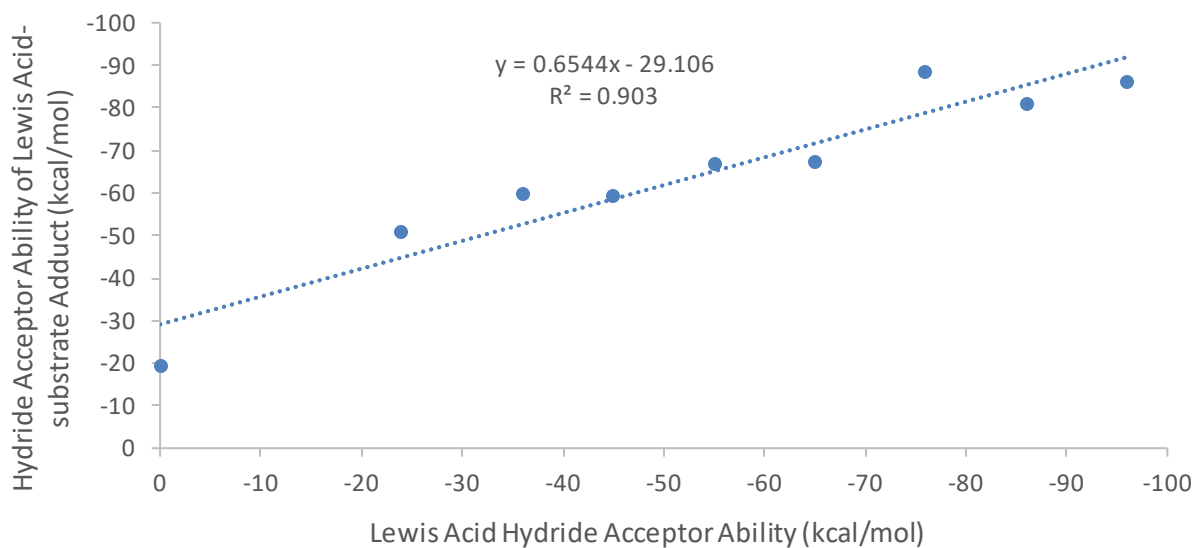


Figure S5. Plot showing the effect of Lewis acid strength on the resulting ΔG_{H-} of the benzaldehyde-Lewis acid adduct.

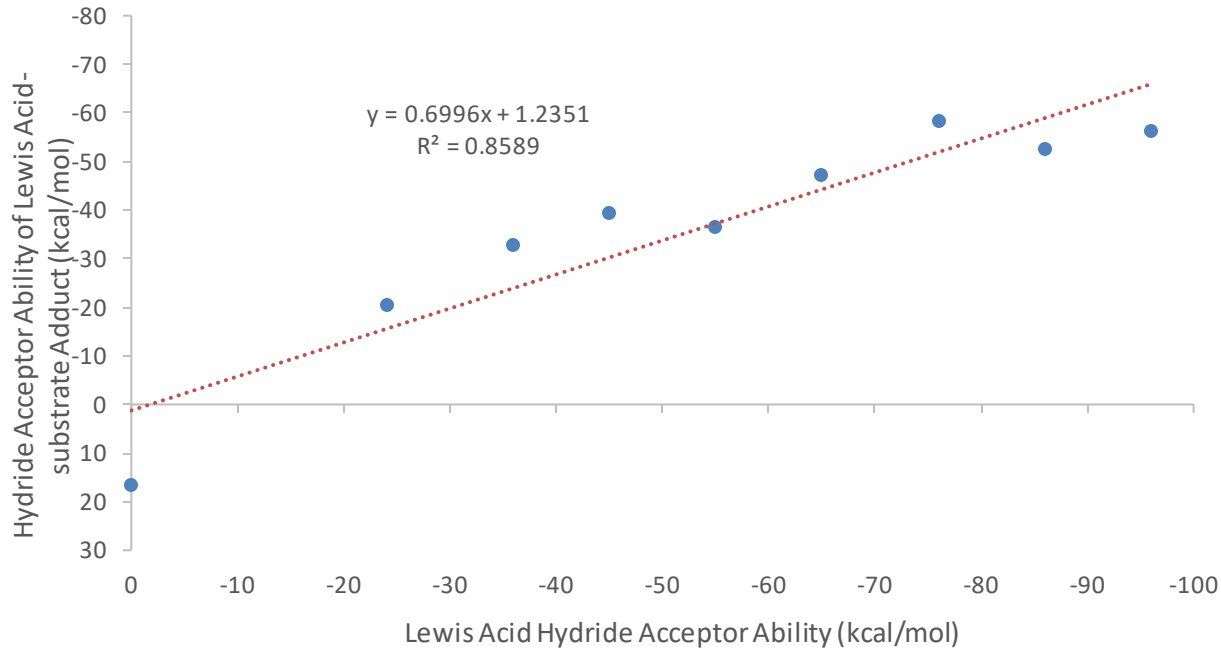


Figure S6. Plot showing the effect of Lewis acid strength on the resulting ΔG_{H-} of the *N*-piperidino-cyclohex-1-ene-Lewis acid adduct.

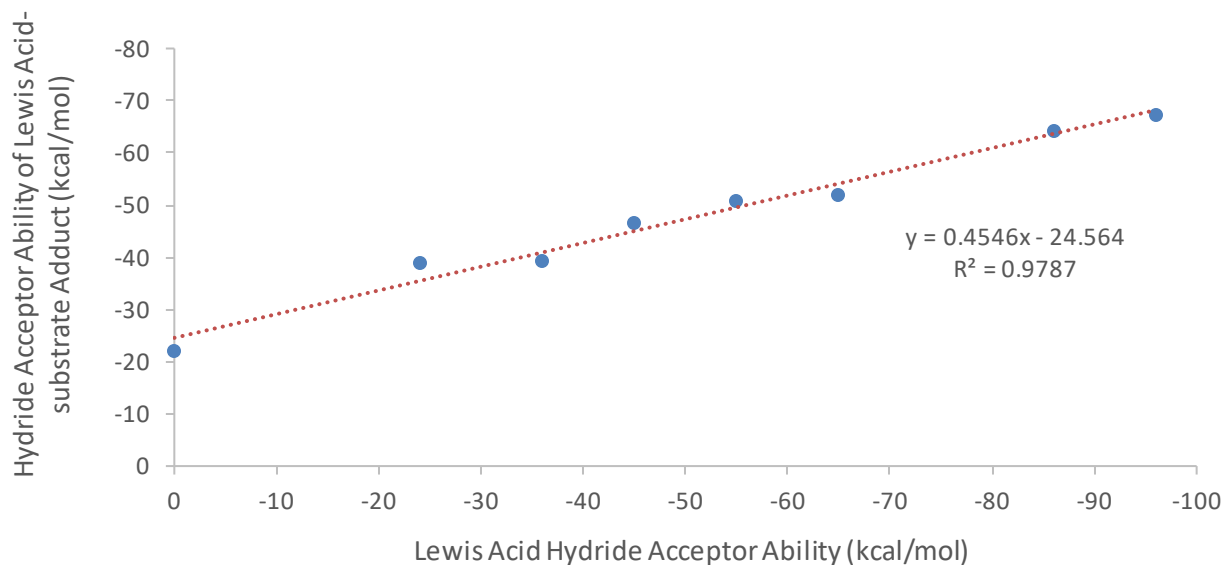


Figure S7. Plot showing the effect of Lewis acid strength on the resulting ΔG_{H^-} of the phenyl-(1-phenyl-ethylidene)-amine-Lewis acid adduct.

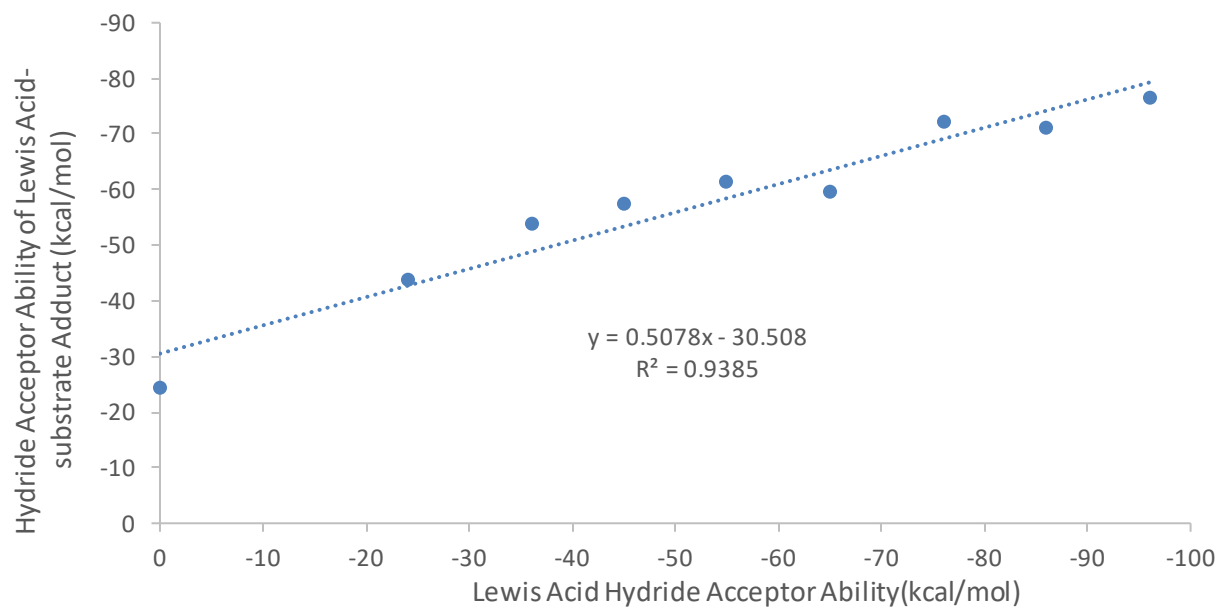


Figure S8. Plot showing the effect of Lewis acid strength on the resulting ΔG_{H^-} of the N-benzylidene-aniline-Lewis acid adduct.

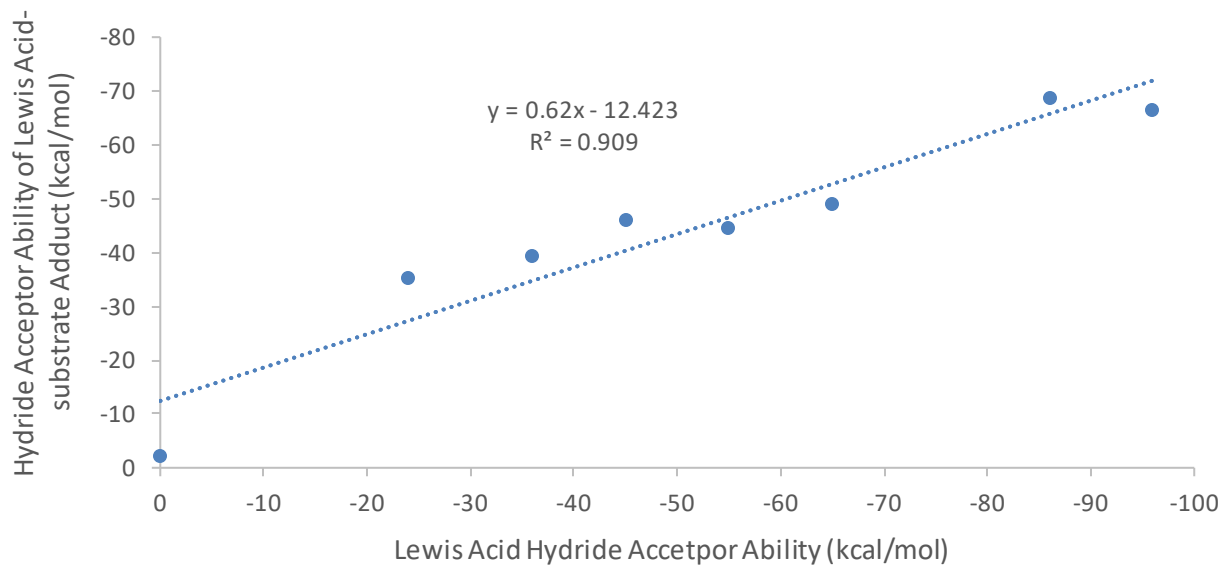


Figure S9. Plot showing the effect of Lewis acid strength on the resulting ΔG_{H^-} of the phenyl-tert-butyl-(1-phenyl-ethylidene)-amine-Lewis acid adduct.

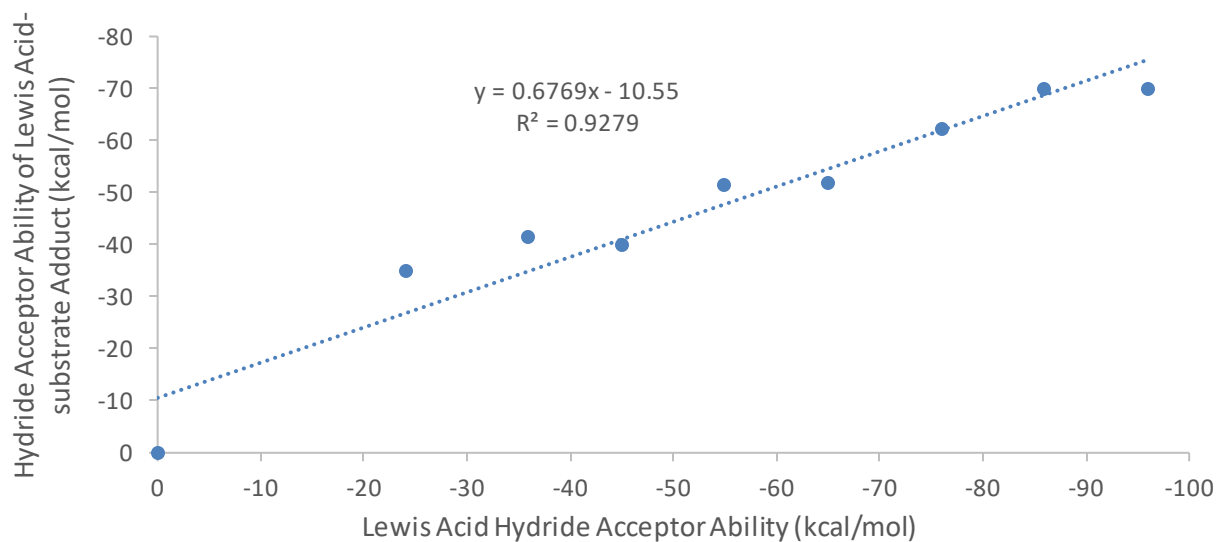


Figure S10. Plot showing the effect of Lewis acid strength on the resulting ΔG_{H^-} of the N-benzylidene tert-butylamine-Lewis acid adduct.

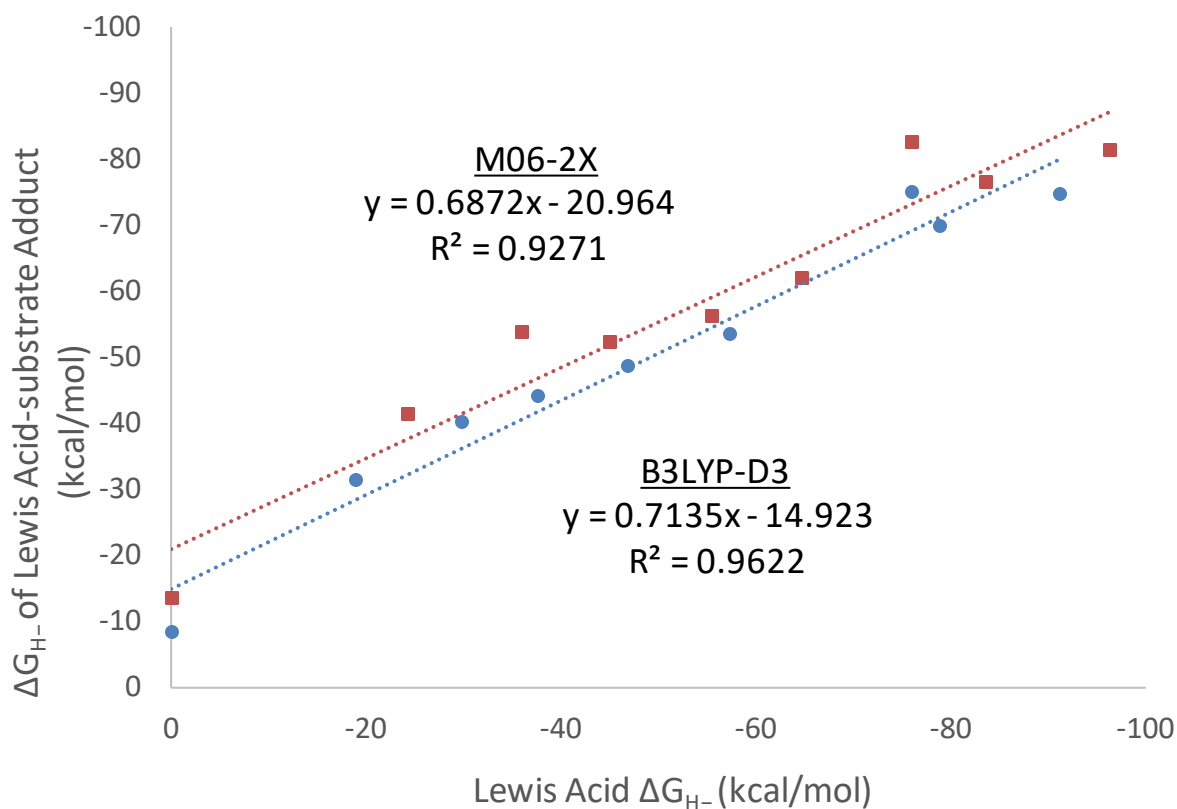


Figure S11. Comparison of the effect of Lewis acid strength on the resulting ΔG_{H-} of the Actone-Lewis acid adduct using the M06-2X (orange squares) and B3LYP-D3 (blue circles) functionals.

2) Energies for the Optimized Lewis Acid-Acetone Adducts.

Table S1. Computed energies for the optimized structures of the Lewis acid-Acetone adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
Acetone	-193.0606922	0.058907	0.089203
Acetonium	-193.3895994	0.069626	0.103635
Isopropoxide	-193.6272207	0.066497	0.099462
Isopropanol	-194.2647114	0.082143	0.11574
Acetone-BEt ₃	-455.4773745	0.24891	0.307399
[Isopropoxide-BEt ₃] ⁻	-456.1391822	0.261637	0.317228
Acetone-BPh ₃	-912.6076601	0.31606	0.388653
[Isopropoxide-BPh ₃] ⁻	-913.2958562	0.326882	0.399229
Acetone-B(C ₆ F ₅)Ph ₂	-1408.607839	0.269908	0.352654
[Isopropoxide-B(C ₆ F ₅)Ph ₂] ⁻	-1409.300482	0.282295	0.363397
Acetone-B(C ₆ F ₅) ₂ Ph	-1904.604383	0.224372	0.316466
[Isopropoxide-B(C ₆ F ₅) ₂ Ph] ⁻	-1905.308151	0.236733	0.327522
Acetone-B(C ₆ F ₅) ₃	-2400.608215	0.179601	0.280654
[Isopropoxide-B(C ₆ F ₅) ₃] ⁻	-2401.321383	0.189791	0.291529
[Acetone-SiEt ₃] ⁺	-719.9058506	0.241449	0.305285
Isopropoxide-SiEt ₃	-720.7581932	0.256028	0.317315
[Acetone-SiPhH ₂] ⁺	-715.0604031	0.155288	0.209995
Isopropoxide-SiPhH ₂	-715.9204102	0.16878	0.222343

Table S2. Computed energies for the optimized structures of the Lewis acid-Acetone adducts. All single point energy calculations were implemented using the M06-2X/6-311++G(d,p) at 298K

in acetonitrile, using the PCM solvation model and the geometries optimized at the M06-2X/6-31G(d,p) level of theory.

Lewis Acid-Base Adduct	Solvation Energy MeCN (Hartrees)
Acetone	-193.1265453
Acetonium	-193.5292344
Isopropoxide	-193.8102836
Isopropanol	-194.3276116
Acetone-BEt ₃	-455.5957547
[Isopropoxide-BEt ₃] ⁻	-456.3288335
Acetone-BPh ₃	-912.8365346
[Isopropoxide-BPh ₃] ⁻	-913.5875172
Acetone-B(C ₆ F ₅)Ph ₂	-1409.020298
[Isopropoxide-B(C ₆ F ₅)Ph ₂] ⁻	-1409.770394
Acetone-B(C ₆ F ₅) ₂ Ph	-1905.201822
[Isopropoxide-B(C ₆ F ₅) ₂ Ph] ⁻	-1905.958196
Acetone-B(C ₆ F ₅) ₃	-2401.38719
[Isopropoxide-B(C ₆ F ₅) ₃] ⁻	-2402.150554
[Acetone-SiEt ₃] ⁺	-720.1021159
Isopropoxide-SiEt ₃	-720.8931373
[Acetone-SiPhH ₂] ⁺	-715.2578434
Isopropoxide-SiPhH ₂	-716.0553339

3) Energies for the Optimized Lewis Acid-Cyclohexanone Adducts.

Table S3. Computed energies for the optimized structures of the Lewis acid-Cyclohexanone adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
Cyclohexanone	-309.7544142	0.122209	0.159915
Cyclohexanonium	-310.0896285	0.134678	0.173045
Cyclohexanoxide	-310.3243806	0.130185	0.167611
Cyclohexanol	-310.9573977	0.146357	0.184323
Cyclohexanone-BEt ₃	-572.1688751	0.314625	0.376667
[Cyclohexanoxide-BEt ₃] ⁻	-572.837695	0.323337	0.385568
Cyclohexanone-BPh ₃	-1029.301424	0.382701	0.457963
[Cyclohexanoxide-BPh ₃] ⁻	-1029.988147	0.390779	0.46769
Cyclohexanone-B(C ₆ F ₅)Ph ₂	-1525.304884	0.33719	0.421947
[Cyclohexanoxide-B(C ₆ F ₅)Ph ₂] ⁻	-1525.998636	0.345544	0.432008
Cyclohexanone-B(C ₆ F ₅) ₂ Ph	-2021.304022	0.291804	0.385988
[Cyclohexanoxide-B(C ₆ F ₅) ₂ Ph] ⁻	-2022.003807	0.300393	0.395932
Cyclohexanone-B(C ₆ F ₅) ₃	-2517.32241	0.245629	0.350048
[Cyclohexanoxide-B(C ₆ F ₅) ₃] ⁻	-2518.015956	0.256042	0.36021
[Cyclohexanone-SiEt ₃] ⁺	-836.6025256	0.30912	0.374642
Cyclohexanoxide-SiEt ₃	-837.4500906	0.320484	0.385929
[Cyclohexanone-SiPhH ₂] ⁺	-831.76278	0.224474	0.279561
Cyclohexanoxide-SiPhH ₂	-832.6141605	0.234199	0.291111

Table S4. Computed energies for the optimized structures of the Lewis acid-Cyclohexanone adducts. All single point energy calculations were implemented using the M06-2X/6-311++G(d,p) at 298K in acetonitrile, using the PCM solvation model and the geometries optimized at the M06-2X/6-31G(d,p) level of theory.

Lewis Acid-Base Adduct	Solvation Energy MeCN (Hartrees)
Cyclohexanone	-309.8411028
Cyclohexanonium	-310.2454249
Cyclohexanoxide	-310.526392
Cyclohexanol	-311.044139
Cyclohexanone-BEt ₃	-572.311006
[Cyclohexanoxide-BEt ₃] ⁻	-573.0475906
Cyclohexanone-BPh ₃	-1029.553778
[Cyclohexanoxide-BPh ₃] ⁻	-1030.302569
Cyclohexanone-B(C ₆ F ₅)Ph ₂	-1525.73961
[Cyclohexanoxide-B(C ₆ F ₅)Ph ₂] ⁻	-1526.492183
Cyclohexanone-B(C ₆ F ₅) ₂ Ph	-2021.92298
[Cyclohexanoxide-B(C ₆ F ₅) ₂ Ph] ⁻	-2022.678254
Cyclohexanone-B(C ₆ F ₅) ₃	-2518.104683
[Cyclohexanoxide-B(C ₆ F ₅) ₃] ⁻	-2518.869327
[Cyclohexanone-SiEt ₃] ⁺	-836.8185265
Cyclohexanoxide-SiEt ₃	-837.6091351
[Cyclohexanone-SiPhH ₂] ⁺	-831.9769836
Cyclohexanoxide-SiPhH ₂	-832.7736888

4) Energies for the Optimized Lewis Acid-Cyclohexathione Adducts.

Table S5. Computed energies for the optimized structures of the Lewis acid-Cyclohexathione adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
Cyclohexathione	-632.7025456	0.119416	0.158193
Cyclohexathionium	-633.0362978	0.128573	0.167936
Cyclohexathioxide	-633.3427884	0.130023	0.168599
Cyclohexathioli	-633.9203608	0.14029	0.17983
Cyclohexathione-BEt ₃	-895.1093939	0.310127	0.374282
[Cyclohexanoxide-BEt ₃] ⁻	-895.8036569	0.32178	0.384248
Cyclohexathione-BPh ₃	-1352.242463	0.378854	0.45552
[Cyclohexathioxide-BPh ₃] ⁻	-1352.948663	0.388338	0.46585
Cyclohexanthione-B(C ₆ F ₅)Ph ₂	-1848.242682	0.333278	0.419324
[Cyclohexanthioxide-B(C ₆ F ₅)Ph ₂] ⁻	-1848.95455	0.343089	0.429948
Cyclohexanthione-B(C ₆ F ₅) ₂ Ph	-2344.240008	0.287804	0.383355
[Cyclohexanthioxide-B(C ₆ F ₅) ₂ Ph] ⁻	-2344.959936	0.297188	0.393958
Cyclohexanthione-B(C ₆ F ₅) ₃	-2840.238765	0.241558	0.34731
[Cyclohexanthioxide-B(C ₆ F ₅) ₃] ⁻	-2840.968444	0.251816	0.35803
[Cyclohexanthione-SiEt ₃] ⁺	-1159.537345	0.305344	0.372313
Cyclohexanthioxide-SiEt ₃	-1160.399153	0.317624	0.384221
[Cyclohexanthione-SiPhH ₂] ⁺	-1154.696495	0.220533	0.27683
Cyclohexanthioxide-SiPhH ₂	-1155.565548	0.230862	0.288911

Table S6. Computed energies for the optimized structures of the Lewis acid-Cyclohexathione adducts. All single point energy calculations were implemented using the M06-2X/6-311++G(d,p) at 298K in acetonitrile, using the PCM solvation model and the geometries optimized at the M06-2X/6-31G(d,p) level of theory.

Lewis Acid-Base Adduct	Solvation Energy MeCN (Hartrees)
Cyclohexathione	-632.7898619
Cyclohexathionium	-633.1954251
Cyclohexathioxide	-633.5356545
Cyclohexathioli	-634.007578
Cyclohexathione-BEt ₃	-895.257053
[Cyclohexanoxide-BEt ₃] ⁻	-896.0221986
Cyclohexathione-BPh ₃	-1352.500265
[Cyclohexathioxide-BPh ₃] ⁻	-1353.271729
Cyclohexanthione-B(C ₆ F ₅)Ph ₂	-1848.683645
[Cyclohexanthioxide-B(C ₆ F ₅)Ph ₂] ⁻	-1849.457251
Cyclohexanthione-B(C ₆ F ₅) ₂ Ph	-2344.865368
[Cyclohexanthioxide-B(C ₆ F ₅) ₂ Ph] ⁻	-2345.642458
Cyclohexanthione-B(C ₆ F ₅) ₃	-2841.047374
[Cyclohexanthioxide-B(C ₆ F ₅) ₃] ⁻	-2841.829837
[Cyclohexanthione-SiEt ₃] ⁺	-1159.759254
Cyclohexanthioxide-SiEt ₃	-1160.565831
[Cyclohexanthione-SiPhH ₂] ⁺	-1154.919454
Cyclohexanthioxide-SiPhH ₂	-1155.730901

5) Energies for the Optimized Lewis Acid-Acetophenone Adducts.

Table S7. Computed energies for the optimized structures of the Acetophenone-Lewis acid adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
Acetophenone	-384.7296306	0.106604	0.14733
Acetophenonium	-385.0745089	0.11991	0.160347
Phenylethanoxide	-385.3106824	0.114907	0.156324
Phenylethanol	-385.9279543	0.129749	0.172282
Acetophenone-BEt ₃	-647.1490873	0.297226	0.363944
[Phenylethanoxide-BEt ₃] ⁻	-647.8143421	0.308509	0.373545
Acetophenone-BPh ₃	-1104.276124	0.364451	0.445704
[Phenylethanoxide-BPh ₃] ⁻	-1104.965464	0.376299	0.45556
Acetophenone-B(C ₆ F ₅)Ph ₂	-1600.272139	0.318812	0.409714
[Phenylethanoxide-B(C ₆ F ₅)Ph ₂] ⁻	-1600.976631	0.330356	0.419655
Acetophenone-B(C ₆ F ₅) ₂ Ph	-2096.277209	0.274584	0.373901
[Phenylethanoxide-B(C ₆ F ₅) ₂ Ph] ⁻	-2096.989303	0.285776	0.383993
Acetophenone-B(C ₆ F ₅) ₃	-2592.278393	0.229108	0.337896
[Phenylethanoxide-B(C ₆ F ₅) ₃] ⁻	-2592.995545	0.23955	0.347912
[Acetophenone-SiEt ₃] ⁺	-911.5821828	0.290862	0.362413
Phenylethanoxide-SiEt ₃	-912.4204223	0.302663	0.373335
[Acetophenone-SiPhH ₂] ⁺	-906.7409904	0.20615	0.267402
Phenylethanoxide-SiPhH ₂	-907.5878936	0.220264	0.278667

Table S8. Computed energies for the optimized structures of the Lewis acid-Acetophenone adducts. All single point energy calculations were implemented using the M06-2X/6-311++G(d,p) at 298K in acetonitrile, using the PCM solvation model and the geometries optimized at the M06-2X/6-31G(d,p) level of theory.

Lewis Acid-Base Adduct	Solvation Energy MeCN (Hartrees)
Acetophenone	-384.8365972
Acetophenonium	-385.2382225
Phenylethanoxide	-385.5239909
Phenylethanol	-386.0365074
Acetophenone-BEt ₃	-647.3092264
[Phenylethanoxide-BEt ₃] ⁻	-648.0439035
Acetophenone-BPh ₃	-1104.545882
[Phenylethanoxide-BPh ₃] ⁻	-1105.299575
Acetophenone-B(C ₆ F ₅)Ph ₂	-1600.728967
[Phenylethanoxide-B(C ₆ F ₅)Ph ₂] ⁻	-1601.492849
Acetophenone-B(C ₆ F ₅) ₂ Ph	-2096.91468
[Phenylethanoxide-B(C ₆ F ₅) ₂ Ph] ⁻	-2097.683604
Acetophenone-B(C ₆ F ₅) ₃	-2593.097508
[Phenylethanoxide-B(C ₆ F ₅) ₃] ⁻	-2593.870379
[Acetophenone-SiEt ₃] ⁺	-911.8125131
Phenylethanoxide-SiEt ₃	-912.6008537
[Acetophenone-SiPhH ₂] ⁺	-906.9705935
Phenylethanoxide-SiPhH ₂	-907.7679836

6) Energies for the Optimized Lewis Acid-Benzaldehyde Adducts.

Table S9. Computed energies for the optimized structures of the Lewis acid-Benzaldehyde adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
Benzaldehyde	-345.4274796	0.080615	0.118354
Benzaldehyde + H ⁺	-345.7617608	0.093952	0.131953
Benzylalcoholoxide	-346.0080049	0.088137	0.126387
Benzyl alcohol	-346.6261274	0.101684	0.142616
Benzaldehyde-BEt ₃	-607.8432018	0.271606	0.334746
[Benzylalcoholoxide-BEt ₃] ⁻	-608.5174345	0.28102	0.343994
Benzaldehyde-BPh ₃	-1064.970991	0.337491	0.416132
[Benzylalcoholoxide-BPh ₃] ⁻	-1065.665499	0.346743	0.42592
Benzaldehyde-B(C ₆ F ₅)Ph ₂	-1560.972267	0.292857	0.380477
[Benzylalcoholoxide-B(C ₆ F ₅)Ph ₂] ⁻	-1561.667347	0.303017	0.390553
Benzaldehyde-B(C ₆ F ₅) ₂ Ph	-2056.971758	0.247306	0.344408
[Benzylalcoholoxide-B(C ₆ F ₅) ₂ Ph] ⁻	-2057.684927	0.256971	0.35448
Benzaldehyde-B(C ₆ F ₅) ₃	-2552.967934	0.200108	0.308272
[Benzylalcoholoxide-B(C ₆ F ₅) ₃] ⁻	-2553.693009	0.211945	0.318541
[Benzaldehyde-SiEt ₃] ⁺	-872.2747044	0.265816	0.33325
Benzylalcoholoxide-SiEt ₃	-873.1236619	0.279944	0.344515
[Benzaldehyde-SiPhH ₂] ⁺	-867.4303633	0.180444	0.23833
Benzylalcoholoxide-SiPhH ₂	-868.2820936	0.189072	0.249281

Table S10. Computed energies for the optimized structures of the Lewis acid-Benzaldehyde adducts. All single point energy calculations were implemented using the M06-2X/6-311++G(d,p) at 298K in acetonitrile, using the PCM solvation model and the geometries optimized at the M06-2X/6-31G(d,p) level of theory.

Lewis Acid-Base Adduct	Solvation Energy MeCN (Hartrees)
------------------------	----------------------------------

Benzaldehyde	-345.5230587
Benzaldehyde + H ⁺	-345.9233009
Benzylalcoholoxide	-346.2155102
Benzyl alcohol	-346.7260847
Benzaldehyde-BEt ₃	-607.99508
[Benzylalcoholoxide-BEt ₃] ⁻	-608.7394556
Benzaldehyde-BPh ₃	-1065.232796
[Benzylalcoholoxide-BPh ₃] ⁻	-1065.991807
Benzaldehyde-B(C ₆ F ₅)Ph ₂	-1561.417459
[Benzylalcoholoxide-B(C ₆ F ₅)Ph ₂] ⁻	-1562.176416
Benzaldehyde-B(C ₆ F ₅) ₂ Ph	-2057.599459
[Benzylalcoholoxide-B(C ₆ F ₅) ₂ Ph] ⁻	-2058.369755
Benzaldehyde-B(C ₆ F ₅) ₃	-2553.784606
[Benzylalcoholoxide-B(C ₆ F ₅) ₃] ⁻	-2554.558338
[Benzaldehyde-SiEt ₃] ⁺	-872.4976465
Benzylalcoholoxide-SiEt ₃	-873.2947896
[Benzaldehyde-SiPhH ₂] ⁺	-867.65406
Benzylalcoholoxide-SiPhH ₂	-868.4542648

7) Energies for the Optimized Lewis Acid-*N*-Piperidino-Cyclohex-1-ene Adducts.

Table S11. Computed energies for the optimized structures of the Lewis acid-*N*-piperidino-cyclohex-1-ene adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
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<i>N</i> -Piperidino-cyclohex-1-ene	-485.1450309	0.251996	0.300584
<i>N</i> -Piperidino-cyclohex-1-ene + H ⁺	-485.5481583	0.264993	0.314834
<i>N</i> -Cyclohexyl-Piperidinium	-485.6829292	0.258305	0.306906
<i>N</i> -Cyclohexyl-Piperidine	-486.3659366	0.275772	0.324557
<i>N</i> -Piperidino-cyclohex-1-ene-BEt ₃	-747.5533658	0.441201	0.516186
[1-cyclohexylidenepiperidin-1-ium-BEt ₃] ⁻	-748.1925602	0.455455	0.526259
<i>N</i> -Piperidino-cyclohex-1-ene-BPh ₃	-1204.681114	0.517284	0.599504
[1-cyclohexylidenepiperidin-1-ium-BPh ₃] ⁻	-1205.338177	0.524318	0.608642
<i>N</i> -Piperidino-cyclohex-1-ene-B(C ₆ F ₅)Ph ₂	-1700.669739	0.468895	0.56345
[1-cyclohexylidenepiperidin-1-ium-B(C ₆ F ₅)Ph ₂] ⁻	-1701.348323	0.479643	0.572862
<i>N</i> -Piperidino-cyclohex-1-ene-B(C ₆ F ₅) ₂ Ph	-2196.682731	0.426491	0.527803
[1-cyclohexylidenepiperidin-1-ium-B(C ₆ F ₅) ₂ Ph] ⁻	-2197.357661	0.434647	0.537577
<i>N</i> -Piperidino-cyclohex-1-ene-B(C ₆ F ₅) ₃	-2692.680786	0.379968	0.491626
[1-cyclohexylidenepiperidin-1-ium-B(C ₆ F ₅) ₃] ⁻	-2693.377632	0.387162	0.500873
[<i>N</i> -Piperidino-cyclohex-1-ene-SiEt ₃] ⁺	-1012.00567	0.44373	0.516674
P 1-cyclohexylidenepiperidin-1-ium-SiEt ₃	-1012.804442	0.449522	0.525485
[<i>N</i> -Piperidino-cyclohex-1-ene-SiPhH ₂] ⁺	-1007.167774	0.352648	0.420921
1-cyclohexylidenepiperidin-1-ium-SiPhH ₂	-1007.975623	0.362995	0.430427

Table S12. Computed energies for the optimized structures of the Lewis acid-*N*-Piperidino-cyclohex-1-ene adducts. All single point energy calculations were implemented using the M06-2X/6-311++G(d,p) at 298K in acetonitrile, using the PCM solvation model and the geometries optimized at the M06-2X/6-31G(d,p) level of theory.

Lewis Acid-Base Adduct	Solvation Energy MeCN (Hartrees)
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<i>N</i> -Piperidino-cyclohex-1-ene	-485.2577776
<i>N</i> -Piperidino-cyclohex-1-ene + H ⁺	-485.7192364
<i>N</i> -Cyclohexyl-Piperidinium	-485.8945158
<i>N</i> -Cyclohexyl-Piperidine	-486.4770842
<i>N</i> -Piperidino-cyclohex-1-ene-BEt ₃	-747.724761
[1-cyclohexylidenepiperidin-1-ium-BEt ₃] ⁻	-748.4260137
<i>N</i> -Piperidino-cyclohex-1-ene-BPh ₃	-1204.965118
[1-cyclohexylidenepiperidin-1-ium-BPh ₃] ⁻	-1205.678899
<i>N</i> -Piperidino-cyclohex-1-ene-B(C ₆ F ₅)Ph ₂	-1701.141007
[1-cyclohexylidenepiperidin-1-ium-B(C ₆ F ₅)Ph ₂] ⁻	-1701.869206
<i>N</i> -Piperidino-cyclohex-1-ene-B(C ₆ F ₅) ₂ Ph	-2197.337798
[1-cyclohexylidenepiperidin-1-ium-B(C ₆ F ₅) ₂ Ph] ⁻	-2198.058725
<i>N</i> -Piperidino-cyclohex-1-ene-B(C ₆ F ₅) ₃	-2693.520413
[1-cyclohexylidenepiperidin-1-ium-B(C ₆ F ₅) ₃] ⁻	-2694.257131
[<i>N</i> -Piperidino-cyclohex-1-ene-SiEt ₃] ⁺	-1012.250311
P 1-cyclohexylidenepiperidin-1-ium-SiEt ₃	-1012.994073
[<i>N</i> -Piperidino-cyclohex-1-ene-SiPhH ₂] ⁺	-1007.412273
1-cyclohexylidenepiperidin-1-ium-SiPhH ₂	-1008.166716

8) Energies for the Optimized Lewis Acid-Phenyl-(1-phenyl-ethylidene)-amine Adducts.

Table S13. Computed energies for the optimized structures of the Lewis acid-Phenyl-(1-phenyl-ethylidene)-amine adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
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Phenyl-(1-phenyl-ethylidene)-amine	-595.8177379	0.19331	0.246765
Phenyl-(1-phenyl-ethylidene)-ammonium	-596.2027915	0.20681	0.260575
Phenyl-(1-phenyl-ethylidene)-amide	-596.4304514	0.202568	0.255654
<i>N</i> -Phenyl- α -methylbenzylamine	-597.0273718	0.217635	0.271314
Phenyl-(1-phenyl-ethylidene)-amine-BE ₃	-848.1780946	0.431379	0.505593
[Phenyl-(1-phenyl-ethylidene)-amide-BE ₃] ⁻	-848.7665731	0.446437	0.51928
Phenyl-(1-phenyl-ethylidene)-amine-BPh ₃	-1299.835723	0.497068	0.583217
[Phenyl-(1-phenyl-ethylidene)-amide-BPh ₃] ⁻	-1300.427707	0.510202	0.596373
Phenyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅)Ph ₂	-1811.367661	0.412174	0.508517
[Phenyl-(1-phenyl-ethylidene)-amide-B(C ₆ F ₅)Ph ₂] ⁻	-1812.048605	0.423031	0.518496
Phenyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅) ₂ Ph	-2307.364117	0.365342	0.472334
[Phenyl-(1-phenyl-ethylidene)-amide-B(C ₆ F ₅) ₂ Ph] ⁻	-2308.056652	0.377514	0.482447
Phenyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅) ₃	-2803.37227	0.320623	0.436582
[Phenyl-(1-phenyl-ethylidene)-amide-B(C ₆ F ₅) ₃] ⁻	-2804.069432	0.333016	0.44686
[Phenyl-(1-phenyl-ethylidene)-amine-SiEt ₃] ⁺	-1109.699722	0.425771	0.50237
Phenyl-(1-phenyl-ethylidene)-amide-SiEt ₃	-1110.451342	0.438839	0.517018
[Phenyl-(1-phenyl-ethylidene)-amine-SiPhH ₂] ⁺	-1117.845076	0.294322	0.366234
Phenyl-(1-phenyl-ethylidene)-amide-SiPhH ₂	-1118.664832	0.307108	0.376806

Table S15. Computed energies for the optimized structures of the Lewis acid-Phenyl-(1-phenyl-ethylidene)-amine. All single point energy calculations were implemented using the M06-2X/6-311++G(d,p) at 298K in acetonitrile, using the PCM solvation model and the geometries optimized at the M06-2X/6-31G(d,p) level of theory.

Lewis Acid-Base Adduct	Solvation Energy MeCN (Hartrees)
Phenyl-(1-phenyl-ethylidene)-amine	-595.9615847

Phenyl-(1-phenyl-ethylidene)-ammonium	-596.3999474
Phenyl-(1-phenyl-ethylidene)-amide	-596.6636605
<i>N</i> -Phenyl- α -methylbenzylamine	-597.1734968
Phenyl-(1-phenyl-ethylidene)-amine-BEt ₃	-858.4290915
[Phenyl-(1-phenyl-ethylidene)-amide-BEt ₃] ⁻	-859.1608238
Phenyl-(1-phenyl-ethylidene)-amine-BPh ₃	-1315.67265
[Phenyl-(1-phenyl-ethylidene)-amide-BPh ₃] ⁻	-1316.402666
Phenyl-(1-phenyl-ethylidene)-amine -B(C ₆ F ₅)Ph ₂	-1811.86376
[Phenyl-(1-phenyl-ethylidene)-amide-B(C ₆ F ₅)Ph ₂] ⁻	-1812.603464
Phenyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅) ₂ Ph	-2308.043864
[Phenyl-(1-phenyl-ethylidene)-amide-B(C ₆ F ₅) ₂ Ph] ⁻	-2308.791352
Phenyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅) ₃	-2804.233639
[Phenyl-(1-phenyl-ethylidene)-amide-B(C ₆ F ₅) ₃] ⁻	-2804.983184
[Phenyl-(1-phenyl-ethylidene)-amine-SiEt ₃] ⁺	-1122.946519
Phenyl-(1-phenyl-ethylidene)-amide-SiEt ₃	-1123.716354
[Phenyl-(1-phenyl-ethylidene)-amine-SiPhH ₂] ⁺	-1118.115341
Phenyl-(1-phenyl-ethylidene)-amide-SiPhH ₂	-1118.888674

9) Energies for the Optimized Lewis Acid-Benzylidene Aniline Adducts.

Table S16. Computed energies for the optimized structures of the Benzylidene Aniline -Lewis acid adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
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Benzylidene Aniline	-556.519463	0.167155	0.21704
Benzylidene Anilinium	-556.897624	0.180246	0.231036
Benzylidene Anilide	-557.1328412	0.175376	0.225748
<i>N</i> -phenyl-benzylamine	-557.7299655	0.190078	0.241602
Benzylidene Aniline-BEt ₃	-818.943679	0.36297	0.434463
[Benzylidene Anilide-BEt ₃] ⁻	-819.6089427	0.370292	0.44323
Benzylidene Aniline-BPh ₃	-1276.068328	0.429391	0.515867
[Benzylidene Anilide-BPh ₃] ⁻	-1276.75534	0.439093	0.525412
Benzylidene Aniline-B(C ₆ F ₅)Ph ₂	-1772.072732	0.384913	0.480256
[Benzylidene Anilide-B(C ₆ F ₅)Ph ₂] ⁻	-1772.765359	0.394274	0.489586
Benzylidene Aniline-B(C ₆ F ₅) ₂ Ph	-2268.067578	0.337333	0.443739
[Benzylidene Anilide-B(C ₆ F ₅) ₂ Ph] ⁻	-2268.77611	0.349104	0.453707
Benzylidene Aniline-B(C ₆ F ₅) ₃	-2764.072051	0.29207	0.407391
[Benzylidene Anilide-B(C ₆ F ₅) ₃] ⁻	-2764.781646	0.303802	0.417698
[Benzylidene Aniline-SiEt ₃] ⁺	-1083.378934	0.355622	0.432183
Benzylidene Anilide-SiEt ₃	-1084.203705	0.367323	0.443488
[Benzylidene Aniline-SiPhH ₂] ⁺	-1078.536005	0.2682	0.336907
Benzylidene Anilide-SiPhH ₂	-1079.370568	0.279216	0.347991

Table S17. Computed energies for the optimized structures of the Lewis acid-Benzylidene Aniline. All single point energy calculations were implemented using the M06-2X/6-311++G(d,p) at 298K in acetonitrile, using the PCM solvation model and the geometries optimized at the M06-2X/6-31G(d,p) level of theory.

Lewis Acid-Base Adduct	Solvation Energy MeCN (Hartrees)
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Benzylidene Aniline	-556.6550157
Benzylidene Anilinium	-557.0888027
Benzylidene Anilide	-557.3562834
<i>N</i> -phenyl-benzylamine	-557.8680876
Benzylidene Aniline-BEt ₃	-819.1380806
[Benzylidene Anilide-BEt ₃] ⁻	-819.8692476
Benzylidene Aniline-BPh ₃	-1276.372261
[Benzylidene Anilide-BPh ₃] ⁻	-1277.121994
Benzylidene Aniline-B(C ₆ F ₅)Ph ₂	-1772.557387
[Benzylidene Anilide-B(C ₆ F ₅)Ph ₂] ⁻	-1773.312412
Benzylidene Aniline-B(C ₆ F ₅) ₂ Ph	-2268.737785
[Benzylidene Anilide-B(C ₆ F ₅) ₂ Ph] ⁻	-2269.501804
Benzylidene Aniline-B(C ₆ F ₅) ₃	-2764.926339
[Benzylidene Anilide-B(C ₆ F ₅) ₃] ⁻	-2765.687427
[Benzylidene Aniline-SiEt ₃] ⁺	-1083.640089
Benzylidene Anilide-SiEt ₃	-1084.419554
[Benzylidene Aniline-SiPhH ₂] ⁺	-1078.798741
Benzylidene Anilide-SiPhH ₂	-1079.586299

10) Energies for the Optimized Lewis Acid- Tert-butyl-(1-phenyl-ethylidene)-amine Adducts.

Table S18. Computed energies for the optimized structures of the Lewis acid-Tert-butyl-(1-phenyl-ethylidene)-amine adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
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Tert-butyl-(1-phenyl-ethylidene)-amine	-522.0323117	0.225209	0.279426
Tert-butyl-(1-phenyl-ethylidene)-ammonium	-522.6041158	0.231902	0.286072
Tert-butyl-(1-phenyl-ethylidene)-amide	-522.6041158	0.231902	0.286072
N-tert-butyl- α -methylbenzylamine	-523.2439321	0.249342	0.303638
Tert-butyl-(1-phenyl-ethylidene)-amine-BEt ₃	-784.4331951	0.425259	0.497821
[Tert-butyl-(1-phenyl-ethylidene)-amide-BEt ₃] ⁻	-785.0883013	0.432785	0.505751
Tert-butyl-(1-phenyl-ethylidene)-amine -BPh ₃	-1241.569386	0.491971	0.578338
[Tert-butyl-(1-phenyl-ethylidene)-amide-BPh ₃] ⁻	-1242.238584	0.502952	0.587397
Tert-butyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅)Ph ₂	-1737.563063	0.4469	0.542893
[Tert-butyl-(1-phenyl-ethylidene)-amide-B(C ₆ F ₅)Ph ₂] ⁻	-1738.245004	0.457325	0.551512
Tert-butyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅) ₂ Ph	-2233.563682	0.400148	0.506346
[Tert-butyl-(1-phenyl-ethylidene)-amide-B(C ₆ F ₅) ₂ Ph] ⁻	-2234.245415	0.411542	0.515682
Tert-butyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅) ₃	-2729.5636	0.354342	0.470396
[Tert-butyl-(1-phenyl-ethylidene)-amide-B(C ₆ F ₅) ₃] ⁻	-2730.255994	0.365959	0.479908
[Tert-butyl-(1-phenyl-ethylidene)-amine-SiEt ₃] ⁺	-1048.887529	0.419694	0.495567
Tert-butyl-(1-phenyl-ethylidene)-amide-SiEt ₃	-1049.710836	0.429954	0.505752
[Tert-butyl-(1-phenyl-ethylidene)-amine-SiPhH ₂] ⁺	-1044.054877	0.329353	0.399284
Tert-butyl-(1-phenyl-ethylidene)-amide-SiPhH ₂	-1044.880605	0.341995	0.410105

Table S19. Computed energies for the optimized structures of the Lewis acid-Tert-butyl-(1-phenyl-ethylidene)-amine. All single point energy calculations were implemented using the M06-2X/6-311++G(d,p) at 298K in acetonitrile, using the PCM solvation model and the geometries optimized at the M06-2X/6-31G(d,p) level of theory.

Lewis Acid-Base Adduct	Solvation Energy MeCN (Hartrees)
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Tert-butyl-(1-phenyl-ethylidene)-amine	-522.1574677
Tert-butyl-(1-phenyl-ethylidene)-ammonium	-522.6103172
Tert-butyl-(1-phenyl-ethylidene)-amide	-522.8192771
N-tert-butyl- α -methylbenzylamine	-523.3704599
Tert-butyl-(1-phenyl-ethylidene)-amine-BEt ₃	-784.6168512
[Tert-butyl-(1-phenyl-ethylidene)-amide-BEt ₃] ⁻	-785.3346579
Tert-butyl-(1-phenyl-ethylidene)-amine-BPh ₃	-1241.86192
[Tert-butyl-(1-phenyl-ethylidene)-amide-BPh ₃] ⁻	-1242.58994
Tert-butyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅)Ph ₂	-1738.039619
[Tert-butyl-(1-phenyl-ethylidene)-amide-B(C ₆ F ₅)Ph ₂] ⁻	-1738.778084
Tert-butyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅) ₂ Ph	-2234.222345
[Tert-butyl-(1-phenyl-ethylidene)-amide-B(C ₆ F ₅) ₂ Ph] ⁻	-2234.959034
Tert-butyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅) ₃	-2730.404853
[Tert-butyl-(1-phenyl-ethylidene)-amide-B(C ₆ F ₅) ₃] ⁻	-2731.148953
[Tert-butyl-(1-phenyl-ethylidene)-amine-SiEt ₃] ⁺	-1049.140869
Tert-butyl-(1-phenyl-ethylidene)-amide-SiEt ₃	-1049.914905
[Tert-butyl-(1-phenyl-ethylidene)-amine-SiPhH ₂] ⁺	-1044.307904
Tert-butyl-(1-phenyl-ethylidene)-amide-SiPhH ₂	-1045.08473

11) Energies for the Optimized Lewis Acid-*N*-benzylidene tert-butylamine Adducts.

Table S20. Computed energies for the optimized structures of the Lewis acid-*N*-benzylidene tert-butylamine adducts. All calculations were implemented using the M06-2X/6-31g(d,p) at 298K.

Lewis Acid-Base Adduct	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
<i>N</i> -benzylidene tert-butylamine	-482.7413682	0.199022	0.249697
<i>N</i> -benzylidene tert-butylammonium	-483.129157	0.2123	0.263855
<i>N</i> -benzylidene tert-butylamide	-483.3073782	0.205818	0.256666
<i>N</i> -tert-butyl-benzylamine	-483.949135	0.221585	0.274231
<i>N</i> -benzylidene tert-butylamine-BEt ₃	-745.1485588	0.397416	0.467416
[<i>N</i> -benzylidene tert-butylamide-BEt ₃] ⁻	-745.8052033	0.406112	0.475543
<i>N</i> -benzylidene tert-butylamine-amine-BPh ₃	-1202.274111	0.464524	0.549825
[<i>N</i> -benzylidene tert-butylamide-BPh ₃] ⁻	-1202.946598	0.471844	0.55766
<i>N</i> -benzylidene tert-butylamine-B(C ₆ F ₅)Ph ₂	-1698.281889	0.417588	0.512718
[<i>N</i> -benzylidene tert-butylamide-B(C ₆ F ₅)Ph ₂] ⁻	-1698.951016	0.42628	0.521812
<i>N</i> -benzylidene tert-butylamine-B(C ₆ F ₅) ₂ Ph	-2194.269872	0.372876	0.477494
[<i>N</i> -benzylidene tert-butylamide-B(C ₆ F ₅) ₂ Ph] ⁻	-2194.960998	0.381364	0.485819
<i>N</i> -benzylidene tert-butylamine-B(C ₆ F ₅) ₃	-2690.276016	0.329094	0.440483
[<i>N</i> -benzylidene tert-butylamide-B(C ₆ F ₅) ₃] ⁻	-2690.969253	0.337	0.450146
[<i>N</i> -benzylidene tert-butylamine-SiEt ₃] ⁺	-1009.588522	0.38973	0.465824
<i>N</i> -benzylidene tert-butylamide-SiEt ₃	-1010.418923	0.403184	0.475504
[<i>N</i> -benzylidene tert-butylamine-SiPhH ₂] ⁺	-1009.592708	0.392604	0.465896
<i>N</i> -benzylidene tert-butylamide-SiPhH ₂	-1010.418923	0.403184	0.475504

Table S21. Computed energies for the optimized structures of the Lewis acid-Tert-butyl-(1-phenyl-ethylidene)-amine. All single point energy calculations were implemented using the M06-2X/6-311++G(d,p) at 298K in acetonitrile, using the PCM solvation model and the geometries optimized at the M06-2X/6-31G(d,p) level of theory.

Lewis Acid-Base Adduct	Solvation Energy MeCN
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	(Hartrees)
<i>N</i> -benzylidene tert-butylamine	-482.8583034
<i>N</i> -benzylidene tert-butylammonium	-483.3042236
<i>N</i> -benzylidene tert-butylamide	-483.516873
<i>N</i> -tert-butyl-benzylamine	-484.0673397
<i>N</i> -benzylidene tert-butylamine-BE ₃	-745.3236553
[<i>N</i> -benzylidene tert-butylamide-BE ₃] ⁻	-746.0422979
<i>N</i> -benzylidene tert-butylamine-amine-BPh ₃	-1202.563988
[<i>N</i> -benzylidene tert-butylamide-BPh ₃] ⁻	-1203.290806
<i>N</i> -benzylidene tert-butylamine-B(C ₆ F ₅)Ph ₂	-1698.749141
[<i>N</i> -benzylidene tert-butylamide-B(C ₆ F ₅)Ph ₂] ⁻	-1699.476183
<i>N</i> -benzylidene tert-butylamine-B(C ₆ F ₅) ₂ Ph	-2194.919724
[<i>N</i> -benzylidene tert-butylamide-B(C ₆ F ₅) ₂ Ph] ⁻	-2195.66484
<i>N</i> -benzylidene tert-butylamine-B(C ₆ F ₅) ₃	-2691.109634
[<i>N</i> -benzylidene tert-butylamide-B(C ₆ F ₅) ₃] ⁻	-2691.854724
[<i>N</i> -benzylidene tert-butylamine-SiEt ₃] ⁺	-1009.832359
<i>N</i> -benzylidene tert-butylamide-SiEt ₃	-1010.614598
[<i>N</i> -benzylidene tert-butylamine-SiPhH ₂] ⁺	-1005.006567
<i>N</i> -benzylidene tert-butylamide-SiPhH ₂	-1005.781337

12) Computed ΔG_{H-} values of Lewis Acid-Substrate Adducts.

Table S22. Computed ΔG_{H-} values (kcal/mol) of Lewis Acid-Substrate Adducts. All calculations were implemented using the M06-2X/6-31g(d,p)//M06-2X/6-311++g(d,p) level of theory in MeCN at 298K.

Complex	ΔG_{H-} in MeCN
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Acetone	-12.0
Cyclohexanone	-14.2
Cyclohexathione	-50.7
Benzaldehyde	-19.1
Acetophenone	-15.5
<i>N</i> -Piperidino-cyclohex-1-ene	16.7
Phenyl-(1-phenyl-ethylidene)-amine	-22.2
<i>N</i> -Benzylidene Aniline	-24.3
Tert-butyl-(1-phenyl-ethylidene)-amine	-2.4
<i>N</i> -benzylidene tert-butylamine	0.0
Isopropanol	-82.5
Cyclohexanol	-83.2
Cyclohexathiol	-91.6
Benzyl Alcohol	-88.3
Phenylethanol	-82.1
<i>N</i> -cyclohexyl-piperidine	-58.2
<i>N</i> -Phenyl-methylbenzylamine	-68.0
<i>N</i> -phenyl-benzylamine	-72.2
<i>N</i> -tert-butyl-benzylamine	-62.4
<i>N</i> -Tert-butyl-methylbenzylamine	
Acetone-BEt ₃	-41.4
Acetone-BPh ₃	-53.8
Acetone-B(C ₆ F ₅)Ph ₂	-52.3
Acetone-B(C ₆ F ₅) ₂ Ph	-56.2
Acetone-B(C ₆ F ₅) ₃	-62.0
[Acetone-SiEt ₃] ⁺	-76.6
[Acetone-SiPhH ₂] ⁺	-81.3
Cyclohexanone-BEt ₃	-46.1
Cyclohexanone-BPh ₃	-54.2
Cyclohexanone-B(C ₆ F ₅)Ph ₂	-56.4
Cyclohexanone-B(C ₆ F ₅) ₂ Ph	-57.9
Cyclohexanone B(C ₆ F ₅) ₃	-62.6
[Cyclohexanone-SiEt ₃] ⁺	-78.3
[Cyclohexanone-SiPhH ₂] ⁺	-83.2

Complex	ΔG_{H-} in MeCN
Cyclohexathione-BEt ₃	-62.2
Cyclohexathione-BPh ₃	-67.5
Cyclohexathione-B(C ₆ F ₅)Ph ₂	-68.5
Cyclohexathione -B(C ₆ F ₅) ₂ Ph	-71.1

(Cyclohexathione-B(C ₆ F ₅) ₃)	-74.0
[Cyclohexathione-SiEt ₃] ⁺	-87.8
[Cyclohexathione-SiPhH ₂] ⁺	-92.1
Benzaldehyde-BEt ₃	-50.6
Benzaldehyde-BPh ₃	-59.8
Benzaldehyde-B(C ₆ F ₅)Ph ₂	-59.2
Benzaldehyde-B(C ₆ F ₅) ₂ Ph	-66.7
Benzaldehyde-B(C ₆ F ₅) ₃	-67.5
[Benzaldehyde-SiEt ₃] ⁺	-80.7
[Benzaldehyde-SiPhH ₂] ⁺	-86.1
Acetophenone-BEt ₃	-43.3
Acetophenone-BPh ₃	-54.9
Acetophenone-B(C ₆ F ₅)Ph ₂	-61.5
Acetophenone-B(C ₆ F ₅) ₂ Ph	-64.9
Acetophenone-B(C ₆ F ₅) ₃	-67.8
[Acetophenone-SiEt ₃] ⁺	-76.6
[Acetophenone-SiPhH ₂] ⁺	-80.9
N-Piperidino-cyclohex-1-ene-BEt ₃	-20.5
N-Piperidino-cyclohex-1-ene-BPh ₃	-32.9
N-Piperidino-cyclohex-1-ene-B(C ₆ F ₅)Ph ₂	-39.6
N-Piperidino-cyclohex-1-ene-B(C ₆ F ₅) ₂ Ph	-36.6
N-Piperidino-cyclohex-1-ene-B(C ₆ F ₅) ₃	-47.1
[N-Piperidino-cyclohex-1-ene-SiEt ₃] ⁺	-52.4
[N-Piperidino-cyclohex-1-ene-SiPhH ₂] ⁺	-56.3
Phenyl-(1-phenyl-ethylidene)-amine-BEt ₃	-39.1
Phenyl-(1-phenyl-ethylidene)-amine-BPh ₃	-39.2
Phenyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅)Ph ₂	-46.7
Phenyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅) ₂ Ph	-50.8
Phenyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅) ₃	-51.9
[Phenyl-(1-phenyl-ethylidene)-amine-SiEt ₃] ⁺	-64.2
[Phenyl-(1-phenyl-ethylidene)-amine-SiPhH ₂] ⁺	-67.4
Benzylidene Aniline-BEt ₃	-43.6
Benzylidene Aniline-BPh ₃	-53.7
Benzylidene Aniline-B(C ₆ F ₅)Ph ₂	-57.3
Complex	ΔG_{H-} in MeCN
Benzylidene Aniline-B(C ₆ F ₅) ₂ Ph	-61.4
Benzylidene Aniline-B(C ₆ F ₅) ₃	-59.6
[Benzylidene Aniline-SiEt ₃] ⁺	-71.1
[Benzylidene Aniline-SiPhH ₂] ⁺	-76.6

Tert-butyl-(1-phenyl-ethylidene)-amine-BEt ₃	-35.1
Tert-butyl-(1-phenyl-ethylidene)-amine-BPh ₃	-39.3
Tert-butyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅)Ph ₂	-46.2
Tert-butyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅) ₂ Ph	-44.5
Tert-butyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅) ₃	-49.0
[Tert-butyl-(1-phenyl-ethylidene)-amine-SiEt ₃] ⁺	-68.6
[Tert-butyl-(1-phenyl-ethylidene)-amine-SiPhH ₂] ⁺	-66.6
<i>N</i> -benzylidene tert-butylamine-BEt ₃	-34.9
<i>N</i> -benzylidene tert-butylamine-BPh ₃	-41.3
<i>N</i> -benzylidene tert-butylamine-B(C ₆ F ₅)Ph ₂	-40.1
<i>N</i> -benzylidene tert-butylamine-B(C ₆ F ₅) ₂ Ph	-51.6
<i>N</i> -benzylidene tert-butylamine-B(C ₆ F ₅) ₃	-51.9
[<i>N</i> -benzylidene tert-butylamine-SiEt ₃] ⁺	-69.8
[<i>N</i> -benzylidene tert-butylamine-SiPhH ₂] ⁺	-69.9

13) Computed Binding Affinities of Lewis Acid-Substrate Adducts.

Table S23. Computed $\Delta G_{\text{H-}}$ values (kcal/mol) of Lewis Acid-Substrate Adducts. All calculations were implemented using the M06-2X/6-31g(d,p)//M06-2X/6-311++g(d,p) level of theory in MeCN at 298K.

Complex	Binding Affinity
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Acetone-BEt ₃	8.45
Acetone-BPh ₃	4.55
Acetone-B(C ₆ F ₅)Ph ₂	0.41
Acetone-B(C ₆ F ₅) ₂ Ph	-2.90
Acetone-B(C ₆ F ₅) ₃	-9.41
[Acetone-SiEt ₃] ⁺	-27.36
[Acetone-SiPhH ₂] ⁺	-34.34
Cyclohexanone-BEt ₃	9.48
Cyclohexanone-BPh ₃	4.91
Cyclohexanone-B(C ₆ F ₅)Ph ₂	-0.13
Cyclohexanone-B(C ₆ F ₅) ₂ Ph	-4.50
Cyclohexanone B(C ₆ F ₅) ₃	-9.60
[Cyclohexanone-SiEt ₃] ⁺	-25.84
[Cyclohexanone-SiPhH ₂] ⁺	-33.58
Cyclohexathione-BEt ₃	10.17
Cyclohexathione-BPh ₃	5.73
Cyclohexathione-B(C ₆ F ₅)Ph ₂	2.18
Cyclohexathione -B(C ₆ F ₅) ₂ Ph	-1.21
(Cyclohexathione-B(C ₆ F ₅) ₃)	-6.54
[Cyclohexathione-SiEt ₃] ⁺	-21.36
[Cyclohexathione-SiPhH ₂] ⁺	-30.30
Benzaldehyde-BEt ₃	7.31
Benzaldehyde-BPh ₃	4.54
Benzaldehyde-B(C ₆ F ₅)Ph ₂	0.78
Benzaldehyde-B(C ₆ F ₅) ₂ Ph	-2.83
Benzaldehyde-B(C ₆ F ₅) ₃	-10.73
[Benzaldehyde-SiEt ₃] ⁺	-25.07
[Benzaldehyde-SiPhH ₂] ⁺	-31.99
Acetophenone-BEt ₃	6.52
Acetophenone-BPh ₃	5.25
Acetophenone-B(C ₆ F ₅)Ph ₂	1.86
Acetophenone-B(C ₆ F ₅) ₂ Ph	-3.26
Complex	Binding Affinity
Acetophenone-B(C ₆ F ₅) ₃	-8.62
[Acetophenone-SiEt ₃] ⁺	-26.68
[Acetophenone-SiPhH ₂] ⁺	-34.23
N-Piperidino-cyclohex-1-ene-BEt ₃	9.35
N-Piperidino-cyclohex-1-ene-BPh ₃	11.32

N-Piperidino-cyclohex-1-ene-B(C ₆ F ₅)Ph ₂	10.72
N-Piperidino-cyclohex-1-ene-B(C ₆ F ₅) ₂ Ph	-0.21
N-Piperidino-cyclohex-1-ene-B(C ₆ F ₅) ₃	-6.09
[N-Piperidino-cyclohex-1-ene-SiEt ₃] ⁺	-32.23
[N-Piperidino-cyclohex-1-ene-SiPhH ₂] ⁺	-46.22
Phenyl-(1-phenyl-ethylidene)-amine-BEt ₃	39.68
Phenyl-(1-phenyl-ethylidene)-amine-BPh ₃	33.12
Phenyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅)Ph ₂	0.06
Phenyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅) ₂ Ph	-3.17
Phenyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅) ₃	-12.42
[Phenyl-(1-phenyl-ethylidene)-amine-SiEt ₃] ⁺	-29.83
[Phenyl-(1-phenyl-ethylidene)-amine-SiPhH ₂] ⁺	-44.70
Benzylidene Aniline-BEt ₃	3.41
Benzylidene Aniline-BPh ₃	3.19
Benzylidene Aniline-B(C ₆ F ₅)Ph ₂	-0.76
Benzylidene Aniline-B(C ₆ F ₅) ₂ Ph	-4.64
Benzylidene Aniline-B(C ₆ F ₅) ₃	-13.46
[Benzylidene Aniline-SiEt ₃] ⁺	-29.60
[Benzylidene Aniline-SiPhH ₂] ⁺	-39.21
Tert-butyl-(1-phenyl-ethylidene)-amine-BEt ₃	21.35
Tert-butyl-(1-phenyl-ethylidene)-amine-BPh ₃	14.49
Tert-butyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅)Ph ₂	14.83
Tert-butyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅) ₂ Ph	10.00
Tert-butyl-(1-phenyl-ethylidene)-amine-B(C ₆ F ₅) ₃	4.63
[Tert-butyl-(1-phenyl-ethylidene)-amine-SiEt ₃] ⁺	-24.35
[Tert-butyl-(1-phenyl-ethylidene)-amine-SiPhH ₂] ⁺	-43.29
<i>N</i> -benzylidene tert-butylamine-BEt ₃	16.14
<i>N</i> -benzylidene tert-butylamine-BPh ₃	12.99
<i>N</i> -benzylidene tert-butylamine-B(C ₆ F ₅)Ph ₂	6.99
<i>N</i> -benzylidene tert-butylamine-B(C ₆ F ₅) ₂ Ph	11.06
<i>N</i> -benzylidene tert-butylamine-B(C ₆ F ₅) ₃	2.32
[<i>N</i> -benzylidene tert-butylamine-SiEt ₃] ⁺	-21.28
[<i>N</i> -benzylidene tert-butylamine-SiPhH ₂] ⁺	-40.02

14) 3D Coordinates of All Computed Structures

The 3D coordinates are organized so that they can be readily visualized in a Mercury. For each complex, the first number is the number of atoms, followed by the complex name, and the 3D coordinates.

C	-0.00000	0.18568	-0.00000	H	-1.80627	-0.14766	1.87241
C	-1.28744	-0.61305	-0.00002	H	-0.34818	-1.08434	1.93220
C	1.28743	-0.61307	0.00002	H	-3.08873	-2.61508	-1.04983
O	0.00002	1.39500	0.00000	H	-3.36010	-0.88150	-0.84816
H	-1.32813	-1.26301	-0.87958	H	-2.93096	-1.87365	0.54429
H	-1.32911	-1.26109	0.88092	H	-0.03449	0.89596	3.37241
H	-2.13967	0.06543	-0.00116	H	0.96398	1.18802	1.94545
H	1.32813	-1.26297	0.87963	H	-0.59851	1.97332	2.09481
H	1.32906	-1.26117	-0.88088				
H	2.13968	0.06539	0.00109				
				33			
11				Isopropoxide + BEt ₃			
Isopropoxide				C	-2.23492	0.13792	0.28889
C	-1.25826	-0.63694	-0.08640	C	-3.44184	0.97554	-0.14078
C	0.00003	0.19073	0.33622	C	-2.47429	-1.33926	-0.05318
C	1.25775	-0.63782	-0.08639	O	-1.12424	0.67249	-0.33239
O	0.00063	1.41369	-0.15163	B	0.30218	0.19948	-0.07705
H	-1.30040	-1.65554	0.33383	C	1.17947	1.54855	-0.46753
H	-2.15571	-0.08975	0.22439	C	2.60743	1.68873	0.07185
H	-1.27866	-0.70519	-1.18304	C	0.50743	-0.22875	1.51063
H	0.00001	0.09851	1.48205	C	1.74911	-1.07347	1.82443
H	2.15541	-0.09089	0.22418	C	0.62755	-1.06397	-1.11269
H	1.29936	-1.65635	0.33400	C	2.07643	-1.22936	-1.58941
H	1.27788	-0.70619	-1.18301	H	-2.16213	0.20920	1.39327
				H	-3.26202	2.02647	0.10124
32				H	-4.36754	0.64773	0.34728
Acetone + BEt ₃				H	-3.56789	0.89726	-1.22626
C	1.86945	-0.37724	-0.32047	H	-1.65267	-1.95678	0.31638
C	3.10750	0.09390	-1.02249	H	-3.41351	-1.70487	0.38185
C	2.00523	-1.46168	0.70498	H	-2.51767	-1.45522	-1.14210
O	0.80148	0.15626	-0.60726	H	1.20000	1.67390	-1.56374
B	-0.79732	-0.05980	-0.05612	H	0.59612	2.40424	-0.09527
C	-1.52805	1.26357	-0.65569	H	3.26125	0.87604	-0.26616
C	-0.66723	2.52229	-0.83593	H	3.08997	2.63193	-0.22560
C	-1.25299	-1.43454	-0.78016	H	2.61202	1.66116	1.16876
C	-0.75140	-0.13118	1.56254	H	-0.35923	-0.81169	1.86277
C	-2.73803	-1.72196	-0.52287	H	0.51717	0.67230	2.14859
C	-0.06970	1.03506	2.28667	H	1.84289	-1.32738	2.89075
H	3.87188	0.35303	-0.28362	H	2.67623	-0.56898	1.53103
H	3.51024	-0.72584	-1.62633	H	1.71846	-2.01956	1.26999
H	2.88197	0.95008	-1.65620	H	0.29799	-2.03188	-0.69642
H	1.98112	-0.99496	1.69608	H	-0.00244	-0.90528	-2.00242
H	1.16352	-2.15078	0.64524	H	2.20616	-2.05381	-2.30658
H	2.95183	-1.99019	0.58734	H	2.43061	-0.31567	-2.08167
H	-2.36874	1.50886	0.01025	H	2.76114	-1.42210	-0.75453
H	-1.99178	1.03208	-1.62581				
H	-1.26608	3.39149	-1.12696	44			
H	0.08796	2.37073	-1.61327	Acetone + BPh ₃			
H	-0.12916	2.78726	0.08031	C	1.09569	0.68314	2.31618
H	-0.67283	-2.30900	-0.44666	C	1.13325	0.60704	3.80957
H	-1.09053	-1.35825	-1.86470	C	2.14192	1.48359	1.61269

O	0.19456	0.06730	1.73686	C	-2.04475	3.33802	1.18908
B	-0.09525	-0.07699	0.11396	C	-2.35679	3.84076	-0.07085
C	-1.20635	-1.24377	0.07564	C	-1.93661	3.13984	-1.20117
C	-2.31329	-1.20285	0.93661	C	-1.21877	1.95578	-1.05951
C	-3.31276	-2.16818	0.89159	C	1.35536	0.14323	-0.50140
C	-3.23799	-3.20374	-0.03936	C	-1.05297	-1.16524	-0.21445
C	-2.15889	-3.25968	-0.91445	C	1.96290	-0.90685	-1.20615
C	-1.15592	-2.29208	-0.85020	C	3.21146	-0.77724	-1.81701
C	-0.70818	1.34211	-0.35260	C	3.90114	0.42920	-1.74515
C	1.32929	-0.49449	-0.52848	C	3.32047	1.49996	-1.06615
C	-0.96930	2.43927	0.47619	C	2.07307	1.35187	-0.46671
C	-1.53690	3.61707	-0.01211	C	-1.94626	-1.79016	0.67143
C	-1.86280	3.72658	-1.35836	C	-2.88445	-2.72832	0.25013
C	-1.62764	2.64472	-2.20617	C	-2.97153	-3.07371	-1.09812
C	-1.06681	1.47579	-1.70507	C	-2.11506	-2.45915	-2.00690
C	2.00065	0.25414	-1.50328	C	-1.17938	-1.52239	-1.56592
C	3.25886	-0.11775	-1.97611	H	0.79270	-1.02067	3.49753
C	3.88626	-1.25400	-1.47368	H	2.49090	0.66266	2.69286
C	3.23880	-2.02299	-0.50786	H	3.15312	-0.92314	3.16301
C	1.97688	-1.64802	-0.05457	H	2.99372	-0.49059	1.44701
H	2.13647	0.31732	4.13605	H	0.11974	-2.86712	1.98831
H	0.94037	1.60516	4.21701	H	1.81459	-3.01991	2.51173
H	0.38899	-0.09758	4.17638	H	1.42941	-2.44973	0.87682
H	2.89953	0.78657	1.23319	H	-1.07351	1.76117	2.29692
H	1.71608	1.99747	0.74950	H	-2.36383	3.87597	2.07986
H	2.61061	2.18713	2.30188	H	-2.91791	4.76646	-0.17341
H	-2.39274	-0.38942	1.65592	H	-2.16932	3.52086	-2.19333
H	-4.15501	-2.11278	1.57540	H	-0.89449	1.42432	-1.95379
H	-4.01820	-3.95774	-0.08210	H	1.44469	-1.86151	-1.27740
H	-2.09337	-4.06003	-1.64588	H	3.64638	-1.62077	-2.34870
H	-0.31286	-2.35650	-1.53417	H	4.87488	0.53721	-2.21639
H	-0.74489	2.38546	1.54085	H	3.84424	2.45146	-1.00592
H	-1.72772	4.44621	0.66316	H	1.63308	2.19613	0.06098
H	-2.30333	4.64058	-1.74397	H	-1.88755	-1.51408	1.72261
H	-1.88911	2.71221	-3.25806	H	-3.55530	-3.19050	0.97157
H	-0.90685	0.63311	-2.37555	H	-3.70016	-3.80697	-1.43480
H	1.53619	1.15794	-1.89113	H	-2.17459	-2.71066	-3.06380
H	3.75260	0.48449	-2.73323	H	-0.52256	-1.05586	-2.29861
H	4.86837	-1.54304	-1.83522				
H	3.71449	-2.91781	-0.11683				
H	1.47162	-2.26751	0.68502				
				44			
				Acetone + B(C ₆ F ₅)Ph ₂			
				C	-2.05044	-0.69312	2.20820
				C	-2.02207	-1.04295	3.66016
				C	-3.36528	-0.57032	1.51568
				O	-0.96183	-0.50321	1.65243
				B	-0.65578	-0.09051	0.10917
				C	0.95976	0.11064	0.12807
				C	1.80672	-0.73693	0.83899
				C	3.19018	-0.62124	0.82936
				C	3.78392	0.36581	0.05561
45							
Isopropoxide + BPh ₃							
C	1.10282	-0.97524	2.43832				
C	2.52651	-0.39861	2.43093				
C	1.11271	-2.41745	1.92246				
O	0.17606	-0.13580	1.81729				
B	-0.05328	0.01542	0.35151				
C	-0.89052	1.42306	0.19701				
C	-1.32276	2.15008	1.31362				

C	2.98493	1.21163	-0.69807	C	1.53651	-1.95494	-1.02715
C	1.60264	1.06559	-0.65456	C	2.51593	-2.71853	-1.66109
C	-1.03359	-1.34271	-0.83013	C	3.81748	-2.23518	-1.76541
C	-1.49081	1.27867	-0.09314	C	4.11746	-0.98033	-1.23850
C	-1.34119	-2.62732	-0.36781	C	3.12582	-0.23446	-0.60684
C	-1.59806	-3.68075	-1.24480	C	-1.86137	-0.10687	1.04988
C	-1.54059	-3.47268	-2.61848	C	-3.21071	-0.29148	0.76350
C	-1.21283	-2.20863	-3.10566	C	-3.61188	-0.51128	-0.54355
C	-0.96037	-1.16504	-2.22154	C	-2.65038	-0.53882	-1.53980
C	-2.54084	1.42613	-1.00658	C	-1.31457	-0.34959	-1.20385
C	-3.28590	2.60275	-1.08069	F	-1.59645	0.12600	2.34692
C	-3.00063	3.66506	-0.22852	F	-4.13274	-0.24617	1.73666
C	-1.96017	3.54472	0.69122	F	-4.90667	-0.68766	-0.83968
C	-1.21877	2.36880	0.74851	F	-3.02210	-0.73458	-2.81337
F	1.30194	-1.74171	1.57381	F	-0.46509	-0.35204	-2.24919
F	5.10886	0.49040	0.02822	H	1.15696	-0.85459	3.65583
F	0.89778	1.89124	-1.43980	H	3.42941	-0.76454	2.55425
F	3.95080	-1.45302	1.54297	H	2.97798	-2.34467	3.24141
F	3.54707	2.14960	-1.46073	H	2.92336	-2.08190	1.48474
H	-2.66261	-0.35016	4.21452	H	-0.70274	-1.97244	2.51453
H	-2.44695	-2.04385	3.78906	H	0.57019	-3.13392	2.93830
H	-1.00199	-1.01671	4.03923	H	0.39907	-2.58877	1.26219
H	-3.58799	0.49996	1.41957	H	0.88566	2.36594	2.16488
H	-3.30738	-0.97673	0.50426	H	1.04347	4.80648	1.71167
H	-4.15183	-1.05617	2.09344	H	1.17167	5.62678	-0.63073
H	-1.36275	-2.82816	0.70232	H	1.13678	3.98829	-2.50090
H	-1.83384	-4.66585	-0.85323	H	0.97402	1.57034	-2.02827
H	-1.73901	-4.28975	-3.30484	H	0.52542	-2.35537	-0.96439
H	-1.15057	-2.03811	-4.17620	H	2.26248	-3.69108	-2.07649
H	-0.69070	-0.18602	-2.61413	H	4.58635	-2.82517	-2.25758
H	-2.79215	0.60042	-1.66803	H	5.12764	-0.58555	-1.31908
H	-4.09268	2.68744	-1.80274	H	3.37529	0.74050	-0.19223
H	-3.58004	4.58150	-0.28219				
H	-1.72381	4.37051	1.35579	44			
H	-0.39984	2.29278	1.46275	Acetone + B(C ₆ F ₅) ₂ Ph			
				C	0.67669	1.71856	2.43232
45				C	0.36703	1.93773	3.87584
Isopropoxide + B(C ₆ F ₅)Ph ₂				C	1.87903	2.37138	1.84016
C	1.29796	-1.12616	2.59596	O	-0.08484	0.97511	1.79925
C	2.74727	-1.61362	2.45684	B	-0.05868	0.59586	0.23600
C	0.32494	-2.27274	2.30595	C	-1.37358	-0.34668	0.07393
O	1.05886	0.05222	1.88216	C	-2.57861	0.01809	0.66885
B	0.76769	0.18534	0.44639	C	-3.75940	-0.69419	0.50807
C	0.91022	1.78410	0.11008	C	-3.76822	-1.81890	-0.30390
C	0.93435	2.73068	1.14271	C	-2.59860	-2.20684	-0.94016
C	1.02586	4.09825	0.88586	C	-1.43857	-1.46769	-0.74562
C	1.09790	4.56170	-0.42540	C	-0.31156	1.92854	-0.63307
C	1.07701	3.64112	-1.47178	C	1.36804	-0.17474	0.04495
C	0.98421	2.27768	-1.20162	C	-0.77646	3.13703	-0.10693
C	1.80795	-0.69910	-0.46760	C	-1.07860	4.22398	-0.92790
C	-0.84611	-0.15958	0.09523	C	-0.93433	4.11530	-2.30557

C	-0.49437	2.91157	-2.85585	C	3.72126	-1.58842	-0.42455
C	-0.19319	1.83779	-2.02825	C	3.60392	-0.27966	-0.85626
C	2.48614	0.33959	-0.60823	C	2.41883	0.41715	-0.62578
C	3.68781	-0.35206	-0.73453	F	-2.66417	0.71108	1.98450
C	3.80978	-1.61609	-0.18089	F	-4.80608	-0.74958	1.49378
C	2.73224	-2.16675	0.50000	F	-4.85681	-2.50941	-0.58472
C	1.55460	-1.44108	0.60226	F	-2.65184	-2.76815	-2.17564
F	-2.64733	1.11832	1.43703	F	-0.47247	-1.33192	-1.70646
F	-4.88941	-2.51388	-0.47616	F	0.52998	-2.06983	1.13285
F	-0.35016	-1.88945	-1.40903	F	2.75947	-3.43872	0.67133
F	2.48093	1.57664	-1.12587	F	4.84846	-2.27706	-0.63720
F	4.72279	0.20003	-1.36591	F	4.63016	0.30345	-1.48998
F	4.95117	-2.28768	-0.28492	F	2.43106	1.69277	-1.05229
F	2.84261	-3.37349	1.05138	H	0.55824	1.83739	3.60046
F	0.55943	-2.02068	1.28492	H	0.97041	3.53360	1.87192
F	-4.88017	-0.30237	1.11447	H	2.48939	3.08255	2.67755
F	-2.59752	-3.27862	-1.73193	H	2.11954	2.48021	1.05015
H	1.26565	1.78046	4.47893	H	2.64009	0.78264	3.90553
H	0.07214	2.98481	4.00682	H	2.77058	0.25829	2.22158
H	-0.44113	1.28347	4.19761	H	1.56358	-0.49338	3.28457
H	2.70710	1.65531	1.92808	H	0.21447	1.18851	-2.33112
H	1.74151	2.60041	0.78328	H	-0.53853	3.10879	-3.68052
H	2.14203	3.26544	2.40694	H	-1.63775	5.05228	-2.58705
H	-0.93318	3.24110	0.96582	H	-1.99371	5.02751	-0.12696
H	-1.43591	5.15056	-0.48888	H	-1.23966	3.07789	1.21398
H	-1.16953	4.95725	-2.94874				
H	-0.38705	2.81288	-3.93162				
H	0.14409	0.90169	-2.47093				

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Acetone + B(C₆F₅)₃

45				C	-0.31977	-0.93946	2.88472
Isopropoxide + B(C ₆ F ₅) ₂ Ph				C	-0.10381	-0.69900	4.33811
C	1.01395	1.50218	2.65479	C	-0.82087	-2.27151	2.44154
C	1.68627	2.72320	2.02357	O	-0.06778	0.00021	2.11634
C	2.06440	0.44636	3.03569	B	-0.08142	-0.00801	0.52470
O	-0.04967	0.96722	1.91620	C	0.48493	1.46306	0.14808
B	-0.06983	0.69879	0.47731	C	1.66462	1.89594	0.74884
C	-1.40370	-0.26876	0.20852	C	2.26846	3.11210	0.46599
C	-2.56747	-0.15517	0.96751	C	1.68938	3.94659	-0.48028
C	-3.71925	-0.89790	0.72246	C	0.52583	3.54890	-1.12167
C	-3.75425	-1.79049	-0.33556	C	-0.04905	2.32323	-0.80433
C	-2.63299	-1.91875	-1.13848	C	1.01559	-1.08400	-0.01372
C	-1.50561	-1.15778	-0.85715	C	-1.63431	-0.28553	0.13651
C	-0.40994	2.00900	-0.44238	C	1.96603	-1.77980	0.72032
C	1.31679	-0.12036	0.02874	C	2.94459	-2.58114	0.14142
C	-0.25364	2.03783	-1.83565	C	3.00437	-2.69114	-1.23823
C	-0.68376	3.11649	-2.60289	C	2.08124	-2.00484	-2.01915
C	-1.30252	4.20655	-1.99239	C	1.12418	-1.22107	-1.39613
C	-1.49649	4.19172	-0.61390	C	-2.12973	-1.41767	-0.50084
C	-1.06245	3.10279	0.14083	C	-3.47659	-1.60393	-0.79340
C	1.49705	-1.43883	0.44787	C	-4.39199	-0.62594	-0.43620
C	2.65295	-2.17578	0.23807	C	-3.94995	0.51790	0.21607

C	-2.59766	0.65862	0.48863
F	2.28092	1.10659	1.64507
F	2.24932	5.11615	-0.77238
F	-1.16405	2.00327	-1.47042
F	-1.31547	-2.43355	-0.82893
F	-3.89173	-2.71601	-1.39596
F	-5.68314	-0.78819	-0.70061
F	-4.82202	1.45692	0.57495
F	-2.22213	1.77608	1.12374
F	1.97606	-1.73417	2.07212
F	3.81939	-3.23553	0.90325
F	3.93211	-3.45014	-1.81077
F	2.13118	-2.10343	-3.34434
F	0.25438	-0.56739	-2.17683
F	3.39298	3.47805	1.07960
F	-0.02975	4.34120	-2.03618
H	-0.88306	-1.17487	4.93669
H	0.85043	-1.17782	4.59053
H	-0.03297	0.36733	4.54560
H	-1.91497	-2.24492	2.52904
H	-0.56528	-2.50318	1.40867
H	-0.45033	-3.04469	3.11678

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Isopropoxide + B(C₆F₅)₃

C	-0.67886	-0.82754	3.05620
C	-1.32852	-2.08775	2.47591
C	-1.67517	-0.07919	3.93965
O	-0.16323	0.09519	2.13221
B	-0.07826	-0.02492	0.69207
C	0.61200	1.40364	0.20027
C	1.80027	1.79313	0.81800
C	2.48296	2.96265	0.50817
C	1.98635	3.79907	-0.47980
C	0.82339	3.44374	-1.14096
C	0.17114	2.26265	-0.79877
C	1.00061	-1.15204	0.11266
C	-1.60034	-0.22805	0.05614
C	1.19389	-1.26538	-1.26167
C	2.15099	-2.07684	-1.84913
C	2.99400	-2.82061	-1.03384
C	2.85356	-2.73551	0.34007
C	1.87471	-1.90518	0.88285
C	-2.55695	0.74292	0.34420
C	-3.89408	0.64742	-0.01431
C	-4.33170	-0.47363	-0.70455
C	-3.42292	-1.47009	-1.01605
C	-2.09232	-1.32918	-0.63184
F	2.37257	1.01413	1.74563
F	3.62030	3.28622	1.13794
F	2.62829	4.93006	-0.79548

F	0.34102	4.23887	-2.10501
F	-0.93663	1.99941	-1.50965
F	-2.20278	1.85826	0.99837
F	-4.76450	1.61883	0.28886
F	-5.61573	-0.59056	-1.06101
F	-3.83677	-2.56365	-1.66950
F	-1.30324	-2.37689	-0.92885
F	0.41056	-0.55892	-2.09452
F	2.28140	-2.15118	-3.17970
F	3.92886	-3.61189	-1.57276
F	3.66400	-3.44881	1.13325
F	1.81473	-1.88938	2.22320
H	0.15797	-1.16198	3.68769
H	-0.71650	-2.53761	1.68932
H	-1.45211	-2.82633	3.27494
H	-2.31808	-1.87409	2.06070
H	-2.05457	-0.71567	4.74693
H	-2.51976	0.26159	3.33134
H	-1.19645	0.80132	4.37485

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Acetone + proton

C	0.135630	0.238016	-0.560400
O	0.294754	0.972469	-1.586565
C	0.417713	-1.209189	-0.592373
C	-0.345876	0.922361	0.649031
H	0.642075	0.510148	-2.374060
H	1.017998	-1.514646	-1.451128
H	0.894926	-1.517732	0.341946
H	-0.553242	-1.724890	-0.629990
H	-0.812257	1.877601	0.409200
H	-1.010230	0.272096	1.222543
H	0.538526	1.108551	1.277809

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Isopropanol

C	-0.00139	0.04587	0.36883
C	-1.32169	-0.54850	-0.08882
C	1.18987	-0.77970	-0.10292
O	0.04821	1.35973	-0.16671
H	0.00610	0.08872	1.47009
H	-2.15214	0.07931	0.24071
H	-1.45604	-1.55528	0.31476
H	-1.34146	-0.60038	-1.18126
H	2.13404	-0.33006	0.22264
H	1.14879	-1.79694	0.29645
H	1.19297	-0.83059	-1.19558
H	0.88135	1.76136	0.10339

32				H	-2.22434	-2.07771	-1.61954
Acetone + [SiEt ₃] ⁺				H	-1.09609	-1.19084	-2.64799
Si	0.74550	0.05715	0.02991	H	-0.00902	1.37870	2.01530
C	1.62887	1.58091	-0.56263	H	-1.73980	1.12617	2.04681
C	1.24958	2.86554	0.18969	H	-1.14121	3.54125	1.47326
C	1.03363	-1.44583	-1.04235	H	-2.04383	2.77338	0.16528
C	2.54900	-1.64146	-1.25612	H	-0.29747	2.96645	0.02993
C	0.80010	-0.24213	1.86847	H	-0.43075	-2.46185	0.26110
C	-0.19135	-1.28960	2.39412	H	-1.78923	-1.91424	1.21642
O	-0.99078	0.59835	-0.20337	H	0.00799	-2.75800	2.73708
C	-2.10328	0.07088	-0.42409	H	-0.20185	-1.02427	2.98621
C	-3.28276	0.96445	-0.51697	H	1.16741	-1.62277	2.05119
C	-2.26920	-1.39612	-0.60978	H	1.91712	0.27679	0.88571
H	1.44507	1.69206	-1.63855	H	3.61402	-1.26035	-0.11501
H	2.70565	1.39180	-0.46621	H	2.00019	-2.00256	-0.13247
H	1.77767	3.72509	-0.22684	H	2.66624	-1.30637	-1.61951
H	1.51273	2.80172	1.24859	H	3.80552	1.31603	-0.37950
H	0.17786	3.07030	0.12017	H	2.31426	2.27357	-0.51707
H	0.53999	-1.32155	-2.01384	H	2.82720	1.23995	-1.86293
H	0.61076	-2.34518	-0.58164				
H	2.73996	-2.54830	-1.83241				
H	3.08352	-1.74185	-0.30634	24			
H	2.98712	-0.80336	-1.80354	Acetone + [SiPhH ₂] ⁺			
H	0.65319	0.71427	2.38259	C	-3.15370	0.45075	-1.17044
H	1.82840	-0.54896	2.10173	C	-3.78818	0.61143	0.06025
H	-0.06373	-1.44227	3.46734	C	-3.13999	0.26056	1.24330
H	-0.05200	-2.26204	1.91105	C	-1.84918	-0.25151	1.19808
H	-1.22907	-0.97398	2.24030	C	-1.19510	-0.41141	-0.03517
H	-2.98658	2.01101	-0.55535	C	-1.86308	-0.06114	-1.22083
H	-3.89115	0.68969	-1.38386	Si	0.50013	-1.07618	-0.09550
H	-3.90720	0.78716	0.36830	O	1.61237	0.35422	-0.00620
H	-1.55643	-1.96450	-0.01220	C	2.86721	0.41238	0.02587
H	-3.29128	-1.70134	-0.38328	C	3.49362	1.74870	0.10230
H	-2.08287	-1.61654	-1.66972	C	3.69410	-0.82298	-0.00456
				H	-3.66749	0.71793	-2.08721
				H	-4.79793	1.00666	0.09705
33				H	-3.64320	0.38025	2.19632
Isopropoxide + [SiEt ₃] ⁺				H	-1.35556	-0.53324	2.12476
Si	-0.72800	-0.01567	0.10573	H	-1.38042	-0.19417	-2.18573
C	-2.09798	0.05587	-1.17148	H	0.93490	-1.84353	1.08475
C	-2.06519	-1.13029	-2.14428	H	0.91846	-1.67251	-1.37595
C	-0.90247	1.36319	1.37717	H	2.74668	2.53797	0.15719
C	-1.10737	2.73925	0.73040	H	4.16157	1.77766	0.97101
C	-0.74018	-1.69011	0.97722	H	4.13436	1.88170	-0.77805
C	0.10352	-1.78023	2.25601	H	3.40623	-1.44418	-0.86013
O	0.67413	0.21936	-0.77578	H	4.75769	-0.59626	-0.05274
C	1.97710	0.16265	-0.20966	H	3.48970	-1.40615	0.90247
C	2.60633	-1.18547	-0.53399				
C	2.78518	1.32136	-0.77300	25			
H	-1.99565	0.99674	-1.72529	Isopropoxide + [SiPhH ₂] ⁺			
H	-3.06762	0.10467	-0.65927	C	-3.62226	-0.67806	-0.14901
H	-2.83778	-1.04760	-2.91404				

C	-3.81426	0.70166	-0.13577	O	-2.76562	-0.54413	-0.00034
C	-2.72029	1.55544	-0.02181	H	1.62461	-2.38795	0.00006
C	-1.43551	1.02954	0.08561	H	3.31365	-0.56851	-0.00018
C	-1.22530	-0.35513	0.07860	H	2.56692	1.80173	-0.00020
C	-2.33604	-1.19922	-0.04651	H	0.13815	2.33854	-0.00004
Si	0.49651	-1.04454	0.25670	H	-0.86269	-1.77405	0.00010
O	1.52995	0.18463	-0.15421	H	-2.14924	1.25788	-0.88006
C	2.88860	0.22544	0.27270	H	-2.14944	1.25702	0.88107
C	3.70357	-0.83961	-0.44958				
C	3.40519	1.62670	-0.00457				
H	-4.47326	-1.34494	-0.24537	36			
H	-4.81641	1.11055	-0.21945	Benzaldehyde + BEt ₃			
H	-2.86853	2.63082	-0.01902	C	-2.18334	0.11733	1.15288
H	-0.58013	1.69512	0.16313	C	-3.52900	0.09108	1.48415
H	-2.19842	-2.27842	-0.07246	C	-4.49293	0.00169	0.47671
H	0.80348	-1.46606	1.65145	C	-4.11895	-0.06165	-0.86403
H	0.63911	-2.24151	-0.61198	C	-2.77145	-0.03515	-1.20237
H	2.92629	0.03310	1.35659	C	-1.80617	0.05461	-0.19500
H	4.75471	-0.79173	-0.15233	C	-0.39659	0.07636	-0.56775
H	3.33344	-1.84473	-0.22355	O	0.50550	0.14357	0.26458
H	3.63570	-0.68372	-1.53017	B	2.13428	0.15042	-0.24557
H	4.43895	1.73299	0.33469	C	2.27072	-1.09719	-1.28523
H	2.78745	2.36651	0.50916	C	2.91882	0.04547	1.15717
H	3.36455	1.82801	-1.07881	C	2.27832	1.58625	-0.98155
				C	1.48354	-2.38823	-1.01896
14				C	2.14771	2.82084	-0.08599
Benzaldehyde				C	2.87904	-1.30222	1.88259
C	-1.73255	1.05605	-0.00002	H	-1.41071	0.18516	1.91173
C	-2.20725	-0.25341	0.00003	H	-3.83416	0.13927	2.52366
C	-1.31728	-1.32936	0.00005	H	-5.54521	-0.01893	0.74160
C	0.05079	-1.09619	0.00003	H	-4.87463	-0.13161	-1.63847
C	0.52853	0.21697	-0.00001	H	-2.46141	-0.08446	-2.24273
C	-0.36116	1.29072	-0.00004	H	-0.13685	0.03194	-1.63593
C	1.98918	0.47129	-0.00003	H	2.05742	-0.76960	-2.31530
O	2.82852	-0.39783	-0.00001	H	3.34173	-1.34766	-1.29626
H	-2.42893	1.88788	-0.00004	H	2.54630	0.82508	1.83693
H	-3.27672	-0.43878	0.00005	H	3.96869	0.31434	0.96504
H	-1.69666	-2.34590	0.00009	H	1.55820	1.66146	-1.81379
H	0.77061	-1.90859	0.00005	H	3.26301	1.59721	-1.47129
H	0.02483	2.30740	-0.00007	H	1.74899	-3.18040	-1.72644
H	2.27718	1.54421	-0.00006	H	0.39865	-2.24505	-1.11641
				H	1.65511	-2.77270	-0.01077
15				H	2.21171	3.75848	-0.64782
Benzylalkoxide				H	1.19043	2.82306	0.44942
C	1.29872	-1.34874	0.00007	H	2.93500	2.83853	0.67355
C	2.25226	-0.33087	-0.00005	H	3.39869	-1.27387	2.84630
C	1.82984	1.00041	-0.00011	H	1.84667	-1.61603	2.07857
C	0.46974	1.29898	-0.00002	H	3.34870	-2.08997	1.28382
C	-0.49233	0.28547	0.00011				
C	-0.05991	-1.03912	0.00014	37			
C	-2.02448	0.53861	0.00019	Benzylalcoxide + BEt ₃			
				C	2.88052	-1.44620	0.01295

C	4.20264	-1.01579	0.05539	C	0.573658	2.154090	-1.513734
C	4.49924	0.33960	-0.08339	C	0.532984	3.519171	-1.778858
C	3.46167	1.25099	-0.26322	C	0.831413	4.431359	-0.767229
C	2.13837	0.81629	-0.30365	C	1.167092	3.963599	0.498565
C	1.83356	-0.53760	-0.16431	C	1.193064	2.591932	0.754629
C	0.38871	-1.00309	-0.18435	C	1.388485	-2.183892	-1.243500
O	-0.45823	-0.00334	-0.59983	C	2.089413	-2.974615	-2.148386
B	-1.90107	-0.09448	-0.12962	C	3.116766	-2.418039	-2.908382
C	-2.69610	1.06221	-0.98170	C	3.430377	-1.072116	-2.752212
C	-2.51899	-1.58172	-0.49539	C	2.712921	-0.287753	-1.849393
C	-1.97104	0.15743	1.51468	C	2.261133	-1.172926	1.902690
C	-2.18443	2.49103	-0.77822	C	2.509163	-1.535647	3.225539
C	-0.86819	1.06014	2.08349	C	1.636352	-1.140811	4.234266
C	-3.98445	-1.76968	-0.09035	C	0.517896	-0.375120	3.911220
H	2.64990	-2.50520	0.11589	C	0.287514	-0.015253	2.587155
H	5.00443	-1.73668	0.19342	H	-2.431287	-2.231542	-0.535551
H	5.53071	0.67973	-0.05321	H	-4.781101	-3.060353	-0.726256
H	3.68521	2.30904	-0.37311	H	-6.663271	-1.465633	-0.533156
H	1.30723	1.49954	-0.44460	H	-6.237299	0.943934	-0.152630
H	0.33288	-1.90545	-0.82708	H	-3.896200	1.765640	0.036969
H	0.14638	-1.36138	0.83662	H	-1.522329	1.390094	0.043226
H	-2.61902	0.81353	-2.05273	H	0.360244	1.450516	-2.317817
H	-3.77247	1.04277	-0.74759	H	0.279802	3.873742	-2.773990
H	-2.41929	-1.77679	-1.57634	H	0.808708	5.498006	-0.969432
H	-1.93033	-2.37108	0.00271	H	1.410499	4.666255	1.290242
H	-2.94996	0.59291	1.77639	H	1.457810	2.243342	1.749477
H	-1.93967	-0.79953	2.06583	H	0.602534	-2.636238	-0.641300
H	-2.63445	3.22353	-1.46453	H	1.841627	-4.026605	-2.258868
H	-2.38977	2.84004	0.24109	H	3.669971	-3.031572	-3.613218
H	-1.09770	2.52759	-0.91892	H	4.233513	-0.629538	-3.334469
H	-0.85809	2.03878	1.59238	H	2.967020	0.764079	-1.742807
H	-0.96481	1.23557	3.16497	H	2.946586	-1.496253	1.123592
H	0.12509	0.62873	1.91207	H	3.384270	-2.131319	3.468697
H	-4.11738	-1.57296	0.98091	H	1.824032	-1.426039	5.265057
H	-4.63443	-1.06567	-0.62275	H	-0.169926	-0.059647	4.690505
H	-4.37246	-2.77974	-0.28633	H	-0.587012	0.597586	2.362681

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Benzylaldehyde + BPh₃

C	-3.276054	-1.555172	-0.454236
C	-4.581847	-2.007423	-0.559602
C	-5.642854	-1.105058	-0.450173
C	-5.407083	0.251443	-0.235867
C	-4.100418	0.711294	-0.129485
C	-3.037515	-0.191169	-0.238451
C	-1.677503	0.315037	-0.122932
O	-0.696271	-0.426250	-0.212423
B	0.894092	0.058794	0.021280
C	1.674393	-0.819684	-1.075710
C	1.147253	-0.401444	1.548408
C	0.897306	1.651221	-0.239948

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Benzylalcooxide + BPh₃

C	-3.169019	-1.386610	-0.294552
C	-4.423637	-1.993175	-0.314590
C	-5.550092	-1.299123	0.117056
C	-5.413792	0.012466	0.570241
C	-4.160931	0.615594	0.588433
C	-3.024966	-0.075761	0.159144
C	-1.660511	0.581116	0.202957
O	-0.713943	-0.218640	-0.409198
B	0.728275	0.073492	-0.143946
C	1.561809	-0.929335	-1.131838
C	1.082400	-0.279299	1.420561
C	1.060331	1.648117	-0.511842

C	1.430591	2.032162	-1.810376	C	-0.11628	1.26183	1.68364
C	1.623906	3.365169	-2.168220	C	0.58868	2.04595	-0.83324
C	1.450186	4.375043	-1.225063	C	0.46975	1.86761	-2.21953
C	1.079740	4.031251	0.072581	C	0.77497	2.88440	-3.11785
C	0.891825	2.691813	0.412507	C	1.21974	4.11781	-2.64593
C	0.922053	-1.597047	-2.185703	C	1.35538	4.31740	-1.27597
C	1.615440	-2.426984	-3.066908	C	1.03992	3.29272	-0.38530
C	2.986672	-2.615313	-2.918535	C	0.88670	-1.70901	0.48018
C	3.650090	-1.963984	-1.879852	C	1.69368	-2.83416	0.39719
C	2.943283	-1.139287	-1.007740	C	2.97495	-2.70269	-0.11859
C	2.179928	0.250782	2.115969	C	3.41651	-1.45477	-0.53034
C	2.487378	-0.128571	3.422534	C	2.57016	-0.35384	-0.43233
C	1.687862	-1.055163	4.086676	C	-1.02340	2.31446	1.90200
C	0.585378	-1.594555	3.426472	C	-1.42369	2.68665	3.18152
C	0.298113	-1.210896	2.118876	C	-0.91347	2.01439	4.29108
H	-2.277276	-1.907029	-0.628088	C	-0.00884	0.97409	4.10580
H	-4.521687	-3.015501	-0.670145	C	0.37527	0.60343	2.81735
H	-6.527214	-1.773522	0.100001	F	4.65087	-1.31966	-1.01276
H	-6.286255	0.565607	0.907560	F	3.77408	-3.76228	-0.20669
H	-4.055621	1.640763	0.938497	F	1.25806	-4.02462	0.81130
H	-1.730110	1.577891	-0.270590	F	-0.33562	-1.90082	1.02270
H	-1.409730	0.770868	1.264643	F	3.08547	0.81078	-0.82953
H	1.573878	1.256696	-2.560435	H	-4.26540	-1.14022	1.33261
H	1.912933	3.618663	-3.185969	H	-6.28272	-2.09888	0.23427
H	1.602738	5.416442	-1.497584	H	-6.39763	-2.20747	-2.23575
H	0.938357	4.807820	0.821353	H	-4.52531	-1.37074	-3.62134
H	0.610361	2.443120	1.435253	H	-2.50106	-0.41033	-2.51614
H	-0.147878	-1.449177	-2.307009	H	-2.09926	-0.10796	1.22727
H	1.083505	-2.928607	-3.872886	H	0.13856	0.90442	-2.60349
H	3.532207	-3.262163	-3.601291	H	0.67232	2.71647	-4.18604
H	4.721164	-2.103253	-1.749541	H	1.46192	4.91476	-3.34233
H	3.478413	-0.647105	-0.196878	H	1.70715	5.27305	-0.89855
H	2.804467	0.993920	1.621194	H	1.15183	3.46555	0.68203
H	3.348686	0.304600	3.926685	H	-1.41366	2.85901	1.04351
H	1.918378	-1.350671	5.107181	H	-2.12514	3.50472	3.31594
H	-0.050730	-2.315816	3.935175	H	-1.21633	2.30427	5.29254
H	-0.564717	-1.635490	1.607184	H	0.39797	0.44834	4.96432
				H	1.08433	-0.21151	2.69511

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Benzaldehyde + B(C₆F₅)Ph₂

C	-4.33219	-1.19534	0.24961
C	-5.45735	-1.73054	-0.36450
C	-5.51825	-1.79049	-1.75538
C	-4.46210	-1.31950	-2.54006
C	-3.33549	-0.78739	-1.93389
C	-3.27234	-0.72721	-0.53459
C	-2.10511	-0.17748	0.13316
O	-1.12292	0.21937	-0.50283
B	0.26070	0.84012	0.17686
C	1.26890	-0.43660	0.06084

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Benzylalcooxide + B(C₆F₅)Ph₂

C	3.56688	-1.52000	-1.81700
C	4.68003	-2.08189	-1.20043
C	5.34521	-1.38181	-0.19519
C	4.89354	-0.11961	0.17958
C	3.77864	0.43672	-0.44265
C	3.09801	-0.25940	-1.44123
C	1.82420	0.29417	-2.05542
O	0.66612	-0.25689	-1.50889
B	0.09327	0.25762	-0.23821
C	-1.51327	-0.20532	-0.25504

C	0.18878	1.89806	-0.22653	O	-1.05429	-0.83596	-0.22422
C	0.72655	-0.46158	1.09016	B	0.12707	0.03770	0.42271
C	0.50079	0.01122	2.39294	C	1.48401	-0.66526	-0.12915
C	1.00505	-0.64394	3.51530	C	0.02794	-0.09828	2.02800
C	1.75130	-1.81091	3.36651	C	-0.19605	1.52164	-0.16757
C	1.96631	-2.31922	2.08727	C	0.67621	2.32876	-0.89380
C	1.45114	-1.65615	0.97584	C	0.33090	3.59318	-1.36277
C	-1.98731	-1.32635	-0.93521	C	-0.93657	4.09786	-1.11822
C	-3.32072	-1.72752	-0.92142	C	-1.84599	3.33053	-0.40419
C	-4.24957	-1.00961	-0.18699	C	-1.45592	2.07905	0.04760
C	-3.82514	0.09657	0.53049	C	1.59667	-1.75137	-0.98770
C	-2.48463	0.46207	0.48818	C	2.81927	-2.32373	-1.33231
C	1.04189	2.64373	0.59687	C	3.99081	-1.80509	-0.80894
C	1.16233	4.03037	0.48235	C	3.92882	-0.71602	0.05263
C	0.42373	4.71974	-0.47348	C	2.69219	-0.18117	0.37145
C	-0.43045	4.00549	-1.31336	C	-0.26625	0.96671	2.88624
C	-0.53659	2.62418	-1.18569	C	-0.35098	0.79018	4.26620
F	-4.71039	0.79417	1.25768	C	-0.15314	-0.46955	4.82285
F	-5.53596	-1.38477	-0.16269	C	0.14230	-1.54856	3.99220
F	-3.71918	-2.81099	-1.60543	C	0.23830	-1.35587	2.61752
F	-1.17164	-2.11842	-1.64303	F	5.05074	-0.20464	0.55624
F	-2.16107	1.53016	1.23959	F	5.16580	-2.34064	-1.12874
H	3.02963	-2.07053	-2.58611	F	2.86434	-3.36976	-2.15884
H	5.02799	-3.06717	-1.49834	F	0.51677	-2.33400	-1.54311
H	6.20988	-1.82024	0.29472	F	2.67519	0.87865	1.18860
H	5.40336	0.42774	0.96708	F	1.20803	4.31933	-2.05211
H	3.40873	1.41352	-0.14087	F	-1.27917	5.30213	-1.56368
H	1.84220	1.39120	-1.96992	F	-3.07064	3.79602	-0.16174
H	1.82897	0.05067	-3.12878	F	-2.38576	1.38473	0.73761
H	-0.09070	0.91505	2.52809	F	1.91308	1.92404	-1.19656
H	0.81534	-0.24360	4.50878	H	-1.92892	-2.15254	-2.14180
H	2.15408	-2.32126	4.23782	H	-3.68874	-3.48852	-3.31670
H	2.53955	-3.23395	1.95435	H	-5.77762	-4.07552	-2.12759
H	1.61265	-2.06279	-0.01851	H	-6.14125	-3.36009	0.21319
H	1.63022	2.12484	1.35099	H	-4.38884	-2.03283	1.38162
H	1.83592	4.57229	1.14231	H	-2.18644	-1.01097	1.43401
H	0.51199	5.79901	-0.56630	H	-0.41606	1.96113	2.47406
H	-1.01239	4.52996	-2.06776	H	-0.57081	1.63855	4.90705
H	-1.19873	2.07684	-1.85550	H	-0.22007	-0.60947	5.89722
				H	0.31014	-2.53365	4.41700
				H	0.49342	-2.20361	1.98183

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Benzaldehyde + B(C₆F₅)₂Ph

C	-2.86113	-2.41666	-1.65310
C	-3.83803	-3.16133	-2.29385
C	-5.01571	-3.49366	-1.61874
C	-5.22419	-3.09313	-0.29964
C	-4.24765	-2.35304	0.35309
C	-3.07272	-2.00994	-0.32663
C	-2.06493	-1.23790	0.36904

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Benzylalcooxide + B(C₆F₅)₂Ph

C	3.14090	-2.36753	-1.23350
C	4.13116	-3.25391	-1.65482
C	5.47089	-2.87770	-1.63828
C	5.81955	-1.60207	-1.19604
C	4.83193	-0.71805	-0.77659
C	3.48543	-1.09146	-0.78943
C	2.42284	-0.12497	-0.31375

O	1.15524	-0.65963	-0.50757	C	1.47509	3.50323	0.05714
B	0.05341	-0.08114	0.26923	C	0.52496	2.44746	-0.19623
C	-1.32783	-0.88986	-0.15463	O	0.74399	1.29715	0.20312
C	0.19951	-0.36698	1.87165	B	-0.07758	-0.02563	-0.05692
C	-0.02647	1.55153	-0.08098	C	-0.03489	-0.74762	1.39938
C	0.71963	2.50020	0.61355	C	0.81961	-0.89267	-1.09249
C	0.75506	3.85357	0.28893	C	-1.55696	0.40579	-0.56838
C	0.02839	4.31205	-0.79614	C	-2.32940	1.23271	0.24685
C	-0.71369	3.40706	-1.53900	C	-3.62302	1.62861	-0.04772
C	-0.71415	2.06569	-1.17759	C	-4.20779	1.17596	-1.22450
C	-2.59855	-0.34645	0.01220	C	-3.48318	0.35643	-2.07461
C	-3.78071	-1.02693	-0.24151	C	-2.18031	-0.00747	-1.74153
C	-3.72511	-2.34459	-0.66855	C	1.18338	-0.86040	2.06726
C	-2.48814	-2.94501	-0.82582	C	1.32846	-1.48243	3.29877
C	-1.32802	-2.22199	-0.55933	C	0.21449	-2.04490	3.90634
C	0.99312	-1.43421	2.31050	C	-1.01619	-1.97542	3.27147
C	1.08180	-1.77670	3.65907	C	-1.11876	-1.33850	2.03959
C	0.36135	-1.05895	4.60990	C	0.41554	-2.20245	-1.33687
C	-0.44697	-0.00084	4.19656	C	1.12101	-3.08682	-2.13518
C	-0.52204	0.33392	2.84764	C	2.30678	-2.66192	-2.72360
F	-2.42094	-4.22367	-1.22107	C	2.75115	-1.36776	-2.50749
F	-4.85009	-3.02642	-0.91699	C	2.00727	-0.51165	-1.70084
F	-4.96995	-0.43297	-0.07520	F	-2.08804	-2.51950	3.84386
F	-2.74177	0.92309	0.43811	F	0.32818	-2.64764	5.08543
F	-0.19009	-2.92093	-0.69961	F	2.51865	-1.55103	3.89392
F	1.49372	4.71350	1.00292	F	2.30371	-0.36002	1.51567
F	0.04908	5.60748	-1.12980	F	-2.33675	-1.32467	1.48536
F	-1.41096	3.83732	-2.59865	F	-4.30175	2.42995	0.77048
F	-1.44283	1.26172	-1.96767	F	-5.44573	1.54025	-1.53686
F	1.49042	2.14728	1.65554	F	-4.03136	-0.06797	-3.21006
H	2.09075	-2.63903	-1.23946	F	-1.55233	-0.78057	-2.63126
H	3.85199	-4.24603	-1.99859	F	-1.79237	1.70170	1.38810
H	6.23973	-3.57087	-1.96713	F	3.88492	-0.95022	-3.07001
H	6.86234	-1.29755	-1.17920	F	3.00499	-3.49092	-3.49327
H	5.10413	0.27774	-0.43224	F	0.68423	-4.32682	-2.34247
H	2.60897	0.10357	0.74918	F	-0.73070	-2.63432	-0.79244
H	2.54620	0.83111	-0.85664	F	2.50676	0.72928	-1.54811
H	1.54722	-2.00559	1.56685	H	2.90424	2.17635	0.96432
H	1.71249	-2.60657	3.96861	H	4.55740	4.01301	1.37696
H	0.42604	-1.32158	5.66246	H	4.01400	6.32530	0.68467
H	-1.01721	0.56433	4.92986	H	1.85906	6.84323	-0.41435
H	-1.16005	1.16064	2.53810	H	0.21808	5.01894	-0.82796
				H	-0.39372	2.65834	-0.75854

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Benzaldehyde + B(C₆F₅)₃

C	2.69828	3.20341	0.67899
C	3.60656	4.22491	0.90129
C	3.29710	5.52992	0.50750
C	2.08362	5.82652	-0.11295
C	1.16807	4.80977	-0.34395

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Benzylalcoholoxide + B(C₆F₅)₃

C	-3.10438	-1.97920	-1.91999
C	-4.23413	-2.50939	-2.53853
C	-4.50365	-3.87392	-2.47031
C	-3.63152	-4.71173	-1.77841
C	-2.50065	-4.18238	-1.16488

C	-2.22872	-2.81451	-1.22695	C	-0.01748	-1.11460	-0.00003
C	-1.01138	-2.24627	-0.53241	C	-0.47650	0.22864	0.00001
O	-0.74180	-0.96236	-0.99415	C	0.43795	1.31185	0.00003
B	0.08730	-0.10756	-0.15720	C	-1.84370	0.53209	0.00004
C	-0.67490	0.38583	1.23261	O	-2.73178	-0.40010	0.00003
C	1.50717	-0.91119	0.14140	H	2.50971	1.86600	0.00002
C	0.29930	1.30405	-0.98656	H	3.30344	-0.47634	-0.00006
C	1.48380	2.01595	-1.13655	H	1.71544	-2.37097	-0.00010
C	1.57365	3.21936	-1.82908	H	-0.73431	-1.92897	-0.00005
C	0.43514	3.77106	-2.39235	H	0.06951	2.33391	0.00007
C	-0.77674	3.11355	-2.24777	H	-2.18160	1.57018	0.00008
C	-0.82102	1.91521	-1.54637	H	-3.64827	-0.07730	0.00005
C	0.02488	1.14822	2.16349				
C	-0.54614	1.71760	3.29014	16			
C	-1.90499	1.54221	3.51594	Benzylalcohol			
C	-2.65142	0.80509	2.61344	C	-1.35057	1.35068	0.00654
C	-2.03282	0.25236	1.49304	C	-2.29607	0.33089	-0.00604
C	1.86708	-1.52890	1.33173	C	-1.87552	-0.99809	-0.01143
C	3.00947	-2.31104	1.48222	C	-0.51840	-1.29712	-0.00459
C	3.84215	-2.51656	0.39648	C	0.43362	-0.27549	0.00972
C	3.52023	-1.93529	-0.82171	C	0.01081	1.05111	0.01510
C	2.37088	-1.16481	-0.92232	C	1.90085	-0.63163	0.02722
F	-3.96250	0.63573	2.82431	O	2.67568	0.54476	-0.04195
F	-2.48422	2.08117	4.59455	H	-1.67163	2.38769	0.00960
F	0.18206	2.43581	4.15391	H	-3.35525	0.56715	-0.01270
F	1.33921	1.36147	1.98039	H	-2.60588	-1.80098	-0.02278
F	-2.84104	-0.43911	0.67624	H	-0.19234	-2.33504	-0.01118
F	2.74641	3.85278	-1.95367	H	0.75447	1.83933	0.02389
F	0.50160	4.92820	-3.05971	H	2.11464	-1.30077	-0.82047
F	-1.88728	3.65007	-2.76857	H	2.11781	-1.19668	0.94704
F	-2.03950	1.37222	-1.39883	H	3.60444	0.29915	0.00315
F	2.63509	1.56942	-0.61285				
F	4.31801	-2.13109	-1.87855				
F	4.94154	-3.26814	0.51722				
F	3.30167	-2.87870	2.65927	36			
F	1.10500	-1.41696	2.43329	Benzylaldehyde + [SiEt ₃] ⁺			
F	2.12157	-0.63603	-2.12853	C	2.57117	-1.09607	-0.43648
H	-2.87699	-0.91946	-1.95631	C	3.92109	-1.33885	-0.59742
H	-4.91003	-1.85084	-3.07670	C	4.85720	-0.44984	-0.05232
H	-5.38562	-4.28351	-2.95414	C	4.45719	0.68600	0.65524
H	-3.82965	-5.77842	-1.72214	C	3.10679	0.94083	0.82259
H	-1.81495	-4.83832	-0.63219	C	2.16003	0.05005	0.27773
H	-1.19639	-2.25291	0.55719	C	0.78195	0.34357	0.46631
H	-0.15482	-2.92345	-0.70056	O	-0.13743	-0.39602	0.02000
				Si	-1.93234	-0.15993	0.10510
				C	-2.39280	-0.16262	-1.70228
15				C	-2.50691	-1.64419	1.06613
Benzaldehyde + proton				C	-2.18491	1.46644	0.99148
C	1.79412	1.05252	0.00001	C	-4.04374	-1.75007	1.04682
C	2.23656	-0.27503	-0.00004	C	-1.89312	2.73873	0.17994
C	1.33911	-1.35476	-0.00006	C	-1.36840	0.51034	-2.63114

H	1.82385	-1.76719	-0.84650	H	-0.40130	1.96188	1.07784
H	4.25833	-2.21285	-1.14237	H	1.29027	-0.30598	1.67469
H	5.91617	-0.64863	-0.18316	H	0.93120	-1.58285	2.83752
H	5.19785	1.36040	1.06843	H	0.06992	-0.04585	2.92274
H	2.77410	1.81894	1.36928	H	-2.20861	3.66318	0.71067
H	0.50201	1.24763	1.02064	H	-2.01242	2.74213	-0.78490
H	-3.36744	0.33478	-1.79073	H	-3.35749	2.39032	0.29280
H	-2.55866	-1.20028	-2.01432	H	-2.73071	-2.03193	-1.72537
H	-2.14220	-1.58653	2.09786	H	-4.29826	-2.37159	-0.98099
H	-2.06155	-2.54346	0.62542	H	-2.80848	-2.80111	-0.13834
H	-3.24132	1.46552	1.29276				
H	-1.63464	1.46333	1.94192				
H	-4.51628	-0.88019	1.51215	28			
H	-4.42827	-1.83620	0.02637	Benzylaldehyde + [SiPhH ₂] ⁺			
H	-4.37622	-2.63233	1.59659	C	2.67894	0.90149	-0.69801
H	-2.51916	2.78523	-0.71491	C	3.87083	1.59447	-0.63012
H	-0.85118	2.79663	-0.15359	C	4.90285	1.12360	0.19344
H	-2.09640	3.63429	0.77028	C	4.75712	-0.03861	0.95529
H	-1.18155	1.55065	-2.35012	C	3.56747	-0.74252	0.89701
H	-0.41204	-0.01940	-2.61482	C	2.52430	-0.27475	0.06967
H	-1.72631	0.51094	-3.66230	C	1.32140	-1.02228	0.03330
				O	0.33108	-0.68955	-0.68267
				Si	-1.24376	-1.53746	-0.79570
37				C	-2.53853	-0.39908	-0.18577
Benzylalcooxide + [SiEt ₃] ⁺				C	-3.15039	0.51572	-1.05903
C	2.37595	1.30248	-0.28853	C	-4.13177	1.38150	-0.59173
C	3.53979	0.86749	0.34464	C	-4.51391	1.33847	0.74800
C	3.88777	-0.47891	0.30910	C	-3.92085	0.43132	1.62427
C	3.07477	-1.38823	-0.36839	C	-2.93856	-0.43539	1.16033
C	1.92051	-0.94977	-1.00635	H	1.86243	1.24151	-1.32603
C	1.55921	0.39977	-0.96728	H	4.01138	2.49904	-1.21017
C	0.28697	0.85434	-1.64619	H	5.83672	1.67487	0.24009
O	-0.82074	0.03716	-1.33400	H	5.56873	-0.38385	1.58469
Si	-1.48522	-0.07501	0.20932	H	3.43249	-1.64899	1.48062
C	-3.23827	-0.65916	-0.11486	H	1.23550	-1.92888	0.64542
C	-0.60281	-1.34003	1.29981	H	-1.28820	-1.84157	-2.23150
C	-1.44621	1.62859	1.01044	H	-0.98932	-2.70228	0.07590
C	0.48324	-0.78862	2.23283	H	-2.86804	0.54743	-2.10833
C	-2.29910	2.66649	0.26936	H	-4.60397	2.08322	-1.27043
C	-3.27495	-2.04372	-0.77686	H	-5.28451	2.01112	1.10981
H	2.09478	2.35226	-0.24811	H	-4.23000	0.39575	2.66308
H	4.16606	1.57841	0.87403	H	-2.49266	-1.15001	1.84799
H	4.78769	-0.82175	0.80935				
H	3.34370	-2.43944	-0.39717	29			
H	1.27511	-1.65132	-1.52790	Benzylalcooxide + [SiPhH ₂] ⁺			
H	0.09075	1.90309	-1.37893	C	3.91423	-0.81766	0.31476
H	0.41053	0.81438	-2.73465	C	4.96476	0.08990	0.24702
H	-3.73880	0.07437	-0.75770	C	4.72354	1.40770	-0.13753
H	-3.79431	-0.67454	0.83150	C	3.42869	1.80611	-0.45280
H	-0.18324	-2.11980	0.65224	C	2.37548	0.89564	-0.38754
H	-1.38055	-1.83671	1.89694	C	2.61386	-0.42110	-0.00318
H	-1.78803	1.53144	2.04899				

C	1.49609	-1.43560	0.05875	C	-1.17142	0.00000	0.29343
O	0.24276	-0.80649	-0.10009	O	-2.43070	-0.00000	-0.07920
Si	-1.17633	-1.65960	0.02873	H	-0.88771	-2.14666	0.17219
C	-2.53137	-0.38480	0.03386	H	-0.44687	-1.27112	-1.29446
C	-3.82779	-0.69861	-0.39255	H	1.16756	-1.28600	1.31941
C	-4.84092	0.25521	-0.36012	H	1.63407	-2.15754	-0.14041
C	-4.56640	1.54285	0.09395	H	2.87538	0.00000	0.04238
C	-3.28024	1.87432	0.51305	H	1.81939	0.00000	-1.37295
C	-2.27078	0.91634	0.48385	H	1.16756	1.28600	1.31941
H	4.10395	-1.84435	0.62016	H	1.63407	2.15754	-0.14040
H	5.97143	-0.22891	0.49811	H	-0.88771	2.14666	0.17218
H	5.54180	2.11867	-0.18850	H	-0.44687	1.27112	-1.29446
H	3.23431	2.83131	-0.75209	H	-0.97079	0.00000	1.42983
H	1.36281	1.19624	-0.63201				
H	1.64435	-2.18639	-0.73267				
H	1.53959	-1.96732	1.02137				
H	-1.13051	-2.46340	1.27908	39			
H	-1.35986	-2.60043	-1.10653	Cyclohexanone + BEt ₃			
H	-4.05113	-1.69673	-0.76353	C	-2.11327	0.81517	-1.33364
H	-5.84092	-0.00238	-0.69434	C	-3.17214	0.95585	-0.21860
H	-5.35417	2.28936	0.11652	C	-3.63181	-0.41341	0.28585
H	-3.06437	2.87963	0.86082	C	-2.44674	-1.25119	0.77004
H	-1.26555	1.17926	0.80304	C	-1.38426	-1.40880	-0.33905
				C	-0.99118	-0.04256	-0.81856
17				O	0.13685	0.43938	-0.74577
Cyclohexanone				C	1.18149	-0.41662	1.52226
C	-0.38838	1.28169	0.35922	B	1.57936	-0.09642	-0.01908
C	1.00488	1.25958	-0.28955	C	2.54720	1.19803	-0.20834
C	1.77886	0.00000	0.10432	C	2.05136	-1.37610	-0.89138
C	1.00488	-1.25958	-0.28955	C	3.43801	-1.86179	-0.44727
C	-0.38837	-1.28169	0.35922	C	0.55369	0.73301	2.31759
C	-1.15059	0.00000	0.07080	C	1.87425	2.57310	-0.32566
O	-2.28170	-0.00000	-0.35929	H	-1.71150	1.78107	-1.64414
H	-0.99228	2.12588	0.02046	H	-2.56693	0.31769	-2.19965
H	-0.27183	1.35862	1.44924	H	-2.73725	1.52594	0.61114
H	0.89311	1.28662	-1.38064	H	-4.01598	1.53772	-0.59889
H	1.55815	2.15966	-0.00562	H	-4.35672	-0.28766	1.09536
H	2.76545	0.00000	-0.36932	H	-4.14718	-0.94590	-0.52441
H	1.94621	0.00000	1.19003	H	-1.97907	-0.77207	1.63899
H	0.89312	-1.28662	-1.38064	H	-2.77402	-2.24426	1.08875
H	1.55816	-2.15966	-0.00561	H	-0.51564	-1.96785	-0.00214
H	-0.99228	-2.12588	0.02045	H	-1.83565	-1.93261	-1.19167
H	-0.27183	-1.35862	1.44924	H	0.54899	-1.31157	1.62187
18				H	2.12419	-0.69554	2.01508
Cyclohexanolate				H	3.18926	1.06369	-1.09123
C	-0.36614	-1.25418	-0.19609	H	3.24120	1.22090	0.64551
C	1.10658	-1.26170	0.22074	H	1.35876	-2.22858	-0.83088
C	1.82179	0.00000	-0.27258	H	2.09963	-1.10169	-1.95530
C	1.10658	1.26170	0.22074	H	3.80622	-2.69105	-1.05984
C	-0.36614	1.25418	-0.19609	H	4.17503	-1.05450	-0.50827
				H	3.42044	-2.20560	0.59237
				H	0.27353	0.43911	3.33502

H	1.24653	1.57598	2.39876	Cyclohexanone + BPh ₃			
H	-0.35267	1.11925	1.83003	C	-2.09146	1.39579	-0.61883
H	2.60519	3.38844	-0.32674	C	-3.40492	0.75960	-0.10555
H	1.17427	2.76003	0.49545	C	-4.27491	0.26933	-1.26436
H	1.29826	2.64798	-1.25306	C	-3.49815	-0.69400	-2.16331
				C	-2.22339	-0.01923	-2.72425
				C	-1.41726	0.43297	-1.54566
40				O	-0.30666	-0.08143	-1.36498
Cyclohexanolate + BEt ₃				C	1.77906	-1.11213	-0.34213
C	1.53960	0.48855	0.93157	B	0.60781	-0.06700	0.01891
C	2.93582	1.09652	0.77657	C	-0.43815	-0.60103	1.13709
C	3.92788	0.05691	0.24691	C	1.18543	1.42506	0.20517
C	3.43151	-0.55212	-1.06793	C	2.22569	-2.07348	0.57188
C	2.02227	-1.12879	-0.91517	C	3.28630	-2.92888	0.27345
C	1.02182	-0.08820	-0.39791	C	3.92177	-2.84609	-0.96080
O	-0.21896	-0.68112	-0.29889	C	-0.85189	0.13752	2.25266
C	-1.33038	1.64157	-0.81650	C	-1.82282	-0.34245	3.13265
B	-1.49289	0.13795	-0.14816	C	-2.41097	-1.58516	2.91468
C	-1.89301	0.29583	1.46035	C	1.06639	2.45820	-0.73234
C	-2.62917	-0.70408	-0.99688	C	1.64050	3.71263	-0.52580
C	-2.76804	-2.17971	-0.60865	C	2.35829	3.96692	0.63720
C	-2.60624	2.48719	-0.74344	C	3.49641	-1.89603	-1.88851
C	-1.51492	-0.88974	2.35559	C	2.44615	-1.04087	-1.57366
H	0.82249	1.22614	1.30579	C	2.50587	2.95292	1.58240
H	1.57325	-0.32897	1.66567	C	1.93247	1.70544	1.36140
H	2.88689	1.93540	0.06726	C	-2.01143	-2.34840	1.81806
H	3.29141	1.51017	1.72833	C	-1.03675	-1.85969	0.95167
H	4.92300	0.50037	0.11433	H	-1.43243	1.69380	0.19340
H	4.03236	-0.74416	0.99253	H	-2.33613	2.28242	-1.21942
H	3.41610	0.23459	-1.83579	H	-3.15478	-0.07559	0.55821
H	4.13219	-1.31998	-1.41943	H	-3.93424	1.50296	0.49610
H	1.64998	-1.52472	-1.86599	H	-5.16789	-0.22677	-0.87314
H	2.03111	-1.96536	-0.20213	H	-4.61910	1.12509	-1.86028
H	1.02113	0.74925	-1.12636	H	-3.20258	-1.57699	-1.58326
H	-0.52438	2.21210	-0.32260	H	-4.11065	-1.04235	-2.99897
H	-1.02565	1.56084	-1.87397	H	-1.62788	-0.70164	-3.33227
H	-1.41862	1.20047	1.88328	H	-2.51201	0.85160	-3.32392
H	-2.97622	0.47925	1.56065	H	1.73048	-2.15949	1.53656
H	-3.61962	-0.22675	-0.92241	H	3.61198	-3.66365	1.00415
H	-2.35450	-0.65496	-2.06415	H	4.74408	-3.51374	-1.19972
H	-3.36209	-2.76964	-1.32278	H	-0.41435	1.11759	2.43187
H	-1.77576	-2.63793	-0.53318	H	-2.12236	0.25691	3.98751
H	-3.25191	-2.28793	0.36933	H	-3.16863	-1.95995	3.59606
H	-2.48784	3.49904	-1.15731	H	0.52399	2.28824	-1.66137
H	-3.42741	2.00803	-1.28854	H	1.52965	4.48919	-1.27721
H	-2.93891	2.59787	0.29587	H	2.80596	4.94166	0.80383
H	-1.69879	-0.70788	3.42494	H	3.98987	-1.82061	-2.85331
H	-2.06919	-1.79309	2.08041	H	2.13446	-0.29285	-2.30083
H	-0.45586	-1.13644	2.23116	H	3.07446	3.13481	2.48963
				H	2.07271	0.91812	2.10021
51				H	-2.45408	-3.32527	1.64511

H	-0.71971	-2.47068	0.10773	H	1.05368	-0.80198	-2.73492
				H	2.07161	3.45977	2.90578
52				H	1.62187	1.11193	2.31583
Cyclohexanolate + BPh ₃				H	-1.45134	-1.17413	4.18241
C	-2.53755	0.95256	-0.24007	H	-0.72854	0.43300	2.46424
C	-4.02491	0.69513	0.01222				
C	-4.74848	0.33107	-1.28725	51			
C	-4.08208	-0.86943	-1.96542	Cyclohexanone + B(C ₆ F ₅)Ph ₂			
C	-2.58935	-0.61904	-2.18983	C	1.65832	-2.13474	-0.25610
C	-1.86673	-0.26671	-0.88760	C	3.02537	-2.26544	0.45639
O	-0.52121	-0.07238	-1.17815	C	4.15366	-2.49222	-0.55182
C	1.91362	-0.51776	-0.80093	C	4.17686	-1.38624	-1.60808
B	0.51534	-0.01586	-0.10192	C	2.82127	-1.30070	-2.35073
C	0.12515	-1.03125	1.13843	C	1.77055	-1.08125	-1.31006
C	0.75006	1.53524	0.39315	O	1.14702	-0.01176	-1.32982
C	3.11169	-0.62443	-0.07737	C	-0.13632	2.08503	-0.76510
C	4.29853	-1.05483	-0.66362	B	0.22321	0.63951	-0.15890
C	4.32563	-1.39608	-2.01573	C	1.20897	0.65464	1.12216
C	0.35017	-2.41216	1.00743	C	-1.13268	-0.25544	-0.00383
C	-0.05358	-3.33116	1.97316	C	-0.15197	3.23799	0.02779
C	-0.70480	-2.89365	3.12518	C	-0.51153	4.47708	-0.49945
C	0.42645	2.59311	-0.47166	C	-0.86270	4.58890	-1.84126
C	0.67149	3.92458	-0.14603	C	0.97749	-0.03939	2.31513
C	1.26403	4.24923	1.07353	C	1.91811	-0.06355	3.34435
C	3.15283	-1.30099	-2.75934	C	3.12465	0.61662	3.20321
C	1.97049	-0.87048	-2.15563	C	-1.55072	-1.32448	-0.78710
C	1.60716	3.22395	1.95058	C	-2.77292	-1.96847	-0.62652
C	1.35267	1.89557	1.60871	C	-3.64750	-1.53263	0.35562
C	-0.94417	-1.53252	3.28927	C	-0.85870	3.45362	-2.64959
C	-0.53460	-0.62698	2.30962	C	-0.50468	2.22089	-2.11078
H	-2.01922	1.20515	0.68991	C	-3.28297	-0.46264	1.16235
H	-2.41282	1.81293	-0.91268	C	-2.05344	0.14887	0.96316
H	-4.12738	-0.13564	0.72481	F	-0.76444	-1.81713	-1.77088
H	-4.49530	1.56936	0.47752	F	-4.82093	-2.13524	0.52735
H	-5.80883	0.12448	-1.09634	F	-3.10612	-2.99574	-1.40860
H	-4.70887	1.19259	-1.96888	F	-4.11470	-0.03490	2.11016
H	-4.20472	-1.75165	-1.32169	F	-1.75614	1.18054	1.76344
H	-4.58327	-1.09928	-2.91353	C	3.37640	1.32921	2.03173
H	-2.10265	-1.49466	-2.63265	C	2.42681	1.34673	1.01300
H	-2.44793	0.21627	-2.89030	H	0.85632	-1.91555	0.44579
H	-2.00072	-1.11686	-0.19105	H	1.43006	-3.07218	-0.77831
H	3.10981	-0.36337	0.98033	H	3.21115	-1.35273	1.03427
H	5.20613	-1.12624	-0.06796	H	2.96358	-3.09179	1.16910
H	5.24924	-1.73219	-2.48068	H	5.11463	-2.52733	-0.03062
H	0.86055	-2.76871	0.11460	H	4.02105	-3.46398	-1.04540
H	0.14136	-4.39182	1.83047	H	4.37357	-0.42179	-1.12386
H	-1.01977	-3.60485	3.88475	H	4.97065	-1.55110	-2.34105
H	-0.03125	2.34103	-1.42594	H	2.79637	-0.48353	-3.07274
H	0.40311	4.71470	-0.84440	H	2.62757	-2.25018	-2.86250
H	1.45671	5.28667	1.33523	H	0.12252	3.16264	1.07704
H	3.15905	-1.56580	-3.81497	H	-0.51551	5.35630	0.13803

H	-1.13997	5.55335	-2.25577	H	2.75748	-1.57887	-2.50479
H	0.04659	-0.58839	2.44354	H	2.86605	-0.22362	0.21789
H	1.70830	-0.61356	4.25686	H	-1.37833	2.86770	0.49265
H	3.85940	0.59924	4.00216	H	-2.24322	4.75244	-0.84487
H	-1.13478	3.53125	-3.69717	H	-1.64174	4.95845	-3.24895
H	-0.51115	1.34004	-2.75103	H	1.88737	2.90282	0.19611
H	4.30801	1.87573	1.91707	H	3.19109	3.63091	2.16391
H	2.62634	1.91789	0.10763	H	3.07162	2.33969	4.28638
52				H	-0.15983	3.25411	-4.28552
Cyclohexanolate + B(C ₆ F ₅)Ph ₂				H	0.70760	1.36717	-2.91786
C	1.82673	-2.08452	0.03088	H	1.62684	0.31926	4.40214
C	2.99897	-2.93026	0.53378	H	0.32893	-0.39024	2.44049
C	3.99450	-3.21663	-0.59371	51			
C	4.48297	-1.91352	-1.23247	Cyclohexanone + B(C ₆ F ₅) ₂ Ph			
C	3.30735	-1.05824	-1.70849	C	-3.14717	0.28124	-0.74363
C	2.31960	-0.76473	-0.57832	C	-4.26067	-0.64928	-0.20600
O	1.30141	0.02704	-1.10292	C	-4.90104	-1.45627	-1.33667
C	-0.27269	1.96501	-1.11639	C	-3.84490	-2.24146	-2.11564
B	0.30248	0.70013	-0.25140	C	-2.76764	-1.29317	-2.69719
C	1.00041	1.19687	1.14896	C	-2.18910	-0.53715	-1.54638
C	-1.03098	-0.29174	0.02744	O	-0.99336	-0.72255	-1.27538
C	-1.11004	2.94399	-0.55892	C	1.26754	-0.92348	-0.19632
C	-1.59939	4.00959	-1.31045	B	-0.20981	-0.30871	0.06658
C	-1.26259	4.12838	-2.65803	C	-1.07524	-1.03208	1.22073
C	1.82645	2.33147	1.12051	C	-0.07742	1.30943	0.16384
C	2.56457	2.74421	2.22768	C	2.00992	-1.63244	0.74264
C	2.49995	2.02305	3.41783	C	3.29684	-2.09756	0.48775
C	-1.36782	-1.36511	-0.79728	C	3.88747	-1.84264	-0.74034
C	-2.50117	-2.15363	-0.62105	C	-1.70036	-0.35820	2.27362
C	-3.38325	-1.87011	0.40825	C	-2.53343	-1.02232	3.17420
C	-0.43222	3.17156	-3.23540	C	-2.75716	-2.38921	3.04108
C	0.05307	2.11039	-2.47114	C	-0.46501	2.25967	-0.77262
C	-3.11412	-0.79722	1.24153	C	-0.22763	3.62173	-0.62461
C	-1.96866	-0.03900	1.02686	C	0.44671	4.07772	0.49744
F	-0.60452	-1.71421	-1.84538	C	3.19185	-1.11765	-1.69914
F	-4.48105	-2.61617	0.59036	C	1.91338	-0.66870	-1.40399
F	-2.75969	-3.18004	-1.44473	C	0.87175	3.16604	1.45526
F	-3.96388	-0.50137	2.23580	C	0.61158	1.81661	1.26459
F	-1.81181	0.99936	1.87080	F	-1.12252	1.90064	-1.89437
C	1.69050	0.89202	3.47992	F	0.68242	5.37625	0.65658
C	0.95879	0.49499	2.36186	F	-0.63871	4.48600	-1.55160
H	1.12992	-1.87040	0.84787	F	1.52644	3.59243	2.53256
H	1.26659	-2.62932	-0.73934	F	1.05998	0.96876	2.19965
H	3.51407	-2.38538	1.33766	C	-2.13565	-3.08806	2.00657
H	2.63779	-3.86885	0.97010	C	-1.30870	-2.41260	1.11441
H	4.84272	-3.80406	-0.22147	F	1.51523	-1.89723	1.95417
H	3.49610	-3.82515	-1.36130	F	3.96745	-2.78179	1.41396
H	5.05981	-1.34870	-0.48676	F	5.11625	-2.28227	-0.99737
H	5.16613	-2.12781	-2.06307	F	3.75972	-0.85409	-2.87621
H	3.65237	-0.10626	-2.12568				

F	1.29357	0.06284	-2.34425
H	-2.64601	0.81393	0.06204
H	-3.58619	1.01063	-1.43528
H	-3.82756	-1.32282	0.54218
H	-5.00334	-0.03207	0.30576
H	-5.64539	-2.14378	-0.92499
H	-5.43165	-0.78151	-2.02112
H	-3.35685	-2.96092	-1.44657
H	-4.29237	-2.80923	-2.93521
H	-1.97448	-1.83336	-3.21545
H	-3.24153	-0.58654	-3.38780
H	-1.54813	0.71265	2.39181
H	-3.00667	-0.47054	3.98075
H	-3.40399	-2.90869	3.74105
H	-2.29117	-4.15777	1.90195
H	-0.82230	-2.97098	0.31531

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Cyclohexanolate + B(C₆F₅)₂Ph

C	-3.30937	-0.09742	-0.40731
C	-4.76863	-0.55795	-0.35717
C	-5.26795	-0.94703	-1.75137
C	-4.37023	-2.02095	-2.37234
C	-2.90559	-1.57888	-2.38475
C	-2.41462	-1.20212	-0.98688
O	-1.06336	-0.86460	-1.09857
C	1.32500	-0.81788	-0.36687
B	-0.25115	-0.48374	0.06080
C	-0.72570	-1.31436	1.38682
C	-0.20846	1.16951	0.30367
C	2.29928	-1.39838	0.43934
C	3.60481	-1.63667	0.01472
C	3.98950	-1.26485	-1.26148
C	-0.65764	-2.71650	1.34084
C	-1.12809	-3.51929	2.37378
C	-1.69803	-2.93467	3.50463
C	-0.69739	2.12792	-0.58029
C	-0.56020	3.49929	-0.37504
C	0.11991	3.96545	0.73730
C	3.06534	-0.64919	-2.09211
C	1.77379	-0.42992	-1.62974
C	0.66239	3.05142	1.62782
C	0.50229	1.69436	1.38159
F	-1.33825	1.79181	-1.70908
F	0.26022	5.28034	0.94603
F	-1.06679	4.37756	-1.25144
F	1.34357	3.48951	2.69520
F	1.10158	0.86393	2.25180
C	-1.78873	-1.54923	3.57699
C	-1.30881	-0.76021	2.53039
F	2.03854	-1.77006	1.70009

F	4.49696	-2.21679	0.82995
F	5.24063	-1.48476	-1.68493
F	3.43761	-0.25997	-3.31976
F	0.96200	0.22833	-2.46695
H	-2.95764	0.17253	0.59387
H	-3.22225	0.79255	-1.03995
H	-4.85022	-1.42706	0.31067
H	-5.40384	0.22734	0.06860
H	-6.30755	-1.29392	-1.70797
H	-5.25445	-0.05581	-2.39412
H	-4.46235	-2.94327	-1.78165
H	-4.70868	-2.26183	-3.38705
H	-2.25756	-2.36673	-2.78281
H	-2.77614	-0.69976	-3.03036
H	-2.54074	-2.08635	-0.33314
H	-0.22208	-3.18355	0.45780
H	-1.05276	-4.60146	2.30110
H	-2.06825	-3.55421	4.31710
H	-2.23392	-1.07852	4.45009
H	-1.40103	0.32180	2.60915

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Cyclohexanone + B(C₆F₅)₃

C	-1.74396	-2.02541	1.55218
C	-3.27150	-1.76445	1.56132
C	-3.78659	-1.53926	2.98406
C	-3.02874	-0.40218	3.67104
C	-1.50564	-0.68381	3.69364
C	-1.08616	-0.89824	2.27859
O	-0.32411	-0.06073	1.77029
C	1.10545	1.33230	0.24609
B	0.10649	0.05727	0.24414
C	-1.31118	0.28781	-0.52190
C	0.97675	-1.24234	-0.19316
C	1.06177	2.40356	-0.63782
C	1.98666	3.44157	-0.61094
C	3.01009	3.42256	0.32488
C	-1.89196	-0.55851	-1.45912
C	-3.14452	-0.33187	-2.02221
C	-3.87091	0.78612	-1.64202
C	1.45033	-2.26091	0.62139
C	2.29379	-3.27020	0.16857
C	2.70856	-3.26776	-1.15336
C	3.10106	2.36477	1.21974
C	2.15992	1.34796	1.15529
C	2.27006	-2.26144	-2.00659
C	1.42988	-1.27881	-1.50977
F	1.09121	-2.33678	1.92072
F	3.51510	-4.22248	-1.60462
F	2.70470	-4.23011	0.99587
F	2.66330	-2.25174	-3.27737

F	1.02781	-0.31988	-2.35426	F	-2.92310	4.00342	-2.68569
C	-3.33948	1.65706	-0.69853	F	-2.32198	4.48629	-0.07550
C	-2.08631	1.39090	-0.16638	F	-2.12487	1.66709	-3.84352
F	0.10641	2.48538	-1.57139	F	-0.75195	-0.14036	-2.41232
F	1.89842	4.45123	-1.47476	C	3.15952	-0.67852	-2.02167
F	3.90054	4.40884	0.36373	C	2.01385	-0.11090	-1.46996
F	4.08604	2.33259	2.11623	F	-0.53978	-2.72384	-1.03137
F	2.30105	0.33035	2.02052	F	-2.63332	-4.28266	-0.59797
F	-1.28817	-1.69929	-1.82451	F	-4.55949	-3.56616	1.19147
F	-3.65433	-1.18630	-2.90621	F	-4.33399	-1.20692	2.53641
F	-5.06933	1.01760	-2.16523	F	-2.25446	0.39850	2.10079
F	-4.03173	2.72867	-0.31916	F	1.23388	-2.50973	1.06963
F	-1.62533	2.25165	0.75150	F	3.42175	-3.63416	0.03535
H	-1.35529	-2.15322	0.54253	F	4.73707	-2.43713	-2.02941
H	-1.53332	-2.93550	2.12588	F	3.80765	-0.07576	-3.02627
H	-3.48607	-0.88375	0.94378	F	1.65640	1.07159	-2.00377
H	-3.76798	-2.61619	1.09011	H	1.96060	2.01792	0.14559
H	-4.85576	-1.31104	2.95844	H	1.28274	2.93767	1.48666
H	-3.66955	-2.46125	3.56772	H	4.17342	1.92508	1.31438
H	-3.20259	0.53890	3.13468	H	3.67079	3.59291	1.05844
H	-3.37371	-0.25712	4.69752	H	4.53465	3.25537	3.38908
H	-0.93873	0.14323	4.12210	H	2.83448	3.72590	3.39273
H	-1.31212	-1.59878	4.26446	H	3.90718	0.87982	3.69682
				H	3.18684	1.85040	4.97708
52				H	1.53073	0.20511	4.00979
Cyclohexanolate + B(C ₆ F ₅) ₃				H	0.99858	1.86657	3.74926
C	2.03059	2.18029	1.22607	H	2.46914	0.14567	1.72107
C	3.42728	2.67713	1.60849				
C	3.52716	2.91876	3.11708	18			
C	3.15539	1.65571	3.89886	Cyclohexanone + proton			
C	1.77604	1.13599	3.48869	C	-0.32588	-1.29168	0.43764
C	1.69015	0.88978	1.98358	C	1.04169	-1.24059	-0.31505
O	0.41793	0.37844	1.71550	C	1.80840	0.03391	0.02886
C	-1.24178	-1.09697	0.56226	C	0.98833	1.27848	-0.30249
B	0.00269	-0.01261	0.37697	C	-0.38130	1.26063	0.45097
C	1.29403	-0.67838	-0.42723	C	-1.03309	-0.03090	0.16582
C	-0.73208	1.21103	-0.47641	O	-2.16668	-0.11612	-0.41264
C	-1.42694	-2.29386	-0.11988	H	-0.93759	-2.14622	0.14667
C	-2.51904	-3.13312	0.08001	H	-0.12166	-1.33244	1.51520
C	-3.50098	-2.77351	0.98708	H	1.59856	-2.13612	-0.03386
C	1.82857	-1.87346	0.05015	H	0.85566	-1.29867	-1.39239
C	2.96387	-2.48039	-0.46606	H	2.74438	0.05958	-0.53506
C	3.63700	-1.87499	-1.51739	H	2.07785	0.03531	1.09163
C	-1.19279	2.40159	0.07502	H	1.50428	2.19508	-0.01100
C	-1.91483	3.34745	-0.65157	H	0.80071	1.33793	-1.37953
C	-2.22774	3.10574	-1.97767	H	-0.17973	1.29913	1.52876
C	-3.37772	-1.57562	1.67397	H	-1.01347	2.11052	0.17871
C	-2.27150	-0.76744	1.44286	H	-2.58442	0.74582	-0.60249
C	-1.81568	1.91728	-2.56482				
C	-1.09991	1.00693	-1.80371	19			
F	-0.96943	2.72425	1.35703	Cyclohexanol			

C	0.33930	1.24696	-0.18926	H	1.89016	-0.94958	2.06627
C	-1.13746	1.27236	0.21307	H	3.38180	-2.16631	0.26909
C	-1.85889	0.01654	-0.28290	H	4.29867	-0.69655	-0.07542
C	-1.16182	-1.25026	0.22056	H	4.28071	-2.01796	-1.23862
C	0.31547	-1.26295	-0.17821	H	3.64776	1.52274	1.27182
C	1.03170	-0.01576	0.32162	H	3.56271	3.11504	0.52437
O	2.37267	-0.09875	-0.12477	H	3.88840	1.69869	-0.47291
H	0.85784	2.13643	0.19164	H	0.13870	-2.75732	2.18411
H	0.43322	1.26071	-1.28300	H	1.01286	-2.85505	0.65572
H	-1.21367	1.32147	1.30787	H	-0.60577	-2.16150	0.69949
H	-1.62030	2.17381	-0.17678				
H	-2.90603	0.02861	0.03623	40			
H	-1.85950	0.01376	-1.38111	Cyclohexanolate + [SiEt ₃] ⁺			
H	-1.24292	-1.29318	1.31522	C	-1.74821	-0.74818	0.78125
H	-1.66313	-2.14271	-0.16656	C	-3.14725	-1.35634	0.64695
H	0.82617	-2.14946	0.20987	C	-4.21597	-0.26607	0.54306
H	0.41112	-1.28665	-1.27161	C	-3.91049	0.68585	-0.61590
H	0.99369	-0.01268	1.42609	C	-2.51100	1.28843	-0.47680
H	2.83237	0.69865	0.16098	C	-1.44375	0.20443	-0.37524
				O	-0.18965	0.84269	-0.21885
39				Si	1.29561	0.07209	-0.20684
Cyclohexanone + [SiEt ₃] ⁺				C	1.70595	-0.57729	1.52177
C	-1.73481	1.23411	0.52856	C	1.28902	-1.33769	-1.45865
C	-2.76018	0.37117	1.31948	C	2.52007	1.41123	-0.68595
C	-3.95665	0.00422	0.44253	C	3.20841	-0.61636	1.83924
C	-3.51119	-0.72056	-0.82643	C	2.58501	-2.16029	-1.44689
C	-2.49132	0.13438	-1.63249	C	2.38627	2.65654	0.20181
C	-1.38402	0.49510	-0.71256	H	-1.66959	-0.17821	1.71698
O	-0.23064	0.07214	-0.97041	H	-0.99127	-1.54136	0.82273
Si	1.34906	0.09242	-0.05146	H	-3.18314	-1.98069	-0.25631
C	2.42973	-0.87005	-1.21963	H	-3.35193	-2.01803	1.49437
C	1.79712	1.89472	0.14750	H	-5.20650	-0.71536	0.41847
C	0.94666	-0.84333	1.51438	H	-4.23941	0.30484	1.48091
C	3.66641	-1.46801	-0.52346	H	-3.97573	0.13147	-1.56211
C	3.31134	2.06264	0.38136	H	-4.65924	1.48245	-0.66677
C	0.33958	-2.23032	1.24944	H	-2.27295	1.94391	-1.32016
H	-0.85479	1.47579	1.12508	H	-2.45230	1.89875	0.43391
H	-2.22581	2.16839	0.23073	H	-1.44694	-0.37709	-1.31419
H	-2.26025	-0.53668	1.67802	H	1.18939	0.06010	2.25014
H	-3.06774	0.93943	2.19971	H	1.27450	-1.57932	1.64354
H	-4.64320	-0.63113	1.00790	H	1.11814	-0.91365	-2.45618
H	-4.51031	0.91256	0.17585	H	0.43481	-1.99832	-1.26034
H	-3.04743	-1.68032	-0.57145	H	3.54194	1.01446	-0.63667
H	-4.35767	-0.93789	-1.48090	H	2.34484	1.67947	-1.73470
H	-2.10045	-0.39515	-2.50176	H	3.40036	-1.02780	2.83441
H	-2.98827	1.05695	-1.95528	H	3.75981	-1.22975	1.11953
H	2.73303	-0.22042	-2.04881	H	3.64553	0.38625	1.80799
H	1.82753	-1.67098	-1.66451	H	2.58305	-2.93491	-2.21896
H	1.24419	2.34145	0.98130	H	2.72474	-2.65964	-0.48285
H	1.50071	2.44037	-0.75653	H	3.46327	-1.52904	-1.61943
H	0.29667	-0.25003	2.16840	H	3.09244	3.44073	-0.08578

H	1.37548	3.06728	0.13541	C	-3.70058	-1.58985	0.34074
H	2.57099	2.41708	1.25475	C	-3.53735	-1.05207	-0.93258
				C	-2.64727	0.00104	-1.13183
31				H	2.23361	0.80995	-1.61166
Cyclohexanone + [SiPhH ₂] ⁺				H	0.72873	-0.11539	-1.69956
C	1.36122	0.00670	-1.39840	H	1.86529	-2.13946	-0.84128
C	1.03580	-1.44935	-0.93498	H	2.68827	-1.55451	-2.28177
C	2.22677	-2.06026	-0.19756	H	4.31887	-2.16900	-0.47769
C	2.65265	-1.18878	0.98244	H	4.41942	-0.45505	-0.87392
C	3.00876	0.25724	0.51099	H	2.90631	-1.65751	1.49774
C	1.80751	0.75043	-0.19635	H	4.41189	-0.75233	1.59383
O	1.14430	1.68117	0.33995	H	2.43952	0.71156	2.14341
Si	-0.51161	2.28536	-0.01469	H	3.27190	1.28410	0.69752
C	-1.56466	0.78187	0.10321	H	0.74912	-0.41929	0.74507
C	-1.69012	0.10968	1.33058	H	-1.18684	3.20390	0.31991
C	-2.38946	-1.09045	1.40696	H	-0.60116	2.17365	-1.78697
C	-2.97538	-1.62652	0.26036	H	-1.52494	0.37398	2.05042
C	-2.87053	-0.96356	-0.96108	H	-3.09829	-1.49641	2.40575
C	-2.16686	0.23445	-1.04024	H	-4.39148	-2.41216	0.49847
H	0.50535	0.47283	-1.88819	H	-4.09929	-1.45508	-1.76929
H	2.20077	-0.03385	-2.10127	H	-2.51910	0.40814	-2.13246
H	0.15115	-1.42609	-0.28786				
H	0.77364	-2.02472	-1.82532	17			
H	1.95934	-3.05770	0.16118	Acetophenone			
H	3.06905	-2.18573	-0.88836	C	-1.69497	-0.20486	-0.00065
H	1.84504	-1.13058	1.72127	C	-0.20171	-0.05601	-0.00031
H	3.52939	-1.59543	1.49036	O	-2.20493	-1.30591	0.00008
H	3.25838	0.91204	1.34609	C	-2.54668	1.04707	0.00045
H	3.84842	0.19965	-0.18935	C	0.42636	1.19171	-0.00028
H	-0.62879	3.27890	1.05586	C	1.81565	1.27512	-0.00005
H	-0.42415	2.84602	-1.37328	C	2.58175	0.11275	0.00020
H	-1.24839	0.52510	2.23399	C	1.95960	-1.13546	0.00020
H	-2.48772	-1.60215	2.35829	C	0.57385	-1.21908	-0.00005
H	-3.52492	-2.55998	0.32200	H	-3.59512	0.75321	0.00122
H	-3.34019	-1.37676	-1.84711	H	-2.33559	1.65759	-0.88248
H	-2.09246	0.74536	-1.99792	H	-2.33416	1.65722	0.88331
				H	-0.16384	2.10271	-0.00045
32				H	2.29974	2.24614	-0.00005
Cyclohexanolate + [SiPhH ₂] ⁺				H	3.66516	0.17878	0.00039
C	1.67295	-0.01353	-1.14926	H	2.55843	-2.04037	0.00039
C	2.47528	-1.31550	-1.23529	H	0.06166	-2.17544	-0.00008
C	3.77197	-1.22193	-0.42809				
C	3.48059	-0.84795	1.02710	18			
C	2.68148	0.45445	1.10756	1-phenylethanolate			
C	1.39063	0.36252	0.30417	C	-1.81768	-1.21456	0.27890
O	0.72857	1.61800	0.40998	C	-2.59638	-0.06372	0.15519
Si	-0.72055	1.95643	-0.32155	C	-1.97834	1.14760	-0.15753
C	-1.91477	0.53888	-0.06662	C	-0.59738	1.19986	-0.33708
C	-2.09092	-0.01990	1.20839	C	0.19251	0.05397	-0.20740
C	-2.97413	-1.07502	1.41311	C	-0.43836	-1.15211	0.09572

C	1.74149	0.01800	-0.38175	H	-4.34073	0.97548	-1.26617
C	2.33344	0.94349	0.73400	H	-2.53443	2.69801	-1.02158
O	2.25218	-1.19500	-0.36195	H	-0.91014	2.62595	-0.34966
H	-2.29690	-2.16362	0.51445	H	-2.14095	3.63154	0.42368
H	-3.67427	-0.10894	0.29359				
H	-2.57810	2.04991	-0.26342	40			
H	-0.11945	2.14587	-0.59260	1-phenylethanolate + BEt ₃			
H	0.23302	-2.00636	0.15876	C	-3.761872	-0.695609	-0.249935
H	1.89298	0.61903	-1.34107	C	-4.001930	0.653394	-0.499516
H	3.42038	0.97194	0.60346	C	-2.984335	1.582176	-0.285204
H	1.94616	1.97338	0.73541	C	-1.739779	1.168153	0.179761
H	2.12289	0.48363	1.70672	C	-1.493239	-0.180730	0.439602
				C	-2.514929	-1.104810	0.216941
				C	-0.146924	-0.608412	1.023005
				C	-0.313687	-0.768485	2.541690
39				O	0.852031	0.312053	0.795014
Acetophenone + BEt ₃				C	3.002527	-0.721280	-0.265294
C	4.29491	-0.55852	-0.52475	B	1.693689	0.277240	-0.478979
C	4.55059	0.70992	-0.00926	C	2.209429	1.831047	-0.665175
C	3.50106	1.51315	0.43642	C	0.852615	-0.121449	-1.850292
C	2.19507	1.05005	0.36567	C	2.718302	2.482990	0.622521
C	1.93239	-0.22639	-0.14826	C	0.528578	-1.589421	-2.159383
C	2.98885	-1.02914	-0.59205	C	2.753481	-2.014941	0.517555
C	0.52611	-0.68991	-0.21957	H	-4.543903	-1.429889	-0.425622
C	0.21656	-2.08876	-0.66101	H	-4.971278	0.977963	-0.867997
O	-0.35419	0.11939	0.08367	H	-3.162031	2.634719	-0.490711
C	-2.37884	1.47119	0.77412	H	-0.918497	1.863813	0.328817
B	-2.04978	0.02784	0.12608	H	-2.322239	-2.160325	0.404289
C	-2.45295	-1.21475	1.09603	H	0.091084	-1.602368	0.605111
C	-2.47182	-0.13572	-1.42793	H	0.625618	-1.122704	2.975508
C	-1.55311	-1.43791	2.31647	H	-1.118289	-1.466649	2.797380
C	-3.99171	-0.00964	-1.59360	H	-0.545590	0.209907	2.974823
C	-1.97264	2.67457	-0.08136	H	3.431892	-0.976385	-1.249439
H	5.11226	-1.18023	-0.87345	H	3.802835	-0.174462	0.259828
H	5.57134	1.07434	0.04562	H	3.002946	1.869943	-1.430187
H	3.70389	2.50001	0.83801	H	1.385934	2.447615	-1.066057
H	1.36343	1.65775	0.70614	H	-0.077706	0.464146	-1.913076
H	2.79709	-2.01670	-0.99826	H	1.473622	0.248833	-2.683696
H	0.84919	-2.80090	-0.12633	H	3.041447	3.526547	0.493906
H	-0.83220	-2.31339	-0.48865	H	1.932868	2.459208	1.384945
H	0.43380	-2.17927	-1.73069	H	3.570511	1.928147	1.034704
H	-1.90545	1.55489	1.76385	H	0.090375	-1.728886	-3.158444
H	-3.45923	1.52003	0.97133	H	1.434268	-2.207452	-2.116866
H	-3.46431	-0.98225	1.45894	H	-0.187069	-2.016977	-1.446127
H	-2.57185	-2.16539	0.55333	H	3.665104	-2.605598	0.692056
H	-1.98162	0.62420	-2.05285	H	2.325092	-1.779617	1.499184
H	-2.15999	-1.10870	-1.83679	H	2.038765	-2.672955	0.007831
H	-1.95882	-2.18354	3.00741				
H	-0.55202	-1.78649	2.02993	51			
H	-1.41359	-0.50803	2.87740	Acetophenone + BPh ₃			
H	-4.31385	-0.14541	-2.63107	C	-5.40647	0.46737	0.47168
H	-4.51633	-0.75504	-0.98561				

C	-5.62262	-0.84884	0.07088	52			
C	-4.54269	-1.68774	-0.20486	1-phenylethanolate + BPh ₃			
C	-3.24603	-1.21246	-0.07888	C	4.469758	-0.772257	-0.195371
C	-3.02160	0.10881	0.33634	C	4.788062	0.554012	-0.472466
C	-4.10947	0.94695	0.60841	C	3.849149	1.368213	-1.104860
C	-1.62639	0.58387	0.44720	C	2.604146	0.858505	-1.453751
C	-1.29948	1.95709	0.94003	C	2.280120	-0.472885	-1.183582
O	-0.74444	-0.21572	0.09178	C	3.224431	-1.281703	-0.555946
B	0.87697	-0.02561	-0.06010	C	0.911911	-1.005593	-1.595017
C	1.26943	-1.34854	-0.89787	C	0.952352	-1.422110	-3.067809
C	1.48515	-0.07246	1.43491	O	-0.078935	-0.042484	-1.435125
C	1.06519	1.36210	-0.87150	B	-0.776454	0.043880	-0.105561
C	2.88145	0.01084	1.57198	C	-1.957807	-1.097718	-0.039508
C	3.50334	-0.04406	2.81386	C	0.299888	-0.130010	1.130511
C	2.74067	-0.19936	3.97101	C	-1.487950	1.514096	-0.066248
C	1.35921	-0.30421	3.86485	C	0.556141	-1.358856	1.756224
C	0.74718	-0.24118	2.61202	C	1.585379	-1.525881	2.684022
C	2.10159	-1.31796	-2.02198	C	2.403942	-0.451226	3.016644
C	2.45632	-2.48485	-2.70029	C	2.170926	0.787879	2.421398
C	1.97424	-3.71611	-2.27010	C	1.132555	0.937200	1.506789
C	1.14593	-3.77463	-1.14957	C	-2.612304	-1.454049	1.150819
C	0.81088	-2.60593	-0.47501	C	-3.650822	-2.381555	1.180984
C	1.80041	2.45443	-0.39450	C	-4.075207	-2.993872	0.002883
C	1.88176	3.65103	-1.10626	C	-3.450549	-2.658069	-1.195298
C	1.21595	3.78848	-2.32062	C	-2.414989	-1.724360	-1.206832
C	0.48059	2.71606	-2.82303	C	-1.652337	2.272380	-1.233648
C	0.41765	1.52292	-2.10820	C	-2.291408	3.511613	-1.226600
H	-6.24780	1.11967	0.67816	C	-2.790116	4.036510	-0.036921
H	-6.63662	-1.22212	-0.03033	C	-2.636912	3.307119	1.140850
H	-4.71483	-2.71045	-0.52184	C	-1.995796	2.071069	1.117160
H	-2.39226	-1.84455	-0.30045	H	5.185288	-1.407626	0.319591
H	-3.95314	1.97567	0.91283	H	5.755250	0.955718	-0.183176
H	-1.26652	2.63380	0.07694	H	4.084400	2.409460	-1.309331
H	-2.04442	2.31102	1.65122	H	1.837353	1.490326	-1.894156
H	-0.31050	1.95788	1.39693	H	2.963057	-2.308383	-0.308956
H	3.49107	0.11264	0.67571	H	0.702781	-1.904528	-0.987910
H	4.58493	0.02687	2.88180	H	-0.004588	-1.865102	-3.357404
H	3.22174	-0.24631	4.94297	H	1.753416	-2.144523	-3.255673
H	0.75364	-0.43944	4.75643	H	1.128185	-0.536795	-3.687355
H	-0.33627	-0.34322	2.56677	H	-0.064177	-2.216185	1.499747
H	2.47743	-0.36171	-2.37829	H	1.752159	-2.498722	3.142032
H	3.10630	-2.42989	-3.56888	H	3.214552	-0.575410	3.730483
H	2.24421	-4.62546	-2.79859	H	2.807211	1.635465	2.665448
H	0.77270	-4.73302	-0.79962	H	0.971621	1.908456	1.041599
H	0.18560	-2.66591	0.41539	H	-2.286612	-0.996354	2.084419
H	2.31014	2.37325	0.56286	H	-4.130572	-2.631141	2.125058
H	2.46102	4.47927	-0.70840	H	-4.883346	-3.720999	0.020277
H	1.27287	4.72048	-2.87472	H	-3.774599	-3.124091	-2.123789
H	-0.03590	2.80906	-3.77411	H	-1.940035	-1.451619	-2.146774
H	-0.14582	0.68645	-2.51947	H	-1.259937	1.867145	-2.163011
				H	-2.400136	4.072314	-2.152995

H	-3.288761	5.002647	-0.025658
H	-3.014964	3.706693	2.079509
H	-1.869174	1.523004	2.050271

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Acetophenone + B(C₆F₅)Ph₂

C	-5.00584	-1.21465	0.91218
C	-5.63912	-2.08091	0.02082
C	-5.00604	-2.46568	-1.15929
C	-3.73933	-1.97966	-1.45580
C	-3.10059	-1.10575	-0.56675
C	-3.73913	-0.72910	0.62478
C	-1.74978	-0.58269	-0.83842
C	-1.00237	-0.96858	-2.07651
O	-1.26669	0.17337	0.02386
C	1.22491	-0.42248	0.00874
B	0.19226	0.84487	0.09847
C	0.20219	1.55821	1.54358
C	0.27150	1.97129	-1.05633
C	1.32024	1.56112	2.38375
C	1.32151	2.24973	3.59557
C	0.19020	2.95073	4.00036
C	-0.93492	2.96746	3.17829
C	-0.91838	2.28686	1.96529
C	-0.79191	2.33794	-1.88612
C	-0.68422	3.38488	-2.80382
C	0.50257	4.09794	-2.90748
C	1.57438	3.76367	-2.07881
C	1.45146	2.72426	-1.16734
C	1.19829	-1.38543	1.01982
C	2.05013	-2.48138	1.06424
C	2.98049	-2.65720	0.04921
C	3.02848	-1.74665	-0.99483
C	2.15455	-0.66366	-0.99957
F	0.29620	-1.29321	2.00420
F	1.97678	-3.36736	2.05698
F	3.80230	-3.70266	0.06669
F	3.89513	-1.92583	-1.99158
F	2.21703	0.12678	-2.07990
H	-5.50009	-0.92334	1.83232
H	-6.62983	-2.46063	0.24891
H	-5.49945	-3.14346	-1.84695
H	-3.25205	-2.28893	-2.37386
H	-3.22375	-0.06426	1.31011
H	-1.67401	-0.96293	-2.93638
H	-0.16889	-0.29386	-2.26193
H	-0.62121	-1.98882	-1.94774
H	2.21193	1.00999	2.09057
H	2.20508	2.23296	4.22687
H	0.18507	3.48342	4.94628

H	-1.82038	3.51921	3.48068
H	-1.79471	2.33113	1.31987
H	-1.74554	1.81523	-1.82095
H	-1.53201	3.64262	-3.43182
H	0.59343	4.91211	-3.61954
H	2.50449	4.32024	-2.14328
H	2.29168	2.48678	-0.51719

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1-phenylethanolate + B(C₆F₅)Ph₂

C	4.97361	-0.16042	0.33201
C	5.30051	-1.48649	0.06950
C	4.52333	-2.22235	-0.82480
C	3.42933	-1.63215	-1.44665
C	3.09054	-0.30063	-1.18966
C	3.87638	0.42577	-0.29684
C	1.85450	0.32914	-1.82202
C	1.84498	0.16658	-3.34098
O	0.67476	-0.23628	-1.33265
C	-1.57066	-0.19526	-0.19369
B	0.02971	0.27161	-0.09215
C	0.12882	1.91052	-0.06793
C	0.59802	-0.45046	1.26371
C	1.02414	2.62938	0.73579
C	1.17486	4.01301	0.62695
C	0.42562	4.72695	-0.30305
C	-0.46816	4.03979	-1.12325
C	-0.60414	2.65988	-1.00216
C	1.26630	-1.67948	1.17762
C	1.72579	-2.35444	2.30606
C	1.50888	-1.82160	3.57490
C	0.81887	-0.61738	3.69526
C	0.37091	0.04945	2.55592
C	-2.56505	0.44311	0.54477
C	-3.90599	0.07846	0.53082
C	-4.30753	-0.99788	-0.24344
C	-3.35653	-1.68561	-0.97816
C	-2.02314	-1.28530	-0.93570
F	-2.26268	1.48107	1.34501
F	-4.81354	0.74707	1.25747
F	-5.59376	-1.37287	-0.27329
F	-3.73359	-2.73938	-1.71818
F	-1.18757	-2.04681	-1.65465
H	5.56611	0.41670	1.03613
H	6.15059	-1.94870	0.56299
H	4.76790	-3.26124	-1.02874
H	2.80475	-2.21599	-2.11798
H	3.60413	1.45605	-0.07912
H	1.90043	1.40645	-1.60166
H	0.99126	0.71374	-3.74909
H	2.76739	0.54568	-3.79226

H	1.72532	-0.88736	-3.60869	F	-2.87990	0.20866	0.20736
H	1.62538	2.08873	1.46413	H	-3.89070	3.96771	-2.01105
H	1.88086	4.53390	1.26978	H	-2.97426	6.26244	-2.20226
H	0.53730	5.80445	-0.39115	H	-0.73160	6.79155	-1.29339
H	-1.05786	4.58345	-1.85776	H	0.59718	5.03683	-0.18354
H	-1.29858	2.13522	-1.65742	H	-2.54701	2.18661	-0.90329
H	1.42487	-2.10524	0.19110	H	0.98521	3.68016	1.48589
H	2.25582	-3.29776	2.19518	H	1.26186	1.93230	1.71728
H	1.86751	-2.34104	4.46001	H	1.95383	2.76300	0.31243
H	0.62978	-0.19637	4.68026	H	-1.42854	1.61794	2.30848
H	-0.17464	0.98429	2.66919	H	-1.81316	1.38433	4.71938
51				H	-0.85462	-0.53817	5.96222
Acetophenone + B(C ₆ F ₅) ₂ Ph				H	0.49975	-2.23070	4.74685
C	-2.90707	4.19417	-1.61487	H	0.90475	-1.98878	2.32836
C	-2.39059	5.48549	-1.71916	52			
C	-1.13036	5.78713	-1.20531	1-phenylethanolate + B(C ₆ F ₅) ₂ Ph			
C	-0.38560	4.79876	-0.57641	C	5.91846	-0.01437	-0.79344
C	-0.89673	3.49774	-0.47858	C	5.95113	-1.32368	-1.26948
C	-2.16243	3.19595	-1.00389	C	4.75639	-1.97635	-1.56182
C	-0.12347	2.42251	0.15948	C	3.53528	-1.32833	-1.38681
C	1.08688	2.71849	0.98408	C	3.49706	-0.01556	-0.91554
O	-0.52538	1.25909	-0.04244	C	4.69880	0.63199	-0.61957
C	1.54513	-0.22635	-0.03434	C	2.17012	0.71654	-0.77248
B	0.01603	-0.11936	0.53317	C	2.03705	1.72788	-1.92168
C	-1.00436	-1.21865	-0.10567	O	1.11104	-0.19533	-0.81006
C	-0.19511	-0.14720	2.13096	C	-1.06092	-1.27878	-0.13229
C	1.76549	-0.42629	-1.39788	B	0.02879	-0.06940	0.17844
C	3.02418	-0.52584	-1.97217	C	-0.64725	1.45169	0.00525
C	4.14785	-0.41095	-1.16482	C	0.50187	-0.35268	1.71508
C	3.98721	-0.18914	0.19332	C	-2.41184	-1.19402	0.19265
C	2.70461	-0.09727	0.72616	C	-3.32352	-2.22732	0.02630
C	-0.97242	0.77877	2.83211	C	-2.88604	-3.44317	-0.47475
C	-1.20703	0.64721	4.20139	C	-1.54670	-3.59309	-0.79030
C	-0.67434	-0.43090	4.89734	C	-0.66878	-2.52846	-0.60512
C	0.08617	-1.37991	4.21411	C	1.69751	-1.02917	1.98097
C	0.31507	-1.23761	2.85182	C	2.08075	-1.35739	3.28188
C	-0.61741	-2.50046	-0.48196	C	1.26245	-1.02486	4.35682
C	-1.50319	-3.46449	-0.94649	C	0.05681	-0.36582	4.11648
C	-2.85371	-3.16239	-1.03683	C	-0.31065	-0.03975	2.81534
C	-3.29342	-1.90453	-0.65254	C	-0.20415	2.56667	0.71084
C	-2.37211	-0.97636	-0.18667	C	-0.64355	3.86610	0.46817
F	0.72325	-0.53065	-2.23265	C	-1.56839	4.09671	-0.53482
F	3.16547	-0.72213	-3.28171	C	-2.03578	3.02311	-1.27839
F	5.36444	-0.49564	-1.69285	C	-1.56516	1.74659	-1.00111
F	5.05696	-0.04952	0.97532	F	-2.92062	-0.05446	0.69979
F	2.64628	0.17376	2.03859	F	-4.61469	-2.06718	0.34608
F	0.67034	-2.87273	-0.40109	F	-3.74357	-4.45738	-0.64291
F	-1.06854	-4.67300	-1.30083	F	-1.10650	-4.76918	-1.25812
F	-3.71876	-4.07042	-1.48094	F	0.61269	-2.80235	-0.89622
F	-4.59057	-1.60261	-0.71928	F	0.72784	2.45947	1.67323

F	-0.17341	4.89578	1.18433	F	2.66337	-2.40824	3.31842
F	-2.00340	5.33636	-0.78701	F	0.49217	-3.38352	4.64629
F	-2.92708	3.23523	-2.25518	F	-2.00884	-2.75714	3.78249
F	-2.05351	0.77322	-1.78557	F	-2.35802	-1.18906	1.66545
H	6.84390	0.50036	-0.55058	F	-1.84957	0.24670	-2.49704
H	6.90119	-1.83297	-1.40279	F	-4.16125	1.54330	-2.63604
H	4.77365	-3.00053	-1.92388	F	-5.14371	2.85944	-0.46478
H	2.59227	-1.82597	-1.58558	F	-3.75108	2.83211	1.87319
H	4.67369	1.65101	-0.23865	F	-1.43696	1.49982	2.04348
H	2.19100	1.26122	0.18565	F	-1.64196	-2.10623	-1.02680
H	1.11605	2.30694	-1.82014	F	-0.93003	-3.91790	-2.88685
H	2.88754	2.41660	-1.94821	F	1.49811	-3.73416	-4.10277
H	2.00137	1.17931	-2.86749	F	3.19420	-1.71177	-3.43041
H	2.33655	-1.30860	1.14622	H	3.87319	5.92523	-0.47161
H	3.02034	-1.87655	3.45455	H	5.28379	5.06223	1.37212
H	1.55647	-1.27879	5.37183	H	4.85184	2.82054	2.33488
H	-0.59461	-0.10586	4.94740	H	2.98166	1.43160	1.44525
H	-1.25714	0.47096	2.64078	H	2.02859	4.54933	-1.36380
				H	-0.09770	3.11104	-1.69329
				H	1.40932	2.68028	-2.53010
				H	0.16507	1.43987	-2.21097
51							
Acetophenone + B(C ₆ F ₅) ₃				52			
C	3.67890	4.94431	-0.05262	1-phenylethanolate + B(C ₆ F ₅) ₃			
C	4.46887	4.45714	0.98808	C	4.82962	-0.90770	1.35793
C	4.22491	3.19738	1.53452	C	5.18422	0.41656	1.59570
C	3.18063	2.42254	1.05127	C	4.22147	1.31520	2.05636
C	2.38606	2.90928	0.00300	C	2.91637	0.89039	2.27399
C	2.64411	4.16803	-0.55546	C	2.54851	-0.43476	2.02357
C	1.29172	2.06919	-0.49228	C	3.51757	-1.32887	1.57367
C	0.66009	2.32809	-1.82130	C	1.10394	-0.86389	2.25775
O	0.92057	1.14586	0.26134	C	0.86658	-1.02348	3.75945
B	-0.12965	0.00225	-0.00311	O	0.19570	0.08889	1.77696
C	-1.54922	0.77137	-0.19941	B	-0.25748	0.01836	0.38726
C	-0.02423	-0.91171	1.33638	C	-1.16148	1.37679	0.13272
C	0.38088	-0.92712	-1.23907	C	-1.34192	-1.20572	0.08360
C	-1.09932	-1.45050	2.03452	C	1.06868	-0.09551	-0.60075
C	-0.94498	-2.27517	3.14358	C	-1.83273	-1.35819	-1.21128
C	0.32887	-2.59852	3.58597	C	-2.81637	-2.26526	-1.57066
C	1.43316	-2.09719	2.91102	C	-3.37185	-3.07850	-0.59175
C	1.23239	-1.28446	1.80524	C	-2.92710	-2.96253	0.71298
C	1.61287	-0.88708	-1.87763	C	-1.93592	-2.03329	1.02475
C	2.00314	-1.81106	-2.84217	C	1.96595	0.96944	-0.64126
C	1.14283	-2.84108	-3.18511	C	3.22237	0.90797	-1.22184
C	-0.09826	-2.93088	-2.56491	C	3.62963	-0.27205	-1.82700
C	-0.44309	-1.98682	-1.61204	C	2.77113	-1.35612	-1.83534
C	-2.08811	1.47940	0.87347	C	1.52505	-1.24961	-1.22272
C	-3.28511	2.17715	0.81217	C	-2.15077	1.68877	1.06423
C	-3.99891	2.19109	-0.37895	C	-2.98961	2.79126	0.95685
C	-3.49840	1.51607	-1.48144	C	-2.87285	3.62970	-0.14092
C	-2.29465	0.82825	-1.37148	C	-1.92609	3.34418	-1.11026
F	2.50744	0.08712	-1.60617				
F	2.33914	-0.85429	1.16712				

C	-1.10476	2.23055	-0.96286
F	1.65152	2.12944	-0.04491
F	-1.57180	-2.00182	2.31617
F	-3.45661	-3.74293	1.66421
F	-4.32416	-3.96312	-0.90873
F	-3.24168	-2.36721	-2.83600
F	-1.33482	-0.59170	-2.19634
F	-0.23669	2.02506	-1.96381
F	-1.81620	4.14046	-2.18131
F	-3.67217	4.69513	-0.26706
F	-3.91924	3.04484	1.88721
F	-2.36451	0.89347	2.12080
F	0.79448	-2.38039	-1.22768
F	3.15825	-2.50588	-2.40479
F	4.84329	-0.36361	-2.38038
F	4.05380	1.95542	-1.18511
H	5.56790	-1.61006	0.98141
H	6.19934	0.75253	1.40730
H	4.48732	2.35449	2.22547
H	2.14429	1.59032	2.57925
H	3.23333	-2.35678	1.35757
H	0.95008	-1.83984	1.76362
H	-0.15959	-1.34089	3.94263
H	1.56244	-1.75044	4.18960
H	1.02759	-0.05831	4.24930

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Acetophenone + proton

C	0.16514	-0.01053	-0.00001
C	1.58687	-0.07055	0.00001
C	2.52127	1.08569	0.00007
O	2.11218	-1.25686	-0.00001
C	-0.57785	-1.21858	-0.00004
C	-1.95709	-1.17445	-0.00005
C	-2.61186	0.06256	-0.00003
C	-1.89284	1.26122	0.00000
C	-0.51108	1.23267	0.00001
H	2.02289	2.04935	-0.00016
H	3.16329	1.02138	0.88632
H	3.16371	1.02118	-0.88586
H	3.08408	-1.25231	0.00001
H	-0.05782	-2.16960	-0.00005
H	-2.53066	-2.09389	-0.00007
H	-3.69691	0.09216	-0.00003
H	-2.41597	2.21014	0.00002
H	0.03458	2.16834	0.00004

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Phenylethanol

C	-2.04739	-1.10106	-0.20727
C	-2.61908	0.11925	0.14635

C	-1.80623	1.23512	0.32229
C	-0.42736	1.13627	0.15094
C	0.14856	-0.08312	-0.20177
C	-0.67118	-1.19846	-0.38171
C	1.64884	-0.22682	-0.33790
O	2.19775	1.05685	-0.57301
C	2.24814	-0.84891	0.92355
H	-2.67452	-1.97480	-0.35366
H	-3.69325	0.19952	0.27861
H	-2.24711	2.18977	0.59206
H	0.21312	2.00201	0.27584
H	-0.22656	-2.14968	-0.66665
H	1.85282	-0.88936	-1.19445
H	3.15727	0.97630	-0.55495
H	3.33245	-0.96992	0.82122
H	1.81387	-1.83231	1.11998
H	2.04405	-0.19984	1.77920

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Acetophenone + [SiEt₃]⁺

C	4.510173	-0.831661	-0.037029
C	4.732091	0.528607	-0.257103
C	3.662767	1.423808	-0.346597
C	2.366273	0.959462	-0.220762
C	2.129987	-0.412252	0.009790
C	3.215955	-1.304719	0.104720
C	0.766813	-0.874274	0.131245
C	0.401970	-2.268378	0.520787
O	-0.155711	-0.041046	-0.130020
C	-2.334489	1.515168	-1.043284
Si	-1.953283	-0.019011	-0.048184
C	-2.613485	-1.583697	-0.828343
C	-2.289774	0.143579	1.781988
C	-1.722536	1.426562	2.408628
C	-1.227303	2.581240	-1.062489
C	-4.120848	-1.422409	-1.109967
H	5.347302	-1.517222	0.025501
H	5.748285	0.895942	-0.358695
H	3.848930	2.478424	-0.514216
H	1.524288	1.640126	-0.284397
H	3.055573	-2.364569	0.265469
H	1.211673	-2.790576	1.023051
H	-0.470827	-2.249747	1.176900
H	0.125581	-2.822767	-0.384450
H	-3.258769	1.940231	-0.630240
H	-2.579517	1.218802	-2.069829
H	-2.453947	-2.449548	-0.176680
H	-2.081745	-1.785298	-1.766519
H	-3.380530	0.116905	1.905985
H	-1.918460	-0.742053	2.312706
H	-1.933327	1.464931	3.479130

H	-0.637041	1.492175	2.282626
H	-2.165334	2.317273	1.954522
H	-1.575716	3.489214	-1.558752
H	-0.351544	2.221644	-1.609110
H	-0.906119	2.859092	-0.053926
H	-4.528360	-2.330407	-1.558170
H	-4.315285	-0.598193	-1.801517
H	-4.684832	-1.231177	-0.192001

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1-phenylethanolate + [SiEt₃]⁺

C	-4.640516	0.159700	0.683997
C	-4.919580	-0.706961	-0.370558
C	-3.887780	-1.135902	-1.199880
C	-2.582546	-0.701222	-0.982106
C	-2.299182	0.167882	0.069494
C	-3.336909	0.592714	0.900797
C	-0.896147	0.697972	0.291313
C	-0.770786	2.126401	-0.240518
O	0.030678	-0.161007	-0.342826
C	2.288213	-1.858369	-0.428680
Si	1.694245	-0.100939	-0.153550
C	2.481046	1.058460	-1.424537
C	2.106997	0.446568	1.604114
C	1.665537	-0.578032	2.658263
C	3.812982	-1.993196	-0.320778
C	3.754138	1.761921	-0.933598
H	-5.437543	0.493012	1.341308
H	-5.935324	-1.049830	-0.540035
H	-4.098055	-1.815845	-2.019816
H	-1.769680	-1.038915	-1.615190
H	-3.119721	1.263800	1.729451
H	-0.705296	0.710308	1.376560
H	0.217482	2.542461	-0.016447
H	-1.527481	2.774027	0.209770
H	-0.915418	2.122196	-1.324815
H	1.792905	-2.511995	0.298891
H	1.946875	-2.192200	-1.415817
H	1.740454	1.804047	-1.734556
H	2.701298	0.469079	-2.324007
H	3.189675	0.611986	1.675153
H	1.649314	1.424304	1.806123
H	1.842806	-0.219942	3.676393
H	0.599868	-0.814904	2.569472
H	2.212471	-1.518650	2.539437
H	4.141802	-3.028307	-0.448825
H	4.320008	-1.393757	-1.084449
H	4.177081	-1.653112	0.655496
H	4.205165	2.377499	-1.717227
H	4.512848	1.043925	-0.603923
H	3.539067	2.416021	-0.082675

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Acetophenone + [SiPhH₂]⁺

C	4.33592	-1.44539	0.02994
C	4.89419	-0.43716	0.81780
C	4.17785	0.72864	1.10428
C	2.89987	0.88892	0.60330
C	2.32443	-0.12150	-0.19966
C	3.05881	-1.29262	-0.48195
C	0.99161	0.06819	-0.70889
C	0.28041	-0.89263	-1.59663
O	0.37948	1.13522	-0.35738
Si	-1.25850	1.72971	-0.69838
C	-2.47098	0.51670	-0.03337
C	-2.68903	0.41432	1.35051
C	-3.60903	-0.49912	1.85245
C	-4.32630	-1.31397	0.97813
C	-4.12802	-1.21887	-0.39791
C	-3.20496	-0.30859	-0.90160
H	4.90032	-2.34566	-0.18295
H	5.89760	-0.56043	1.21242
H	4.62283	1.50435	1.71654
H	2.33265	1.78759	0.81568
H	2.63870	-2.08619	-1.08767
H	0.91406	-1.68640	-1.97846
H	-0.55426	-1.32834	-1.03240
H	-0.15206	-0.34548	-2.44105
H	-1.19169	3.01581	0.00311
H	-1.29942	1.83985	-2.16818
H	-2.14814	1.05685	2.04126
H	-3.77462	-0.57015	2.92189
H	-5.04930	-2.02112	1.37095
H	-4.69685	-1.84663	-1.07511
H	-3.06534	-0.23333	-1.97804

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1-phenylethanolate + [SiPhH₂]⁺

C	0.347973	1.803799	-1.114995
C	0.192981	2.844993	-0.199173
C	-0.803099	2.773855	0.768185
C	-1.638174	1.658300	0.826331
C	-1.489882	0.615642	-0.085043
C	-0.492848	0.699811	-1.061604
C	-2.370146	-0.616800	-0.005065
C	-3.316956	-0.726688	-1.190167
O	-1.592672	-1.810750	0.025232
Si	-0.491025	-2.104205	1.241690
C	1.144936	-1.235666	1.001921
C	1.429350	-0.026469	1.649296
C	2.615069	0.657071	1.401136
C	3.539505	0.137304	0.499375
C	3.278215	-1.065739	-0.150359

C	2.092201	-1.745294	0.102646
H	1.136859	1.847277	-1.859292
H	0.854569	3.704701	-0.237319
H	-0.926191	3.579814	1.485037
H	-2.406835	1.593997	1.593093
H	-0.354349	-0.130113	-1.750051
H	-2.959481	-0.554311	0.923387
H	-3.931577	-1.624440	-1.094637
H	-2.742432	-0.794711	-2.117902
H	-3.964577	0.151861	-1.244330
H	-1.077240	-1.656976	2.534678
H	-0.274635	-3.567737	1.214809
H	0.702295	0.399686	2.336300
H	2.812768	1.599647	1.901926
H	4.465565	0.668861	0.303259
H	3.998729	-1.472589	-0.851973
H	1.897795	-2.684792	-0.410790

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Cyclohexanethione

C	-0.05308	-1.26022	0.52434
C	-1.33143	-1.25917	-0.33647
C	-2.16264	-0.00000	-0.09034
C	-1.33143	1.25917	-0.33647
C	-0.05308	1.26022	0.52434
C	0.73615	0.00000	0.27883
S	2.26383	0.00000	-0.27413
H	0.56374	-2.13732	0.32395
H	-0.34618	-1.27748	1.58416
H	-1.04214	-1.30729	-1.39337
H	-1.91419	-2.15964	-0.12083
H	-3.04762	-0.00000	-0.73434
H	-2.52299	-0.00000	0.94710
H	-1.04214	1.30729	-1.39337
H	-1.91419	2.15964	-0.12083
H	0.56374	2.13732	0.32395
H	-0.34618	1.27748	1.58416

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Cyclohexathiolate

C	-0.04157	1.24852	-0.15118
C	-1.53511	1.25949	0.20248
C	-2.23280	0.00000	-0.31751
C	-1.53511	-1.25949	0.20248
C	-0.04157	-1.24852	-0.15118
C	0.68772	-0.00000	0.36559
S	2.46091	0.00000	-0.06924
H	0.45898	2.13980	0.24129
H	0.08072	1.27831	-1.24343
H	-1.64817	1.29789	1.29630

H	-2.02791	2.15728	-0.19566
H	-3.29620	0.00000	-0.04177
H	-2.18854	-0.00000	-1.41632
H	-1.64817	-1.29789	1.29630
H	-2.02791	-2.15728	-0.19566
H	0.45898	-2.13980	0.24128
H	0.08072	-1.27830	-1.24344
H	0.57347	-0.00000	1.46490

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Cyclohexathione + BEt₃

C	2.62970	-0.74158	-1.28655
C	3.52789	-0.87566	-0.03536
C	3.77461	0.48361	0.62070
C	2.45794	1.18973	0.94666
C	1.57247	1.31656	-0.31311
C	1.35821	-0.05397	-0.87623
S	-0.06011	-0.85998	-0.91292
C	-1.28387	0.56095	1.49583
B	-1.73974	0.19232	-0.01408
C	-2.89420	-0.94931	-0.14110
C	-2.00740	1.46316	-0.98220
C	-3.30746	2.18177	-0.58713
C	-0.89777	-0.57910	2.44300
C	-2.54876	-2.43671	0.03066
H	2.42299	-1.71677	-1.73046
H	3.14463	-0.11679	-2.02812
H	3.03088	-1.54573	0.67658
H	4.47089	-1.34924	-0.32280
H	4.36835	0.35596	1.53091
H	4.36416	1.11256	-0.05919
H	1.90362	0.62382	1.70580
H	2.63863	2.18792	1.35526
H	0.62979	1.81061	-0.09240
H	2.11299	1.90827	-1.06430
H	-0.49416	1.32461	1.51380
H	-2.16058	1.07164	1.92471
H	-3.42520	-0.83395	-1.09688
H	-3.63451	-0.67855	0.62805
H	-1.19244	2.20011	-0.96593
H	-2.09746	1.13709	-2.02767
H	-3.52923	3.02523	-1.24877
H	-4.16247	1.49930	-0.62679
H	-3.25075	2.57303	0.43393
H	-0.58748	-0.21200	3.42734
H	-1.73767	-1.26188	2.60181
H	-0.06926	-1.17843	2.04253
H	-3.44795	-3.04934	0.15080
H	-1.90967	-2.61857	0.90017
H	-2.01572	-2.82760	-0.84227

40				S	-0.37855	-0.25061	-1.74566
	Cyclohexathiolate + BEt ₃			C	2.00323	-1.00764	-0.37920
C	1.64719	0.28844	0.94836	B	0.75372	-0.07084	0.03847
C	2.96703	1.06689	0.97541	C	-0.24184	-0.68355	1.15447
C	4.11879	0.21004	0.44369	C	1.20472	1.46292	0.24065
C	3.80353	-0.31897	-0.95812	C	2.40448	-2.11813	0.37404
C	2.47315	-1.07991	-0.98087	C	3.52955	-2.86696	0.02764
C	1.31921	-0.21912	-0.45848	C	4.27799	-2.52642	-1.09362
S	-0.24697	-1.15160	-0.53389	C	-0.64626	0.04314	2.28297
C	-1.25116	1.62816	-0.88561	C	-1.52890	-0.48837	3.22384
B	-1.68968	0.22431	-0.16093	C	-2.03593	-1.77363	3.05909
C	-1.93513	0.46606	1.45594	C	0.85083	2.56655	-0.54357
C	-3.01186	-0.41004	-0.89435	C	1.33188	3.84882	-0.27420
C	-3.52240	-1.74590	-0.34429	C	2.18567	4.06238	0.80086
C	-2.32194	2.72303	-0.79033	C	3.90366	-1.42221	-1.85809
C	-1.63843	-0.68797	2.41890	C	2.78900	-0.67574	-1.49487
H	0.82032	0.90501	1.31544	C	2.56124	2.98112	1.59712
H	1.71777	-0.58089	1.61778	C	2.08250	1.70765	1.31257
H	2.86807	1.96391	0.34735	C	-1.64640	-2.52457	1.95025
H	3.18978	1.41573	1.99127	C	-0.76345	-1.98312	1.02041
H	5.05735	0.77851	0.43858	H	-1.50556	1.50322	0.23674
H	4.26682	-0.64376	1.12026	H	-2.72320	2.19423	-0.85598
H	3.74156	0.53151	-1.65188	H	-3.04569	-0.39675	0.74608
H	4.61990	-0.95918	-1.31584	H	-3.82296	1.14167	1.10476
H	2.24110	-1.42492	-1.99388	H	-5.35799	-0.42905	-0.15166
H	2.55142	-1.97716	-0.35034	H	-5.06950	1.06131	-1.04586
H	1.22853	0.65412	-1.12035	H	-3.64933	-1.61369	-1.50531
H	-0.33054	2.02672	-0.42812	H	-4.85170	-0.88807	-2.57555
H	-1.01006	1.45721	-1.94658	H	-2.53370	-0.47099	-3.42963
H	-1.36243	1.34561	1.79955	H	-3.34269	1.05079	-2.98262
H	-2.99142	0.76123	1.58747	H	1.83349	-2.39905	1.25497
H	-3.83478	0.31994	-0.81331	H	3.81915	-3.71919	0.63549
H	-2.81466	-0.52078	-1.97137	H	5.15043	-3.11140	-1.36833
H	-4.37132	-2.15085	-0.91326	H	-0.26456	1.05152	2.42657
H	-2.72959	-2.50339	-0.35098	H	-1.82074	0.10424	4.08602
H	-3.85380	-1.63743	0.69529	H	-2.72353	-2.19032	3.78868
H	-1.99876	3.68273	-1.21701	H	0.18788	2.43431	-1.39630
H	-3.23810	2.42788	-1.31397	H	1.03843	4.67945	-0.90957
H	-2.59831	2.90776	0.25503	H	2.56126	5.05814	1.01470
H	-1.93205	-0.46428	3.45493	H	4.48662	-1.14081	-2.73003
H	-2.15339	-1.60578	2.11629	H	2.52467	0.20186	-2.08468
H	-0.57135	-0.92972	2.41286	H	3.23519	3.13138	2.43534
				H	2.40023	0.87081	1.93221
51				H	-2.02828	-3.53221	1.81399
	Cyclohexathione + BPh ₃			H	-0.46336	-2.58619	0.16461
C	-2.32124	1.25869	-0.44129	52			
C	-3.46063	0.50903	0.28974		Cyclohexathiolate + BPh ₃		
C	-4.58865	0.14603	-0.67578	C	-2.52509	1.09839	-0.33531
C	-4.05599	-0.65916	-1.86104	C	-3.93723	1.00082	0.24987
C	-2.93223	0.10925	-2.59542	C	-4.95867	0.65038	-0.83506
C	-1.86097	0.42705	-1.59431				

C	-4.56230	-0.63574	-1.56511	51			
C	-3.14063	-0.54187	-2.13003	Cyclohexathione + B(C ₆ F ₅)Ph ₂			
C	-2.12907	-0.20499	-1.03116	C	2.06990	-1.89817	-0.20957
S	-0.44089	-0.17979	-1.73253	C	3.29911	-1.77711	0.72162
C	2.18843	-0.65192	-0.63327	C	4.59673	-2.03674	-0.04327
B	0.74384	-0.08196	-0.12660	C	4.71704	-1.10263	-1.24722
C	0.04702	-1.02476	1.00465	C	3.49127	-1.23822	-2.18054
C	1.00036	1.45106	0.38418	C	2.25722	-0.97795	-1.37000
C	2.98093	-1.51190	0.14064	S	1.32388	0.32008	-1.71243
C	4.24771	-1.92804	-0.27158	C	-0.61188	2.12486	-0.73004
C	4.76703	-1.49209	-1.48597	B	-0.00246	0.74138	-0.15985
C	-0.05173	-2.41381	0.79806	C	0.96499	0.86080	1.12652
C	-0.72356	-3.25232	1.68114	C	-1.17571	-0.38246	-0.03753
C	-1.33739	-2.72524	2.81837	C	-0.61103	3.30637	0.02121
C	0.59503	2.60444	-0.29998	C	-1.18942	4.47714	-0.46557
C	0.90033	3.88637	0.15987	C	-1.78229	4.49439	-1.72419
C	1.63101	4.05768	1.33126	C	0.80317	0.07920	2.27774
C	4.00603	-0.63014	-2.27503	C	1.67209	0.17781	3.36392
C	2.74738	-0.21948	-1.84822	C	2.73611	1.07359	3.32735
C	2.05811	2.92969	2.03113	C	-1.37052	-1.56039	-0.74987
C	1.74929	1.65839	1.55700	C	-2.46590	-2.39953	-0.56601
C	-1.26029	-1.35689	3.05190	C	-3.43164	-2.06899	0.36943
C	-0.57497	-0.52900	2.15939	C	-1.80393	3.32969	-2.48836
H	-1.79895	1.33731	0.44689	C	-1.23027	2.16524	-1.98886
H	-2.48053	1.91600	-1.06959	C	-3.28528	-0.90412	1.11132
H	-3.94467	0.21973	1.02325	C	-2.17949	-0.09611	0.89207
H	-4.21350	1.94000	0.74382	F	-0.48502	-1.97250	-1.67818
H	-5.96386	0.55350	-0.40668	F	-4.48327	-2.86057	0.56061
H	-5.00023	1.47379	-1.56240	F	-2.58773	-3.51674	-1.28369
H	-4.60893	-1.47471	-0.85716	F	-4.20308	-0.57719	2.01900
H	-5.27878	-0.85618	-2.36613	F	-2.08565	1.00989	1.63914
H	-2.85543	-1.48063	-2.61625	C	2.91630	1.87416	2.20004
H	-3.10120	0.24188	-2.90009	C	2.04065	1.76613	1.12361
H	-2.16031	-1.01019	-0.28362	H	1.14695	-1.69230	0.32935
H	2.59314	-1.87050	1.09195	H	2.02062	-2.91958	-0.61098
H	4.82926	-2.59695	0.35905	H	3.31094	-0.77084	1.15640
H	5.75169	-1.81547	-1.81372	H	3.17765	-2.48227	1.54855
H	0.40230	-2.83228	-0.09823	H	5.45501	-1.89889	0.62111
H	-0.77732	-4.32009	1.48161	H	4.62225	-3.07889	-0.38794
H	-1.86925	-3.37462	3.50892	H	4.77907	-0.06318	-0.90278
H	0.02478	2.48208	-1.21789	H	5.62283	-1.31133	-1.82324
H	0.56457	4.75577	-0.40125	H	3.55903	-0.55417	-3.02851
H	1.86880	5.05439	1.69411	H	3.44637	-2.26714	-2.56028
H	4.39889	-0.27562	-3.22523	H	-0.16266	3.30610	1.01082
H	2.17257	0.46317	-2.47187	H	-1.17827	5.37747	0.14146
H	2.63635	3.04385	2.94528	H	-2.22963	5.40681	-2.10619
H	2.09980	0.78800	2.11101	H	-0.01591	-0.63503	2.32816
H	-1.73519	-0.92779	3.93126	H	1.51530	-0.44519	4.23942
H	-0.52533	0.53798	2.36622	H	3.41517	1.15364	4.17045
				H	-2.27114	3.32895	-3.46851
				H	-1.27007	1.25795	-2.59245

H	3.73599	2.58561	2.16300	H	2.54337	3.92669	2.19966
H	2.19019	2.40618	0.25542	H	2.82615	2.41612	4.15781
52				H	-2.80138	2.61670	-3.80639
Cyclohexathiolate + B(C ₆ F ₅)Ph ₂				H	-1.19547	1.01288	-2.84242
C	2.40937	-1.55869	-0.29579	H	1.73256	0.18264	4.13588
C	3.60672	-2.14903	0.45515	H	0.38212	-0.51848	2.20925
C	4.86275	-2.13847	-0.41965	51			
C	5.16286	-0.72582	-0.92754	Cyclohexathione + B(C ₆ F ₅) ₂ Ph			
C	3.95583	-0.12914	-1.65915	C	-3.30057	0.34996	-0.56613
C	2.70976	-0.13530	-0.76926	C	-4.31797	-0.50255	0.22898
S	1.32383	0.65482	-1.66149	C	-5.32795	-1.16786	-0.70548
C	-1.11495	1.93824	-0.90255	C	-4.61752	-2.00231	-1.77088
B	-0.08825	0.82586	-0.29109	C	-3.61191	-1.14181	-2.57098
C	0.67468	1.28484	1.06913	C	-2.65865	-0.51753	-1.59675
C	-1.01873	-0.52906	-0.04036	S	-1.07721	-0.91880	-1.66169
C	-1.63915	2.99556	-0.14613	C	1.38154	-0.94524	-0.24207
C	-2.54982	3.90575	-0.68221	B	-0.08580	-0.30600	0.05169
C	-2.97243	3.78074	-2.00208	C	-0.94769	-0.99755	1.22616
C	1.31158	2.53811	1.11380	C	0.06614	1.30861	0.15002
C	2.06861	2.94845	2.20611	C	2.10513	-1.71637	0.66576
C	2.22929	2.10416	3.30494	C	3.38966	-2.18266	0.40186
C	-1.05202	-1.71779	-0.76795	C	4.00594	-1.86492	-0.79877
C	-1.93950	-2.76048	-0.50378	C	-1.52285	-0.26385	2.26939
C	-2.86274	-2.64220	0.51904	C	-2.30666	-0.87182	3.25050
C	-2.47748	2.73171	-2.77481	C	-2.53445	-2.24285	3.21051
C	-1.56979	1.82990	-2.22745	C	-0.41015	2.30118	-0.69833
C	-2.88488	-1.47547	1.26723	C	-0.15205	3.65564	-0.51188
C	-1.98505	-0.46176	0.96837	C	0.62303	4.06386	0.56139
F	-0.22044	-1.95135	-1.79174	C	3.33496	-1.07724	-1.72420
F	-3.72028	-3.63598	0.78272	C	2.05874	-0.62954	-1.41971
F	-1.91141	-3.88068	-1.23941	C	1.12766	3.11139	1.43707
F	-3.77674	-1.34058	2.25819	C	0.84640	1.77195	1.21172
F	-2.08582	0.63975	1.72858	F	-1.17391	2.00032	-1.76347
C	1.61679	0.85602	3.29005	F	0.87712	5.35410	0.75408
C	0.85031	0.46429	2.19129	F	-0.64469	4.55897	-1.35823
H	1.52451	-1.55195	0.34879	F	1.87298	3.48992	2.47259
H	2.16465	-2.17850	-1.16774	F	1.35936	0.88988	2.07934
H	3.78816	-1.54988	1.35873	C	-1.96444	-3.00113	2.18754
H	3.38428	-3.16945	0.78904	C	-1.18459	-2.38228	1.21742
H	5.72279	-2.53889	0.13075	F	1.60165	-2.03585	1.85849
H	4.69979	-2.79989	-1.28237	F	4.03739	-2.92303	1.29961
H	5.41271	-0.08529	-0.07051	F	5.23228	-2.30542	-1.06030
H	6.04143	-0.73475	-1.58421	F	3.92104	-0.75271	-2.87544
H	4.16924	0.89428	-1.98505	F	1.45701	0.15320	-2.33325
H	3.74665	-0.71664	-2.56426	H	-2.56999	0.80895	0.09708
H	2.92200	0.47932	0.11712	H	-3.83582	1.14576	-1.10155
H	-1.32797	3.10485	0.88963	H	-3.76887	-1.26287	0.79637
H	-2.93257	4.71453	-0.06412	H	-4.81553	0.14421	0.95686
H	-3.68146	4.48855	-2.42349	H	-6.00720	-1.80235	-0.12851
H	1.21875	3.19282	0.24971	H	-5.94296	-0.40095	-1.19430

H	-4.07012	-2.82316	-1.29186
H	-5.33154	-2.44803	-2.46883
H	-3.08309	-1.73765	-3.31723
H	-4.15840	-0.34010	-3.08392
H	-1.36608	0.81141	2.31904
H	-2.73635	-0.27136	4.04658
H	-3.14308	-2.72042	3.97183
H	-2.12238	-4.07484	2.15295
H	-0.73686	-2.99297	0.43435

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Cyclohexathiolate + B(C₆F₅)₂Ph

C	-3.40604	0.26221	-0.64314
C	-4.84457	0.14111	-0.13188
C	-5.73308	-0.56647	-1.15816
C	-5.15479	-1.93345	-1.53313
C	-3.70778	-1.81165	-2.02257
C	-2.83054	-1.11521	-0.97836
S	-1.10948	-1.05085	-1.59148
C	1.47183	-0.90635	-0.33108
B	-0.07887	-0.42322	-0.03079
C	-0.77146	-1.12130	1.26134
C	0.04551	1.21762	0.14685
C	2.30692	-1.58217	0.55649
C	3.62131	-1.93358	0.25704
C	4.16862	-1.58027	-0.96381
C	-0.81085	-2.52332	1.36335
C	-1.50105	-3.17373	2.37756
C	-2.19854	-2.43565	3.33595
C	-0.43122	2.23003	-0.68343
C	-0.20911	3.58542	-0.44072
C	0.52833	3.98220	0.66032
C	3.39318	-0.87060	-1.86774
C	2.08689	-0.54314	-1.53068
C	1.03903	3.01406	1.51163
C	0.79566	1.67666	1.23308
F	-1.14836	1.97431	-1.78135
F	0.74625	5.27997	0.90096
F	-0.70085	4.51354	-1.27167
F	1.76111	3.38114	2.57793
F	1.33671	0.79307	2.08675
C	-2.18129	-1.04891	3.26129
C	-1.47222	-0.41008	2.24089
F	1.89760	-1.92967	1.78217
F	4.36928	-2.59811	1.14784
F	5.43049	-1.90874	-1.26391
F	3.91803	-0.49774	-3.04188
F	1.41599	0.18479	-2.43463
H	-2.77680	0.75076	0.10817
H	-3.37347	0.88851	-1.54365
H	-4.83985	-0.43428	0.80468

H	-5.25143	1.13132	0.10463
H	-6.75562	-0.67507	-0.77697
H	-5.79407	0.05473	-2.06291
H	-5.17813	-2.58459	-0.64848
H	-5.77668	-2.41423	-2.29796
H	-3.29370	-2.79934	-2.25117
H	-3.68131	-1.22928	-2.95421
H	-2.84490	-1.72339	-0.06426
H	-0.29886	-3.11091	0.60357
H	-1.50480	-4.25995	2.42064
H	-2.74803	-2.93935	4.12649
H	-2.71949	-0.45667	3.99709
H	-1.48143	0.67769	2.20557

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Cyclohexathione + B(C₆F₅)₃

C	2.28944	1.86762	1.21585
C	3.72814	1.38558	0.91068
C	4.59809	1.43102	2.16635
C	3.97445	0.60475	3.29101
C	2.52790	1.06286	3.58972
C	1.74080	1.01847	2.31425
S	0.47427	-0.00413	2.19455
C	-1.40555	-1.14636	0.39690
B	-0.18959	-0.07787	0.25357
C	1.12369	-0.60180	-0.54572
C	-0.83173	1.32282	-0.25515
C	-1.57931	-2.28850	-0.37942
C	-2.68683	-3.12067	-0.26030
C	-3.68263	-2.81452	0.65546
C	1.78618	0.08221	-1.56053
C	2.93035	-0.39988	-2.19034
C	3.45811	-1.62236	-1.80787
C	-1.03475	2.50638	0.44087
C	-1.69619	3.60487	-0.10052
C	-2.19451	3.53608	-1.39072
C	-3.56171	-1.67727	1.44207
C	-2.44293	-0.87308	1.28711
C	-2.01959	2.37091	-2.12816
C	-1.35493	1.30363	-1.54826
F	-0.57831	2.66348	1.69626
F	-2.82837	4.57587	-1.92199
F	-1.85269	4.71665	0.61645
F	-2.48913	2.29381	-3.37061
F	-1.19648	0.19972	-2.29132
C	2.83767	-2.34387	-0.79440
C	1.69763	-1.82599	-0.20083
F	-0.67725	-2.64019	-1.30048
F	-2.80294	-4.20389	-1.02467
F	-4.74488	-3.60251	0.77795
F	-4.51312	-1.36680	2.31975

F	-2.37301	0.22750	2.05736	F	3.68035	-3.59385	0.73031
F	1.38367	1.29985	-1.95388	F	5.37832	-2.58673	-1.14528
F	3.52649	0.31399	-3.14281	F	4.62220	-0.41599	-2.61369
F	4.55153	-2.09645	-2.39367	F	2.23760	0.70783	-2.22239
F	3.33470	-3.51838	-0.41491	F	-0.49487	-2.88839	-0.76652
F	1.13581	-2.55883	0.77098	F	-2.46546	-4.26226	0.37140
H	1.66569	1.86140	0.32342	F	-4.03907	-3.10685	2.27242
H	2.33333	2.89797	1.59295	F	-3.56515	-0.52270	3.01351
H	3.68100	0.35750	0.53005	F	-1.61599	0.86651	1.91237
H	4.14254	2.00727	0.11218	H	-2.07518	1.76793	-0.17898
H	5.60006	1.05483	1.94069	H	-2.17941	2.54296	-1.75522
H	4.71273	2.47161	2.49574	H	-4.50149	1.24658	-0.22021
H	3.95231	-0.45346	3.00443	H	-4.24541	2.97952	-0.40145
H	4.56207	0.67978	4.20979	H	-5.95152	2.13448	-2.04015
H	2.06748	0.44401	4.36209	H	-4.53605	2.79551	-2.85893
H	2.54743	2.10275	3.94030	H	-5.08013	-0.16884	-2.34340
52				H	-5.18376	0.64067	-3.90498
Cyclohexathiolate + B(C ₆ F ₅) ₃				H	-3.00844	-0.58739	-3.65402
C	-2.61251	1.75038	-1.13179	H	-2.74229	1.14717	-3.82641
C	-4.10349	2.01397	-0.89973	H	-2.80633	-0.38702	-1.19700
C	-4.88158	1.97323	-2.21689	18			
C	-4.65417	0.64606	-2.94500	Cyclohexanethione + proton			
C	-3.16132	0.37885	-3.16218	C	-0.08925	1.26833	0.59012
C	-2.39589	0.40863	-1.83593	C	-1.33450	1.25941	-0.35680
S	-0.63695	0.03965	-2.16884	C	-2.16611	-0.00291	-0.15179
C	1.59875	-0.88083	-0.58506	C	-1.32637	-1.25939	-0.35712
B	0.16792	-0.09201	-0.38319	C	-0.08029	-1.26063	0.58690
C	-0.93004	-0.92982	0.49680	C	0.64938	0.00825	0.35847
C	0.62767	1.32632	0.32265	S	2.17851	-0.08245	-0.29119
C	2.05544	-1.96072	0.16627	H	0.52426	2.15747	0.43562
C	3.30409	-2.54743	-0.01460	H	-0.45207	1.25925	1.62565
C	4.17374	-2.03589	-0.96267	H	-1.90790	2.16289	-0.13911
C	-1.22091	-2.25544	0.16147	H	-0.98989	1.33057	-1.39392
C	-2.24318	-2.99432	0.73666	H	-3.00163	-0.00458	-0.85731
C	-3.04631	-2.41171	1.70766	H	-2.59999	-0.00389	0.85489
C	0.71152	2.58924	-0.25651	H	-1.89451	-2.16625	-0.14000
C	1.21683	3.70189	0.41663	H	-0.98145	-1.32887	-1.39426
C	1.68226	3.57756	1.71281	H	-0.43671	-1.26315	1.62454
C	3.78236	-0.93751	-1.71182	H	0.54383	-2.14088	0.42154
C	2.52719	-0.38294	-1.49960	H	2.42279	1.23823	-0.39735
C	1.63537	2.33517	2.32925	19			
C	1.12511	1.25708	1.62493	Cyclohexanethiol			
F	0.30269	2.83135	-1.50527	C	-0.07407	1.26060	-0.17097
F	2.17097	4.63826	2.36414	C	-1.56291	1.26446	0.19051
F	1.26356	4.89540	-0.18822	C	-2.25461	-0.00280	-0.31633
F	2.08590	2.19657	3.58204	C	-1.55832	-1.25603	0.21835
F	1.11504	0.07788	2.26917	C	-0.06923	-1.25924	-0.13973
C	-2.80144	-1.10324	2.08013	C	0.61493	0.00987	0.37491
C	-1.75848	-0.40046	1.48042	S	2.38395	-0.07670	-0.09863
F	1.31006	-2.50308	1.13875				

H	0.41688	2.16018	0.21657	H	-0.51673	3.07516	1.85584
H	0.04558	1.27416	-1.26190	H	-1.37939	2.91209	0.32677
H	-1.67093	1.32315	1.28197	H	0.30448	2.40454	0.44508
H	-2.04361	2.15672	-0.22298				
H	-3.31073	-0.00212	-0.02853	40			
H	-2.22291	-0.01466	-1.41405	Cyclohexathiolate + [SiEt ₃] ⁺			
H	-1.66630	-1.29138	1.31068	C	-1.84474	-0.65852	0.82662
H	-2.03591	-2.15854	-0.17585	C	-3.12800	-1.46903	0.61523
H	0.42507	-2.14488	0.27232	C	-4.35135	-0.55480	0.52716
H	0.04575	-1.30090	-1.23133	C	-4.16902	0.49160	-0.57373
H	0.56087	0.01464	1.47029	C	-2.88674	1.30166	-0.36151
H	2.73841	1.10975	0.42050	C	-1.66447	0.38268	-0.27907
				S	-0.17864	1.44399	-0.03528
39				Si	1.46768	0.04478	-0.17913
Cyclohexathione + [SiEt ₃] ⁺				C	1.83052	-0.81475	1.47242
C	1.77292	-1.04141	0.75791	C	1.09336	-1.23154	-1.51993
C	2.63438	0.00112	1.52930	C	2.93987	1.11864	-0.66094
C	3.99923	0.17623	0.86715	C	3.30782	-1.18938	1.66678
C	3.85561	0.55359	-0.60498	C	2.19983	-2.28600	-1.66489
C	2.98843	-0.48873	-1.37012	C	3.17036	2.29453	0.29801
C	1.68466	-0.59362	-0.65631	H	-1.88299	-0.13632	1.79163
S	0.32528	-0.05212	-1.43042	H	-0.97884	-1.32933	0.86430
Si	-1.50281	-0.10535	-0.03783	H	-3.04036	-2.04528	-0.31628
C	-2.74793	0.65402	-1.21389	H	-3.24716	-2.19542	1.42559
C	-1.83226	-1.90096	0.38699	H	-5.25621	-1.14450	0.34844
C	-1.10289	1.02554	1.40179	H	-4.48770	-0.04407	1.48981
C	-3.95704	1.24663	-0.46498	H	-4.11994	-0.01387	-1.54766
C	-3.29001	-2.09277	0.84947	H	-5.03130	1.16505	-0.61054
C	-0.64848	2.43161	0.98384	H	-2.74864	2.02879	-1.16749
H	0.79761	-1.17397	1.22388	H	-2.96027	1.86934	0.57579
H	2.30123	-2.00279	0.77395	H	-1.55280	-0.12976	-1.24299
H	2.09655	0.95667	1.55082	H	1.50185	-0.15603	2.28407
H	2.73057	-0.34283	2.56182	H	1.20648	-1.71458	1.54513
H	4.56560	0.94974	1.39293	H	0.94647	-0.69727	-2.46631
H	4.57243	-0.75427	0.95632	H	0.14169	-1.72994	-1.29710
H	3.38555	1.53890	-0.70257	H	3.83361	0.48231	-0.69893
H	4.82737	0.60702	-1.10074	H	2.77949	1.48861	-1.68005
H	2.85950	-0.20544	-2.41557	H	3.46406	-1.72021	2.61033
H	3.49011	-1.46298	-1.31979	H	3.67474	-1.83488	0.86258
H	-3.07643	-0.11084	-1.92732	H	3.94375	-0.29922	1.68137
H	-2.26656	1.44025	-1.80763	H	1.99094	-2.97810	-2.48558
H	-1.14719	-2.24128	1.17074	H	2.29848	-2.88116	-0.75169
H	-1.63801	-2.52396	-0.49317	H	3.17265	-1.82486	-1.86484
H	-0.37571	0.56233	2.07771	H	4.06074	2.86854	0.02654
H	-2.03482	1.09262	1.98097	H	2.31782	2.98005	0.28952
H	-3.65494	2.05775	0.20356	H	3.29964	1.95076	1.32986
H	-4.47769	0.49607	0.13562				
H	-4.67893	1.65708	-1.17353	31			
H	-3.53227	-1.46449	1.71218	Cyclohexathione + [SiPhH ₂] ⁺			
H	-3.46210	-3.13004	1.14321	C	1.23360	-0.29602	-1.34187
H	-3.99512	-1.85618	0.04836	C	0.81220	-1.65582	-0.69932

C	-1.204251	1.517500	0.127695
N	-0.187489	0.488990	0.138383
C	1.105342	1.095537	0.371095
C	1.462714	2.047423	-0.770694
C	0.401784	3.141226	-0.910272
C	-0.503778	-0.646023	1.157760
C	0.610545	-1.485195	1.663133
C	1.286983	-2.296857	0.581035
C	0.264645	-3.217356	-0.099440
C	-0.894081	-2.379874	-0.642947
C	-1.549833	-1.537188	0.454298
H	-1.766215	3.283753	-1.011782
H	-1.066155	1.961438	-1.964484
H	-2.191344	1.053220	0.029435
H	-1.217628	2.085592	1.088426
H	1.841962	0.297030	0.472560
H	1.125166	1.668641	1.328100
H	2.452094	2.493380	-0.604090
H	1.510482	1.462695	-1.698093
H	0.430636	3.775863	-0.012274
H	0.608097	3.792615	-1.769405
H	-0.994945	-0.122276	2.005791
H	1.322880	-0.915071	2.277024
H	1.782489	-1.737539	-0.263687
H	2.090511	-2.918656	1.008775
H	0.717453	-3.800132	-0.918195
H	-0.120722	-3.922522	0.649897
H	-0.500376	-1.688028	-1.400251
H	-1.643113	-3.015765	-1.138536
H	-2.370949	-0.956106	0.008005
H	-1.988033	-2.193338	1.215360

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Piperidino-Cyclohex-1-ene + BEt₃

C	-2.192369	-2.241877	-0.194945
C	-1.275023	-1.095379	-0.597428
N	-1.598559	0.106121	0.192811
C	-3.040260	0.328747	0.454688
C	-3.893153	-0.411148	-0.570548
C	-3.664749	-1.928765	-0.520775
C	-0.655666	0.902604	0.625867
C	0.768825	0.840583	0.210030
C	0.691968	1.744777	-1.073220
C	0.285744	3.174828	-0.685338
C	-1.027546	3.220531	0.105835
C	-1.038446	2.198802	1.281287
B	1.922092	-0.465077	0.260383
C	1.801116	-1.154533	1.748506
C	0.547567	-1.972847	2.075482
C	1.936356	-1.604566	-0.930855
C	1.947156	-1.075390	-2.368456

C	3.344625	0.383468	0.212323
C	4.616615	-0.462146	0.090226
H	-2.060896	-2.418618	0.877497
H	-1.855084	-3.149496	-0.702036
H	-0.230462	-1.318706	-0.412094
H	-1.386305	-0.850909	-1.661543
H	-3.249111	1.397242	0.402848
H	-3.265744	-0.018592	1.470669
H	-4.941841	-0.163416	-0.386146
H	-3.650909	-0.019759	-1.564583
H	-4.315870	-2.379882	0.233825
H	-3.948942	-2.364410	-1.482736
H	1.266613	1.488206	0.943608
H	-0.024360	1.333640	-1.797784
H	1.669228	1.740398	-1.560690
H	0.188654	3.808343	-1.574115
H	1.088205	3.605298	-0.073755
H	-1.863406	2.980123	-0.565580
H	-1.214349	4.222305	0.503371
H	-2.001696	2.194562	1.793236
H	-0.268409	2.463264	2.007917
H	1.914755	-0.380049	2.525030
H	2.670440	-1.816269	1.880848
H	0.599521	-2.462386	3.055190
H	0.377812	-2.763304	1.332737
H	-0.354036	-1.343256	2.092592
H	1.162935	-2.386455	-0.854561
H	2.864863	-2.170265	-0.769050
H	2.734237	-0.322748	-2.499785
H	0.999032	-0.584553	-2.625192
H	2.115684	-1.857927	-3.117547
H	3.369455	1.125035	-0.602717
H	3.421176	0.981188	1.135956
H	4.688589	-0.933434	-0.896260
H	5.528202	0.130351	0.231250
H	4.634908	-1.269111	0.831939

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N-Cyclohexylidene-Piperidine + BEt₃

C	3.060633	-1.857458	0.669912
C	1.981243	-0.902392	1.189154
N	1.735966	0.150818	0.220405
C	2.079360	-0.152294	-1.153103
C	3.602279	-0.343838	-1.270849
C	4.163912	-1.058895	-0.023270
C	0.625199	1.072341	0.487377
C	-0.697103	0.850304	-0.300453
C	-1.625061	2.061499	-0.058554
C	-0.998657	3.441993	-0.263046
C	0.223072	3.606614	0.631725

H	-2.099130	1.444047	2.149960
H	1.198309	1.789383	-4.012710
H	-0.426314	3.660680	-4.232984
H	-2.355211	3.781743	-2.669837
H	-2.646279	2.084123	-0.918677
H	-0.639783	-1.514790	-2.632173
H	-0.202984	-3.902788	-3.018504
H	-0.071982	-5.482626	-1.107049
H	-0.483047	-4.639036	1.198642
H	-0.964366	-2.255007	1.572904

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N-Cyclohexylidene-Piperidine + BPh₃

C	3.714950	-1.590776	0.271420
C	2.433330	-0.790994	0.042533
N	2.614759	0.583271	0.492645
C	3.642659	1.214307	-0.323234
C	4.991590	0.520989	-0.138886
C	4.882606	-0.963185	-0.489364
C	1.406093	1.441739	0.581185
C	0.081167	0.757081	1.003682
C	0.265169	0.054576	2.369199
C	1.269186	0.773470	3.291365
C	1.220045	2.276097	3.029110
C	1.706690	2.581787	1.599960
B	-0.970317	-0.002490	-0.084484
C	-2.495955	-0.003228	0.579144
C	-3.480393	-0.848586	0.030974
C	-1.027016	0.904300	-1.462536
C	0.068995	0.991578	-2.344142
C	-0.628572	-1.589297	-0.392559
C	-4.800719	-0.859782	0.469803
C	-5.203084	-0.013852	1.502034
C	-4.262721	0.838617	2.068819
C	-2.944459	0.839974	1.607902
C	0.061740	1.774296	-3.496096
C	-1.064942	2.526857	-3.820007
C	-2.165856	2.477351	-2.971469
C	-2.140063	1.682536	-1.824291
C	-0.230429	-2.116277	-1.631308
C	0.079127	-3.465589	-1.813377
C	-0.013020	-4.358810	-0.751632
C	-0.453219	-3.884180	0.483012
C	-0.764346	-2.537074	0.642872
H	3.553810	-2.627707	-0.043904
H	3.934332	-1.595293	1.346872
H	1.608901	-1.252839	0.579066
H	2.176179	-0.849248	-1.032904
H	3.730261	2.269806	-0.048818
H	3.360911	1.190590	-1.398009
H	5.289961	0.629202	0.911428

H	5.753493	1.013351	-0.755379
H	5.823721	-1.485881	-0.280950
H	4.693479	-1.059219	-1.567887
H	1.237660	1.917700	-0.396395
H	-0.520936	1.655547	1.216369
H	-0.714493	0.002958	2.862437
H	0.583418	-0.985660	2.243758
H	1.055334	0.550577	4.343996
H	2.284276	0.419542	3.077477
H	1.826178	2.829577	3.756377
H	0.186286	2.622834	3.160412
H	1.242475	3.509851	1.244368
H	2.787012	2.761343	1.633307
H	-3.190796	-1.521369	-0.774095
H	0.971132	0.427850	-2.115118
H	-5.519586	-1.533020	0.007834
H	-6.230808	-0.020203	1.856113
H	-4.553021	1.508644	2.875282
H	-2.249006	1.532737	2.077550
H	0.939286	1.799052	-4.138456
H	-1.081136	3.142148	-4.716014
H	-3.055129	3.059625	-3.203330
H	-3.020965	1.666378	-1.187535
H	-0.160110	-1.454292	-2.489834
H	0.390523	-3.818749	-2.794176
H	0.232735	-5.409008	-0.886581
H	-0.564017	-4.569465	1.320487
H	-1.144401	-2.201343	1.605473

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Piperidino-Cyclohex-1-ene + B(C₆F₅)Ph₂

C	-2.884544	1.433434	1.666587
C	-1.959487	1.620155	0.469101
N	-2.562276	1.042784	-0.748243
C	-3.838015	1.720759	-1.064168
C	-4.826615	1.508514	0.084273
C	-4.260259	2.041550	1.399870
C	-2.048357	0.080393	-1.459798
C	-0.870171	-0.792276	-1.128266
C	-1.491111	-2.217602	-1.338767
C	-1.670463	-2.549652	-2.825762
C	-1.995403	-1.277040	-3.622164
C	-2.759919	-0.272507	-2.764248
B	0.256041	-0.727667	0.138878
C	1.254873	-1.995747	-0.190786
C	1.466808	-3.064839	0.690010
C	1.233233	0.612885	-0.006762
C	1.090276	1.674713	-0.892904
C	-0.404949	-0.856213	1.632979
C	2.285478	-4.144519	0.359507
C	2.927389	-4.188695	-0.873414

C	2.753789	-3.132125	-1.764099	N	-2.709667	-0.619908	-0.693834
C	1.936066	-2.059597	-1.418066	C	-3.513867	-0.097812	0.397393
C	2.007524	2.710277	-1.042028	C	-4.705235	-1.027459	0.638747
C	3.155127	2.713338	-0.269163	C	-4.178572	-2.419195	0.996809
C	3.354610	1.683881	0.640878	C	-1.977749	0.258139	-1.607001
C	2.410863	0.671439	0.746579	C	-0.800598	1.188156	-1.162894
C	-0.110054	0.010934	2.697095	C	-0.067068	1.603604	-2.471155
C	-0.699816	-0.112005	3.954649	C	-0.976225	1.710121	-3.711731
C	-1.620689	-1.125384	4.201098	C	-2.369895	2.164010	-3.290014
C	-1.927141	-2.016180	3.176197	C	-3.016013	1.090600	-2.397450
C	-1.326409	-1.878525	1.925778	B	0.263738	0.838942	0.083974
F	-0.006376	1.780268	-1.686537	C	1.422918	2.038010	0.110808
F	1.787304	3.692872	-1.920475	C	2.540013	1.969962	-0.744002
F	4.049847	3.692824	-0.388868	C	-0.574295	0.816390	1.499667
F	4.452051	1.678663	1.398200	C	-0.576066	-0.245970	2.417925
F	2.675455	-0.282350	1.645813	C	1.176051	-0.559811	-0.058467
H	-2.409467	1.890797	2.538219	C	3.521463	2.954981	-0.794341
H	-2.961531	0.360416	1.880825	C	3.434420	4.071306	0.033643
H	-0.993455	1.166458	0.635648	C	2.357468	4.165902	0.907548
H	-1.811893	2.684156	0.245263	C	1.382317	3.168349	0.941882
H	-4.249286	1.356924	-1.999593	C	-1.346671	-0.244174	3.580243
H	-3.610398	2.786423	-1.181592	C	-2.149306	0.849886	3.888906
H	-5.033979	0.434827	0.170768	C	-2.164890	1.932698	3.013649
H	-5.767042	2.004338	-0.174436	C	-1.400227	1.902486	1.849847
H	-4.944859	1.823367	2.223838	C	2.133786	-0.823089	0.930338
H	-4.173460	3.134291	1.333961	C	2.998963	-1.908446	0.924030
H	-0.226332	-0.643277	-2.009102	C	2.962145	-2.804182	-0.134118
H	-0.836226	-2.953220	-0.869996	C	2.058902	-2.584067	-1.155991
H	-2.454893	-2.279229	-0.817021	C	1.210493	-1.479603	-1.100198
H	-0.746947	-2.992548	-3.211380	F	2.262658	0.000313	1.979957
H	-2.462723	-3.294250	-2.954415	F	3.878710	-2.096954	1.916837
H	-2.588303	-1.503592	-4.512291	F	3.789554	-3.856262	-0.165671
H	-1.075238	-0.805047	-3.978919	F	2.016612	-3.426204	-2.198087
H	-2.927302	0.647412	-3.333578	F	0.405021	-1.363056	-2.176019
H	-3.750338	-0.678429	-2.515470	H	-2.785867	-3.886149	0.201677
H	0.988184	-3.052173	1.665510	H	-3.790293	-3.082824	-1.019172
H	2.424783	-4.951697	1.073340	H	-1.508354	-2.231368	-1.208631
H	3.563845	-5.028855	-1.134185	H	-1.458953	-1.843802	0.519110
H	3.263200	-3.139738	-2.723948	H	-3.847123	0.916502	0.162179
H	1.843845	-1.233046	-2.123844	H	-2.949762	-0.035364	1.337990
H	0.593024	0.826393	2.541495	H	-5.315626	-1.078906	-0.272019
H	-0.435278	0.586016	4.744428	H	-5.330762	-0.635420	1.450034
H	-2.082552	-1.227610	5.178352	H	-4.999589	-3.128465	1.157103
H	-2.631541	-2.825018	3.350557	H	-3.625338	-2.342725	1.944028
H	-1.568447	-2.611935	1.162440	H	-1.547742	-0.441356	-2.329302
				H	-1.287691	2.109446	-0.797446
				H	0.413215	2.572451	-2.302014
				H	0.742375	0.897532	-2.688992
				H	-0.540230	2.400016	-4.444086
				H	-1.057358	0.737251	-4.214738
				H	-3.006989	2.375382	-4.157122

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N-Cyclohexylidene-Piperidine + $B(C_6F_5)_2$

C	-3.227825	-2.925524	-0.089938
C	-2.120631	-1.901696	-0.364895

H	-2.273505	3.106843	-2.737178
H	-3.714731	1.571677	-1.703761
H	-3.610255	0.394017	-3.001485
H	2.649705	1.105904	-1.396739
H	0.028306	-1.126547	2.214076
H	4.359644	2.847427	-1.479021
H	4.197338	4.844979	0.004763
H	2.276790	5.017736	1.579350
H	0.579677	3.271583	1.664775
H	-1.318976	-1.103825	4.245700
H	-2.752497	0.858137	4.792673
H	-2.786879	2.798154	3.230104
H	-1.465381	2.754396	1.176543

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Piperidino-Cyclohex-1-ene + B(C₆F₅)₂Ph

C	-0.225908	-4.075267	0.856808
C	-0.154582	-2.657007	0.288033
N	1.227479	-2.160954	0.456987
C	2.220443	-2.996249	-0.241662
C	2.194761	-4.427224	0.286894
C	0.782545	-5.005037	0.181496
C	1.525201	-1.123837	1.181558
C	0.519305	-0.149164	1.699099
C	0.082305	-0.794074	3.050224
C	1.335082	-1.366413	3.776827
C	2.645086	-0.708561	3.312440
C	2.890108	-0.949084	1.785948
B	-0.314063	0.735544	0.507517
C	-0.804447	2.178104	1.101437
C	-1.342548	3.123660	0.212953
C	0.953603	0.964954	-0.563003
C	1.271338	0.108006	-1.614463
C	-1.665161	0.125176	-0.218286
C	-1.784668	4.371313	0.637654
C	-1.711500	4.717455	1.985600
C	-1.181796	3.803906	2.888605
C	-0.734434	2.559364	2.445142
C	2.421701	0.188128	-2.386597
C	3.342585	1.192339	-2.129398
C	3.089930	2.075407	-1.091414
C	1.928377	1.939293	-0.334033
C	-2.017046	0.368140	-1.545039
C	-3.224241	-0.020113	-2.115146
C	-4.170683	-0.671581	-1.340270
C	-3.888014	-0.915859	-0.005053
C	-2.670205	-0.499219	0.513923
F	0.469021	-0.937086	-1.914682
F	2.656349	-0.709301	-3.348756
F	4.457751	1.290899	-2.849414
F	3.975403	3.030492	-0.806832

F	1.825934	2.783462	0.700452
F	-1.188515	1.035459	-2.366867
F	-3.481894	0.236454	-3.398088
F	-5.331064	-1.056045	-1.868147
F	-4.782059	-1.540040	0.764407
F	-2.467406	-0.778881	1.818927
H	-1.247447	-4.442524	0.724285
H	-0.034688	-4.033398	1.936892
H	-0.822860	-1.987991	0.817473
H	-0.399626	-2.637488	-0.775895
H	3.202703	-2.533547	-0.165443
H	1.924551	-2.956780	-1.297289
H	2.523911	-4.424799	1.333959
H	2.910950	-5.028023	-0.280670
H	0.743820	-6.001776	0.628920
H	0.518351	-5.116784	-0.877808
H	1.157025	0.681730	2.028884
H	-0.411557	-0.033496	3.657152
H	-0.652405	-1.589213	2.909298
H	1.231908	-1.262269	4.860112
H	1.411010	-2.445284	3.579898
H	3.495045	-1.118573	3.863773
H	2.620549	0.364259	3.520862
H	3.387007	-0.082730	1.334172
H	3.523328	-1.826875	1.645576
H	-1.403069	2.878737	-0.845700
H	-2.187526	5.076630	-0.083637
H	-2.060904	5.687643	2.324999
H	-1.112512	4.057922	3.942691
H	-0.304098	1.885524	3.180334

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N-Cyclohexylidene-Piperidine +
B(C₆F₅)₂Ph

C	1.818404	-3.819356	-0.418588
C	0.951972	-2.684219	0.132715
N	1.639332	-2.011177	1.220786
C	2.904067	-1.436576	0.801538
C	3.844383	-2.543424	0.321537
C	3.190643	-3.292295	-0.841878
C	0.796073	-1.345368	2.217686
C	0.131407	0.054986	1.990757
C	-0.959124	0.197346	3.093539
C	-0.639271	-0.531058	4.412342
C	0.865082	-0.517479	4.654464
C	1.569338	-1.334356	3.559141
B	-0.415058	0.629576	0.510619
C	-1.197172	2.091793	0.709613
C	-2.512865	2.119017	1.210884
C	0.916535	0.873834	-0.471101
C	1.168464	0.304353	-1.720487

C	-1.586868	-0.275537	-0.266041
C	-3.232910	3.294803	1.398411
C	-2.667066	4.521647	1.063190
C	-1.384600	4.534981	0.528816
C	-0.676376	3.345695	0.356831
C	2.344288	0.474709	-2.445453
C	3.350097	1.284529	-1.948954
C	3.150813	1.904824	-0.727232
C	1.968606	1.685606	-0.031205
C	-2.114235	0.221283	-1.465073
C	-3.175854	-0.339816	-2.154854
C	-3.799954	-1.469424	-1.642505
C	-3.332693	-2.003486	-0.458671
C	-2.257860	-1.400520	0.195510
F	0.289938	-0.523604	-2.316174
F	2.516544	-0.151578	-3.616426
F	4.483595	1.469994	-2.633624
F	4.103830	2.699854	-0.224734
F	1.904411	2.332270	1.148112
F	-1.571448	1.309766	-2.029173
F	-3.614416	0.192437	-3.302760
F	-4.834314	-2.025136	-2.284366
F	-3.920870	-3.090028	0.060867
F	-1.919206	-2.015146	1.348680
H	1.309857	-4.296563	-1.264258
H	1.947320	-4.575305	0.366445
H	0.009993	-3.084478	0.518692
H	0.694203	-2.003589	-0.695183
H	3.354209	-0.883897	1.630282
H	2.792393	-0.726495	-0.030073
H	4.035754	-3.237412	1.149662
H	4.802426	-2.109444	0.010983
H	3.831266	-4.107502	-1.198153
H	3.061118	-2.593159	-1.681917
H	-0.024810	-2.053795	2.355125
H	0.911040	0.779554	2.262082
H	-1.094414	1.263292	3.303011
H	-1.923520	-0.165971	2.725409
H	-1.179846	-0.061684	5.242776
H	-0.983339	-1.573025	4.369522
H	1.120579	-0.909191	5.646046
H	1.210850	0.523425	4.630182
H	2.578201	-0.934808	3.411070
H	1.693111	-2.376843	3.876664
H	-3.003798	1.179266	1.452358
H	-4.243767	3.249340	1.796320
H	-3.221601	5.446068	1.200195
H	-0.927713	5.476488	0.233292
H	0.307944	3.417687	-0.092326

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Piperidino-Cyclohex-1-ene + B(C ₆ F ₅) ₃			
C	3.628954	-2.323914	1.485471
C	2.742704	-1.500464	0.549485
N	2.959826	-0.069702	0.851596
C	4.354343	0.332594	0.592847
C	5.303635	-0.445181	1.501951
C	5.102982	-1.951892	1.319264
C	2.052514	0.697912	1.377980
C	0.618509	0.314609	1.574730
C	0.693169	-0.480767	2.916482
C	1.644528	0.250425	3.906962
C	1.799159	1.741758	3.571311
C	2.422520	1.935850	2.146917
B	-0.328166	0.058889	0.191479
C	-1.930827	0.344351	0.499835
C	-2.815066	0.272295	-0.578842
C	0.260338	1.268845	-0.791501
C	1.402793	1.146587	-1.581769
C	-0.338267	-1.443858	-0.489441
C	-4.187465	0.451333	-0.484155
C	-4.750301	0.741584	0.749490
C	-3.919170	0.856352	1.850132
C	-2.548997	0.668997	1.701929
C	1.995268	2.184794	-2.286754
C	1.435984	3.451905	-2.228543
C	0.310147	3.644680	-1.445151
C	-0.236737	2.573096	-0.743928
C	-0.230523	-1.756421	-1.844632
C	-0.320040	-3.052652	-2.343727
C	-0.570426	-4.109858	-1.483384
C	-0.741048	-3.849037	-0.132320
C	-0.642947	-2.539656	0.317316
F	-2.340995	0.037425	-1.812288
F	2.054498	-0.031797	-1.668667
F	-4.963633	0.358701	-1.563510
F	-6.063738	0.918505	0.870151
F	-4.431830	1.158886	3.044156
F	-1.838687	0.864126	2.833671
F	3.106077	1.973423	-2.996638
F	1.983824	4.466304	-2.891829
F	-0.230661	4.858394	-1.350650
F	-1.277692	2.891531	0.040345
F	-0.058420	-0.806956	-2.770573
F	-0.184802	-3.283865	-3.649563
F	-0.657389	-5.354290	-1.946916
F	-1.008801	-4.845016	0.713745
F	-0.857727	-2.356284	1.633775
H	3.465816	-3.382934	1.266469
H	3.311187	-2.154517	2.522006
H	1.689888	-1.727602	0.672257
H	3.011133	-1.669353	-0.495546

H	4.454239	1.410715	0.696034
H	4.530919	0.089658	-0.461255
H	5.104425	-0.161793	2.543654
H	6.333110	-0.154647	1.274302
H	5.721071	-2.506039	2.030533
H	5.435510	-2.238281	0.313406
H	0.169612	1.266004	1.876044
H	-0.312289	-0.548583	3.325299
H	1.036026	-1.507048	2.760324
H	1.284289	0.136913	4.932532
H	2.642309	-0.211223	3.880235
H	2.446051	2.237370	4.299377
H	0.824388	2.233783	3.622693
H	1.989930	2.814597	1.655809
H	3.499818	2.079067	2.232670

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N-Cyclohexylidene-Piperidine + B(C₆F₅)₃

C	-4.853535	-1.494108	-0.141200
C	-3.341251	-1.272271	-0.033663
N	-2.772076	-1.065993	-1.345789
C	-3.338913	0.054601	-2.063585
C	-4.844311	-0.144216	-2.254044
C	-5.512064	-0.335336	-0.891100
C	-1.435342	-1.556051	-1.691444
C	-0.276735	-0.506901	-1.711591
C	0.873234	-1.016322	-2.639604
C	0.962230	-2.543586	-2.697935
C	-0.296554	-3.130384	-3.354160
C	-1.521310	-2.248623	-3.068398
B	0.376322	0.007219	-0.268520
C	1.417083	1.292588	-0.469217
C	2.149134	1.727253	0.636778
C	-0.728592	0.681635	0.763080
C	-1.538062	1.707548	0.275763
C	1.187519	-1.287821	0.373413
C	2.981960	2.835106	0.644605
C	3.107497	3.592825	-0.510507
C	2.395526	3.218373	-1.635218
C	1.569613	2.096443	-1.593414
C	-2.537300	2.335988	1.004962
C	-2.717965	1.994378	2.336342
C	-1.879711	1.047393	2.900691
C	-0.899988	0.434347	2.123927
C	0.526468	-2.343683	0.998186
C	1.128599	-3.528875	1.397476
C	2.485447	-3.708087	1.180853
C	3.200395	-2.691943	0.571102
C	2.549039	-1.523611	0.188548
F	2.068416	1.045862	1.792663
F	-1.374774	2.159762	-0.982077

F	3.657193	3.185377	1.746601
F	3.902991	4.668306	-0.534042
F	2.500931	3.943035	-2.756600
F	0.924049	1.839702	-2.743590
F	-3.314809	3.267935	0.440167
F	-3.662684	2.590581	3.071170
F	-2.007293	0.746151	4.198620
F	-0.101564	-0.410716	2.791458
F	-0.796250	-2.271962	1.240088
F	0.416774	-4.495472	1.988644
F	3.090796	-4.840380	1.553703
F	4.511668	-2.844383	0.350849
F	3.340899	-0.621509	-0.420426
H	-5.284771	-1.600556	0.861244
H	-5.034144	-2.429075	-0.686816
H	-2.867196	-2.143213	0.421797
H	-3.168882	-0.417354	0.648100
H	-2.842243	0.150095	-3.033883
H	-3.190274	1.014083	-1.538671
H	-5.009122	-1.034603	-2.874393
H	-5.274046	0.718688	-2.776746
H	-6.590602	-0.498932	-0.999059
H	-5.382707	0.586893	-0.305213
H	-1.220724	-2.342980	-0.958188
H	-0.708722	0.366951	-2.207378
H	0.730292	-0.645302	-3.663709
H	1.834276	-0.607391	-2.309094
H	1.860336	-2.857456	-3.242380
H	1.063955	-2.942988	-1.682970
H	-0.471603	-4.146202	-2.980189
H	-0.151944	-3.218267	-4.437884
H	-1.602792	-1.473739	-3.842652
H	-2.445907	-2.833353	-3.107749

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Piperidino-Cyclohex-1-ene + proton

C	-1.009129	2.707348	-0.364445
C	-1.359258	1.347924	0.242447
N	-0.122329	0.531355	0.347185
C	0.830767	1.173005	1.289340
C	1.259031	2.526307	0.719948
C	0.044797	3.426036	0.480518
C	0.134074	-0.521537	-0.365439
C	1.389835	-1.332249	-0.233121
C	1.005145	-2.705016	0.374893
C	-0.044349	-3.410948	-0.483173
C	-1.265143	-2.520679	-0.713796
C	-0.850330	-1.150418	-1.307330
H	-1.925912	3.298586	-0.432206
H	-0.644235	2.553383	-1.386814

H	-2.114698	0.820720	-0.330835
H	-1.733306	1.463567	1.264381
H	1.674970	0.518533	1.479773
H	0.286721	1.301872	2.230093
H	1.955909	2.988790	1.423596
H	1.804610	2.357954	-0.216044
H	-0.394772	3.704174	1.446305
H	0.352112	4.353684	-0.007335
H	2.177004	-0.854093	0.343822
H	1.778077	-1.492611	-1.244863
H	0.623540	-2.550648	1.391209
H	1.912881	-3.306661	0.459515
H	-0.349615	-4.345011	-0.004663
H	0.397853	-3.678740	-1.450694
H	-1.797614	-2.354133	0.230185
H	-1.970150	-2.991302	-1.402701
H	-1.720554	-0.537194	-1.526023
H	-0.325930	-1.322000	-2.253727

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N-Cyclohexyl-Piperidine

C	-0.955745	2.789467	-1.341685
C	-1.186355	1.557117	-0.469630
N	-0.094623	0.604585	-0.633458
C	1.168230	1.198292	-0.206350
C	1.503555	2.408992	-1.074586
C	0.382021	3.444229	-0.996931
C	-0.382754	-0.709113	-0.051428
C	-0.349440	-0.775432	1.484930
C	-0.783110	-2.158472	1.979332
C	0.091041	-3.258424	1.374260
C	0.085791	-3.185936	-0.154681
C	0.515203	-1.799595	-0.643464
H	-1.781992	3.495766	-1.208367
H	-0.951272	2.473708	-2.391370
H	-2.120887	1.062245	-0.755918
H	-1.297432	1.883893	0.584071
H	1.962768	0.450963	-0.287967
H	1.129811	1.521868	0.852809
H	2.455913	2.842260	-0.751226
H	1.623116	2.071537	-2.110551
H	0.333523	3.842515	0.025943
H	0.584081	4.290694	-1.660999
H	-1.411018	-0.948161	-0.364770
H	0.673775	-0.576236	1.832796
H	-0.990900	0.002441	1.914929
H	-0.746690	-2.199998	3.072992
H	-1.829464	-2.331387	1.691707
H	1.121429	-3.136341	1.735565
H	-0.247826	-4.243962	1.710545
H	0.741312	-3.954783	-0.576623

H	-0.927955	-3.398964	-0.520951
H	1.557838	-1.631158	-0.342252
H	0.479016	-1.732568	-1.735258

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Piperidino-Cyclohex-1-ene + [SiEt₃]⁺

C	-1.713191	-2.356841	-0.720850
C	-1.454348	-0.914001	-1.167683
N	-1.828975	0.062148	-0.123340
C	-3.283233	0.047969	0.211269
C	-3.908006	-1.308723	-0.124571
C	-2.924651	-2.425238	0.223399
C	-1.009916	0.942092	0.370300
C	0.450829	1.015801	0.061875
C	0.547299	2.013812	-1.133038
C	-0.017707	3.370231	-0.690483
C	-1.426955	3.254141	-0.101116
C	-1.530651	2.181514	1.031115
Si	1.678043	-0.481914	0.203203
C	1.122201	-1.451938	1.726244
C	0.709538	-0.571754	2.914032
C	1.896543	-1.582880	-1.312229
C	2.204532	-0.806682	-2.601044
C	3.312022	0.398663	0.545187
C	4.529884	-0.535353	0.500086
H	-0.824415	-2.772388	-0.240271
H	-1.894221	-2.949592	-1.622234
H	-0.425000	-0.733945	-1.466067
H	-2.088460	-0.659849	-2.024027
H	-3.772365	0.870904	-0.320491
H	-3.364727	0.224254	1.285147
H	-4.834679	-1.395819	0.447054
H	-4.184762	-1.361724	-1.182532
H	-2.595448	-2.299516	1.262412
H	-3.403513	-3.403620	0.158787
H	0.855957	1.588698	0.910581
H	-0.010610	1.627258	-1.995764
H	1.590141	2.111880	-1.448484
H	-0.038049	4.067059	-1.533445
H	0.655261	3.800158	0.061121
H	-2.138521	2.986075	-0.892527
H	-1.755516	4.211133	0.311445
H	-2.557198	2.117400	1.387611
H	-0.885578	2.457939	1.868471
H	1.960278	-2.097316	2.018685
H	0.304507	-2.137359	1.474155
H	0.489426	-1.170542	3.800765
H	-0.194018	0.009645	2.689132
H	1.496177	0.138455	3.187730
H	1.054820	-2.267364	-1.462923
H	2.746197	-2.233909	-1.067097

H	3.057374	-0.132944	-2.465964
H	1.354655	-0.192738	-2.920032
H	2.447627	-1.479302	-3.426633
H	3.451116	1.220786	-0.168635
H	3.244043	0.873940	1.532603
H	4.690528	-0.933226	-0.506090
H	5.441864	-0.010468	0.793244
H	4.412191	-1.387090	1.177862

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N-Cyclohexylidene-Piperidine + [SiEt₃]⁺

C	-3.202238	-1.797277	-0.907722
C	-2.461619	-0.522004	-1.293745
N	-1.467819	-0.214096	-0.270312
C	-1.953133	-0.405859	1.105222
C	-3.479494	-0.417703	1.198625
C	-4.062290	-1.559836	0.350204
C	-0.716631	1.013634	-0.525179
C	0.595604	1.067074	0.281869
C	1.373063	2.358327	-0.047243
C	0.537128	3.619175	0.179730
C	-0.750471	3.560740	-0.639311
C	-1.543751	2.296865	-0.308023
Si	1.774322	-0.444717	0.174205
C	2.558729	-0.596035	1.894682
C	1.579295	-1.142060	2.942604
C	0.998319	-2.115412	-0.260870
C	0.653549	-2.261667	-1.746499
C	3.127371	-0.107373	-1.114405
C	4.140719	-1.253698	-1.230571
H	-2.448948	-2.570947	-0.716894
H	-3.818303	-2.145166	-1.741546
H	-1.940340	-0.653606	-2.249433
H	-3.199485	0.287261	-1.450233
H	-1.553322	0.383375	1.749353
H	-1.564219	-1.355453	1.508429
H	-3.788693	-0.513237	2.244062
H	-3.858180	0.548430	0.844233
H	-4.109133	-2.478695	0.943529
H	-5.091201	-1.316662	0.066010
H	-0.442871	0.974538	-1.593944
H	0.323704	1.136418	1.348167
H	1.690807	2.331690	-1.099503
H	2.292262	2.406383	0.550280
H	1.117971	4.511156	-0.079204
H	0.285366	3.699093	1.246158
H	-0.495932	3.559092	-1.708286
H	-1.362545	4.451534	-0.462617
H	-2.459175	2.258291	-0.909397
H	-1.855447	2.337219	0.746138
H	2.935862	0.386353	2.208068

H	3.435615	-1.252533	1.835673
H	2.031532	-1.202728	3.937119
H	1.237057	-2.146548	2.673692
H	0.687601	-0.510540	3.028014
H	0.099089	-2.266172	0.344510
H	1.712432	-2.896795	0.037123
H	1.551388	-2.226697	-2.372490
H	-0.006358	-1.451937	-2.069832
H	0.143301	-3.207177	-1.957615
H	2.652326	0.070790	-2.088774
H	3.650542	0.822774	-0.862926
H	3.652924	-2.197171	-1.496725
H	4.900707	-1.051815	-1.991412
H	4.663005	-1.417155	-0.282604

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Piperidino-Cyclohex-1-ene + [SiPhH₂]⁺

C	-1.093182	0.213086	2.494256
C	-0.779065	0.429024	1.019173
N	-0.685011	-0.868714	0.294468
C	-0.497980	-2.057419	1.163728
C	0.511979	-1.722381	2.258790
C	-0.009773	-0.616460	3.194399
C	-0.706194	-0.937320	-1.013525
C	-0.633837	0.263773	-1.851645
C	-1.388640	0.216092	-3.209555
C	-1.997907	-1.153645	-3.497580
C	-0.969569	-2.236416	-3.193897
C	-0.699250	-2.292010	-1.685994
Si	1.293634	0.494787	-2.133174
C	1.548367	2.023560	-3.143194
C	1.421254	3.294940	-2.564039
C	1.579218	4.441957	-3.333356
C	1.867293	4.330945	-4.692781
C	1.999206	3.076766	-5.282200
C	1.840542	1.928589	-4.511795
H	-1.197439	1.195619	2.960445
H	-2.070690	-0.272320	2.579451
H	-1.568941	1.017702	0.548582
H	0.172030	0.961299	0.896346
H	-1.470567	-2.336867	1.582879
H	-0.138645	-2.884840	0.558249
H	1.443514	-1.413275	1.772044
H	0.736464	-2.637782	2.810938
H	-0.423299	-1.048961	4.108328
H	0.818857	0.028405	3.497745
H	-0.893882	1.168903	-1.300518
H	-2.163194	0.986334	-3.197006
H	-0.709367	0.485136	-4.027054
H	-2.890111	-1.311604	-2.877515
H	-2.320985	-1.201759	-4.539772

H	-0.044167	-2.028173	-3.741763
H	-1.312613	-3.221611	-3.516975
H	-1.465652	-2.905053	-1.198555
H	0.263980	-2.779120	-1.484654
H	1.768702	-0.721355	-2.829476
H	1.876928	0.570203	-0.770578
H	1.208420	3.395188	-1.501250
H	1.485358	5.421091	-2.875839
H	1.994339	5.226142	-5.292589
H	2.230851	2.993525	-6.338636
H	1.954155	0.953534	-4.979935

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N-Cyclohexylidene-Piperidine + [SiPhH₂]⁺

C	-1.296129	-0.785603	2.252752
C	-0.670344	0.047906	1.133053
N	0.185959	-0.752715	0.243524
C	0.751913	-1.940829	0.882717
C	1.091436	-1.632797	2.336358
C	-0.192798	-1.377678	3.148939
C	-0.355317	-1.021984	-1.088680
C	-0.367066	0.262929	-1.930483
C	-0.729858	-0.058929	-3.387392
C	-2.077063	-0.783583	-3.468722
C	-2.091624	-2.043090	-2.599115
C	-1.719496	-1.727287	-1.146154
Si	1.302876	1.134215	-1.702172
C	1.558137	2.359995	-3.109738
C	1.186422	3.703873	-2.968693
C	1.299965	4.601653	-4.027316
C	1.794073	4.168713	-5.254555
C	2.174783	2.838792	-5.417117
C	2.057202	1.947907	-4.354011
H	-1.988618	-0.173960	2.839182
H	-1.888847	-1.589753	1.800674
H	-1.449690	0.531648	0.537188
H	-0.074659	0.858430	1.577018
H	0.061637	-2.804676	0.852348
H	1.650061	-2.229782	0.324558
H	1.733638	-0.744886	2.348689
H	1.670224	-2.452662	2.770493
H	-0.545617	-2.311469	3.598654
H	0.026690	-0.694009	3.975281
H	0.376538	-1.697273	-1.562329
H	-1.145932	0.936537	-1.538893
H	-0.750077	0.857115	-3.986937
H	0.051506	-0.699777	-3.824505
H	-2.866165	-0.101029	-3.124588
H	-2.310076	-1.039568	-4.507907
H	-1.367467	-2.764693	-3.001924
H	-3.073545	-2.525583	-2.643928

H	-2.485466	-1.071968	-0.707252
H	-1.701155	-2.647822	-0.550284
H	2.387453	0.118702	-1.762960
H	1.360252	1.909365	-0.437904
H	0.805514	4.058817	-2.013192
H	1.006306	5.638468	-3.894392
H	1.885325	4.865944	-6.081772
H	2.565289	2.497985	-6.371229
H	2.362872	0.912964	-4.495865

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N-benzylidene aniline

C	-4.08232	1.03445	-0.38600
C	-4.60334	-0.17757	0.05722
C	-3.74498	-1.21349	0.43050
C	-2.37021	-1.03942	0.36250
C	-1.84060	0.17749	-0.08309
C	-2.70370	1.21022	-0.45587
C	-0.38655	0.38638	-0.16410
N	0.44916	-0.52405	0.14310
C	1.82569	-0.22987	0.08412
C	2.68446	-1.21884	-0.40690
C	4.05010	-0.98058	-0.48971
C	4.58009	0.23336	-0.05434
C	3.73257	1.20723	0.46613
C	2.36144	0.98184	0.53612
H	-4.74787	1.84051	-0.67676
H	-5.67816	-0.31759	0.11279
H	-4.15420	-2.15739	0.77585
H	-1.68272	-1.82879	0.64756
H	-2.28983	2.15398	-0.80206
H	-0.06095	1.37585	-0.51890
H	2.25453	-2.16158	-0.72819
H	4.70632	-1.74877	-0.88614
H	5.64887	0.41211	-0.10658
H	4.14040	2.14552	0.82868
H	1.70356	1.72726	0.97260

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N-benzylidene anilide

C	-3.60222	1.38524	0.00018
C	-4.58515	0.39832	0.00006
C	-4.20437	-0.94305	-0.00013
C	-2.85482	-1.28235	-0.00016
C	-1.86109	-0.29883	-0.00006
C	-2.25176	1.04057	0.00010
C	-0.39130	-0.67838	0.00003
N	0.45499	0.46681	0.00001
C	1.76111	0.20838	-0.00003
C	2.38332	-1.08792	0.00006
C	3.76549	-1.23834	0.00015

C	4.63158	-0.14737	0.00007	H	-1.35217	-2.86671	1.17911
C	4.05330	1.13445	-0.00009	H	-2.87151	0.77126	-1.04333
C	2.68737	1.30969	-0.00022	H	-2.38744	-0.63841	-1.97265
H	-3.89142	2.43358	0.00037	H	-3.17727	-0.85530	2.12752
H	-5.63775	0.66892	0.00010	H	-1.58808	-0.21245	2.40251
H	-4.96110	-1.72376	-0.00024	H	-2.34182	1.96113	1.20825
H	-2.55798	-2.33015	-0.00028	H	-3.93980	1.24895	1.05789
H	-1.45252	1.77447	0.00014	H	-3.27763	1.58834	2.65667
H	-0.23614	-1.35347	-0.87440	H	-1.70303	-4.35433	-0.79030
H	-0.23628	-1.35334	0.87459	H	-0.70596	-3.02017	-1.36896
H	1.76188	-1.97812	0.00010	H	-2.42252	-3.02863	-1.70576
H	4.17893	-2.24763	0.00028	H	-4.90586	-0.40951	-1.75430
H	5.70920	-0.28032	0.00028	H	-4.32050	-1.93193	-1.08070
H	4.69787	2.01363	-0.00025	H	-4.75057	-0.60886	-0.00554
H	2.25152	2.30598	-0.00046				

48

47				<i>N</i> -benzylidene anilide + BEt ₃			
<i>N</i> -benzylidene aniline + BEt ₃				C	3.57102	-0.67667	-1.40130
C	4.07923	0.24738	-0.61790	C	4.61688	-0.96068	-0.52531
C	4.86180	-0.75905	-0.05442	C	4.33391	-1.22074	0.81281
C	4.25288	-1.85960	0.54081	C	3.01637	-1.19683	1.26270
C	2.86696	-1.94585	0.56860	C	1.96042	-0.92268	0.39103
C	2.06723	-0.92575	0.03231	C	2.25565	-0.65738	-0.94777
C	2.69285	0.17628	-0.57408	C	0.52476	-0.97972	0.88854
C	0.61625	-1.16752	0.12397	N	-0.43225	-0.23088	0.10662
N	-0.38224	-0.36518	0.03572	C	-0.17596	1.12464	0.01533
C	-0.14784	1.04549	-0.09047	C	0.68172	1.81669	0.90437
C	-0.40934	1.69639	-1.29222	C	0.94011	3.17624	0.76261
C	-0.16575	3.06410	-1.38939	C	0.37353	3.91613	-0.26919
C	0.32233	3.77229	-0.29400	C	-0.44986	3.24649	-1.17725
C	0.56902	3.11115	0.90748	C	-0.70730	1.89164	-1.05069
C	0.33611	1.74482	1.01334	B	-1.90337	-0.93274	0.05180
B	-1.97410	-0.86452	0.25892	C	-3.07494	0.08244	-0.50840
C	-1.98192	-2.49268	0.35508	C	-1.78098	-2.26498	-0.91053
C	-2.83612	-0.32597	-1.01619	C	-2.28878	-1.38493	1.59653
C	-2.42500	-0.18586	1.68585	C	-2.40012	-0.20449	2.56662
C	-3.02169	1.22760	1.65413	C	-4.49287	-0.46937	-0.30834
C	-1.68306	-3.26890	-0.93537	C	-1.49200	-1.95302	-2.38105
C	-4.28039	-0.84365	-0.96725	H	3.78241	-0.46301	-2.44541
H	4.55247	1.09815	-1.09636	H	5.64327	-0.97171	-0.88087
H	5.94409	-0.68820	-0.08836	H	5.14048	-1.43550	1.50883
H	4.85367	-2.65274	0.97239	H	2.79701	-1.39112	2.31091
H	2.38905	-2.81241	1.01718	H	1.43377	-0.42291	-1.61729
H	2.10814	0.96865	-1.02305	H	0.22118	-2.02967	0.84775
H	0.34760	-2.20248	0.31565	H	0.51977	-0.72070	1.96551
H	-0.78887	1.13050	-2.13513	H	1.15283	1.28266	1.72229
H	-0.36262	3.57618	-2.32531	H	1.60128	3.66070	1.47785
H	0.50502	4.83853	-0.37465	H	0.58076	4.97626	-0.37765
H	0.94176	3.65976	1.76589	H	-0.88352	3.78708	-2.01567
H	0.51791	1.21255	1.94147	H	-1.30723	1.38244	-1.79399
H	-2.99922	-2.75693	0.67357	H	-2.96010	0.28247	-1.58318

H	-3.01974	1.07069	-0.02892	H	6.45213	2.27266	0.44974
H	-2.70593	-2.85994	-0.84513	H	4.93586	3.73680	-0.86348
H	-0.99353	-2.94244	-0.54059	H	2.52825	3.19115	-1.01376
H	-3.24211	-1.93517	1.58856	H	3.16772	-0.30100	1.42079
H	-1.56359	-2.10700	2.00349	H	0.68062	2.09408	-0.28271
H	-2.58928	-0.50114	3.60766	H	0.35987	-1.45235	2.31425
H	-1.48163	0.39709	2.55411	H	1.44545	-3.66384	2.56223
H	-3.21069	0.47137	2.26783	H	2.78964	-4.61195	0.70587
H	-5.26023	0.15118	-0.79029	H	3.04494	-3.33091	-1.40902
H	-4.75160	-0.53627	0.75429	H	1.97053	-1.10605	-1.64357
H	-4.58558	-1.48181	-0.72074	H	-2.51544	0.90132	-2.52434
H	-1.26143	-2.84042	-2.98610	H	-3.39543	3.08490	-3.20337
H	-0.63843	-1.26743	-2.45818	H	-3.08733	5.07472	-1.74834
H	-2.34489	-1.45254	-2.85465	H	-1.92662	4.81432	0.43741
				H	-1.09279	2.61983	1.13731
				H	-0.40323	0.11991	-2.82277
				H	-0.25825	-1.70259	-4.46828
				H	-0.97285	-4.00232	-3.84903
				H	-1.82979	-4.43810	-1.55917
				H	-1.97189	-2.61349	0.08149
				H	-3.63973	-0.98242	0.37973
				H	-4.89922	-1.21216	2.48099
				H	-3.89014	-0.48726	4.63341
				H	-1.60685	0.49538	4.63862
				H	-0.35043	0.71775	2.54391
59							
<i>N</i> -benzylidene aniline + BPh ₃							
C	4.88949	0.90423	1.01387				
C	5.39730	2.03112	0.36845				
C	4.54958	2.85243	-0.36868				
C	3.19838	2.54238	-0.45650				
C	2.68262	1.39323	0.16006				
C	3.54442	0.57626	0.91005				
C	1.23274	1.19996	0.00173				
N	0.50965	0.14587	0.13479				
C	1.13731	-1.14057	0.33361				
C	0.96302	-1.85801	1.51248				
C	1.57316	-3.10502	1.64111				
C	2.32726	-3.63623	0.60042				
C	2.47482	-2.91694	-0.58427				
C	1.88318	-1.66882	-0.72028				
B	-1.15314	0.11470	-0.14496				
C	-1.87368	-0.15105	1.28444				
C	-1.66240	1.57658	-0.66579				
C	-1.24044	-1.08304	-1.24268				
C	-2.35217	1.75459	-1.87381				
C	-2.86219	2.99405	-2.26140				
C	-2.69543	4.10805	-1.44717				
C	-2.03967	3.96199	-0.22640				
C	-1.55301	2.71582	0.15462				
C	-0.74265	-0.87606	-2.54046				
C	-0.64687	-1.90443	-3.47399				
C	-1.04520	-3.19366	-3.12799				
C	-1.52905	-3.43452	-1.84597				
C	-1.61972	-2.39364	-0.92287				
C	-3.17555	-0.67457	1.31408				
C	-3.89495	-0.79880	2.49951				
C	-3.33333	-0.38973	3.70667				
C	-2.05386	0.15690	3.70815				
C	-1.34715	0.27634	2.51247				
H	5.54725	0.27400	1.60265				
				60			
				<i>N</i> -benzylidene anilide + BPh ₃			
				C	4.28385	-0.03017	0.99293
				C	5.36402	-0.11263	0.11850
				C	5.13634	-0.06882	-1.25553
				C	3.83867	0.05462	-1.74167
				C	2.74790	0.13099	-0.87120
				C	2.98581	0.09242	0.50231
				C	1.33608	0.22228	-1.43453
				N	0.30474	0.63844	-0.50844
				C	0.20135	2.00437	-0.32032
				C	1.19367	2.91238	-0.76822
				C	1.06272	4.28562	-0.58642
				C	-0.04565	4.83049	0.04969
				C	-1.02539	3.95145	0.51388
				C	-0.91435	2.58203	0.33971
				B	-0.79441	-0.38926	0.00676
				C	-2.24826	-0.00359	-0.67164
				C	-0.37916	-1.91249	-0.48188
				C	-0.85590	-0.45485	1.65278
				C	-1.02403	-2.60408	-1.51701
				C	-0.63260	-3.88510	-1.91308
				C	0.43033	-4.52017	-1.28077
				C	1.08878	-3.86305	-0.24174
				C	0.67963	-2.59219	0.14862

C	-0.17550	0.41400	2.51982	C	-1.88652	-4.07345	0.42456
C	-0.22667	0.27863	3.90857	C	-2.30168	-3.12359	1.35563
C	-0.97199	-0.74199	4.48857	C	-2.00174	-1.78000	1.16786
C	-1.65095	-1.63255	3.65874	B	0.40006	0.62284	0.51721
C	-1.57965	-1.48939	2.27620	C	1.67043	-0.10409	-0.21892
C	-3.49604	-0.20028	-0.06241	C	0.56383	2.21015	0.20761
C	-4.69710	0.08031	-0.71500	C	0.15386	0.23024	2.07352
C	-4.69123	0.57332	-2.01599	C	0.93807	3.11267	1.21286
C	-3.46803	0.78919	-2.64776	C	1.20348	4.45384	0.93717
C	-2.27909	0.50873	-1.98015	C	1.10061	4.93608	-0.36274
H	4.45053	-0.05890	2.06597	C	0.75357	4.05872	-1.38813
H	6.37558	-0.20638	0.50273	C	0.50461	2.72004	-1.10318
H	5.97139	-0.12718	-1.94835	C	-0.76026	0.97972	2.83060
H	3.66268	0.09323	-2.81511	C	-1.15706	0.59275	4.10871
H	2.13717	0.16193	1.17674	C	-0.64711	-0.57678	4.66811
H	1.36389	0.89365	-2.30863	C	0.25564	-1.34447	3.93786
H	1.07922	-0.76648	-1.82150	C	0.64204	-0.94360	2.66122
H	2.09781	2.54422	-1.23710	C	2.89963	-0.23891	0.42642
H	1.85709	4.93487	-0.94752	C	4.04307	-0.73580	-0.18921
H	-0.14264	5.90252	0.18904	C	4.00282	-1.08831	-1.52955
H	-1.90483	4.33890	1.02210	C	2.81988	-0.92153	-2.23330
H	-1.69772	1.93809	0.71614	C	1.70777	-0.41690	-1.57410
H	-1.85651	-2.12879	-2.02987	F	0.61456	-0.22469	-2.35024
H	-1.16326	-4.38683	-2.71904	F	2.76350	-1.22628	-3.53083
H	0.74046	-5.51581	-1.58737	F	5.08742	-1.56434	-2.13616
H	1.91892	-4.34581	0.26802	F	5.18161	-0.85753	0.49215
H	1.19355	-2.10469	0.97478	F	3.04335	0.14148	1.70160
H	0.41041	1.22871	2.10254	H	-5.62761	-1.77002	-1.99373
H	0.31943	0.97781	4.53744	H	-7.01629	0.27232	-2.19224
H	-1.01653	-0.84977	5.56916	H	-6.03360	2.49207	-1.65951
H	-2.22499	-2.44911	4.09050	H	-3.67962	2.64697	-0.93315
H	-2.08349	-2.22173	1.64714	H	-3.30353	-1.63496	-1.25297
H	-3.53474	-0.56864	0.95960	H	-1.67579	1.85148	-0.58409
H	-5.64180	-0.08338	-0.20129	H	-0.32081	-2.01270	-1.78012
H	-5.62411	0.79434	-2.52796	H	-0.83536	-4.40702	-1.42358
H	-3.44194	1.18568	-3.66013	H	-2.12270	-5.12179	0.57368
H	-1.33219	0.69976	-2.48298	H	-2.85622	-3.42614	2.23745
				H	-2.30551	-1.03228	1.89387
59				H	1.04087	2.75649	2.23358
<i>N</i> -benzylidene aniline + B(C ₆ F ₅)Ph ₂				H	1.49489	5.12118	1.74283
C	-5.20438	-0.80164	-1.74970	H	1.30247	5.98049	-0.57948
C	-5.98469	0.34770	-1.86401	H	0.69169	4.41464	-2.41237
C	-5.43677	1.59151	-1.56577	H	0.27188	2.04793	-1.92733
C	-4.11361	1.67595	-1.15465	H	-1.18365	1.88707	2.40219
C	-3.32143	0.52465	-1.01340	H	-1.86412	1.20044	4.66592
C	-3.88442	-0.72587	-1.32511	H	-0.95195	-0.88657	5.66305
C	-1.94736	0.79769	-0.56961	H	0.65367	-2.26272	4.35928
N	-1.01450	0.02074	-0.14703	H	1.32211	-1.57886	2.09927
C	-1.28387	-1.38936	0.03701				
C	-0.85181	-2.32959	-0.89351	60			
C	-1.16220	-3.67369	-0.69395	<i>N</i> -benzylidene anilide + B(C ₆ F ₅)Ph ₂			

C	5.35646	-1.08726	-2.02149	H	-0.64234	4.50407	-2.61016
C	5.92011	-0.90415	-0.76033	H	1.69502	5.26307	-2.23753
C	5.09064	-0.64159	0.32632	H	3.19493	3.90706	-0.78194
C	3.71036	-0.56011	0.15674	H	2.36009	1.85356	0.28004
C	3.13685	-0.73661	-1.10196	H	-1.33256	2.68716	1.57307
C	3.97750	-1.00658	-2.18578	H	-1.04734	3.55435	3.85773
C	1.63738	-0.61800	-1.33306	H	0.52803	2.44012	5.43164
N	0.80745	-0.64222	-0.14463	H	1.78600	0.43441	4.67206
C	0.56929	-1.90264	0.38270	H	1.45463	-0.45193	2.40239
C	-0.40471	-2.11642	1.39083				
C	-0.65085	-3.38008	1.90516	59			
C	0.04736	-4.50063	1.45695	<i>N</i> -benzylidene aniline + B(C ₆ F ₅) ₂ Ph			
C	1.01539	-4.31113	0.47816	C	5.58188	0.09189	-1.51941
C	1.27776	-3.05104	-0.04879	C	6.23403	1.23705	-1.06327
B	-0.09986	0.59423	0.21833	C	5.53559	2.19150	-0.33008
C	-1.66446	0.20977	-0.24469	C	4.18824	1.99556	-0.05880
C	0.39051	1.94554	-0.58212	C	3.52690	0.83466	-0.48878
C	0.03083	1.03898	1.79481	C	4.24046	-0.12034	-1.23371
C	-0.42631	2.73643	-1.39877	C	2.10671	0.77626	-0.13255
C	0.02864	3.91949	-1.98541	N	1.27222	-0.20176	-0.11141
C	1.33418	4.34687	-1.77799	C	1.74412	-1.54997	-0.31723
C	2.17265	3.58537	-0.96338	C	2.51715	-2.12961	0.68864
C	1.69841	2.42062	-0.37244	C	3.01774	-3.41511	0.51055
C	-0.65586	2.17482	2.25628	C	2.75436	-4.11300	-0.66511
C	-0.49278	2.67399	3.54225	C	1.98417	-3.52264	-1.66392
C	0.39072	2.05245	4.42570	C	1.47041	-2.23942	-1.49607
C	1.09375	0.93298	3.99792	B	-0.22668	0.06571	0.55734
C	0.91118	0.44019	2.70367	C	-1.27839	-1.05988	0.01735
C	-1.90513	-0.08800	-1.58604	C	-0.84601	1.49455	0.03480
C	-3.14196	-0.44793	-2.10363	C	0.14572	0.06702	2.13664
C	-4.23091	-0.54229	-1.25065	C	-1.97273	1.95523	0.72230
C	-4.05012	-0.28039	0.09580	C	-2.68284	3.09422	0.37154
C	-2.78953	0.08216	0.56420	C	-2.28503	3.82711	-0.73858
F	-2.71814	0.26815	1.89297	C	-1.19282	3.39856	-1.47369
F	-5.08853	-0.38708	0.93529	C	-0.51173	2.24769	-1.08770
F	-5.43424	-0.88931	-1.72180	C	0.39108	-1.11992	2.84350
F	-3.29873	-0.70507	-3.40889	C	0.86946	-1.11289	4.15083
F	-0.90259	-0.02771	-2.48021	C	1.11956	0.09524	4.79705
H	5.99248	-1.29614	-2.87728	C	0.88423	1.28843	4.12207
H	6.99591	-0.96926	-0.62669	C	0.40863	1.26644	2.81244
H	5.51871	-0.50170	1.31479	C	-1.47481	-1.18428	-1.35753
H	3.05511	-0.35765	0.99848	C	-2.39162	-2.03755	-1.94842
H	3.53862	-1.15446	-3.17060	C	-3.22445	-2.79098	-1.13213
H	1.46061	0.32177	-1.85794	C	-3.11640	-2.66374	0.24265
H	1.33443	-1.41107	-2.03479	C	-2.17091	-1.79896	0.79103
H	-0.96263	-1.27961	1.78754	F	-2.18476	-1.71216	2.12274
H	-1.41084	-3.48544	2.67512	F	-3.92997	-3.35949	1.03530
H	-0.15367	-5.48633	1.86412	F	-4.12184	-3.61444	-1.66551
H	1.59099	-5.15723	0.11048	F	-2.49462	-2.12347	-3.27482
H	2.06161	-2.96297	-0.79016	F	-0.73489	-0.43132	-2.19711
H	-1.45453	2.43310	-1.58145	F	-2.43398	1.26277	1.77016

F	-3.74465	3.48147	1.07557	C	1.74311	-2.09163	0.77658
F	-2.94978	4.92227	-1.09510	C	2.89763	-2.85840	0.68810
F	-0.80431	4.08301	-2.54957	C	3.99574	-2.35432	0.00979
F	0.51994	1.90452	-1.88149	C	3.90727	-1.09757	-0.56283
H	6.12393	-0.64408	-2.10317	C	2.73004	-0.36655	-0.43818
H	7.28498	1.38724	-1.28785	F	2.74830	0.82847	-1.05702
H	6.03413	3.08854	0.01993	F	4.95320	-0.60125	-1.23456
H	3.63524	2.74498	0.50039	F	5.11852	-3.07293	-0.09512
H	3.75504	-1.01432	-1.60249	F	2.96260	-4.07371	1.24595
H	1.69186	1.72620	0.20122	F	0.72513	-2.66435	1.44242
H	2.71751	-1.56847	1.59522	F	-1.69837	1.61071	-1.52257
H	3.61896	-3.86696	1.29221	F	-1.56319	4.21408	-1.87366
H	3.14896	-5.11394	-0.80362	F	0.37578	5.69892	-0.65969
H	1.78113	-4.05918	-2.58462	F	2.19952	4.46039	0.94765
H	0.89699	-1.76364	-2.28047	F	2.08469	1.82795	1.33373
H	0.19665	-2.07629	2.36471	H	-5.65347	0.50199	-0.88213
H	1.03895	-2.05231	4.66873	H	-7.13492	-1.17782	0.19054
H	1.48666	0.10527	5.81855	H	-6.13181	-3.15977	1.30687
H	1.06358	2.23854	4.61650	H	-3.67337	-3.44473	1.34553
H	0.22688	2.21498	2.31000	H	-3.18509	0.20012	-0.83253
				H	-1.48548	-1.81673	1.39207
				H	-1.54661	-2.87163	0.00412
60				H	0.80233	0.27120	-2.08362
<i>N</i> -benzylidene anilide + B(C ₆ F ₅) ₂ Ph				H	1.01456	-0.14319	-4.45574
C	-5.22457	-0.36507	-0.38800	H	-0.47022	-1.78004	-5.61935
C	-6.05668	-1.30618	0.21099	H	-2.19643	-2.97811	-4.27390
C	-5.49348	-2.41747	0.83579	H	-2.44047	-2.56822	-1.90192
C	-4.11216	-2.57686	0.85697	H	-2.26466	0.83431	1.47053
C	-3.26888	-1.63285	0.26330	H	-2.98710	1.20717	3.79320
C	-3.84033	-0.52651	-0.36401	H	-1.43122	0.72859	5.67825
C	-1.76416	-1.84488	0.33879	H	0.84993	-0.12394	5.18451
N	-0.93924	-0.89256	-0.38464	H	1.55948	-0.50212	2.86341
C	-0.82626	-1.12230	-1.74948				
C	0.13674	-0.44924	-2.53832				
C	0.25479	-0.68592	-3.89932	59			
C	-0.56974	-1.59902	-4.55403	<i>N</i> -benzylidene aniline + B(C ₆ F ₅) ₃			
C	-1.52732	-2.26508	-3.79863	C	-3.49975	4.37467	1.43160
C	-1.65990	-2.03866	-2.43292	C	-3.70673	5.29247	0.40152
B	0.11953	-0.04747	0.39519	C	-3.02682	5.15748	-0.80595
C	1.59857	-0.81382	0.23766	C	-2.13945	4.10316	-0.98102
C	0.19822	1.55145	-0.07119	C	-1.95940	3.15383	0.03327
C	-0.30087	0.11057	1.97278	C	-2.63706	3.30307	1.25242
C	-0.70490	2.24034	-0.87282	C	-0.98001	2.09637	-0.22638
C	-0.66142	3.61771	-1.08350	N	-0.93193	0.90484	0.25576
C	0.31795	4.37594	-0.46959	C	-2.07723	0.36016	0.95906
C	1.24402	3.74110	0.34594	C	-3.26776	0.25459	0.23730
C	1.15749	2.37045	0.52795	C	-4.37770	-0.33749	0.82384
C	-1.57505	0.61488	2.28469	C	-4.29992	-0.82914	2.12584
C	-1.98800	0.82826	3.59516	C	-3.10639	-0.72870	2.83201
C	-1.11819	0.56064	4.65145	C	-1.98287	-0.14102	2.25257
C	0.15704	0.08159	4.37258	B	0.25748	-0.16726	-0.09496
C	0.55261	-0.13832	3.05302	C	-0.61647	-1.43565	-0.62880

C	1.17327	-0.43681	1.22940	C	-3.30645	2.08074	0.43156
C	1.32139	0.44731	-1.18443	C	-1.32243	1.78758	-1.15803
C	2.08060	-1.49353	1.18243	N	-0.49488	1.38496	-0.03514
C	3.01394	-1.75073	2.17391	C	-0.01093	2.42817	0.74756
C	3.08359	-0.90392	3.27357	C	0.93890	2.20566	1.77184
C	2.22080	0.17696	3.35494	C	1.43146	3.24513	2.54596
C	1.30432	0.39677	2.33210	C	1.01073	4.55901	2.35117
C	2.06176	1.58884	-0.86904	C	0.07264	4.79814	1.35467
C	3.08053	2.10780	-1.65375	C	-0.43056	3.76684	0.56863
C	3.43187	1.44416	-2.82040	B	0.23244	0.00507	-0.05648
C	2.75150	0.28884	-3.17024	C	0.15838	-0.85711	1.36186
C	1.72899	-0.19040	-2.35621	C	1.80130	0.29408	-0.53198
C	-0.87761	-2.60554	0.07327	C	-0.53939	-1.05587	-1.07389
C	-1.76588	-3.57910	-0.37582	C	2.01056	0.83893	-1.79658
C	-2.45139	-3.38673	-1.56395	C	3.24504	1.22734	-2.29096
C	-2.24668	-2.21834	-2.28712	C	4.36865	1.08233	-1.48995
C	-1.35134	-1.28144	-1.80109	C	4.22280	0.55117	-0.22149
F	-1.24059	-0.13292	-2.49704	C	2.95960	0.17128	0.22446
F	-2.92421	-2.00285	-3.41479	C	0.03133	-1.82324	-2.08472
F	-3.30933	-4.30320	-2.00190	C	-0.67851	-2.76373	-2.82780
F	-1.97557	-4.68359	0.33845	C	-2.01814	-2.98481	-2.56186
F	-0.31174	-2.84199	1.26316	C	-2.63181	-2.26304	-1.54859
F	2.07296	-2.31168	0.12183	C	-1.88516	-1.33934	-0.83177
F	3.84806	-2.78370	2.07903	C	0.83415	-2.07513	1.42701
F	3.97103	-1.12942	4.23741	C	0.76445	-2.95209	2.49749
F	2.28020	1.00161	4.40030	C	-0.03791	-2.62766	3.58235
F	0.50588	1.47258	2.48259	C	-0.74200	-1.43676	3.56609
F	1.77712	2.27007	0.25792	C	-0.63942	-0.58625	2.46707
F	4.40590	1.91258	-3.59238	F	-1.35933	0.54004	2.55479
F	1.16188	-1.32631	-2.76918	F	-1.52100	-1.11519	4.60519
F	3.72244	3.21790	-1.29482	F	-0.12710	-3.45514	4.62832
F	3.08620	-0.36256	-4.28123	F	1.44750	-4.10254	2.49680
H	-4.01253	4.49703	2.37927	F	1.61597	-2.45038	0.40065
H	-4.38995	6.12269	0.54751	F	0.96962	0.98815	-2.63599
H	-3.17562	5.87857	-1.60197	F	3.36929	1.73034	-3.52483
H	-1.58696	4.00395	-1.91124	F	5.57241	1.45178	-1.93840
H	-2.46969	2.59740	2.05786	F	5.29467	0.41265	0.56752
H	-0.19104	2.35114	-0.92767	F	2.92903	-0.31450	1.47951
H	-3.30109	0.61833	-0.78566	F	1.32610	-1.71369	-2.40930
H	-5.29901	-0.42555	0.25826	F	-2.71051	-3.88359	-3.26729
H	-5.16490	-1.29725	2.58306	F	-2.52998	-0.69657	0.15227
H	-3.03728	-1.11561	3.84285	F	-0.07292	-3.46270	-3.79415
H	-1.06051	-0.06438	2.80900	F	-3.92101	-2.47656	-1.26819
60				H	-5.03916	2.37531	1.66373
<i>N</i> -benzylidene anilide + B(C ₆ F ₅) ₃				H	-6.39893	3.37459	-0.15746
C	-4.61482	2.49350	0.67096	H	-5.40700	3.64293	-2.42126
C	-5.37889	3.05469	-0.34876	H	-3.07680	2.92151	-2.84167
C	-4.82264	3.20518	-1.61685	H	-2.70604	1.63776	1.21784
C	-3.51366	2.79690	-1.85248	H	-1.38275	0.95773	-1.86309
C	-2.74387	2.22621	-0.83543	H	-0.83675	2.60077	-1.72123
				H	1.30161	1.20648	1.96884

H	2.16285	3.01596	3.31641
H	1.40023	5.36797	2.96050
H	-0.28655	5.80841	1.17590
H	-1.17398	4.01452	-0.17737

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N-benzyl aniline

C	-3.66297	1.19286	0.64540
C	-4.57117	0.41406	-0.06931
C	-4.13661	-0.74725	-0.70037
C	-2.79886	-1.12695	-0.61841
C	-1.88545	-0.35633	0.09954
C	-2.32884	0.80963	0.73039
C	-0.43907	-0.77639	0.21213
N	0.43983	0.35029	-0.03689
C	1.82143	0.17587	-0.04497
C	2.63677	1.19616	-0.56283
C	4.01682	1.07303	-0.55171
C	4.62585	-0.06495	-0.02151
C	3.82360	-1.07709	0.49046
C	2.43457	-0.97042	0.47774
H	-3.99619	2.09993	1.13969
H	-5.61220	0.71330	-0.13536
H	-4.83677	-1.35611	-1.26335
H	-2.45929	-2.02983	-1.11894
H	-1.61494	1.41205	1.28472
H	-0.24101	-1.62127	-0.46791
H	-0.24793	-1.14034	1.23018
H	0.10122	0.96467	-0.76614
H	2.16964	2.09025	-0.96750
H	4.62427	1.87515	-0.95958
H	5.70604	-0.15835	-0.01214
H	4.27782	-1.97311	0.90246
H	1.83418	-1.78179	0.87280

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N-benzylidene aniline + proton

C	-4.10409	1.04408	-0.40550
C	-4.62893	-0.17747	0.01148
C	-3.78648	-1.21903	0.41752
C	-2.41532	-1.04466	0.39975
C	-1.87430	0.18321	-0.03062
C	-2.72958	1.22870	-0.42213
C	-0.46263	0.43701	-0.10214
N	0.47568	-0.44769	0.05687
C	1.88464	-0.20114	0.04486
C	2.39165	1.01629	0.49456
C	3.76468	1.22483	0.44155
C	4.61009	0.22497	-0.03592
C	4.08708	-0.99538	-0.45909
C	2.71618	-1.21765	-0.41949

H	-4.76409	1.84708	-0.71211
H	-5.70399	-0.32215	0.03038
H	-4.20901	-2.15864	0.75415
H	-1.77794	-1.85371	0.74616
H	-2.30936	2.17678	-0.74514
H	-0.12317	1.44683	-0.32490
H	0.20156	-1.41949	0.18532
H	1.73867	1.77309	0.91744
H	4.17533	2.16397	0.79430
H	5.68076	0.39281	-0.06576
H	4.74520	-1.77566	-0.82370
H	2.29834	-2.15950	-0.76318

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N-benzylidene aniline + [SiEt₃]⁺

C	3.91578	-0.21087	-0.99226
C	4.69805	-1.10284	-0.25641
C	4.10307	-2.11968	0.48979
C	2.72120	-2.24606	0.50318
C	1.92680	-1.31852	-0.18955
C	2.53318	-0.31212	-0.95727
C	0.48823	-1.50106	-0.14328
N	-0.42856	-0.58546	-0.21210
C	-1.80455	-1.05160	-0.27122
C	-2.35220	-1.72457	0.81572
C	-3.67723	-2.14661	0.74605
C	-4.43432	-1.88805	-0.39378
C	-3.87116	-1.20692	-1.47132
C	-2.54777	-0.77989	-1.41535
Si	-0.26369	1.29175	0.06405
C	0.00845	2.10787	-1.61079
C	1.15722	3.13096	-1.60526
C	-1.91009	1.77631	0.81046
C	1.09879	1.53213	1.32694
C	0.89400	0.70711	2.60545
C	-1.85893	3.24281	1.27618
H	4.38685	0.55367	-1.60015
H	5.77915	-1.01705	-0.28265
H	4.71687	-2.82057	1.04378
H	2.25110	-3.04886	1.06428
H	1.92487	0.35726	-1.55632
H	0.12743	-2.52900	-0.05429
H	-1.75471	-1.89508	1.70718
H	-4.11749	-2.67087	1.58686
H	-5.46651	-2.21631	-0.44260
H	-4.45992	-1.01118	-2.36055
H	-2.09248	-0.25539	-2.25064
H	0.17299	1.35163	-2.38748
H	-0.92982	2.60670	-1.88236
H	1.27038	3.59641	-2.58635
H	0.97620	3.93018	-0.88095

H	2.11409	2.66789	-1.34285	H	-4.14166	-1.12350	0.58480
H	-2.16908	1.12039	1.64892	H	1.01674	-2.52023	-0.20401
H	-2.70197	1.64405	0.06538	H	0.14191	-2.70551	-1.71669
H	2.09618	1.36741	0.91354	H	-1.80906	-0.29968	2.03030
H	1.05616	2.60294	1.57063	H	-2.09411	-2.02393	1.95501
H	1.64789	0.95483	3.35526	H	-0.23161	-1.45785	3.57188
H	-0.08744	0.89217	3.05298	H	0.36812	-2.47219	2.25870
H	0.97526	-0.36741	2.40854	H	0.69943	-0.74591	2.25028
H	-2.84267	3.57617	1.61221	H	0.04032	-4.84698	-0.42239
H	-1.54742	3.91729	0.47084	H	-1.57708	-4.16333	-0.58514
H	-1.16545	3.37622	2.11114	H	-0.70664	-4.01392	0.94142

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N-benzylidene anilide + [SiEt₃]⁺

C	3.50745	0.64933	1.30590
C	4.63702	0.09630	0.71047
C	4.55005	-0.42336	-0.57928
C	3.33960	-0.38811	-1.26350
C	2.20140	0.16991	-0.67584
C	2.29682	0.68669	0.61684
C	0.90248	0.20818	-1.46268
N	-0.31902	0.27927	-0.66872
C	-0.83220	1.54867	-0.36272
C	-0.06643	2.71948	-0.51533
C	-0.59959	3.96872	-0.21569
C	-1.90125	4.10140	0.25393
C	-2.66688	2.95037	0.41797
C	-2.15037	1.69841	0.11219
Si	-1.11136	-1.22880	-0.16211
C	-2.76052	-1.44336	-1.08187
C	-3.95199	-1.85573	-0.20792
C	0.01559	-2.66635	-0.62783
C	-1.35897	-1.24631	1.71053
C	-0.06149	-1.49287	2.49200
C	-0.58719	-3.99524	-0.14657
H	3.56527	1.05384	2.31157
H	5.57878	0.06525	1.24866
H	5.42363	-0.86471	-1.04866
H	3.27225	-0.80519	-2.26591
H	1.41606	1.11911	1.08262
H	0.91898	1.05535	-2.15988
H	0.86510	-0.68448	-2.09397
H	0.96568	2.65730	-0.84122
H	0.02460	4.84774	-0.34469
H	-2.30998	5.07758	0.48947
H	-3.68831	3.02242	0.77901
H	-2.79117	0.83093	0.23124
H	-2.98720	-0.50847	-1.60697
H	-2.60486	-2.19345	-1.86817
H	-4.87042	-1.95094	-0.79407
H	-3.77368	-2.81761	0.28380

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N-benzylidene aniline + [SiPhH₂]⁺

C	-2.85656	1.70640	-1.28207
C	-3.40854	2.53096	-0.29957
C	-2.64040	2.96486	0.78060
C	-1.31667	2.56629	0.88337
C	-0.76894	1.69170	-0.07192
C	-1.54259	1.28295	-1.17158
C	0.60807	1.30450	0.11891
N	1.21441	0.23355	-0.30852
C	2.64517	0.14118	-0.05578
C	3.50383	0.03859	-1.14547
C	4.87160	-0.06349	-0.91222
C	5.36220	-0.06844	0.39209
C	4.48743	0.02680	1.47112
C	3.11606	0.12759	1.25290
Si	0.48058	-1.35092	-0.98485
C	-1.15196	-1.64943	-0.17845
C	-1.28874	-1.58670	1.21577
C	-2.52047	-1.82393	1.81470
C	-3.62652	-2.13736	1.02591
C	-3.50286	-2.21411	-0.35903
C	-2.27236	-1.96621	-0.95922
H	-3.45186	1.40376	-2.13594
H	-4.43999	2.85514	-0.38968
H	-3.06976	3.62230	1.52766
H	-0.70463	2.91262	1.71133
H	-1.10356	0.68239	-1.96179
H	1.23260	1.99356	0.69188
H	3.11054	0.05982	-2.15776
H	5.55364	-0.13357	-1.75208
H	6.42901	-0.15034	0.56733
H	4.86843	0.01387	2.48613
H	2.42044	0.17744	2.08578
H	1.54993	-2.28989	-0.61940
H	0.37800	-1.16509	-2.44513
H	-0.43056	-1.35226	1.84336
H	-2.61902	-1.77280	2.89366
H	-4.58643	-2.32798	1.49423

H	-4.36325	-2.46559	-0.96980	C	-1.66402	-1.09193	-0.00040
H	-2.18913	-2.01821	-2.04260	C	-1.21284	0.23226	-0.00038
				C	-2.14138	1.27421	-0.00004
40				C	0.23234	0.54576	-0.00072
<i>N</i> -benzylidene anilide + [SiPhH ₂] ⁺				N	1.11267	-0.36582	0.00055
C	-4.04926	-0.95780	-1.32969	C	2.54389	-0.04820	0.00011
C	-4.99401	-1.60157	-0.53836	C	3.12279	-0.71757	-1.25220
C	-4.67749	-1.93568	0.77773	C	3.12293	-0.71523	1.25361
C	-3.42314	-1.62788	1.29062	C	2.89368	1.44215	-0.00121
C	-2.46697	-0.98515	0.49964	H	-4.22256	1.81821	0.00068
C	-2.79130	-0.64994	-0.81335	H	-5.01336	-0.53204	0.00067
C	-1.09926	-0.68724	1.09495	H	-3.37226	-2.39093	-0.00006
N	-0.16198	-0.01031	0.21045	H	-0.92586	-1.88698	-0.00067
C	-0.24780	1.38815	0.08695	H	-1.78963	2.30307	-0.00009
C	-1.35756	2.10989	0.55375	H	0.47236	1.61790	-0.00208
C	-1.40515	3.49412	0.41980	H	4.21178	-0.61301	-1.27317
C	-0.36681	4.19301	-0.18576	H	2.71077	-0.25867	-2.15573
C	0.73562	3.48235	-0.65370	H	2.86775	-1.77990	-1.26006
C	0.80273	2.10267	-0.51443	H	4.21184	-0.60982	1.27481
Si	0.83692	-0.98765	-0.84602	H	2.71026	-0.25520	2.15627
C	2.62293	-0.98954	-0.27992	H	2.86871	-1.77774	1.26312
C	3.61149	-1.67111	-1.00305	H	2.50314	1.94870	0.88719
C	4.93367	-1.68309	-0.57082	H	3.98057	1.55972	-0.00140
C	5.28874	-1.00876	0.59611	H	2.50305	1.94723	-0.89040
C	4.32084	-0.32501	1.32612				
C	2.99771	-0.31744	0.89009	28			
H	-4.28952	-0.68878	-2.35337	<i>N</i> -benzylidene tert-butylamide			
H	-5.97276	-1.84089	-0.94116	C	2.53721	1.42305	-0.17428
H	-5.40923	-2.43724	1.40316	C	3.54199	0.58971	0.31874
H	-3.17764	-1.89177	2.31709	C	3.29017	-0.77490	0.45176
H	-2.06123	-0.13076	-1.42813	C	2.04764	-1.29245	0.09007
H	-1.21890	-0.09173	2.00918	C	1.03303	-0.46682	-0.40051
H	-0.64938	-1.63549	1.41130	C	1.29773	0.89722	-0.52697
H	-2.19991	1.59142	0.99715	C	-0.34335	-1.01545	-0.86168
H	-2.27692	4.02654	0.78751	N	-1.37870	-0.07282	-1.05657
H	-0.41365	5.27127	-0.29058	C	-2.21740	0.11467	0.09629
H	1.56378	4.00589	-1.12106	C	-3.12684	1.30951	-0.22307
H	1.69451	1.57927	-0.84871	C	-3.13955	-1.10983	0.36407
H	0.74975	-0.48084	-2.23745	C	-1.47927	0.43100	1.42535
H	0.27049	-2.35528	-0.77766	H	2.72670	2.48976	-0.27862
H	3.34984	-2.19992	-1.91776	H	4.50880	0.99900	0.60173
H	5.68775	-2.21523	-1.14216	H	4.06304	-1.43305	0.84413
H	6.32035	-1.01552	0.93382	H	1.85090	-2.35972	0.19699
H	4.59624	0.20352	2.23334	H	0.46569	1.49398	-0.89949
H	2.24348	0.22483	1.45658	H	-0.55265	-1.86555	-0.16164
				H	-0.10251	-1.52647	-1.81913
27				H	-3.86042	1.51132	0.57063
<i>N</i> -benzylidene tert-butylamine				H	-2.50753	2.20010	-0.37579
C	-3.50680	1.00257	0.00037	H	-3.65476	1.10882	-1.16102
C	-3.94961	-0.31645	0.00038	H	-3.83284	-0.95959	1.20582
C	-3.02519	-1.36254	-0.00002	H	-2.53856	-1.99964	0.58632

H	-3.71836	-1.31534	-0.54250
H	-0.80083	-0.38688	1.69772
H	-0.87071	1.33452	1.30675
H	-2.17327	0.58425	2.26558

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N-benzylidene tert-butylamine + BEt₃

C	-0.168089	-2.816370	3.943573
C	0.657562	-3.923453	3.774160
C	1.538916	-3.973691	2.695741
C	1.581047	-2.929083	1.780116
C	0.717569	-1.839364	1.921582
C	-0.134287	-1.770092	3.025025
C	0.830577	-0.699966	0.970301
N	0.108907	-0.344342	-0.025871
C	-1.108838	-1.143923	-0.452994
B	0.573077	1.124569	-0.786498
C	-1.446329	-0.897644	-1.929512
C	-0.906344	-2.663496	-0.313692
C	-2.296246	-0.693622	0.407612
C	3.244908	1.424764	-0.074401
C	1.776089	1.851125	0.075101
C	1.930741	-0.517661	-2.434746
C	1.097968	0.764179	-2.294447
C	-1.070776	2.649531	0.681375
C	-0.717706	2.132381	-0.721067
H	-0.837736	-2.760659	4.795454
H	0.625838	-4.739418	4.488460
H	2.196400	-4.827366	2.568637
H	2.266012	-2.963972	0.937318
H	-0.761153	-0.895880	3.170934
H	1.679574	-0.055712	1.173484
H	-2.389194	-1.412501	-2.133582
H	-1.573856	0.152846	-2.167344
H	-0.686296	-1.318269	-2.589685
H	-1.683925	-3.155846	-0.903496
H	-0.991073	-3.025354	0.709953
H	0.063059	-2.969957	-0.718925
H	-2.114639	-0.889100	1.466391
H	-2.504270	0.368888	0.272250
H	-3.180941	-1.262676	0.106973
H	3.914112	2.081695	0.491455
H	3.558534	1.467262	-1.121885
H	3.445822	0.401058	0.267971
H	1.534457	1.931234	1.146432
H	1.724243	2.892628	-0.276381
H	2.344429	-0.641733	-3.441349
H	1.340513	-1.417249	-2.218913
H	2.771331	-0.531654	-1.733997
H	1.731551	1.612557	-2.594563
H	0.294864	0.749495	-3.041004

H	-0.296760	3.320913	1.063272
H	-2.017452	3.200607	0.701205
H	-1.156930	1.828314	1.406658
H	-1.629551	1.740068	-1.186011
H	-0.448509	2.994991	-1.348540

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N-benzylidene tert-butylamide + BEt₃

C	0.930939	-3.276627	3.802445
C	1.841924	-3.989680	3.027003
C	2.104429	-3.567500	1.724974
C	1.464860	-2.445998	1.204122
C	0.551515	-1.722198	1.972024
C	0.294972	-2.155611	3.275244
C	-0.116594	-0.451770	1.438161
N	-0.205145	-0.296964	0.005882
C	-1.443367	-0.888409	-0.536542
B	0.532586	0.956633	-0.686805
C	-1.437459	-0.920169	-2.071421
C	-1.611247	-2.354564	-0.084123
C	-2.724824	-0.126980	-0.110907
C	2.934878	0.877131	0.680992
C	1.659442	1.648994	0.321973
C	2.029429	-0.843031	-2.127437
C	1.327320	0.519681	-2.090709
C	-1.093986	2.950720	0.134979
C	-0.496777	2.210985	-1.069728
H	0.711493	-3.597942	4.817674
H	2.339250	-4.866657	3.432221
H	2.812576	-4.116917	1.109975
H	1.644459	-2.104492	0.189161
H	-0.422180	-1.604500	3.882059
H	0.461085	0.376337	1.857280
H	-1.096468	-0.386814	1.947774
H	-2.360345	-1.397181	-2.423046
H	-1.387228	0.080411	-2.497440
H	-0.589968	-1.495465	-2.449737
H	-2.503274	-2.789657	-0.550790
H	-1.726392	-2.447652	1.000070
H	-0.738605	-2.945733	-0.379087
H	-2.810508	-0.051815	0.978056
H	-2.725286	0.884111	-0.521562
H	-3.620537	-0.647713	-0.473362
H	3.582432	1.427021	1.379225
H	3.532953	0.678351	-0.215099
H	2.718882	-0.094494	1.141355
H	1.209762	2.019284	1.256903
H	1.972022	2.569297	-0.199211
H	2.501077	-1.061084	-3.096974
H	1.325956	-1.655741	-1.914862
H	2.813889	-0.915815	-1.366239

H	2.088536	1.295349	-2.283552
H	0.661560	0.576984	-2.966850
H	-0.324195	3.526747	0.660434
H	-1.897515	3.653336	-0.130129
H	-1.508020	2.242797	0.865492
H	-1.319387	1.897200	-1.729426
H	0.068847	2.940777	-1.673231

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N-benzylidene tert-butylamine + BPh₃

C	1.56375	0.12055	-0.01035
N	0.52047	-0.51132	0.40736
C	0.64455	-1.78415	1.21913
C	1.40364	-1.47817	2.53345
C	-0.70185	-2.38077	1.65661
C	1.30266	-2.85194	0.31923
C	3.04083	0.01348	0.09008
C	3.85721	-0.96608	0.68560
C	5.24052	-0.85230	0.64783
C	5.85106	0.23419	0.02493
C	5.06463	1.21572	-0.56705
C	3.68114	1.10062	-0.53445
B	-0.98969	0.09562	-0.09422
C	-1.79249	0.61722	1.21610
C	-3.14083	0.99396	1.09416
C	-3.85346	1.55036	2.15203
C	-3.22963	1.77462	3.37735
C	-1.88312	1.45696	3.51696
C	-1.18430	0.89514	2.44855
C	-1.63614	-1.12717	-0.95580
C	-2.91396	-1.66520	-0.74540
C	-3.41454	-2.70855	-1.52249
C	-2.64406	-3.25682	-2.54387
C	-1.36947	-2.74804	-2.77862
C	-0.88577	-1.70221	-1.99526
C	-0.76245	1.42726	-1.03403
C	-0.36893	2.64778	-0.44862
C	-0.16636	3.80286	-1.19587
C	-0.38210	3.78727	-2.57357
C	-0.80208	2.60891	-3.17791
C	-0.98417	1.45172	-2.41783
H	1.30574	0.98969	-0.60468
H	0.68715	-1.17806	3.30061
H	1.90586	-2.38298	2.88930
H	2.14377	-0.68334	2.44847
H	-0.46296	-3.19818	2.34543
H	-1.26643	-2.79461	0.82434
H	-1.32136	-1.65952	2.18911
H	2.15924	-2.49073	-0.24840
H	1.62089	-3.69963	0.93378

H	0.56399	-3.20890	-0.40128
H	3.43350	-1.82533	1.18287
H	5.84663	-1.62283	1.11210
H	6.93310	0.31207	0.00292
H	5.52301	2.06859	-1.05550
H	3.07275	1.87242	-0.99843
H	-3.63774	0.87343	0.13440
H	-4.89637	1.82191	2.01638
H	-3.78180	2.20890	4.20489
H	-1.37133	1.65291	4.45507
H	-0.12419	0.68844	2.57817
H	-3.52376	-1.28642	0.06948
H	-4.40798	-3.09985	-1.32290
H	-3.03042	-4.07177	-3.14815
H	-0.75296	-3.16439	-3.57026
H	0.11436	-1.31915	-2.19936
H	-0.22291	2.69062	0.62949
H	0.14116	4.72062	-0.70259
H	-0.23731	4.68770	-3.16286
H	-0.99298	2.58486	-4.24700
H	-1.32117	0.55128	-2.92131

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N-benzylidene tert-butylamide + BPh₃

C	-5.20191	-0.58575	-1.11826
C	-5.45837	-0.22501	0.19962
C	-4.39091	-0.04176	1.08111
C	-3.08314	-0.20606	0.64255
C	-2.81173	-0.56202	-0.68346
C	-3.88598	-0.75630	-1.55054
C	-1.36795	-0.75919	-1.13108
N	-0.46024	0.32428	-0.82222
C	-0.64910	1.53758	-1.66078
C	-1.13172	1.20330	-3.09304
C	-1.71364	2.49330	-1.07109
C	0.64754	2.35344	-1.82603
B	0.82388	-0.00655	0.03979
C	0.49418	-1.22991	1.14632
C	0.64668	-2.58512	0.78858
C	0.38136	-3.63761	1.66036
C	-0.04147	-3.37810	2.96187
C	-0.18466	-2.05488	3.36246
C	0.08300	-1.01346	2.47167
C	2.07390	-0.61172	-0.86387
C	3.27570	-1.04052	-0.26747
C	4.31291	-1.61528	-0.99537
C	4.17893	-1.80966	-2.37053
C	2.99380	-1.42779	-2.98951
C	1.96963	-0.84351	-2.24100
C	1.28018	1.32095	0.90994

C	2.58551	1.82992	0.98707	C	3.68423	-2.22135	0.45628
C	2.90563	2.96451	1.73372	B	-0.28536	0.60554	0.20111
C	1.91962	3.64315	2.44319	C	-0.32848	0.47877	1.83015
C	0.61047	3.16830	2.39040	C	-0.33568	-0.78582	2.45113
C	0.31116	2.03533	1.63832	C	-0.47431	-0.93532	3.82525
H	-6.02442	-0.73083	-1.81362	C	-0.64092	0.18992	4.63256
H	-6.48039	-0.08744	0.54112	C	-0.66785	1.44881	4.04590
H	-4.58382	0.23112	2.11498	C	-0.51154	1.58708	2.66530
H	-2.24286	-0.06481	1.31762	C	-0.12172	2.13489	-0.32542
H	-3.68557	-1.03858	-2.58266	C	-0.93122	2.76070	-1.28055
H	-1.01474	-1.65519	-0.61839	C	-0.66044	4.04517	-1.75088
H	-1.38589	-1.03399	-2.19961	C	0.43472	4.75210	-1.26492
H	-1.19098	2.13006	-3.67238	C	1.24938	4.16547	-0.29852
H	-0.44481	0.52754	-3.61248	C	0.96901	2.88002	0.15328
H	-2.12992	0.75589	-3.09721	C	-1.61960	-0.23171	-0.24888
H	-1.82714	3.37621	-1.71413	C	-1.63394	-1.59466	-0.52390
H	-1.41013	2.83536	-0.08003	C	-2.78582	-2.33947	-0.73207
H	-2.68855	2.00541	-0.99029	C	-4.02075	-1.71571	-0.63052
H	1.48801	1.71789	-2.11568	C	-4.06956	-0.36739	-0.31145
H	0.49520	3.10507	-2.60932	C	-2.88570	0.33319	-0.10885
H	0.91793	2.88037	-0.91163	F	-0.47017	-2.28220	-0.60384
H	0.99190	-2.82187	-0.21621	F	-2.71574	-3.64078	-1.01688
H	0.51174	-4.66364	1.32407	F	-5.14220	-2.40547	-0.82560
H	-0.24687	-4.19273	3.65148	F	-5.24846	0.23954	-0.18085
H	-0.49901	-1.82550	4.37820	F	-3.01621	1.61167	0.26967
H	-0.01760	0.00297	2.83961	H	1.74488	-0.20504	1.48430
H	3.38674	-0.93359	0.81095	H	0.37358	-0.09991	-3.77762
H	5.22525	-1.92483	-0.49029	H	-0.45696	-1.15857	-2.64008
H	4.98281	-2.26259	-2.94507	H	-0.57586	0.61121	-2.47654
H	2.86263	-1.58756	-4.05761	H	2.49371	0.84809	-3.39725
H	1.04364	-0.56124	-2.73592	H	3.12958	1.08372	-1.76805
H	3.37579	1.34642	0.41940	H	1.64268	1.92235	-2.26837
H	3.93161	3.32564	1.75218	H	3.18634	-1.48010	-2.05829
H	2.16400	4.52991	3.02220	H	1.67599	-2.37316	-1.74217
H	-0.17939	3.68673	2.92948	H	1.99612	-1.68853	-3.33859
H	-0.72056	1.69369	1.58699	H	4.28954	1.10337	0.07716
				H	6.61510	0.26216	-0.01105
				H	7.06886	-2.16716	0.19925
				H	5.18617	-3.75096	0.52680
				H	2.85732	-2.91103	0.59898
				H	-0.22853	-1.67917	1.83536
				H	-0.46712	-1.92731	4.26715
				H	-0.75873	0.08089	5.70617
				H	-0.81403	2.33166	4.66113
				H	-0.54838	2.58100	2.22980
				H	-1.79807	2.23761	-1.67606
				H	-1.30947	4.49380	-2.49688
				H	0.64854	5.75188	-1.62967
				H	2.10246	4.70822	0.09793
				H	1.62224	2.43672	0.90560
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<i>N</i> -benzylidene tert-butylamine +							
$B(C_6F_5)_2$							
C	2.02954	-0.36751	0.44650				
N	1.11290	-0.11200	-0.41138				
C	1.37862	-0.22064	-1.91310				
C	0.08191	-0.21615	-2.73025				
C	2.21178	0.99475	-2.35038				
C	2.11815	-1.52186	-2.26504				
C	3.42494	-0.85792	0.28820				
C	4.48587	0.03775	0.14824				
C	5.79470	-0.43731	0.10947				
C	6.04877	-1.79954	0.23203				
C	4.99185	-2.68964	0.41417				

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N-benzylidene tert-butylamide +
B(C₆F₅)Ph₂

C	5.10948	-0.50835	-1.68825
C	5.41644	-0.14325	-0.38210
C	4.38277	0.07748	0.52950
C	3.05742	-0.07204	0.13896
C	2.73662	-0.43976	-1.17262
C	3.77718	-0.65112	-2.07646
C	1.27844	-0.57112	-1.59787
N	0.42369	-1.31855	-0.70078
C	0.60375	-2.79346	-0.78179
C	0.87992	-3.26893	-2.22982
C	1.80699	-3.29398	0.05277
C	-0.63457	-3.57347	-0.29709
B	-0.75293	-0.56661	0.01533
C	-0.35550	1.09650	0.20818
C	-0.63051	2.02130	-0.81016
C	-0.48203	3.39829	-0.70373
C	-0.01779	3.94584	0.48045
C	0.30983	3.08993	1.51378
C	0.14293	1.71482	1.35598
C	-2.15915	-0.50398	-0.85926
C	-3.25982	0.25850	-0.42959
C	-4.43872	0.35475	-1.16360
C	-4.55864	-0.31251	-2.38154
C	-3.48182	-1.06105	-2.84617
C	-2.31055	-1.14450	-2.09395
C	-1.05338	-1.22902	1.50555
C	-2.32756	-1.59435	1.96239
C	-2.53171	-2.24983	3.17900
C	-1.45307	-2.57303	3.99266
C	-0.16988	-2.22316	3.57264
C	0.01040	-1.56734	2.36058
F	-1.01981	1.60987	-2.02826
F	-0.77036	4.20261	-1.73561
F	0.13537	5.26860	0.60931
F	0.78980	3.58941	2.66104
F	0.55541	1.00891	2.42193
H	5.90578	-0.68807	-2.40550
H	6.45182	-0.03352	-0.07279
H	4.61390	0.36504	1.55127
H	2.25149	0.08214	0.85139
H	3.53689	-0.94078	-3.09790
H	0.88981	0.44197	-1.69124
H	1.26640	-0.95309	-2.62939
H	0.89566	-4.36286	-2.24865
H	0.10991	-2.92991	-2.92979
H	1.85377	-2.92826	-2.59531
H	1.90238	-4.38299	-0.04765

H	1.66509	-3.06584	1.11015
H	2.74436	-2.84146	-0.28064
H	-1.55687	-3.18572	-0.73565
H	-0.52615	-4.62277	-0.59395
H	-0.73646	-3.54711	0.78715
H	-3.18335	0.80208	0.51220
H	-5.26429	0.95609	-0.78988
H	-5.47443	-0.24078	-2.96227
H	-3.55040	-1.57495	-3.80236
H	-1.46680	-1.70848	-2.48266
H	-3.19391	-1.39887	1.33835
H	-3.54093	-2.51990	3.48127
H	-1.60468	-3.09066	4.93630
H	0.69157	-2.46666	4.19007
H	1.01966	-1.31526	2.04997

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N-benzylidene tert-butylamine +
B(C₆F₅)₂Ph

C	1.03546	1.46597	0.32385
N	0.63797	0.62411	1.21759
C	1.16499	0.67363	2.63028
C	0.63465	-0.43209	3.55200
C	2.68872	0.43103	2.56053
C	0.69538	2.00361	3.25216
C	1.94690	2.62414	0.20719
C	2.74141	3.27312	1.17257
C	3.52660	4.36203	0.82219
C	3.55037	4.83365	-0.48936
C	2.78079	4.20395	-1.46036
C	1.99170	3.11609	-1.11174
B	-0.37195	-0.53307	0.51822
C	0.71958	-1.35353	-0.41228
C	0.96360	-1.09588	-1.76187
C	1.92884	-1.74646	-2.52032
C	2.73803	-2.70105	-1.92406
C	2.57375	-2.96741	-0.57434
C	1.59446	-2.28737	0.13996
C	-1.27565	-1.44047	1.50758
C	-2.22920	-0.82006	2.33474
C	-3.11511	-1.54836	3.11711
C	-3.10202	-2.94250	3.06562
C	-2.20495	-3.58175	2.21982
C	-1.30914	-2.83686	1.45101
C	-1.52522	0.27097	-0.34164
C	-2.05614	1.51455	-0.01543
C	-3.14593	2.08627	-0.66354
C	-3.77260	1.38924	-1.68288
C	-3.30103	0.12977	-2.02968
C	-2.21180	-0.39823	-1.35401

C	4.44483	1.11877	0.58857	H	-0.25728	0.76358	4.60104
C	3.37574	0.50403	1.23025	H	-1.72490	0.78941	3.60179
C	2.23851	1.24647	1.56481	H	-1.79168	-2.47635	3.68232
C	2.21795	2.62385	1.33641	H	-1.34429	-2.52179	1.97649
C	1.19338	0.54983	2.36011	H	-2.51799	-1.32220	2.58190
N	0.20840	-0.18278	1.98514	H	1.47839	-1.19535	4.21281
C	-0.45773	-0.91276	3.17861	H	0.19337	-2.29414	4.69942
C	-1.02645	0.14261	4.13510	H	0.99316	-2.52300	3.13464
C	-1.59890	-1.85967	2.80047				
C	0.62946	-1.77475	3.84315	62			
B	-0.16828	-0.23385	0.35497	<i>N</i> -benzylidene tert-butylamide + B(C ₆ F ₅) ₃			
C	1.11689	-0.99685	-0.31379	C	4.92833	-0.48129	1.15246
C	2.07357	-0.43805	-1.15534	C	5.00543	-1.85313	0.93058
C	3.18894	-1.13324	-1.61137	C	3.88493	-2.64714	1.16783
C	3.39052	-2.44765	-1.22521	C	2.69923	-2.07475	1.61740
C	2.46541	-3.05292	-0.38417	C	2.60520	-0.69805	1.82986
C	1.36892	-2.31926	0.03880	C	3.73888	0.08610	1.60316
C	-2.77976	-0.35901	0.46286	C	1.34730	-0.07151	2.41417
C	-1.60366	-0.94133	-0.00924	N	0.05672	-0.44587	1.84344
C	-4.05561	-0.74556	0.09345	C	-0.89943	-0.87696	2.90252
C	-4.20236	-1.76246	-0.84183	C	-0.99638	0.10750	4.09866
C	-3.07037	-2.36208	-1.36558	C	-2.35661	-1.02824	2.43324
C	-1.80555	-1.94310	-0.95538	C	-0.46162	-2.26074	3.42506
C	-0.42535	1.29091	-0.19810	B	-0.33443	-0.01444	0.40870
C	-0.74154	2.42240	0.54063	C	1.00749	0.20635	-0.59402
C	-1.05731	3.65292	-0.02349	C	1.84485	1.30859	-0.40081
C	-1.12707	3.77459	-1.40083	C	2.96062	1.61244	-1.16578
C	-0.87589	2.65863	-2.18894	C	3.28193	0.81205	-2.24708
C	-0.55164	1.45791	-1.57795	C	2.46040	-0.26209	-2.53172
F	2.04100	0.85575	-1.49035	C	1.35322	-0.52999	-1.72954
F	4.10273	-0.51450	-2.35843	C	-1.32321	-1.20684	-0.22934
F	4.46168	-3.11731	-1.63850	C	-2.65905	-1.09970	-0.60744
F	2.63447	-4.31755	-0.00137	C	-3.45322	-2.17368	-0.99847
F	0.50469	-2.95931	0.85083	C	-2.92166	-3.45023	-1.01431
F	-2.69774	0.61066	1.39697	C	-1.59901	-3.62265	-0.63721
F	-5.12969	-0.16334	0.62422	C	-0.84698	-2.51700	-0.26655
F	-5.41323	-2.15614	-1.22068	C	-1.05450	1.49731	0.22078
F	-3.19314	-3.33143	-2.26940	C	-1.07071	2.50955	1.16974
F	-0.78558	-2.57380	-1.54597	C	-1.58744	3.78294	0.94095
F	-0.71861	2.40557	1.89221	C	-2.08720	4.10266	-0.30835
F	-1.28893	4.70833	0.75867	C	-2.04881	3.14522	-1.31254
F	-1.43265	4.94062	-1.96147	C	-1.52538	1.89326	-1.03083
F	-0.96065	2.74942	-3.51425	F	1.64074	2.16084	0.62298
F	-0.35750	0.40582	-2.38527	F	3.74297	2.64987	-0.84257
H	3.25961	4.29771	0.49715	F	4.35280	1.07578	-3.00131
H	5.22787	2.95864	-0.20217	F	2.72334	-1.03062	-3.59532
H	5.30851	0.52852	0.30059	F	0.62417	-1.56630	-2.16859
H	3.40554	-0.56252	1.44085	F	-3.33064	0.06255	-0.51485
H	1.37185	3.21725	1.66049	F	-4.73747	-1.98626	-1.32846
H	1.35782	0.63292	3.43342	F	-3.66778	-4.49682	-1.38189
H	-1.56378	-0.36965	4.93731	F	-1.06020	-4.84822	-0.64870

F	0.42385	-2.78484	0.06333	H	-3.94353	1.62905	-0.00053
F	-0.52679	2.33371	2.38608	H	-2.46224	1.95538	0.89417
F	-1.58046	4.70824	1.90995				
F	-2.58484	5.32035	-0.55189				
F	-2.50356	3.44900	-2.53489	29			
F	-1.48356	1.02929	-2.06010	(<i>N</i> - <i>tert</i> -butyl)benzylamine			
H	5.78953	0.15301	0.96175	C	2.97119	-1.39649	0.02453
H	5.92773	-2.29939	0.57056	C	3.94356	-0.41427	-0.14978
H	3.93351	-3.71891	0.99749	C	3.56982	0.92628	-0.17385
H	1.82258	-2.68843	1.78752	C	2.23117	1.27892	-0.02468
H	3.67253	1.16268	1.74652	C	1.25218	0.30167	0.15784
H	1.36542	-0.39829	3.45786	C	1.63446	-1.04166	0.17800
H	1.48656	1.01554	2.46006	C	-0.19583	0.69529	0.35963
H	-1.50840	-0.39072	4.92949	N	-1.09065	-0.28053	-0.24623
H	-0.02918	0.45288	4.46689	C	-2.53621	-0.07134	-0.06373
H	-1.57574	0.98931	3.82262	C	-3.22829	-1.14313	-0.90819
H	-2.99109	-1.10081	3.32293	C	-2.89249	-0.28861	1.40972
H	-2.51905	-1.93347	1.84718	C	-3.00757	1.31965	-0.51538
H	-2.69152	-0.16117	1.85642	H	3.25563	-2.44413	0.04067
H	0.53826	-2.23549	3.87112	H	4.98563	-0.69247	-0.27078
H	-1.15735	-2.63396	4.18587	H	4.31930	1.69853	-0.31629
H	-0.44149	-2.96835	2.58987	H	1.94080	2.32634	-0.05297
				H	0.86616	-1.79729	0.30542
28				H	-0.33513	1.72427	-0.01258
<i>N</i> -benzylidene <i>tert</i> -butylamine + proton				H	-0.40516	0.72570	1.43618
C	3.09584	-1.35338	0.00000	H	-0.88928	-0.32225	-1.24388
C	3.98669	-0.27408	0.00011	H	-4.31425	-1.08836	-0.79236
C	3.51725	1.03707	0.00005	H	-2.99637	-1.00901	-1.97091
C	2.14995	1.27434	-0.00008	H	-2.88841	-2.13684	-0.60513
C	1.24799	0.19760	-0.00010	H	-3.97876	-0.28056	1.53904
C	1.73215	-1.12396	-0.00012	H	-2.48119	0.49747	2.04949
C	-0.15640	0.52883	0.00002	H	-2.50341	-1.25213	1.74949
N	-1.13697	-0.31058	-0.00003	H	-2.72443	1.50285	-1.55787
C	-2.60866	-0.03042	0.00004	H	-4.09622	1.40230	-0.44027
C	-3.17213	-0.68790	-1.26231	H	-2.57233	2.11137	0.10167
C	-3.17191	-0.68697	1.26297				
C	-2.86355	1.47031	-0.00058	49			
H	3.47429	-2.36904	-0.00003	<i>N</i> -benzylidene <i>tert</i> -butylamine + [SiEt ₃] ⁺			
H	5.05497	-0.46320	0.00019	C	0.077253	-3.956486	2.856302
H	4.21316	1.86786	0.00006	C	0.939428	-3.713192	3.926665
H	1.77359	2.29337	-0.00008	C	1.611124	-2.498245	4.016487
H	1.05817	-1.97628	-0.00037	C	1.419865	-1.538078	3.034356
H	-0.42657	1.58224	0.00026	C	0.529951	-1.748974	1.960149
H	-0.91048	-1.30405	-0.00006	C	-0.135228	-2.990845	1.886122
H	-4.25570	-0.55279	-1.28191	C	0.502713	-0.617237	1.031432
H	-2.74987	-0.23752	-2.16380	N	-0.222820	-0.212855	0.027577
H	-2.97163	-1.76362	-1.27526	C	-1.483254	-0.913753	-0.443360
H	-4.25556	-0.55252	1.28225	Si	0.482405	1.278049	-0.929758
H	-2.75000	-0.23544	2.16405	C	-2.250670	-0.036054	-1.440934
H	-2.97075	-1.76255	1.27706	C	-1.072875	-2.206774	-1.173887
H	-2.46243	1.95447	-0.89591	C	-2.438527	-1.104256	0.746506
				C	2.788012	2.864236	-0.920120

C	2.110318	1.743181	-0.107194	C	3.053403	0.361440	0.925579
C	0.390354	1.717366	-3.748355	C	1.734659	1.143524	0.904592
C	0.832928	0.697415	-2.686108	C	2.005793	-1.073606	-2.103716
C	-1.255675	2.873132	0.677638	C	1.487526	0.369169	-2.048294
C	-0.711976	2.710814	-0.748654	C	-1.027380	2.971574	0.564857
H	-0.435507	-4.908522	2.778159	C	-0.404453	2.443151	-0.735058
H	1.091762	-4.476035	4.682988	H	2.438426	-2.020965	4.677740
H	2.290312	-2.304104	4.838787	H	3.457819	-3.778107	3.248318
H	1.962998	-0.599435	3.101919	H	2.567257	-4.172509	0.965308
H	-0.814044	-3.221840	1.078999	H	0.692548	-2.788126	0.109221
H	1.327445	0.055278	1.250573	H	0.552656	-0.667843	3.821292
H	-3.102353	-0.621646	-1.796404	H	-0.750676	0.083776	2.027551
H	-2.647228	0.864073	-0.967864	H	-1.599269	-1.373803	1.608781
H	-1.664826	0.235957	-2.321571	H	-2.490109	-0.910814	-2.852926
H	-1.914519	-2.904807	-1.191532	H	-1.513580	0.500988	-2.458595
H	-0.214757	-2.703968	-0.721609	H	-0.735471	-1.075729	-2.716315
H	-0.807543	-1.986165	-2.210569	H	-2.890202	-2.742499	-1.270807
H	-2.023112	-1.635621	1.597020	H	-2.061775	-2.815540	0.286607
H	-2.777853	-0.127490	1.100555	H	-1.131442	-2.950791	-1.213094
H	-3.316569	-1.654653	0.399807	H	-3.267209	-0.415519	0.734955
H	3.750423	3.129268	-0.477925	H	-2.961479	0.871547	-0.443773
H	2.978504	2.556748	-1.952859	H	-3.941842	-0.536994	-0.893052
H	2.181046	3.773165	-0.945732	H	3.713998	0.728496	1.717252
H	1.962142	2.087629	0.923751	H	3.590245	0.468535	-0.022788
H	2.786400	0.880231	-0.067100	H	2.893120	-0.705363	1.101478
H	0.666273	1.380949	-4.749836	H	1.246613	1.071957	1.883344
H	-0.693465	1.869023	-3.736695	H	1.965277	2.211801	0.776849
H	0.857170	2.694188	-3.588777	H	2.610426	-1.253473	-2.997938
H	0.378557	-0.277319	-2.886740	H	1.179203	-1.791920	-2.108670
H	1.915173	0.533804	-2.753955	H	2.620194	-1.311804	-1.230230
H	-1.856637	3.779965	0.769889	H	2.337928	1.065707	-2.058367
H	-1.888163	2.027942	0.968145	H	0.907624	0.599504	-2.949224
H	-0.446959	2.942766	1.412662	H	-0.266618	3.126487	1.336777
H	-0.132706	3.602581	-1.021965	H	-1.541013	3.926178	0.415898
H	-1.525290	2.660593	-1.476986	H	-1.760290	2.264526	0.969007
				H	-1.174615	2.373356	-1.511814
				H	0.332308	3.165677	-1.112929

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N-benzylidene tert-butylamide + [SiEt₃]⁺

C	2.051238	-2.205295	3.680418
C	2.623682	-3.190058	2.879199
C	2.123516	-3.409644	1.597823
C	1.062724	-2.645483	1.119021
C	0.484719	-1.655144	1.914094
C	0.988069	-1.446857	3.198799
C	-0.676385	-0.821272	1.405622
N	-0.610954	-0.506785	-0.023657
C	-1.795282	-0.922769	-0.814246
Si	0.494671	0.787939	-0.491357
C	-1.610719	-0.575333	-2.295767
C	-1.979961	-2.447323	-0.739631
C	-3.067152	-0.210992	-0.320923

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N-benzylidene tert-butylamine + [SiPhH₂]⁺

N	0.691666	1.001852	0.023706
C	1.234229	-0.174685	-0.131153
C	0.681009	-1.327011	0.604149
C	2.436820	-0.393513	-0.987159
C	1.367101	2.178862	-0.496604
C	0.931449	2.766185	-1.680711
C	1.587357	3.900238	-2.147865
C	2.653625	4.439397	-1.429533
C	3.071539	3.845557	-0.242091
C	2.427887	2.705714	0.232953

C	0.614916	-1.271508	2.000822
C	0.108341	-2.356298	2.708237
C	-0.368355	-3.470226	2.021744
C	-0.311572	-3.519171	0.628788
C	0.239408	-2.462916	-0.083658
Si	-1.004309	1.308004	0.771089
C	-2.114845	-0.065843	0.236473
C	-2.364562	-0.270403	-1.129351
C	-3.151736	-1.335021	-1.552334
C	-3.708665	-2.200960	-0.612101
C	-3.481848	-2.000831	0.747029
C	-2.684949	-0.940845	1.169541
H	3.325485	-0.379916	-0.344537
H	2.384751	-1.392485	-1.424734
H	2.552465	0.369300	-1.756472
H	0.096863	2.338833	-2.228927
H	1.261755	4.365207	-3.071759
H	3.156918	5.327103	-1.796322
H	3.898362	4.267696	0.318200
H	2.738462	2.231976	1.159695
H	0.990234	-0.399027	2.528769
H	0.084288	-2.329840	3.792213
H	-0.779085	-4.309081	2.573831
H	-0.688509	-4.386784	0.098601
H	0.279850	-2.497711	-1.168417
H	-0.815830	1.408142	2.227757
H	-1.299528	2.610631	0.154563
H	-1.946601	0.406523	-1.872825
H	-3.342508	-1.484571	-2.609759
H	-4.329217	-3.028129	-0.941392
H	-3.922570	-2.671250	1.477707
H	-2.500091	-0.803194	2.231836

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N-benzylidene tert-butylamide +
[SiH₂Ph]⁺

C	-1.864387	-1.435777	2.564788
C	-1.514321	-1.018057	3.844976
C	-0.613655	0.033694	4.000996
C	-0.069930	0.656964	2.883014
C	-0.413098	0.242786	1.594206
C	-1.317123	-0.808119	1.447355
C	0.242611	0.912709	0.395245
N	-0.395481	0.648769	-0.885506
C	-1.410714	1.632189	-1.334924
Si	0.293379	-0.515653	-1.983859
C	-2.235420	1.023784	-2.474685
C	-2.380336	1.988358	-0.199773
C	-0.716921	2.905383	-1.843346

C	3.058862	-1.037573	-1.544533
C	1.749537	-1.361782	-1.164507
C	4.155602	-1.647825	-0.940466
C	3.957547	-2.597952	0.057311
C	2.663663	-2.937408	0.447173
C	1.571589	-2.325989	-0.160830
H	-2.570121	-2.250532	2.433563
H	-1.942529	-1.504230	4.715683
H	-0.337757	0.371710	4.995099
H	0.632222	1.478552	3.009363
H	-1.603328	-1.117289	0.445157
H	0.295402	1.994052	0.579968
H	1.285038	0.575520	0.363372
H	-0.706705	-1.544787	-2.374594
H	0.798180	0.108872	-3.240446
H	-3.004944	1.733288	-2.791274
H	-1.621353	0.800217	-3.354254
H	-2.727713	0.103080	-2.147975
H	-3.119073	2.707091	-0.567420
H	-1.871762	2.443427	0.654567
H	-2.906219	1.098720	0.155806
H	-0.051986	2.664960	-2.678768
H	-1.451209	3.641943	-2.185254
H	-0.119142	3.371130	-1.054002
H	3.224924	-0.297901	-2.324338
H	5.162412	-1.382647	-1.247933
H	4.810280	-3.075046	0.530348
H	2.506021	-3.678941	1.224046
H	0.567966	-2.599697	0.156653

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Phenyl-(1-phenyl-ethylidene)-amine

C	-4.18984	0.78541	-0.12387
C	-4.57848	-0.50923	0.20156
C	-3.60918	-1.49346	0.39588
C	-2.26303	-1.18351	0.26619
C	-1.86066	0.11640	-0.06608
C	-2.83895	1.09623	-0.25900
C	-0.40466	0.42892	-0.19295
C	-0.02890	1.80538	-0.69283
N	0.42101	-0.49868	0.10535
C	1.81275	-0.30532	0.08374
C	2.59509	-1.12568	-0.73633
C	3.97863	-0.99658	-0.73753
C	4.60317	-0.07243	0.09817
C	3.82893	0.72665	0.93484
C	2.44203	0.61644	0.92868
H	-4.93705	1.55797	-0.27351
H	-5.63119	-0.75253	0.30415
H	-3.90697	-2.50571	0.64996
H	-1.49598	-1.93468	0.41699

H	-2.55579	2.11299	-0.50985	C	-2.51096	2.47912	0.56762
H	-0.58509	2.03031	-1.60679	N	-0.39608	-0.19781	-0.08561
H	-0.28986	2.57028	0.04566	C	0.48108	-1.17928	0.02029
H	1.03799	1.87309	-0.89963	C	0.02760	-2.64758	0.07671
H	2.09865	-1.85459	-1.36828	C	1.98591	-0.98682	0.06452
H	4.57411	-1.62942	-1.38806	C	2.73521	-1.42056	-1.04580
H	5.68419	0.01732	0.10317	C	4.12765	-1.33717	-1.02823
H	4.30524	1.44189	1.59812	C	4.78616	-0.84928	0.10747
H	1.83320	1.22858	1.58760	C	4.04667	-0.45074	1.22372
29				C	2.64843	-0.51985	1.20832
Phenyl-(1-phenyl-ethylidene)-amide				C	-1.82035	-0.64811	-0.12058
C	3.51671	1.55329	0.03787	C	-2.49276	-0.92473	1.07653
C	4.50949	0.64327	-0.31876	C	-3.82590	-1.34471	1.02670
C	4.16370	-0.68774	-0.54554	C	-4.47339	-1.49000	-0.20474
C	2.83984	-1.09549	-0.40817	C	-3.78959	-1.21652	-1.39514
C	1.83624	-0.19076	-0.04794	C	-2.45758	-0.79488	-1.36057
C	2.19204	1.14152	0.16925	H	0.44224	3.03814	1.20384
C	0.39175	-0.64977	0.12781	H	1.65952	1.78365	1.14083
C	0.32804	-1.59203	1.35432	H	0.55087	1.73756	3.34435
N	-0.47665	0.47713	0.27787	H	0.09809	0.26075	2.48468
C	-1.77518	0.27055	0.06169	H	-1.04534	1.59901	2.59339
C	-2.67823	1.38101	0.22085	H	0.39153	1.26044	-2.44220
C	-4.03461	1.28120	0.00396	H	1.77510	0.92587	-1.41201
C	-4.63108	0.07126	-0.39082	H	2.10111	3.07218	-2.58536
C	-3.79057	-1.02788	-0.55214	H	1.97354	3.35393	-0.84013
C	-2.41978	-0.95400	-0.33475	H	0.60182	3.71639	-1.89757
H	3.77728	2.59495	0.21011	H	-1.23324	3.17440	-0.99002
H	5.54143	0.96727	-0.42535	H	-2.05142	1.69133	-1.38973
H	4.92637	-1.40711	-0.83356	H	-3.39743	3.00700	0.19403
H	2.57263	-2.13477	-0.59222	H	-2.85418	1.55911	1.05098
H	1.38484	1.81936	0.42650	H	-2.04910	3.11087	1.33354
H	0.16189	-1.26724	-0.76789	H	-0.36535	-2.87397	1.07735
H	-0.70246	-1.92596	1.50380	H	-0.76533	-2.84023	-0.65558
H	0.97573	-2.47206	1.25243	H	0.88436	-3.29928	-0.12172
H	0.63778	-1.02910	2.24005	H	2.21806	-1.80485	-1.92979
H	-2.22902	2.32459	0.52115	H	4.70218	-1.65781	-1.90168
H	-4.65619	2.16603	0.14213	H	5.87810	-0.78836	0.12281
H	-5.70110	-0.00414	-0.55814	H	4.55731	-0.08314	2.11823
H	-4.21600	-1.98538	-0.85480	H	2.07699	-0.21993	2.08877
H	-1.82679	-1.85296	-0.47511	H	-1.97487	-0.80069	2.03117
50				H	-4.36019	-1.55729	1.95704
Phenyl-(1-phenyl-ethylidene)-amine +				H	-5.51625	-1.81740	-0.23769
BEt ₃				H	-4.29569	-1.33053	-2.35798
B	-0.10661	1.44471	-0.23839	H	-1.90668	-0.57607	-2.27976
C	0.57578	1.95000	1.15238	51			
C	0.01327	1.35359	2.46824	Phenyl-(1-phenyl-ethylidene)-amide +			
C	0.89781	1.57184	-1.51805	BEt ₃			
C	1.42351	3.01361	-1.72424	B	-1.53072	-1.09185	0.03977
C	-1.51023	2.19541	-0.57993	C	-2.66374	-1.07641	1.24469
				C	-3.24020	0.27210	1.74825

C	-0.90319	-2.62483	0.04529	Phenyl-(1-phenyl-ethylidene)-amine +			
C	-1.89872	-3.70523	-0.45278	BPh ₃			
C	-2.07982	-0.81327	-1.49803	B	0.18741	0.52917	0.27555
C	-3.61808	-0.85142	-1.68111	C	1.54781	0.61127	1.17079
N	-0.35868	-0.05299	0.36888	C	0.18201	1.68952	-0.85945
C	0.78764	-0.50923	1.19621	C	-1.11724	0.51721	1.23363
C	0.92597	0.26554	2.54414	N	0.26393	-0.90271	-0.53047
C	2.12340	-0.60046	0.39944	C	-0.70587	-1.66056	-1.02290
C	3.38242	-0.62815	1.01738	C	-0.35360	-2.97501	-1.73948
C	4.54852	-0.76932	0.25686	C	-2.17416	-1.34816	-0.91112
C	4.47304	-0.88635	-1.13237	C	-3.04836	-2.42058	-0.64066
C	3.22210	-0.85982	-1.76020	C	-4.42057	-2.20058	-0.52595
C	2.06048	-0.71916	-0.99974	C	-4.93958	-0.91256	-0.70649
C	-0.36458	1.31169	0.04127	C	-4.08058	0.15230	-0.99673
C	-1.56201	1.97334	-0.37874	C	-2.70166	-0.05707	-1.09310
C	-1.57798	3.31813	-0.71998	C	1.65267	-1.41511	-0.73477
C	-0.41739	4.10015	-0.66226	C	2.15680	-2.38415	0.14340
C	0.76621	3.48433	-0.25286	C	3.46536	-2.84226	-0.02898
C	0.80257	2.13572	0.08785	C	4.25587	-2.33919	-1.06908
H	-2.21847	-1.56028	2.12636	C	3.74177	-1.37015	-1.93725
H	-3.51713	-1.70963	0.96836	C	2.43544	-0.89811	-1.77463
H	-3.84096	0.13833	2.65909	C	-0.01984	1.47920	-2.23612
H	-3.88846	0.74299	1.00156	C	-0.01614	2.53038	-3.16128
H	-2.43621	0.97922	1.98034	C	0.19125	3.84088	-2.73092
H	-0.00483	-2.69268	-0.58463	C	0.40356	4.08448	-1.36920
H	-0.59604	-2.95040	1.04943	C	0.40299	3.02586	-0.45903
H	-1.45530	-4.71045	-0.43321	C	-1.48974	-0.63379	1.95954
H	-2.79455	-3.72669	0.17741	C	-2.57539	-0.64072	2.83794
H	-2.22186	-3.50612	-1.47958	C	-3.32821	0.52171	3.02898
H	-1.72697	0.14337	-1.89860	C	-2.98023	1.67961	2.32999
H	-1.66253	-1.56996	-2.17590	C	-1.89357	1.67026	1.44927
H	-3.91491	-0.69546	-2.72776	C	1.61327	0.11745	2.48704
H	-4.02556	-1.81679	-1.36096	C	2.78620	0.17610	3.24719
H	-4.10646	-0.07674	-1.07964	C	3.94371	0.74127	2.70810
H	0.54997	-1.54453	1.47852	C	3.91004	1.24993	1.40641
H	1.28871	1.28598	2.39858	C	2.73108	1.18372	0.66003
H	-0.06224	0.31027	3.01399	H	-0.11705	-3.75354	-1.00150
H	1.60778	-0.26011	3.22098	H	-1.20288	-3.30311	-2.34587
H	3.45885	-0.53648	2.10285	H	0.52403	-2.83290	-2.38044
H	5.52209	-0.78726	0.75400	H	-2.64615	-3.42644	-0.49445
H	5.38455	-0.99500	-1.72520	H	-5.08817	-3.03569	-0.29730
H	3.15535	-0.94720	-2.84805	H	-6.01686	-0.74033	-0.62256
H	1.06795	-0.68296	-1.46152	H	-4.48261	1.15884	-1.14214
H	-2.48397	1.40011	-0.41170	H	-2.03238	0.77688	-1.31988
H	-2.52339	3.77367	-1.02805	H	1.53023	-2.75529	0.95934
H	-0.43888	5.15778	-0.92709	H	3.87048	-3.59245	0.65608
H	1.69174	4.06524	-0.20300	H	5.28001	-2.70006	-1.19889
H	1.75630	1.69790	0.37259	H	4.36243	-0.97140	-2.74478
				H	2.02431	-0.12564	-2.43002
				H	-0.18804	0.46631	-2.61125
				H	-0.17654	2.32244	-4.22284

H	0.19397	4.66570	-3.44788
H	0.57650	5.10586	-1.01862
H	0.59594	3.23491	0.59720
H	-0.92495	-1.56035	1.82218
H	-2.83713	-1.55519	3.37738
H	-4.17837	0.52309	3.71571
H	-3.56188	2.59534	2.46818
H	-1.65055	2.58490	0.90232
H	0.71820	-0.31726	2.93892
H	2.79543	-0.21728	4.26743
H	4.86233	0.79177	3.29836
H	4.80678	1.70150	0.97338
H	2.72788	1.59363	-0.35369

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Phenyl-(1-phenyl-ethylidene)-amide +
BPh₃

B	-0.80005	-0.37976	0.02951
C	-1.71547	0.51128	1.05806
C	-1.96356	-0.96697	-0.97346
C	0.00455	-1.55282	0.84848
N	0.20653	0.50611	-0.78419
C	1.18452	-0.10046	-1.74634
C	0.73217	-1.44550	-2.37175
C	2.59197	-0.25992	-1.09073
C	2.99816	-1.44433	-0.45447
C	4.26097	-1.54243	0.13757
C	5.14330	-0.45912	0.10375
C	4.75335	0.72524	-0.52720
C	3.49107	0.82017	-1.11908
C	0.47026	1.88082	-0.53047
C	0.76179	2.79872	-1.58029
C	1.00684	4.14622	-1.33307
C	0.96855	4.65628	-0.03267
C	0.68140	3.78021	1.01851
C	0.44744	2.42820	0.78282
C	-1.93325	0.16237	2.40396
C	-2.79785	0.88573	3.23524
C	-3.48597	1.99310	2.74033
C	-2.87297	-1.96991	-0.57588
C	-3.92994	-2.38814	-1.39036
C	-4.13191	-1.79678	-2.63988
C	0.91642	-1.18730	1.86498
C	1.66185	-2.12287	2.58611
C	1.52932	-3.48695	2.31019
C	0.64275	-3.88881	1.31018
C	-0.10113	-2.93694	0.60234
C	-3.27507	-0.77133	-3.04916
C	-2.22197	-0.36751	-2.22411
C	-3.30639	2.35948	1.40141

C	-2.44613	1.62616	0.58420
H	1.33303	0.59934	-2.58510
H	0.47159	-2.16903	-1.59765
H	-0.13989	-1.29571	-3.01225
H	1.55422	-1.84818	-2.97443
H	2.31751	-2.29769	-0.41117
H	4.55357	-2.47203	0.63313
H	6.12994	-0.53729	0.56712
H	5.43588	1.57855	-0.56036
H	3.19019	1.74902	-1.61067
H	0.77655	2.44516	-2.61171
H	1.21917	4.81293	-2.17353
H	1.15986	5.71363	0.15781
H	0.65518	4.15338	2.04609
H	0.23986	1.76483	1.62173
H	-1.40754	-0.70140	2.81889
H	-2.93420	0.58091	4.27659
H	-4.15979	2.56245	3.38490
H	-2.76091	-2.42554	0.41173
H	-4.60696	-3.17501	-1.04625
H	-4.95568	-2.12058	-3.28024
H	1.05383	-0.12661	2.09046
H	2.35754	-1.78904	3.36084
H	2.11199	-4.22544	2.86592
H	0.52916	-4.95158	1.07882
H	-0.78438	-3.28916	-0.17447
H	-3.43395	-0.28347	-4.01499
H	-1.56541	0.44540	-2.54863
H	-3.84593	3.21981	0.99607
H	-2.33033	1.92304	-0.46216

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Phenyl-(1-phenyl-ethylidene)-amine +
B(C₆F₅)Ph₂

B	-0.01237	-0.25337	0.54940
C	1.05764	-1.16229	1.39003
C	0.71883	1.14827	0.06924
C	-1.37566	-0.00857	1.38966
C	0.78660	1.70755	-1.20357
C	1.47449	2.87662	-1.51517
C	2.13585	3.56394	-0.51272
C	2.09197	3.06616	0.78222
C	1.39967	1.89101	1.04059
C	-2.34083	-1.01864	1.52601
C	-3.52369	-0.82720	2.23204
C	-3.77103	0.39384	2.85567
C	-2.81911	1.40358	2.76715
C	-1.64577	1.20018	2.04342
C	0.64081	-2.07702	2.36500
C	1.53705	-2.93313	3.00603
C	2.89176	-2.88564	2.69864

C	3.34192	-1.95974	1.75915	C	1.68476	0.40831	1.40398
C	2.43697	-1.11494	1.12769	C	1.51404	1.83026	-0.68547
F	0.16316	1.13447	-2.26228	C	-0.82069	0.78711	0.41620
F	1.49360	3.33565	-2.76728	N	0.82357	-0.74254	-0.90088
F	2.79431	4.68752	-0.78294	C	-0.09641	-0.88003	-2.04222
F	2.71261	3.72019	1.76213	C	-0.19715	0.34544	-2.95144
F	1.39376	1.48753	2.31522	C	-1.47259	-1.40645	-1.59907
H	-2.17842	-1.97863	1.03542	C	-2.68218	-0.80334	-1.94645
H	-4.25469	-1.62847	2.29211	C	-3.89876	-1.32287	-1.50056
H	-4.69274	0.55172	3.40714	C	-3.92588	-2.46060	-0.70314
H	-2.99153	2.35805	3.25602	C	-2.72404	-3.08065	-0.36027
H	-0.93571	2.01895	1.97843	C	-1.51568	-2.56148	-0.80667
H	-0.40862	-2.12634	2.63936	C	1.75076	-1.78370	-0.76574
H	1.17325	-3.63191	3.75399	C	2.54255	-2.21067	-1.85135
H	3.59252	-3.55065	3.19435	C	3.45102	-3.25618	-1.72691
H	4.39912	-1.89746	1.51791	C	3.61845	-3.90697	-0.50768
H	2.81467	-0.41352	0.38645	C	2.84760	-3.49708	0.57913
N	-0.33514	-1.12942	-0.86193	C	1.92318	-2.46746	0.45470
C	-1.37644	-1.16540	-1.63506	C	1.19193	0.66435	2.68971
C	-1.36949	-2.02673	-2.87688	C	2.01019	0.65897	3.82155
C	-2.62244	-0.40018	-1.39407	C	3.36826	0.39332	3.70232
C	-3.83142	-1.10185	-1.50049	C	1.38444	3.13066	-0.17227
C	-5.03542	-0.48075	-1.19892	C	2.12337	4.20217	-0.66085
C	-5.04683	0.85962	-0.82193	C	3.05196	4.00475	-1.68282
C	-3.85388	1.57313	-0.75502	C	-1.46222	-0.17653	1.19941
C	-2.64474	0.94950	-1.03750	C	-2.81393	-0.17286	1.50737
C	0.78065	-1.96607	-1.26679	C	-3.61398	0.85213	1.02598
C	0.87655	-3.25500	-0.74723	C	-3.03940	1.83591	0.24407
C	1.97965	-4.03762	-1.06187	C	-1.67702	1.78160	-0.04525
C	2.97744	-3.53844	-1.89799	C	3.23251	2.72194	-2.18841
C	2.86086	-2.25833	-2.42752	C	2.47688	1.66042	-1.68884
C	1.75894	-1.46315	-2.11605	C	3.89715	0.15474	2.43379
H	-1.09752	-3.06033	-2.65243	C	3.07078	0.17795	1.31733
H	-2.33263	-1.98811	-3.37970	F	-0.77237	-1.22442	1.67869
H	-0.60736	-1.63895	-3.55926	F	-3.36102	-1.15277	2.23609
H	-3.82605	-2.15342	-1.77221	F	-4.92572	0.86916	1.28850
H	-5.96159	-1.04259	-1.25447	F	-3.80463	2.81863	-0.25263
H	-5.98534	1.34871	-0.58243	F	-1.25426	2.75269	-0.87689
H	-3.85834	2.61713	-0.46143	H	0.30385	-1.68595	-2.66906
H	-1.72007	1.50537	-0.96105	H	-0.56952	1.22972	-2.42912
H	0.11394	-3.61151	-0.06221	H	0.78693	0.59581	-3.34922
H	2.06798	-5.03211	-0.63798	H	-0.86330	0.12864	-3.79322
H	3.84370	-4.14750	-2.13335	H	-2.68398	0.10310	-2.54384
H	3.63185	-1.86654	-3.08271	H	-4.82491	-0.81762	-1.76117
H	1.65913	-0.46350	-2.52170	H	-4.87026	-2.85430	-0.33969
				H	-2.72960	-3.96422	0.27122
				H	-0.58112	-3.03032	-0.51191
				H	2.44828	-1.69205	-2.80266
				H	4.04576	-3.55017	-2.58808
				H	4.33408	-4.71705	-0.40598
				H	2.95528	-3.99541	1.53886
63							
Phenyl-(1-phenyl-ethylidene)-amide +							
B(C ₆ F ₅)Ph ₂							
B	0.78406	0.53411	0.02490				

H	1.31451	-2.16805	1.29946
H	0.13632	0.88576	2.82537
H	1.57839	0.86251	4.79865
H	4.00946	0.38214	4.57978
H	0.68461	3.30410	0.64398
H	1.98249	5.19498	-0.24012
H	3.63357	4.83803	-2.06819
H	3.96663	2.54395	-2.97096
H	2.64577	0.65838	-2.07990
H	4.95949	-0.04274	2.31482
H	3.51454	0.00934	0.33798

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Phenyl-(1-phenyl-ethylidene)-amine +
B(C₆F₅)₂Ph

B	-0.195465	-0.205597	0.299011
C	1.407586	-0.468631	0.640484
C	-0.469977	1.421020	0.184041
C	-1.207776	-0.902701	1.371099
N	-0.410778	-0.847413	-1.228820
C	-1.472363	-1.273160	-1.845324
C	-1.370054	-1.726325	-3.283367
C	-2.823902	-1.357067	-1.244208
C	-3.530183	-2.551032	-1.450477
C	-4.765207	-2.753026	-0.850072
C	-5.326704	-1.747690	-0.067513
C	-4.650328	-0.543826	0.107528
C	-3.403959	-0.346643	-0.473341
C	0.823519	-0.873263	-1.995184
C	1.615255	-2.019435	-1.948215
C	2.840353	-2.028766	-2.602708
C	3.266433	-0.900751	-3.304411
C	2.459330	0.230199	-3.357395
C	1.228579	0.251238	-2.702791
C	-1.061798	2.126135	-0.858729
C	-1.242475	3.506698	-0.871334
C	-0.817158	4.259976	0.207792
C	-0.213409	3.613490	1.277971
C	-0.050423	2.238018	1.237285
C	-1.577268	-2.254313	1.278896
C	-2.508593	-2.833868	2.130308
C	-3.099321	-2.074158	3.138554
C	-2.735707	-0.741110	3.276754
C	-1.810797	-0.170991	2.401944
C	1.882066	-1.659795	1.189101
C	3.222085	-1.926009	1.448423
C	4.180941	-0.975345	1.144739
C	3.774094	0.219024	0.572536
C	2.424191	0.442489	0.335733
F	-1.515128	1.500277	-1.972166
F	-1.823545	4.099239	-1.914639

F	-0.984656	5.578698	0.222094
F	0.210778	4.319020	2.324007
F	0.571707	1.691017	2.291763
F	1.057946	-2.690628	1.425610
F	3.588370	-3.100662	1.962636
F	5.469146	-1.211638	1.376053
F	4.679323	1.140451	0.243855
F	2.156478	1.610363	-0.271606
H	-0.645769	-2.535664	-3.402023
H	-2.342054	-2.032913	-3.660948
H	-1.009178	-0.887316	-3.884889
H	-3.089612	-3.346594	-2.044199
H	-5.286536	-3.693493	-0.991964
H	-6.291871	-1.901226	0.403896
H	-5.082960	0.242225	0.716536
H	-2.879363	0.583601	-0.308105
H	1.282725	-2.871925	-1.361548
H	3.468640	-2.911718	-2.553026
H	4.228573	-0.905263	-3.805066
H	2.788222	1.109757	-3.900218
H	0.595438	1.130171	-2.728148
H	-1.139409	-2.874291	0.500048
H	-2.777211	-3.878697	2.004956
H	-3.828820	-2.520089	3.807607
H	-3.176375	-0.133454	4.061564
H	-1.577616	0.879228	2.535029

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Phenyl-(1-phenyl-ethylidene)-amide +
B(C₆F₅)₂Ph

B	0.312637	-0.343602	0.575528
C	1.567316	-0.489763	-0.524138
C	0.849364	-1.374232	1.743193
C	-1.138699	-0.830688	-0.089698
N	0.109393	1.133568	1.071096
C	-1.077979	1.512333	1.860560
C	-1.382529	0.597852	3.046780
C	-2.308812	1.775163	0.975216
C	-3.559859	1.200203	1.201840
C	-4.640492	1.473762	0.361231
C	-4.489327	2.334197	-0.719019
C	-3.247634	2.927687	-0.947603
C	-2.175283	2.654888	-0.108148
C	0.984051	2.200196	0.803703
C	1.477303	3.012598	1.843780
C	2.339582	4.071706	1.594527
C	2.758740	4.354357	0.295823
C	2.279064	3.565896	-0.746107
C	1.394505	2.519314	-0.503697
C	1.522432	-1.149268	-1.751183
C	2.626241	-1.333835	-2.581054

C	3.868399	-0.873862	-2.186650	C	0.912422	-0.372127	2.456206
C	0.863728	-2.760457	1.523448	C	0.829398	-0.853016	3.880343
C	1.425720	-3.651432	2.430932	C	2.255326	0.131020	2.052667
C	2.016622	-3.174578	3.600528	C	3.318732	-0.782514	2.052658
C	-1.584436	-0.195475	-1.250272	C	4.585157	-0.373128	1.660484
C	-2.830188	-0.376433	-1.823663	C	4.811632	0.958999	1.311006
C	-3.722970	-1.258481	-1.231650	C	3.770759	1.877580	1.373135
C	-3.340475	-1.924916	-0.084816	C	2.490576	1.469378	1.741357
C	-2.077064	-1.696180	0.460655	C	-1.355404	-0.878827	2.243214
C	2.046945	-1.803232	3.831663	C	-1.787642	-2.177452	1.984605
C	1.478932	-0.924995	2.908914	C	-2.973290	-2.625245	2.559125
C	3.983544	-0.244280	-0.957358	C	-3.718749	-1.785053	3.382074
C	2.858249	-0.088790	-0.160735	C	-3.272924	-0.491310	3.635945
F	0.387221	-1.688831	-2.229543	C	-2.087176	-0.032781	3.070741
F	2.495648	-1.967859	-3.754147	C	-0.466843	2.581298	0.706453
F	4.940001	-1.042852	-2.969526	C	-0.693586	3.912279	0.375750
F	-0.782689	0.680171	-1.879959	C	-0.719207	4.284017	-0.957988
F	-3.194714	0.299242	-2.919312	C	-0.506878	3.318166	-1.933636
F	-4.945229	-1.430907	-1.746083	C	-0.281820	2.006021	-1.549153
F	-4.200004	-2.759228	0.517457	C	1.569839	-2.024042	-0.363802
F	-1.855786	-2.349178	1.617207	C	2.739058	-2.661921	-0.740522
F	5.181418	0.188472	-0.546518	C	3.750980	-1.915944	-1.328555
F	3.081225	0.495147	1.023312	C	3.559327	-0.558932	-1.519907
H	-0.854260	2.493885	2.294210	C	2.360907	0.034676	-1.132406
H	-1.600294	-0.429659	2.748386	C	-1.483662	-1.688779	-1.619757
H	-0.524265	0.566019	3.718677	C	-2.666566	-2.173447	-2.172068
H	-2.239421	0.988981	3.604935	C	-3.881563	-1.631794	-1.790161
H	-3.695146	0.500828	2.020997	C	-3.893890	-0.600067	-0.863534
H	-5.595901	0.988780	0.542411	C	-2.692431	-0.143883	-0.343914
H	-5.323908	2.532394	-1.384550	F	-0.458745	2.311987	2.033606
H	-3.112306	3.596017	-1.792818	F	-0.893537	4.821552	1.330142
H	-1.205947	3.102577	-0.306392	F	-0.935901	5.550041	-1.300931
H	1.196306	2.775930	2.867133	F	-0.526310	3.660336	-3.219707
H	2.707215	4.666801	2.426431	F	-0.081528	1.113679	-2.527853
H	3.443402	5.173842	0.101075	F	0.648430	-2.797170	0.243032
H	2.579559	3.777353	-1.768928	F	2.909559	-3.965830	-0.520564
H	0.996654	1.936517	-1.325453	F	4.899390	-2.491921	-1.672440
H	0.416357	-3.150314	0.608931	F	4.538704	0.183525	-2.034001
H	1.407016	-4.719142	2.227082	F	2.308394	1.359871	-1.312146
H	2.457630	-3.864364	4.315123	F	-0.374825	-2.266237	-2.095935
H	2.523158	-1.413638	4.728170	F	-2.631951	-3.149367	-3.077951
H	1.541460	0.147101	3.081284	F	-5.017463	-2.086368	-2.308820
				F	-5.048834	-0.049565	-0.492877
				F	-2.795126	0.870174	0.530486
62				H	0.124918	-1.674873	4.005481
Phenyl-(1-phenyl-ethylidene)-amine +				H	1.823079	-1.137950	4.225215
B(C ₆ F ₅) ₃				H	0.491086	-0.020141	4.506985
B	-0.085442	-0.031475	0.026179	H	3.139229	-1.822720	2.312430
C	-1.438606	-0.680623	-0.656754	H	5.395221	-1.094013	1.620313
C	-0.232793	1.580002	-0.222014	H	5.800535	1.276813	0.998619
C	1.312453	-0.667454	-0.543348	H	3.945084	2.917835	1.121065
N	-0.107963	-0.404645	1.657640				

H	1.686207	2.188279	1.801448
H	-1.206411	-2.818425	1.334667
H	-3.314419	-3.634705	2.356107
H	-4.646130	-2.136753	3.821222
H	-3.852024	0.171459	4.269848
H	-1.746937	0.982136	3.236376

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Phenyl-(1-phenyl-ethylidene)-amide +
B(C₆F₅)₃

B	-0.156374	0.085028	-0.157565
C	-1.121409	-0.741139	0.923993
C	-1.173296	1.378211	-0.478162
C	1.268645	0.579275	0.536034
N	0.236363	-0.756097	-1.402578
C	1.234147	-0.261864	-2.370492
C	1.048626	1.188197	-2.820159
C	2.671696	-0.568293	-1.919787
C	2.981781	-1.879525	-1.533668
C	4.259286	-2.218179	-1.107731
C	5.266095	-1.253006	-1.066135
C	4.976900	0.046503	-1.462919
C	3.690917	0.383829	-1.889323
C	-0.374742	-1.970948	-1.762188
C	-0.409428	-3.060183	-0.873665
C	-1.026028	-4.256927	-1.225947
C	-1.596119	-4.420762	-2.485089
C	-1.543645	-3.360539	-3.387886
C	-0.952271	-2.155422	-3.032067
C	-0.899039	-0.900237	2.290574
C	-1.787343	-1.544320	3.149412
C	-2.983828	-2.037436	2.662593
C	-1.974802	1.531474	-1.603551
C	-2.894328	2.565894	-1.761090
C	-3.074145	3.485572	-0.743362
C	1.826867	1.850367	0.534508
C	3.109612	2.137502	0.995598
C	3.900899	1.119054	1.491453
C	-2.331346	3.353989	0.421205
C	-1.426339	2.309571	0.528527
C	-3.278937	-1.866892	1.319057
C	-2.367425	-1.215117	0.501452
C	3.393842	-0.171741	1.523615
C	2.111850	-0.402615	1.056143
F	0.200887	-0.428580	2.894551
F	-1.497813	-1.676034	4.449578
F	-3.846688	-2.655632	3.474990
F	-1.918291	0.671966	-2.635614
F	-3.620979	2.668544	-2.881326
F	-3.956802	4.481820	-0.874993
F	1.170573	2.909921	0.020534

F	3.590668	3.386661	0.937949
F	5.146829	1.366611	1.907378
F	-2.510931	4.222499	1.423959
F	-0.774402	2.212538	1.699922
F	-4.442987	-2.311960	0.834076
F	-2.754730	-1.049168	-0.770307
F	4.153832	-1.171729	1.982522
F	1.694889	-1.678400	1.111188
H	1.103385	-0.869115	-3.273312
H	1.142649	1.903225	-1.999789
H	0.062476	1.306938	-3.266080
H	1.797072	1.437940	-3.578708
H	2.194579	-2.627958	-1.538382
H	4.469358	-3.235943	-0.792636
H	6.260615	-1.511964	-0.716175
H	5.745433	0.813408	-1.420014
H	3.482273	1.412340	-2.166549
H	0.067718	-2.950371	0.093233
H	-1.040499	-5.076117	-0.512050
H	-2.069900	-5.357904	-2.760182
H	-1.990411	-3.463671	-4.373178
H	-0.964072	-1.320550	-3.725641

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Phenyl-(1-phenyl-ethylidene)-amine +
proton

C	-3.954096	-1.322410	0.910898
C	-3.870479	-2.504288	0.176948
C	-2.675683	-2.863416	-0.446473
C	-1.569154	-2.033469	-0.349778
C	-1.646686	-0.835693	0.384028
C	-2.846199	-0.494644	1.028368
C	-0.477659	0.041348	0.469460
C	-0.195240	0.841008	1.694637
N	0.327506	0.090618	-0.558325
C	1.594229	0.762694	-0.668756
C	2.594547	0.526444	0.271057
C	3.817973	1.170302	0.120535
C	4.031818	2.023203	-0.960181
C	3.025515	2.234388	-1.900949
C	1.796243	1.599863	-1.762762
H	-4.884532	-1.045265	1.393079
H	-4.736011	-3.153310	0.098500
H	-2.603981	-3.796326	-0.993910
H	-0.627712	-2.350832	-0.790362
H	-2.934613	0.429882	1.587329
H	-1.125224	1.251673	2.088657
H	0.206260	0.177721	2.468352
H	0.515118	1.644661	1.506772
H	0.016131	-0.397556	-1.396158
H	2.428026	-0.166547	1.089642

H	4.607564	0.994026	0.842106
H	4.989337	2.518958	-1.074391
H	3.195410	2.894432	-2.743900
H	1.001593	1.762538	-2.484421

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N-Phenyl- α -methylbenzylamine

C	-3.513088	-1.208466	-1.128650
C	-3.575083	-2.600054	-1.187074
C	-2.411622	-3.343824	-1.031915
C	-1.190670	-2.704160	-0.818894
C	-1.118327	-1.312768	-0.759136
C	-2.296303	-0.572866	-0.915732
C	0.193041	-0.565793	-0.548218
C	1.385740	-1.471355	-0.234370
N	-0.022649	0.450231	0.476219
C	0.914921	1.441208	0.748741
C	0.854921	2.118785	1.978210
C	1.732884	3.152965	2.263925
C	2.699347	3.543412	1.337892
C	2.766646	2.874441	0.121114
C	1.892832	1.833005	-0.178011
H	-4.415908	-0.618053	-1.249351
H	-4.524850	-3.098520	-1.351905
H	-2.448562	-4.427801	-1.073598
H	-0.295112	-3.304167	-0.698807
H	-2.243414	0.510290	-0.859416
H	0.401747	-0.029830	-1.483806
H	2.270581	-0.861828	-0.038108
H	1.610762	-2.143133	-1.067133
H	1.183182	-2.074667	0.656121
H	-0.490252	0.089838	1.298591
H	0.102072	1.825789	2.705530
H	1.661690	3.658276	3.222256
H	3.386838	4.350704	1.563838
H	3.513672	3.159091	-0.613632
H	1.974964	1.329248	-1.134679

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Phenyl-(1-phenyl-ethylidene)-amine + [SiEt₃]⁺

Si	0.02609	1.40989	-0.13613
C	0.37211	2.05279	1.58821
C	-0.36756	1.31712	2.72940
C	1.47653	1.56159	-1.31267
C	1.54439	2.96509	-1.96333
C	-1.51290	2.20199	-0.84390
C	-2.68222	2.39354	0.14950
N	-0.35927	-0.41933	-0.04197
C	0.51732	-1.41971	-0.06536

C	0.03398	-2.86578	-0.20061
C	1.99481	-1.18765	0.05258
C	2.85630	-1.75503	-0.90621
C	4.23360	-1.55119	-0.80493
C	4.75842	-0.81863	0.26962
C	3.90428	-0.28714	1.24470
C	2.52265	-0.46218	1.13506
C	-1.80372	-0.80556	-0.09543
C	-2.47544	-1.10905	1.09555
C	-3.82981	-1.45468	1.03767
C	-4.49345	-1.50133	-0.19470
C	-3.80375	-1.21171	-1.37919
C	-2.45025	-0.86373	-1.33766
H	0.06234	3.10483	1.59420
H	1.45001	2.04767	1.78003
H	-0.12966	1.78201	3.69301
H	-0.07524	0.26200	2.78588
H	-1.45331	1.36411	2.59090
H	1.40027	0.80419	-2.10101
H	2.41204	1.37442	-0.77691
H	2.44414	3.04615	-2.58371
H	1.58651	3.75444	-1.20345
H	0.67520	3.14902	-2.60432
H	-1.20637	3.19079	-1.20496
H	-1.86011	1.64926	-1.72213
H	-3.51149	2.90957	-0.34752
H	-3.05654	1.43484	0.52298
H	-2.37366	3.00305	1.00613
H	-0.41184	-3.18278	0.75426
H	-0.73362	-2.94716	-0.98097
H	0.88410	-3.51707	-0.42791
H	2.44534	-2.32919	-1.74261
H	4.90278	-1.97265	-1.56166
H	5.84075	-0.67236	0.35334
H	4.31658	0.26249	2.09662
H	1.85774	-0.07448	1.90941
H	-1.94765	-1.07190	2.05238
H	-4.36733	-1.68912	1.96197
H	-5.55380	-1.77096	-0.23342
H	-4.32049	-1.25882	-2.34301
H	-1.89887	-0.64807	-2.25756

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Phenyl-(1-phenyl-ethylidene)-amide + [SiEt₃]⁺

Si	-1.43378	-1.07070	0.04745
C	-2.77091	-1.22017	1.36306
C	-3.33968	0.09870	1.93192
C	-0.58716	-2.74661	-0.01354
C	-1.51653	-3.83813	-0.59556

C	-2.09302	-0.68939	-1.67170
C	-3.62897	-0.80291	-1.79910
N	-0.22185	0.13393	0.49857
C	0.95865	-0.30591	1.28893
C	1.18430	0.58279	2.54940
C	2.24582	-0.48698	0.43167
C	3.50036	-0.67266	1.03151
C	4.63876	-0.88499	0.24814
C	4.53864	-0.91710	-1.14590
C	3.29192	-0.73640	-1.75298
C	2.15603	-0.52599	-0.96754
C	-0.29170	1.49907	0.08912
C	-1.54173	2.08852	-0.21892
C	-1.63319	3.41531	-0.63313
C	-0.48789	4.20838	-0.74415
C	0.75409	3.64443	-0.43997
C	0.85884	2.31437	-0.03616
H	-2.34501	-1.79573	2.19304
H	-3.59545	-1.82172	0.96522
H	-3.98673	-0.10116	2.79439
H	-3.93947	0.63042	1.18506
H	-2.53462	0.76723	2.25865
H	0.32331	-2.68820	-0.61957
H	-0.28155	-3.05847	0.99064
H	-1.00806	-4.80879	-0.62462
H	-2.41979	-3.95029	0.01543
H	-1.82813	-3.59180	-1.61690
H	-1.78100	0.31345	-1.97814
H	-1.62986	-1.38772	-2.37729
H	-3.95185	-0.58008	-2.82286
H	-3.97205	-1.81405	-1.55074
H	-4.13456	-0.10109	-1.12613
H	0.70700	-1.31045	1.67187
H	1.57061	1.57012	2.28480
H	0.22942	0.70844	3.07129
H	1.89068	0.09710	3.22970
H	3.59398	-0.65432	2.11968
H	5.61005	-1.02685	0.73014
H	5.42973	-1.08157	-1.75742
H	3.20473	-0.75760	-2.84286
H	1.17891	-0.37139	-1.43296
H	-2.45054	1.49564	-0.12029
H	-2.61596	3.83718	-0.86155
H	-0.56236	5.25004	-1.06282
H	1.66287	4.24668	-0.52747
H	1.84192	1.89137	0.16682

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Phenyl-(1-phenyl-ethylidene)-amine +
[SiPhH₂]⁺

C	-3.552190	3.742471	1.415731
C	-3.680638	2.367764	1.605995
C	-2.556043	1.554810	1.557549
C	-1.292212	2.121014	1.339063
C	-1.163414	3.507181	1.184687
C	-2.297005	4.309642	1.200775
C	-0.103359	1.253826	1.324227
C	1.054260	1.611391	2.200846
N	-0.098890	0.157889	0.614024
C	0.977187	-0.805993	0.787431
C	2.093969	-0.767655	-0.042721
C	3.081550	-1.733178	0.119942
C	2.942369	-2.724013	1.090755
C	1.814982	-2.754014	1.906731
C	0.820397	-1.789600	1.758335
Si	-1.327207	-0.348074	-0.710272
C	-0.348201	-1.143716	-2.051363
C	0.070516	-0.380549	-3.151641
C	0.849927	-0.953111	-4.152484
C	1.211411	-2.295118	-4.065283
C	0.793701	-3.068733	-2.983078
C	0.017478	-2.497197	-1.982503
H	-4.432173	4.375998	1.445872
H	-4.654406	1.930751	1.796991
H	-2.649972	0.486542	1.734813
H	-0.187745	3.952974	1.016523
H	-2.200289	5.379578	1.054398
H	1.051771	2.679888	2.412627
H	0.923571	1.091838	3.158357
H	2.008336	1.295297	1.779241
H	2.172549	-0.009877	-0.816292
H	3.955817	-1.716585	-0.521178
H	3.714148	-3.476617	1.208647
H	1.705895	-3.525235	2.661132
H	-0.066876	-1.799147	2.385075
H	-1.964578	0.906769	-1.135651
H	-2.222926	-1.278882	-0.000205
H	-0.217227	0.665192	-3.234839
H	1.166096	-0.357344	-5.002121
H	1.814453	-2.743161	-4.848324
H	1.070027	-4.116123	-2.924467
H	-0.295062	-3.106886	-1.137346

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Phenyl-(1-phenyl-ethylidene)-amide +
[SiPhH₂]⁺

C	-3.723047	3.492985	1.442345
C	-3.523619	2.206072	1.936960
C	-2.269598	1.610799	1.848750
C	-1.201129	2.289682	1.255948
C	-1.410672	3.578173	0.764543

C	-2.662587	4.179123	0.857840	C	-3.00607	0.38200	1.27757
C	0.173662	1.648839	1.195553	C	-2.99763	-1.74024	-0.01114
C	0.736232	1.551572	2.618715	C	-3.00522	0.39849	-1.27216
N	0.097139	0.320372	0.554591	H	4.39919	1.50859	-0.00971
C	1.256092	-0.497254	0.613165	H	5.01004	-0.89658	-0.00281
C	2.541636	0.036355	0.451501	H	3.21796	-2.61727	0.00641
C	3.658325	-0.792167	0.459048	H	0.82940	-1.91801	0.00839
C	3.515252	-2.168960	0.609701	H	2.04620	2.18904	-0.00706
C	2.241263	-2.706548	0.770824	H	-0.00866	2.50326	0.88690
C	1.124450	-1.878709	0.789122	H	-0.02149	2.50714	-0.87635
Si	-1.071066	0.033183	-0.737020	H	-1.52828	2.27660	0.01577
C	-0.414592	-1.254172	-1.926827	H	-4.09640	0.29962	1.32105
C	0.835939	-1.128029	-2.549855	H	-2.74790	1.44025	1.34209
C	1.292674	-2.091761	-3.440899	H	-2.59038	-0.12316	2.15403
C	0.501651	-3.203155	-3.731065	H	-4.09161	-1.77194	-0.01159
C	-0.742613	-3.345137	-3.126905	H	-2.62857	-2.26065	-0.89893
C	-1.192948	-2.376973	-2.231219	H	-2.62894	-2.27222	0.86990
H	-4.701712	3.957332	1.509722	H	-2.58769	-0.09432	-2.15476
H	-4.346721	1.664662	2.392563	H	-4.09538	0.31512	-1.31826
H	-2.112734	0.604165	2.227995	H	-2.74859	1.45788	-1.32213
H	-0.586343	4.109600	0.295701				
H	-2.810908	5.180531	0.466259	31			
H	0.818740	2.323854	0.609373	Tert-butyl-(1-phenyl-ethylidene)-amide			
H	0.110549	0.882068	3.215750	C	2.62641	-1.18715	-0.76778
H	1.757323	1.167276	2.631608	C	3.30641	-0.76055	0.37886
H	0.726456	2.541738	3.081290	C	2.80100	0.31078	1.10360
H	2.662904	1.106428	0.308773	C	1.63283	0.95846	0.68718
H	4.645598	-0.357994	0.333463	C	0.93325	0.53455	-0.44419
H	4.387184	-2.814388	0.605740	C	1.45677	-0.55491	-1.15808
H	2.113924	-3.777390	0.894959	C	-0.40684	1.11115	-0.94441
H	0.131201	-2.296488	0.929182	C	-0.69080	2.50020	-0.29929
H	-1.311703	1.319266	-1.436216	N	-1.48342	0.17727	-1.02892
H	-2.371705	-0.483563	-0.241334	C	-1.90903	-0.53283	0.14895
H	1.472065	-0.276404	-2.317975	C	-1.03194	-1.76132	0.54276
H	2.266561	-1.981072	-3.907564	C	-2.09333	0.29692	1.44802
H	0.858876	-3.957584	-4.425372	C	-3.29582	-1.09363	-0.22234
H	-1.361268	-4.209465	-3.347974	H	3.01060	-2.02680	-1.34281
H	-2.164289	-2.502443	-1.757911	H	4.21582	-1.26240	0.69916
				H	3.31713	0.65153	1.99876
30				H	1.26041	1.80318	1.26124
Tert-butyl-(1-phenyl-ethylidene)-amine				H	0.86989	-0.91174	-2.00169
C	3.62427	0.74873	-0.00550	H	-0.17931	1.37720	-1.99663
C	3.96651	-0.59815	-0.00175	H	-1.63949	2.85483	-0.71196
C	2.95922	-1.56305	0.00339	H	0.09698	3.23219	-0.53447
C	1.62512	-1.18213	0.00469	H	-0.79974	2.46749	0.78876
C	1.26679	0.17214	0.00118	H	-1.51973	-2.39324	1.30131
C	2.28433	1.13101	-0.00390	H	-0.84984	-2.36532	-0.35314
C	-0.18922	0.55282	0.00244	H	-0.06026	-1.45333	0.94184
C	-0.46960	2.04277	0.00762	H	-2.58084	-0.28952	2.24126
N	-1.02234	-0.40819	-0.00120	H	-2.70661	1.18146	1.24105
C	-2.48727	-0.29205	-0.00153	H	-1.12354	0.63023	1.83661

H	-3.19818	-1.68796	-1.13649
H	-3.73126	-1.71828	0.57140
H	-3.97158	-0.26052	-0.44135

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Tert-butyl-(1-phenyl-ethylidene)-amine +
BEt₃

C	3.74397	-0.25443	1.47188
C	4.74109	-0.36329	0.50719
C	4.39578	-0.56459	-0.82834
C	3.05919	-0.65178	-1.19754
C	2.05298	-0.49647	-0.23989
C	2.40326	-0.31979	1.10158
C	0.60253	-0.63594	-0.58354
C	0.31237	-1.99662	-1.15695
N	-0.30219	0.25750	-0.35884
C	0.07937	1.72060	-0.20125
C	0.16226	2.10809	1.28913
C	-0.98590	2.52620	-0.96962
C	1.39891	2.12757	-0.89399
B	-2.00391	-0.27708	-0.13634
C	-1.94767	-1.69178	0.68879
C	-1.05453	-1.71035	1.93566
C	-2.63856	-0.37619	-1.63659
C	-4.04666	-0.98616	-1.61467
C	-2.88008	0.82635	0.75841
C	-3.86660	0.25248	1.78987
H	4.00709	-0.11867	2.51567
H	5.78547	-0.30225	0.79472
H	5.17020	-0.65630	-1.58267
H	2.79528	-0.79639	-2.24134
H	1.62131	-0.23699	1.84970
H	0.46936	-2.76714	-0.39617
H	-0.68237	-2.08247	-1.57355
H	1.05623	-2.17551	-1.93980
H	-0.43159	1.44353	1.91637
H	1.19803	2.06545	1.63620
H	-0.20119	3.12919	1.43615
H	-0.94971	2.26037	-2.03028
H	-0.74492	3.58838	-0.87724
H	-1.99634	2.37495	-0.61319
H	2.30086	1.85324	-0.35179
H	1.45496	1.72359	-1.90961
H	1.39052	3.21790	-0.97284
H	-2.97862	-1.85989	1.01927
H	-1.73386	-2.58094	0.08623
H	0.00778	-1.81359	1.68130
H	-1.15235	-0.77894	2.50858
H	-1.29212	-2.53592	2.61498
H	-2.70929	0.62803	-2.07816
H	-2.02885	-0.95233	-2.34621

H	-4.03216	-2.00374	-1.20916
H	-4.49544	-1.03559	-2.61236
H	-4.72128	-0.39661	-0.98435
H	-2.28186	1.57098	1.29066
H	-3.49071	1.41739	0.05912
H	-4.44676	1.05362	2.26058
H	-4.58208	-0.43770	1.33145
H	-3.36090	-0.29613	2.59056

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Tert-butyl-(1-phenyl-ethylidene)-amide +
BEt₃

C	3.26851	0.13401	-1.65494
C	4.35812	0.39664	-0.82443
C	4.22562	0.19656	0.54451
C	3.02265	-0.26813	1.07678
C	1.92518	-0.53840	0.25603
C	2.07108	-0.32348	-1.11995
C	0.60286	-1.11907	0.77839
C	0.47993	-1.01800	2.31663
N	-0.53827	-0.70163	-0.01584
C	-1.41814	-1.81342	-0.41669
C	-2.39566	-1.39554	-1.53016
C	-0.63689	-3.00936	-1.02415
C	-2.26220	-2.37862	0.75184
B	-1.01186	0.84562	-0.05667
C	0.12028	1.86188	0.62605
C	-1.10325	1.36686	-1.66250
C	-2.45184	1.09937	0.74671
C	-2.38903	0.96044	2.27194
C	-2.37241	2.09247	-2.13007
C	-0.36208	3.31912	0.68259
H	3.34910	0.30327	-2.72554
H	5.29257	0.76412	-1.23945
H	5.05915	0.41043	1.20886
H	2.94075	-0.39711	2.15103
H	1.19657	-0.47705	-1.74492
H	0.74559	-2.19538	0.61441
H	-0.46273	-1.46585	2.63225
H	1.28811	-1.56969	2.81322
H	0.49159	0.01206	2.67521
H	-3.13562	-2.19229	-1.67178
H	-2.92007	-0.47299	-1.29503
H	-1.86906	-1.25472	-2.47766
H	-1.32939	-3.65941	-1.57094
H	-0.14392	-3.63753	-0.27586
H	0.12116	-2.64494	-1.72529
H	-1.61495	-2.78119	1.53799
H	-2.88740	-1.59415	1.18528
H	-2.91194	-3.19656	0.41213
H	0.44551	1.59503	1.64105

H	1.03955	1.85526	0.02609
H	-0.91948	0.52907	-2.34660
H	-0.25629	2.04811	-1.85078
H	-2.79940	2.11999	0.52368
H	-3.27332	0.45875	0.38891
H	-3.33947	1.20027	2.77033
H	-2.11737	-0.05837	2.56864
H	-1.62304	1.62041	2.69774
H	-2.34600	2.36467	-3.19515
H	-2.53197	3.01919	-1.56557
H	-3.27397	1.48532	-1.97644
H	0.42700	4.01171	1.00619
H	-0.70595	3.65878	-0.30205
H	-1.20459	3.44417	1.37279

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Tert-butyl-(1-phenyl-ethylidene)-amine + BPh₃

C	-4.92552	-1.08506	-0.26713
C	-5.76562	0.02229	-0.32505
C	-5.23696	1.30373	-0.17422
C	-3.87223	1.47619	0.01800
C	-3.01901	0.36973	0.01596
C	-3.55392	-0.91472	-0.09257
C	-1.55381	0.51323	0.29427
C	-1.35950	0.90985	1.73565
N	-0.59480	0.26535	-0.53934
C	-0.83699	0.15825	-2.04352
C	-2.08341	0.91207	-2.54585
C	0.36396	0.81185	-2.75963
C	-0.94833	-1.31460	-2.44270
B	0.97116	0.00357	0.14573
C	1.54917	1.47260	0.56008
C	0.91073	2.69646	0.31371
C	1.47519	3.92207	0.66849
C	2.71400	3.96316	1.29679
C	3.38298	2.76725	1.54945
C	2.81130	1.55472	1.17794
C	1.24514	-0.89465	2.66061
C	0.66514	-1.02066	1.39165
C	0.96940	-1.78776	3.69536
C	0.09408	-2.85039	3.49580
C	-0.49546	-3.01064	2.24440
C	-0.20727	-2.11060	1.22199
C	2.06954	-0.75180	-0.83183
C	2.12968	-2.14680	-0.97920
C	3.10631	-2.78109	-1.74718
C	4.09285	-2.03453	-2.37985
C	4.08725	-0.64994	-2.22935
C	3.09802	-0.03296	-1.47038
H	-5.33532	-2.08583	-0.35406

H	-6.83235	-0.11126	-0.47060
H	-5.89079	2.16907	-0.20122
H	-3.45877	2.47482	0.13185
H	-2.89778	-1.77656	-0.02258
H	-2.03486	1.75181	1.92233
H	-1.69046	0.08320	2.37332
H	-0.34655	1.18782	1.99700
H	-2.00418	0.96212	-3.63368
H	-3.02769	0.42315	-2.31921
H	-2.10958	1.93944	-2.16808
H	0.04216	1.16085	-3.74278
H	1.18062	0.11207	-2.90651
H	0.74213	1.67238	-2.20126
H	-1.85421	-1.76835	-2.03152
H	-1.00596	-1.37515	-3.53395
H	-0.07318	-1.87965	-2.11890
H	-0.06439	2.70606	-0.17220
H	0.94354	4.84415	0.45143
H	3.15796	4.91281	1.57850
H	4.35833	2.77998	2.02704
H	3.37352	0.63855	1.34532
H	1.90667	-0.05786	2.86525
H	1.43481	-1.64433	4.66634
H	-0.12650	-3.54326	4.30171
H	-1.17911	-3.83588	2.06457
H	-0.68135	-2.26259	0.25192
H	1.40397	-2.77292	-0.46958
H	3.10165	-3.86379	-1.83410
H	4.86159	-2.52276	-2.97106
H	4.85598	-0.04693	-2.70399
H	3.11768	1.05005	-1.38460

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Tert-butyl-(1-phenyl-ethylidene)-amide + BPh₃

C	-3.99546	1.41639	0.12682
C	-4.78889	0.29395	-0.10427
C	-4.34531	-0.94859	0.33402
C	-3.12260	-1.07160	0.99080
C	-2.30715	0.03954	1.21048
C	-2.77552	1.28585	0.77916
C	-0.97120	-0.02695	1.96393
C	-0.70903	-1.41654	2.56752
N	0.17165	0.54562	1.25330
C	0.90185	1.55371	2.06485
C	1.23327	1.07813	3.50602
C	2.25211	1.96380	1.44996
C	0.07807	2.85492	2.21115
B	0.68309	-0.04020	-0.13221
C	-0.49350	-0.95799	-0.90049
C	-1.44212	-0.42754	-1.79241

C	-2.40771	-1.20868	-2.42259	Tert-butyl-(1-phenyl-ethylidene)-amine +			
C	-2.46239	-2.58114	-2.19591	B(C ₆ F ₅)Ph ₂			
C	-1.51963	-3.15268	-1.34757	C	3.57151	1.33420	1.40231
C	-0.55706	-2.35377	-0.73189	C	3.45955	2.51530	0.66824
C	2.23838	1.36349	-1.88480	C	2.20550	3.06978	0.44352
C	1.05355	1.22531	-1.14499	C	1.05939	2.43631	0.91825
C	2.50026	2.47537	-2.68681	C	1.16369	1.23491	1.62095
C	1.57371	3.50817	-2.78635	C	2.43468	0.71138	1.89732
C	0.38366	3.40738	-2.06803	C	-0.05615	0.56983	2.18544
C	0.14372	2.29172	-1.27034	C	0.07527	0.48374	3.69180
C	1.96985	-1.08266	-0.01117	N	-1.04559	0.14803	1.46119
C	2.49713	-1.70225	-1.16271	C	-2.32270	-0.28233	2.18852
C	3.53634	-2.62541	-1.11447	C	-2.79277	0.84774	3.14757
C	4.09092	-2.99256	0.11234	C	-3.53592	-0.49234	1.26475
C	3.57817	-2.42598	1.27311	C	-2.06464	-1.64674	2.85166
C	2.54000	-1.49390	1.19869	B	-0.88487	-0.02074	-0.22770
H	-4.32755	2.39661	-0.20495	C	-1.43781	1.37341	-0.87112
H	-5.73771	0.38801	-0.62480	C	0.70713	-0.43578	-0.49592
H	-4.94072	-1.83764	0.14516	C	-2.08150	2.36580	-0.11867
H	-2.78330	-2.05777	1.28836	C	-2.64612	3.50585	-0.69410
H	-2.15553	2.16025	0.95080	C	-2.58987	3.68791	-2.06938
H	-1.16904	0.62417	2.82598	C	-1.97542	2.71237	-2.85319
H	0.18028	-1.37536	3.19957	C	-1.42406	1.58198	-2.26202
H	-1.55226	-1.75145	3.18402	C	-1.75119	-1.29553	-0.84387
H	-0.52868	-2.16085	1.78984	C	1.55826	0.12757	-1.44631
H	1.68439	1.90594	4.06478	C	2.84954	-0.32820	-1.70953
H	0.35063	0.75627	4.06511	C	3.37181	-1.38881	-0.99236
H	1.95351	0.25590	3.50192	C	2.59213	-1.95550	0.00385
H	2.81468	2.53368	2.19878	C	1.31658	-1.46587	0.22579
H	2.12784	2.59742	0.57242	C	-1.45161	-2.64393	-0.57978
H	2.84645	1.09336	1.16434	C	-2.19259	-3.69813	-1.11135
H	-0.87425	2.68103	2.72476	C	-3.26165	-3.44692	-1.96389
H	0.63206	3.60290	2.79177	C	-3.57150	-2.12620	-2.27037
H	-0.12690	3.27278	1.22170	C	-2.83204	-1.08348	-1.71889
H	-1.44036	0.63677	-2.00215	F	1.20591	1.20564	-2.15601
H	-3.12768	-0.73782	-3.08804	F	3.59237	0.27147	-2.63949
H	-3.21744	-3.19453	-2.68150	F	4.60839	-1.82592	-1.22061
H	-1.52390	-4.22604	-1.17024	F	3.09624	-2.91218	0.78775
H	0.18481	-2.84125	-0.10363	F	0.71480	-1.97602	1.33146
H	3.00544	0.59819	-1.80736	H	4.54630	0.89285	1.58276
H	3.44171	2.53814	-3.22846	H	4.34893	2.99886	0.27818
H	1.77566	4.37783	-3.40633	H	2.10758	3.99329	-0.11673
H	-0.35556	4.20364	-2.12391	H	0.08770	2.86889	0.72121
H	-0.78095	2.24178	-0.70076	H	2.53146	-0.22844	2.43400
H	2.05367	-1.46223	-2.12804	H	0.95509	-0.13819	3.88687
H	3.90916	-3.07150	-2.03382	H	0.30887	1.47836	4.08130
H	4.89996	-3.71698	0.15893	H	-0.76360	0.06986	4.23421
H	3.98206	-2.71096	2.24228	H	-3.50882	1.48693	2.62579
H	2.14189	-1.07554	2.11705	H	-3.31317	0.40336	4.00155
				H	-2.01252	1.50076	3.53054
				H	-4.41663	-0.47726	1.91477

H	-3.52209	-1.44696	0.74709	F	-1.15128	-1.51476	1.63595
H	-3.64050	0.31466	0.53663	F	-3.59732	-0.83539	2.16367
H	-1.22708	-1.67010	3.54729	F	-4.61234	1.56491	1.34272
H	-2.96857	-1.95478	3.38511	F	-2.99920	3.26954	-0.05400
H	-1.86554	-2.38168	2.06835	F	-0.55085	2.64645	-0.63272
H	-2.14055	2.26586	0.96319	H	-2.66417	-3.89848	-0.18773
H	-3.12969	4.24573	-0.06283	H	-4.75949	-2.60188	-0.53287
H	-3.02372	4.57096	-2.52792	H	-4.65561	-0.41039	-1.70139
H	-1.93152	2.83009	-3.93178	H	-2.50355	0.48557	-2.47060
H	-0.97635	0.82952	-2.90436	H	-0.50074	-2.98275	-0.96664
H	-0.63070	-2.90607	0.07406	H	0.29184	-1.43880	-3.00627
H	-1.92264	-4.72005	-0.86113	H	0.92082	0.89716	-3.41701
H	-3.83824	-4.26450	-2.38533	H	-0.76128	0.56575	-3.85566
H	-4.39917	-1.90059	-2.93652	H	-0.36985	1.46466	-2.37221
H	-3.13589	-0.07086	-1.95934	H	3.61438	-1.56494	-3.47007

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Tert-butyl-(1-phenyl-ethylidene)-amide +
B(C₆F₅)Ph₂

C	-2.63573	-2.94179	-0.70124
C	-3.81069	-2.21847	-0.89559
C	-3.75024	-0.99228	-1.55046
C	-2.52798	-0.48689	-1.98977
C	-1.33787	-1.18764	-1.77323
C	-1.41989	-2.43207	-1.14111
C	0.03272	-0.68823	-2.24847
C	-0.06064	0.64058	-3.01516
N	1.08928	-0.73394	-1.23444
C	2.31588	-1.42003	-1.73490
C	2.76460	-0.95342	-3.14795
C	3.55186	-1.21696	-0.83687
C	2.08666	-2.94599	-1.83678
B	1.00831	0.10771	0.10418
C	-0.61675	0.50736	0.46924
C	-1.50134	-0.29918	1.19517
C	-2.82034	0.02552	1.49384
C	-3.34195	1.23603	1.07917
C	-2.52014	2.09088	0.36976
C	-1.20727	1.72143	0.09320
C	2.57449	-0.30377	2.29304
C	1.64694	-0.79126	1.36063
C	3.18228	-1.11726	3.25276
C	2.88601	-2.47253	3.31669
C	1.96668	-2.99570	2.40774
C	1.37224	-2.16727	1.46331
C	1.76616	1.58149	0.07836
C	1.66150	2.45945	1.17448
C	2.25821	3.71503	1.19385
C	2.99218	4.15707	0.09315
C	3.10462	3.32382	-1.01339
C	2.49852	2.06633	-1.00881

F	-1.15128	-1.51476	1.63595
F	-3.59732	-0.83539	2.16367
F	-4.61234	1.56491	1.34272
F	-2.99920	3.26954	-0.05400
F	-0.55085	2.64645	-0.63272
H	-2.66417	-3.89848	-0.18773
H	-4.75949	-2.60188	-0.53287
H	-4.65561	-0.41039	-1.70139
H	-2.50355	0.48557	-2.47060
H	-0.50074	-2.98275	-0.96664
H	0.29184	-1.43880	-3.00627
H	0.92082	0.89716	-3.41701
H	-0.76128	0.56575	-3.85566
H	-0.36985	1.46466	-2.37221
H	3.61438	-1.56494	-3.47007
H	1.98604	-1.06179	-3.90724
H	3.09576	0.08805	-3.14574
H	4.43730	-1.54578	-1.39308
H	3.50078	-1.80099	0.08076
H	3.68934	-0.16767	-0.56814
H	1.25557	-3.18984	-2.50821
H	2.98157	-3.44771	-2.22444
H	1.86863	-3.35684	-0.84834
H	2.87485	0.73801	2.25543
H	3.90330	-0.68489	3.94286
H	3.36178	-3.11220	4.05557
H	1.71709	-4.05407	2.43250
H	0.66648	-2.60012	0.76352
H	1.07393	2.14707	2.03763
H	2.14548	4.35639	2.06490
H	3.45923	5.13834	0.09829
H	3.65999	3.65369	-1.88855
H	2.57840	1.44117	-1.89149

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Tert-butyl-(1-phenyl-ethylidene)-amine +
B(C₆F₅)₂Ph

C	5.52684	0.70460	-1.71666
C	6.43960	-0.18497	-1.15679
C	6.03036	-1.05890	-0.15152
C	4.70851	-1.05645	0.27771
C	3.78148	-0.20442	-0.32620
C	4.19865	0.70634	-1.29809
C	2.37914	-0.16093	0.19915
C	2.40537	0.59074	1.50835
N	1.32609	-0.66695	-0.35640
C	1.40331	-1.50487	-1.64278
C	2.73389	-2.25646	-1.85253
C	0.32363	-2.61413	-1.62469

C	1.17262	-0.55194	-2.81679	H	-1.08013	0.33581	3.07097
B	-0.14097	-0.34335	0.41791				
C	0.05640	-1.06533	1.88257	65			
C	0.84328	-2.22474	2.00607	Tert-butyl-(1-phenyl-ethylidene)-amide +			
C	1.07940	-2.84636	3.22747	B(C ₆ F ₅) ₂ Ph			
C	0.53772	-2.31738	4.39572	C	2.18206	-3.26249	1.52128
C	-0.24031	-1.16976	4.31074	C	3.48013	-3.01709	1.07841
C	-0.47423	-0.56120	3.07773	C	3.97988	-1.71968	1.13170
C	-1.57372	1.76927	1.06670	C	3.18172	-0.67700	1.59886
C	-0.38548	1.30468	0.49553	C	1.86276	-0.90126	2.00180
C	-1.94405	3.10611	1.14463	C	1.39300	-2.21715	1.98711
C	-1.12084	4.07551	0.59554	C	0.93744	0.20950	2.51644
C	0.05015	3.67435	-0.02526	C	1.70447	1.51507	2.78454
C	0.37480	2.32463	-0.07442	N	-0.32055	0.38166	1.77424
C	-1.49847	-0.86171	-0.37370	C	-1.50124	0.44298	2.68616
C	-2.09564	-0.13088	-1.40324	C	-1.30644	1.40169	3.89311
C	-3.30176	-0.46460	-2.00712	C	-2.79593	0.92607	1.99727
C	-3.99767	-1.57835	-1.56690	C	-1.81595	-0.94432	3.29363
C	-3.45655	-2.34236	-0.54489	B	-0.37722	0.66810	0.22930
C	-2.24246	-1.97612	0.02290	C	1.05134	0.20978	-0.59316
F	-2.47349	0.90323	1.56286	C	1.28307	-0.99508	-1.26669
F	-3.09139	3.45640	1.72186	C	2.45532	-1.32070	-1.94551
F	-1.45150	5.36153	0.65337	C	3.48809	-0.40825	-2.02059
F	0.85112	4.57930	-0.58786	C	3.31405	0.81855	-1.40856
F	1.51185	2.05986	-0.75760	C	2.13230	1.09494	-0.73205
F	-1.50146	0.96514	-1.91499	C	-2.73067	0.32391	-1.19987
F	-3.79454	0.28280	-2.99383	C	-1.68094	-0.20246	-0.44008
F	-5.15519	-1.91718	-2.12498	C	-3.84912	-0.39737	-1.61629
F	-4.09908	-3.42956	-0.12149	C	-3.98952	-1.72491	-1.26276
F	-1.77857	-2.82374	0.94764	C	-2.99373	-2.30280	-0.49418
H	5.84764	1.40488	-2.48070	C	-1.89103	-1.54754	-0.11850
H	7.47158	-0.18691	-1.49110	C	-0.50689	2.27032	-0.18088
H	6.74221	-1.74092	0.30134	C	-0.39005	2.69341	-1.51744
H	4.38210	-1.73963	1.05789	C	-0.38977	4.03217	-1.88153
H	3.48989	1.40953	-1.72090	C	-0.50287	5.02282	-0.90395
H	2.90181	-0.06526	2.23390	C	-0.61148	4.64170	0.42646
H	3.04182	1.46811	1.37235	C	-0.60776	3.28726	0.76908
H	1.44733	0.87804	1.91807	F	0.36855	-1.97222	-1.32994
H	2.57273	-2.93741	-2.69038	F	2.58289	-2.51552	-2.53491
H	3.57645	-1.62632	-2.11952	F	4.62483	-0.70366	-2.65995
H	2.99727	-2.86201	-0.97974	F	4.29959	1.72557	-1.45029
H	0.68712	-3.46234	-2.20642	F	2.13778	2.31528	-0.16668
H	-0.60801	-2.28906	-2.08139	F	-2.79614	1.61860	-1.54485
H	0.10971	-2.97740	-0.61747	F	-4.80696	0.19880	-2.33932
H	0.25465	0.02271	-2.69432	F	-5.05947	-2.43030	-1.64486
H	2.00898	0.14351	-2.92122	F	-3.10353	-3.58415	-0.11884
H	1.09602	-1.13824	-3.73746	F	-1.02000	-2.22383	0.64282
H	1.29780	-2.66626	1.12164	H	1.77967	-4.27105	1.49848
H	1.68915	-3.74446	3.26609	H	4.09479	-3.82736	0.69791
H	0.72184	-2.79169	5.35437	H	4.99077	-1.50973	0.79232
H	-0.66927	-0.73560	5.20892	H	3.58646	0.33029	1.60999

H	0.38034	-2.40923	2.32143
H	0.65891	-0.17030	3.50731
H	1.04804	2.23892	3.26894
H	2.56068	1.33384	3.44581
H	2.06304	1.97423	1.86495
H	-2.18081	1.32535	4.54810
H	-0.43084	1.15571	4.49829
H	-1.22373	2.44503	3.57799
H	-3.49726	1.25744	2.77038
H	-3.28924	0.12780	1.44188
H	-2.61891	1.76489	1.32070
H	-0.98454	-1.31950	3.90071
H	-2.69512	-0.88381	3.94619
H	-2.01736	-1.67291	2.50796
H	-0.29320	1.93982	-2.29875
H	-0.29658	4.31050	-2.92847
H	-0.49884	6.07367	-1.18083
H	-0.68928	5.39680	1.20528
H	-0.65834	3.00792	1.81583

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Tert-butyl-(1-phenyl-ethylidene)-amine +
B(C₆F₅)₃

C	-5.18673	-3.00048	-0.76804
C	-6.22041	-2.07377	-0.85922
C	-5.94692	-0.71427	-0.72158
C	-4.64166	-0.28290	-0.51797
C	-3.59527	-1.20877	-0.48610
C	-3.87686	-2.57309	-0.56393
C	-2.21893	-0.74044	-0.10122
C	-2.20212	-0.66961	1.40785
N	-1.23337	-0.44207	-0.88715
C	-1.40890	-0.61157	-2.41997
C	-2.70506	0.06561	-2.91174
C	-0.26895	0.00639	-3.24357
C	-1.40140	-2.11234	-2.73721
B	0.16216	0.10068	-0.10218
C	-0.37115	1.47024	0.65068
C	-0.95914	2.46283	-0.13030
C	-1.47550	3.65234	0.35566
C	-1.41321	3.90432	1.71930
C	-0.85024	2.95130	2.55070
C	-0.34866	1.76988	2.01003
C	1.83515	-0.74912	1.70815
C	0.73745	-1.07224	0.90925
C	2.49207	-1.65258	2.53019
C	2.06521	-2.97275	2.56480
C	0.99271	-3.35414	1.77525
C	0.36741	-2.41158	0.96788
C	1.49604	0.39801	-1.02332
C	2.20455	-0.68030	-1.55887

C	3.44110	-0.58873	-2.17259
C	4.05730	0.65320	-2.26034
C	3.40747	1.75944	-1.74393
C	2.15939	1.61730	-1.13915
F	-1.02795	2.29226	-1.46370
F	-2.01550	4.55018	-0.46697
F	-1.90222	5.03422	2.21859
F	-0.81007	3.15728	3.86538
F	0.09396	0.88346	2.91542
F	2.30976	0.50396	1.70041
F	3.52661	-1.26905	3.27421
F	2.67799	-3.85937	3.34226
F	0.57316	-4.61931	1.78385
F	-0.65281	-2.88862	0.22053
F	1.63525	-1.90233	-1.56716
F	4.03222	-1.66628	-2.68569
F	5.24481	0.77504	-2.84272
F	3.97999	2.95895	-1.81796
F	1.63943	2.75683	-0.66842
H	-5.39686	-4.06196	-0.84437
H	-7.23945	-2.40955	-1.01860
H	-6.75124	0.01209	-0.76800
H	-4.42639	0.77718	-0.41155
H	-3.07322	-3.29518	-0.45556
H	-2.87997	0.14163	1.69954
H	-2.65361	-1.59588	1.77290
H	-1.24641	-0.52680	1.88955
H	-2.60680	0.24595	-3.98351
H	-3.59294	-0.54501	-2.77226
H	-2.84400	1.03509	-2.42759
H	-0.59923	-0.01700	-4.28400
H	0.63501	-0.59120	-3.19714
H	-0.05346	1.03935	-2.98137
H	-0.51041	-2.58481	-2.32113
H	-2.28911	-2.62150	-2.36780
H	-1.37917	-2.22943	-3.82451

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Tert-butyl-(1-phenyl-ethylidene)-amide +
B(C₆F₅)₃

C	-4.37137	1.33887	0.95418
C	-5.10579	0.22523	0.55171
C	-4.60931	-1.04616	0.82114
C	-3.37945	-1.20103	1.45843
C	-2.60971	-0.09333	1.82326
C	-3.14810	1.17583	1.59375
C	-1.25525	-0.20723	2.53608
C	-0.97803	-1.63831	3.02110
N	-0.11188	0.44064	1.87019
C	0.66956	1.29606	2.81733
C	0.94671	0.63117	4.19356
C	2.05799	1.69501	2.27471

C	-0.08540	2.60770	3.13169	H	0.50508	3.23057	3.81398
B	0.31586	0.15272	0.40565	H	-0.27929	3.17910	2.22436
C	-0.91006	-0.61613	-0.49173				
C	-1.82043	0.00245	-1.35539	31			
C	-2.81292	-0.65967	-2.07230	Tert-butyl-(1-phenyl-ethylidene)-amine +			
C	-2.92564	-2.03400	-1.99530	proton			
C	-2.02681	-2.71427	-1.19676	C	3.02342	-1.50639	0.24776
C	-1.06012	-2.00977	-0.49006	C	3.97188	-0.55901	-0.13727
C	1.99550	1.87713	-0.97145	C	3.58905	0.75545	-0.39787
C	0.76987	1.60296	-0.35450	C	2.25787	1.12931	-0.27340
C	2.36252	3.11344	-1.49713	C	1.29396	0.17514	0.08412
C	1.49875	4.18805	-1.40709	C	1.68829	-1.14557	0.35372
C	0.28012	3.99253	-0.78227	C	-0.11830	0.57169	0.16371
C	-0.04550	2.73615	-0.28686	C	-0.46539	1.97837	0.53231
C	1.57813	-0.95583	0.16948	N	-1.02203	-0.31759	-0.11943
C	1.89230	-1.35343	-1.13255	C	-2.52875	-0.28102	-0.10247
C	2.78413	-2.36031	-1.45785	C	-2.94939	-1.61772	-0.72023
C	3.43035	-3.04792	-0.43923	C	-3.02372	-0.20102	1.34370
C	3.16574	-2.69682	0.86991	C	-3.04891	0.86716	-0.97090
C	2.25576	-1.67560	1.14025	H	3.32801	-2.52077	0.47877
F	-1.81238	1.32147	-1.58130	H	5.01492	-0.84431	-0.22182
F	-3.65694	0.03051	-2.84632	H	4.32875	1.49035	-0.69427
F	-3.87994	-2.68521	-2.66673	H	1.96788	2.15353	-0.48382
F	-2.10564	-4.04683	-1.09065	H	0.96835	-1.87944	0.70691
F	-0.27276	-2.81675	0.25174	H	-0.48938	2.58609	-0.38003
F	2.98944	0.97484	-1.03961	H	-1.43708	2.05431	1.01223
F	3.56450	3.27626	-2.06412	H	0.29824	2.38469	1.19421
F	1.83660	5.38489	-1.89591	H	-0.64961	-1.21439	-0.42591
F	-0.57398	5.01550	-0.65525	H	-4.03822	-1.68729	-0.72539
F	-1.23815	2.69812	0.32112	H	-2.60202	-1.70317	-1.75429
F	1.32042	-0.72476	-2.17560	H	-2.56670	-2.46225	-0.13806
F	3.03585	-2.67906	-2.73393	H	-4.11483	-0.25787	1.34006
F	4.29918	-4.02436	-0.72399	H	-2.74496	0.73043	1.83962
F	3.77769	-3.34554	1.86999	H	-2.64123	-1.03779	1.93318
F	2.06402	-1.44137	2.45072	H	-2.58870	0.84692	-1.96227
H	-4.75077	2.33906	0.76670	H	-4.12606	0.73638	-1.09786
H	-6.05484	0.34717	0.03855	H	-2.89319	1.84942	-0.52425
H	-5.17066	-1.92656	0.51968				
H	-3.00577	-2.20359	1.64148	32			
H	-2.57824	2.04419	1.90187	<i>N</i> -tert-butyl-alpha-methylbenzylamine			
H	-1.43810	0.37649	3.44560	C	1.720649	-1.050931	3.530484
H	-0.05438	-1.66119	3.59731	C	0.733902	-1.982754	3.838960
H	-1.79788	-1.99686	3.65503	C	-0.266442	-2.260067	2.909978
H	-0.85370	-2.33382	2.19231	C	-0.279810	-1.611142	1.679213
H	1.43478	1.37057	4.83726	C	0.707320	-0.674483	1.362190
H	0.03718	0.31602	4.71023	C	1.704445	-0.401606	2.298834
H	1.61165	-0.22563	4.10429	C	0.723530	-0.000849	0.000994
H	2.69177	1.99133	3.11658	N	-0.652736	0.360894	-0.346697
H	2.00566	2.54859	1.59817	C	-0.920205	1.204941	-1.530415
H	2.55502	0.87136	1.75880	C	1.352841	-0.948396	-1.025320
H	-1.04606	2.40946	3.62023	C	0.155913	2.270016	-1.781886

C	-2.255744	1.901851	-1.250810	H	-3.78873	-1.34620	1.41088
C	-1.099068	0.326157	-2.775632	H	-3.08228	0.15486	0.84989
H	2.500650	-0.824464	4.250810	H	-2.31972	-0.74254	2.17732
H	0.742014	-2.488197	4.799502	H	-3.01048	-1.06451	-1.60335
H	-1.039832	-2.984782	3.145854	H	-2.30069	-2.67329	-1.70453
H	-1.060687	-1.810896	0.951919	H	-3.77587	-2.42524	-0.77560
H	2.473393	0.329691	2.060571	H	1.68176	1.50496	-0.57676
H	1.380386	0.882749	0.084405	H	0.85435	0.89399	-1.99613
H	-1.045172	0.829176	0.466545	H	1.21067	-0.56320	1.90640
H	0.675727	-1.785838	-1.218572	H	3.43380	0.40423	2.40934
H	2.294914	-1.341461	-0.634239	H	5.17945	0.47297	0.64628
H	1.567590	-0.443926	-1.970497	H	4.71471	-0.46943	-1.59866
H	0.289376	2.904394	-0.898761	H	2.51196	-1.44534	-2.10402
H	1.122941	1.821520	-2.029632	H	1.41289	3.29335	-2.25196
H	-0.135251	2.911232	-2.619455	H	-0.33770	3.11422	-2.26581
H	-2.167342	2.586603	-0.399683	H	0.48374	3.72191	-0.82295
H	-3.025031	1.158918	-1.019843	H	-3.08928	0.80187	-1.04387
H	-2.580764	2.481745	-2.118643	H	-1.94610	1.54937	-2.12816
H	-0.172531	-0.167345	-3.073376	H	-3.46966	3.28350	-1.27652
H	-1.437854	0.934831	-3.620413	H	-1.91740	3.59826	-0.50702
H	-1.846676	-0.445768	-2.575258	H	-3.20305	2.79724	0.39620

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Tert-butyl-(1-phenyl-ethylidene)-amine +
[SiEt₃]⁺

C	0.42538	-3.04306	-0.90368
C	0.37228	-1.64229	-0.37027
C	1.70259	-1.03865	-0.13784
N	-0.70987	-0.98271	-0.04879
C	-2.02839	-1.71127	0.24659
C	-1.77002	-3.02200	1.01479
C	-2.84043	-0.83944	1.22097
C	-2.81492	-1.97670	-1.04065
Si	-0.71596	0.95196	-0.10162
C	0.74282	1.56260	-1.13284
C	1.97251	-0.51756	1.13468
C	3.22470	0.01664	1.41818
C	4.20619	0.04574	0.43004
C	3.94761	-0.48897	-0.83264
C	2.70913	-1.05063	-1.11190
C	0.55342	3.00312	-1.64349
C	-2.24658	1.49049	-1.07529
C	-2.73016	2.87045	-0.58719
C	-0.70745	1.55199	1.68891
C	0.29171	2.68790	1.95673
H	1.20452	-3.06965	-1.66910
H	0.75483	-3.72573	-0.11412
H	-0.50539	-3.39550	-1.33319
H	-2.69023	-3.29332	1.53582
H	-1.50966	-3.86817	0.38304
H	-0.99352	-2.88514	1.77419

H	-3.78873	-1.34620	1.41088
H	-3.08228	0.15486	0.84989
H	-2.31972	-0.74254	2.17732
H	-3.01048	-1.06451	-1.60335
H	-2.30069	-2.67329	-1.70453
H	-3.77587	-2.42524	-0.77560
H	1.68176	1.50496	-0.57676
H	0.85435	0.89399	-1.99613
H	1.21067	-0.56320	1.90640
H	3.43380	0.40423	2.40934
H	5.17945	0.47297	0.64628
H	4.71471	-0.46943	-1.59866
H	2.51196	-1.44534	-2.10402
H	1.41289	3.29335	-2.25196
H	-0.33770	3.11422	-2.26581
H	0.48374	3.72191	-0.82295
H	-3.08928	0.80187	-1.04387
H	-1.94610	1.54937	-2.12816
H	-3.46966	3.28350	-1.27652
H	-1.91740	3.59826	-0.50702
H	-3.20305	2.79724	0.39620
H	-1.71912	1.88014	1.95215
H	-0.49437	0.70835	2.35346
H	0.30792	2.94551	3.01804
H	1.30910	2.40932	1.66431
H	0.02374	3.59446	1.40798

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Tert-butyl-(1-phenyl-ethylidene)-amide +
[SiEt₃]⁺

C	-0.49210	-1.44735	-2.24376
C	-0.62808	-1.40166	-0.71617
C	-1.92747	-0.74802	-0.23719
N	0.58420	-0.87084	-0.07239
C	1.38527	-1.88807	0.65887
C	2.71518	-1.30510	1.15344
C	0.61869	-2.40541	1.88948
C	1.74845	-3.07423	-0.25467
Si	0.94199	0.85785	-0.07673
C	-0.21492	1.80710	-1.24574
C	-2.04924	-0.30878	1.08505
C	-3.22862	0.26652	1.54742
C	-4.32029	0.41042	0.69544
C	-4.21775	-0.03241	-0.61903
C	-3.03475	-0.60704	-1.07912
C	-0.16632	3.32056	-0.98251
C	0.76822	1.61134	1.66454
C	1.76642	2.73021	1.98831
C	2.66824	1.23979	-0.77390
C	2.97415	0.45388	-2.05399
H	0.48643	-1.85907	-2.49885

H	-1.25735	-2.08056	-2.70200	C	-2.39410	-0.44990	1.18806
H	-0.56819	-0.44814	-2.68145	C	-3.17121	-1.56027	1.50005
H	-0.72043	-2.44474	-0.39257	C	-4.14934	-1.99390	0.60632
H	3.21884	-2.05341	1.77174	C	-4.35188	-1.31875	-0.59502
H	3.37731	-1.06112	0.31998	C	-3.56843	-0.21217	-0.90989
H	2.57810	-0.41216	1.77065	H	4.45142	-2.42947	-1.61145
H	-0.38171	-2.76448	1.62954	H	4.51999	-3.19949	0.74349
H	0.50857	-1.60715	2.63081	H	2.74730	-2.50524	2.33153
H	1.15974	-3.23225	2.36073	H	0.93344	-0.99251	1.57695
H	2.29759	-2.72147	-1.13267	H	2.63021	-0.94772	-2.38009
H	2.38701	-3.77785	0.28841	H	-0.89923	-1.45160	-1.45155
H	0.87304	-3.63056	-0.59976	H	-0.99459	0.05449	-2.40299
H	0.10064	1.61708	-2.27922	H	0.34039	-1.09607	-2.64577
H	-1.24988	1.46537	-1.16786	H	1.70567	4.17219	0.24103
H	-1.19888	-0.40308	1.75147	H	1.15156	3.46530	-1.28100
H	-3.29195	0.60620	2.57675	H	-0.00324	3.87259	0.01106
H	-5.23936	0.86422	1.05157	H	1.60676	2.80097	2.38396
H	-5.05941	0.07412	-1.29637	H	1.20668	1.08264	2.33151
H	-2.97808	-0.92953	-2.11304	H	-0.06916	2.31010	2.14609
H	-0.79507	3.86536	-1.69260	H	2.90494	1.62296	-0.94396
H	-0.52410	3.56312	0.02284	H	3.29284	2.61035	0.46437
H	0.84837	3.72194	-1.07581	H	3.07732	0.87642	0.66125
H	0.85369	0.81407	2.41370	H	-1.63429	2.72819	0.64641
H	-0.26023	1.98439	1.75854	H	-1.75724	2.27016	-1.75209
H	1.59775	3.15064	2.98428	H	-1.64554	-0.10865	1.90255
H	1.69548	3.55210	1.26899	H	-3.02315	-2.08174	2.43960
H	2.79735	2.36303	1.95626	H	-4.75881	-2.85755	0.85040
H	2.67688	2.31542	-0.99722	H	-5.11839	-1.65409	-1.28527
H	3.46227	1.09082	-0.03590	H	-3.73099	0.30248	-1.85436
H	3.92917	0.74799	-2.49928				
H	3.01178	-0.62288	-1.85901				
H	2.19695	0.60820	-2.81040				
				45			
				Tert-butyl-(1-phenyl-ethylidene)-amide + [SiPhH ₂] ⁺			
				C	2.15190	2.34533	-0.69906
				C	1.42816	1.38951	0.25305
				C	-0.06544	1.67573	0.38381
				N	1.63195	-0.03476	-0.08029
				C	2.90439	-0.70266	0.30528
				C	3.56767	-0.00895	1.50180
				C	2.58849	-2.14083	0.74525
				C	3.91220	-0.73491	-0.85762
				Si	0.60213	-0.68722	-1.33571
				C	-0.76956	2.49519	-0.49605
				C	-2.14288	2.69050	-0.33870
				C	-2.82365	2.06690	0.69946
				C	-2.12784	1.24581	1.58744
				C	-0.76310	1.05711	1.42759
				C	-1.08575	-1.23733	-0.72890
				C	-1.22400	-2.14336	0.33254
				C	-2.47897	-2.50880	0.80656
44							
Tert-butyl-(1-phenyl-ethylidene)-amine + [SiPhH ₂] ⁺							
C	3.68395	-2.11327	-0.91389				
C	3.72266	-2.54334	0.41192				
C	2.73212	-2.14731	1.30806				
C	1.71972	-1.29071	0.89023				
C	1.69207	-0.84482	-0.43624				
C	2.65594	-1.28589	-1.34812				
C	0.55044	-0.00559	-0.85888				
C	-0.31929	-0.63925	-1.90262				
N	0.25406	1.15073	-0.32914				
C	1.23949	2.07798	0.39884				
C	0.99021	3.47505	-0.19932				
C	0.96554	2.05784	1.90310				
C	2.71221	1.74982	0.12472				
Si	-1.53579	1.71176	-0.40567				
C	-2.57864	0.23372	-0.02372				

C	-3.62605	-1.97151	0.22307	H	3.50586	-1.28346	-1.71148
C	-3.50972	-1.07523	-0.83419	H	1.30326	-1.84195	-1.94591
C	-2.24827	-0.71310	-1.30367	H	0.35263	0.31599	-2.40584
H	1.93948	3.38895	-0.44764	H	-0.25354	2.98194	-1.31783
H	3.23207	2.19551	-0.63194	H	-2.67764	3.32892	-1.03510
H	1.85499	2.16727	-1.73721	H	-3.89328	2.21085	0.81518
H	1.83310	1.55888	1.25532	H	-2.65485	0.74107	2.39082
H	4.44505	-0.58951	1.79908	H	-0.21950	0.38998	2.09320
H	3.90897	1.00268	1.26453	H	-0.33700	-2.55968	0.80542
H	2.88945	0.03874	2.35950	H	-2.56635	-3.21039	1.63072
H	3.50569	-2.66408	1.03311	H	-4.60708	-2.25228	0.59407
H	2.11874	-2.71724	-0.05655	H	-4.39980	-0.64878	-1.28701
H	1.91156	-2.12434	1.60507	H	-2.16925	0.00973	-2.11259
H	4.15746	0.27776	-1.18841				
H	4.84097	-1.22840	-0.55233				