Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Computed thermodynamic stabilities of silylium Lewis base adducts

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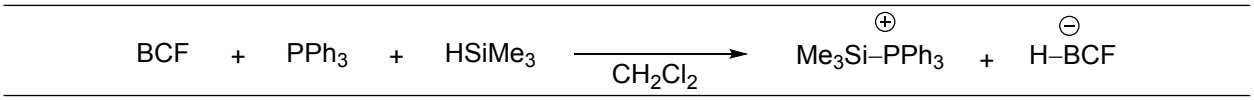
1. Basis set comparisons



Basis set	Time (h)[b]	ΔG (kcal/mol)	ΔΔG (kcal/mol)[c]
6-31G	13.2	-5.52	-2.91
6-31G*	39.6	2.29	4.91
6-31+G*	226.3	-3.12	-0.51
6-31+G**	191.8	-2.61	--
6-311+G*	326.8	-3.17	-0.55
6-311+G**	341.3	-2.48	0.13
6-311++G**	425.8	-2.56	0.05

Table S1. Calculations for the splitting of trimethylsilane with BCF and PPh_3.[a]

[a]All calculations were run using the ωB97X-D functional using the CPCM solvation mode with solvent parameters for dichloromethane. [b]The time listed represents the amount of time for all calculations in the reaction scheme to converge. To make for a fair comparison, the calculations were performed starting from the same structure for each molecule. [c]ΔΔG represents the difference in Gibbs free energy between the other basis set relative to 6-31+G** which was chosen for the paper.

To determine the best basis set for the scope of the paper, several basis sets were screened using the ωB97X-D functional. We aimed to strike a balance between minimized energy and computational cost. Assuming the 6-311++G** basis set gives the most accurate energy for the reaction shown in Table S1, we compared the Gibbs free energies of seven different basis sets. For the paper, we chose 6-31+G** as our basis set as the value for the test calculation comes close to that of the 6-311++G** basis set in less than half the computational time.

2. References

Full Guassian Reference: Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2016**.

3. Table of summarized energies

Compound	Absolute E (a.u.)	# imaginary freq	Zero Point E (a.u.)	G (a.u.)
$Me_3Si–PPh_3^+$	-1445.191	0	-1444.799	-1444.852
PPh_3	-1036.094	0	-1035.818	-1035.863
2-Me-THF	-271.712	0	-271.566	-271.596
$Me_3Si–2\text{-}Me\text{-}THF^+$	-680.803	0	-680.541	-680.580
$Me_2EtSi–PPh_3^+$	-1484.494	0	-1484.072	-1484.129
$Me_2EtSi–2\text{-}Me\text{-}THF^+$	-720.105	0	-719.813	-719.854
$Et_3Si–PPh_3^+$	-1563.097	0	-1562.616	-1562.674
$Et_3Si–2\text{-}Me\text{-}THF^+$	-798.709	0	-798.359	-798.403
$Me_2PhSi–PPh_3^+$	-1636.872	0	-1636.424	-1636.482
$Me_2PhSi–2\text{-}Me\text{-}THF^+$	-872.480	0	-872.163	-872.209
$Ph_3Si–PPh_3^+$	-2020.232	0	-2019.674	-2019.741
$Ph_3Si–2\text{-}Me\text{-}THF^+$	-1255.834	0	-1255.407	-1255.460
P^tBu_3	-814.788	0	-814.415	-814.456
$Me_3Si–P^tBu_3^+$	-1223.898	0	-1223.407	-1223.454
$P(p\text{-tol})_3$	-1154.024	0	-1153.664	-1153.716
$Me_3Si–P(p\text{-tol})_3^+$	-1563.125	0	-1562.650	-1562.711
PCy_3	-1047.016	0	-1046.527	-1046.573
$Me_3Si–PCy_3^+$	-1456.121	0	-1455.514	-1455.567
$P(o\text{-tol})_3$	-1154.008	0	-1153.647	-1153.695
$Me_3Si–P(o\text{-tol})_3^+$	-1563.107	0	-1562.630	-1562.687
$PPh_2(p\text{-tol})$	-1075.404	0	-1075.099	-1075.147
$Me_3Si–PPh_2(p\text{-tol})^+$	-1484.502	0	-1484.082	-1484.138
$PPh_2i\text{-Pr}$	-923.027	0	-922.746	-922.790
$Me_3Si–PPh_2i\text{-Pr}^+$	-1332.126	0	-1331.730	-1331.780
$PPh_2(o\text{-biphenyl})$	-1267.086	0	-1266.728	-1266.781
$Me_3Si–PPh_2(o\text{-biphenyl})^+$	-1676.184	0	-1675.709	-1675.768
$P(p\text{-F-Ph})_3$	-1333.739	0	-1333.487	-1333.537
$Me_3Si–P(p\text{-F-Ph})_3^+$	-1742.832	0	-1742.464	-1742.522
$P(1\text{-naphthyl})_3$	-1496.887	0	-1496.468	-1496.522
$Me_3Si–P(1\text{-naphthyl})_3^+$	-1905.981	0	-1905.445	-1905.506
$PPh_2(C_6F_5)$	-1532.126	0	-1531.890	-1531.941
$Me_3Si–PPh_2(C_6F_5)^+$	-1941.211	0	-1940.860	-1940.920
$P(p\text{-}CF_3\text{-Ph})_3$	-2047.008	0	-2046.717	-2046.782
$Me_3Si–P(p\text{-}CF_3\text{-Ph})_3^+$	-2456.093	0	-2455.687	-2455.760
$P(^tBu)_2(o\text{-biphenyl})$	-1119.553	0	-1119.131	-1119.180
$Me_3Si–P(^tBu)_2(o\text{-biphenyl})^+$	-1528.639	0	-1528.098	-1528.152
$P(\text{mesityl})_3$	-1389.863	0	-1389.334	-1389.394

$Me_3Si–P(mesityl)_3^+$	-1798.950	0	-1798.302	-1798.365
Me_2O	-154.991	0	-154.910	-154.936
$Me_3Si–OMe_2^+$	-564.072	0	-563.875	-563.913
MeOEt	-194.301	0	-194.192	-194.220
$Me_3Si–OMeEt^+$	-603.384	0	-603.158	-603.197
MeO*i*Pr	-233.611	0	-233.474	-233.504
$Me_3Si–OMe*i*Pr^+$	-642.692	0	-642.439	-642.478
MeO*t*Bu	-272.920	0	-272.754	-272.786
$Me_3Si–OMe*t*Bu^+$	-681.999	0	-681.716	-681.755
$(MeOCH_2)_2$	-308.788	0	-308.645	-308.677
$Me_3Si–(MeOCH_2)_2^+$	-717.866	0	-717.608	-717.650
1,2-epoxybutane	-232.373	0	-232.258	-232.286
$Me_3Si–1,2\text{-epoxybutane}^+$	-641.457	0	-641.226	-641.265
Anisole	-346.680	0	-346.545	-346.576
$Me_3Si–anisole^+$	-755.752	0	-755.503	-755.544
2-pentanone	-271.727	0	-271.584	-271.617
$Me_3Si–2\text{-pentanone}^+$	-680.812	0	-680.554	-680.596
Cyclohexenone	-308.596	0	-308.468	-308.498
$Me_3Si–cyclohexenone^+$	-717.687	0	-717.444	-717.484
Cyclohexeneoxide	-309.786	0	-309.633	-309.622
$Me_3Si–cyclohexeneoxide^+$	-718.873	0	-718.606	-718.646
$AsPh_3$	-2928.587	0	-2928.311	-2928.357
$Me_3Si–AsPh_3^+$	-3337.685	0	-3337.293	-3337.349
Cyclohexanone	-309.828	0	-309.676	-309.706
$Me_3Si–cyclohexanone^+$	-718.913	0	-718.646	-718.687
Dabco	-345.260	0	-345.074	-345.105
$Me_3Si–Dabco^+$	-754.373	0	-754.070	-754.109
Cis-2,5-Me_2-THF	-311.025	0	-310.851	-310.883
$Me_3Si–Cis\text{-}2,5\text{-}Me_2\text{-}THF^+$	-720.117	0	-719.827	-719.867
trans-2,5-Me_2-THF	-311.025	0	-310.851	-310.883
$Me_3Si–trans\text{-}2,5\text{-}Me_2\text{-}THF^+$	-720.111	0	-719.821	-719.862
Dioxane	-307.591	0	-307.467	-307.496
$Me_3Si–dioxane^+$	-716.671	0	-716.432	-716.470
3-penten-2-one	-270.493	0	-270.375	-270.408
$Me_3Si–3\text{-penten-2one}^+$	-679.583	0	-679.350	-679.392
Methylbutyrate	-346.939	0	-346.790	-346.824
$Me_3Si–methylbutyrate^+$	-756.022	0	-755.758	-755.801
Et_2O	-233.612	0	-233.475	-233.504
$Me_3Si–OEt_2^+$	-642.695	0	-642.441	-642.481
EtOH	-155.011	0	-154.931	-154.956
$Me_3Si–ethanol^+$	-564.093	0	-563.897	-563.935
Hexylmethylether	-351.525	0	-351.302	-351.339

Me_3Si–hexylmethylether$^+$	-760.609	0	-760.268	-760.314
H-PPh_3^+	-1036.527	0	-1036.239	-1036.286
Imine	-657.118	0	-656.914	-656.954
iPrCOOH	-307.645	0	-307.525	-307.556
Me_3Si–iPrCOOH$^+$	-716.730	0	-716.495	-716.537
iPrCOO-$SiMe_3$	-716.322	0	-716.100	-716.142
Lutidine	-326.841	0	-326.696	-326.728
Me_3Si–lutidine$^+$	-735.931	0	-735.667	-735.707
Methylcrotonate	-345.705	0	-345.850	-345.613
Me_3Si–methylcrotonate$^+$	-754.790	0	-754.551	-754.596
Methyl-(E)-3-(oxiran-2-yl)acrylate	-458.957	0	-458.821	-458.856
Me_3Si–Methyl-(E)-3-(oxiran-2-yl)acrylate$^+$	-868.039	0	-867.788	-867.834
$MeOSiMe_3$	-524.371	0	-524.217	-524.251
Me_3Si–$MeOSiMe_3^+$	-933.458	0	-933.187	-933.230
$EtOSiMe_3$	-563.682	0	-563.498	-563.535
Me_3Si–$EtOSiMe_3^+$	-972.770	0	-972.470	-972.514
N-Me-acetamide	-248.476	0	-248.373	-248.403
Me_3Si–N-Me-acetamide$^+$	-657.574	0	-657.355	-675.396
N-Me-piperidine	-291.153	0	-290.964	-290.995
Me_3Si–N-Me-piperidine$^+$	-700.265	0	-699.959	-699.998
N,N-dimethylaniline	-366.123	0	-365.947	-365.981
Me_3Si–N,N,-dimethylaniline$^+$	-775.217	0	-774.925	-774.966
THF	-232.400	0	-232.282	-232.311
Me_3Si–THF$^+$	-641.490	0	-641.257	-641.296
Tetrahydropyran	-271.713	0	-271.566	-271.594
Me_3Si–tetrahydropyran$^+$	-680.800	0	-680.536	-680.575
Tetrahydrothiophene	-555.388	0	-555.274	-555.302
Me_3Si–tetrahydrothiophene$^+$	-964.471	0	-964.241	-964.279
4H-chromene	-422.862	0	-422.714	-422.747
Me_3Si–4H-chromene$^+$	-831.925	0	-831.663	-831.704
Chroman	-424.096	0	-423.925	-423.957
Me_3Si–chroman$^+$	-833.168	0	-832.881	-832.923
Isochroman	-424.089	0	-423.918	-423.950
Me_3Si–isochroman$^+$	-833.172	0	-832.885	-832.927
N,N-dimethylacetamide	-287.770	0	-287.638	-287.669
Me_3Si–N,N-dimethylacetamide$^+$	-696.873	0	-696.626	-696.669
N-acetyl-pyrrolidine	-365.181	0	-365.012	-365.044
Me_3Si–N-acetyl-pyrrolidine$^+$	-774.287	0	-774.001	-774.044
Benzaldehyde	-345.480	0	-345.369	-345.399
Me_3Si–Benzaldehyde$^+$	-754.564	0	-754.338	-754.380

Benzaldehyde dimethylacetal	-500.480	0	-500.285	-500.323
Me_3Si–Benzaldehyde dimethylacetal$^+$	-909.563	0	-909.252	-909.299
Isosorbide	-1352.743	0	-1352.372	-1352.429
Me_3Si–isosorbide$^+$ Isomer1	-1761.832	0	-1761.344	-1761.406
Me_3Si–isosorbide$^+$ Isomer2	-1761.833	0	-1761.345	-1761.410
Isomannide	-1761.832	0	-1761.343	-1761.404
Me_3Si–isomannide$^+$	-1352.741	0	-1352.368	-1352.420
Alpha-Me-glucose	-2361.018	0	-2360.382	-2360.462
Me_3Si–Alpha-Me-glucose$^+$	-2270.102	0	-2769.350	-2769.434
Beta-Me-glucose	-2361.017	0	-2360.380	-2360.456
Me_3Si–Beta-Me-glucose$^+$	-2770.107	0	-2769.354	-2769.438
Glucose-oxocarbenium$^+$	-2245.700	0	-2245.108	-2245.184
Me_3Si^+	-409.015	0	-408.904	-408.935

4. Optimized Coordinates and Gibbs free energies

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Me_3Si–PPh_3^+. Gibbs free energy: -1444.851922

P	-0.00050700	0.00965100	0.17536700
C	1.58420200	0.60322300	-0.47449900
C	1.62732200	1.52091700	-1.52798000
C	2.77434700	0.10698100	0.07264700
C	2.85776600	1.93876300	-2.02955700
H	0.71084900	1.91095500	-1.95841000
C	3.99877600	0.52622900	-0.43564600
H	2.75569800	-0.61399200	0.88437700
C	4.04064000	1.44289000	-1.48603300
H	2.88852500	2.65257900	-2.84557000
H	4.91758800	0.13702600	-0.01077000
H	4.99654600	1.77109400	-1.88056400
C	-1.30921000	1.08433800	-0.47158800
C	-1.43856100	2.37676800	0.05292600
C	-2.16662200	0.65082500	-1.48647000
C	-2.42279700	3.22823300	-0.43559100
H	-0.76899600	2.73008000	0.83146200
C	-3.15200100	1.50921400	-1.96960300
H	-2.06894700	-0.34622500	-1.90297100
C	-3.28181500	2.79294500	-1.44490000
H	-2.52084700	4.22756700	-0.02580700
H	-3.81805200	1.17111800	-2.75603300
H	-4.05173100	3.45766700	-1.82235900
C	-0.27571900	-1.66806000	-0.45540700
C	0.59956500	-2.24067100	-1.38169900
C	-1.38338300	-2.39253800	0.00443500
C	0.36636300	-3.53420800	-1.84364000

H	1.45910100	-1.68774300	-1.74531000
C	-1.61142400	-3.68139000	-0.46403700
H	-2.07754200	-1.95536000	0.71604700
C	-0.73498500	-4.25335900	-1.38665600
H	1.04802500	-3.97592300	-2.56240700
H	-2.47164600	-4.23753600	-0.10777500
H	-0.91252700	-5.26043300	-1.74903300
Si	-0.01181200	0.00755900	2.50877900
C	0.72018300	-1.64059800	2.99706800
H	0.62490100	-1.74745900	4.08323300
H	0.18971300	-2.47404900	2.52807700
H	1.78155300	-1.71770900	2.74585600
C	-1.80892000	0.18772300	2.98800400
H	-1.86310400	0.28355800	4.07811300
H	-2.25866200	1.08224600	2.54844700
H	-2.40626800	-0.68145400	2.69956300
C	1.03328700	1.46804400	3.02524600
H	1.16759100	1.42138200	4.11165000
H	2.02327600	1.44974600	2.56187000
H	0.55450400	2.42226600	2.78942300

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PPh_3. Gibbs free energy: -1035.86317

P	-0.05237900	-0.04147700	-1.25474200
C	0.56823600	1.51906600	-0.49374000
C	1.43682000	1.56641700	0.60205500
C	0.13004700	2.72402400	-1.05946400
C	1.85230500	2.79108000	1.12417700
H	1.79208900	0.64557000	1.05446200
C	0.53332900	3.94768100	-0.53013400
H	-0.53616900	2.70659800	-1.91867700
C	1.39850200	3.98347700	0.56333300
H	2.52898700	2.81111300	1.97301300
H	0.17868200	4.87144800	-0.97653700
H	1.72093300	4.93552100	0.97321700
C	1.02104200	-1.30351600	-0.44798700
C	2.26784200	-1.54664200	-1.04014900
C	0.67140700	-2.01846300	0.70265800
C	3.15430700	-2.46545400	-0.48409300
H	2.55061500	-1.00987900	-1.94251900
C	1.55288300	-2.94942900	1.25232200
H	-0.29055500	-1.85036100	1.17731200
C	2.79665800	-3.17170600	0.66431500
H	4.11898500	-2.63576600	-0.95176500
H	1.26704500	-3.49704500	2.14521900
H	3.48254200	-3.89454400	1.09498000
C	-1.65577500	-0.27661500	-0.37729700
C	-2.02182800	0.41934800	0.78013700
C	-2.55226100	-1.20943100	-0.91549000

C	-3.25415400	0.18426000	1.38814700
H	-1.34362700	1.14883400	1.21216600
C	-3.77866600	-1.45456200	-0.30148700
H	-2.29020400	-1.74886700	-1.82246800
C	-4.13343100	-0.75472200	0.85148700
H	-3.52479700	0.73355600	2.28469100
H	-4.46052300	-2.18349900	-0.72834400
H	-5.09263400	-0.93646800	1.32598900

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2-Me-THF. Gibbs free energy: -271.596066

C	1.35061200	-0.83310900	-0.20690500
O	-0.01015200	-1.13983400	0.11512900
C	-0.74117200	0.06260800	0.40649100
C	0.12452400	1.19690900	-0.14022000
C	1.53712300	0.65665500	0.08563200
H	2.00829400	-1.47313000	0.38914000
H	1.51934400	-1.05228200	-1.26902300
H	-0.81807000	0.15902300	1.50062800
H	-0.06993500	1.33353200	-1.21094900
H	-0.06638700	2.14499800	0.36828900
H	2.28813600	1.11576400	-0.56126500
H	1.84044300	0.80955700	1.12653100
C	-2.13287400	-0.03881900	-0.18761700
H	-2.66723600	-0.90129100	0.22060100
H	-2.70793500	0.86284000	0.04633900
H	-2.07471400	-0.14579700	-1.27560500

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Me_3Si–2-Me-THF^+. Gibbs free energy: -680.579885

C	1.05464100	-1.43260900	-0.55170300
O	0.36055000	-0.23151500	-0.04403400
C	1.35391900	0.81085500	0.40304100
C	2.69595100	0.12639300	0.16467000
C	2.38665700	-1.36990300	0.16128400
H	0.44274100	-2.29447000	-0.29629800
H	1.13795100	-1.32148500	-1.63439300
H	1.14713800	0.93754500	1.46712500
H	3.10144200	0.43406100	-0.80412000
H	3.40933500	0.40926500	0.93987500
H	3.14379800	-1.95244800	-0.36542100
H	2.28814400	-1.75808600	1.17826600
C	1.15675800	2.09214500	-0.37264100
H	0.20062100	2.57391200	-0.16101000
H	1.94741100	2.78741100	-0.07700500
H	1.24284400	1.91034600	-1.44703900
Si	-1.44609900	-0.05000700	0.04132200
C	-1.93485600	0.73178100	-1.57041800
H	-3.02771600	0.77871600	-1.62894800
H	-1.54678900	1.74798900	-1.67434300

H	-1.57870200	0.13316300	-2.41431400
C	-2.07394100	-1.78672300	0.24151600
H	-1.61731900	-2.29172600	1.09767500
H	-3.15190700	-1.72516000	0.42941700
H	-1.93251800	-2.39409800	-0.65645700
C	-1.71430700	0.99114500	1.55669000
H	-1.31700000	2.00491300	1.46608700
H	-2.79488700	1.07606200	1.71667600
H	-1.28252300	0.51780800	2.44334800

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$Me_2EtSi–PPh_3^+$. Gibbs free energy: -1484.128609

P	-0.00440300	-0.00789300	0.17802000
C	1.57869600	0.59329600	-0.46948300
C	1.62068700	1.54467200	-1.49237300
C	2.76945700	0.07330400	0.05427700
C	2.85064900	1.97263900	-1.98700100
H	0.70405600	1.95307600	-1.90513400
C	3.99303200	0.50296500	-0.44685000
H	2.75179600	-0.67350500	0.84245100
C	4.03391800	1.45370100	-1.46666200
H	2.88054400	2.71223200	-2.77969400
H	4.91208900	0.09573800	-0.03975500
H	4.98929200	1.79020400	-1.85545700
C	-1.31873900	1.06407600	-0.46160200
C	-1.48331900	2.33856600	0.09522500
C	-2.14321500	0.64631300	-1.51029600
C	-2.46827700	3.18827700	-0.39496500
H	-0.84264300	2.67929100	0.90286100
C	-3.12955600	1.50245600	-1.99496800
H	-2.01969800	-0.33750800	-1.95080900
C	-3.29325400	2.76903700	-1.43864100
H	-2.59295600	4.17373000	0.04032000
H	-3.76961800	1.17631500	-2.80760200
H	-4.06366800	3.43230900	-1.81760900
C	-0.27740300	-1.68192600	-0.46329700
C	0.59392800	-2.24532600	-1.39880900
C	-1.38378700	-2.41017800	-0.00645600
C	0.35837000	-3.53399200	-1.87298300
H	1.45182300	-1.68879500	-1.76073900
C	-1.61417500	-3.69411200	-0.48720600
H	-2.07529900	-1.97944300	0.71172700
C	-0.74163000	-4.25710500	-1.41907500
H	1.03686600	-3.96847600	-2.59911400
H	-2.47338800	-4.25349700	-0.13357400
H	-0.92133700	-5.26012700	-1.79147300
Si	0.00438600	-0.01514100	2.50942700
C	0.72513800	-1.67006000	2.99614100
H	0.61942500	-1.78758700	4.08011700

H	0.19530200	-2.49800200	2.51661600
H	1.78836200	-1.74910600	2.75288500
C	-1.78530300	0.17355600	3.01580300
H	-1.82796200	0.24415500	4.10832700
H	-2.23489500	1.07959900	2.60085300
H	-2.39190300	-0.68546800	2.71618000
C	1.07868000	1.44023500	3.01313400
H	2.07019100	1.32506400	2.56120700
H	0.66141100	2.36873000	2.60682700
C	1.20784100	1.55203700	4.54264400
H	1.65868600	0.65334700	4.97483400
H	1.84278000	2.40080000	4.81180800
H	0.23505800	1.70329100	5.02042500

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Me_2EtSi–2-Me-THF^+. Gibbs free energy: -719.854163

C	1.09638300	-1.40691800	-0.74308500
O	0.62423200	-0.06939100	-0.31595800
C	1.79157500	0.75208100	0.18335200
C	2.97330700	-0.20404100	0.05176400
C	2.35707500	-1.60235200	0.06678300
H	0.30267500	-2.12380400	-0.53787900
H	1.27491600	-1.33878900	-1.81677500
H	1.56275400	0.95713200	1.23156100
H	3.48931900	-0.02604400	-0.89656100
H	3.68373500	-0.04521500	0.86422300
H	3.00710500	-2.35311800	-0.38464700
H	2.11042400	-1.91636700	1.08494700
C	1.89617000	2.01336000	-0.63843100
H	1.03448400	2.66832600	-0.50768600
H	2.78789800	2.55639400	-0.31206900
H	2.00981900	1.76999300	-1.69775700
Si	-1.06983100	0.09444500	0.33362500
C	-1.29473100	1.90110200	0.69616700
H	-2.27534000	2.01540100	1.17220300
H	-0.55037300	2.29433900	1.39384300
H	-1.29541700	2.50535400	-0.21478600
C	-2.12072100	-0.51990300	-1.07821000
H	-1.94028800	-1.58787600	-1.24381300
H	-1.80888600	-0.00079500	-1.99214700
C	-1.08802500	-0.97111000	1.85750200
H	-0.34647900	-0.63518200	2.58854800
H	-2.07460300	-0.89720900	2.32785400
H	-0.90631500	-2.02589600	1.63255500
C	-3.62063500	-0.28146600	-0.82110700
H	-4.21526100	-0.65128700	-1.66044800
H	-3.96466600	-0.79998200	0.07935500
H	-3.84411300	0.78299100	-0.70201300

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$Et_3Si–PPh_3^+$. Gibbs free energy: -1562.674398

P	0.02187900	-0.14425800	0.17781400
C	1.55827700	0.56406300	-0.47625400
C	1.53207000	1.57039800	-1.44497500
C	2.78302400	0.07441800	-0.00437800
C	2.72995500	2.08393600	-1.93766000
H	0.58853000	1.95567800	-1.81745000
C	3.97405900	0.58926400	-0.50325700
H	2.81560400	-0.71378200	0.74239000
C	3.94721700	1.59588100	-1.46862700
H	2.70825900	2.86523100	-2.68956500
H	4.91985000	0.20568600	-0.13631400
H	4.87685300	2.00001600	-1.85535800
C	-1.36158300	0.88582100	-0.38729500
C	-1.58530700	2.12112000	0.23338700
C	-2.18978200	0.47048000	-1.43444900
C	-2.63504900	2.93013200	-0.18623500
H	-0.94059000	2.46463900	1.03583700
C	-3.24128400	1.28483400	-1.84799800
H	-2.02241600	-0.48167300	-1.92625800
C	-3.46606200	2.51006700	-1.22443700
H	-2.80331900	3.88564900	0.29827000
H	-3.88426800	0.95833500	-2.65816500
H	-4.28788800	3.14021800	-1.54783300
C	-0.18233700	-1.79178500	-0.56011200
C	0.74820600	-2.28359800	-1.47926400
C	-1.29120100	-2.56966900	-0.20486700
C	0.56999500	-3.54926900	-2.03439500
H	1.60826000	-1.68997900	-1.76903000
C	-1.46563300	-3.82840800	-0.76633100
H	-2.02201300	-2.20161100	0.50655700
C	-0.53308400	-4.32104200	-1.67944200
H	1.29505100	-3.92628300	-2.74753800
H	-2.32730300	-4.42505100	-0.48716000
H	-0.66908400	-5.30517500	-2.11535400
Si	0.12371500	-0.11979300	2.51870900
C	0.98949300	-1.67281500	3.12949600
H	0.92726400	-1.57342500	4.22285000
C	-1.62505200	0.13607500	3.16418300
H	-1.52957200	-0.01528200	4.24837200
H	-1.86258200	1.19884500	3.03522600
C	1.18395900	1.38692800	2.90974300
H	2.17523500	1.25738100	2.46172400
H	0.75456000	2.28273100	2.44700800
C	1.31941900	1.60685300	4.42748900
H	1.79590900	0.75236000	4.91775300
H	1.93422400	2.48781000	4.63232100
H	0.34641600	1.76715300	4.90213900

C	-2.77825700	-0.71868700	2.62719500
H	-2.97052500	-0.51007300	1.56957200
H	-2.58450800	-1.78933900	2.74066800
H	-3.70203800	-0.49639000	3.16844000
H	2.05644100	-1.57552600	2.89383700
C	0.48119200	-3.05827000	2.71232600
H	-0.59090000	-3.17578700	2.89583200
H	0.66039300	-3.24724300	1.65146200
H	0.99866000	-3.83749200	3.27919900

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Et_3Si–2-Me-THF^+. Gibbs free energy: -798.403282

C	1.40659900	-0.84168000	-1.43603700
O	0.77516800	0.10579100	-0.48864700
C	1.84018300	0.81273500	0.32008200
C	3.13648400	0.18941500	-0.19001100
C	2.73017800	-1.15936800	-0.78012600
H	0.73847100	-1.69376900	-1.54931800
H	1.50672500	-0.31074500	-2.38337500
H	1.63951300	0.53056900	1.35548600
H	3.57180600	0.82820700	-0.96444600
H	3.85843100	0.09661800	0.62271100
H	3.45208000	-1.53287900	-1.50776100
H	2.59910000	-1.91512300	-0.00070100
C	1.73482100	2.30275000	0.10542700
H	0.83006000	2.72713300	0.53988700
H	2.59400600	2.77369100	0.59172400
H	1.77197800	2.53781100	-0.96146700
Si	-0.92344000	-0.24624600	0.08666400
C	-1.42041700	1.19012300	1.17058500
H	-2.21262000	0.78994300	1.81833200
H	-0.60866600	1.45456200	1.85784000
C	-1.89704600	-0.34287100	-1.50148600
H	-1.46801600	-1.09320600	-2.17403300
H	-1.81212100	0.62205300	-2.01523200
C	-0.78907900	-1.86368500	1.00788400
H	-1.82015200	-2.12406900	1.28405800
H	-0.46502000	-2.65342300	0.31942900
C	-3.37793600	-0.67625600	-1.23686500
H	-3.94150900	-0.67799100	-2.17345800
H	-3.49221300	-1.66430300	-0.78099400
H	-3.85005500	0.05374200	-0.57148600
C	0.09552600	-1.84926100	2.26396400
H	0.03579800	-2.80685000	2.78790800
H	1.14855600	-1.68327800	2.01643400
H	-0.21079800	-1.06896500	2.96760200
C	-1.94150000	2.43063800	0.42704100
H	-2.85699900	2.20432300	-0.12667000
H	-2.17325400	3.23219300	1.13323700

H	-1.21515800	2.81964200	-0.29258000

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$Me_2PhSi–PPh_3^+$. Gibbs free energy: -1636.48249

P	-0.06537800	-0.04757600	0.20344100
C	1.56675200	0.53331000	-0.33639500
C	1.74058300	1.79463700	-0.90853100
C	2.67851200	-0.27734900	-0.06993000
C	3.02481300	2.24659400	-1.20509200
H	0.88690900	2.42800600	-1.12436100
C	3.95641800	0.18106000	-0.36759100
H	2.55175000	-1.26598900	0.36179800
C	4.13039200	1.44611300	-0.92988900
H	3.15747000	3.22633800	-1.65105200
H	4.81484700	-0.44826300	-0.15920100
H	5.12894800	1.80472400	-1.15652800
C	-1.35456100	1.03334300	-0.47342800
C	-1.51460800	2.32311000	0.05087600
C	-2.19762600	0.58349200	-1.49467000
C	-2.50880800	3.15657800	-0.44979000
H	-0.86474400	2.68658600	0.84066800
C	-3.19179500	1.42463200	-1.98880500
H	-2.08586600	-0.41455000	-1.90517300
C	-3.34899100	2.70720400	-1.46768400
H	-2.62774700	4.15385700	-0.04029900
H	-3.84575900	1.07315200	-2.77953100
H	-4.12655500	3.35784500	-1.85391300
C	-0.30286300	-1.71243400	-0.46879900
C	0.33918800	-2.09120900	-1.65341400
C	-1.16893200	-2.60416000	0.17370000
C	0.11792200	-3.35816100	-2.18436000
H	1.00847100	-1.40524900	-2.16219200
C	-1.38591400	-3.86938300	-0.36329400
H	-1.68358600	-2.32039900	1.08554100
C	-0.74102800	-4.24679800	-1.53980800
H	0.61762800	-3.64918700	-3.10186400
H	-2.05544100	-4.55826700	0.13993200
H	-0.90803500	-5.23469900	-1.95588300
Si	-0.08437900	0.01189900	2.53561500
C	0.99917400	-1.41519500	3.05629700
H	0.92341900	-1.52534300	4.14319600
H	0.68381100	-2.35555700	2.59532300
H	2.05009600	-1.23982400	2.81018200
C	-1.87098800	-0.11231500	3.06051500
H	-1.93996300	0.11509000	4.12972400
H	-2.50678700	0.59418600	2.51905200
H	-2.27078800	-1.11864800	2.91184900
C	0.65575500	1.68498600	2.91863900
C	2.02523600	1.93135300	2.72774100

C	-0.14932500	2.73650900	3.38596600
C	2.56934900	3.18767100	2.98010800
H	2.68194200	1.14263900	2.37079900
C	0.39263200	3.99447100	3.64128500
H	-1.21236400	2.58167000	3.54990200
C	1.75188400	4.22228500	3.43336100
H	3.62902200	3.35883400	2.82056300
H	-0.24657600	4.79478600	4.00004100
H	2.17500600	5.20293300	3.62641900

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Me_2PhSi–2-Me-THF^+. Gibbs free energy: -872.208859

C	0.89712800	-1.49114200	-0.81904200
O	1.24648600	-0.24092200	-0.10963900
C	2.65254000	-0.30596800	0.42939400
C	3.10969000	-1.70110300	0.01575700
C	1.82260200	-2.50100200	-0.17973200
H	-0.16327500	-1.66726700	-0.65334500
H	1.10184200	-1.32495100	-1.87831200
H	2.52770600	-0.22365500	1.51053600
H	3.66722900	-1.64258600	-0.92416400
H	3.76397700	-2.12772800	0.77739400
H	1.96360000	-3.36985600	-0.82407400
H	1.41259900	-2.83537400	0.77692600
C	3.48348400	0.82171900	-0.13671700
H	3.15388900	1.80356300	0.20775400
H	4.51348100	0.68251200	0.20337400
H	3.47524500	0.79690100	-1.22958600
Si	0.11276800	1.16732000	0.09467700
C	0.43343500	2.26202900	-1.36870600
H	-0.32444100	3.05121400	-1.40845900
H	1.41456300	2.73860000	-1.29879500
H	0.38974100	1.69977600	-2.30623800
C	0.57214300	1.85920700	1.75514800
H	1.55907000	2.32783700	1.76236200
H	-0.16220300	2.63001700	2.01200800
H	0.54065800	1.09567300	2.53753100
C	-1.56147100	0.36407500	0.06981400
C	-2.05515500	-0.29389400	1.20864400
C	-2.35936600	0.39174700	-1.08491800
C	-3.30298200	-0.91093800	1.19131900
H	-1.46504400	-0.33052100	2.12052800
C	-3.60864500	-0.22449500	-1.10467200
H	-2.00783800	0.89432600	-1.98186700
C	-4.07941500	-0.87772400	0.03307200
H	-3.67081200	-1.41458100	2.07932700
H	-4.21248400	-0.19505200	-2.00586800
H	-5.05206800	-1.35901300	0.01843500

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$Ph_3Si–PPh_3^{+\cdot}$ Gibbs free energy: -2019.740903

P	0.05716200	-0.04158600	0.25324400
C	1.68272700	0.41733800	-0.40778600
C	1.80188200	1.43685900	-1.35689700
C	2.82987600	-0.23374600	0.06917400
C	3.06245900	1.80800800	-1.81867200
H	0.92190200	1.94394000	-1.73729700
C	4.08369000	0.14343800	-0.39805800
H	2.75295500	-1.03135600	0.80093600
C	4.20158700	1.16715500	-1.33796000
H	3.15009400	2.59955300	-2.55494800
H	4.96772800	-0.36110200	-0.02367600
H	5.18180200	1.46247100	-1.69733800
C	-1.18505500	1.09934300	-0.41261200
C	-1.19521900	2.43217100	0.02348700
C	-2.13005700	0.66066300	-1.34430000
C	-2.15413700	3.31199400	-0.46543100
H	-0.45983900	2.78939700	0.73737100
C	-3.08762500	1.54922400	-1.82772500
H	-2.12583600	-0.36557700	-1.69509300
C	-3.10349700	2.87018200	-1.38697400
H	-2.15955700	4.34133700	-0.12366800
H	-3.82029800	1.20509900	-2.54955000
H	-3.85314900	3.55856100	-1.76281700
C	-0.35160200	-1.72926400	-0.27185000
C	0.53595900	-2.47978700	-1.04771700
C	-1.55318600	-2.30201900	0.17096200
C	0.22969400	-3.80124200	-1.36495100
H	1.46342500	-2.04596700	-1.40485200
C	-1.85021600	-3.62104200	-0.15084400
H	-2.25756600	-1.72671200	0.76314000
C	-0.95609000	-4.37389800	-0.91189800
H	0.92164800	-4.38157000	-1.96557600
H	-2.77851400	-4.06044300	0.19769100
H	-1.18585100	-5.40633100	-1.15342000
Si	0.07464900	0.02994100	2.58895400
C	0.50937600	1.79586300	3.00148400
C	1.69076600	2.38510300	2.51735200
C	-0.36191800	2.58067900	3.77189200
C	1.98139100	3.71990400	2.78179100
H	2.39070500	1.80585800	1.92118600
C	-0.06906100	3.91635300	4.04107400
H	-1.27950100	2.15272300	4.16522800
C	1.09882600	4.48831900	3.54086900
H	2.89416200	4.16009200	2.39380600
H	-0.75367900	4.50948500	4.63853900
H	1.32220500	5.53093300	3.74311000
C	-1.66406600	-0.46409300	3.04720500

C	-2.76541900	0.30649500	2.63382000
C	-1.90845300	-1.65428300	3.74859600
C	-4.06683100	-0.10999600	2.89698300
H	-2.61524400	1.23809600	2.09489400
C	-3.21126500	-2.07158400	4.01365100
H	-1.08070600	-2.26929600	4.08884500
C	-4.29108200	-1.30438800	3.58166500
H	-4.90418200	0.49533800	2.56548400
H	-3.38120800	-2.99847600	4.55169400
H	-5.30602000	-1.63333400	3.78059600
C	1.38446900	-1.21472900	3.05302300
C	1.27374800	-2.56556100	2.67761100
C	2.53600100	-0.80568400	3.74302200
C	2.28655300	-3.47301200	2.97251700
H	0.39549000	-2.92013400	2.14501900
C	3.54999100	-1.71432900	4.03958100
H	2.65184300	0.23035300	4.04775400
C	3.42839700	-3.04669800	3.65070000
H	2.18389900	-4.51095300	2.67321400
H	4.43494200	-1.38005600	4.57119300
H	4.21945500	-3.75392400	3.87849000

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Ph_3Si–2-Me-THF^+. Gibbs free energy: -1255.460198

C	-1.11448300	-0.27742500	2.49777800
O	-0.22646600	0.41842800	1.53755300
C	0.14936400	1.78578700	2.07778900
C	-0.72245300	1.91065800	3.32615300
C	-1.83410500	0.87187700	3.16173700
H	-1.74272300	-0.95626800	1.92438000
H	-0.46938400	-0.83379100	3.17974800
H	-0.15649600	2.47620600	1.29127800
H	-0.12711300	1.68804000	4.21655400
H	-1.10976300	2.92628700	3.41829000
H	-2.26868800	0.57065000	4.11578800
H	-2.63337400	1.24069400	2.51323600
C	1.63647400	1.83136400	2.32605900
H	2.20936700	1.72412800	1.40376100
H	1.87472500	2.80615600	2.76137400
H	1.93664100	1.05731200	3.03719800
Si	-0.00424600	-0.14569900	-0.16549500
C	-1.71039000	-0.70566400	-0.64768600
C	-2.82475100	0.13904900	-0.50024400
C	-1.91170100	-1.98755000	-1.18075100
C	-4.09481500	-0.28012200	-0.88277000
H	-2.71378100	1.13071700	-0.06902800
C	-3.18251400	-2.40657100	-1.57103400
H	-1.07672600	-2.67403200	-1.28782600
C	-4.27344100	-1.55322900	-1.42439500

H	-4.94305200	0.38502600	-0.75853000
H	-3.31943900	-3.40000500	-1.98537400
H	-5.26350500	-1.88045000	-1.72543900
C	0.63212400	1.32921800	-1.09674000
C	2.01527700	1.48589500	-1.28660100
C	-0.23202600	2.28766900	-1.65154700
C	2.52033200	2.57745100	-1.98801600
H	2.70726200	0.74707700	-0.89042000
C	0.27134500	3.38155900	-2.34952800
H	-1.30753000	2.18371400	-1.54765700
C	1.64803200	3.52845100	-2.51498500
H	3.59117800	2.68429000	-2.12572800
H	-0.41016500	4.11489800	-2.76794300
H	2.04057500	4.38052200	-3.06063500
C	1.25724100	-1.50092500	-0.03668800
C	1.84607200	-1.87131700	1.18015400
C	1.66372000	-2.16565800	-1.20641000
C	2.80535300	-2.88056200	1.23174000
H	1.56966300	-1.36752600	2.10091900
C	2.61977600	-3.17600500	-1.15678900
H	1.23951400	-1.89303400	-2.16999100
C	3.19073100	-3.53512300	0.06389600
H	3.25310500	-3.15142100	2.18228700
H	2.92131500	-3.67930700	-2.06952200
H	3.93861000	-4.32047700	0.10306500

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P^tBu_3. Gibbs free energy: -814.455735

P	-0.00014400	0.00016200	0.70509400
C	1.44859900	1.05506800	0.00844600
C	2.68889100	0.76568500	0.88333100
C	1.81961500	0.84949200	-1.46899500
C	1.14342300	2.54988500	0.22470000
H	2.47214800	0.93122800	1.94351700
H	3.07071100	-0.24808900	0.77080200
H	3.49531100	1.45092800	0.59349400
H	0.97869500	1.03796300	-2.13947800
H	2.62208100	1.54855400	-1.73799000
H	2.19185700	-0.15746800	-1.66791300
H	2.05285800	3.12479100	0.01267600
H	0.36460100	2.92695200	-0.43977200
H	0.85631500	2.76122100	1.25978300
C	-1.63768600	0.72714600	0.00833700
C	-2.01176300	1.94123700	0.88727200
C	-1.64286800	1.15583500	-1.46772500
C	-2.77902500	-0.28651700	0.21725300
H	-2.06721800	1.66156000	1.94420200
H	-1.31790600	2.77561300	0.79494000
H	-3.00113800	2.30606300	0.58424100

H	-1.37444000	0.33824000	-2.13997900
H	-2.65170800	1.49182600	-1.73992800
H	-0.96485700	1.98941800	-1.66148100
H	-3.73164200	0.21546000	0.00950500
H	-2.71683500	-1.14318700	-0.45544300
H	-2.81874600	-0.65122300	1.24867800
C	0.18856700	-1.78141500	0.00868400
C	-0.67855500	-2.71095300	0.88693600
C	-0.17604500	-2.00216900	-1.46844200
C	1.63696000	-2.26288900	0.22113100
H	-0.42664000	-2.60111800	1.94666700
H	-1.74843300	-2.54024500	0.77492300
H	-0.48399400	-3.75235500	0.60162500
H	0.40148800	-1.36250700	-2.13908600
H	0.03762100	-3.04465500	-1.73763100
H	-1.23607700	-1.83062500	-1.66616700
H	1.67776700	-3.33980100	0.01884600
H	2.34830000	-1.78355700	-0.45325900
H	1.97135700	-2.10983800	1.25225300

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$Me_3Si–P^tBu_3^+$. Gibbs free energy: -1223.45397

P	0.27588100	-0.00032900	0.00016100
C	0.87363900	-1.14685400	1.40928300
C	0.69507800	-2.62869900	1.02645100
C	2.35369100	-0.91446000	1.76312500
C	0.01639000	-0.91327200	2.67009200
H	-0.32816100	-2.87035300	0.73460800
H	1.37699200	-2.95239900	0.24027300
H	0.92497700	-3.22403700	1.91561200
H	2.53119800	0.06157600	2.21539700
H	2.64005900	-1.66806500	2.50382600
H	3.02063600	-1.03000100	0.90823000
H	0.42177400	-1.54439300	3.46715200
H	0.03428200	0.11298200	3.03141900
H	-1.02245600	-1.21519500	2.52310300
C	0.87042300	1.79400800	0.28925300
C	0.68610900	2.20388200	1.76324500
C	2.35172700	1.98835400	-0.08357800
C	0.01297100	2.76838900	-0.54453500
H	-0.33742200	2.06831800	2.11587400
H	1.36779900	1.68852500	2.43961400
H	0.91177400	3.27246600	1.83443900
H	2.53516700	1.88427300	-1.15332000
H	2.63089500	3.01060000	0.19158600
H	3.01922500	1.31322600	0.45292200
H	0.41531400	3.77473600	-0.39151700
H	0.03462300	2.57221900	-1.61475900
H	-1.02692400	2.78873500	-0.21269100

C	0.87566600	-0.64586700	-1.69669000
C	0.69447700	0.42685400	-2.78775900
C	2.35715900	-1.06392900	-1.67291400
C	0.02217500	-1.85654400	-2.12704800
H	-0.32939200	0.79847200	-2.85168900
H	1.37376100	1.27148500	-2.67392100
H	0.92646100	-0.04299900	-3.74866500
H	2.53746100	-1.94276400	-1.05318300
H	2.64405500	-1.32843100	-2.69581500
H	3.02153500	-0.26377700	-1.34484000
H	0.42930400	-2.22761900	-3.07284200
H	0.04226500	-2.68427700	-1.42096000
H	-1.01760500	-1.58128200	-2.31489300
Si	-2.08149500	-0.00271800	-0.00145300
C	-2.70979700	1.05230400	1.41611800
H	-3.79664500	0.90782200	1.43634100
H	-2.32174800	0.75368500	2.39205800
H	-2.52635100	2.11996100	1.27481700
C	-2.70513900	0.69889900	-1.62521900
H	-2.52224100	0.04106000	-2.47800400
H	-3.79179900	0.79315700	-1.51215400
H	-2.31169300	1.69157800	-1.85347900
C	-2.70638400	-1.75915700	0.20240600
H	-3.79445300	-1.70395000	0.07721600
H	-2.32485800	-2.45088200	-0.55138300
H	-2.51419700	-2.17491100	1.19417500

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P(*p*-tol)$_3$. Gibbs free energy: -1153.715656

P	-0.01940300	-0.01086300	1.45826200
C	-1.63654200	-0.34465200	0.64485700
C	-1.79173100	-1.09238800	-0.52673400
C	-2.78255600	0.19722600	1.24033700
C	-3.05296300	-1.28315800	-1.08718900
H	-0.92351800	-1.52824000	-1.01221100
C	-4.03949700	0.01373100	0.67127300
H	-2.69324500	0.77324300	2.15842100
C	-4.19708100	-0.73369000	-0.50074800
H	-3.14690900	-1.86468800	-2.00085700
H	-4.91193700	0.45234200	1.14872600
C	1.09055700	-1.23112100	0.63938400
C	1.25331800	-2.47852100	1.25533800
C	1.77509800	-0.99046900	-0.55618600
C	2.06215000	-3.45737200	0.68547100
H	0.74230200	-2.68890100	2.19186100
C	2.59104700	-1.96970000	-1.11909000
H	1.67170800	-0.03255500	-1.05751800
C	2.74921000	-3.21784500	-0.50981400
H	2.16879800	-4.41879800	1.18129900

H	3.11001800	-1.75921300	-2.05076800
C	0.50216800	1.56042900	0.65125200
C	-0.11315200	2.12049500	-0.47253300
C	1.60385000	2.22633700	1.20336200
C	0.36714000	3.30467100	-1.02953400
H	-0.97012500	1.63003800	-0.92490500
C	2.08813500	3.40121600	0.63668200
H	2.09621000	1.81816500	2.08297700
C	1.47480500	3.96356500	-0.48821800
H	-0.12578900	3.71890600	-1.90544800
H	2.95147000	3.89176500	1.07881800
C	-5.56272100	-0.96721100	-1.09458900
H	-5.50437700	-1.11515500	-2.17612800
H	-6.02220500	-1.86312900	-0.66262100
H	-6.23188200	-0.12585400	-0.89558900
C	3.65859200	-4.26530400	-1.09993500
H	3.82372000	-4.09366700	-2.16661700
H	4.63581100	-4.25031500	-0.60510400
H	3.24148800	-5.26808100	-0.97182700
C	1.97371900	5.25813400	-1.07768600
H	1.47483300	6.11349900	-0.60874400
H	3.04891300	5.37811000	-0.92042600
H	1.77445500	5.30924700	-2.15147800

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$Me_3Si–P(p\text{-tol})_3^+$. Gibbs free energy: -1562.710617

P	-0.00951500	0.00831100	0.43169100
C	0.54801500	-1.60158700	-0.17895700
C	1.50232500	-1.69472900	-1.19599700
C	-0.01368700	-2.77118200	0.34630100
C	1.88362000	-2.94248000	-1.67724600
H	1.94635300	-0.79932800	-1.61886000
C	0.37387800	-4.01171100	-0.14424400
H	-0.76671100	-2.72458500	1.12741800
C	1.32976400	-4.11859100	-1.16128200
H	2.62384700	-3.00057800	-2.46970000
H	-0.07462100	-4.90976800	0.26963800
C	1.13066900	1.26757600	-0.19215700
C	2.40976800	1.37377600	0.37070500
C	0.76985700	2.11362800	-1.24230100
C	3.30738000	2.31363800	-0.11442300
H	2.71809500	0.71549200	1.17765000
C	1.67957800	3.05381200	-1.71999500
H	-0.21363700	2.04229400	-1.69525900
C	2.95655400	3.17123300	-1.16626400
H	4.29574700	2.38473600	0.32993200
H	1.38670800	3.70478600	-2.53824200
C	-1.64993600	0.33371500	-0.26204900
C	-2.20405200	-0.50807000	-1.22752400

C	-2.37264800	1.45404300	0.17174400
C	-3.46511100	-0.23132700	-1.75019200
H	-1.66108100	-1.37955000	-1.57818400
C	-3.62599100	1.72083600	-0.35925200
H	-1.95894200	2.13031500	0.91416500
C	-4.19469000	0.88179000	-1.32783400
H	-3.88297400	-0.89596900	-2.50026400
H	-4.17357500	2.59392400	-0.01664700
C	1.77056300	-5.46411800	-1.67241500
H	1.99276200	-5.42566900	-2.74181900
H	2.68129600	-5.78632900	-1.15652700
H	1.00459500	-6.22449500	-1.50312800
C	3.93779500	4.19512000	-1.67125300
H	3.58153300	4.67173000	-2.58683900
H	4.09583100	4.97599800	-0.92025800
H	4.90947000	3.73590600	-1.87412600
C	-5.55762100	1.18602300	-1.88963000
H	-6.30809000	1.20799300	-1.09363000
H	-5.56556600	2.16812600	-2.37218900
H	-5.86176500	0.43991700	-2.62650600
Si	-0.08634500	0.03970400	2.76003900
C	0.12992400	1.83379500	3.23728900
H	0.20299800	1.89295400	4.32885200
H	1.04411600	2.25919900	2.81415100
H	-0.71775800	2.45019800	2.92536400
C	1.32380300	-1.04713400	3.33042100
H	1.23834100	-1.17571400	4.41504100
H	1.28745000	-2.03764000	2.86887200
H	2.29999900	-0.60061600	3.12261000
C	-1.76750200	-0.64335700	3.20837400
H	-1.90447300	-0.53161600	4.28958800
H	-2.57388000	-0.10004500	2.70772300
H	-1.86247900	-1.70591100	2.96805100

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PCy_3. Gibbs free energy: -1046.572961

P	-0.35311500	0.01269100	0.31545800
C	-1.70640100	-0.74502900	-0.77712800
C	-2.40522500	-1.95413100	-0.12307600
C	-2.80390500	0.25272900	-1.19424100
H	-1.21090600	-1.08515100	-1.69522000
C	-3.27002700	-1.55336700	1.07729500
H	-1.69133400	-2.73222600	0.16218900
H	-3.05373300	-2.40814500	-0.88606100
C	-3.67253600	0.70129600	-0.01487600
H	-2.38328500	1.11114000	-1.72374700
H	-3.44617300	-0.26087500	-1.92392600
C	-4.31472800	-0.50274400	0.68364000
H	-2.62923500	-1.15092100	1.87229300

H	-3.76521600	-2.44031300	1.48811200
H	-4.44876300	1.39029100	-0.36674900
H	-3.05860400	1.25648300	0.70619600
H	-4.87480200	-0.17553100	1.56679600
H	-5.04149700	-0.96290800	-0.00087800
C	0.72037400	-1.52737700	0.53926900
C	1.08301900	-2.44110300	-0.64960700
C	1.90997800	-1.38979100	1.51994400
H	-0.02918500	-2.08068000	1.11989300
C	2.43969100	-2.15199700	-1.29324200
H	0.29685900	-2.43053100	-1.41000000
H	1.11394900	-3.47120600	-0.26450300
C	3.28617400	-1.17103700	0.88184700
H	1.70291300	-0.60480800	2.25684400
H	1.96427200	-2.33120200	2.08480800
C	3.55880000	-2.16642300	-0.24881100
H	2.41576200	-1.18426800	-1.80724800
H	2.63815300	-2.90491400	-2.06459500
H	4.05250500	-1.27151300	1.65924300
H	3.37794700	-0.15275400	0.49743800
H	4.52383800	-1.94725500	-0.71932900
H	3.63498000	-3.17900700	0.17268000
C	0.33561100	1.27226400	-0.91870500
C	-0.38512800	2.62869600	-0.70294200
C	1.84820600	1.53509900	-0.87908200
H	0.08763900	0.90460900	-1.92339800
C	0.07768600	3.37794700	0.55163900
H	-1.46976700	2.50482800	-0.65743500
H	-0.18134900	3.25289600	-1.58487100
C	2.31248800	2.24046500	0.39819500
H	2.40209400	0.61019400	-1.03420200
H	2.09045300	2.18217900	-1.73484500
C	1.59357600	3.57892400	0.57240200
H	-0.22078400	2.81027100	1.44220500
H	-0.43610800	4.34440100	0.60483500
H	3.39789900	2.38924400	0.36371000
H	2.10655500	1.60681500	1.27111700
H	1.90119200	4.06082500	1.50712200
H	1.88454200	4.25314900	-0.24547300

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$Me_3Si–PCy_3^+$. Gibbs free energy: -1455.566893

P	-0.25011600	-0.06081900	0.40462600
C	-1.64528500	-1.11786900	-0.30015000
C	-2.21073300	-2.20296300	0.64005700
C	-2.80655200	-0.41703300	-1.03112400
H	-1.07719300	-1.63190300	-1.08192100
C	-3.34766500	-1.72371400	1.54527200
H	-1.42721200	-2.68092100	1.23553200

H	-2.59938800	-2.99148700	-0.01622900
C	-3.90680400	0.10123100	-0.10831600
H	-2.45209000	0.36239400	-1.70797400
H	-3.24155300	-1.18716300	-1.68134100
C	-4.46257800	-1.02654200	0.76371600
H	-2.96167400	-1.03615000	2.30331500
H	-3.74741300	-2.58336500	2.09227000
H	-4.70522000	0.54243200	-0.71309900
H	-3.52268200	0.90414300	0.53083200
H	-5.21620600	-0.63775900	1.45622200
H	-4.96792800	-1.75887900	0.12048800
C	1.06613600	-1.38689400	0.63763800
C	1.44974000	-2.25812300	-0.57810700
C	2.33434500	-1.02663600	1.43918700
H	0.47762500	-2.03203300	1.30116900
C	2.59227500	-1.70452600	-1.42976000
H	0.58985000	-2.49306600	-1.20916200
H	1.77228300	-3.21751800	-0.15335800
C	3.49658800	-0.47527300	0.61377000
H	2.10946100	-0.35340800	2.26695800
H	2.66104900	-1.96650400	1.90238000
C	3.82512600	-1.37607000	-0.58116600
H	2.25635100	-0.82270000	-1.98471800
H	2.85497200	-2.45165500	-2.18539600
H	4.37317200	-0.39396800	1.26465100
H	3.27692900	0.54282400	0.28087800
H	4.59723200	-0.91023300	-1.20180300
H	4.24795700	-2.31665500	-0.20341700
C	0.00706300	1.20061500	-0.95684200
C	-0.99646800	2.37868700	-0.86638800
C	1.41730500	1.74934600	-1.22603100
H	-0.26235400	0.59661800	-1.83224900
C	-0.54107700	3.55009300	0.00857300
H	-1.98333400	2.04857600	-0.53426300
H	-1.12965600	2.74003200	-1.89362000
C	1.86206100	2.86565200	-0.28504500
H	2.15116900	0.94809600	-1.25201400
H	1.38214300	2.15502900	-2.24562200
C	0.87207100	4.02946000	-0.31955500
H	-0.58244200	3.26921400	1.06457200
H	-1.26092900	4.36622300	-0.10981100
H	2.85973500	3.20446600	-0.58226000
H	1.95821500	2.48780400	0.73976500
H	1.17413200	4.81053700	0.38545900
H	0.88329400	4.48007400	-1.32056100
Si	-0.58135800	0.75924000	2.58292300
C	-0.49786900	-0.77287300	3.66504500
H	0.52078500	-1.16448800	3.73357700

H	-0.80192600	-0.46968000	4.67350800
H	-1.15901800	-1.58370100	3.35277000
C	-2.22114400	1.65439300	2.74344400
H	-3.08043600	0.98269300	2.78176100
H	-2.17910000	2.19241200	3.69779000
H	-2.39263600	2.39543900	1.95924200
C	0.79059200	1.93252900	3.10082600
H	0.70276700	2.92426200	2.65361700
H	0.66836700	2.05032400	4.18474300
H	1.80191600	1.56072800	2.92648900

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P(*o*-tol)$_3$. Gibbs free energy: -1153.69451

P	-0.04857100	-0.03248400	-0.92309100
C	0.68801800	1.55365900	-0.33233100
C	1.61827200	1.79025000	0.70258700
C	0.24291300	2.63833800	-1.10588300
C	2.04879000	3.10625700	0.91576400
C	0.65896500	3.94179400	-0.85873700
H	-0.45478700	2.45331700	-1.91948800
C	1.57833200	4.17537900	0.15929300
H	2.76696800	3.29609400	1.70905200
H	0.28206700	4.75849400	-1.46601500
H	1.93270300	5.18111200	0.36275800
C	0.99359100	-1.41322500	-0.27997800
C	2.14191000	-1.58511100	-1.07058000
C	0.78016100	-2.28390700	0.81010800
C	3.09837300	-2.55250800	-0.78452500
H	2.29315500	-0.93321000	-1.92804900
C	1.74001500	-3.27292600	1.06267600
C	2.89094900	-3.40877600	0.29231200
H	3.98443700	-2.64322000	-1.40455300
H	1.58250900	-3.94750700	1.90011400
H	3.61530000	-4.18099800	0.53173600
C	-1.73838600	-0.19150000	-0.19931400
C	-2.32277200	0.47630700	0.89828900
C	-2.51517900	-1.10640400	-0.92897100
C	-3.65352400	0.17988300	1.22023700
C	-3.82585700	-1.40812900	-0.57640100
H	-2.07515400	-1.59874300	-1.79309400
C	-4.40136500	-0.75312400	0.50779400
H	-4.10977400	0.68856900	2.06534700
H	-4.39265600	-2.13227500	-1.15270500
H	-5.42767300	-0.95898100	0.79548900
C	-1.59402600	1.47262900	1.76510200
H	-0.66162400	1.06068700	2.15972600
H	-1.33353100	2.38037600	1.21406900
H	-2.21683000	1.75912200	2.61572800
C	2.15955800	0.71844500	1.61608200

H	1.35845700	0.12714700	2.06666400
H	2.80896900	0.01854300	1.08300900
H	2.73695800	1.17006000	2.42595900
C	-0.40210600	-2.19930600	1.74373200
H	-0.49551600	-1.20563900	2.19057100
H	-1.34545400	-2.40720400	1.23210900
H	-0.29087700	-2.92025800	2.55685800

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$Me_3Si–P(o\text{-tol})_3^+$. Gibbs free energy: -1562.6866

P	0.00861100	-0.01798500	0.02420800
C	1.61960400	0.65536700	-0.50111600
C	1.84188900	1.56489200	-1.55541900
C	2.70241700	0.16199100	0.24245400
C	3.16355000	1.96439400	-1.78955900
C	4.00417800	0.56066300	-0.02364000
H	2.53686400	-0.56612900	1.02974800
C	4.23158800	1.48089900	-1.04253100
H	3.35626800	2.66713500	-2.59451000
H	4.82508400	0.15876900	0.55950200
H	5.23981800	1.81490500	-1.26406100
C	-1.36530700	1.04217800	-0.53552000
C	-1.43143200	2.26515500	0.14924600
C	-2.29468100	0.75175200	-1.55486700
C	-2.40552600	3.20766000	-0.14433900
H	-0.69489000	2.50449100	0.90948000
C	-3.27881900	1.71348600	-1.81708500
C	-3.34385000	2.92077900	-1.13110600
H	-2.42885200	4.14984300	0.39160400
H	-4.00636100	1.50834200	-2.59642600
H	-4.11956100	3.63866900	-1.37578400
C	-0.19986900	-1.75043200	-0.50324900
C	0.48941900	-2.39083800	-1.55372500
C	-1.16866700	-2.45134100	0.23096300
C	0.18420000	-3.73584600	-1.79591900
C	-1.46331900	-3.77905900	-0.04199800
H	-1.72475500	-1.95216900	1.01750000
C	-0.77073800	-4.42770900	-1.05959600
H	0.70499100	-4.24730900	-2.59966900
H	-2.22170500	-4.29619300	0.53507000
H	-0.97664100	-5.46857500	-1.28597500
Si	-0.03412300	0.01597100	2.39023100
C	0.76125200	-1.56998900	2.98487400
H	0.57126600	-1.63801100	4.06227900
H	0.33754900	-2.45911900	2.51217200
H	1.84469200	-1.58014000	2.84101800
C	-1.83352400	0.13212100	2.89085500
H	-1.85475300	0.32004400	3.97054800
H	-2.34942900	0.95863200	2.39564400

H	-2.39111500	-0.78956900	2.70662300
C	0.93368300	1.52075500	2.93926500
H	1.11801200	1.40499900	4.01353900
H	1.90196000	1.60682500	2.44044200
H	0.38261200	2.45410800	2.79933000
C	-2.27764800	-0.48912800	-2.41319800
H	-1.30149800	-0.65043300	-2.87881400
H	-2.52144800	-1.38916100	-1.84376200
H	-3.01062600	-0.39138500	-3.21570000
C	1.49361500	-1.72393800	-2.46055100
H	1.10021200	-0.80307100	-2.89893400
H	2.41717800	-1.46905200	-1.93510700
H	1.74946700	-2.39376100	-3.28312900
C	0.77314500	2.10138600	-2.47546700
H	0.12463500	1.31084300	-2.86075000
H	0.13144200	2.83143300	-1.97512200
H	1.23714400	2.59199100	-3.33266000

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PPh_2(*p*-tol). Gibbs free energy: -1075.14702

P	-0.02484900	-0.01583600	1.45494800
C	-1.64209400	-0.34581900	0.63558800
C	-1.79589500	-1.13651200	-0.50830900
C	-2.78033700	0.23415300	1.21194100
C	-3.05761200	-1.33396100	-1.06853800
H	-0.92878900	-1.60076200	-0.96815400
C	-4.03951400	0.04776600	0.64630200
H	-2.68184800	0.83805700	2.11078800
C	-4.18076400	-0.73979800	-0.49609000
H	-3.16063600	-1.95068700	-1.95609100
H	-4.91000300	0.50860900	1.10267900
C	1.09033800	-1.22881100	0.63461100
C	1.26822400	-2.47085800	1.25688900
C	1.76125300	-0.99005000	-0.56928300
C	2.07909600	-3.44704600	0.68525900
H	0.76740000	-2.67920600	2.19924000
C	2.57938600	-1.96635700	-1.13351300
H	1.64576300	-0.03617500	-1.07569000
C	2.75274500	-3.20959700	-0.51790000
H	2.19746600	-4.40471300	1.18559400
H	3.08815500	-1.75785200	-2.07118100
C	0.49839000	1.55979400	0.65316700
C	-0.12659500	2.12847100	-0.46175300
C	1.60710000	2.21168000	1.20997400
C	0.35391900	3.31682900	-1.01269600
H	-0.98943200	1.64354700	-0.90844500
C	2.09554200	3.39063700	0.65308200
H	2.09670400	1.79057900	2.08478200
C	1.46740900	3.94747300	-0.46093500

H	-0.14071400	3.74595000	-1.87872300
H	2.96038000	3.87762200	1.09275100
C	3.66437800	-4.25368400	-1.11032800
H	3.82217600	-4.08448000	-2.17847400
H	4.64431200	-4.23125000	-0.62125200
H	3.25371500	-5.25834800	-0.97648200
H	-5.16161000	-0.89303700	-0.93512900
H	1.84245900	4.86928700	-0.89446800

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$Me_3Si–PPh_2$(*p*-tol)$^+$. Gibbs free energy: -1484.138497

P	-0.01198100	0.00553400	0.42698200
C	0.55053000	-1.60519500	-0.18724200
C	1.51827400	-1.69290900	-1.19179200
C	-0.02029900	-2.77071600	0.33963900
C	1.91086200	-2.94270100	-1.66556900
H	1.96465300	-0.79571400	-1.60771500
C	0.37464600	-4.01451200	-0.13994400
H	-0.78041900	-2.71677400	1.11313100
C	1.34127500	-4.10084600	-1.14186000
H	2.66204500	-3.00756300	-2.44520700
H	-0.07146700	-4.91416900	0.26967600
C	1.12777800	1.27060600	-0.19666900
C	2.41189600	1.36012700	0.35576600
C	0.74514600	2.13744600	-1.22375400
C	3.30541700	2.31394900	-0.11825600
H	2.72633600	0.68250000	1.14389600
C	1.64547500	3.09163900	-1.69273700
H	-0.24585900	2.07061500	-1.66025100
C	2.92101500	3.18166600	-1.14077000
H	4.29833200	2.38128400	0.31280000
H	1.34626000	3.76451400	-2.48906400
C	-1.65284100	0.32768700	-0.26483000
C	-2.20336800	-0.50672400	-1.23980000
C	-2.38018400	1.43938200	0.18148500
C	-3.46505400	-0.22983500	-1.75848100
H	-1.65816500	-1.37341100	-1.59860400
C	-3.63525400	1.70675100	-0.34681000
H	-1.97080400	2.10839400	0.93279200
C	-4.19890500	0.87747500	-1.32553600
H	-3.88206700	-0.88982600	-2.51318400
H	-4.18731500	2.57187900	0.00811000
C	-5.55124500	1.19054600	-1.90728500
H	-6.23737200	1.55454800	-1.13810600
H	-5.46486100	1.97355900	-2.66816800
H	-5.99414400	0.31142600	-2.38039900
Si	-0.08115700	0.03231800	2.75806800
C	0.14172900	1.82522500	3.23472900
H	0.21568600	1.88293700	4.32631900

H	1.05747800	2.24750500	2.81183500
H	-0.70376900	2.44519000	2.92416800
C	1.32768800	-1.05983700	3.32015100
H	1.24697500	-1.18630500	4.40541400
H	1.28442500	-2.05106600	2.86087800
H	2.30475100	-0.61791600	3.10711300
C	-1.76241700	-0.64828700	3.20831600
H	-1.89475000	-0.53917300	4.29039300
H	-2.56991400	-0.10229600	2.71261900
H	-1.86028800	-1.71005600	2.96587100
H	3.61884700	3.92750700	-1.50664600
H	1.64960200	-5.07206600	-1.51448300

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PPh_2*i*-Pr. Gibbs free energy: -922.7895

P	-0.00429900	-0.04645300	1.46143100
C	-1.65923200	-0.31935800	0.68972200
C	-1.88252300	-0.97941800	-0.52534500
C	-2.76654600	0.19130300	1.38122100
C	-3.17185900	-1.11803000	-1.03696700
H	-1.05261500	-1.39491200	-1.08821900
C	-4.05536900	0.06587800	0.86647600
H	-2.61897500	0.69350900	2.33419400
C	-4.26140000	-0.59148300	-0.34543000
H	-3.32262500	-1.63391500	-1.98026900
H	-4.89814200	0.47467400	1.41521400
C	0.51280100	1.53221000	0.65205000
C	0.25666700	1.82839200	-0.69300800
C	1.24154100	2.45211900	1.41428200
C	0.72600800	3.00965000	-1.26219300
H	-0.31703600	1.13651700	-1.30346000
C	1.71627100	3.63488300	0.84632700
H	1.44266400	2.24209500	2.46152000
C	1.45967500	3.91467400	-0.49384300
H	0.52059300	3.22337600	-2.30671000
H	2.28376300	4.33484700	1.45175600
H	-5.26442100	-0.69809400	-0.74661400
H	1.82691000	4.83412500	-0.93913700
C	1.10571100	-1.25958200	0.56855400
C	0.75015200	-2.69621300	0.96569000
C	2.57073500	-0.95005700	0.89610500
H	0.96918600	-1.13501600	-0.51284600
H	-0.29141300	-2.94430100	0.74139300
H	1.38840300	-3.40295200	0.42466200
H	0.91112200	-2.85258000	2.03834400
H	2.85849200	0.05436500	0.57236600
H	2.75943500	-1.02963600	1.97293100
H	3.22375300	-1.66758300	0.38804800

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$Me_3Si–PPh_2$*i*-Pr^+. Gibbs free energy: -1331.780338

P	0.02488200	0.26468500	0.38437500
C	-1.45391100	-0.76068200	0.12777300
C	-2.43242500	-0.93004000	1.11119400
C	-1.60721600	-1.38421900	-1.11836300
C	-3.55849300	-1.70657100	0.84384000
H	-2.33261200	-0.47413800	2.08933500
C	-2.73199100	-2.15802300	-1.37827900
H	-0.84151100	-1.28804500	-1.88211900
C	-3.71187800	-2.31588100	-0.39836100
H	-4.31337500	-1.83397100	1.61222600
H	-2.84118600	-2.63946100	-2.34397300
C	1.45148600	-0.81122700	0.06876200
C	1.38034000	-2.17129700	0.39272600
C	2.64019400	-0.27817100	-0.44103500
C	2.49188800	-2.98715800	0.20542000
H	0.46221100	-2.59695900	0.78557700
C	3.74835900	-1.09961400	-0.62698200
H	2.71807900	0.77417300	-0.69296800
C	3.67430000	-2.45323600	-0.30499200
H	2.43101800	-4.04106200	0.45457300
H	4.66543300	-0.68063400	-1.02655800
H	-4.59121300	-2.91753500	-0.60281500
H	4.53764900	-3.09322300	-0.45377300
C	0.09303400	0.80459200	2.15353000
C	-0.90417000	1.93440600	2.44386300
C	1.51903100	1.20220100	2.55333300
H	-0.18651400	-0.09077400	2.72188000
H	-1.91724900	1.72057500	2.09488800
H	-0.95136600	2.09353700	3.52424600
H	-0.57777700	2.87357100	1.98814100
H	2.22447300	0.37632600	2.44217600
H	1.88446800	2.05291000	1.96986600
H	1.51125100	1.50161400	3.60493600
Si	-0.10541800	2.04168700	-1.11586700
C	1.11240400	3.36057700	-0.58981900
H	1.02432800	4.18736100	-1.30382900
H	0.89683500	3.75872900	0.40494500
H	2.15031600	3.01773300	-0.61149900
C	-1.88460200	2.60073600	-0.99872400
H	-2.05969000	3.34347000	-1.78497800
H	-2.57934700	1.77071000	-1.15794000
H	-2.10984000	3.06876000	-0.03734900
C	0.30035700	1.31802600	-2.79158600
H	-0.48567300	0.64475700	-3.14358700
H	0.36964400	2.14724300	-3.50466600
H	1.25403800	0.78391700	-2.80403300

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PPh_2(*o*-biphenyl). Gibbs free energy: -1266.781078

P	-0.45016200	0.00777000	-0.80191100
C	-0.23869900	1.58063600	0.13367200
C	-0.22923500	1.66085900	1.53091300
C	-0.05988000	2.75189700	-0.61069700
C	-0.04441500	2.88549800	2.16873800
H	-0.35851000	0.76054900	2.12489300
C	0.11800800	3.97950600	0.02493600
H	-0.04799500	2.70306400	-1.69665000
C	0.12942800	4.04775800	1.41729900
H	-0.03600500	2.93261100	3.25339000
H	0.25883000	4.87917000	-0.56589300
H	0.27680400	5.00116600	1.91481700
C	0.05016900	-1.25289000	0.45772600
C	1.41813700	-1.56909200	0.58942500
C	-0.88002800	-1.94242200	1.24468900
C	1.81226500	-2.55691800	1.49701500
C	-0.47558200	-2.92360300	2.14697700
H	-1.93710800	-1.71548100	1.15008000
C	0.87554600	-3.23357600	2.27401600
H	2.86882100	-2.79022100	1.59340800
H	-1.21624400	-3.44275300	2.74707000
H	1.20091400	-3.99697000	2.97351600
C	-2.28409400	-0.18452100	-0.82124200
C	-3.16832600	0.58479700	-0.05671300
C	-2.81141500	-1.15465400	-1.68477800
C	-4.54509700	0.38295600	-0.14818300
H	-2.78595800	1.34602400	0.61584700
C	-4.18540800	-1.36666700	-1.76701600
H	-2.14186700	-1.75255800	-2.29835500
C	-5.05660900	-0.59446400	-0.99961100
H	-5.21685600	0.99075500	0.45010700
H	-4.57490700	-2.12514300	-2.43879600
H	-6.12858200	-0.74999400	-1.07000700
C	2.47049400	-0.87865800	-0.21619300
C	3.06795300	-1.53062700	-1.30065400
C	2.89263000	0.41334700	0.11350600
C	4.05412200	-0.89549600	-2.05278700
H	2.75072500	-2.53733200	-1.55816000
C	3.87831900	1.04975200	-0.63830000
H	2.44297000	0.92405500	0.95936900
C	4.45840400	0.39901100	-1.72611800
H	4.50344800	-1.40932500	-2.89692800
H	4.19012000	2.05565400	-0.37445500
H	5.22370100	0.89560100	-2.31431500

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Me_3Si–PPh_2(*o*-biphenyl)$^+$. Gibbs free energy: -1675.767643

P	0.61684100	0.02061400	0.06160200

C	0.43753700	1.64953200	-0.71387700
C	0.29939500	1.74332500	-2.10329500
C	0.48133700	2.81032500	0.06472200
C	0.19001500	2.99297200	-2.70451200
H	0.26583300	0.84662300	-2.71446700
C	0.37212900	4.05771200	-0.54328100
H	0.60843600	2.75696800	1.14093700
C	0.22203100	4.14914600	-1.92558400
H	0.07520000	3.06295500	-3.78072900
H	0.40238100	4.95550600	0.06443100
H	0.12978900	5.12185600	-2.39698000
C	-0.13171300	-1.23064300	-1.03753400
C	-1.52015200	-1.47576400	-1.08274800
C	0.73200000	-1.97376300	-1.85536100
C	-1.98359900	-2.49538000	-1.92284600
C	0.24502800	-2.96916300	-2.69360800
H	1.79823800	-1.78063800	-1.83984300
C	-1.11879300	-3.24014500	-2.71666900
H	-3.05095000	-2.68800000	-1.96256600
H	0.93139800	-3.53035800	-3.31789900
H	-1.51285700	-4.01959000	-3.36012400
C	2.40283900	-0.33508900	0.11908800
C	3.34039400	0.62263800	-0.27195900
C	2.83490000	-1.56477200	0.63539700
C	4.70221800	0.35133100	-0.14552400
H	3.02078300	1.57772500	-0.67473100
C	4.19328100	-1.82916900	0.75720500
H	2.11723700	-2.32455700	0.93021300
C	5.12910000	-0.86909500	0.36952800
H	5.42644700	1.09804100	-0.45255700
H	4.52113600	-2.78310800	1.15594500
H	6.18955600	-1.07484400	0.46999100
C	-2.55701000	-0.71131900	-0.32844700
C	-3.40143200	-1.38952700	0.56051200
C	-2.80697800	0.63893900	-0.59996500
C	-4.46471800	-0.73081600	1.17139800
H	-3.23031600	-2.44257000	0.76409100
C	-3.87368400	1.29699500	0.00942500
H	-2.19204300	1.17150700	-1.31687100
C	-4.70549800	0.61500500	0.89427000
H	-5.10805100	-1.27102700	1.85815400
H	-4.05723100	2.34231800	-0.21650000
H	-5.53832500	1.12703100	1.36505800
Si	-0.03613500	-0.05511900	2.31376100
C	-0.36212400	-1.86844400	2.63230700
H	0.56839100	-2.43813100	2.70154500
H	-0.88098400	-1.95768600	3.59301500
H	-0.99582400	-2.32129500	1.86598400

C	1.48508500	0.56403000	3.21224500
H	1.72058900	1.60469800	2.97099000
H	1.27527500	0.51048700	4.28672400
H	2.36716800	-0.04760800	3.00727200
C	-1.50510200	1.04880000	2.62062000
H	-1.42938700	2.01472900	2.11614900
H	-2.43766400	0.57164200	2.31699400
H	-1.54987700	1.23381300	3.70005500

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P(*p*-F-Ph)$_3$. Gibbs free energy: -1333.536838

P	0.07264100	0.03480500	1.44101100
C	1.67836100	-0.16884600	0.56199700
C	2.02493000	0.51430100	-0.60873600
C	2.60240100	-1.06544000	1.11607500
C	3.25858100	0.30716700	-1.22260200
H	1.33094800	1.21863700	-1.05561900
C	3.83425400	-1.29717300	0.51113600
H	2.36067400	-1.59555500	2.03338900
C	4.13379200	-0.59993900	-0.64889200
H	3.53509200	0.83407500	-2.12887100
H	4.55149100	-1.99367500	0.93026200
C	-0.63407700	1.52244800	0.61595300
C	-0.38867500	2.76574600	1.21279500
C	-1.38969800	1.48040300	-0.56189900
C	-0.86378700	3.94520000	0.64538900
H	0.18077600	2.82038700	2.13653200
C	-1.88220200	2.64726600	-1.14094800
H	-1.59897200	0.52937900	-1.04147800
C	-1.60291500	3.85566000	-0.52315000
H	-0.67731700	4.91067800	1.10153900
H	-2.46697500	2.62350700	-2.05361700
C	-0.94176900	-1.31217000	0.69828900
C	-0.56127100	-2.06772500	-0.41594300
C	-2.17593300	-1.58312000	1.30494800
C	-1.39188000	-3.06590900	-0.92275900
H	0.39102200	-1.88393400	-0.90301200
C	-3.02586900	-2.56541600	0.80629600
H	-2.48545100	-1.01809300	2.18015100
C	-2.60919600	-3.28786100	-0.30110500
H	-1.10402700	-3.65702900	-1.78490500
H	-3.98393900	-2.77506800	1.26803700
F	5.33305000	-0.81022700	-1.24066400
F	-2.07722900	4.99432000	-1.08044500
F	-3.42252000	-4.25342500	-0.79025400

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$Me_3Si–P(p\text{-}F\text{-}Ph)_3^+$. Gibbs free energy: -1742.521915

P	-0.00202200	-0.00905100	0.39098700
C	0.81721900	-1.48442200	-0.26543900

C	1.73342100	-1.38749800	-1.31789500
C	0.51758100	-2.73730800	0.28628200
C	2.35143700	-2.52953000	-1.81530200
H	1.97149800	-0.42533600	-1.75824200
C	1.12638200	-3.88497000	-0.20307300
H	-0.20156700	-2.83504900	1.09333600
C	2.03485200	-3.75189400	-1.24384700
H	3.06662700	-2.47569500	-2.62738300
H	0.90964500	-4.86137900	0.21317800
C	0.88364500	1.44304000	-0.23146100
C	2.15843500	1.72235000	0.27989600
C	0.32509400	2.27752300	-1.20437300
C	2.87250600	2.82314100	-0.17225300
H	2.61367300	1.07927500	1.02636500
C	1.02958800	3.38589300	-1.66332000
H	-0.65804000	2.07286200	-1.61403300
C	2.28659600	3.63304100	-1.13516000
H	3.85932600	3.05306400	0.21103400
H	0.61492200	4.04603000	-2.41580000
C	-1.69445900	0.03462900	-0.25244000
C	-2.11935200	-0.87565100	-1.22511000
C	-2.58777700	0.99472900	0.24265800
C	-3.42505300	-0.83236000	-1.70248000
H	-1.43962200	-1.62383400	-1.61807600
C	-3.89218400	1.05038400	-0.22886800
H	-2.27479600	1.71676800	0.99025200
C	-4.28165600	0.12991000	-1.19218900
H	-3.77317500	-1.53081100	-2.45406200
H	-4.59623700	1.78669900	0.13972300
F	2.63405900	-4.85860300	-1.71791000
F	2.97040400	4.70452100	-1.57499700
F	-5.54597900	0.17483100	-1.64858300
Si	-0.01465300	-0.01769500	2.72739400
C	-1.51612000	-1.02089800	3.20611600
H	-1.66175000	-0.91776700	4.28703900
H	-2.42234600	-0.66386000	2.70910800
H	-1.39216000	-2.08487500	2.98748100
C	1.59979300	-0.80971500	3.23393400
H	1.57867600	-0.95290300	4.32000300
H	1.74194500	-1.78865400	2.76820700
H	2.46311000	-0.18146200	2.99898300
C	-0.14029100	1.78207300	3.21050400
H	0.01287700	1.85397000	4.29293200
H	0.62389600	2.39250200	2.72149500
H	-1.12310700	2.20530400	2.98680200

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P(1-naphthyl)$_3$. Gibbs free energy: -1496.522113

P	0.12963700	-0.74349000	0.12147700

C	0.53949400	0.05558500	-1.48797600
C	-0.16851500	1.24995600	-1.85801300
C	1.45383000	-0.48314600	-2.36655000
C	-1.11926600	1.87692000	-1.00525900
C	0.09967300	1.85325700	-3.12133100
C	1.70657200	0.11170000	-3.62611700
H	1.99976300	-1.38163700	-2.09653800
C	-1.76315800	3.02945100	-1.38250400
H	-1.34322100	1.43625900	-0.03877500
C	-0.58292000	3.04581000	-3.48553800
C	1.04708400	1.25419400	-3.99499500
H	2.43215000	-0.34324700	-4.29279700
C	-1.49273800	3.62469300	-2.63707100
H	-2.48539200	3.48692800	-0.71383800
H	-0.36855400	3.49444900	-4.45160500
H	1.24039700	1.71893700	-4.95773000
H	-2.00605300	4.53676500	-2.92419700
C	1.05877000	0.30217600	1.32423300
C	0.80844600	0.12710900	2.72789200
C	1.94878700	1.27126100	0.91568200
C	-0.08903300	-0.85328400	3.23595000
C	1.49527800	0.95608800	3.66311100
C	2.61992200	2.09874700	1.84676600
H	2.14949200	1.41070600	-0.14170200
C	-0.29208000	-1.00053300	4.58609600
H	-0.62935400	-1.49261800	2.54460900
C	1.26534600	0.77996000	5.05469200
C	2.40111300	1.94321900	3.19001100
H	3.31395800	2.85117300	1.48629400
C	0.39312800	-0.17627500	5.50965500
H	-0.98586900	-1.75280200	4.94777700
H	1.79731100	1.41888900	5.75417500
H	2.91771300	2.57071300	3.91095700
H	0.22554200	-0.30357900	6.57428800
C	1.13803600	-2.28706600	0.08464000
C	0.63326900	-3.42726300	-0.62974000
C	2.32096700	-2.40202000	0.78206300
C	-0.56945900	-3.39169000	-1.38907600
C	1.37057600	-4.64741100	-0.59817900
C	3.04418800	-3.61788700	0.81808900
H	2.71877500	-1.54767800	1.31982000
C	-1.01379600	-4.49807200	-2.07064800
H	-1.14886900	-2.47436900	-1.42981600
C	0.88498100	-5.77646300	-1.31193100
C	2.58027700	-4.71615000	0.14423100
H	3.97074800	-3.66866700	1.38089100
C	-0.27970800	-5.70699600	-2.03371600
H	-1.93652700	-4.44590500	-2.63982000

H	1.45589400	-6.70026400	-1.27626900
H	3.13006700	-5.65296100	0.16559400
H	-0.64146700	-6.57538000	-2.57483900

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$Me_3Si–P(1\text{-naphthyl})_3^+$. Gibbs free energy: -1905.505543

P	0.27412700	-0.44818600	0.08555100
C	0.59511400	0.13096200	-1.61429700
C	0.03783800	1.35608300	-2.11256000
C	1.36096900	-0.66562400	-2.44013000
C	-0.68421400	2.27664700	-1.30914100
C	0.24035100	1.68030200	-3.48535000
C	1.57695800	-0.32059400	-3.79171600
H	1.80427500	-1.58108900	-2.06530400
C	-1.21554700	3.42449500	-1.84251000
H	-0.80045900	2.09550300	-0.24710800
C	-0.32334900	2.87340700	-4.01166600
C	1.01349200	0.81695000	-4.30581000
H	2.18100700	-0.97028700	-4.41487100
C	-1.04409100	3.72446100	-3.21321100
H	-1.76518900	4.10843200	-1.20431600
H	-0.16750800	3.10075000	-5.06200100
H	1.15928500	1.07883400	-5.34953000
H	-1.47127700	4.63246700	-3.62498200
C	1.17036000	0.65144300	1.23046500
C	1.03593000	0.51418000	2.65285300
C	1.94888300	1.66040700	0.70325900
C	0.33065700	-0.54729800	3.27792300
C	1.66723400	1.48096700	3.48744500
C	2.58991300	2.59868700	1.54146900
H	2.07383400	1.75743200	-0.36926900
C	0.21808500	-0.62135800	4.64386900
H	-0.10314600	-1.33896200	2.67815400
C	1.52992600	1.38279200	4.89800200
C	2.43607300	2.52054100	2.90011700
H	3.19078700	3.38359000	1.09621200
C	0.81485600	0.36014800	5.46752200
H	-0.32393800	-1.44660100	5.09376100
H	2.01019800	2.13254700	5.51969400
H	2.91090500	3.24952900	3.55007500
H	0.71657100	0.29182700	6.54551200
C	0.99794600	-2.11527700	0.23591300
C	0.41971300	-3.24323100	-0.43687500
C	2.10418700	-2.28269600	1.04223700
C	-0.65815300	-3.14419300	-1.35527100
C	0.97694900	-4.53202200	-0.19435000
C	2.66242600	-3.56152200	1.25635800
H	2.56005300	-1.43131400	1.53504900
C	-1.18386500	-4.25882300	-1.95955100

H	-1.06259800	-2.17308100	-1.61620200
C	0.40983200	-5.66896300	-0.82990100
C	2.09938200	-4.66163000	0.66596400
H	3.52957600	-3.66023500	1.89951000
C	-0.65229800	-5.54029700	-1.68820900
H	-2.00580700	-4.15286200	-2.65987200
H	0.84141000	-6.64499400	-0.62930500
H	2.51418800	-5.65028300	0.83843800
H	-1.07760100	-6.41432600	-2.16948400
Si	-2.05204700	-0.46283700	0.58642400
C	-2.39274200	1.04878500	1.63817000
H	-3.32831300	0.85127800	2.17432200
H	-1.61778800	1.24065200	2.38423500
H	-2.54120400	1.94993800	1.03856700
C	-2.97241200	-0.40075300	-1.04402200
H	-3.95164900	0.04670900	-0.83871500
H	-2.48143000	0.21522500	-1.80111100
H	-3.14200800	-1.39965300	-1.45380700
C	-2.41120100	-2.04338900	1.52582300
H	-2.24928800	-1.92241900	2.59972500
H	-3.47335800	-2.26602000	1.37194000
H	-1.83900600	-2.90484800	1.17351400

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$PPh_2(C_6F_5)$. Gibbs free energy: -1531.94085

P	-0.82990300	0.18780100	-1.24479100
C	-1.65651000	1.49877500	-0.25755600
C	-1.15442300	2.05477600	0.92311900
C	-2.87107600	1.97904700	-0.76761000
C	-1.85605700	3.06095700	1.58514000
H	-0.21089900	1.71532200	1.33658800
C	-3.57957200	2.97355300	-0.09821800
H	-3.26923300	1.57167200	-1.69365700
C	-3.07119600	3.51880900	1.08008400
H	-1.44998100	3.48536600	2.49784400
H	-4.52075500	3.33031200	-0.50420600
H	-3.61607600	4.30174500	1.59791400
C	0.84796600	0.09220400	-0.46428300
C	1.92907100	0.60676800	-1.18135700
C	1.15582600	-0.48908600	0.76758000
C	3.23762400	0.54315700	-0.72257500
C	2.45479900	-0.57487300	1.24936100
C	3.50109300	-0.05524700	0.50045000
C	-1.60748500	-1.36779900	-0.63732900
C	-2.66432200	-1.40445900	0.27610800
C	-1.14458000	-2.56785400	-1.19184000
C	-3.23767800	-2.62201800	0.63951600
H	-3.03713600	-0.48588400	0.71837800
C	-1.70557700	-3.78500500	-0.81403100

H	-0.33742700	-2.55587900	-1.92044000
C	-2.75683100	-3.81453800	0.10188600
H	-4.05573900	-2.63721400	1.35295100
H	-1.32781000	-4.70774700	-1.24306100
H	-3.20187400	-4.76133900	0.39090500
F	1.73273300	1.19686900	-2.36648200
F	4.23820300	1.04907800	-1.44540100
F	4.74816100	-0.12524100	0.95630700
F	0.19395300	-0.97727600	1.55685400
F	2.70350800	-1.13858200	2.43294300

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$Me_3Si–PPh_2(C_6F_5)^+$. Gibbs free energy: -1940.919959

P	0.71532200	-0.10336600	-0.18042900
C	1.27767600	-1.21814300	1.12991100
C	0.42352700	-1.63755300	2.15295200
C	2.60568100	-1.66370000	1.09383600
C	0.89838000	-2.50551700	3.13320200
H	-0.60497900	-1.29500900	2.19654600
C	3.07243700	-2.52570700	2.07888000
H	3.28512900	-1.33675400	0.31255800
C	2.21758200	-2.95013000	3.09602500
H	0.23277600	-2.83214200	3.92456900
H	4.10098700	-2.86791800	2.04861100
H	2.58155800	-3.62902400	3.85981900
C	-1.08749500	0.08770000	0.02532300
C	-1.92908700	-0.92544400	-0.43790900
C	-1.70503200	1.18538700	0.63220700
C	-3.30826400	-0.85620000	-0.34667700
C	-3.08722500	1.28017900	0.73138300
C	-3.89042000	0.26104400	0.23898100
C	1.49197600	1.51750300	0.04488000
C	2.26791600	1.79126100	1.17298700
C	1.31370200	2.49096200	-0.94512800
C	2.86273100	3.04316100	1.30867100
H	2.40569100	1.04280000	1.94594500
C	1.90553500	3.73941700	-0.79852800
H	0.70807900	2.29019500	-1.82397100
C	2.68151000	4.01502800	0.32758000
H	3.46395200	3.25753800	2.18550100
H	1.76344600	4.49467300	-1.56368700
H	3.14593900	4.98905200	0.43904300
F	-1.39438600	-2.02442600	-0.97922800
F	-4.06805800	-1.84495600	-0.80411800
F	-5.20703300	0.34729600	0.33762500
F	-0.99693800	2.17925600	1.15948300
F	-3.64258400	2.34025900	1.30901300
Si	1.30147400	-0.92364300	-2.31345300
C	1.48735700	-2.77073600	-2.13988200

H	1.82358100	-3.15809000	-3.10854300
H	2.24364700	-3.03365900	-1.39580100
H	0.55167200	-3.26918400	-1.88098100
C	2.93402200	-0.08292700	-2.65771400
H	3.32557100	-0.50304400	-3.59125900
H	2.82369600	0.99552800	-2.79190100
H	3.67905800	-0.26156300	-1.87749400
C	-0.05485800	-0.37246000	-3.47172700
H	0.26124600	-0.61737100	-4.49200900
H	-0.99980500	-0.88666000	-3.28256400
H	-0.22661900	0.70652400	-3.43009700

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P(*p*-CF_3-Ph)$_3$. Gibbs free energy: -2046.781507

P	-0.00747400	0.03033700	-1.85805300
C	1.63210400	-0.16787900	-1.03692300
C	1.83301600	-0.88535900	0.14690200
C	2.72980800	0.44782000	-1.64994900
C	3.10047600	-0.98120800	0.71152800
H	0.99903400	-1.37279400	0.64108900
C	3.99865900	0.36461200	-1.08682300
H	2.59706600	0.99714100	-2.57752400
C	4.17990300	-0.35034300	0.09568800
H	3.24077900	-1.53676900	1.63217300
H	4.83916200	0.85007000	-1.57023400
C	-0.98115100	-1.30794200	-1.04447400
C	-0.87916800	-2.58963100	-1.59999000
C	-1.79434700	-1.11981600	0.07682800
C	-1.55339100	-3.66586600	-1.03582100
H	-0.26362200	-2.75424600	-2.47983500
C	-2.48232500	-2.19041700	0.64061600
H	-1.89228800	-0.13721200	0.52621600
C	-2.35378800	-3.46240200	0.08778900
H	-1.45664500	-4.65378200	-1.47229600
H	-3.10482400	-2.03097300	1.51402300
C	-0.67077800	1.53342900	-1.02116700
C	-0.08489000	2.13452600	0.09693100
C	-1.83251800	2.09806900	-1.56283900
C	-0.64999500	3.27097700	0.66774900
H	0.81580100	1.71862300	0.53562600
C	-2.40991700	3.22563400	-0.99078900
H	-2.29612000	1.65326800	-2.43881800
C	-1.81481800	3.81040300	0.12632300
H	-0.18589000	3.72568400	1.53597200
H	-3.31323500	3.64722300	-1.41718700
C	-2.39577100	5.06693600	0.71242700
C	5.55838800	-0.49706800	0.67807600
C	-3.12498800	-4.61338900	0.67141100
F	-3.72621200	5.15870200	0.51869800

F	-1.85070900	6.17698400	0.15950200
F	-2.18355600	5.16043200	2.04050300
F	6.35035300	0.55693700	0.39863300
F	5.53859500	-0.63073900	2.01902500
F	6.19245900	-1.59164700	0.19379900
F	-2.48520600	-5.79009600	0.51813400
F	-4.33622600	-4.75781700	0.08214300
F	-3.35859800	-4.46073500	1.98986100

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$Me_3Si–P(p\text{-}CF_3\text{-}Ph)_3^+$. Gibbs free energy: -2455.760363

P	-0.01825700	0.02528800	0.93231700
C	1.07703900	1.31376600	0.27103600
C	0.67412400	2.13079500	-0.78921700
C	2.34991100	1.46250800	0.82939400
C	1.54408200	3.09429400	-1.28418200
H	-0.30773600	2.02042500	-1.23578300
C	3.22043500	2.42486900	0.33166900
H	2.68271400	0.82692200	1.64348200
C	2.81127600	3.23766300	-0.72153700
H	1.23174000	3.72827400	-2.10675100
H	4.20599200	2.53750400	0.76654200
C	-1.67721300	0.29547600	0.24399600
C	-2.41674500	1.40439100	0.67617400
C	-2.21454400	-0.58203700	-0.69703900
C	-3.68520200	1.63088600	0.16433800
H	-2.00998100	2.10291700	1.40015200
C	-3.49082100	-0.35618500	-1.20687400
H	-1.65265300	-1.44215800	-1.04301700
C	-4.21827300	0.74596300	-0.77472600
H	-4.25426300	2.49145000	0.49806500
H	-3.90542000	-1.04012600	-1.93730900
C	0.58142900	-1.57255900	0.31124600
C	1.52313700	-1.63280400	-0.71830800
C	0.06539000	-2.75108900	0.86089800
C	1.94496000	-2.86783500	-1.19804500
H	1.93038200	-0.72787600	-1.15524900
C	0.48453600	-3.98411800	0.37873600
H	-0.67442500	-2.72329700	1.65401600
C	1.42236900	-4.03663200	-0.65060800
H	2.67405700	-2.91128100	-1.99870900
H	0.07727700	-4.89396600	0.80338900
Si	-0.06987900	0.07230700	3.27511200
C	1.38032400	-0.97111000	3.81666900
H	1.31159300	-1.09975100	4.90262300
H	1.37133900	-1.96437300	3.36027700
H	2.33930200	-0.49362400	3.59871800
C	0.10581000	1.87687800	3.71855200
H	0.17474700	1.94867800	4.80977500

H	1.01326700	2.31682800	3.29638100
H	-0.75347200	2.47309800	3.40031200
C	-1.73038200	-0.65131700	3.72510400
H	-1.85867400	-0.54477700	4.80798900
H	-2.55405200	-0.12348400	3.23659400
H	-1.80479700	-1.71523600	3.48496800
C	1.91442200	-5.37258500	-1.14917300
C	3.73106500	4.29436000	-1.27969700
C	-5.60374000	1.01257400	-1.30673600
F	1.00518800	-6.34744100	-0.97112200
F	3.03426300	-5.75761800	-0.49935300
F	2.21625900	-5.34255100	-2.45995300
F	4.92984700	4.30937900	-0.67528900
F	3.95118000	4.11074000	-2.59788200
F	3.20194300	5.52840100	-1.14543300
F	-5.68233500	2.22519100	-1.89310300
F	-6.52124600	1.00324100	-0.31717400
F	-5.99306200	0.10568300	-2.21689000

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P(^{t}Bu)$_2$(*o*-biphenyl). Gibbs free energy: -1119.180476

P	0.54313800	0.86217000	-0.06196300
C	0.32036400	1.79764500	1.57746400
C	0.83455800	0.82081000	2.65243500
C	1.24397700	3.02648600	1.55447900
C	-1.09761500	2.23297000	1.97062000
H	0.22055500	-0.08503400	2.69822700
H	1.87074700	0.52115800	2.46614200
H	0.78956800	1.30408900	3.63614200
H	0.87688800	3.80302300	0.87741100
H	1.29394300	3.46435200	2.55869900
H	2.26379300	2.76270500	1.25359400
H	-1.05138900	2.77293400	2.92490300
H	-1.55483100	2.89981500	1.23685100
H	-1.75762600	1.37369200	2.11436500
C	0.08422600	1.96646600	-1.54524800
C	-1.01258600	3.02651900	-1.37452100
C	1.38921700	2.68505100	-1.94657500
C	-0.30157000	1.01875000	-2.69529900
H	-1.98221400	2.59677500	-1.11412600
H	-0.75004400	3.76985400	-0.61771900
H	-1.14118900	3.55986000	-2.32489800
H	2.19174000	1.96825500	-2.14683800
H	1.21856500	3.26780700	-2.86022700
H	1.73728300	3.37612700	-1.17369000
H	-0.36218800	1.58858500	-3.63034400
H	0.44618700	0.22953400	-2.83507700
H	-1.27070700	0.54160600	-2.52673800
C	-0.80504900	-0.40964400	0.03554900

C	-0.45123000	-1.76458500	0.20418500
C	-2.17097300	-0.09125400	-0.01625300
C	-1.45312600	-2.73474900	0.34462100
C	0.96726200	-2.23701100	0.22457900
C	-3.15998600	-1.06098100	0.10405100
H	-2.47508600	0.93958100	-0.14915800
C	-2.79964500	-2.39294700	0.29557000
H	-1.16286900	-3.77253700	0.48139100
C	1.67754600	-2.39039200	-0.97050700
C	1.58639200	-2.58371900	1.42774600
H	-4.20626700	-0.77581300	0.05427800
H	-3.56043100	-3.16036300	0.39830700
C	2.98706000	-2.86342000	-0.96159500
H	1.19918000	-2.13177200	-1.91082000
C	2.89981000	-3.05273300	1.44024800
H	1.04181600	-2.47477500	2.36119800
C	3.60434400	-3.19172900	0.24588700
H	3.52509000	-2.97629900	-1.89782600
H	3.37125900	-3.30897700	2.38407400
H	4.62595000	-3.55887500	0.25442200

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$Me_3Si–P(^tBu)_2$(*o*-biphenyl)$^+$. Gibbs free energy: -1528.152075

P	-0.81597600	-0.29329000	0.13025100
C	-0.95509900	-0.68286800	1.98030800
C	-1.52824900	-2.08887900	2.21862100
C	0.41319800	-0.56342200	2.65853200
C	-1.90360800	0.35138600	2.61161900
H	-2.48858900	-2.24593300	1.72568800
H	-0.84151400	-2.87875000	1.91198000
H	-1.69286200	-2.20352500	3.29464000
H	1.15164500	-1.24833600	2.23906500
H	0.79628700	0.45801800	2.59857200
H	0.29234800	-0.80941300	3.71842400
H	-1.89335600	0.20348100	3.69599200
H	-1.59078700	1.38170800	2.42035300
H	-2.93676800	0.22209200	2.28055200
C	-0.11494100	-1.72880500	-0.89381000
C	0.29553800	-1.16036600	-2.26275700
C	1.07317500	-2.43697600	-0.22256100
C	-1.20622400	-2.79002300	-1.13372100
H	-0.55725100	-0.76653100	-2.81616200
H	1.04088400	-0.37418800	-2.18485300
H	0.72885300	-1.97329900	-2.85393600
H	0.77247700	-2.97613400	0.67744900
H	1.45934200	-3.17697200	-0.93093300
H	1.88907800	-1.76651500	0.02973500
H	-0.74714300	-3.60312700	-1.70454000
H	-1.59619800	-3.22234400	-0.21125300

H	-2.03731700	-2.41492000	-1.73232400
Si	-3.03292100	0.10010600	-0.70046200
C	-3.85063200	1.68239500	-0.09223500
H	-3.56765400	2.55623300	-0.68471400
H	-4.92226600	1.51412700	-0.25577100
H	-3.71731700	1.90720500	0.96756800
C	-2.93444000	0.21049800	-2.56645900
H	-2.74495800	-0.74259900	-3.06426500
H	-3.91615300	0.56803900	-2.89932100
H	-2.19035200	0.94172600	-2.89530300
C	-4.12972700	-1.30169500	-0.10606400
H	-5.07296800	-1.18142000	-0.65291900
H	-3.76431700	-2.31052300	-0.29500500
H	-4.36119000	-1.20005100	0.95808300
C	0.18414700	1.27513500	-0.00517600
C	1.58688100	1.48576400	-0.09954500
C	-0.63489100	2.41495200	0.05586500
C	2.05805500	2.80530700	-0.16451200
C	2.69598100	0.47731500	-0.12854600
C	-0.14399700	3.71290900	0.00837500
H	-1.70093900	2.30008800	0.15560200
C	1.22182100	3.91301800	-0.11599100
H	3.12988500	2.95253700	-0.24897600
C	3.28348400	0.03093600	1.05938700
C	3.28230400	0.10810000	-1.34408800
H	-0.83412000	4.54767700	0.06149700
H	1.63978800	4.91246300	-0.16910800
C	4.36438700	-0.84750500	1.03136700
H	2.90180900	0.37665300	2.01238400
C	4.36037000	-0.77235400	-1.37581800
H	2.89943800	0.51787100	-2.27339600
C	4.89206200	-1.26969800	-0.18718600
H	4.79707700	-1.19578000	1.96362500
H	4.79028200	-1.06100200	-2.32942600
H	5.72779900	-1.96145200	-0.20992400

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$P(mesityl)_3$. Gibbs free energy: -1389.393624

P	0.02086100	-0.00579600	0.98038200
C	-1.68706800	-0.37253900	0.39122500
C	-2.06039800	-1.27799400	-0.62830100
C	-2.70473900	0.27797200	1.13108900
C	-3.41691800	-1.52635100	-0.85528000
C	-4.04663100	0.01058800	0.85323200
C	-4.42754400	-0.90094700	-0.12774900
H	-3.69270400	-2.22234400	-1.64476600
H	-4.81369600	0.53205700	1.42158600
C	1.17833800	-1.29308700	0.34647000
C	1.12506800	-2.51758600	1.06001000

C	2.14188300	-1.14248000	-0.67460300
C	2.02334400	-3.53968800	0.75502600
C	3.03502900	-2.18935100	-0.92856300
C	3.00065600	-3.39165800	-0.22783200
H	1.95664100	-4.47810300	1.30136100
H	3.77262600	-2.06199600	-1.71815000
C	0.53569500	1.65280600	0.36071800
C	-0.09955600	2.42091400	-0.64118500
C	1.62602200	2.22023200	1.06585700
C	0.34371800	3.72502500	-0.88192500
C	2.04419200	3.51951000	0.77420300
C	1.40529900	4.29923300	-0.18689100
H	-0.15085900	4.30596200	-1.65762000
H	2.89250700	3.93197700	1.31598200
C	-5.87869300	-1.21247300	-0.38928300
H	-6.06099900	-1.38569100	-1.45366200
H	-6.18225400	-2.11845700	0.14702000
H	-6.52742000	-0.39790400	-0.05647500
C	3.99038100	-4.49319400	-0.50874000
H	4.46388400	-4.36365100	-1.48545600
H	4.78288400	-4.50247800	0.24750600
H	3.50706400	-5.47422900	-0.48717600
C	1.83397700	5.71898800	-0.45523300
H	1.27374600	6.41632300	0.17754400
H	2.89700600	5.86149300	-0.24281600
H	1.64971000	5.99819100	-1.49628100
C	2.39847500	1.44549900	2.10776400
H	1.73932800	1.06859500	2.89644000
H	2.89947400	0.57476400	1.66957500
H	3.16378800	2.07666600	2.56524200
C	-1.21145500	1.91039300	-1.52664700
H	-0.98332500	0.92372300	-1.93686500
H	-2.16070000	1.81830200	-0.99156300
H	-1.36212200	2.59587300	-2.36393400
C	2.24834000	0.07236400	-1.56537200
H	1.27141600	0.39221500	-1.93524700
H	2.68551600	0.93027700	-1.04632700
H	2.87785600	-0.15444800	-2.42922500
C	0.08137800	-2.78390400	2.11911600
H	0.07580000	-2.00070700	2.88363500
H	-0.92555100	-2.81353300	1.68707100
H	0.26370500	-3.74522500	2.60505400
C	-1.07985500	-1.97155200	-1.54367900
H	-0.32980100	-1.27935200	-1.93346800
H	-0.53645400	-2.77412600	-1.03675100
H	-1.60880900	-2.40857000	-2.39391200
C	-2.39711700	1.31111700	2.18953400
H	-1.70428800	0.92383100	2.94322700

H	-1.92686500	2.20003700	1.75356900
H	-3.31365500	1.63103400	2.69056600

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$Me_3Si–P(mesityl)_3^+$. Gibbs free energy: -1798.364771

P	0.01379900	-0.00847800	0.96397600
C	-1.71265900	-0.36345900	0.43423300
C	-2.04016500	-1.34741700	-0.53242200
C	-2.75197900	0.36248900	1.06051200
C	-3.38532100	-1.65713700	-0.73525300
C	-4.07856300	0.01378300	0.81091600
C	-4.42032700	-1.01893300	-0.05521000
H	-3.63267800	-2.41340500	-1.47532600
H	-4.86439900	0.58448000	1.29966100
C	1.17865900	-1.31382700	0.39276300
C	1.08421900	-2.58766200	0.99931700
C	2.18067300	-1.08409100	-0.58355400
C	2.05403100	-3.55057600	0.72502400
C	3.12789900	-2.08330100	-0.81092000
C	3.10914600	-3.30845200	-0.14799900
H	1.96280000	-4.52504900	1.19834400
H	3.89638700	-1.90217600	-1.55772400
C	0.55117200	1.66319900	0.41292300
C	-0.16381900	2.42889600	-0.54312800
C	1.70413500	2.21388600	1.01657900
C	0.21838500	3.75368700	-0.75091600
C	2.04379100	3.54250700	0.76191600
C	1.29262200	4.34549500	-0.08838100
H	-0.33441900	4.34000000	-1.48027800
H	2.93503500	3.94795500	1.23437700
C	-5.85577400	-1.41406200	-0.27059800
H	-5.99990200	-1.87021200	-1.25295800
H	-6.16295900	-2.14623100	0.48385900
H	-6.52234800	-0.55227100	-0.18417200
C	4.17471200	-4.34349600	-0.38623600
H	4.63862800	-4.21981300	-1.36771700
H	4.96308700	-4.25371800	0.36884300
H	3.76554300	-5.35456800	-0.31673400
C	1.63785900	5.79267600	-0.31152600
H	1.03059100	6.43060100	0.33960000
H	2.68869800	5.99038400	-0.08729600
H	1.43899900	6.09155600	-1.34388600
C	2.67092200	1.43509600	1.87710500
H	2.54626300	0.35462000	1.81347300
H	3.69205700	1.64759600	1.54997700
H	2.60398500	1.73542200	2.92630500
C	-1.26830300	1.91322100	-1.43809900
H	-1.07716600	0.90054800	-1.79629000
H	-2.24276500	1.90647800	-0.94402300

H	-1.34677800	2.56093900	-2.31318700
C	2.27137200	0.12882800	-1.48225200
H	1.29436700	0.45224300	-1.84623300
H	2.73705600	0.98629000	-0.99134000
H	2.87753300	-0.12063200	-2.35517600
C	-0.05579200	-3.03428000	1.88486500
H	-0.94451800	-2.40766900	1.81720200
H	-0.36537700	-4.03911400	1.58594300
H	0.25149200	-3.09783800	2.93241400
C	-1.05725400	-2.04770900	-1.44323700
H	-0.28226400	-1.37554600	-1.81538700
H	-0.55529300	-2.88700900	-0.95623000
H	-1.59227100	-2.44166600	-2.30915500
C	-2.54273800	1.57033200	1.94396200
H	-1.55413800	2.01965800	1.85502600
H	-3.25995700	2.34543500	1.66248900
H	-2.72768400	1.33451500	2.99556500
Si	0.04329900	-0.02005500	3.37577900
C	1.59268200	-0.93075100	3.93749500
H	2.33111000	-0.22210000	4.32010000
H	1.31332000	-1.60321800	4.75537900
H	2.07399400	-1.53159500	3.16224300
C	0.06563900	1.76698100	3.96913500
H	-0.90783100	2.04240800	4.38195100
H	0.80756300	1.84936600	4.77029600
H	0.32417500	2.49834900	3.19978100
C	-1.50795000	-0.90649500	3.97007900
H	-1.25666600	-1.90107700	4.34617300
H	-1.93367100	-0.33045700	4.79830400
H	-2.28325300	-1.02097800	3.20865100

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Me_2O. Gibbs free energy: -154.935743

O	0.72547000	-1.06192000	-0.40419400
C	1.70333000	-0.10030500	-0.73586000
H	2.63112800	-0.57942600	-1.08005700
H	1.91241400	0.47810600	0.16556700
H	1.34466500	0.57723000	-1.52403800
C	0.38632600	-1.88069700	-1.50210400
H	-0.36738100	-2.59190500	-1.16034500
H	-0.02723100	-1.28631500	-2.32946400
H	1.26255900	-2.43313700	-1.87075800

22

$Me_3Si–OMe_2^+$. Gibbs free energy: -563.912567

O	0.47195100	-0.60735600	-0.98810300
C	1.82957400	-0.18617900	-0.65724400
H	2.25513500	-0.89075000	0.05839600
H	1.76618100	0.81374700	-0.23624900
Si	-0.91845600	-0.05828300	0.10699800

C	-2.42938600	-0.63988800	-0.79744100
H	-2.57133500	-1.72173000	-0.73336100
H	-3.29637800	-0.16624100	-0.32340900
H	-2.42133600	-0.33502700	-1.84790200
C	-0.58518100	-0.91555700	1.71789400
H	0.37788500	-0.62168600	2.14498600
H	-1.36559600	-0.63470100	2.43349800
H	-0.60842400	-2.00354800	1.60808700
C	-0.71681500	1.78583500	0.13258800
H	0.10334500	2.11587700	0.77528100
H	-0.57229900	2.18954400	-0.87359000
H	-1.64092700	2.21573600	0.53469900
H	2.39798500	-0.16734400	-1.58549800
C	0.43231200	-1.92126200	-1.62220500
H	-0.57603300	-2.06988100	-1.99780900
H	1.14107500	-1.90141000	-2.44817300
H	0.70281100	-2.68063700	-0.88739700

12

MeOEt. Gibbs free energy: -194.220131

O	0.73498500	-1.04640800	-0.40249300
C	1.71649800	-0.08288900	-0.74136300
H	2.62110900	-0.59113300	-1.11022900
H	1.34164900	0.55670800	-1.55569600
C	0.39039000	-1.87339700	-1.49209100
H	-0.36286000	-2.58104700	-1.14185500
H	-0.02632900	-1.28621600	-2.32296600
H	1.26368900	-2.43071100	-1.86031300
C	2.03592400	0.74824700	0.48447500
H	2.79380100	1.49822900	0.24076300
H	1.14215500	1.26568500	0.84490300
H	2.42171100	0.11674700	1.28994000

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$Me_3Si–OMeEt^+$. Gibbs free energy: -603.196623

O	0.81139900	-1.13332100	-0.12289000
C	2.21113600	-0.66040400	-0.12451900
H	2.69282800	-1.20701400	0.68353400
H	2.62461900	-1.00351800	-1.07344800
C	0.07763800	-0.86939800	-1.35349000
H	-0.85813100	-1.42097700	-1.29704700
H	-0.11002400	0.19988900	-1.44489500
H	0.67833900	-1.24222300	-2.18139800
C	2.30764800	0.83653400	0.05013500
H	3.36726300	1.10519900	0.06156100
H	1.83450500	1.37856600	-0.77119300
H	1.86832200	1.16134400	0.99639100
Si	-0.15441200	-1.43424400	1.41696800
C	-1.29417600	0.02653900	1.52609100
H	-1.85936100	-0.04344200	2.46197300

H	-0.74162600	0.97038500	1.53817500
H	-2.01541000	0.04948700	0.70443200
C	-0.98820200	-3.05611700	1.07665000
H	-0.25964800	-3.81873100	0.78800000
H	-1.47929700	-3.38897400	1.99775900
H	-1.75616500	-2.98612500	0.30188300
C	1.12861300	-1.51330300	2.75355500
H	0.59859300	-1.71469200	3.69158000
H	1.84210400	-2.32732600	2.59954100
H	1.67087400	-0.57265400	2.88153600

15

MeO*i*Pr. Gibbs free energy: -233.503718

O	0.66265800	-0.99753400	-0.46694800
C	1.65448200	-0.02837800	-0.80038400
H	2.54860000	-0.56189400	-1.16233200
C	0.43253900	-1.97037200	-1.46323200
H	-0.24074900	-2.71506500	-1.03470600
H	-0.04003200	-1.54524200	-2.35781400
H	1.36941300	-2.46353300	-1.75944900
C	1.99771100	0.70160200	0.48816000
H	2.78533200	1.43926000	0.30955900
H	1.11630100	1.22460900	0.87396900
H	2.34569700	-0.00250700	1.24873300
C	1.17417900	0.93095900	-1.88701500
H	0.96425400	0.41446400	-2.82758200
H	0.26431100	1.44537300	-1.56004000
H	1.94379400	1.68246300	-2.08774600

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$Me_3Si–OMe$*i*Pr^+. Gibbs free energy: -642.478167

O	0.77447500	-1.05268100	-0.36736600
C	1.79461400	0.02897900	-0.62468600
H	2.02283800	-0.11649600	-1.68120900
C	0.28320500	-1.65826900	-1.60087400
H	-0.45265900	-2.41247200	-1.33525300
H	-0.17021800	-0.88334400	-2.21947700
H	1.13042400	-2.12758400	-2.09824700
C	3.03305000	-0.25387900	0.19574500
H	3.82780700	0.40564800	-0.16281600
H	2.88596000	-0.05216100	1.25700100
H	3.35893300	-1.28736300	0.06189600
C	1.16513300	1.39043200	-0.42362100
H	0.25682900	1.50193900	-1.02018100
H	0.93757300	1.58999100	0.62601800
H	1.88163900	2.14605300	-0.75557100
Si	-0.28374000	-1.24864000	1.12658500
C	0.67951600	-0.63865000	2.59048800
H	0.94439900	0.41949900	2.54871200
H	0.01691900	-0.77341100	3.45425500

H	1.57777200	-1.23462900	2.76896800
C	-1.80895500	-0.26191400	0.74097500
H	-2.54908500	-0.44232900	1.52836100
H	-1.60423500	0.81143100	0.70929500
H	-2.25787100	-0.56210700	-0.21051500
C	-0.55496600	-3.08619000	1.20776500
H	0.38028000	-3.63444800	1.06204100
H	-0.92453300	-3.31844800	2.21275300
H	-1.29840800	-3.44939200	0.49388000

18

MeO*t*Bu. Gibbs free energy: -272.785926

O	1.18053700	-1.34873500	-0.54432700
C	1.84542600	-0.07895200	-0.66962500
C	0.29183100	-1.72119900	-1.57641200
H	-0.06107200	-2.72484800	-1.33180300
H	-0.57553400	-1.05208300	-1.63579100
H	0.78130000	-1.75590500	-2.55768700
C	2.61029200	0.06427800	0.64414000
H	3.17462300	1.00126900	0.65893800
H	1.91576700	0.06267600	1.48956300
H	3.31238500	-0.76581900	0.76792200
C	0.83344800	1.06196500	-0.81840900
H	0.32277200	1.03368300	-1.78547200
H	0.08240100	1.01306900	-0.02365600
H	1.34867600	2.02431300	-0.74625700
C	2.82224300	-0.09468700	-1.85036000
H	3.39948900	0.83480700	-1.86808700
H	3.51991600	-0.93265000	-1.75677400
H	2.30388200	-0.17702900	-2.81014500

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Me_3Si–OMe*t*Bu$^+$. Gibbs free energy: -681.755246

O	0.88580900	-1.05008000	-0.39790000
C	1.84344000	0.12992400	-0.66410100
C	0.31615100	-1.65959100	-1.60026600
H	0.24189800	-2.72805800	-1.42259500
H	-0.65956600	-1.21858600	-1.80354800
H	0.99029900	-1.48403500	-2.43081400
C	2.31960300	0.64331100	0.68313100
H	2.98225100	1.48935300	0.48792300
H	1.50741000	1.01791500	1.30767100
H	2.89317100	-0.11005000	1.22459200
C	1.06467000	1.19121300	-1.42414800
H	0.70009100	0.82931100	-2.38760700
H	0.22081400	1.56121700	-0.83751900
H	1.73774300	2.02936600	-1.62132000
Si	-0.10770600	-1.32774300	1.14071700
C	1.08249500	-1.62580000	2.53771300
H	1.42875000	-0.71219000	3.02319300

H	0.55097600	-2.22545200	3.28514300
H	1.94843800	-2.20611900	2.20617100
C	-1.22403800	0.15188700	1.29331600
H	-1.95303400	-0.06294200	2.08287900
H	-0.70521500	1.07451100	1.56314100
H	-1.78211600	0.31891300	0.36711100
C	-1.07287600	-2.87737400	0.78250400
H	-0.42937500	-3.73915500	0.58456400
H	-1.63321500	-3.09362300	1.70009200
H	-1.79815000	-2.77017300	-0.02723800
C	3.02461000	-0.43411800	-1.44332000
H	3.80590500	0.32929100	-1.46290000
H	3.42571100	-1.32105100	-0.94764100
H	2.78917500	-0.67177000	-2.48176400

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$(MeOCH_2)_2$. Gibbs free energy: -308.677374

O	0.74595200	-1.03375200	-0.40409800
C	1.72352000	-0.07665100	-0.74711500
H	2.63942400	-0.57021200	-1.10561900
H	1.35633500	0.58316800	-1.54762200
C	0.39701100	-1.86461600	-1.49107800
H	-0.35673600	-2.56808900	-1.13447900
H	-0.02017200	-1.27812500	-2.32142500
H	1.26892500	-2.42431200	-1.85716600
C	2.02933800	0.73971500	0.49476200
H	1.11343400	1.23327500	0.85326600
H	2.39652200	0.07989500	1.29526900
O	3.00690600	1.69681600	0.15174500
C	3.35584700	2.52767900	1.23872500
H	4.10959400	3.23115200	0.88212600
H	2.48393200	3.08737500	1.60481300
H	3.77303000	1.94118900	2.06907200

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$Me_3Si–(MeOCH_2)_2^+$. Gibbs free energy: -717.650333

O	0.80345200	-0.94572600	0.08032000
C	1.17054000	0.41379300	-0.30961000
H	1.40522800	0.38621000	-1.37424000
H	0.29514200	1.04146200	-0.15559600
C	1.42007000	-2.00089500	-0.71659200
H	1.28266900	-2.93926200	-0.18411000
H	0.92685300	-2.02780700	-1.68761200
H	2.48251400	-1.78256000	-0.80923500
C	2.35583900	0.87925600	0.51915800
H	2.08451800	0.92262100	1.58476100
H	3.19901900	0.18063200	0.41284100
O	2.68401000	2.15149600	0.02857400
C	3.77721400	2.74108400	0.71050700
H	3.94725200	3.71600600	0.25375000

H	3.55141200	2.87278600	1.77645300
H	4.68171400	2.12807200	0.60704200
Si	-0.44226500	-1.38005400	1.37418100
C	-1.14778900	0.25713500	1.88231400
H	-1.85877100	0.05995600	2.69281800
H	-0.39285800	0.94581200	2.27171100
H	-1.70001800	0.74198400	1.07285500
C	0.57770800	-2.21979200	2.67587400
H	1.33570500	-1.54400800	3.08188000
H	-0.08228900	-2.52236200	3.49619300
H	1.07193600	-3.11979200	2.29969900
C	-1.62413600	-2.48068000	0.46233400
H	-2.45718200	-2.72406000	1.13084800
H	-2.03298600	-1.97806400	-0.41875200
H	-1.16386900	-3.42281600	0.15268300.

13

1,2-epoxybutane. Gibbs free energy: -232.286417

C	-2.40485300	0.81201800	-0.10539300
C	-1.01820000	0.58089200	-0.51412200
H	-3.07887400	1.36486600	-0.75551700
H	-2.87679600	0.11607100	0.58570600
C	-0.21538400	-0.59722300	-0.02823000
H	-0.70104200	1.00086200	-1.47002400
C	1.26312000	-0.25389200	0.15755800
H	-0.64389400	-0.95523600	0.91469900
H	-0.32377600	-1.40686800	-0.75997800
H	1.82632100	-1.12664900	0.49942200
H	1.70891800	0.08768400	-0.78270200
H	1.38731000	0.54105100	0.89941000
O	-1.33870700	1.58557000	0.45794400

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Me_3Si–1,2-epoxybutane$^+$. Gibbs free energy: -641.265193

C	-2.13738700	0.83714700	-1.50859300
C	-1.02839100	0.95187700	-0.56311600
H	-2.07135600	1.32261400	-2.47615200
H	-2.84016800	0.01687500	-1.41721700
C	-0.78596900	-0.03069400	0.53866800
H	-0.19035900	1.57603800	-0.86529000
C	-0.23082400	0.62727500	1.80109400
H	-1.71323500	-0.57067700	0.75141400
H	-0.07064400	-0.76018800	0.14138900
H	-0.02050200	-0.13108000	2.55802600
H	0.69920600	1.16446300	1.59228300
H	-0.95084900	1.33389200	2.22332700
O	-2.26922300	1.77367000	-0.37768600
Si	-2.43959300	3.59589600	-0.45666800
C	-4.25784300	3.77321300	-0.76311600
H	-4.50882200	4.83740700	-0.82609600

H	-4.55340800	3.30264600	-1.70529100
H	-4.83862400	3.33270000	0.05178100
C	-1.84616400	4.07879800	1.23095000
H	-0.78627900	3.84575300	1.36812600
H	-1.97168200	5.15929600	1.35884900
H	-2.42503700	3.57761900	2.01186900
C	-1.35316800	4.15956000	-1.85440600
H	-1.45259400	5.24834200	-1.93160000
H	-0.29576600	3.94157800	-1.68014600
H	-1.65338100	3.73967600	-2.81846400

16

Anisole. Gibbs free energy: -346.576098

C	-2.53858600	-1.37058600	0.12654600
C	-1.15826700	-1.48845100	0.31471300
C	-0.31201800	-0.43007600	0.01216300
C	-0.83918300	0.76860600	-0.48562700
C	-2.21683200	0.89659300	-0.67959000
C	-3.05477900	-0.17846800	-0.36983500
H	-3.19863000	-2.19781800	0.36563600
H	-0.73772800	-2.41155200	0.70177300
H	0.76060900	-0.51135800	0.15557100
H	-2.64838400	1.81217600	-1.06589800
H	-4.12418600	-0.06983300	-0.52263900
O	0.06662600	1.74851700	-0.74859000
C	-0.40977300	2.98809500	-1.24711500
H	0.47012600	3.61755500	-1.37377500
H	-0.90849000	2.86120300	-2.21439200
H	-1.09734200	3.46252500	-0.53803700

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Me_3Si–anisole$^+$. Gibbs free energy: -755.543649

C	-1.06700900	-2.30381000	0.65361300
C	-0.65474400	-1.34082300	1.57352300
C	-0.36868900	-0.04372600	1.15073200
C	-0.50586100	0.24005500	-0.19796300
C	-0.91822000	-0.68906900	-1.13761500
C	-1.20054200	-1.98005000	-0.69634900
H	-1.28538800	-3.31143300	0.99028800
H	-0.55226800	-1.59350600	2.62292500
H	-0.05001300	0.71875400	1.85291100
H	-1.01032000	-0.40964100	-2.18122900
H	-1.52251800	-2.73005000	-1.41004200
O	-0.20435000	1.55450400	-0.66209600
C	-1.28318400	2.53052500	-0.47489400
H	-0.97960600	3.43886800	-0.98890000
H	-2.17614100	2.10898600	-0.93181000
H	-1.41733300	2.70169500	0.59230300
Si	1.56508600	2.06268500	-0.92365500
C	1.42060500	3.37116500	-2.23002300

H	1.06142200	4.32470800	-1.83402800
H	2.42047200	3.54194000	-2.64433200
H	0.77103800	3.05196400	-3.05001500
C	2.34365200	0.47964800	-1.48772300
H	3.40009600	0.68033000	-1.69831100
H	2.29552800	-0.29987800	-0.72305200
H	1.87964200	0.10819400	-2.40548400
C	2.10783600	2.68040300	0.73872800
H	3.09318200	3.14769300	0.63461100
H	1.42066300	3.43835500	1.12700000
H	2.19504400	1.87067500	1.46813700

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2-pentanone. Gibbs free energy: -271.616831

C	0.79015000	0.88019200	0.09040500
O	-0.00091100	-0.04900400	0.11725300
C	0.32014300	2.31475700	0.08712500
H	-0.74206000	2.37073200	0.32790000
H	0.90076000	2.91711700	0.79165400
H	0.48445900	2.73878500	-0.90977000
C	2.28732300	0.66384600	0.04565800
C	2.72849300	-0.78818600	-0.09459800
H	2.68771100	1.27812400	-0.77253200
C	4.25015200	-0.92440700	-0.12554600
H	2.31840000	-1.37127000	0.73654700
H	4.70027200	-0.53380700	0.79371000
H	4.54824000	-1.97208200	-0.22662100
H	4.67909600	-0.37134800	-0.96834800
H	2.70102300	1.10674700	0.96298200
H	2.29822300	-1.21019200	-1.00943300

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Me_3Si–2-pentanone$^+$. Gibbs free energy: -680.596455

C	0.83472900	0.90938000	0.01234800
O	0.06436400	-0.08229300	0.03350700
C	0.32437000	2.30121500	-0.05353200
H	-0.59377600	2.42652400	0.52161600
H	1.08092800	3.01132900	0.27883000
H	0.09965900	2.51382200	-1.10667000
C	2.29399400	0.65498100	0.02230100
C	2.72503100	-0.80461600	-0.06436300
H	2.72075000	1.26271800	-0.78878000
C	4.24671600	-0.93853300	-0.06051200
H	2.29864100	-1.35747600	0.77826300
H	4.53844600	-1.98997300	-0.12220100
H	4.69191000	-0.41573800	-0.91314200
H	4.67892600	-0.52161500	0.85482900
Si	-1.72970800	-0.34589200	0.04454900
C	-2.23189800	0.11305900	1.77310400
H	-2.10707800	1.17984900	1.97783100

H	-3.29123200	-0.12989500	1.90977200
H	-1.65693400	-0.45690300	2.50848800
C	-2.43780400	0.71549300	-1.30763900
H	-1.87932500	0.59763500	-2.24119000
H	-3.46502600	0.38215400	-1.49314300
H	-2.47634200	1.77583700	-1.04648100
C	-1.78393300	-2.16160500	-0.32256400
H	-1.24843100	-2.73352200	0.44049800
H	-2.82407000	-2.50312800	-0.33894500
H	-1.33987200	-2.37609600	-1.29891300
H	2.66907500	1.13321800	0.94037700
H	2.31295900	-1.24944800	-0.97573900

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Cyclohexenone. Gibbs free energy: -308.497558

C	-3.25335900	-0.81927000	-1.21595400
C	-1.72839000	-0.87484800	-1.11868000
C	-1.13711600	0.48053000	-0.86534400
C	-1.83186700	1.50905200	-0.35261000
C	-3.23864000	1.36163400	0.06386300
C	-3.84887700	-0.01921200	-0.05585400
H	-0.08599300	0.62283100	-1.10692300
H	-1.42035700	-1.54298100	-0.30117700
H	-1.29504900	-1.29701000	-2.03080200
H	-3.53319100	-0.34321300	-2.16320400
H	-3.67247800	-1.82907300	-1.22800100
H	-1.37586800	2.48212600	-0.19530100
H	-3.64536400	-0.53297600	0.89480700
H	-4.93323400	0.08567600	-0.14054900
O	-3.86789700	2.30677400	0.52864700

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Me_3Si–cyclohexenone$^+$. Gibbs free energy: -717.484112

C	-3.46029700	-0.79391900	-1.11006500
C	-1.97734900	-1.02952200	-1.38919600
C	-1.17941200	0.22056900	-1.26868200
C	-1.58216500	1.31523900	-0.57790700
C	-2.80851400	1.27109300	0.15710100
C	-3.64919900	0.03911500	0.15688800
H	-0.20503800	0.24727200	-1.74952000
H	-1.55167500	-1.74979100	-0.67289100
H	-1.81779700	-1.46741300	-2.37825800
H	-3.90902700	-0.26911600	-1.95991900
H	-3.98345000	-1.74562700	-1.00230300
H	-0.95928000	2.19992300	-0.53250100
H	-3.33283900	-0.53142500	1.04386900
H	-4.69001200	0.32461100	0.32251400
O	-3.21445800	2.23289100	0.88323900
Si	-2.58331000	3.85405300	1.30933500
C	-2.48611200	4.80084800	-0.28979400

H	-2.27192200	5.85100800	-0.06295600
H	-1.70105900	4.43865800	-0.95874100
H	-3.44255800	4.76221500	-0.81972300
C	-0.95444100	3.55933200	2.15978000
H	-1.05837100	2.81117100	2.95142700
H	-0.16611300	3.23689100	1.47456600
H	-0.62850900	4.49610100	2.62484600
C	-3.92066900	4.44990700	2.44828700
H	-3.67723300	5.45421600	2.81023400
H	-4.88390200	4.49866900	1.93224300
H	-4.02009000	3.79040300	3.31539400

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Cyclohexeneoxide. Gibbs free energy: -309.662423

C	-3.23922700	-0.37642200	-0.98305100
C	-1.70478900	-0.36152500	-0.97550200
C	-1.12076500	1.03015200	-0.82647800
C	-1.95854400	2.17583500	-0.44112100
C	-3.43800600	2.00631500	-0.19447700
C	-3.82326800	0.55039500	0.08468300
H	-1.32521300	-0.97454600	-0.14889100
H	-1.32044500	-0.80725800	-1.89853500
H	-3.59999900	-0.04927700	-1.96728800
H	-3.59635400	-1.40118900	-0.83967200
H	-1.64112900	3.17240400	-0.74805600
H	-3.74241900	2.65850900	0.63215900
H	-3.96258500	2.36289500	-1.09039700
H	-3.45469600	0.25290200	1.07350700
H	-4.91403000	0.46201200	0.10901300
H	-0.20771900	1.23115600	-1.38528400
O	-1.08004700	1.56361900	0.50934500

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Me_3Si–cyclohexeneoxide$^+$. Gibbs free energy: -718.646463

C	-3.36269400	0.03531300	-1.36875800
C	-2.01058800	-0.48965100	-0.86641700
C	-1.10393200	0.60357400	-0.36264600
C	-1.59432800	1.96976800	-0.13431500
C	-3.02522400	2.33351000	-0.39458500
C	-3.94358500	1.10847700	-0.44586900
H	-2.14456000	-1.21020200	-0.05252700
H	-1.48111700	-1.01684200	-1.66450300
H	-3.23400300	0.46054500	-2.37130100
H	-4.05722900	-0.80285300	-1.46507700
H	-0.86345300	2.77338200	-0.12320200
H	-3.34999200	3.05786700	0.35782300
H	-3.03133700	2.85198300	-1.36108500
H	-4.08351100	0.70318700	0.56249900
H	-4.92761400	1.42123600	-0.80394700
H	-0.03348400	0.47084900	-0.48768800

O	-1.42788200	1.05196900	1.02906300
Si	-0.30860200	1.22146800	2.45187700
C	1.25201300	1.99140900	1.79928500
H	1.08857800	3.00241800	1.41556100
H	1.96650500	2.06715800	2.62665800
H	1.72247900	1.38486000	1.01988200
C	-1.31640700	2.31813400	3.55485800
H	-0.78578700	2.48321200	4.49826000
H	-1.48822200	3.29292800	3.08854800
H	-2.28284900	1.85977400	3.78225100
C	-0.13645700	-0.54704600	2.98143400
H	-1.11277300	-0.98814900	3.20071300
H	0.35559600	-1.14535500	2.20876900
H	0.47381600	-0.60022600	3.88909300

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$AsPh_3$. Gibbs free energy: -2928.357134

As	0.14972600	-0.06685900	-1.18563600
C	0.95355900	1.45011800	-0.27266100
C	1.60475500	1.36746800	0.95930700
C	0.87938100	2.68818100	-0.91864600
C	2.15899600	2.50497200	1.54529500
H	1.68044500	0.41214200	1.47015000
C	1.42790000	3.82826500	-0.33516200
H	0.38881200	2.76835500	-1.88572000
C	2.06785200	3.73783600	0.90090600
H	2.65925700	2.42745900	2.50572700
H	1.35918700	4.78415800	-0.84513200
H	2.50009400	4.62365000	1.35574100
C	0.89467400	-1.52934900	-0.14341200
C	2.09205600	-2.08178800	-0.60854300
C	0.30656500	-2.05911300	1.00670900
C	2.70242100	-3.13290900	0.07215600
H	2.55560400	-1.69003500	-1.51068800
C	0.91231100	-3.11333700	1.68990500
H	-0.62748100	-1.64748900	1.37812600
C	2.11270800	-3.64967000	1.22551800
H	3.63247700	-3.55167700	-0.29961800
H	0.44716500	-3.51470100	2.58511400
H	2.58279100	-4.47234500	1.75537000
C	-1.64942500	0.00144800	-0.45259100
C	-2.62260100	-0.77134800	-1.09409700
C	-2.01965600	0.78138700	0.64420100
C	-3.93844400	-0.78122700	-0.63644200
H	-2.35438100	-1.37320500	-1.95924200
C	-3.33651100	0.77840000	1.10309600
H	-1.27903200	1.39459600	1.14914700
C	-4.29722800	-0.00566900	0.46598500
H	-4.68280200	-1.38854700	-1.14216600

H	-3.61127900	1.38739300	1.95900500
H	-5.32262000	-0.00736600	0.82251200

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$Me_3Si–AsPh_3^+$. Gibbs free energy: -3337.348791

As	0.14654600	-0.06186600	-1.03360700
C	1.01156200	1.47239900	-0.29626200
C	1.81571300	1.36400100	0.83779100
C	0.82554500	2.71260000	-0.91106100
C	2.42939800	2.50049800	1.35969400
H	1.96602800	0.40182500	1.31719900
C	1.43570300	3.84663100	-0.38569800
H	0.19963800	2.80738100	-1.79322500
C	2.23952000	3.73863000	0.74894900
H	3.05339100	2.41789400	2.24311100
H	1.28681800	4.80963700	-0.86186100
H	2.71871300	4.62206700	1.15764400
C	0.90087900	-1.59380200	-0.18007100
C	2.10507900	-2.11389400	-0.65847000
C	0.26427500	-2.18402100	0.91175800
C	2.67544800	-3.22326700	-0.04288700
H	2.60881200	-1.66166000	-1.50701100
C	0.83730300	-3.29463300	1.52687700
H	-0.67308800	-1.78376600	1.28550400
C	2.03943400	-3.81345300	1.04880400
H	3.60969700	-3.62769100	-0.41703800
H	0.34489700	-3.75338700	2.37756900
H	2.48132600	-4.68174600	1.52625200
C	-1.68657300	0.02129400	-0.50276200
C	-2.58908400	-0.88764400	-1.06015900
C	-2.12331200	0.96661000	0.42434100
C	-3.92786300	-0.85480200	-0.68482600
H	-2.25793300	-1.63074600	-1.77943200
C	-3.46604600	1.00058300	0.79484400
H	-1.42581100	1.67504700	0.85986000
C	-4.36576200	0.09196700	0.24132900
H	-4.62708700	-1.56398300	-1.11449700
H	-3.80657600	1.73542500	1.51634400
H	-5.41128700	0.12199200	0.52977400
Si	0.37033400	-0.14861600	-3.43131600
C	0.08774800	-1.94324800	-3.86299200
H	0.32190400	-2.09190500	-4.92265200
H	0.72579800	-2.60951500	-3.27555200
H	-0.95478700	-2.23392700	-3.70685900
C	-0.96903900	0.99488200	-4.05133100
H	-0.74678200	2.04304800	-3.83388600
H	-1.04771300	0.88681200	-5.13844400
H	-1.94124600	0.74756100	-3.61490900
C	2.10543200	0.45671600	-3.76286900

H	2.23351500	0.58324700	-4.84324500
H	2.29235200	1.42202600	-3.28361100
H	2.86064400	-0.25400100	-3.41672400

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Cyclohexanone. Gibbs free energy: -309.706092

C	-0.39931100	-0.26426700	-0.98912300
C	0.30095300	0.10249700	0.32086800
C	-0.12121300	1.49483000	0.79442000
C	-1.64730300	1.59596300	0.96256900
C	-2.38479800	1.12824300	-0.27281900
C	-1.92973800	-0.19466300	-0.84831900
H	0.36168700	1.74301400	1.74432700
H	0.04893800	-0.63889700	1.09092300
H	1.38679000	0.06673200	0.18612600
H	-0.07827200	0.42751200	-1.77807500
H	-0.11442900	-1.26986500	-1.31301000
H	-1.95982500	0.93802000	1.78567600
H	-2.25867200	-0.97462100	-0.14729700
H	-2.43696800	-0.36303000	-1.80125400
O	-3.30014100	1.77027100	-0.76488100
H	-1.96624200	2.61245600	1.20489800
H	0.21081600	2.24280600	0.06351400

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Me_3Si–cyclohexanone$^+$. Gibbs free energy: -718.687165

C	-0.73981600	-0.41447200	-0.98689700
C	0.36832900	0.06113200	-0.04889300
C	0.14506900	1.51324800	0.36853100
C	-1.23254300	1.70609400	1.04023300
C	-2.32136600	1.11108300	0.22236400
C	-2.13249200	-0.24841800	-0.34302600
H	0.91025800	1.84343000	1.07429400
H	0.40105800	-0.57959000	0.84121800
H	1.33742300	-0.03198000	-0.54675900
H	-0.70868800	0.15476400	-1.92242100
H	-0.60959000	-1.46747000	-1.24604000
H	-1.24738600	1.15384200	1.99113000
H	-2.20924000	-0.93462100	0.51355600
H	-2.94772700	-0.47511300	-1.03120500
O	-3.41146600	1.69335600	-0.00666000
Si	-4.14173500	3.28819600	0.46594700
C	-3.04826100	4.58170900	-0.30085900
H	-3.55562300	5.54962900	-0.22264200
H	-2.07810000	4.67628100	0.19341500
H	-2.88464300	4.37535200	-1.36260400
C	-4.19854600	3.27010700	2.32371500
H	-4.65711400	2.34765700	2.69191400
H	-3.21263500	3.38173800	2.78209100
H	-4.81917400	4.10834100	2.65900800

C	-5.79959300	3.13098900	-0.34701200
H	-6.38123100	4.04155200	-0.16962100
H	-5.69458000	2.99901600	-1.42770900
H	-6.35926100	2.28348400	0.05862100
H	-1.42735800	2.75439000	1.26519800
H	0.20666600	2.16940500	-0.50673300

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Dabco. Gibbs free energy: -345.104723

C	1.19516200	0.77570100	-0.69421800
C	1.19516200	-0.78253400	-0.68644400
H	1.18729900	1.16876800	-1.71608400
H	2.08154200	1.17640100	-0.19184400
H	1.19989300	-1.18592300	-1.70428500
H	2.07553100	-1.17795500	-0.16948000
C	-1.19516200	0.78253400	-0.68644400
H	-2.07553100	1.17795500	-0.16948000
H	-1.19989300	1.18592300	-1.70428500
C	-1.19516200	-0.77570100	-0.69421800
H	-2.08154200	-1.17640100	-0.19184400
H	-1.18729900	-1.16876800	-1.71608400
C	-0.00668100	-0.77886800	1.38074900
H	-0.89679200	-1.16961600	1.88439900
H	0.87064500	-1.18486900	1.89469700
C	0.00668100	0.77886800	1.38074900
H	-0.87064500	1.18486900	1.89469700
H	0.89679200	1.16961600	1.88439900
N	-0.00369700	-1.28398900	0.00029700
N	0.00369700	1.28398900	0.00029700

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$Me_3Si–Dabco^+$. Gibbs free energy: -754.108643

C	-2.19326500	1.05646600	0.88067300
C	-0.65954700	0.93436300	1.05841400
H	-2.45641500	2.02286600	0.44444100
H	-2.68443500	0.98152200	1.85315400
H	-0.15788000	1.89790700	0.95351400
H	-0.39563100	0.50816800	2.02720500
C	-2.19195000	0.23431900	-1.35505800
H	-2.45541100	-0.62548200	-1.97529600
H	-2.68229000	1.11462700	-1.77620100
C	-0.65859800	0.44906700	-1.33633900
H	-0.15588700	-0.12307400	-2.11794700
H	-0.39581700	1.50163200	-1.44993200
C	-0.65891400	-1.38252500	0.28144000
H	-0.39336100	-2.00770100	-0.57196600
H	-0.15798100	-1.77241800	1.16903100
C	-2.19267500	-1.29106500	0.47441900
H	-2.68226700	-2.09561100	-0.07841400
H	-2.45736400	-1.39853300	1.52880400

N	-0.12397800	0.00023700	0.00151200
N	-2.69171900	-0.00020600	-0.00011500
Si	1.79003100	-0.00004400	-0.00019200
C	2.28961600	1.61705800	-0.77763800
H	3.37354500	1.72067000	-0.65751800
H	2.07027300	1.64680200	-1.84819300
H	1.82558000	2.48275200	-0.29665000
C	2.28758000	-1.48155700	-1.01317300
H	3.37169700	-1.43154600	-1.16213400
H	2.06534800	-2.42344600	-0.50447500
H	1.82330000	-1.49569000	-2.00332800
C	2.29509400	-0.13626800	1.78708500
H	3.37947700	-0.28963500	1.81251100
H	2.07624800	0.77474100	2.35047900
H	1.83466200	-0.98730400	2.29688200

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Cis-2,5-Me_2-THF. Gibbs free energy: -310.882615

C	-1.18580600	0.17061900	0.48035800
O	0.07321300	0.86414700	0.51167500
C	1.15586800	-0.05843800	0.35424600
C	0.55256800	-1.21073100	-0.44250400
C	-0.85163800	-1.30015700	0.15753700
H	-1.64519100	0.25662500	1.47315000
H	1.45790000	-0.42495900	1.34912900
H	0.50966900	-0.94219000	-1.50480700
H	1.12482200	-2.13634600	-0.34304100
H	-1.58400300	-1.74410400	-0.52173300
H	-0.83400600	-1.89909300	1.07342700
C	-2.08629600	0.83270900	-0.55110900
H	-3.08374900	0.38234600	-0.52758500
H	-2.18603500	1.90259400	-0.34655700
H	-1.66991300	0.70837500	-1.55660700
C	2.32532800	0.65045800	-0.29840700
H	2.66091900	1.49325800	0.31261100
H	3.16403200	-0.04268900	-0.41589400
H	2.03971400	1.02624000	-1.28621900

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Me_3Si–Cis-2,5-Me_2-THF^+. Gibbs free energy: -719.867308

C	1.14484100	1.24371800	-0.21885900
O	0.27974400	0.02259500	-0.11942200
C	1.08238800	-1.24008700	-0.27663000
C	2.51280300	-0.72627800	-0.30138800
C	2.40243600	0.68708000	-0.86743400
H	0.60961200	1.92571600	-0.87742500
H	0.78576100	-1.63563000	-1.25067600
H	2.92743200	-0.71571500	0.71095700
H	3.13735500	-1.37588300	-0.91644300
H	3.27036600	1.30390700	-0.62871700

H	2.28265400	0.65958400	-1.95338000
C	1.32194400	1.83306900	1.16340000
H	1.90678000	2.75260800	1.07771300
H	0.35998300	2.08871700	1.61402900
H	1.84872200	1.14437100	1.82843800
C	0.77354500	-2.20591900	0.84343700
H	-0.23872600	-2.61034000	0.78812600
H	1.46723800	-3.04691200	0.75756300
H	0.92462500	-1.73233600	1.81683500
Si	-1.53619100	0.06494500	-0.09480000
C	-2.04077300	-1.26089100	-1.29493200
H	-1.80022900	-2.27115100	-0.95434500
H	-3.12803800	-1.20495600	-1.41840100
H	-1.58598300	-1.09883200	-2.27667800
C	-1.97458300	1.77292400	-0.68080200
H	-3.06860800	1.83897000	-0.68649900
H	-1.60516000	2.56012500	-0.01781700
H	-1.62736900	1.96460400	-1.69988600
C	-2.02009900	-0.23373900	1.67419400
H	-1.50397600	0.45906000	2.34538800
H	-3.09696000	-0.05996100	1.77711400
H	-1.81177200	-1.25519700	2.00075900

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trans-2,5-Me_2-THF. Gibbs free energy: -310.882825

C	1.10702300	-0.12504700	-0.41885300
O	0.00003000	-0.93960300	0.00006300
C	-1.10701000	-0.12510600	0.41885700
C	-0.76246000	1.29309700	-0.04027400
C	0.76242600	1.29313400	0.04030100
H	1.14737500	-0.15339000	-1.51817800
H	-1.14745000	-0.15345200	1.51818300
H	-1.09300600	1.44280600	-1.07522700
H	-1.23560500	2.05478300	0.58417200
H	1.23548900	2.05483200	-0.58419600
H	1.09301000	1.44286900	1.07523300
C	2.39941100	-0.68659400	0.14342800
H	2.55778700	-1.71473900	-0.19428100
H	3.24874200	-0.08208300	-0.19133000
H	2.37405900	-0.67767500	1.23802900
C	-2.39940700	-0.68660500	-0.14349600
H	-2.55788400	-1.71474000	0.19418400
H	-3.24868700	-0.08200500	0.19122400
H	-2.37397400	-0.67766000	-1.23809400

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Me_3Si–trans-2,5-Me_2-THF^+. Gibbs free energy: -719.86168

C	1.20323600	1.08620700	0.46422000
O	0.32718100	0.01238100	-0.10495700
C	1.18734400	-1.19436100	-0.34957600

C	2.58795200	-0.60070000	-0.56311800
C	2.43714200	0.91530000	-0.39740000
H	1.38746600	0.78562300	1.49991800
H	0.77797300	-1.63376000	-1.25758800
H	3.27095900	-1.00474500	0.18781700
H	2.97684600	-0.86305500	-1.54738200
H	3.30696900	1.37083300	0.07867700
H	2.27283800	1.40638100	-1.36080800
C	0.55862300	2.44752800	0.40895500
H	-0.32124300	2.52512400	1.05004800
H	1.29669000	3.16117900	0.78502600
H	0.30357600	2.73028800	-0.61434500
C	1.10487600	-2.14313600	0.82786300
H	0.09882500	-2.53463800	0.98704600
H	1.76494600	-2.99088700	0.62446300
H	1.44972600	-1.65999600	1.74607300
Si	-1.49621500	-0.07791100	-0.07309300
C	-1.92496100	-0.10141800	1.73410400
H	-1.61242700	0.81538700	2.24217500
H	-3.01131000	-0.18922500	1.84245500
H	-1.46406000	-0.95386400	2.24118500
C	-1.88831500	-1.64544900	-0.99500200
H	-2.98144600	-1.72269400	-1.02391600
H	-1.53953200	-1.59775200	-2.03094400
H	-1.50904300	-2.55777300	-0.53102900
C	-2.13922800	1.38551100	-1.02286400
H	-1.58301500	1.53133900	-1.95333000
H	-3.17801400	1.15972800	-1.29040900
H	-2.13717500	2.31733200	-0.45526800

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Dioxane: Gibbs free energy: -307.495603

C	-4.43416400	0.63680000	-1.26697300
C	-2.50230400	1.95243000	-1.26339400
C	-2.57763400	2.05816600	0.25110100
C	-4.50949300	0.74253600	0.24752200
H	-1.46305200	1.94874400	-1.59977800
H	-5.03451900	1.43640000	-1.72689400
H	-4.81190500	-0.33016800	-1.60691400
H	-1.97727800	1.25856600	0.71102100
H	-2.19989200	3.02513500	0.59104200
H	-3.98808100	-0.11030900	0.70810600
H	-5.54874500	0.74622300	0.58390600
H	-3.02371600	2.80527500	-1.72397900
O	-3.92430700	1.95828300	0.69389500
O	-3.08749000	0.73668300	-1.70976800

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Me_3Si–dioxane$^+$. Gibbs free energy: -716.469714

C	-4.13972800	0.00754800	-0.93702300

C	-2.29043500	1.35774600	-1.39597400
C	-2.59602600	2.25939800	-0.21815200
C	-4.52400000	0.85462600	0.25777200
H	-1.20977100	1.31317300	-1.53969000
H	-4.67118800	0.35070000	-1.83506300
H	-4.41505400	-1.02963700	-0.73924000
H	-2.11865700	1.91937400	0.70256700
H	-2.32866000	3.29700000	-0.41365300
H	-4.04502700	0.51577500	1.17817500
H	-5.60102500	0.91344600	0.39402900
H	-2.75479200	1.75621200	-2.30875000
O	-4.04396000	2.22788700	0.03746700
Si	-5.08556600	3.72409700	-0.23173300
C	-4.97180000	4.02599300	-2.05869800
H	-5.54445500	4.92749500	-2.30317000
H	-3.94132700	4.19261900	-2.38560800
H	-5.39406500	3.19206300	-2.62633900
C	-6.76243500	3.21331300	0.37115100
H	-6.74296000	2.85548800	1.40442200
H	-7.39849000	4.10565200	0.34374800
H	-7.22970600	2.45992900	-0.26871100
C	-4.24606500	4.99720200	0.82576400
H	-4.89235600	5.88069200	0.87308000
H	-4.09915900	4.63091100	1.84566000
H	-3.28324700	5.31779400	0.41902500
O	-2.74058900	0.03986000	-1.14870600

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3-penten-2-one. Gibbs free energy: -270.408009

C	-1.08426100	0.14472000	0.00050500
O	-1.26483600	1.35733200	0.00035800
C	-2.24156000	-0.82228300	-0.00057500
H	-2.18527000	-1.46725000	-0.88416400
H	-2.18071900	-1.47665400	0.87566800
H	-3.19009000	-0.28494000	0.00440800
C	0.27215300	-0.45661300	0.00100600
C	1.38107300	0.29441200	-0.00052000
H	0.33675500	-1.54294000	0.00245700
C	2.77809900	-0.23000200	-0.00018800
H	1.25882900	1.37723000	-0.00220400
H	3.31901500	0.13640300	-0.87957900
H	3.32000700	0.14036000	0.87692400
H	2.80713700	-1.32227100	0.00226900

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Me_3Si–3-penten-2one$^+$. Gibbs free energy: -679.391541

C	0.85941200	0.88921800	0.00290600
O	0.07053300	-0.11060500	-0.01545100
C	0.32931800	2.27864400	-0.00489600
H	-0.51728000	2.37916400	0.67745700

H	1.10122100	3.00064000	0.25598500
H	-0.02814400	2.50132700	-1.01738500
C	2.27310500	0.65145800	0.00302800
C	2.78195300	-0.60242700	-0.00881000
H	2.92275400	1.51977700	0.01475900
C	4.22585800	-0.92712200	-0.00828000
H	2.08618000	-1.43962300	-0.01728800
H	4.45756700	-1.55129500	0.86229700
H	4.46137300	-1.53576900	-0.88879300
H	4.85766600	-0.03798600	0.00092800
Si	-1.69836600	-0.35804200	0.00519400
C	-2.20240000	-0.00950200	1.76142200
H	-2.07775300	1.04273100	2.03199700
H	-3.26151000	-0.26075700	1.88410600
H	-1.62575700	-0.62225600	2.46024300
C	-2.44749300	0.78006700	-1.26312700
H	-1.90585600	0.73312900	-2.21282700
H	-3.47452500	0.44788000	-1.45167700
H	-2.49256400	1.81987600	-0.92946400
C	-1.79176800	-2.14975600	-0.46863200
H	-1.24780900	-2.77475600	0.24548200
H	-2.83723400	-2.47493100	-0.48040300
H	-1.37337000	-2.31320200	-1.46619900

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Methylbutyrate. Gibbs free energy: -346.823658

C	-0.75981700	2.15606200	-0.88017100
O	-0.04110900	2.55004600	-1.77726600
C	-1.04061200	0.71247300	-0.54703400
C	-0.49014100	-0.27619200	-1.56997300
H	-0.60934400	0.52305100	0.44421100
C	-0.77582300	-1.72236100	-1.16869400
H	-0.93360400	-0.06757500	-2.54957900
H	-0.38672200	-2.42070500	-1.91513300
H	-0.30880400	-1.96280700	-0.20745900
H	-1.85226200	-1.90002800	-1.07087500
C	-1.18214400	4.38744500	-0.24139900
H	-1.49254900	4.68322400	-1.24533300
H	-1.79307100	4.88605700	0.50857800
H	-0.12761100	4.63050000	-0.09676600
O	-1.39965300	2.98442700	-0.04399200
H	-2.12374700	0.59602000	-0.42909700
H	0.58860900	-0.12452500	-1.67776800

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Me_3Si–methylbutyrate$^+$. Gibbs free energy: -755.800841

C	0.15345800	1.74909000	-0.67012100
O	1.19463900	1.47676100	-1.32843700
C	-1.02518400	0.84203600	-0.73052100
C	-0.89441400	-0.29464300	-1.74329700

H	-1.17352600	0.44718400	0.28421400
C	-2.14326900	-1.17347500	-1.74527100
H	-0.73247400	0.12914700	-2.73895600
H	-2.04432200	-1.97361000	-2.48289100
H	-2.30412500	-1.63545800	-0.76595900
H	-3.03677700	-0.59317500	-1.99729500
C	-0.96563500	3.24874800	0.83215300
H	-1.25619400	2.45719400	1.52153700
H	-0.61069400	4.11867300	1.37641800
H	-1.78287800	3.52081400	0.16498900
O	0.17604500	2.82369300	0.04334400
H	-1.90918400	1.45623300	-0.94134900
H	-0.01240400	-0.89532200	-1.50354800
Si	2.75320300	2.38322700	-1.45459100
C	2.30673000	4.02507000	-2.20274100
H	1.68637500	4.62396600	-1.53099600
H	3.22714400	4.58396700	-2.40422200
H	1.77924000	3.89396000	-3.15212100
C	3.69642000	1.25820800	-2.58892300
H	3.83050700	0.26939800	-2.14078300
H	3.18519500	1.14337100	-3.54903400
H	4.68786500	1.68211500	-2.77997900
C	3.43250500	2.46575400	0.27347500
H	4.43481300	2.90638300	0.23733200
H	2.81215800	3.08727100	0.92425300
H	3.52007500	1.46776100	0.71295000

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Et_2O. Gibbs free energy: -233.504207

C	0.00000000	2.38240700	0.40661000
C	0.00000000	1.17994100	-0.51504100
H	-0.88827400	2.38049100	1.04530700
H	0.88827400	2.38049100	1.04530700
H	0.00000000	3.30553100	-0.18061700
H	0.88793800	1.19205000	-1.16655400
H	-0.88793800	1.19205000	-1.16655400
O	0.00000000	0.00000000	0.26842400
C	0.00000000	-1.17994100	-0.51504100
C	0.00000000	-2.38240700	0.40661000
H	0.88793800	-1.19205000	-1.16655400
H	-0.88793800	-1.19205000	-1.16655400
H	0.00000000	-3.30553100	-0.18061700
H	0.88827400	-2.38049100	1.04530700
H	-0.88827400	-2.38049100	1.04530700

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$Me_3Si–OEt_2^+$. Gibbs free energy: -642.48091

C	-1.64895900	1.93239500	-0.41326900
C	-1.26777800	1.16804200	0.83386100
H	-0.77270100	2.28163600	-0.96379200

H	-2.27050100	1.33415400	-1.08133900
H	-2.22005800	2.81298900	-0.10684800
H	-2.13894700	0.84274800	1.40267000
H	-0.61828200	1.74242900	1.49341400
O	-0.52280500	-0.06840700	0.52130900
C	-1.28127900	-1.33022500	0.62374100
C	-2.36935500	-1.43281900	-0.41819800
H	-1.66355800	-1.36330300	1.64505100
H	-0.53541300	-2.11459900	0.50654200
H	-2.82192900	-2.42413000	-0.33203200
H	-3.15862500	-0.69403000	-0.26410200
H	-1.96402800	-1.32550700	-1.42689600
Si	1.19560300	-0.06087200	-0.11329300
C	1.00264200	-0.28809800	-1.94507500
H	0.43191600	0.52729300	-2.39771600
H	1.99363400	-0.31065500	-2.41109200
H	0.50591500	-1.23533700	-2.17575300
C	1.86773500	1.58354100	0.42389800
H	1.86099700	1.68706600	1.51267800
H	2.91292900	1.62320600	0.09647300
H	1.35437400	2.43845000	-0.02210000
C	2.01487900	-1.48548300	0.75340200
H	1.80931300	-1.47543100	1.82766700
H	1.73488000	-2.45887400	0.34262400
H	3.09678000	-1.37277100	0.62001700

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EtOH. Gibbs free energy: -154.956083

C	-2.51905900	0.69095900	-0.00003000
C	-1.00415000	0.70972000	-0.00001000
H	-2.90892300	1.71321600	-0.00001200
H	-2.89940200	0.17773000	-0.88832300
H	-2.89942400	0.17769000	0.88822900
H	-0.63123900	1.23678100	-0.88814800
H	-0.63126200	1.23674200	0.88816000
O	-0.53975800	-0.63931000	-0.00003500
H	0.42200200	-0.63487900	-0.00002200

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Me_3Si–ethanol$^+$. Gibbs free energy: -563.934993

C	-2.33831500	0.70586600	0.35393400
C	-1.00267500	0.64311300	-0.34103200
H	-2.76926200	1.69562800	0.18303900
H	-3.03327200	-0.03645600	-0.04761300
H	-2.22587600	0.55509600	1.42936100
H	-1.06928100	0.77220800	-1.42153500
H	-0.28936100	1.35461900	0.07266700
O	-0.38382500	-0.68180300	-0.10324000
H	-0.93944200	-1.40136200	-0.43880300
Si	1.43372600	-0.97712200	-0.00816300

C	2.09943200	-0.22605500	-1.56732400
H	1.92969400	0.85392800	-1.60473400
H	3.18082500	-0.39429000	-1.61208100
H	1.64881900	-0.68633400	-2.45130500
C	1.89283700	-0.09108100	1.55366100
H	1.32818600	-0.47708900	2.40662400
H	2.95827800	-0.25471700	1.74833300
H	1.73440100	0.98853900	1.47961600
C	1.48342300	-2.82776900	0.07646500
H	1.09253400	-3.28958900	-0.83476400
H	2.52620300	-3.14330500	0.18801400
H	0.92590100	-3.20487900	0.93849000

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Hexylmethylether. Gibbs free energy: -351.339336

C	2.94307100	3.31051800	0.00000000
C	1.50710900	2.78755800	0.00000000
H	2.97144000	4.40460400	0.00000000
H	3.48671000	2.96060700	0.88469000
H	3.48671000	2.96060700	-0.88469000
C	1.43154200	1.26080600	0.00000000
H	0.97550100	3.17512300	0.87881200
H	0.97550100	3.17512300	-0.87881200
C	0.00000000	0.72464100	0.00000000
H	1.96354000	0.87225500	-0.87952200
H	1.96354000	0.87225500	0.87952200
H	-0.53075100	1.11317200	0.87994000
H	-0.53075100	1.11317200	-0.87994000
C	-0.06201800	-0.80290200	0.00000000
C	-1.48786100	-1.32330400	0.00000000
H	0.45852000	-1.19549200	0.88220500
H	0.45852000	-1.19549200	-0.88220500
H	-2.02870500	-0.95882800	0.88867500
H	-2.02870500	-0.95882800	-0.88867500
O	-1.46742900	-2.73857200	0.00000000
C	-2.76182800	-3.29920400	0.00000000
H	-2.64725300	-4.38451200	0.00000000
H	-3.32723400	-2.99692900	0.89322700
H	-3.32723400	-2.99692900	-0.89322700

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Me_3Si–hexylmethylether$^+$. Gibbs free energy: -760.313752

C	5.81281400	-0.61423200	-0.51376100
C	4.71219300	-0.00486100	0.35322700
H	6.79304000	-0.51744700	-0.03751900
H	5.62857400	-1.67976500	-0.68963000
H	5.86351900	-0.11866100	-1.48947500
C	3.32673400	-0.11930600	-0.28291700
H	4.70047300	-0.49952500	1.33283700
H	4.93515900	1.05302400	0.54201800

C	2.22191400	0.48146200	0.58593000
H	3.33362200	0.38177700	-1.26027400
H	3.10270500	-1.17718100	-0.47587600
H	2.20572600	-0.02983900	1.55711600
H	2.44850100	1.53615100	0.78779000
C	0.84187500	0.37592500	-0.06966600
C	-0.22307200	0.93612700	0.85011900
H	0.62643600	-0.67460800	-0.29514600
H	0.84406300	0.92065000	-1.02014100
H	-0.33651400	0.35530900	1.76495000
H	-0.03392000	1.97696800	1.11797500
O	-1.55914200	0.93749400	0.22182000
C	-1.84247200	2.11837100	-0.58363500
H	-2.83101200	1.99141500	-1.01879500
H	-1.83397400	2.98000700	0.08206400
H	-1.09014000	2.20604400	-1.36681900
Si	-2.53393900	-0.59832300	-0.04411400
C	-1.85847000	-1.77519900	1.22035500
H	-2.42064200	-2.71094900	1.12350000
H	-0.80224900	-2.01154400	1.06825800
H	-2.00404700	-1.40655000	2.23951300
C	-4.27587400	-0.05784700	0.29863600
H	-4.67411500	0.61698300	-0.46348700
H	-4.91141700	-0.95043800	0.31091000
H	-4.35352500	0.42432900	1.27714500
C	-2.19088500	-1.05617500	-1.80997200
H	-2.49752700	-0.26663900	-2.50217500
H	-1.13115500	-1.27133300	-1.97224300
H	-2.76184700	-1.95719400	-2.05934500

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H-PPh_3^+. Gibbs free energy: -1036.285033

P	-0.03020800	-0.02892900	-0.88320200
C	0.59624600	1.57995600	-0.38508600
C	1.57460500	1.67833100	0.60865600
C	0.05492500	2.73097800	-0.97225800
C	2.01044400	2.93650700	1.01607000
H	1.99598200	0.78693200	1.06225500
C	0.49847700	3.98125600	-0.55776500
H	-0.70719100	2.65817200	-1.74245800
C	1.47394800	4.08313000	0.43499200
H	2.76943300	3.01737900	1.78624300
H	0.08359100	4.87529300	-1.00987600
H	1.81754000	5.06124200	0.75500200
C	1.06261300	-1.34239000	-0.32994500
C	2.28808200	-1.53009200	-0.98174500
C	0.70824100	-2.13230900	0.76785500
C	3.15971100	-2.51223100	-0.52561000
H	2.56442500	-0.91675500	-1.83429800

C	1.58980000	-3.11224600	1.21610000
H	-0.24397700	-1.98929800	1.26872400
C	2.81081600	-3.30025100	0.57202400
H	4.10959800	-2.66298500	-1.02643100
H	1.31967000	-3.72816000	2.06678700
H	3.49494900	-4.06504900	0.92419900
C	-1.69983600	-0.27758600	-0.27126800
C	-2.14630500	0.43500400	0.84620500
C	-2.52390800	-1.22283400	-0.89463700
C	-3.42409000	0.19460700	1.34271200
H	-1.50898100	1.17188000	1.32483200
C	-3.79940400	-1.45245500	-0.39098800
H	-2.17804400	-1.77552700	-1.76297100
C	-4.24674200	-0.74564100	0.72564500
H	-3.77572900	0.74365400	2.20909100
H	-4.44427200	-2.17982600	-0.87159000
H	-5.24288300	-0.92719300	1.11510200
H	-0.07666000	-0.06756800	-2.28102400

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Imine. Gibbs free energy: -656.954123

C	-0.98208800	0.78832900	0.19999400
O	-1.64976800	-0.32016100	0.56880000
N	0.20496300	0.70024100	-0.25387700
C	-1.77718600	2.05086000	0.39570700
H	-1.32553800	2.65975700	1.18578600
H	-1.77547700	2.65060300	-0.51905700
H	-2.80520600	1.81972000	0.67275500
C	0.88385300	1.92938300	-0.63359800
H	0.88187000	2.68118900	0.16687800
H	1.92450400	1.70261300	-0.87517200
H	0.42867700	2.38845700	-1.52152900
Si	-1.01658300	-1.91822000	0.47978500
C	0.48650900	-2.09324100	1.58117500
H	1.36109900	-1.60564800	1.14417700
H	0.29814300	-1.65027400	2.56490900
H	0.71362500	-3.15519000	1.72854200
C	-0.67075500	-2.38133500	-1.29999700
H	-0.47392300	-3.45705200	-1.37100700
H	-1.53485000	-2.15529700	-1.93376500
H	0.19585300	-1.84156500	-1.68934600
C	-2.44247200	-2.92483800	1.15662700
H	-3.35563000	-2.75829900	0.57600300
H	-2.20427800	-3.99335300	1.11317000
H	-2.64761400	-2.66679000	2.20079500

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iPrCOOH. Gibbs free energy: -307.555966

C	-1.42621900	1.07666800	-0.45056000
C	-0.61558500	-0.22277300	-0.41303900

H	-0.63536700	-0.68143000	-1.40505800
H	-0.97173500	1.82341100	-1.10738700
H	-2.42951000	0.86298500	-0.82777600
H	-1.55617100	1.51784400	0.54542300
C	-1.19867500	-1.22696900	0.59645200
H	-0.64787600	-2.17078900	0.58099300
H	-1.17328200	-0.82524200	1.61459000
H	-2.24186900	-1.43285100	0.34218400
C	0.86133900	-0.01931200	-0.11396200
O	1.19503300	0.90727700	0.80365100
H	0.41898600	1.37763300	1.13420600
O	1.74392500	-0.67193200	-0.62746600

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Me_3Si–iPrCOOH$^+$. Gibbs free energy: -716.5369

C	3.48960100	-0.67226700	-0.23586100
C	2.33821400	0.31203700	-0.43567900
H	2.25282800	0.56538400	-1.49930100
H	3.35375000	-1.59791500	-0.80340200
H	4.40978300	-0.21085700	-0.59843900
H	3.64795000	-0.90485500	0.82326300
C	2.54288700	1.62238600	0.35048700
H	1.73124900	2.32874500	0.16917400
H	2.61453200	1.42510200	1.42339700
H	3.47879200	2.07771700	0.02176100
C	0.99458800	-0.25922500	-0.09260500
O	0.83764800	-1.42800100	0.44286900
H	1.67812000	-1.88949200	0.59375300
O	-0.03870200	0.41752600	-0.32282200
Si	-1.79040800	0.04980800	-0.01129900
C	-2.16123600	-1.44415800	-1.05096100
H	-3.23134400	-1.66636300	-0.97672300
H	-1.92805200	-1.26066500	-2.10376000
H	-1.60917600	-2.32453100	-0.71181900
C	-1.91503400	-0.21427100	1.82316600
H	-1.39214500	-1.11948600	2.14194200
H	-1.51363000	0.64187300	2.37299000
H	-2.97181400	-0.32193900	2.09070300
C	-2.56322200	1.62322500	-0.61465900
H	-2.19320000	2.48490200	-0.05169100
H	-2.35960000	1.78243800	-1.67734900
H	-3.64868500	1.57007400	-0.48000500

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iPrCOO-$SiMe_3$. Gibbs free energy: -716.142184

C	-2.33954000	-1.14802900	0.41153900
C	-1.10950200	-0.73911100	-0.40877200
H	-1.27058800	-1.00795400	-1.45648300
H	-3.24425800	-0.64489800	0.05748100
H	-2.49555300	-2.22717100	0.32418800

H	-2.19798600	-0.90556400	1.46864700
C	0.15929100	-1.43598700	0.09968400
H	1.04024100	-1.14017700	-0.47796900
H	0.33801900	-1.19683100	1.15204600
H	0.04196200	-2.51973800	0.00908800
C	-0.93293800	0.76643100	-0.39912200
O	-0.74607000	1.27210900	0.81753400
O	-0.95699100	1.45775700	-1.40442800
Si	-0.52669900	2.96357700	1.13768400
C	-2.06163700	3.88293100	0.59958200
H	-2.95277000	3.47166700	1.08457900
H	-1.97956500	4.93865500	0.88067300
H	-2.19680100	3.82397100	-0.48357500
C	1.01785900	3.55039300	0.26573900
H	1.21857900	4.59538500	0.52662400
H	1.88617400	2.95424700	0.56461300
H	0.90430700	3.48111900	-0.81935500
C	-0.32557200	2.98174400	2.99439000
H	0.54573800	2.39455400	3.30160900
H	-0.18536700	4.00818100	3.35011600
H	-1.21085400	2.56930600	3.48869800

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Lutidine. Gibbs free energy: -326.728259

C	1.15759400	0.26677100	-0.00615100
C	1.19845700	-1.12989600	-0.00850100
C	0.00000000	-1.83471800	0.00000000
C	-1.19845700	-1.12989600	0.00850100
C	-1.15759400	0.26677100	0.00615100
N	0.00000000	0.94372900	0.00000000
H	0.00000000	-2.92043700	0.00000000
H	2.15162500	-1.64786800	-0.01529100
H	-2.15162500	-1.64786800	0.01529100
C	-2.41647700	1.09177000	-0.00386600
H	-2.51595000	1.61585200	-0.95990100
H	-3.30419200	0.47232100	0.14165300
H	-2.38101200	1.84914800	0.78383800
C	2.41647700	1.09177000	0.00386600
H	2.38101200	1.84914700	-0.78383800
H	2.51595000	1.61585300	0.95990100
H	3.30419200	0.47232100	-0.14165300

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Me_3Si–lutidine$^+$. Gibbs free energy: -735.707285

C	-1.07369100	-1.18831000	0.07287300
C	-2.44661000	-1.19393700	-0.12720200
C	-3.13906300	-0.00252900	-0.26935600
C	-2.44460100	1.18618000	-0.11930500
C	-1.07137000	1.17581200	0.07989000
N	-0.37916700	-0.00678800	0.08535700

H	-4.20942500	-0.00104300	-0.44160300
H	-2.96366300	-2.14524600	-0.15012700
H	-2.95890100	2.13919800	-0.13585400
C	-0.38659100	2.48567000	0.34479200
H	-0.06720100	2.96677800	-0.58174500
H	-1.10079400	3.15131900	0.83122400
H	0.47291600	2.38573200	1.00659300
C	-0.38984700	-2.49859700	0.33527300
H	-0.00136000	-2.94462500	-0.58190400
H	0.42078900	-2.40684400	1.05870500
H	-1.12367600	-3.19023900	0.75057900
Si	1.54128400	0.00578500	-0.04461900
C	2.05810300	1.46784800	-1.09329100
H	1.37801500	1.63383500	-1.93446900
H	2.18213300	2.40243300	-0.54599600
H	3.03220900	1.20182900	-1.51696900
C	2.14438700	0.05049000	1.71741300
H	1.81479300	-0.82862900	2.27857900
H	3.23959200	0.05487100	1.71103800
H	1.80659800	0.94249900	2.25178200
C	2.12940900	-1.49353400	-0.99637300
H	2.20525600	-2.41096100	-0.41325400
H	1.52916300	-1.68238400	-1.89143000
H	3.13900000	-1.23655900	-1.33626900

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Methylcrotonate. Gibbs free energy: -345.612744

C	0.67053400	0.70271600	0.17827600
O	0.60402600	1.91105500	0.32325100
C	-0.47473100	-0.21835600	0.03542300
C	-1.73277800	0.23397100	0.06543300
H	-0.24826600	-1.27272400	-0.09294700
C	-2.95100800	-0.61843900	-0.06424300
H	-1.88921600	1.30356700	0.19822300
H	-3.57939500	-0.51589800	0.82708100
H	-3.55635200	-0.28660300	-0.91473100
H	-2.70140700	-1.67337000	-0.19994300
C	3.02491100	0.82293800	0.26315600
H	3.03724300	1.33547300	1.22713100
H	3.84857900	0.11464800	0.19883800
H	3.08797900	1.55756700	-0.54198200
O	1.83443600	0.03782700	0.13080900

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Me_3Si–methylcrotonate$^+$. Gibbs free energy: -754.595585

C	0.79300100	0.44485500	-0.01770600
O	-0.06510000	-0.49512100	0.00621300
C	2.20431500	0.14758900	-0.03443200
C	2.63055800	-1.13071600	-0.02422700
H	2.90759000	0.97045300	-0.05395400

C	4.05543600	-1.54034200	-0.03734700
H	1.88804800	-1.92572100	-0.00431700
H	4.26610900	-2.15070300	0.84774200
H	4.24207900	-2.18302000	-0.90459600
H	4.73765800	-0.68934200	-0.06161800
C	1.16783600	2.82303400	-0.05262100
H	1.76510000	2.82381900	-0.96421500
H	0.47402800	3.65868100	-0.05322600
H	1.79095300	2.84655900	0.84125300
O	0.31777000	1.65010500	-0.02582900
Si	-1.85321700	-0.40435900	0.03354300
C	-2.29905500	0.49497600	1.59953000
H	-2.01923600	1.55060600	1.55380100
H	-3.38238800	0.43546100	1.75013900
H	-1.81426600	0.03698800	2.46691400
C	-2.34834000	0.46490400	-1.53459200
H	-1.88039700	-0.00241900	-2.40629100
H	-3.43431500	0.39202500	-1.65744300
H	-2.07800200	1.52375700	-1.51321100
C	-2.27420600	-2.21268900	0.05730800
H	-1.85604700	-2.70199800	0.94189800
H	-3.36175300	-2.33832000	0.08181800
H	-1.89364700	-2.71726400	-0.83561800

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Methyl-(E)-3-(oxiran-2-yl)acrylate. Gibbs free energy: -458.856373

C	0.64164800	0.57840200	0.17004600
O	0.47917100	1.73911300	-0.15769100
C	-0.46294400	-0.29977500	0.63115400
C	-1.71172200	0.17542700	0.68911600
H	-0.25721000	-1.32412400	0.91966600
C	-2.86630900	-0.63911400	1.11100300
H	-1.91395400	1.20691800	0.40716100
H	-2.64620200	-1.61830100	1.53222100
C	2.18215500	-1.27662800	0.46824700
H	1.64369800	-1.97883900	-0.17205600
H	3.25222000	-1.38801900	0.30409100
H	1.95669000	-1.46196500	1.52083500
O	1.88561100	0.07847500	0.10965000
C	-4.18475800	-0.43750800	0.48605400
H	-4.29794900	0.31655000	-0.28959100
H	-4.87716800	-1.27475500	0.44957800
O	-3.91086500	0.07058400	1.78646000

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Me_3Si–Methyl-(E)-3-(oxiran-2-yl)acrylate$^+$. Gibbs free E: -867.834248

C	1.11573100	0.09540700	0.33040900
O	1.62639600	1.10432300	-0.24926900
C	-0.28252600	-0.22072500	0.14150700
C	-1.04764500	0.55413300	-0.64857400

H	-0.69321300	-1.08488600	0.64789900
C	-2.46644700	0.28431100	-0.90999800
H	-0.62087400	1.42568200	-1.14021300
H	-2.96067900	-0.44914400	-0.27744800
C	1.46334800	-1.78228000	1.79600000
H	1.09903900	-2.52703500	1.08919000
H	2.35479000	-2.14321100	2.30044300
H	0.70112600	-1.50221800	2.52229200
O	1.90718900	-0.60343000	1.07784800
C	-2.99579400	0.50585500	-2.27326700
H	-2.32954100	0.85850700	-3.05679700
H	-3.84524100	-0.09428700	-2.58810700
O	-3.25122200	1.43244000	-1.23196300
Si	3.30363200	1.73980700	-0.18259600
C	3.15965000	3.16847100	-1.35944000
H	4.12456500	3.68040500	-1.43633700
H	2.87738900	2.82665700	-2.35966700
H	2.41693200	3.89310700	-1.01334000
C	4.40390600	0.36948000	-0.79159400
H	4.04844400	-0.02577700	-1.74792200
H	5.41305800	0.76665000	-0.94570700
H	4.46600700	-0.44996200	-0.07121300
C	3.57968300	2.23345000	1.58874800
H	4.55643100	2.72111800	1.67783500
H	2.81737000	2.94383600	1.92186800
H	3.57170800	1.36711100	2.25552800

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$MeOSiMe_3$. Gibbs free energy: -524.251478

O	0.54167800	-0.83575200	-0.71575500
C	1.87647300	-0.57774100	-0.32141700
H	2.53944300	-1.20284400	-0.92478800
H	2.04078500	-0.81916400	0.73675600
Si	-0.76303500	-0.09428400	0.04902300
C	-2.26762100	-0.66150000	-0.90590400
H	-2.37529600	-1.74998800	-0.85775100
H	-3.17591500	-0.21289500	-0.48918400
H	-2.19644800	-0.37002200	-1.95876200
C	-0.84400200	-0.64917600	1.84145500
H	0.05827400	-0.36267200	2.39259900
H	-1.70074700	-0.18452300	2.34239400
H	-0.95837100	-1.73582300	1.91357900
C	-0.56193500	1.77145500	-0.02663600
H	0.32073300	2.10325900	0.53078800
H	-0.46287600	2.11819200	-1.06066300
H	-1.43652700	2.26295400	0.41400300
H	2.14587000	0.47340300	-0.48577200

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$Me_3Si–MeOSiMe_3^+$. Gibbs free energy: -933.23013

O	0.03018600	0.24296400	0.49471700
C	0.08438400	1.58626000	1.08070800
H	0.57553300	1.51698000	2.04811800
H	-0.93372600	1.94390200	1.21829100
Si	-1.58119300	-0.18672400	-0.22910700
C	-1.45774600	-1.93073600	-0.85460200
H	-1.35265200	-2.65464800	-0.04321900
H	-2.41166800	-2.13375500	-1.35598900
H	-0.66720700	-2.09095200	-1.59099000
C	-2.78129000	-0.04811900	1.18514100
H	-3.02713900	0.98429100	1.44589100
H	-3.71215400	-0.54470100	0.89022800
H	-2.39781100	-0.55666700	2.07472500
C	-1.81052400	1.06738000	-1.58160500
H	-1.82699900	2.09168100	-1.19855300
H	-1.01976800	0.98798200	-2.33363900
H	-2.76916500	0.88304400	-2.07818700
Si	1.62987000	-0.57631900	0.17855500
C	2.86312900	0.33939800	1.22687200
H	2.64560100	0.25009400	2.29505400
H	3.83418700	-0.13780300	1.05037900
H	2.96478100	1.39574000	0.96684700
C	1.43112400	-2.33472500	0.74873500
H	0.82931100	-2.39126000	1.66072600
H	0.99298800	-2.98692600	-0.00862300
H	2.42902400	-2.72023400	0.98534000
C	1.91755500	-0.34440900	-1.64355100
H	2.89796200	-0.76169200	-1.89822800
H	1.17262700	-0.85317800	-2.26087100
H	1.92566900	0.71732900	-1.90786000
H	0.62240100	2.24915400	0.40391500

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$EtOSiMe_3$. Gibbs free energy: -563.534775

O	0.57457800	-0.64272500	-0.80600900
C	1.86903500	-0.82368300	-0.25214800
C	2.60886900	0.48658500	-0.02205100
H	2.42758300	-1.44488500	-0.95961300
H	1.79907200	-1.38456200	0.69015900
H	3.63556200	0.28442300	0.29940200
H	2.64376500	1.07519000	-0.94377100
H	2.12686600	1.08842600	0.75486000
Si	-0.73655600	0.02487300	0.01129000
C	-2.25268300	-0.70326000	-0.81074100
H	-2.29026100	-1.78946000	-0.67944500
H	-3.16460600	-0.27518900	-0.38012700
H	-2.25388200	-0.48810300	-1.88461000
C	-0.64678900	-0.44093300	1.82872500
H	0.23320100	-0.00544300	2.31451100

H	-1.53400000	-0.06873900	2.35280800
H	-0.60689600	-1.52740600	1.96107800
C	-0.74908800	1.89440400	-0.17528800
H	0.11253400	2.35890000	0.31470900
H	-0.73204100	2.17837900	-1.23301500
H	-1.65780200	2.31336700	0.27208800

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$Me_3Si–EtOSiMe_3^+$. Gibbs free energy: -972.51417

O	0.00169400	0.36829100	0.26278600
C	-0.01697900	1.76768100	0.75843300
C	-0.38958100	2.74148300	-0.33424200
H	0.98166100	1.96516400	1.14824900
H	-0.70909700	1.78836000	1.59845400
H	-0.33053300	3.75249800	0.07786500
H	0.29711900	2.67400200	-1.17999500
H	-1.40865900	2.58652100	-0.69462800
Si	-1.59524500	-0.45535900	-0.03051400
C	-1.42211600	-2.19579000	0.60635000
H	-0.79299400	-2.24904400	1.49987600
H	-2.42415100	-2.53571200	0.89102900
H	-1.03796200	-2.88839500	-0.14448900
C	-2.84324500	0.48310800	0.98229600
H	-2.96510100	1.53072600	0.69782900
H	-3.80640500	-0.01334700	0.81523300
H	-2.62858300	0.42293100	2.05333500
C	-1.87717200	-0.32222200	-1.86320600
H	-1.98737000	0.71880800	-2.17892600
H	-1.06550900	-0.77341900	-2.43998500
H	-2.80228700	-0.85173300	-2.11632100
Si	1.67035200	-0.29678500	-0.00707700
C	2.38846800	-0.45220700	1.70065600
H	1.75311900	-1.07475000	2.33753800
H	3.36628400	-0.93977600	1.62034800
H	2.53911400	0.51305100	2.19152400
C	1.50789100	-1.93759600	-0.86494100
H	1.23795300	-2.74365000	-0.18037100
H	0.81478000	-1.93159400	-1.70947200
H	2.50231000	-2.16373000	-1.26749100
C	2.52404000	0.95223400	-1.09000000
H	3.53449900	0.57829500	-1.28991900
H	2.01302300	1.06134900	-2.05113000
H	2.62589400	1.93698000	-0.62663500

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N-Me-acetamide. Gibbs free energy: -248.403202

C	-0.95027000	0.84135200	0.07588500
O	-1.44762700	-0.28383700	-0.03612400
N	0.35871000	1.01549200	0.35342400
C	-1.78130800	2.09353800	-0.08922300

H	-1.20609900	3.01567300	0.01472700
H	-2.25082300	2.07482500	-1.07545600
H	-2.57727700	2.08534800	0.65924600
C	1.26302400	-0.10329200	0.54241200
H	1.29482600	-0.73183700	-0.35184400
H	2.26120200	0.28714200	0.73882200
H	0.94767800	-0.72157300	1.38767000
H	0.72149200	1.95135600	0.43938400

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Me_3Si–N-Me-acetamide$^+$. Gibbs free energy: -657.395714

C	-0.96924700	0.78713300	-0.11600300
O	-1.43460800	-0.41378800	-0.15022800
N	0.33117000	0.90901700	-0.18424800
C	-1.84971600	1.98109900	0.02637200
H	-2.02847500	2.15603600	1.09239800
H	-1.39154500	2.87276000	-0.39869500
H	-2.80764000	1.80682800	-0.46125100
C	1.08300400	2.16232100	-0.15197600
H	0.79327200	2.75982900	0.71298300
H	2.13823500	1.91307100	-0.06831300
H	0.92223700	2.72860500	-1.07134600
Si	-3.05554100	-1.11776600	-0.06946400
C	-3.89897000	-0.68454100	-1.67279500
H	-4.10206700	0.38526600	-1.77448300
H	-3.29757200	-1.00715700	-2.52794400
H	-4.85994800	-1.20840100	-1.72008400
C	-3.88827200	-0.41907500	1.44361600
H	-4.79879400	-0.99606500	1.63909200
H	-3.24309900	-0.50464500	2.32339600
H	-4.18057300	0.62736200	1.32196100
C	-2.65059800	-2.92352100	0.08141700
H	-2.09297300	-3.12732500	1.00021900
H	-3.57685700	-3.50698100	0.10858900
H	-2.05808100	-3.26574200	-0.77216800
H	0.85027100	0.04209600	-0.26979200

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N-Me-piperidine. Gibbs free energy: -290.994701

C	-1.83445800	-1.04454200	-1.16133100
C	-0.30234300	-1.05530600	-1.13349400
C	0.24587400	0.37566100	-1.15944200
C	-0.39281400	1.21143500	-0.04077000
C	-2.38277100	-0.14601400	-0.04290200
H	1.33463100	0.37563800	-1.03458200
H	0.03598200	-1.55052800	-0.21209200
H	0.09609000	-1.63719300	-1.97160400
H	-2.18340000	-0.68158600	-2.13665200
H	-2.23269300	-2.05816900	-1.03970100
H	-0.07844200	0.79945000	0.92839300

H	-0.03930300	2.24744000	-0.08128400
H	-2.11880300	-0.59038300	0.92686900
H	-3.47610800	-0.09583000	-0.08807500
H	0.03881900	0.83442200	-2.13469100
N	-1.85720600	1.22105500	-0.05915500
C	-2.41241900	2.03401300	-1.13291800
H	-3.50116000	2.07459200	-1.02781600
H	-2.02599500	3.05432900	-1.04762100
H	-2.18622000	1.67259900	-2.14970100

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Me_3Si–N-Me-piperidine$^+$. Gibbs free energy: -699.997892

C	-1.77701300	-1.05242000	-1.03952500
C	-0.25256800	-0.95772000	-1.10162000
C	0.18847600	0.50238300	-1.20442700
C	-0.41713400	1.35903700	-0.09666400
C	-2.32425900	-0.19514700	0.09450900
H	1.27464100	0.58786400	-1.10994500
H	0.17437300	-1.40508000	-0.19527600
H	0.13042800	-1.52676500	-1.95245000
H	-2.22471500	-0.76501500	-1.99649400
H	-2.09374100	-2.08095300	-0.84581500
H	-0.02447300	1.03963600	0.87306400
H	-0.16899000	2.41183400	-0.23842400
H	-1.92752200	-0.56114300	1.04429300
H	-3.41452500	-0.23471900	0.13933300
H	-0.06649000	0.91018100	-2.18777900
N	-1.92462900	1.25923000	-0.01076300
C	-2.55590500	1.89074900	-1.21069400
H	-3.63050700	1.71407100	-1.18620300
H	-2.35728400	2.96279000	-1.20133200
H	-2.14836100	1.46674500	-2.12573300
Si	-2.53159200	2.19943100	1.55586400
C	-1.65022800	3.84136700	1.54003400
H	-2.09998000	4.45935100	2.32510800
H	-0.58549800	3.74147200	1.76707500
H	-1.76114900	4.38329800	0.59665700
C	-4.37656500	2.36773700	1.36283500
H	-4.87427000	1.41256400	1.17313400
H	-4.76967400	2.75726700	2.30858200
H	-4.65073400	3.07458900	0.57552100
C	-2.05872500	1.15717100	3.02615000
H	-2.22632400	1.76726500	3.92083200
H	-2.67615500	0.25988600	3.11966000
H	-1.00485800	0.86521300	3.02634400

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N,N-dimethylaniline. Gibbs free energy: -365.980647

N	-1.56974000	-0.00002700	-0.17248500
C	-2.28549800	-1.23975800	0.06809200

H	-3.35492400	-1.06059800	-0.04420900
H	-2.00484600	-2.00243300	-0.66448400
H	-2.10505000	-1.64515200	1.07535100
C	-2.28568300	1.23969900	0.06745800
H	-2.00276400	2.00280700	-0.66374600
H	-3.35486000	1.06104300	-0.04790700
H	-2.10772300	1.64431000	1.07553000
C	-0.18633700	0.00008500	-0.07876600
C	0.54697400	1.20641500	-0.03590200
C	0.54695500	-1.20638100	-0.03623000
C	1.93758800	1.19669800	0.01846900
H	0.03671300	2.16164900	-0.04571700
C	1.93746800	-1.19673700	0.01809900
H	0.03647600	-2.16150300	-0.04648400
C	2.65167500	0.00000800	0.04309200
H	2.46533100	2.14578600	0.04732200
H	2.46529500	-2.14578400	0.04666600
H	3.73568500	-0.00010500	0.08920500

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Me_3Si–N,N,-dimethylaniline$^+$. Gibbs free energy: -774.966081

N	0.48150500	0.65197700	-0.66381100
C	0.77239900	0.40713300	-2.11754700
H	1.80344800	0.69430400	-2.31886000
H	0.64684600	-0.64136600	-2.36850000
H	0.09411200	1.01536700	-2.71751800
C	0.79343000	2.09689400	-0.40432400
H	0.79574200	2.30823600	0.66327300
H	1.78133100	2.31036700	-0.80677300
H	0.05285500	2.71942500	-0.90822800
C	-0.93082900	0.31770400	-0.33565200
C	-1.66800000	1.12086700	0.53346500
C	-1.50422300	-0.83879300	-0.86588700
C	-2.97452200	0.76686800	0.86286600
H	-1.25516500	2.01985300	0.97014600
C	-2.80981300	-1.18320700	-0.52930500
H	-0.95872300	-1.48723200	-1.53842900
C	-3.55152100	-0.38337200	0.33497100
H	-3.53805200	1.40287900	1.53664700
H	-3.24288600	-2.08293900	-0.95238100
H	-4.57052000	-0.65186400	0.59125300
Si	1.64023600	-0.43501800	0.46231300
C	0.97825500	-0.22387700	2.18743000
H	-0.00921600	-0.67837700	2.30078900
H	1.66733400	-0.73852300	2.86646400
H	0.92582100	0.82088200	2.50500800
C	3.34550200	0.27771500	0.22730900
H	3.45037800	1.27141800	0.66999200
H	4.04656000	-0.38824200	0.74276400

H	3.65116600	0.31945400	-0.82192000
C	1.51308400	-2.18887900	-0.14507400
H	2.23203300	-2.77130300	0.44281900
H	0.52547900	-2.62333000	0.02530200
H	1.78506000	-2.30691300	-1.19705900

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THF. Gibbs free energy: -232.310676

C	1.12808200	0.47306800	0.16394000
O	-0.00483400	1.20061400	-0.29489000
C	-1.13650700	0.46194100	0.15038500
C	-0.76725400	-1.01877900	-0.04175300
C	0.78108700	-1.00627400	-0.05985100
H	1.99880100	0.81670000	-0.39759200
H	1.29122000	0.67895700	1.23272200
H	-1.32496700	0.68206100	1.21191900
H	-1.99981500	0.78485100	-0.43451400
H	-1.17010600	-1.63639700	0.76447700
H	-1.16549400	-1.39993900	-0.98517900
H	1.21475300	-1.64162600	0.71603500
H	1.16183500	-1.34926000	-1.02508000

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$Me_3Si–THF^+$. Gibbs free energy: -641.296209

C	1.27624500	-1.20386400	-0.22174900
O	0.45576800	0.03340700	-0.21402100
C	1.29670900	1.22730900	0.04272100
C	2.70100500	0.71568900	-0.20373300
C	2.63113300	-0.73725800	0.27447500
H	0.78593500	-1.92785700	0.42802800
H	1.28507900	-1.55303500	-1.25442900
H	0.96244300	1.99898300	-0.64760600
H	1.12691500	1.52469400	1.07932500
H	2.94263100	0.76571600	-1.26849000
H	3.43276800	1.30507200	0.35007300
H	3.43055400	-1.35452800	-0.13711000
H	2.67602700	-0.78852700	1.36536300
Si	-1.34653900	-0.00106400	0.02493700
C	-1.87276300	1.69720100	-0.50610400
H	-2.96680800	1.74293600	-0.47340900
H	-1.49069700	2.47620000	0.15946700
H	-1.55924300	1.91385200	-1.53132300
C	-1.56951000	-0.35034600	1.83521300
H	-2.64013600	-0.40198800	2.06080400
H	-1.12211800	-1.30611500	2.12328100
H	-1.13374800	0.44184700	2.45090200
C	-1.87893400	-1.37130100	-1.10726900
H	-2.97324200	-1.41909300	-1.10805300
H	-1.54841500	-1.18883100	-2.13376700
H	-1.50586700	-2.34626700	-0.78133700

16
Tetrahydropyran. Gibbs free energy: -271.594208

C	-4.10133100	-0.00164400	-1.23270900
C	-2.57012700	-0.02115200	-1.26184900
C	-2.02932600	1.41184800	-1.23123100
C	-2.64874500	2.18561000	-0.07159400
C	-4.59585500	0.85531000	-0.07162400
H	-0.93868900	1.41801100	-1.12776400
H	-2.19841400	-0.56627000	-0.38333600
H	-2.20575600	-0.55291200	-2.14647700
H	-4.48656600	0.41615500	-2.17112100
H	-4.50669300	-1.01448900	-1.13240100
H	-2.32048300	1.75019300	0.88706300
H	-2.35273300	3.23730100	-0.08847000
H	-4.30958200	0.39069600	0.88668200
H	-5.68311200	0.96218500	-0.08783400
H	-2.27379200	1.92223500	-2.17106500
O	-4.06920200	2.17467000	-0.12841800

29
Me_3Si–tetrahydropyran$^+$. Gibbs free energy: -680.575023

C	-4.32672800	0.05958000	-0.98501900
C	-2.90656100	0.08321200	-1.55701800
C	-2.42489600	1.52418600	-1.74501000
C	-2.56728700	2.32040700	-0.46401800
C	-4.41105800	0.88321500	0.28241900
H	-1.37005600	1.55092600	-2.03424300
H	-2.22960300	-0.44424800	-0.87406800
H	-2.87733600	-0.44660300	-2.51207800
H	-5.04411300	0.44550200	-1.71782600
H	-4.63158900	-0.96179900	-0.73815800
H	-1.96669800	1.91922200	0.35557500
H	-2.33482300	3.37716800	-0.59014100
H	-3.74348400	0.51860200	1.06692400
H	-5.41920500	0.96746300	0.67953400
H	-2.99367000	2.01565000	-2.54162500
O	-3.96459900	2.26226700	0.00636400
Si	-5.04397000	3.73232800	-0.15301700
C	-4.86497000	4.24188400	-1.93034100
H	-5.49421600	5.12200000	-2.10281300
H	-3.83824300	4.51650300	-2.18856700
H	-5.20102700	3.44982000	-2.60571200
C	-6.74185300	3.12505400	0.28239400
H	-6.80756100	2.74777700	1.30656800
H	-7.41730900	3.98521400	0.20719300
H	-7.10518100	2.36260700	-0.41243000
C	-4.31582800	4.91732800	1.07503500
H	-4.88256800	5.85419800	1.04418100
H	-4.38048200	4.51242500	2.08891800

H	-3.27065600	5.15488500	0.85790400

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Tetrahydrothiophene. Gibbs free energy: -555.302344

C	0.05391700	-1.33954400	0.13640800
C	0.05348000	1.33964500	-0.13673200
C	-1.28006500	0.71357700	0.27455900
C	-1.28001800	-0.71379800	-0.27437100
H	0.34490700	-2.16966400	-0.50957400
H	0.02131800	-1.69372400	1.16972200
H	0.34470500	2.16994100	0.50890400
H	0.02083900	1.69323500	-1.17023100
H	-1.35886600	0.68912400	1.36739300
H	-2.11857000	1.30177200	-0.11007500
H	-2.11821900	-1.30225600	0.11049000
H	-1.35915000	-0.68932400	-1.36718400
S	1.30869700	0.00010100	0.00008600

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Me_3Si–tetrahydrothiophene$^+$. Gibbs free energy: -964.279144

C	1.47570000	1.36969300	-0.10904100
C	1.44313000	-1.32460100	-0.47333900
C	2.36699200	-0.80758000	0.62842700
C	2.75996300	0.62122400	0.25266700
H	1.63040700	2.21458600	-0.77859400
H	0.92930800	1.70192900	0.77505300
H	0.77002900	-2.12233500	-0.15700600
H	1.99083600	-1.65157800	-1.35759700
H	1.84969800	-0.81828500	1.59214800
H	3.23965700	-1.45964700	0.70891600
H	3.26049800	1.13471500	1.07670300
H	3.44038700	0.61440300	-0.60401500
S	0.44511200	0.13272900	-1.01646900
Si	-1.48855600	-0.00540300	0.16811000
C	-2.21130900	1.69280300	-0.07050600
H	-2.37605500	1.91218500	-1.12898300
H	-3.18036400	1.73087300	0.43886400
H	-1.57857000	2.47452700	0.35944800
C	-2.39572900	-1.37376700	-0.70711300
H	-1.87274500	-2.33091000	-0.62651400
H	-3.37842900	-1.49135300	-0.23731100
H	-2.55044900	-1.14221400	-1.76438200
C	-1.03153200	-0.40330800	1.92902400
H	-1.95945000	-0.42979400	2.51188600
H	-0.55748000	-1.38437500	2.02100500
H	-0.38256700	0.35247600	2.37962900

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4H-chromene. Gibbs free energy: -422.746599

C	-3.61273600	-0.60064200	-0.04612800
C	-2.26015500	-0.89762800	-0.22761100

C	-1.28742900	0.10146300	-0.22877900
C	-1.66218500	1.42689800	-0.04504400
C	-3.00752500	1.75105900	0.13987900
C	-3.96329900	0.74020100	0.13736200
C	-4.66155000	-1.69106800	-0.04640800
H	-0.24844200	-0.17567000	-0.37399500
H	-0.90494300	2.20408800	-0.04545400
H	-3.30720400	2.78370800	0.28530000
H	-5.01235600	0.98607500	0.28179600
H	-5.40069600	-1.49865000	-0.83487000
C	-4.02853400	-3.03788100	-0.24508800
H	-4.65498100	-3.92278200	-0.25859600
C	-2.71781200	-3.19670000	-0.40798400
H	-2.23120500	-4.15276000	-0.55378700
O	-1.79899900	-2.18016400	-0.41422600
H	-5.22068300	-1.67022800	0.89787700

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Me_3Si–4H-chromene$^+$. Gibbs free energy: -831.703501

C	-3.01911500	-0.31914500	-0.28430400
C	-2.29638900	-0.77944900	-1.37534900
C	-1.86455000	0.02132300	-2.41771100
C	-2.12407300	1.38656600	-2.33395000
C	-2.81881800	1.89957800	-1.23910800
C	-3.27657400	1.05152400	-0.23401700
C	-3.55182400	-1.30086600	0.73101900
H	-1.34992800	-0.40632100	-3.26932600
H	-1.79203100	2.04325400	-3.13004200
H	-3.02172900	2.96307700	-1.17733800
H	-3.84695800	1.45012300	0.59906600
H	-4.49022600	-0.93126500	1.14968100
C	-3.76311800	-2.64176000	0.08595300
H	-4.54697100	-3.30111700	0.44056000
C	-3.04026100	-3.03820700	-0.94681100
H	-3.11135900	-3.94871800	-1.52230700
O	-1.99669200	-2.18161000	-1.44128800
Si	-0.24174400	-2.74481900	-0.99614800
C	0.86206100	-1.77514700	-2.12048200
H	0.84722700	-0.70379000	-1.90867700
H	1.88251400	-2.13697200	-1.94706700
H	0.62575700	-1.94465300	-3.17424900
C	-0.12431800	-2.30150700	0.79920000
H	0.88365800	-2.54807600	1.15032700
H	-0.27914800	-1.23091800	0.96257800
H	-0.83641200	-2.87091600	1.40280200
C	-0.31815500	-4.55498900	-1.38138600
H	0.69778100	-4.95386500	-1.28135100
H	-0.96147100	-5.10924900	-0.69397700
H	-0.64450200	-4.73463400	-2.40976300

H	-2.85604100	-1.40195600	1.57381000

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Chroman. Gibbs free energy: -423.956906

C	-3.62439300	-0.61558000	0.11476300
C	-2.29107000	-0.96058800	-0.14806200
C	-1.33047400	0.02484700	-0.39488300
C	-1.68866800	1.36705300	-0.37136500
C	-3.00914900	1.73359400	-0.10171700
C	-3.95711900	0.74271800	0.13306700
C	-4.66414900	-1.68773500	0.35160500
H	-0.30945700	-0.28090300	-0.60022900
H	-0.93662600	2.12643800	-0.56185700
H	-3.29578300	2.78003900	-0.08108100
H	-4.99045300	1.01874700	0.32970000
H	-5.60150800	-1.40966500	-0.13984700
C	-4.16488700	-3.03967900	-0.15610400
H	-4.79545600	-3.85339400	0.21325600
H	-4.18902500	-3.07191800	-1.25128000
C	-2.73753000	-3.25254100	0.31667400
H	-2.32715200	-4.20265500	-0.02802500
H	-2.68743700	-3.22482000	1.41379200
O	-1.85682500	-2.25372300	-0.20580900
H	-4.87974200	-1.75861700	1.42521300

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Me_3Si–chroman$^+$. Gibbs free energy: -832.923016

C	-3.32166000	-0.66294000	-0.36235400
C	-2.01733700	-0.83860800	0.08427400
C	-1.12181400	0.19971800	0.29113300
C	-1.52903100	1.49215300	-0.02013200
C	-2.81790200	1.71380500	-0.50538000
C	-3.70178700	0.65124400	-0.65625500
C	-4.31588000	-1.79985100	-0.44927400
H	-0.13725000	0.00407400	0.69766600
H	-0.84382400	2.31945500	0.12643900
H	-3.13983400	2.72055500	-0.74880100
H	-4.71339600	0.83289900	-1.00737400
H	-4.75238900	-1.83191800	-1.45111500
C	-3.71967000	-3.16690000	-0.08956400
H	-4.48844300	-3.82514500	0.32266600
H	-3.32240400	-3.66882300	-0.97702900
C	-2.61582600	-3.02338000	0.93154200
H	-2.12801100	-3.95884100	1.19192100
H	-2.92568400	-2.50525200	1.84008700
O	-1.55370600	-2.16477600	0.34946700
Si	-0.29939000	-2.86179700	-0.85997500
C	-0.93603800	-2.31761500	-2.51485400
H	-0.24472000	-2.68586700	-3.28110800
H	-1.92661700	-2.72592100	-2.73253500

H	-0.97805800	-1.22807100	-2.59569700
C	1.30924500	-2.09498600	-0.34784100
H	2.11511000	-2.68849900	-0.79456100
H	1.41683600	-1.06795000	-0.70394000
H	1.44062300	-2.11943900	0.73754000
C	-0.36122300	-4.69034400	-0.55432200
H	0.36888700	-5.14084900	-1.23699900
H	-0.05864400	-4.94969000	0.46410700
H	-1.33214400	-5.14160400	-0.77276000
H	-5.13523200	-1.56675600	0.23902400

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Isochroman. Gibbs free energy: -423.949914

C	-3.60001000	-0.57194200	0.09746600
C	-2.26161000	-0.91008400	-0.13232800
C	-1.32007800	0.09613900	-0.36510700
C	-1.69739800	1.43537800	-0.36703300
C	-3.03095400	1.77723600	-0.13497700
C	-3.97046500	0.77706000	0.09459600
C	-4.61551600	-1.66232700	0.35643700
H	-0.28141600	-0.17259400	-0.54298400
H	-0.95648700	2.20852900	-0.54514300
H	-3.33567100	2.81928200	-0.13552200
H	-5.01055200	1.03983200	0.27153900
H	-5.55622500	-1.43751200	-0.15747600
C	-4.08661900	-3.01534600	-0.10058400
H	-4.71186900	-3.83088600	0.26754100
H	-4.05753700	-3.06981800	-1.19987700
C	-1.83672500	-2.36374400	-0.16595700
H	-1.65493200	-2.66606400	-1.21040900
H	-0.90405700	-2.50191900	0.38680200
O	-2.78337600	-3.23493500	0.42060000
H	-4.83856300	-1.70803400	1.42923800

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Me_3Si–isochroman$^+$. Gibbs free energy: -832.927239

C	-3.13099100	-0.99031100	1.60123300
C	-1.93762800	-1.17173900	0.89550900
C	-0.73412900	-0.68067500	1.40704500
C	-0.71232900	-0.00345400	2.62070500
C	-1.89867500	0.17793500	3.33248800
C	-3.09490100	-0.31587000	2.82472700
C	-4.43758200	-1.54601700	1.07766900
H	0.18948900	-0.83426200	0.85585000
H	0.22528100	0.37510500	3.01365700
H	-1.88965100	0.70175600	4.28261100
H	-4.01902300	-0.17634300	3.37862200
H	-5.23435100	-0.80241000	1.17418300
C	-4.34296500	-1.93986300	-0.37899100
H	-5.16404700	-2.56792900	-0.71510700

H	-4.25206300	-1.08168000	-1.04665100
C	-1.92489500	-1.87488500	-0.43676500
H	-1.94233300	-1.18299400	-1.28219000
H	-1.06090700	-2.53090200	-0.54666700
O	-3.11021600	-2.71926300	-0.59074100
Si	-2.96742000	-4.52071000	-0.20178900
C	-2.16437000	-4.57007100	1.47131900
H	-2.04949500	-5.61906200	1.76612000
H	-1.16957500	-4.11582700	1.47068200
H	-2.77562400	-4.07165900	2.22896800
C	-1.91967500	-5.14070100	-1.60004700
H	-1.78272900	-6.22067600	-1.47855600
H	-2.40964200	-4.96521000	-2.56169200
H	-0.92696100	-4.68330900	-1.62029100
C	-4.72147600	-5.12022600	-0.23555400
H	-5.20079100	-4.94506200	-1.20263700
H	-4.69166700	-6.20397000	-0.07508700
H	-5.33585100	-4.69026200	0.56004300
H	-4.74307700	-2.40944300	1.68049400

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N,N-dimethylacetamide. Gibbs free energy: -287.669423

C	-1.00726100	0.84669100	0.16022800
O	-1.59511900	-0.23631300	0.27323200
N	0.34381800	0.92430400	0.04744700
C	-1.78784200	2.14551200	0.15344900
H	-1.53717300	2.76337200	1.02095300
H	-1.58722700	2.73159400	-0.74760600
H	-2.84840500	1.90088700	0.19256900
C	1.07015400	2.16537800	-0.17237700
H	0.54315200	3.01752000	0.25298400
H	2.04273800	2.09414100	0.32069900
H	1.23617100	2.34499700	-1.24135800
C	1.14032000	-0.28817300	-0.04697500
H	0.49653900	-1.15281200	0.09945000
H	1.61590400	-0.35421300	-1.03216600
H	1.92223500	-0.28245700	0.71871400

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Me_3Si–N,N-dimethylacetamide$^+$. Gibbs free energy: -696.668878

C	-0.21288200	0.45148200	0.20668500
O	-0.23742800	-0.79264300	-0.13716800
N	0.51218200	1.26822800	-0.51723600
C	-0.96540100	0.94358600	1.40109000
H	-0.28541600	1.00245200	2.25697800
H	-1.39232400	1.93112500	1.22856100
H	-1.77118300	0.25593100	1.64874800
C	0.63582300	2.69292000	-0.18861600
H	0.75933400	2.83590100	0.88379300
H	1.52309800	3.07500400	-0.69032800

H	-0.23941800	3.24175100	-0.54411400
C	1.23108400	0.81963700	-1.71243200
H	2.30517900	0.88956700	-1.52879100
H	0.96360500	-0.20579700	-1.94893000
H	0.96086500	1.47508200	-2.54208600
Si	-0.99427500	-2.25741800	0.47889400
C	-0.51902300	-2.41978100	2.27360200
H	0.55515700	-2.26271000	2.41149600
H	-1.06064500	-1.72389700	2.91996800
H	-0.75383500	-3.43580100	2.60937300
C	-0.20770000	-3.54397300	-0.60606200
H	-0.62248000	-4.52968900	-0.37080200
H	-0.40075700	-3.33824300	-1.66311400
H	0.87433100	-3.58365000	-0.44959700
C	-2.82659600	-2.08016400	0.19039500
H	-3.03360100	-1.83769500	-0.85627800
H	-3.31347800	-3.03538100	0.41610800
H	-3.28826400	-1.31709800	0.82338000

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N-acetyl-pyrrolidine. Gibbs free energy: -365.04442

C	-1.90525400	0.95986600	0.16227400
C	-2.26318600	3.16184300	-0.82106100
C	-1.96419700	3.30483700	0.67277800
C	-2.36996700	1.94057600	1.24087900
H	-2.51865900	0.05811300	0.09979600
H	-0.86465700	0.64988100	0.31634900
H	-1.62009300	3.79134200	-1.44061300
H	-3.30862700	3.41291400	-1.04106300
H	-0.89210600	3.47058400	0.82271900
H	-2.50444200	4.14023600	1.12251400
H	-1.91733000	1.73000800	2.21186400
H	-3.45807500	1.88721100	1.35299000
N	-2.01618900	1.73756300	-1.07534700
C	-1.90683800	1.15651400	-2.28622900
O	-1.68222000	-0.05675600	-2.40512800
C	-2.06445800	2.05705700	-3.49181200
H	-2.99070500	2.63665700	-3.43993300
H	-1.23262000	2.76587100	-3.55317700
H	-2.07199300	1.44147700	-4.39062900

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Me_3Si–N-acetyl-pyrrolidine$^+$. Gibbs free energy: -774.043998

C	-2.05936000	1.98297200	0.82640500
C	-2.02938400	3.54976800	-1.05968900
C	-1.92140900	4.31167500	0.26126800
C	-2.55487900	3.35565200	1.27622000
H	-2.74441300	1.16477900	1.04969200
H	-1.07663000	1.74217200	1.24236100
H	-1.23526600	3.79579300	-1.76489500

H	-3.00115700	3.70534600	-1.53795000
H	-0.86911200	4.48575000	0.50506200
H	-2.42561600	5.27719800	0.20659800
H	-2.26441600	3.57028000	2.30535900
H	-3.64622400	3.40091800	1.21064100
N	-1.92556000	2.13500200	-0.63811100
C	-1.72056800	1.12293700	-1.43353500
O	-1.60665400	-0.03875600	-0.87459000
Si	-1.34438000	-1.67807700	-1.45312900
C	-1.09046800	-2.58101300	0.15061800
H	-0.92557900	-3.64587600	-0.04354000
H	-0.21738100	-2.19286600	0.68350400
H	-1.96660800	-2.48465800	0.79863300
C	0.17330700	-1.66481800	-2.53471700
H	0.46693800	-2.70092500	-2.73641000
H	0.00247700	-1.17597100	-3.49771600
H	1.01170700	-1.17098900	-2.03389800
C	-2.89878800	-2.18903600	-2.34585900
H	-2.85186700	-3.26461700	-2.54908600
H	-3.78327400	-2.00174400	-1.72968300
H	-3.02682800	-1.67813900	-3.30449300
C	-1.59166000	1.30214300	-2.90970400
H	-2.13187800	2.18065300	-3.25877200
H	-0.53254300	1.41990300	-3.16003000
H	-1.97541800	0.42485200	-3.42953700

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Benzaldehyde. Gibbs free energy: -345.399467

C	-0.32843800	-1.39166000	0.00167400
C	1.06576500	-1.38845600	0.00224300
C	1.75210800	-0.17703100	0.00181000
C	1.04437500	1.02911100	0.00078900
C	-0.35644900	1.02135000	0.00022100
C	-1.03947800	-0.18806300	0.00067200
H	-0.86520300	-2.33510900	0.00201900
H	1.61301500	-2.32517100	0.00302400
H	2.83904600	-0.16436400	0.00226700
H	-0.89218400	1.96522200	-0.00056600
H	-2.12449600	-0.19960300	0.00023700
C	1.79884400	2.29905900	0.00032500
O	1.29198400	3.40672100	-0.00065300
H	2.90054500	2.19094100	0.00087600

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Me_3Si–Benzaldehyde$^+$. Gibbs free energy: -754.379844

C	-0.43026400	-1.22261500	0.09573300
C	0.78682700	-1.31045600	-0.58207900
C	1.58384500	-0.18254700	-0.70172400
C	1.15465800	1.03490100	-0.13701500
C	-0.07646200	1.11635500	0.54767200

C	-0.86270500	-0.01521900	0.65933300
H	-1.05386800	-2.10583000	0.18765000
H	1.10587100	-2.25230600	-1.01264200
H	2.53284800	-0.23322500	-1.22645600
H	-0.39239200	2.06087900	0.97647400
H	-1.81205500	0.03021500	1.18025700
C	1.99771600	2.17220500	-0.28681500
O	1.69462700	3.30200400	0.18521000
H	2.94088800	2.06410900	-0.83113400
Si	2.60669300	4.85791000	0.09068300
C	1.27450200	6.04126900	-0.42300200
H	1.69928700	7.04572300	-0.52244000
H	0.84345600	5.75771000	-1.38739000
H	0.47590600	6.08135300	0.32297400
C	3.93652100	4.59652300	-1.18265500
H	4.67085500	3.84407900	-0.88055800
H	3.52201700	4.32488000	-2.15824600
H	4.47268400	5.54400900	-1.30672200
C	3.22507500	5.06940900	1.82730300
H	3.74014000	6.03177200	1.91575600
H	2.39848400	5.06078700	2.54348000
H	3.93237800	4.27921800	2.09494300

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Benzaldehyde dimethylacetal. Gibbs free energy: -500.322804

C	-0.48381100	-1.12231800	-0.03760200
C	0.25214100	-0.84128500	1.11577200
C	1.02977400	0.31068000	1.18397800
C	1.07452200	1.19307500	0.10153900
C	0.34142100	0.90835100	-1.04887200
C	-0.43873300	-0.24677800	-1.11985800
H	-1.08622100	-2.02383700	-0.09152100
H	0.22143600	-1.52477000	1.95864300
H	1.61023600	0.52821100	2.07526700
H	0.37969300	1.59005600	-1.89476100
H	-1.00412200	-0.46258800	-2.02102600
C	1.92357600	2.44372200	0.17956200
O	1.36095500	3.29825100	1.12254700
H	1.95762900	2.93869900	-0.80929300
C	1.95131400	4.59115200	1.15496600
H	1.91770800	5.05688200	0.16149500
H	1.35899900	5.18580000	1.85074300
H	2.98834500	4.54533200	1.49935000
O	3.24850300	2.16612900	0.58574700
C	4.01722700	1.50471600	-0.40182000
H	4.05471600	2.08857600	-1.33160200
H	5.02549200	1.40205100	0.00012500
H	3.61391200	0.50842300	-0.62291800

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Me_3Si–Benzaldehyde dimethylacetal$^+$. Gibbs free energy: -909.298812

C	0.60977500	-0.90888400	1.88999800
C	0.98507000	0.18436500	2.67081200
C	1.33242600	1.38916500	2.06721500
C	1.30970000	1.49874500	0.67468400
C	0.91732900	0.40896100	-0.10491900
C	0.57056800	-0.79498500	0.50149300
H	0.34054600	-1.84653800	2.36496400
H	1.00566800	0.09858800	3.75202900
H	1.61335200	2.24223000	2.67544200
H	0.86878400	0.49853100	-1.18652100
H	0.26426800	-1.63799200	-0.10853200
C	1.72002200	2.76273200	-0.01256400
O	1.50802500	3.85690100	0.74232200
H	1.32532300	2.84832300	-1.02742400
C	1.66362800	5.11293700	0.06886800
H	1.03285000	5.14243200	-0.82457700
H	1.34366900	5.87441700	0.77666300
H	2.71042700	5.27203800	-0.20313300
O	3.25003700	2.69772400	-0.31011700
C	4.09320900	2.65707900	0.87780000
H	3.67658000	3.35673300	1.59960500
H	4.11375400	1.64249800	1.27549400
H	5.08562900	2.98744200	0.57944000
Si	3.97803900	2.11856900	-1.88290800
C	4.37448800	0.32997100	-1.58281500
H	3.48138600	-0.24063100	-1.31267100
H	4.79040000	-0.10191800	-2.49944100
H	5.12000000	0.21076400	-0.79120000
C	2.66549400	2.42402100	-3.16127400
H	3.12658400	2.21872700	-4.13446700
H	1.79820800	1.76502600	-3.07259300
H	2.33146700	3.46561300	-3.17468000
C	5.46038500	3.21794900	-2.09798700
H	6.28895600	2.94227700	-1.44037300
H	5.81255900	3.11716100	-3.13048900
H	5.20520300	4.26865800	-1.93171000

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Isosorbide. Gibbs free energy: -1352.429277

C	-0.70961800	1.17550500	-0.03222200
C	0.12940700	2.43885900	0.12123000
C	-0.80036900	3.26623500	1.03608300
C	-2.19230300	2.87627500	0.52155100
C	-1.81453700	5.21362500	0.26561800
C	-2.54598800	4.04148500	-0.40350200
H	-0.59878500	0.52245300	0.84448900
H	-2.47402200	5.68666700	1.00598100
H	-2.10281100	3.83410500	-1.38397100

H	-0.63705400	2.98030800	2.07981900
H	-2.94310600	2.79388000	1.31506000
O	-0.66436700	4.66605400	0.91082900
O	-2.06502200	1.62525700	-0.13995400
H	-0.45716400	0.61481300	-0.93415300
H	1.09680100	2.23726700	0.59662200
H	-1.47919100	5.96949800	-0.44952300
O	0.27405300	3.09843800	-1.11177200
O	-3.93658100	4.23138900	-0.50532400
Si	-4.65627800	5.17792900	-1.70574200
Si	1.66578800	3.07380100	-2.05784000
C	2.02404600	1.31482700	-2.60635700
H	2.90492000	1.28804900	-3.25767500
H	2.22516100	0.66377800	-1.74820700
H	1.17820300	0.89606300	-3.16176500
C	1.24668600	4.17865900	-3.50598600
H	1.04335700	5.20033400	-3.16899400
H	2.07506900	4.21425000	-4.22159900
H	0.36001500	3.80787900	-4.03058600
C	3.10942100	3.74172500	-1.06260700
H	4.00917100	3.78956800	-1.68630300
H	2.89760700	4.74990000	-0.69187100
H	3.33788400	3.10242900	-0.20300000
C	-6.44994900	4.65121600	-1.71463400
H	-6.90371700	4.80023300	-0.72927400
H	-7.01931400	5.24135000	-2.44087900
H	-6.54858600	3.59391500	-1.98028200
C	-4.49762000	6.99509900	-1.26238200
H	-4.92710500	7.19431100	-0.27502500
H	-3.45174200	7.31961100	-1.25295600
H	-5.03129400	7.61197000	-1.99433900
C	-3.81473500	4.84146800	-3.34919800
H	-2.78384400	5.21192400	-3.35951000
H	-3.79647600	3.76989900	-3.57452300
H	-4.35606700	5.34854100	-4.15573500

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Me_3Si–isosorbide$^+$ Isomer1. Gibbs free energy: -1761.40644

C	-0.63950800	1.37122200	-0.25536000
C	0.22961500	2.58291000	0.08186300
C	-0.69608300	3.26547300	1.10563100
C	-2.09578500	2.99555700	0.54783800
C	-1.75548200	5.37275700	0.53859800
C	-2.44177000	4.26069600	-0.24807000
H	-0.52201800	0.58977400	0.50653900
H	-2.38175500	5.72670700	1.35960800
H	-1.96473000	4.16291000	-1.23050300
H	-0.54381200	2.90527400	2.12188100
H	-2.84458600	2.83502100	1.32954500

O	-0.57057100	4.71940700	1.12027200
O	-1.99012600	1.84483400	-0.26421400
H	-0.41163200	0.95570300	-1.23658600
H	1.18509700	2.28030600	0.52353400
H	-1.40143900	6.19807600	-0.07729200
O	0.39276700	3.45533900	-1.00016500
O	-3.81606600	4.48890800	-0.33511700
Si	-4.54091300	4.90153900	-1.81971100
Si	1.61657300	3.38393600	-2.17237700
C	1.60567800	1.71499500	-3.02175300
H	2.36312700	1.70201700	-3.81327300
H	1.84376800	0.90340800	-2.32588300
H	0.63448700	1.50679300	-3.48228900
C	1.16439100	4.76285800	-3.34670400
H	1.12742500	5.73129100	-2.83790100
H	1.90307400	4.83359100	-4.15207200
H	0.18481400	4.57828400	-3.79950000
C	3.27217500	3.66439900	-1.33861900
H	4.07091400	3.62883800	-2.08767200
H	3.32320100	4.63993100	-0.84433400
H	3.48844600	2.88764800	-0.59660100
C	-6.33406500	5.18853100	-1.39418200
H	-6.43932900	5.99367300	-0.66022100
H	-6.89732800	5.46876200	-2.29062400
H	-6.78642700	4.28255400	-0.97865300
C	-3.70102500	6.44843200	-2.46639600
H	-3.77760500	7.26753600	-1.74354600
H	-2.63973400	6.27258800	-2.67558500
H	-4.17061400	6.77541400	-3.40042000
C	-4.30935700	3.47922600	-3.01651200
H	-3.24889200	3.28276000	-3.20786600
H	-4.76020900	2.56208200	-2.62414400
H	-4.78401600	3.70941500	-3.97659700
Si	0.79983500	5.70215600	1.82917000
C	1.31396100	6.78642800	0.41403700
H	0.60446100	7.59831300	0.23200700
H	2.28580200	7.23676500	0.64190800
H	1.41860500	6.19742000	-0.50108400
C	-0.00998700	6.57896700	3.24893700
H	0.73923300	7.18451100	3.77026100
H	-0.80461000	7.25197600	2.91430100
H	-0.42721000	5.86496400	3.96515800
C	2.05639800	4.43426500	2.33064600
H	2.85067000	4.96614300	2.86723200
H	1.65261900	3.68042400	3.01191400
H	2.51835800	3.94093900	1.47243700

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Me_3Si–isosorbide$^+$ Isomer2. Gibbs free energy: -1761.409565

C	-0.97268100	0.84444800	-0.32591500
C	-0.07819900	2.04459600	-0.11187700
C	-0.96371500	2.93453500	0.79438900
C	-2.35593200	2.77195000	0.18821600
C	-1.50057600	4.97429300	-0.19567500
C	-2.47968200	3.93942000	-0.79039500
H	-1.00421400	0.17230300	0.53384900
H	-2.05744000	5.75655300	0.32931600
H	-2.11521600	3.59700800	-1.76537000
H	-0.90678000	2.58994100	1.82978100
H	-3.16864800	2.75838600	0.91482400
O	-0.66183500	4.29999500	0.74805300
O	-2.31943300	1.45718200	-0.47751200
H	-0.76004300	0.31176900	-1.24916700
H	0.84672900	1.74740600	0.39433600
H	-0.87533500	5.42941100	-0.96891100
O	0.13960200	2.67960100	-1.33719800
O	-3.79675200	4.40722700	-0.86959600
Si	-4.34815200	5.39991900	-2.13462600
Si	1.62917700	3.26727700	-1.90071000
C	2.75486700	1.80572700	-2.22728800
H	3.71307200	2.14838700	-2.63327800
H	2.96521300	1.24957900	-1.30714100
H	2.30658200	1.11652000	-2.95027000
C	1.16218500	4.16964000	-3.46750000
H	0.44426600	4.96930700	-3.25727500
H	2.04563800	4.62080600	-3.93123000
H	0.70983800	3.48510800	-4.19223000
C	2.38496800	4.40510100	-0.62172300
H	3.33824000	4.80087400	-0.98947400
H	1.72088400	5.24625400	-0.40263900
H	2.58093800	3.87795900	0.31800800
C	-6.20445500	5.20086300	-2.10243200
H	-6.60532300	5.42448300	-1.10858000
H	-6.67320800	5.88465800	-2.81801500
H	-6.49470700	4.17925400	-2.36803200
C	-3.83175600	7.16946700	-1.79981600
H	-4.20859300	7.51370100	-0.83118100
H	-2.74184900	7.27881800	-1.80357900
H	-4.23322500	7.83285300	-2.57404200
C	-3.59744500	4.79489400	-3.74294900
H	-2.51598200	4.96438900	-3.78132300
H	-3.78398000	3.72706600	-3.89777400
H	-4.04505100	5.33754300	-4.58283500
Si	-3.81590100	0.40445700	-0.64411300
C	-4.28862800	0.02254800	1.11078300
H	-4.67835100	0.90026100	1.63372900
H	-5.07742000	-0.73745500	1.10458600

H	-3.44315300	-0.38037600	1.67638700
C	-3.17773000	-1.04752000	-1.60632300
H	-2.47654000	-1.66041500	-1.03373600
H	-4.03605400	-1.67853300	-1.86287500
H	-2.70569100	-0.73525100	-2.54230800
C	-4.99828000	1.48684100	-1.56663500
H	-4.62796700	1.69848100	-2.57386300
H	-5.95797000	0.96634500	-1.65496200
H	-5.16192300	2.43618000	-1.05058100

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Isomannide. Gibbs free energy: -1352.41992

C	-1.56087600	1.31002600	0.35167400
C	-0.21359600	2.00157900	0.16333700
C	-0.48156700	3.32642300	0.91875700
C	-2.01338400	3.51243100	0.82681400
C	-0.86154700	5.48762700	0.23912200
C	-2.19066600	4.78129500	-0.04247500
H	-1.60562500	0.82140300	1.33609300
H	-0.91753800	6.04240100	1.18748000
H	-0.14944300	3.22664600	1.95937400
H	-2.45409400	3.68786700	1.81584000
O	0.12153400	4.46024400	0.33155900
O	-2.55115800	2.33332700	0.26833500
H	-1.75818300	0.57275300	-0.42800200
H	0.59018400	1.42942400	0.64226400
H	-0.56741600	6.17150600	-0.55851300
O	0.04472800	2.17333100	-1.20313300
H	-3.03690600	5.38406300	0.31143900
O	-2.34059900	4.44215200	-1.39202400
Si	-3.05570900	5.40582500	-2.56755200
Si	1.49347900	2.68610200	-1.89509000
C	-2.97622100	4.36603700	-4.11942400
H	-3.44219300	4.88878100	-4.96163800
H	-1.93714300	4.14857800	-4.38782700
H	-3.49782000	3.41415800	-3.97712800
C	-4.82775800	5.78039600	-2.07344500
H	-5.32508800	6.36602300	-2.85467300
H	-5.39454700	4.85477300	-1.92877200
H	-4.87525900	6.35909100	-1.14455600
C	-2.09888300	7.00814300	-2.77900700
H	-1.04462100	6.80932200	-3.00071700
H	-2.51587800	7.58965000	-3.60899100
H	-2.15047900	7.63017400	-1.87858300
C	2.84047900	2.76694600	-0.59085900
H	3.01015400	1.79122900	-0.12278100
H	3.78199100	3.08255000	-1.05420900
H	2.58548800	3.48959300	0.18993800
C	1.27821000	4.33772200	-2.75447700

H	2.18407200	4.58886500	-3.31831600
H	0.44049300	4.30519300	-3.45931600
H	1.08537100	5.13162700	-2.02849600
C	1.91152500	1.38592100	-3.18415500
H	1.11290900	1.30594100	-3.92983600
H	2.83774500	1.64479300	-3.70978000
H	2.04575200	0.40212400	-2.72189900

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Me_3Si–isomannide$^+$. Gibbs free energy: -1761.403626

C	-1.71768600	1.24960300	0.14434100
C	-0.38855600	1.97046200	0.06590400
C	-0.67839200	3.25099000	0.89566200
C	-2.18064800	3.53518000	0.71835300
C	-0.91061300	5.44850000	0.24904900
C	-2.24795200	4.81257000	-0.14835800
H	-1.87034500	0.73310600	1.09401400
H	-1.02016600	6.00023900	1.19256100
H	-0.43476900	3.07313500	1.94829900
H	-2.70261100	3.65680800	1.66746300
O	0.01158300	4.37573900	0.41454600
O	-2.70903700	2.34204000	0.07005300
H	-1.89380300	0.59230200	-0.70493500
H	0.38598800	1.36527000	0.55062900
H	-0.52265400	6.12000800	-0.51604300
O	-0.09021300	2.23391200	-1.26484400
H	-3.08209200	5.45149400	0.16599900
O	-2.33859100	4.46972000	-1.49845900
Si	-2.79279600	5.52207200	-2.74902000
Si	1.40777700	2.72656600	-1.89035400
C	-2.56475400	4.51557500	-4.30757500
H	-2.62277000	5.17149200	-5.18303800
H	-1.59068300	4.01726900	-4.32282800
H	-3.33959300	3.75036100	-4.41556100
C	-4.58413900	6.02603300	-2.51732600
H	-4.86667700	6.73624300	-3.30250200
H	-5.25869900	5.16652200	-2.58793500
H	-4.75147400	6.52306700	-1.55528200
C	-1.71355800	7.05461500	-2.75748100
H	-0.65299100	6.80955500	-2.87279200
H	-2.00413100	7.69008100	-3.60178200
H	-1.83857100	7.64700600	-1.84476400
C	2.70997300	2.63116600	-0.54595000
H	2.82681400	1.61307700	-0.15942900
H	3.67740500	2.94292200	-0.95507500
H	2.46517400	3.29731800	0.28706300
C	1.27356600	4.45344600	-2.59799800
H	2.16687600	4.68598400	-3.18867600
H	0.40419300	4.53695000	-3.25710800

H	1.18002100	5.19924500	-1.80499300
C	1.77121900	1.51300700	-3.27121800
H	0.97516200	1.52758100	-4.02348100
H	2.71164700	1.76884400	-3.77184700
H	1.85823600	0.49201300	-2.88512500
Si	-4.46720500	1.98850400	-0.30019800
C	-4.44684000	1.66414300	-2.12357300
H	-3.89514200	0.75246400	-2.36989200
H	-5.47260500	1.54596700	-2.48821500
H	-3.98610000	2.50625800	-2.64434800
C	-4.83425000	0.50565900	0.75586900
H	-4.64648100	0.71039200	1.81405000
H	-5.89580500	0.25856400	0.64454200
H	-4.25753900	-0.37360500	0.45514900
C	-5.36281700	3.52089900	0.23389000
H	-6.43346900	3.34312700	0.08272600
H	-5.21261600	3.74184300	1.29424300
H	-5.08797400	4.39309600	-0.36183200

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Alpha-Me-glucose. Gibbs free energy: -2360.461538

C	-2.91621100	0.22328400	-1.07011600
C	-1.48126500	0.78846300	-0.98886200
C	-1.45095800	2.31166300	-0.76748000
C	-2.39450300	2.67165700	0.37619600
C	-3.82208400	0.79709400	0.03241600
H	-0.43562400	2.58801400	-0.45438300
H	-0.97900700	0.58977300	-1.94175300
H	-2.83293400	-0.86299700	-0.91576900
H	-4.85975100	0.63177800	-0.26933400
O	-3.70319200	2.21190200	0.11230900
C	-3.59483500	0.10340600	1.38092100
H	-3.92052700	-0.94080000	1.27331600
H	-2.52804200	0.08636200	1.62650800
O	-4.34384600	0.75590400	2.38273900
O	-3.50052500	0.51315600	-2.31989200
O	-0.82820600	0.11806800	0.07042300
O	-1.79278600	2.95740000	-1.96091100
Si	-3.90158500	0.68580300	4.00505400
Si	0.83089200	0.14651300	0.38395400
Si	-3.38362300	-0.46795500	-3.68194900
Si	-1.13899300	4.39141200	-2.54959800
C	-2.07077300	1.07521400	4.18678200
H	-1.43931600	0.30933100	3.72348900
H	-1.81883200	2.04301100	3.74057800
H	-1.80803800	1.12009200	5.24980000
C	-4.95735400	1.98104900	4.84364000
H	-6.02224700	1.77274300	4.69775800
H	-4.75993300	2.00437300	5.92075300

H	-4.74544500	2.97513400	4.43630400
C	-4.24491100	-1.03389600	4.67367200
H	-3.98618100	-1.09890100	5.73631800
H	-5.30412000	-1.28986300	4.56512700
H	-3.65597000	-1.78683200	4.13812200
C	-4.22583100	-2.10892100	-3.33195200
H	-5.28459700	-1.96120500	-3.09497200
H	-4.16063000	-2.76630900	-4.20613100
H	-3.75714100	-2.62984000	-2.48973400
C	-4.26456100	0.49514100	-5.01986400
H	-3.78273600	1.46606800	-5.17557400
H	-4.24185700	-0.05189800	-5.96862400
H	-5.31167700	0.67120100	-4.75353200
C	-1.58798400	-0.77039900	-4.14622600
H	-1.06002300	0.17325300	-4.32141200
H	-1.05369600	-1.32561900	-3.36712800
H	-1.53909100	-1.36164400	-5.06792100
C	-0.74858800	4.04719200	-4.35125300
H	-0.36035800	4.94385800	-4.84696600
H	0.00156100	3.25419700	-4.44215000
H	-1.64877800	3.72727400	-4.88731900
C	-2.40394000	5.76571500	-2.41387900
H	-3.33224200	5.49187500	-2.92670300
H	-2.63737500	5.96356400	-1.36369100
H	-2.02343100	6.68664000	-2.87018100
C	0.42015400	4.81909000	-1.59461300
H	0.85897700	5.73593100	-2.00397300
H	0.20338700	4.99277500	-0.53551600
H	1.17583700	4.02894900	-1.66810200
C	1.21905000	1.51612900	1.60904000
H	0.51821300	1.48292300	2.45056100
H	2.23161700	1.39262100	2.00964200
H	1.15733600	2.51098700	1.15589300
C	1.74290600	0.40987800	-1.23409800
H	2.82481000	0.39980800	-1.06331700
H	1.50623100	-0.37912700	-1.95597600
H	1.48780400	1.37311300	-1.68995900
C	1.20161600	-1.52000800	1.14623300
H	0.92816800	-2.33094500	0.46370400
H	2.26840800	-1.61137400	1.37740100
H	0.64171900	-1.65215200	2.07823400
H	-2.01972500	2.20854400	1.30519200
O	-2.42875400	4.04876300	0.51741300
C	-3.10359300	4.49347100	1.68410900
H	-2.65176000	4.05704300	2.58448700
H	-2.99239700	5.57783300	1.71578900
H	-4.16553100	4.23260100	1.65129200

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Me_3Si–Alpha-Me-glucose$^+$. Gibbs free energy: -2769.434103

C	0.84365100	-1.50693000	-0.33734500
C	0.95061800	-0.41712700	0.74373200
C	0.65015400	0.99614400	0.20470100
C	-0.70033600	0.89243800	-0.50182400
C	-0.44594300	-1.37480500	-1.16500600
H	0.53420700	1.64926200	1.08214400
H	1.97173200	-0.44028700	1.14741600
H	0.78609500	-2.46038500	0.20803400
H	-0.28465900	-1.87579900	-2.12170300
O	-0.69405700	-0.00896600	-1.54423100
C	-1.66101200	-2.00796600	-0.49205600
H	-1.41468100	-3.05852100	-0.28678300
H	-1.85323100	-1.53047700	0.47666000
O	-2.77253800	-1.93041900	-1.35478500
O	1.96861500	-1.46619600	-1.18206100
O	-0.02864500	-0.67969100	1.72249700
O	1.59584800	1.50301500	-0.68236000
Si	-4.33427600	-1.77863900	-0.73313100
Si	0.24277400	-0.94752400	3.36965600
Si	2.95008900	-2.83301800	-1.36800400
Si	3.12156500	2.13707300	-0.30573700
C	-4.44273100	-0.15451900	0.20473600
H	-3.74081700	-0.13910100	1.04663000
H	-4.22029100	0.68869600	-0.45784200
H	-5.44728700	-0.00773300	0.61583500
C	-5.45478200	-1.79234800	-2.22626100
H	-5.37993200	-2.74439700	-2.76128200
H	-6.49840600	-1.65303200	-1.92500500
H	-5.19077900	-0.98740100	-2.91971100
C	-4.67589000	-3.20448700	0.43630800
H	-5.68119900	-3.12148200	0.86347400
H	-4.60237200	-4.16706600	-0.08017900
H	-3.96073200	-3.20786700	1.26659400
C	1.89033400	-4.26278100	-1.96399300
H	1.41215500	-4.02568700	-2.92022500
H	2.50883300	-5.15561100	-2.10773900
H	1.10573400	-4.52004100	-1.24400700
C	4.23678500	-2.36590900	-2.63779800
H	4.94360700	-1.63122000	-2.24177400
H	4.80360600	-3.25463500	-2.93623200
H	3.76826900	-1.94652500	-3.53390600
C	3.71896800	-3.24365700	0.29353900
H	4.28424900	-2.39158100	0.68616100
H	2.95881600	-3.51550500	1.03381500
H	4.40725500	-4.09077300	0.19920700
C	4.43380100	0.89519000	-0.77819000
H	5.43190100	1.30241600	-0.58236000

H	4.32090900	-0.03492800	-0.21344000
H	4.36450200	0.65472300	-1.84341400
C	3.27384200	3.68699300	-1.34015500
H	3.10497200	3.46344200	-2.39882000
H	2.54921400	4.44622100	-1.03103400
H	4.27691400	4.11599100	-1.24167300
C	3.20178800	2.50507800	1.53221200
H	4.13535900	3.03636500	1.74781200
H	2.37680800	3.13379200	1.88342800
H	3.20929500	1.58295100	2.12311800
C	0.73040900	0.66833400	4.18374500
H	-0.05549800	1.42216400	4.06638500
H	0.89585200	0.51888400	5.25646900
H	1.65539000	1.07173100	3.75960500
C	1.60194400	-2.22300200	3.55550300
H	1.78566900	-2.42830100	4.61572900
H	1.32518900	-3.16501400	3.07059200
H	2.54483800	-1.87640600	3.11847300
C	-1.41261100	-1.55735500	3.98063500
H	-1.69192700	-2.49127200	3.48213300
H	-1.38847100	-1.73938200	5.06014700
H	-2.19186300	-0.81465500	3.77893700
H	-1.49207900	0.68409600	0.22269600
O	-1.07760800	2.17253600	-1.10360700
Si	-1.71493100	3.57740600	-0.10590500
C	-2.29894100	2.81164900	1.48063000
H	-2.66276400	3.63250300	2.10949600
H	-3.13322700	2.12345500	1.32235000
H	-1.51163200	2.29876400	2.03910600
C	-3.09182500	4.24639000	-1.15332400
H	-3.64233700	4.98525400	-0.56049100
H	-2.73892900	4.74482500	-2.05954100
H	-3.79056700	3.45302800	-1.43369800
C	-0.24309500	4.69128800	0.08276800
H	0.13892100	5.03609500	-0.88196100
H	-0.53810200	5.57417100	0.66023600
H	0.56710600	4.19318100	0.62256800
C	-0.62391800	2.42893400	-2.48194100
H	-1.23541800	1.82728100	-3.14786400
H	-0.78471200	3.48994500	-2.65829500
H	0.43124000	2.18013200	-2.53988800

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Beta-Me-glucose. Gibbs free energy: -2360.455616

C	-2.65239900	0.45968900	-0.96878200
C	-1.41292700	1.35796100	-0.80257500
C	-1.78535800	2.83050900	-0.57664400
C	-2.94376300	3.01776200	0.42267600
C	-3.68472200	0.72520400	0.13085000

H	-0.89777000	3.31665700	-0.14845300
H	-0.82322700	1.31494200	-1.72762100
H	-2.31989500	-0.58322300	-0.87342100
H	-3.38181800	4.00858900	0.23929800
H	-4.62653800	0.27794100	-0.19987500
O	-3.99133000	2.11799000	0.23317700
C	-3.31753100	0.08295700	1.46615900
H	-3.07241300	-0.97155000	1.27131600
H	-2.43323200	0.56728700	1.88688900
O	-4.42233000	0.16071300	2.34894900
O	-3.27221400	0.67127800	-2.21750500
O	-0.66560600	0.91460500	0.30904900
O	-2.16171200	3.42832900	-1.79763500
O	-2.50424200	2.94000300	1.76187400
C	-1.97111700	4.14453700	2.27083500
H	-2.69091700	4.96843200	2.16915800
H	-1.76785600	3.97455100	3.32916300
H	-1.03470100	4.42759100	1.77221300
Si	-4.18228500	-0.02036900	4.00511200
Si	0.68997400	-0.07910600	0.22826900
Si	-2.91033700	-0.15717500	-3.63407100
Si	-1.14482500	4.48034800	-2.63131500
C	-3.12389300	1.38261700	4.66379100
H	-2.15217400	1.41735900	4.16051300
H	-3.61400000	2.34848600	4.50587800
H	-2.94849900	1.25353000	5.73785700
C	-5.89698400	0.01507900	4.75290100
H	-6.52106000	-0.78776300	4.34721900
H	-5.84209000	-0.11344800	5.83949100
H	-6.39137300	0.97059800	4.54943900
C	-3.32261300	-1.66058800	4.32431700
H	-3.17780300	-1.81664700	5.39907300
H	-3.91184400	-2.49780800	3.93523500
H	-2.33617600	-1.68911300	3.84797400
C	-2.96323800	-2.00534300	-3.30590400
H	-3.93752000	-2.30694200	-2.90733800
H	-2.79122600	-2.55456900	-4.23831200
H	-2.19274300	-2.31797700	-2.59267300
C	-4.23760600	0.38030500	-4.83502400
H	-4.19716400	1.46330700	-4.99237800
H	-4.10101300	-0.10898300	-5.80546900
H	-5.23387000	0.12561300	-4.45988300
C	-1.21440600	0.31763800	-4.29041600
H	-1.14221700	1.40056300	-4.43540400
H	-0.40283800	0.00641000	-3.62386900
H	-1.04586000	-0.16331400	-5.26085600
C	-1.97871200	4.73441400	-4.28410900
H	-1.37750800	5.38916200	-4.92397900

H	-2.11064200	3.77899300	-4.80257900
H	-2.96465200	5.19319200	-4.15780500
C	-0.99660900	6.07883000	-1.66011100
H	-1.97793000	6.54485600	-1.52320000
H	-0.56313000	5.89973400	-0.66962700
H	-0.34903700	6.79176000	-2.18238200
C	0.55279900	3.69850200	-2.81561100
H	1.22034500	4.36996800	-3.36687100
H	1.01026500	3.50571700	-1.83892400
H	0.50418000	2.75011000	-3.36061900
C	2.05199400	0.81060300	-0.70488800
H	2.28493100	1.77129800	-0.23373000
H	2.96598000	0.20625000	-0.71671300
H	1.76757000	1.00184900	-1.74541200
C	0.27275300	-1.68869200	-0.64482500
H	1.13705300	-2.36207500	-0.61925600
H	-0.56707900	-2.19988700	-0.16191600
H	0.01845800	-1.52541200	-1.69783100
C	1.13090000	-0.37205300	2.02025400
H	0.30468600	-0.86701500	2.54172100
H	2.01845900	-1.00784900	2.10584700
H	1.33790300	0.57466800	2.52957400

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Me_3Si–Beta-Me-glucose$^+$. Gibbs free energy: -2769.437814

C	-2.72214600	0.33708900	-0.76742400
C	-1.34851300	1.02951700	-0.69523500
C	-1.51983000	2.55278400	-0.48131900
C	-2.84877700	2.82177900	0.21881300
C	-3.51809700	0.57709900	0.52913300
H	-0.70671400	2.85312400	0.19013200
H	-0.82565000	0.89791400	-1.64974600
H	-2.57774000	-0.74378000	-0.89195900
H	-3.63847400	3.00086800	-0.51844500
H	-4.58231700	0.60602400	0.26478300
O	-3.17928200	1.84125000	1.12724500
C	-3.29099500	-0.47806400	1.59470300
H	-3.53113000	-1.45929900	1.16282400
H	-2.22977500	-0.47153300	1.87039400
O	-4.12057200	-0.21175100	2.70310800
O	-3.46111600	0.87968600	-1.83794200
O	-0.60859100	0.51070200	0.38357900
O	-1.51414800	3.29036800	-1.67420700
O	-2.73941000	4.04858400	1.01327600
C	-3.52920700	5.16285600	0.49133900
H	-4.58674100	4.95106200	0.64908600
H	-3.21920600	6.05418900	1.02849600
H	-3.29101300	5.26115200	-0.56579100
Si	-3.71303700	-0.78049300	4.24164600

Si	0.51077600	-0.75352600	0.29592100
Si	-3.39762900	0.34871600	-3.44490700
Si	-0.19530100	4.24894200	-2.13972600
C	-2.12998800	0.05123900	4.81435300
H	-1.32083500	-0.06503100	4.08560600
H	-2.28612100	1.12179400	4.97948400
H	-1.79198100	-0.39123100	5.75798200
C	-5.15894900	-0.29653400	5.32065700
H	-6.07900000	-0.79177200	4.99477500
H	-4.97168400	-0.57619800	6.36288700
H	-5.32092400	0.78607700	5.28560300
C	-3.46600300	-2.63751200	4.15659500
H	-3.26378300	-3.04569000	5.15281500
H	-4.35808800	-3.13400800	3.76064100
H	-2.61798100	-2.89622900	3.51256000
C	-3.88636900	-1.46059300	-3.48984000
H	-4.88034900	-1.61008100	-3.05581300
H	-3.90741700	-1.82292000	-4.52357100
H	-3.17501900	-2.08424200	-2.93721300
C	-4.63256900	1.44798500	-4.31305500
H	-4.34040500	2.49964800	-4.22463700
H	-4.69172800	1.20004000	-5.37806000
H	-5.63099800	1.33163300	-3.87957300
C	-1.67794400	0.56941000	-4.16321500
H	-1.30970400	1.58518600	-3.98672800
H	-0.95745500	-0.14035100	-3.74173100
H	-1.70911100	0.40062600	-5.24569700
C	-0.71197900	4.96331800	-3.78373400
H	0.04838900	5.65674900	-4.15810900
H	-0.84758700	4.17336000	-4.52953100
H	-1.65512800	5.51106900	-3.68932300
C	0.06788500	5.57450600	-0.83791800
H	-0.81803200	6.20901700	-0.73015500
H	0.30086600	5.14088400	0.14068600
H	0.90857100	6.21802600	-1.11961300
C	1.31706000	3.15240000	-2.26749400
H	2.19863300	3.73583600	-2.55419600
H	1.53471900	2.67191200	-1.30752500
H	1.17130700	2.36643200	-3.01643800
C	2.04325200	-0.16818500	-0.60612500
H	2.49651000	0.69131800	-0.10177000
H	2.78784100	-0.97105800	-0.64355300
H	1.81421400	0.12070700	-1.63750000
C	-0.24354500	-2.21429500	-0.60754400
H	0.47785000	-3.03845800	-0.63913100
H	-1.14547400	-2.57853500	-0.10430600
H	-0.50021100	-1.96522700	-1.64335900
C	0.84689800	-1.15170900	2.08997800

H	-0.04557300	-1.56898000	2.56876300
H	1.65100800	-1.88958500	2.18033300
H	1.14452800	-0.25298800	2.64028500
Si	-2.27281800	3.96927100	2.82084000
C	-3.78834500	3.38463800	3.71388900
H	-3.63535900	3.50856500	4.79193200
H	-4.66315400	3.97885900	3.43144400
H	-3.98808100	2.33360300	3.49334400
C	-1.83913400	5.74436500	3.16782000
H	-2.71081100	6.39900400	3.24710500
H	-1.32808000	5.76126600	4.13763200
H	-1.14508300	6.14957300	2.42493200
C	-0.77892800	2.87217300	2.88844800
H	-0.94407800	1.89566200	2.42841900
H	0.08390900	3.35136000	2.41583100
H	-0.53566600	2.72025100	3.94654500

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Glucose-oxocarbenium^{+}. Gibbs free energy: -2245.183604

C	-2.71380700	0.34383300	-0.97544100
C	-1.59783100	1.40100800	-0.91251900
C	-2.24453000	2.80427200	-0.97285300
C	-3.66524800	2.84152700	-0.50629000
C	-3.72180400	0.53156200	0.15036800
H	-1.71677500	3.41621700	-0.21616500
H	-0.97018100	1.31076700	-1.80514100
H	-2.28334400	-0.65791500	-0.85588300
H	-4.22816900	3.76669400	-0.63045900
H	-4.60467300	-0.07778600	-0.04263800
O	-4.29712400	1.91242000	0.03779200
C	-3.25860800	0.32712100	1.57880400
H	-2.73245600	-0.63837900	1.59416300
H	-2.53715500	1.10107600	1.85856800
O	-4.37715500	0.31959800	2.42507100
O	-3.41874300	0.49130200	-2.17580700
O	-0.86652900	1.29072600	0.27384700
O	-2.26047200	3.38374000	-2.23790400
Si	-4.17480700	0.11895500	4.10013900
Si	0.53328700	0.35054400	0.51890100
Si	-3.02054300	-0.24716600	-3.65899900
Si	-1.11899800	4.55921100	-2.74360300
C	-3.03845600	1.46962000	4.73457400
H	-2.03841900	1.39779500	4.29317500
H	-3.44179600	2.46346200	4.51474700
H	-2.92457900	1.38238500	5.82065600
C	-5.89720400	0.25468600	4.80443200
H	-6.55621500	-0.50986500	4.38097300
H	-5.87234400	0.11587800	5.89059500
H	-6.33190200	1.23771000	4.59800400

C	-3.41332500	-1.56541400	4.41521600
H	-3.29093300	-1.72685700	5.49186600
H	-4.04852000	-2.36595700	4.02237300
H	-2.42319800	-1.65660300	3.95550400
C	-2.82654300	-2.08589400	-3.36274500
H	-3.73139900	-2.51346100	-2.91916600
H	-2.64293800	-2.59480700	-4.31541100
H	-1.98061200	-2.31109600	-2.70419900
C	-4.47792800	0.15999700	-4.74844400
H	-4.58704000	1.24267700	-4.86752200
H	-4.34226000	-0.27882000	-5.74265000
H	-5.40598500	-0.23634600	-4.32488300
C	-1.43436000	0.48735300	-4.33726700
H	-1.47618300	1.58070400	-4.30644000
H	-0.54835500	0.15633500	-3.78476700
H	-1.30189300	0.18219400	-5.38120400
C	-1.53168500	4.82947200	-4.53967400
H	-0.85393400	5.57377200	-4.97106400
H	-1.42683900	3.90423000	-5.11462100
H	-2.55639900	5.19535700	-4.65645500
C	-1.36192600	6.09328800	-1.70228500
H	-2.36699800	6.50520300	-1.83757100
H	-1.21170500	5.89296500	-0.63593200
H	-0.63788800	6.86080200	-1.99660100
C	0.58288300	3.82866800	-2.48306900
H	1.35198900	4.53412500	-2.81512000
H	0.76789600	3.61635500	-1.42471800
H	0.70954100	2.89969600	-3.04908800
C	2.01440900	1.25166200	-0.18212300
H	2.12631900	2.24270100	0.26927500
H	2.92646300	0.68076400	0.02506200
H	1.93716800	1.37347100	-1.26728300
C	0.33418800	-1.30632500	-0.33569600
H	1.26014300	-1.88082800	-0.22186000
H	-0.47935700	-1.90221900	0.09068500
H	0.15814300	-1.18921600	-1.41075000
C	0.61787100	0.18893200	2.37606000
H	-0.25340400	-0.34714700	2.76606800
H	1.51553900	-0.36380100	2.67247700
H	0.65518400	1.17441600	2.85140600

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Me_3Si^+. Gibbs free energy: -408.934892

Si	0.16595600	0.87225200	0.00416600
C	0.92830600	1.17933400	-1.63264700
H	1.42073800	2.15700600	-1.64180000
H	1.70909600	0.42513800	-1.79623200
H	0.20031600	1.11680300	-2.44310200
C	1.10869400	1.23121100	1.53269800

H	0.68750500	2.13529100	1.99174500
H	0.98579300	0.41852700	2.25545300
H	2.16765200	1.40137600	1.33106800
C	-1.53385700	0.19775100	0.10502000
H	-1.54879800	-0.79230000	-0.36729300
H	-1.88744600	0.11338700	1.13371300
H	-2.21370400	0.83366500	-0.47278800