Electronic Supplementary Information

Rational Selection of Co-Catalysts for the Deaminative Hydrogenation of Amides

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Experimental Details

All manipulations were carried out using standard vacuum, Schlenk line, canula or glovebox techniques. Hydrogen was purchased from Airgas and used as received. The catalysts **Fe^{N}** and **Ru^{PNN}** were prepared as previously described.[1,2] All other chemicals including **RuBH$_4$^{NH}** were purchased from Aldrich, Fisher, VWR, Strem or Cambridge Isotope Laboratories. Amide substrates and additives were purified by sublimation and distillation or vacuum transfer after drying over appropriate drying agents.[3] All other non-volatile solids were dried under vacuum at 50 °C. Solvents were dried and deoxygenated using literature procedures.[3] ^{1}H, ^{13}C and ^{31}P NMR spectra were recorded on Bruker 300 MHz DRX, 500 MHz DRX or 600 MHz spectrometers at ambient temperature, unless otherwise noted. ^{1}H and ^{13}C chemical shifts are referenced to residual solvent signals; ^{31}P chemical shifts are referenced to an external standard of H_3PO_4. Probe temperatures were calibrated using ethylene glycol and methanol as previously described.[4] High pressure catalytic hydrogenation reactions were performed using a Parr 5500 series compact reactor with glass insert.

General procedure and sample spectra for screening the co-catalytic effect

Inside a glovebox, the catalyst (5 μmol) was added as a solution to a glass reactor liner (50 mL). Then amide (7 mmol) and 5 mL of THF were added in succession using a micro syringe. Subsequently, the relevant additive (25 μmol) was added and the Parr reactor sealed and removed from the glovebox. The reactor was pressurized with Commercial grade hydrogen at ambient temperature (450 psi) and heated (100 °C) with mechanical stirring. After 2h heating was stopped, and the reactor was immediately immersed in to a cold ice bath and the H_2 was slowly vented. The products and the remaining reactants were analysed by ^{1}H NMR spectroscopy or GC FID using mesitylene as an internal standard. GC Method: 0.418 mL of mesitylene was added to the reaction solution and the final volume was adjusted to 10 mL by adding THF. An aliquot of 0.02 mL from this mixture was diluted to 0.2 mL and analyzed using a Thermo Fisher GC (Trace 1300; Column – TG 5MS AMINE 30m x 0.25 mm x 0.25 μm; start at 40 °C, ramp 25 °C. hold 2 min). Response factors were calculated using standards. NMR Method: The reaction solution was diluted either to 10 mL or 9 mL. An aliquot of 0.1 mL was mixed with 0.05 mL of 1M mesitylene to prepare the NMR sample.

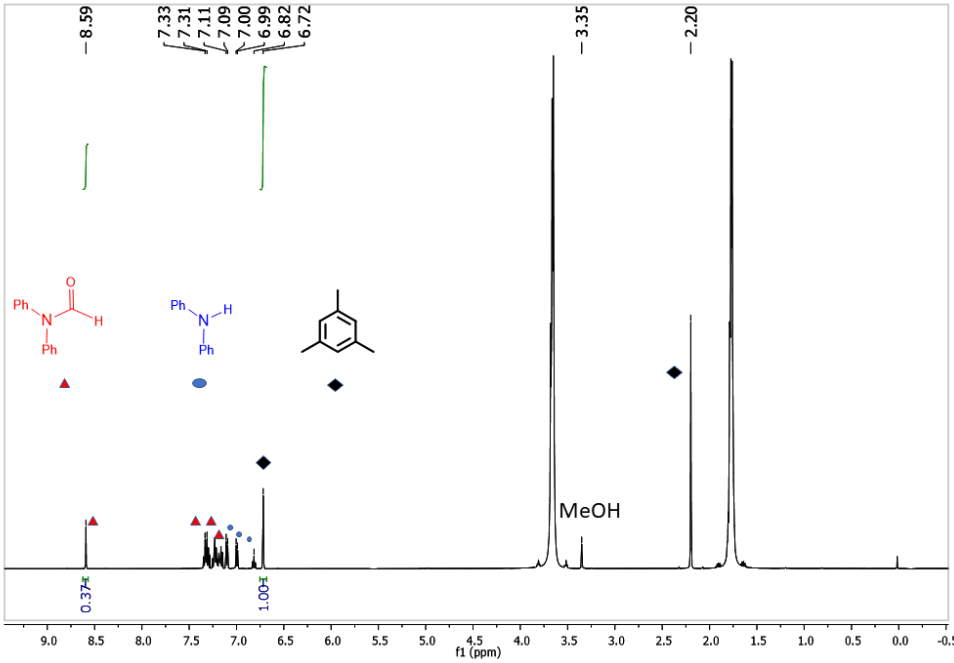
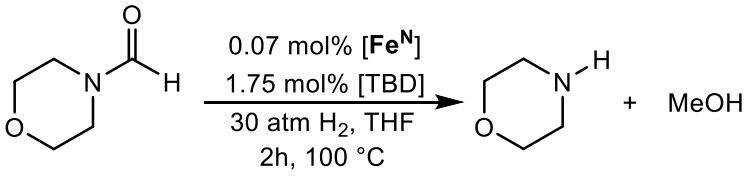


Figure S1: Sample ^{1}H NMR spectrum of product solution from hydrogenation of diphenylformamide using **Fe^{N}** with no additives. The labelled peaks identfy the species present. Two large solvent peaks for residual THF are also observed.



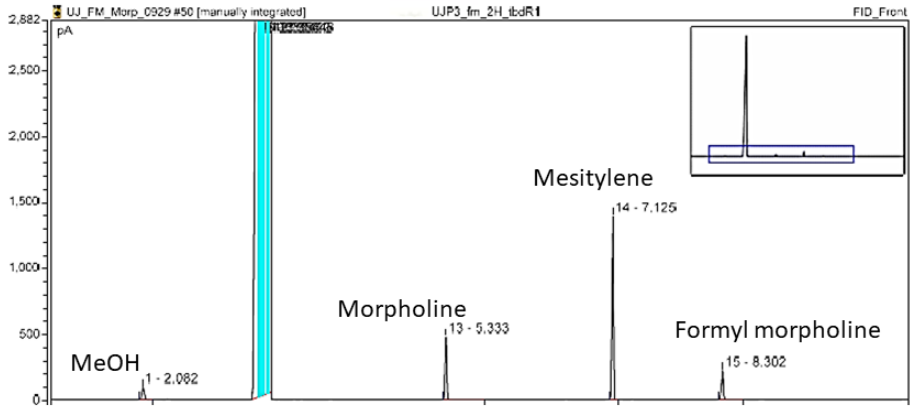


Figure S2: Sample GC-FID chromatogram of product solution from the hydrogenation of formylmorpholine formamide using **Fe^{N}** in the presence of TBD. The labelled peaks identfy the species present along with the off scale solvent signal.

Synthesis of ($^{Ph}PN^{H}P$)RuH(CO)(HCONPh)

Inside the glovebox, a sample of **$RuBH_4^{NH}$** (0.023 g, 0.039 mmol) was transferred to a J-Young tube using 1 mL of THF. Then a solution of NEt_3 in THF (1M, 0.117 mL, 0.117 mmol) was added to the reaction mixture, followed by HCONHPh in THF (1M, 0.043 mL, 0.043 mmol). A drop of deuterated benzene was added, and the tube was tightly closed before it was removed from the glovebox. This mixture was heated at 50 °C and the reaction monitored using ^{31}P NMR spectroscopy until it reached completion. After that, the tube was taken back in to the glovebox and all the volatiles were evaporated under reduced pressure. A near colorless solid was obtained and crystals suitable for X-ray diffraction were obtained by slow diffusion of pentane into a concentrated THF solution of the product. Yield: 0.013 g (40 %). ^1H NMR (THF-d_8; 50 MHz, 23 °C) (two isomers observed): major isomer: 10.98 (s, 1H, N-*H*), 8.02 (s, 1H, *H*CO, overlap with *Ph*H), 8.02(s, 4H, *Ph*H), 7.41(m 10H, *Ph*H), 7.32(s,br 1H, *Ph*H), 7.26-7.22(q,t, 6H, *Ph*H), 6.43(m 2H, *Ph*H), 5.55(d, 2H, *Ph*H), 3.35 (m, 2H, CH_2), 3.02 (t, 2H, CH_2), 2.87 (d, 2H, CH_2), 2.16 (m, 2H, CH_2), -14.24 (t, 1H, Fe-H); $^{31}P\{^1H\}$ NMR (THF-d_8): 58.955; $^{13}C\{^1H\}$ NMR (THF-d_8): δ 174.07 (s, *H*CO), 137.69-137.43 (m, *PhH*), 135.14 (s, *PhH*), 132.39 (s, *PhH*), 130.67 (s, *PhH*), 129.47-128.75 (m, *PhH*), 127.22 (s, *PhH*), 125.67 (s, *PhH*), 121.34 (s, *PhH*), 52.17 (t, *CH_2*), 32.89 (t, *CH_2*).

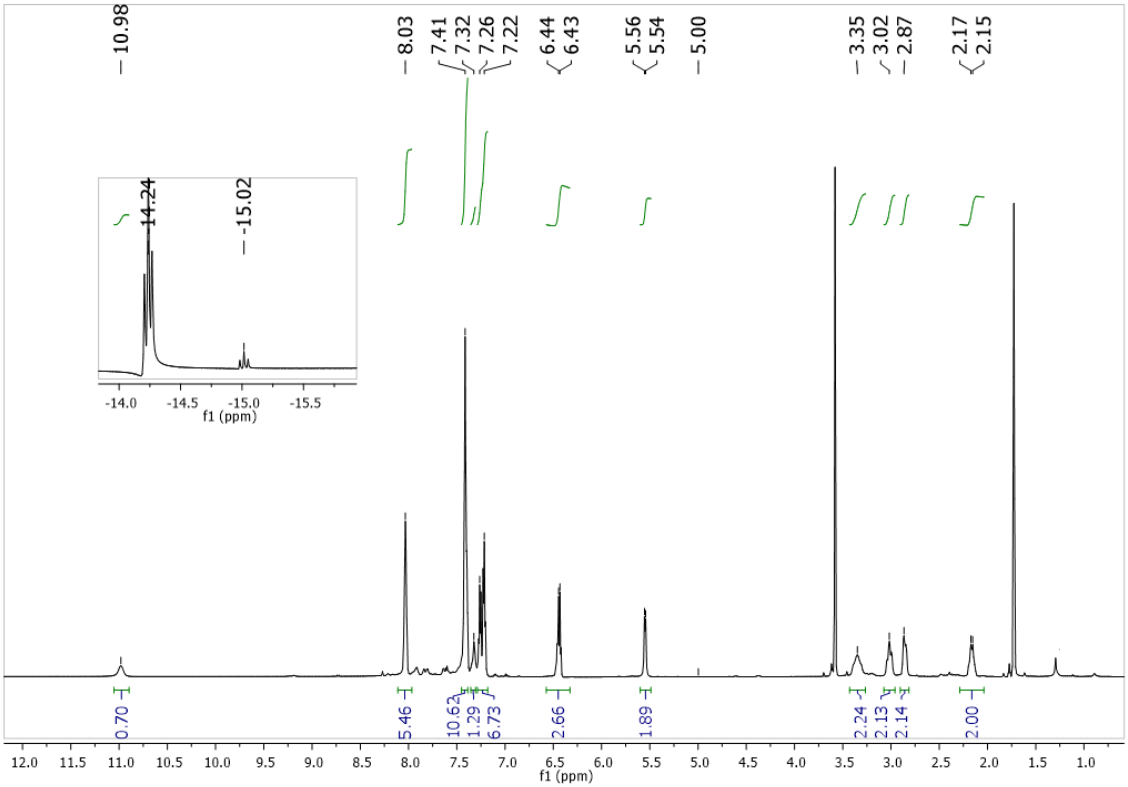


Figure S3: ^1H NMR of ($^{Ph}PN^{H}P$)RuH(CO)(HCONPh) (two isomers observed) in THF-d_8.

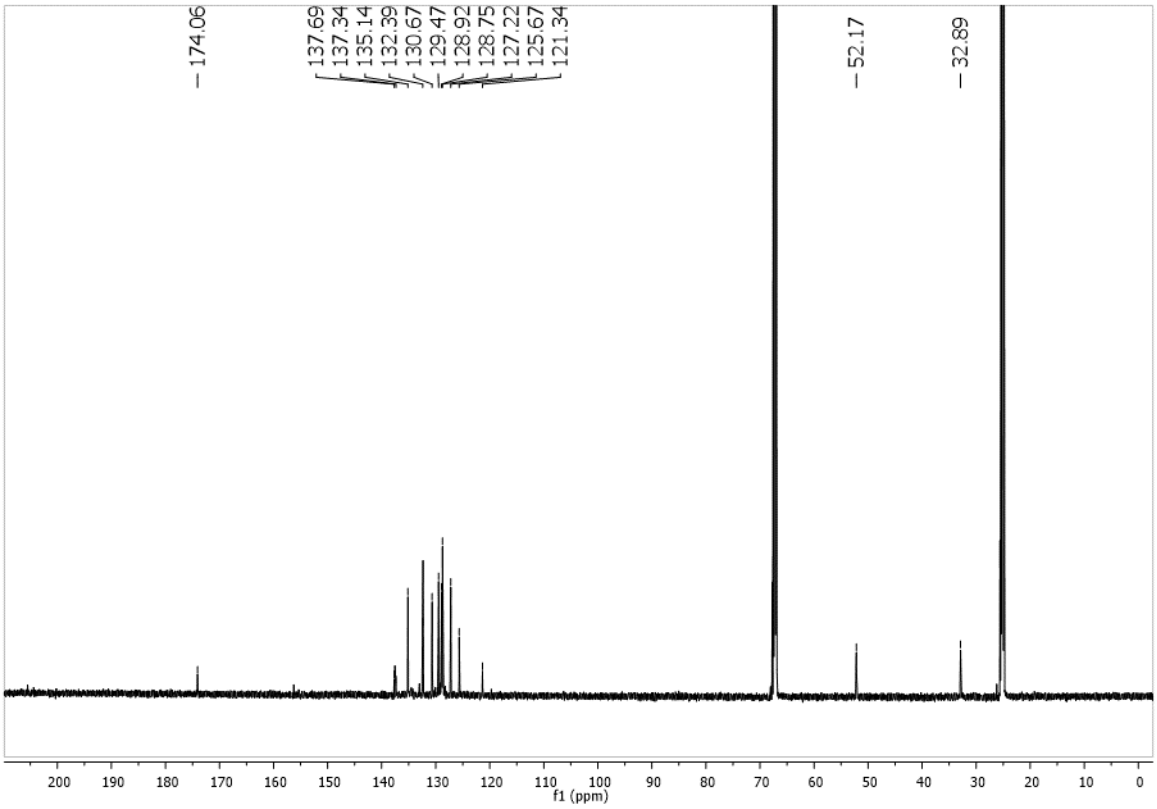


Figure S4: $^{13}C\{^{1}H\}$ NMR of ($^{Ph}PN^{H}P$)RuH(CO)(HCONPh) in THF-d_8.

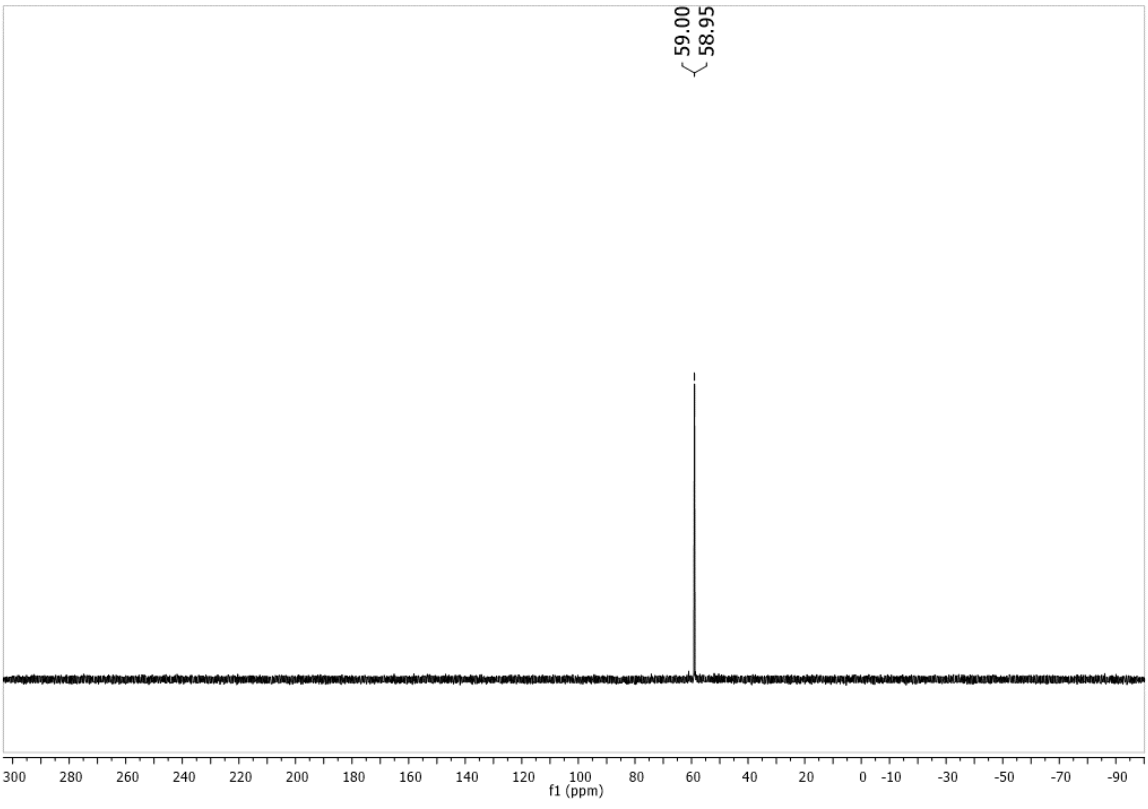


Figure S5: $^{31}P\{^{1}H\}$ NMR of ($^{Ph}PN^{H}P$)RuH(CO)(HCONPh) (two isomers observed) in THF-d_8.

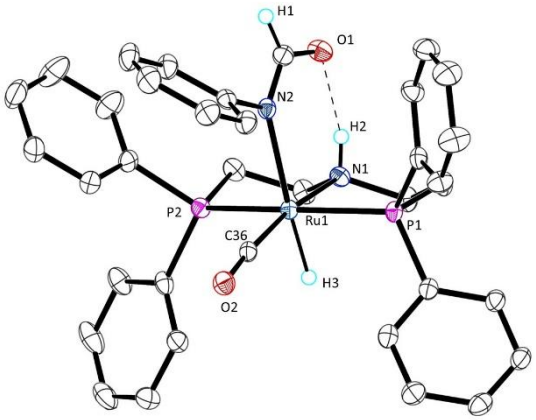
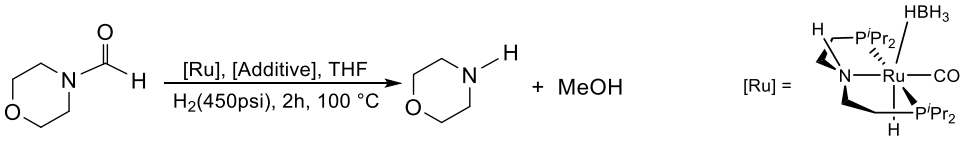


Figure S6: Molecular structure of (^{Ph}PN^{H}P)RuH(CO)(HCONPh) with thermal ellipsoids at 50% probability. Hydrogen atoms and an additional formanilide molecule, co-crystalized with the complex, have been removed for clarity. Selected bond lengths (Å) and angles (deg): Ru(1)−N(2) 2.236(2), Ru(1)−P(2) 2.3082(8), Ru(1)−P(1) 2.3203(8), Ru(1)−N(1) 1.195 (2); P(1)−Ru(1)−P(2) 163.64(3), N(2)−Ru(1)−N(1) 93.01 (9).

Comparative influence of base activator and co-catalysts

Table S1 distinguished the possible roles of the co-catalyst in promoting C–N scission and acting as a base activator. Entries 1 and 2 suggest that TBD can work as an activator, presumably by scavenging BH_3 from (^{Ph}PN^{H}P)RuH(CO)(BH_4). Significantly, comparison of the entries 2, 4, 5 and 6 suggest that the effect of a base catalyst activator saturates at 2 eq per metal and that the influence of TBD as a co-catlayst for C–N bond scission far exceeds any potential influence from acting as a simple catalyst activator.

Table S1: Influence of base activator and co-catalysts on 4-formylmorpholine hydrogenation using (^{Ph}PN^{H}P)RuH(CO)(BH_4).[a]



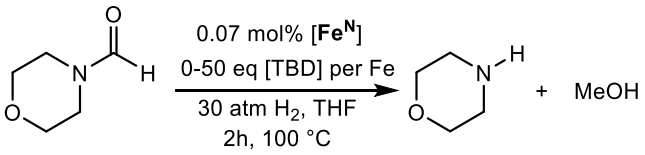
Entry	NEt_3	TBD	HCONHPh	2,6-diisopropyl-4-methylphenol	TON[b] (Con %)
1	2 eq	25 eq	-------	-------	1200 (86%)
2	-------	25 eq	-------	-------	1040 (74%)
3	2 eq	-------	-------	25 eq	822 (59%)
4	2 eq	-------	-------	-------	310 (22%)
5	25 eq	-------	-------	-------	290 (21%)
6	-------	-------	-------	-------	210 (15%)
7	2 eq	-------	25 eq	-------	NR (0%)

[a] Reaction conditions: 30 atm H_2(~ 450 psi), 5 *μmol* of [Ru] (0.018 mol %), 125 *μmol* of each additive, 10 or 125 *μmol* of NEt_3 and 7 mmol of formyl morpholine in 5 mL of THF at 100 °C for 2h. [b] Determined using GC-FID analysis of the products and remaining starting material. Each entry is average of two or more trials.

Discussion of aldehyde hydrogenation

The microkinetic modeling of the catalytic reaction suggests that the intermediate aldehyde is hydrogenated rapidly under the reaction conditions and plays little or no role in the reaction rate (See Reaction 4; Table S2). In the case of formylmorpholine hydrogenation, the intermediate aldehyde is formaldehyde. Given the difficulty in obtaining dry formaldehyde in a non-polymer form we have substituted benzaldehyde for a comparison of the hydrogenation of aldehydes and formamides. Using 0.07mol% of **Fe^{N}**, 100 °C, and 30 atm H_2 in THF, both formylmorpholine and benzaldhyde are hydrogenated to nearly full conversion (>96%). However, although both reactions give high conversion, the uptake of hydrogen gas is noticeably different. The benzaldhyde reaction ceased uptake of hydrogen after *ca* 30 mintues while formylmorphline continued to consume hydrogen for *ca* 90 minutes. While these observations are insufficient to establish reliable rate meaasurements they confirm the computational conclusions that aldehyde hydrogenation is a viable intermediate step in catalysis and that it is facile relative to formamide hydrogenation.

Influence of [TBD] on Catlaysis



Entry	TBD	TON
1	0 eq	320
2	5eq	515
3	10eq	650
4	25eq	830
5	50 eq	965

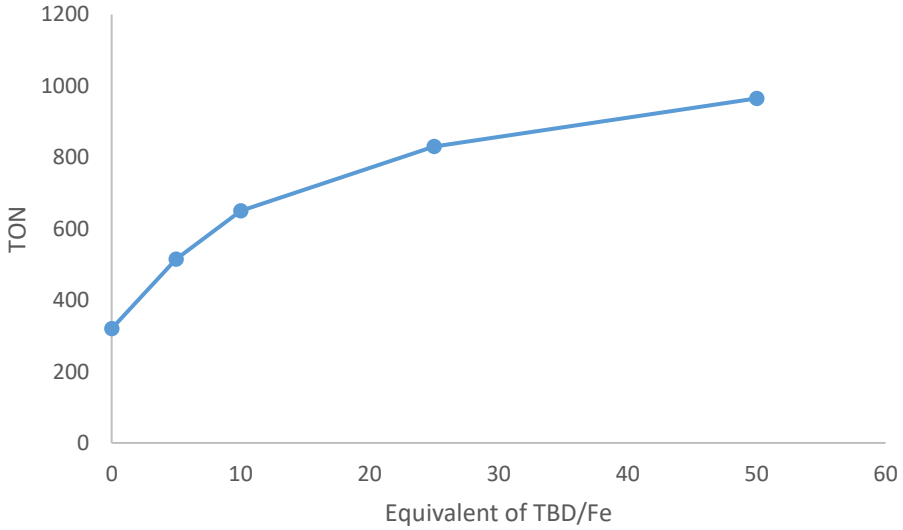


Figure S7: Correlation between TBD loading and TON for formylmorpholine hydrogenation. Experimental conditions: 30 atm H_2(~ 450 psi), 5 *μmol* of [**Fe^{N}**] (0.07 mol %), 0-250 *μmol* of TBD, and 7 mmol of formyl morpholine in 5 mL of THF at 100 °C for 2h. TON determined using GC-FID analysis of the products and remaining starting material. Each point is average of two or more trials.

Computational Details

DFT calculations were carried out with the Gaussian09 software package.[5] The hybrid meta-GGA M06[6] functional was selected on the basis of geometry and energy benchmarks.[7] Structures were fully optimized without any geometry or symmetry constraints, combining the double-z LANL2DZ (on Fe and Ru, including relativistic effects)[8,9] and 6-31+G** (on all other elements)[10,11] basis sets. Vibrational frequencies were computed at the same level of theory to classify all stationary points as either saddle points (transition states, with a single imaginary frequency) or energy minima (reactants, intermediates and products, with only real frequencies). These calculations were also used to obtain the thermochemistry corrections (zero-point, thermal and entropy energies) at the experimental p = 30 atm and T = 373 K conditions. The energy of the optimized geometries was refined by single point calculations with triple-z quality basis sets, including the LANL2TZ[8,9] on Fe and the 6-311+G** on all other elements.[12] The energies reported in the text were obtained by adding the thermochemistry corrections to the refined potential energies. The solvation effects of THF were included in both the geometry optimizations and energy refinements using the continuum SMD model.[13] The ultrafine (99,590) grid was used in all calculations to increase numerical accuracy and to facilitate convergence. Microkinetic models were carried out with the COPASI 4.22 software.[14] A data set collection of input files and computational results is available in the ioChem-BD repository[15] and can be accessed online via https://dx.doi.org/10.19061/iochem-bd-6-14.

The mechanism proposed in Scheme 2 is the result of a thorough mechanistic investigation of the deaminative hydrogenation of DMF by **Fe^{N}**.[7] In this study several mechanisms proposed for the hydrogenation of esters were investigated with fomanilide and DMF. The conclusion of this study was that the mechanism for the hemiaminal C–N bond protonolysis (Step 2 in Scheme 1) depends on the substrate (formanilide or DMF) and the presence of reagents able to assist the proton transfer. In the case of DMF, formanilide could act as a co-catalyst to assist in protonolysis. In contrast, when formanilide is the reactant, the protonolysis is assisted by **Fe^{N}**. This difference originates from the basicity of the $-NMe_2$ group in DMF, which deprotonates formanilide, while NPhH is difficult to protonate but can form an imido intermediate with the Fe-catalyst.

Microkinetic models:

Microkinetic models were constructed to: (1) predict catalytic activity upon using TBD as co-catalyst instead of formanilide, with (^{iPr}PNP)Fe(H)(CO) (**Fe^{N}**) and DMF, and (2) account for the experimental conversions observed with 4-formylmorpholine as substrate.

Microkinetic models were constructed with the COPASI software[14] (version 4.22). Association reactions were assumed to have low energy barriers ($\Delta G^{\ddagger} \leq 5$ kcal mol^{-1}), and thus have no impact on the global kinetics of the reaction. The initial concentrations used in the simulations were those reported in the corresponding experiments[16] (1.4 M of amide, 1mM of catalyst, 0.162 M of hydrogen and 25 mM of co-catalyst). The concentration of hydrogen was kept constant, in line with the effectively constant pressure of hydrogen used in the reactor (30 atm). H_2 concentration was approximated using the molar fraction of H_2 in a saturated solution of H_2 in THF at 33.4 atm and 100 ºC (0.01461 H_2 mol / solution mol) asuming incompresibility of THF and that [H_2] << [THF].[17] As in the experiments, simulations were carried out for a total time of 2 hours at T = 373 K. The models were based on deterministic time course simulations with the LSODA algorithm.[18]

1) DMF with formanilide and TBD as co-catalysts

The DMF conversion *vs* time traces using **Fe^{N}** and formanilide or TBD as co-catalysts were obtained by running a microkinetic model based on the mechanism reported in our previous work[7] (Figure S8). The elementary steps of the mechanism underlying the microkinetic model are given in Figure S9, together with the $\Delta G^{\ddagger}$ values derived from the DFT calculations published in our previous work[7] and presented in Table S2. This model predicts conversions of 12 and 27% for the formanilide and TBD-assisted reactions respectively. The formation of the 1,2-addition adduct with between **Fe^{N}** and the product MeOH (reaction 11) was included in the microkinetic moldel to evaluate the influence of this reaction on DMF conversion. However, the % conversion with and without this reaction were the same, suggesting that the adduct formation with MeOH is not relevant in this process.

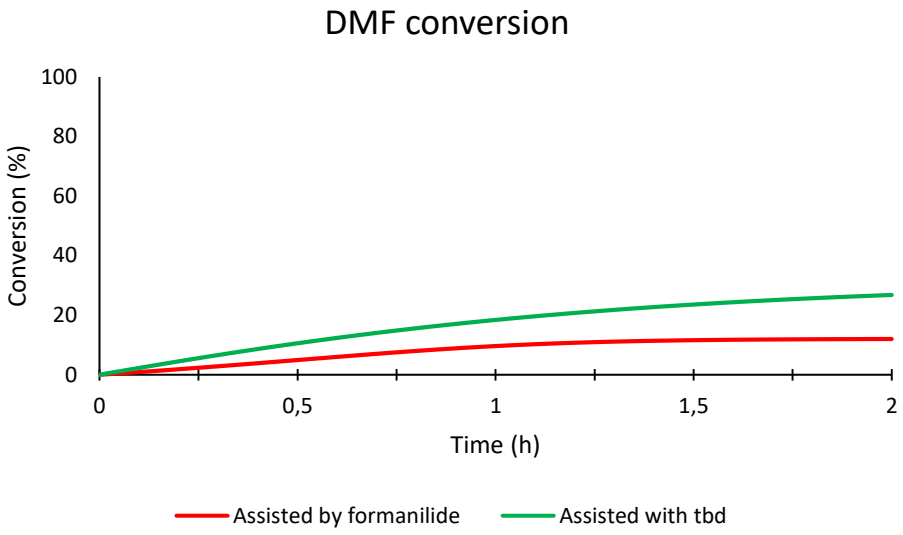


Figure S8: Microkinetic simulations of assisted DMF deaminative hydrogenation.

Reaction 1: $FeH^{NH} + DMF \rightleftharpoons Fe^{NH}DMFH$

Reaction 2: $Fe^{NH}DMFH \rightleftharpoons Hemiaminal^{DMF} + Fe^{N}$

Reaction 3: $Hemiaminal^{DMF} + Formanilide \rightleftharpoons Dimethylamine + Formaldehyde + Formanilide$

Reaction 4: $Formaldehyde + FeH^{NH} \rightleftharpoons Methanol + Fe^{N}$

Reaction 5: $Fe^{N} + Formanilide \rightleftharpoons Adduct^{Formanilide}$

Reaction 6: $Fe^{N} + H_2 + Formanilide \rightleftharpoons FeH^{NH} + Formanilide$

Reaction 7: $Fe^{N} + H_2 \rightleftharpoons FeH^{NH}$

Reaction 8: $Formanilide + FeH^{NH} \rightleftharpoons Aniline + Formaldehyde + Fe^{N}$

Reaction 9: $Hemiaminal^{DMF} + TBD \rightleftharpoons Dimethylamine + Formaldehyde + TBD$

Reaction 10: $Fe^{N} + TBD \rightleftharpoons Adduct^{TBD}$

Reaction 11: $Fe^{N} + Methanol \rightleftharpoons Adduct^{Methanol}$

Figure S9: Implemented reactions in the DMF microkinetic simulations.

	ΔG‡ Forward (kcal mol^{-1})	ΔG‡ Backwards (kcal mol^{-1})
Reaction 1	23.1	0.6
Reaction 2	0.9	2.8
Reaction 3	13.5	10.3
Reaction 4	6.0	11.1
Reaction 5	4.0	16.2
Reaction 6	4.0	14.2
Reaction 7	11.6	21.8
Reaction 8	21.9	6.5
Reaction 9	13.5	10.3
Reaction 10	4.0	5.4
Reaction 11	5.0	11.9

Table S2: Reactions and corresponding Gibbs energies (kcal mol^{-1}) used in the microkinetic model of the deaminative hydrogenation of DMF.

2) 4-formylmorpholine with formanilide and TBD as co-catalyst

The conversions of 4-formylmorpholine *vs* time catalyzed by **Fe^{N}** and using formanilide and TBD as co-catalysts (Figure S10), were obtained by running the microkinetic model shown in Figure S6. In this case, the energies of reactions 1, 2, 3 and 9 were replaced by reactions 12, 13, 14 and 15 (Figure S11), in which 4-formylmorpholine is used instead of DMF (see Table S3). This model predicts conversions of 46 and 56% for the formanilide and TBD-assisted reactions respectively. Experimental conversions of 4-formylmorpholine hydrogenation with 25 eq of formanilide or TBD as co-catalyst could be fitted by correcting the energy of methanol by ± 0.2 kcal mol^{-1}. The similar energies obtained for the reactions 1, 2, 3 and 9 using DMF and 11, 12, 13 and 14 using morpholidine indicate that the same mechanism is expected for the two substrates.

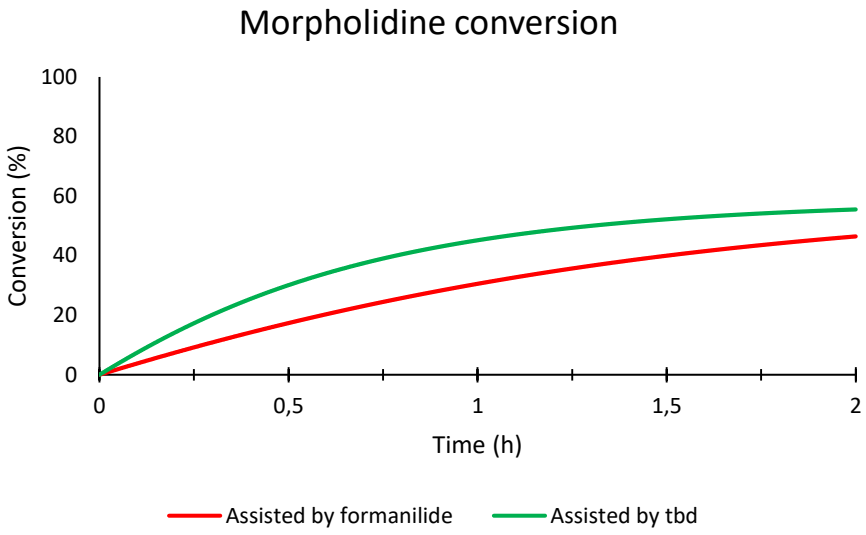


Figure S10: Microkinetic simulations of assisted 4-formylforpholine deaminative hydrogenation

Reaction 12: $\mathbf{FeH^{NH} + Morpholidine \rightleftharpoons Fe^{NH}MorpholidineH}$

Reaction 13: $\mathbf{Fe^{NH}MorpholidineH \rightleftharpoons Hemiaminal^{Morpholidine} + Fe^{N}}$

Reaction 14: $\mathbf{Hemiaminal^{Morpholidine} + Formanilide \rightleftharpoons Morpholine + Formaldehyde + Formanilide}$

Reaction 15: $\mathbf{Hemiaminal^{Morpholidine} + TBD \rightleftharpoons Morpholine + Formaldehyde + TBD}$

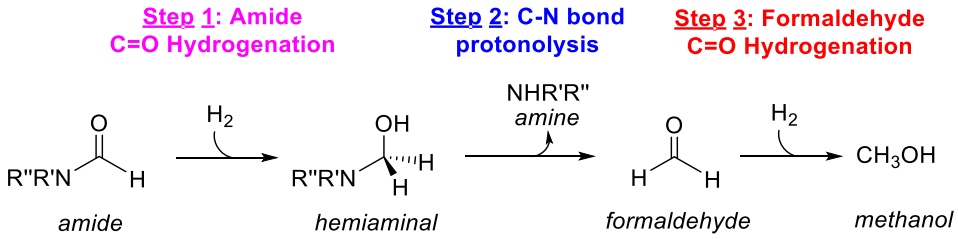
Figure S11: Reactions used together with 4, 5, 6, 7, 8, 10 and 11 to perform the 4-formylmorpholine microkinetic simulations.

	$\Delta G^{\ddagger}$ Forward (kcal mol^{-1})	**$\Delta G^{\ddagger}$ Backwards (kcal mol^{-1})**
Reaction 12	22.5	1.5
Reaction 13	0.5	2.5
Reaction 14	14.6	11.0
Reaction 15	14.6	11.0

Table S3: Reactions and corresponding Gibbs energies (kcal mol^{-1}) used in the microkinetic model of the deaminative hydrogenation of DMF.

Gibbs energies of organic reaction intermediates

The formation of hemiaminal and formaldehyde intermediates from DMF and 4-formylmorpholine is endergonic in both cases by ca 10 kcal/mol (see Figure S12). Therefore their concentration in solution is expected to be very low (eg: 0.1 μM of hemiaminal according to the microkinetic model). This may explain why these species are not observed in the crude ^{1}H NMR spectrum.



DMF	0.0	10.5	13.8	-1.5
Morpholidine	0.0	8.8	12.4	-2.8

Figure S12: Gibbs energies (in kcal mol^{-1}) for the hydrogenation of DMF (R' = Me, R'' = Me) and morpholidine (R'R'' = $O(CH_2)_4$) to amines and methanol calculated in THF solvent (SMD) at 30 atm and 373 K.

Amide influence on $\Delta G_{HT}^{\ddagger}$

The $\Delta G^{\ddagger}_{HT}$ barriers obtained for DMF and 4-formylmorpholine using different co-catalysts were computed to determine the influence of the substrate. As shown in Table S4, similar values were obtained for the three co-catalysts, indicating that DMF can be used as a model for morpholine.

$\Delta G^{\ddagger}_{HT}$ (kcal mol^{-1})	TBD	Triphenylguanidine	Methanol
DMF	21.3	22.3	29.6
4-Formylmorpholine	22.6	21.4	28.1

$\Delta G^{\ddagger}_{HT}$	N-methylformanilide	Formanilide
DMF	25.3	22.6
4-Formylmorpholine	25.4	21.7

Table S4: Comparison between DMF and 4-formylmorpholine of $\Delta G_{HT}^{\ddagger}$ (kcal mol^{-1}).

Cartesian coordinates of optimized geometries, and corresponding corrected Gibbs energies.

Adduct_TBD

Gibbs energy: 1282582.9 kcal mol-1

Atom	X	Y	Z
Fe	0.5940	-0.5199	-0.0708
H	1.4858	-1.6765	0.3536
P	-1.0848	-1.9670	0.1034
P	2.3789	0.7683	0.2391
O	1.3033	-1.3036	-2.7534
N	0.2839	-0.2351	1.9646
C	0.9903	-0.9533	-1.6786
C	-1.6235	-1.7442	1.8602
H	-2.3584	-0.9269	1.8584
H	-2.1127	-2.6340	2.2770
C	-0.4117	-1.3199	2.6667
H	-0.7199	-0.9793	3.6714
H	0.2889	-2.1570	2.8070
C	1.4309	0.2401	2.7450
H	2.1013	-0.6103	2.9366
H	1.0888	0.6111	3.7270
C	2.1441	1.3384	1.9831
H	3.0831	1.6373	2.4674
H	1.4982	2.2270	1.9305
C	-0.7721	-3.8040	-0.0697
H	-1.7698	-4.2671	-0.1480
C	-0.0619	-4.3934	1.1442
H	0.1075	-5.4667	0.9833
H	-0.6340	-4.2896	2.0732
H	0.9221	-3.9266	1.2906
C	0.0310	-4.1287	-1.3251
H	1.0530	-3.7346	-1.2422
H	-0.4078	-3.7228	-2.2426
H	0.1050	-5.2182	-1.4456
C	-2.6632	-1.6669	-0.8481
H	-2.7567	-0.5706	-0.7828
C	-2.5412	-2.0447	-2.3206
H	-2.5768	-3.1343	-2.4583
H	-1.6160	-1.6748	-2.7799
H	-3.3834	-1.6209	-2.8848
C	-3.9040	-2.3051	-0.2350
H	-4.7819	-2.0807	-0.8571
H	-4.1181	-1.9339	0.7740
H	-3.8180	-3.3997	-0.1830
C	4.0936	0.0187	0.1930
H	4.7904	0.8726	0.1714
C	4.4048	-0.8209	1.4268
H	3.7044	-1.6628	1.5198
H	4.3777	-0.2441	2.3585
H	5.4142	-1.2449	1.3354
C	4.3034	-0.8299	-1.0571
H	4.0926	-0.2945	-1.9887
H	3.6604	-1.7203	-1.0311
C	2.5558	2.3825	-0.6831
H	1.5178	2.7534	-0.6920
C	3.4378	3.4082	0.0199
H	4.4681	3.0452	0.1423
H	3.0583	3.6900	1.0082
H	3.4905	4.3262	-0.5819
C	3.0190	2.1911	-2.1238
H	2.8630	3.1177	-2.6926
H	2.4835	1.3882	-2.6455
H	4.0933	1.9637	-2.1678
H	-0.4105	0.5590	1.8817
C	-2.6659	2.1039	2.3391
C	-1.6413	1.7654	0.1663
C	-3.8882	2.7481	0.3278
C	-3.5371	3.1861	1.7307
H	-3.3210	1.2446	2.5999
C	-2.8473	2.5124	-1.8731
H	-4.4717	3.5158	-0.1983
H	-4.4448	3.3477	2.3269
C	-1.4846	2.5653	-2.5123
C	-0.7077	1.3593	-2.0280
H	-3.3967	1.6132	-2.2228
H	-1.5590	2.5511	-3.6073
H	0.3298	1.4347	-2.3850
H	-0.9805	3.4997	-2.2211
H	-1.1269	0.4667	-2.5327
H	-2.9897	4.1389	1.6836
H	-2.2471	2.4493	3.2977
H	-4.5180	1.8341	0.3640
H	-3.4605	3.3847	-2.1407
N	-1.5812	1.6696	1.4894
N	-2.6759	2.5117	-0.4354
N	-0.6972	1.1640	-0.5851
H	5.3453	-1.1758	-1.0999

Adduct_formanilide_NO

Gibbs energy: -1258884.8 kcal mol-1

Atom	X	Y	Z
Fe	-0.9100	0.5424	-0.0395
H	-1.8600	1.2675	0.8830
P	0.4910	2.2615	0.1696
P	-2.1769	-1.2724	0.1700
O	-2.4294	1.6871	-2.2094
O	0.4032	-0.4718	-1.3312
N	0.0493	-0.1752	1.6713
H	0.8174	-0.7189	1.2358
N	1.9876	-1.4871	-0.0108

C	-1.8008	1.2138	-1.3438
C	1.4984	1.7964	1.6574
H	2.3943	1.2707	1.2960
H	1.8361	2.6731	2.2252
C	0.6637	0.8652	2.5143
H	1.2805	0.3982	3.2996
H	-0.1481	1.4116	3.0154
C	-0.7433	-1.1060	2.4941
H	-1.4945	-0.5154	3.0369
H	-0.0959	-1.5858	3.2469
C	-1.4034	-2.1463	1.6115
H	-2.1265	-2.7521	2.1732
H	-0.6436	-2.8300	1.2051
C	-0.1177	3.9761	0.5741
H	0.7886	4.5963	0.6578
C	-0.8495	4.0178	1.9103
H	-1.1915	5.0425	2.1092
H	-0.2151	3.7166	2.7526
H	-1.7356	3.3686	1.8995
C	-1.0084	4.5327	-0.5287
H	-1.9343	3.9488	-0.6143
H	-0.5233	4.5407	-1.5118
H	-1.2939	5.5669	-0.2937
C	1.8019	2.4702	-1.1441
H	2.3958	1.5509	-1.0089
C	1.2380	2.4445	-2.5595
H	0.6033	3.3157	-2.7677
H	0.6499	1.5366	-2.7351
H	2.0617	2.4634	-3.2866
C	2.7164	3.6682	-0.9224
H	3.5647	3.6230	-1.6188
H	3.1282	3.7051	0.0947
H	2.1932	4.6153	-1.1123
C	-3.9786	-1.1570	0.6313
H	-4.3413	-2.1962	0.6724
C	-4.1746	-0.5277	2.0056
H	-3.7733	0.4946	2.0359
H	-3.7044	-1.1061	2.8097
H	-5.2480	-0.4683	2.2310
C	-4.7738	-0.3846	-0.4136
H	-5.8393	-0.3830	-0.1471
H	-4.6863	-0.8073	-1.4214
H	-4.4439	0.6619	-0.4570
C	-2.0550	-2.5604	-1.1743
H	-0.9956	-2.8522	-1.0927
C	-2.9195	-3.7910	-0.9330
H	-3.9858	-3.5690	-1.0765
H	-2.7917	-4.2085	0.0742
H	-2.6556	-4.5789	-1.6515
C	-2.2617	-1.9912	-2.5720
H	-2.0641	-2.7699	-3.3216
H	-1.5789	-1.1563	-2.7639
H	-3.2909	-1.6439	-2.7319
C	1.4809	-1.1082	-1.1627
H	2.0194	-1.3901	-2.0957
C	3.2560	-2.0601	0.0075
C	3.5077	-3.1205	0.8969
H	2.6859	-3.4776	1.5184
C	4.7655	-3.7068	0.9775
H	4.9303	-4.5302	1.6709
C	5.8143	-3.2489	0.1766
H	6.7992	-3.7062	0.2420
C	5.5841	-2.1875	-0.6972
H	6.3957	-1.8064	-1.3154
C	4.3268	-1.5923	-0.7781
H	4.1729	-0.7389	-1.4383

Adduct_Methyl_formanilide_NO

Gibbs energy: -1283527.4 kcal mol-1

Atom	X	Y	Z
Fe	-1.0267	0.2246	-0.0395
H	-2.1250	0.5775	0.9377
P	-0.2053	2.2751	0.2239
P	-1.6467	-1.9067	0.0831
O	-2.9019	0.9441	-2.1113
O	0.4828	-0.3005	-1.3927
N	0.1587	-0.2332	1.6131
H	1.0401	-0.4791	1.1197
N	2.3326	-0.7482	-0.1547
C	-2.1254	0.6459	-1.2882
C	0.9302	2.0877	1.6806
H	1.9382	1.8880	1.2891
H	0.9854	3.0020	2.2858
C	0.4490	0.9058	2.4999
H	1.2049	0.6169	3.2490
H	-0.4749	1.1525	3.0428
C	-0.2674	-1.4061	2.3943
H	-1.1475	-1.1143	2.9849
H	0.5260	-1.6922	3.1054
C	-0.5946	-2.5588	1.4655
H	-1.0740	-3.3872	2.0037
H	0.3285	-2.9498	1.0127
C	-1.2837	3.7183	0.7018
H	-0.5964	4.5715	0.8158
C	-1.9799	3.4838	2.0371
H	-2.5920	4.3599	2.2907
H	-1.2759	3.3279	2.8636
H	-2.6491	2.6140	1.9895
C	-2.3116	4.0377	-0.3757
H	-3.0163	3.2052	-0.5021
H	-1.8600	4.2471	-1.3525
H	-2.8960	4.9215	-0.0862
C	0.9517	2.9025	-1.1010
H	1.7874	2.1881	-1.0127
C	0.3818	2.7630	-2.5077
H	-0.4818	3.4204	-2.6730
H	0.0749	1.7297	-2.7077

H	1.1464	3.0419	-3.2464
C	1.4886	4.3044	-0.8427
H	2.2970	4.5317	-1.5510
H	1.8966	4.4211	0.1698
H	0.7116	5.0677	-0.9851
C	-3.3764	-2.4004	0.5687
H	-3.3828	-3.5019	0.5727
C	-3.7302	-1.9159	1.9696
H	-3.6807	-0.8205	2.0359
H	-3.0760	-2.3366	2.7425
H	-4.7584	-2.2165	2.2127
C	-4.4029	-1.8915	-0.4353
H	-5.4054	-2.2445	-0.1582
H	-4.2065	-2.2280	-1.4602
H	-4.4304	-0.7936	-0.4401
C	-1.1579	-3.0176	-1.3356
H	-0.0585	-2.9759	-1.2698
C	-1.6017	-4.4651	-1.1684
H	-2.6872	-4.5714	-1.2989
H	-1.3355	-4.8796	-0.1874
H	-1.1227	-5.0932	-1.9317
C	-1.5494	-2.4601	-2.6987
H	-1.1345	-3.0981	-3.4917
H	-1.1551	-1.4470	-2.8368
H	-2.6379	-2.4354	-2.8411
C	1.7159	-0.6018	-1.3114
C	3.7048	-0.8784	-0.0088
C	4.2015	-1.8504	0.8808
H	3.4863	-2.5111	1.3726
C	5.5645	-1.9730	1.1278
H	5.9181	-2.7403	1.8149
C	6.4782	-1.1207	0.5047
H	7.5442	-1.2145	0.7007
C	6.0010	-0.1387	-0.3634
H	6.6980	0.5446	-0.8467
C	4.6371	-0.0121	-0.6142
H	4.2778	0.7758	-1.2762
C	2.3784	-0.8376	-2.6506
H	2.5055	0.1176	-3.1779
H	3.3540	-1.3276	-2.5795
H	1.7064	-1.4512	-3.2628

Adduct_Methyl_iPrPhenol

Gibbs energy: -1372745.1 kcal mol-1

Atom	X	Y	Z
Fe	-0.7187	0.5612	-0.0998
H	-1.6852	1.6852	-0.3260
P	0.7839	2.1549	-0.4535
P	-2.5105	-0.5756	0.5760
O	-1.0621	-0.0316	-2.9000
N	-0.5575	1.1348	1.8955
H	0.1845	0.4464	2.0738
C	-0.8964	0.1747	-1.7587
C	1.0963	2.8576	1.2402
H	2.0298	2.4178	1.6157
H	1.2514	3.9438	1.2093
C	-0.0686	2.5044	2.1465
H	0.2125	2.6164	3.2070
H	-0.9162	3.1794	1.9606
C	-1.6904	0.8253	2.7888
H	-2.4166	1.6422	2.6901
H	-1.3495	0.8194	3.8370
C	-2.3166	-0.5015	2.4157
H	-3.2579	-0.6669	2.9563
H	-1.6340	-1.3248	2.6729
C	0.2991	3.6616	-1.4445
H	1.1968	4.3004	-1.4518
C	-0.8353	4.4435	-0.7918
H	-1.0506	5.3402	-1.3887
H	-0.6002	4.7793	0.2252
H	-1.7568	3.8460	-0.7502
C	-0.0805	3.3102	-2.8775
H	-0.9913	2.6968	-2.8989
H	0.7049	2.7635	-3.4122
H	-0.2884	4.2281	-3.4438
C	2.5111	1.7061	-0.9981
H	2.8293	1.0532	-0.1686
C	2.5436	0.8583	-2.2634
H	2.2715	1.4351	-3.1568
H	1.8711	-0.0052	-2.1921
H	3.5594	0.4697	-2.4217
C	3.4738	2.8827	-1.0891
H	4.5006	2.5126	-1.2167
H	3.4627	3.5148	-0.1915
H	3.2501	3.5204	-1.9555
C	-4.2079	0.1119	0.1969
H	-4.9175	-0.6994	0.4272
C	-4.5667	1.3190	1.0556
H	-3.8572	2.1445	0.8975
H	-4.5999	1.0886	2.1269
H	-5.5614	1.6876	0.7705
C	-4.3376	0.4840	-1.2776
H	-5.3704	0.7900	-1.4931
H	-4.0870	-0.3368	-1.9577
H	-3.6810	1.3309	-1.5217
C	-2.6685	-2.4083	0.2795
H	-1.6348	-2.7523	0.4420
C	-3.5863	-3.1231	1.2649
H	-4.6208	-2.7576	1.2010
H	-3.2553	-3.0226	2.3046
H	-3.6096	-4.1970	1.0325
C	-3.0731	-2.7331	-1.1540
H	-2.9744	-3.8124	-1.3332
H	-2.4574	-2.2145	-1.8999
H	-4.1245	-2.4745	-1.3403
C	4.2222	-2.6481	-0.4347
C	4.1104	-1.7805	0.6576

C	2.8957	-1.2194	1.0462
C	1.6967	-1.5093	0.3162
C	1.8033	-2.4259	-0.7679
C	3.0478	-2.9587	-1.1177
H	5.0153	-1.5394	1.2202
H	3.1046	-3.6582	-1.9559
C	0.5569	-2.9003	-1.4799
C	2.7952	-0.3238	2.2598
O	0.5538	-0.9755	0.6861
C	0.1679	-4.2935	-0.9786
H	-0.7737	-4.6354	-1.4324
H	0.9453	-5.0283	-1.2346
H	0.0483	-4.3106	0.1134
C	0.6774	-2.9091	-3.0006
H	0.9857	-1.9309	-3.3914
H	1.4069	-3.6549	-3.3468
H	-0.2866	-3.1633	-3.4637
C	4.0913	0.3700	2.6568
H	3.9026	1.0900	3.4649
H	4.8429	-0.3398	3.0292
H	4.5391	0.9190	1.8159
C	2.2077	-1.0782	3.4544
H	2.0098	-0.3978	4.2965
H	1.2664	-1.5742	3.1846
H	2.9084	-1.8504	3.8038
H	2.0797	0.4653	1.9964
H	-0.2454	-2.2035	-1.2006
C	5.5485	-3.2370	-0.8235
H	6.3067	-2.4614	-0.9994
H	5.9510	-3.8979	-0.0428
H	5.4665	-3.8296	-1.7427

Adduct_Methyl_tBuPhenol

Gibbs energy: -1422003.0 kcal mol-1

Atom	X	Y	Z
Fe	-1.0818	0.0115	-0.0495
H	-2.5450	0.0552	0.1645
P	-1.3234	2.2430	0.1100
P	-1.4201	-2.1877	0.2872
O	-1.7888	-0.0896	-2.8457
N	-0.8030	0.0887	1.9957
H	0.2232	0.0956	1.9161
C	-1.4473	-0.0490	-1.7295
C	-0.9459	2.5601	1.8928
H	0.1221	2.8012	1.9523
H	-1.4913	3.4287	2.2839
C	-1.2560	1.3143	2.6906
H	-0.8005	1.3633	3.6931
H	-2.3402	1.2128	2.8334
C	-1.2270	-1.0849	2.7926
H	-2.3009	-0.9643	2.9842
H	-0.7218	-1.0701	3.7716
C	-0.9693	-2.3867	2.0688
H	-1.5085	-3.2158	2.5454
H	0.0980	-2.6418	2.0919
C	-3.0500	2.9234	-0.1359
H	-2.9250	4.0179	-0.1677
C	-3.9907	2.5838	1.0152
H	-4.9853	3.0002	0.8061
H	-3.6642	2.9925	1.9781
H	-4.1105	1.4961	1.1219
C	-3.6727	2.4528	-1.4462
H	-3.8886	1.3768	-1.4058
H	-3.0408	2.6312	-2.3221
H	-4.6255	2.9738	-1.6101
C	-0.2140	3.4859	-0.7392
H	0.7803	3.0160	-0.6572
C	-0.5573	3.6616	-2.2147
H	-1.4675	4.2642	-2.3362
H	-0.7042	2.7113	-2.7400
H	0.2547	4.1983	-2.7230
C	-0.1668	4.8479	-0.0533
H	0.4936	5.5167	-0.6221
H	0.2229	4.8026	0.9692
H	-1.1560	5.3255	-0.0220
C	-3.1885	-2.7885	0.1625
H	-3.1243	-3.8879	0.1995
C	-4.0563	-2.3241	1.3266
H	-4.1159	-1.2268	1.3662
H	-3.7045	-2.6880	2.2987
H	-5.0794	-2.7003	1.1911
C	-3.8413	-2.3720	-1.1513
H	-4.8273	-2.8472	-1.2415
H	-3.2583	-2.6472	-2.0361
H	-3.9955	-1.2850	-1.1780
C	-0.4192	-3.5548	-0.5033
H	0.6055	-3.1492	-0.4770
C	-0.4395	-4.8661	0.2763
H	-1.4552	-5.2756	0.3662
H	-0.0191	-4.7743	1.2835
H	0.1614	-5.6145	-0.2581
C	-0.8159	-3.8063	-1.9545
H	-0.0542	-4.4266	-2.4453
H	-0.9195	-2.8858	-2.5398
H	-1.7648	-4.3569	-2.0112
C	5.5069	-0.2178	-0.5628
C	4.9822	-0.0952	0.7191
C	3.6134	-0.0133	0.9850
C	2.6438	-0.0703	-0.0968
C	3.2028	-0.1705	-1.4317
C	4.5868	-0.2466	-1.6074
H	5.6885	-0.0617	1.5479
H	4.9885	-0.3323	-2.6161
C	2.3146	-0.1984	-2.6787
C	3.1626	0.1352	2.4413
O	1.3583	-0.0324	0.1507
C	1.4819	1.0831	-2.7409

H	0.8356	1.0840	-3.6311
H	0.8541	1.1742	-1.8505
H	2.1387	1.9642	-2.7998
C	3.0993	-0.2755	-3.9920
H	2.3858	-0.2787	-4.8276
H	3.7653	0.5863	-4.1358
H	3.6996	-1.1918	-4.0745
C	1.4049	-1.4262	-2.6352
H	2.0061	-2.3478	-2.6106
H	0.7709	-1.3984	-1.7448
H	0.7629	-1.4660	-3.5276
C	2.3339	-1.0930	2.8367
H	1.8204	-0.9431	3.7998
H	1.5991	-1.3249	2.0621
H	2.9888	-1.9696	2.9406
C	4.3116	0.2222	3.4490
H	4.9682	1.0825	3.2632
H	3.8882	0.3458	4.4562
H	4.9292	-0.6856	3.4658
C	2.3705	1.4407	2.5839
H	1.8567	1.4982	3.5566
H	3.0502	2.3018	2.5153
H	1.6388	1.5359	1.7778
C	6.9863	-0.2762	-0.8170
H	7.2402	-1.0218	-1.5827
H	7.3881	0.6855	-1.1692
H	7.5390	-0.5394	0.0939

Adduct_Methanol

Gibbs energy: -1080023.3 kcal mol-1

Atom	X	Y	Z
C	-2.4442	-1.2258	-1.6870
H	-3.3732	-1.7987	-1.5734
H	-2.5056	-0.6825	-2.6411
C	-1.2242	-2.1228	-1.6958
H	-1.1991	-2.7730	-0.8109
H	-1.2196	-2.7753	-2.5841
C	1.2084	-2.1174	-1.7064
H	1.1989	-2.7699	-2.5947
H	1.1939	-2.7677	-0.8213
C	2.4243	-1.2149	-1.7082
H	2.4749	-0.6713	-2.6628
H	3.3568	-1.7836	-1.6027
C	-3.2452	1.4627	-1.0455
H	-2.6409	1.7687	-1.9149
C	-3.3453	2.6418	-0.0842
H	-3.7390	3.5209	-0.6124
H	-2.3781	2.9221	0.3498
H	-4.0387	2.4249	0.7402
C	-4.6333	1.0535	-1.5252
H	-5.2587	0.6882	-0.6988
H	-4.6090	0.2777	-2.2991
H	-5.1481	1.9242	-1.9548
C	-3.1664	-0.5735	1.1094
H	-4.2324	-0.4160	0.8773
C	-2.8050	0.2084	2.3686
H	-3.4294	-0.1263	3.2082
H	-2.9452	1.2897	2.2622
H	-1.7561	0.0326	2.6435
C	-2.9373	-2.0613	1.3491
H	-1.8745	-2.2700	1.5353
H	-3.2720	-2.6871	0.5134
H	-3.4949	-2.3814	2.2399
C	3.2191	1.4771	-1.0733
H	2.6060	1.7807	-1.9373
C	4.6047	1.0739	-1.5654
H	5.1122	1.9472	-1.9984
H	4.5768	0.2989	-2.3400
H	5.2387	0.7102	-0.7448
C	3.3227	2.6563	-0.1125
H	4.0245	2.4422	0.7055
H	2.3583	2.9320	0.3304
H	3.7075	3.5373	-0.6439
C	3.1677	-0.5596	1.0820
H	4.2310	-0.3978	0.8407
C	2.9468	-2.0483	1.3238
H	3.5136	-2.3662	2.2095
H	3.2765	-2.6727	0.4851
H	1.8866	-2.2613	1.5194
C	2.8142	0.2209	2.3444
H	1.7685	0.0409	2.6285
H	2.9492	1.3027	2.2366
H	3.4473	-0.1113	3.1784
C	-0.0052	1.5577	0.8289
N	-0.0096	-1.2932	-1.6679
O	-0.0037	2.4390	1.6039
P	-2.2187	0.0604	-0.3703
P	2.2046	0.0702	-0.3894
H	-0.0146	-0.6663	-2.4839
O	-0.0168	1.2694	-2.0724
C	-0.0196	2.6397	-2.0987
H	0.8649	3.1081	-1.6075
H	-0.0228	3.0214	-3.1417
H	-0.9037	3.1045	-1.6033
H	-0.0001	-0.7385	0.8566
Fe	-0.0072	0.2746	-0.2975

Adduct_Methyl_MePhenol

Gibbs energy: -1274188.5 kcal mol-1

Atom	X	Y	Z
Fe	0.1812	0.4735	-0.2215
H	1.0027	1.6489	-0.6841
P	2.1453	-0.5681	-0.0443
P	-1.5532	1.8633	-0.1008

O	-0.1408	-0.0191	-3.0415
N	0.5374	1.0590	1.7444
H	0.0042	0.2647	2.1200
C	-0.0367	0.1309	-1.8833
C	2.5693	-0.3056	1.7406
H	2.1388	-1.1603	2.2831
H	3.6507	-0.3160	1.9276
C	1.9303	0.9845	2.2140
H	1.9640	1.0591	3.3137
H	2.4599	1.8592	1.8115
C	-0.1143	2.3029	2.1877
H	0.4651	3.1437	1.7817
H	-0.0770	2.3778	3.2869
C	-1.5455	2.3306	1.6917
H	-2.0264	3.2977	1.8857
H	-2.1320	1.5592	2.2118
C	3.6104	0.0986	-0.9942
H	4.4035	-0.6586	-0.8815
C	4.1206	1.4188	-0.4278
H	4.9644	1.7760	-1.0338
H	4.4763	1.3356	0.6059
H	3.3410	2.1929	-0.4660
C	3.2900	0.2712	-2.4756
H	2.5493	1.0693	-2.6203
H	2.8962	-0.6368	-2.9448
H	4.1988	0.5603	-3.0205
C	2.2732	-2.4233	-0.1952
H	1.3986	-2.7581	0.3849
C	2.0995	-2.9101	-1.6288
H	2.9998	-2.7182	-2.2290
H	1.2458	-2.4417	-2.1344
H	1.9320	-3.9959	-1.6341
C	3.5259	-3.0255	0.4294
H	3.4912	-4.1197	0.3329
H	3.6198	-2.7989	1.4978
H	4.4421	-2.6860	-0.0735
C	-1.5423	3.4750	-1.0420
H	-2.5704	3.8675	-0.9771
C	-0.5934	4.4995	-0.4298
H	0.4418	4.1292	-0.4279
H	-0.8629	4.7777	0.5958
H	-0.6089	5.4186	-1.0310
C	-1.1797	3.2578	-2.5080
H	-1.2599	4.2070	-3.0549
H	-1.8242	2.5289	-3.0112
H	-0.1428	2.9062	-2.6009
C	-3.2605	1.1557	-0.3146
H	-3.1679	0.2176	0.2560
C	-4.3700	2.0097	0.2871
H	-4.4555	2.9835	-0.2152
H	-4.2339	2.1924	1.3592
H	-5.3361	1.5009	0.1642
C	-3.5754	0.8093	-1.7649
H	-4.4840	0.1936	-1.8113
H	-2.7692	0.2462	-2.2510
H	-3.7689	1.7127	-2.3598
C	-0.7295	-5.0194	1.5521
C	-0.5492	-4.0894	2.5784
C	-0.6778	-2.7126	2.3765
C	-0.9692	-2.2034	1.0781
C	-1.2546	-3.1525	0.0548
C	-1.1106	-4.5171	0.3030
H	-0.3144	-4.4485	3.5843
H	-1.3215	-5.2193	-0.5088
C	-1.7371	-2.6691	-1.2757
H	-2.1042	-3.5016	-1.8885
H	-2.5496	-1.9381	-1.1579
H	-0.9517	-2.1561	-1.8450
C	-0.5491	-1.7736	3.5407
H	0.4120	-1.2372	3.5654
H	-1.3379	-1.0080	3.5270
H	-0.6254	-2.3181	4.4899
C	-0.5520	-6.4934	1.7800
H	0.4062	-6.8618	1.3859
H	-0.5751	-6.7384	2.8491
H	-1.3406	-7.0782	1.2884
O	-1.0394	-0.9111	0.8649

Adduct_triphenylguanidine

Gibbs energy: -1570837.6 kcal mol-1

Atom	X	Y	Z
Fe	-1.6473	-0.3424	-0.0023
H	-2.8805	-1.1373	-0.3404
P	-0.9971	-2.2420	0.9853
P	-2.5022	1.1459	-1.4290
O	-3.2715	0.5586	2.2022
N	-0.8282	-1.2053	-1.7220
H	0.1360	-0.8221	-1.6355
C	-2.5609	0.2265	1.3328
C	-0.0958	-3.1098	-0.3792
H	0.9529	-2.7848	-0.3330
H	-0.1039	-4.2013	-0.2643
C	-0.6998	-2.6716	-1.6964
H	-0.0727	-3.0082	-2.5397
H	-1.7004	-3.1031	-1.8413
C	-1.3680	-0.7667	-3.0177
H	-2.2976	-1.3211	-3.2057
H	-0.6631	-1.0342	-3.8231
C	-1.6192	0.7255	-2.9992
H	-2.1537	1.0593	-3.8984
H	-0.6597	1.2646	-2.9598
C	-2.2844	-3.4799	1.5475
H	-1.7311	-4.2208	2.1482
C	-2.9489	-4.2071	0.3829
H	-3.7010	-4.9059	0.7732
H	-2.2471	-4.7917	-0.2224
H	-3.4723	-3.5009	-0.2772

C	-3.3658	-2.8389	2.4114
H	-3.9856	-2.1595	1.8109
H	-2.9724	-2.2688	3.2590
H	-4.0274	-3.6186	2.8128
C	0.2656	-2.2205	2.3651
H	0.9204	-1.3817	2.0739
C	-0.3531	-1.8970	3.7210
H	-0.8991	-2.7613	4.1224
H	-1.0489	-1.0499	3.6900
H	0.4373	-1.6504	4.4424
C	1.1036	-3.4908	2.4667
H	1.8252	-3.3931	3.2899
H	1.6760	-3.7034	1.5565
H	0.4811	-4.3695	2.6868
C	-4.3256	1.0520	-1.8377
H	-4.5419	1.9680	-2.4108
C	-4.6840	-0.1472	-2.7074
H	-4.4391	-1.0932	-2.2032
H	-4.1837	-0.1334	-3.6825
H	-5.7662	-0.1497	-2.8964
C	-5.1845	1.0393	-0.5775
H	-6.2460	1.1024	-0.8526
H	-4.9684	1.8678	0.1059
H	-5.0422	0.1027	-0.0220
C	-2.1536	2.9717	-1.2822
H	-1.0636	2.9766	-1.1265
C	-2.4626	3.7769	-2.5392
H	-3.5403	3.8122	-2.7485
H	-1.9560	3.3881	-3.4302
H	-2.1296	4.8149	-2.4016
C	-2.8092	3.6054	-0.0618
H	-2.4125	4.6185	0.0909
H	-2.6277	3.0371	0.8592
H	-3.8949	3.7027	-0.1978
N	1.7029	-0.2865	-1.0704
C	1.4861	0.4396	0.0174
C	2.8066	-1.0955	-1.2700
C	3.1984	-1.3397	-2.6016
H	2.6395	-0.8438	-3.3968
C	4.2765	-2.1649	-2.9021
H	4.5597	-2.3183	-3.9426
C	4.9948	-2.7920	-1.8829
H	5.8420	-3.4337	-2.1150
C	4.5982	-2.5893	-0.5599
H	5.1345	-3.0839	0.2491
C	3.5199	-1.7652	-0.2524
H	3.2316	-1.6232	0.7887
N	2.5540	0.8859	0.8107
H	2.3207	1.1083	1.7724
C	3.8373	1.2710	0.4186
C	4.8265	1.3509	1.4095
C	4.1745	1.5932	-0.9030
C	6.1237	1.7314	1.0854
H	4.5656	1.1015	2.4379
C	5.4803	1.9580	-1.2181
H	3.4197	1.5477	-1.6844
C	6.4651	2.0285	-0.2338
H	6.8758	1.7848	1.8705
H	5.7259	2.1961	-2.2516
H	7.4828	2.3135	-0.4907
N	0.2453	0.7570	0.4162
C	0.1615	1.8947	1.2545
C	-0.3106	1.8054	2.5694
C	0.5763	3.1576	0.7938
C	-0.3970	2.9339	3.3835
H	-0.6047	0.8328	2.9557
C	0.4975	4.2830	1.6066
H	0.9764	3.2428	-0.2175
C	0.0007	4.1814	2.9074
H	-0.7715	2.8316	4.4007
H	0.8248	5.2473	1.2208
H	-0.0679	5.0623	3.5422

Adduct_urea_ON

Gibbs energy: -1148756.2 kcal mol-1

Atom	X	Y	Z
Fe	-0.0332	-0.2203	-0.1650
H	0.0271	-1.7245	0.0841
P	-2.2358	-0.3711	0.0487
P	2.1780	-0.2134	0.0596
O	0.0084	-0.8035	-2.9884
N	-0.0326	0.0055	1.9146
C	-0.0106	-0.5523	-1.8429
C	-2.4830	0.0081	1.8468
H	-2.5885	1.0999	1.9305
H	-3.3970	-0.4437	2.2543
C	-1.2511	-0.4547	2.5991
H	-1.2636	-0.0856	3.6378
H	-1.2119	-1.5520	2.6448
C	1.1681	-0.5245	2.5827
H	1.1180	-1.6219	2.5395
H	1.1660	-0.2360	3.6472
C	2.4122	-0.0055	1.8887
H	3.3187	-0.5046	2.2547
H	2.5192	1.0715	2.0778
C	-3.1215	-1.9931	-0.2075
H	-4.1922	-1.7777	-0.0671
C	-2.7124	-3.0469	0.8146
H	-3.2304	-3.9903	0.5943
H	-2.9727	-2.7658	1.8420
H	-1.6324	-3.2454	0.7729
C	-2.8930	-2.5216	-1.6185
H	-1.8329	-2.7637	-1.7734
H	-3.1907	-1.8106	-2.3981
H	-3.4698	-3.4432	-1.7740
C	-3.3098	0.9247	-0.7623
H	-2.9335	1.8393	-0.2781

C	-3.0694	1.0692	-2.2598
H	-3.4478	0.2063	-2.8232
H	-2.0067	1.1860	-2.5005
H	-3.5981	1.9551	-2.6375
C	-4.7968	0.7868	-0.4606
H	-5.3312	1.6847	-0.8000
H	-5.0058	0.6663	0.6100
H	-5.2376	-0.0680	-0.9917
C	3.2014	-1.7218	-0.3407
H	4.2419	-1.4359	-0.1197
C	2.8400	-2.9121	0.5397
H	1.7935	-3.2121	0.3932
H	2.9942	-2.7159	1.6076
H	3.4715	-3.7703	0.2723
C	3.0856	-2.1088	-1.8096
H	3.3382	-1.2896	-2.4932
H	2.0648	-2.4384	-2.0444
C	3.1353	1.2453	-0.6084
H	2.7077	2.0691	-0.0147
C	4.6334	1.1821	-0.3384
H	5.1246	0.4260	-0.9663
H	4.8668	0.9547	0.7100
H	5.0979	2.1490	-0.5755
C	2.8515	1.5462	-2.0745
H	3.3147	2.5030	-2.3528
H	1.7767	1.6261	-2.2732
H	3.2650	0.7797	-2.7430
H	0.0215	1.0393	1.9759
H	3.7615	-2.9456	-2.0322
C	0.2181	2.8521	0.4190
N	-0.1453	1.8409	-0.3631
O	0.4294	2.7656	1.6593
N	0.4409	4.1053	-0.1762
H	-0.0196	4.2865	-1.0599
H	0.3735	4.8768	0.4761
H	-0.2500	2.1428	-1.3274

Adduct_formanilide_ON

Gibbs energy: -1258883.3 kcal mol-1

Atom	X	Y	Z
Fe	0.3323	0.3156	0.0023
H	0.9454	1.6116	-0.4493
P	2.4669	-0.3408	-0.0002
P	-1.4960	1.5804	0.2092
O	-0.0302	-0.1553	-2.8163
O	0.6985	-1.6647	2.7861
N	0.7807	0.9878	1.9470
H	0.6076	0.1114	2.4616
N	-0.5455	-1.4884	0.8391
C	0.0931	-0.0117	-1.6597
C	3.0814	0.1794	1.6690
H	2.9809	-0.6919	2.3283
H	4.1388	0.4729	1.6502
C	2.2039	1.3086	2.1676
H	2.3834	1.4968	3.2393
H	2.4198	2.2435	1.6310
C	-0.0636	2.0636	2.4967
H	0.3594	3.0191	2.1602
H	-0.0082	2.0591	3.5967
C	-1.4954	1.9305	2.0259
H	-2.0863	2.8155	2.2971
H	-1.9723	1.0545	2.4942
C	3.6759	0.4833	-1.1649
H	4.6417	-0.0028	-0.9549
C	3.8343	1.9751	-0.8949
H	4.5744	2.3942	-1.5903
H	4.1833	2.1953	0.1208
H	2.8897	2.5133	-1.0574
C	3.3154	0.2661	-2.6290
H	2.4010	0.8150	-2.8900
H	3.1567	-0.7879	-2.8851
H	4.1210	0.6454	-3.2722
C	2.9227	-2.1526	-0.0099
H	2.4212	-2.4923	0.9100
C	2.3298	-2.9288	-1.1780
H	2.8302	-2.6906	-2.1257
H	1.2588	-2.7339	-1.2999
H	2.4536	-4.0074	-1.0112
C	4.4163	-2.4255	0.1194
H	4.5834	-3.4939	0.3132
H	4.8853	-1.8669	0.9391
H	4.9512	-2.1814	-0.8087
C	-1.5044	3.2415	-0.6542
H	-2.5438	3.6001	-0.5901
C	-0.6078	4.2793	0.0095
H	0.4439	3.9580	0.0087
H	-0.9030	4.5045	1.0411
H	-0.6600	5.2199	-0.5558
C	-1.1207	3.1045	-2.1247
H	-1.2610	4.0671	-2.6351
H	-1.7127	2.3547	-2.6611
H	-0.0620	2.8276	-2.2250
C	-3.2338	0.9431	-0.0348
H	-3.2211	0.0107	0.5489
C	-4.3253	1.8430	0.5337
H	-4.3954	2.7980	-0.0044
H	-4.1888	2.0618	1.5992
H	-5.2990	1.3452	0.4261
C	-3.5344	0.5861	-1.4853
H	-4.4825	0.0344	-1.5447
H	-2.7570	-0.0443	-1.9342
H	-3.6470	1.4870	-2.1042
C	-0.1670	-2.0705	1.9792
H	-0.6783	-3.0323	2.2108
C	-1.6501	-2.1343	0.2344
C	-1.6230	-2.5436	-1.1059
H	-0.7321	-2.3623	-1.7000

C	-2.7106	-3.1919	-1.6837
H	-2.6531	-3.5015	-2.7260
C	-3.8620	-3.4508	-0.9404
H	-4.7118	-3.9551	-1.3957
C	-3.9070	-3.0506	0.3937
H	-4.7981	-3.2371	0.9911
C	-2.8186	-2.3996	0.9707
H	-2.8759	-2.0638	2.0067

Adduct_urea_NO

Gibbs energy: -1148749.6 kcal mol-1

Atom	X	Y	Z
Fe	0.0571	-0.6104	-0.0668
H	0.1294	-2.0342	0.4322
P	-2.1515	-0.7142	0.1470
P	2.2631	-0.4803	0.1528
O	0.1167	-1.7134	-2.7329
N	0.0199	-0.0108	1.9280
C	0.0920	-1.2465	-1.6598
C	-2.4253	-0.1663	1.8987
H	-2.6102	0.9167	1.8753
H	-3.3034	-0.6426	2.3542
C	-1.1618	-0.4588	2.6845
H	-1.1902	0.0394	3.6680
H	-1.0531	-1.5376	2.8673
C	1.2514	-0.2902	2.6861
H	1.2806	-1.3701	2.8911
H	1.2195	0.2272	3.6593
C	2.4662	0.1423	1.8882
H	3.3983	-0.2057	2.3526
H	2.5100	1.2394	1.8371
C	-3.0754	-2.3296	0.0441
H	-4.1339	-2.0753	0.2127
C	-2.6384	-3.3014	1.1340
H	-3.2018	-4.2394	1.0378
H	-2.8184	-2.9155	2.1446
H	-1.5708	-3.5447	1.0447
C	-2.9235	-2.9780	-1.3259
H	-1.8830	-3.2838	-1.4977
H	-3.2190	-2.3183	-2.1502
H	-3.5462	-3.8810	-1.3854
C	-3.1532	0.5322	-0.8152
H	-2.8045	1.4767	-0.3671
C	-2.7931	0.5796	-2.2949
H	-3.0775	-0.3405	-2.8226
H	-1.7180	0.7447	-2.4305
H	-3.3285	1.4090	-2.7782
C	-4.6572	0.4190	-0.6012
H	-5.1631	1.2920	-1.0355
H	-4.9323	0.3752	0.4609
H	-5.0692	-0.4716	-1.0954
C	3.3440	-1.9974	0.1006
H	4.3712	-1.6349	0.2638
C	3.0024	-2.9771	1.2166
H	1.9645	-3.3277	1.1347
H	3.1416	-2.5475	2.2160
H	3.6565	-3.8568	1.1461
C	3.2647	-2.6941	-1.2516
H	3.5085	-2.0319	-2.0908
H	2.2579	-3.0977	-1.4230
C	3.1499	0.8260	-0.8434
H	2.7280	1.7471	-0.4111
C	4.6599	0.8438	-0.6426
H	5.1411	-0.0209	-1.1198
H	4.9458	0.8486	0.4174
H	5.0870	1.7449	-1.1033
C	2.7749	0.8068	-2.3202
H	3.2460	1.6574	-2.8327
H	1.6896	0.8883	-2.4497
H	3.1201	-0.1046	-2.8258
H	-0.0548	1.0216	1.8084
H	3.9670	-3.5381	-1.2813
C	-0.2440	2.5039	-0.1787
N	-0.2190	2.7176	1.1226
O	-0.0490	1.3745	-0.7348
N	-0.5528	3.5365	-1.0790
H	-0.3353	4.4776	-0.7744
H	-0.2626	3.3449	-2.0307
H	-0.4296	3.6926	1.3289

Adduct_triphenylguanidine_2

Gibbs energy: -1570834.9 kcal mol-1

Atom	X	Y	Z
Fe	-1.4225	-0.3501	0.2938
H	-2.6506	-1.1296	0.6597
P	-0.4178	-1.9529	1.4953
P	-2.8355	0.6915	-1.0952
O	-2.2014	1.2439	2.5650
N	-1.2431	-1.7282	-1.2744
H	-0.2936	-1.4413	-1.5962
C	-1.8262	0.6332	1.6393
C	-0.1109	-3.2793	0.2400
H	0.8957	-3.1063	-0.1661
H	-0.1199	-4.2848	0.6796
C	-1.1366	-3.1378	-0.8629
H	-0.8595	-3.7613	-1.7304
H	-2.1297	-3.4702	-0.5273
C	-2.1693	-1.6143	-2.4125
H	-3.0817	-2.1739	-2.1659
H	-1.7257	-2.0987	-3.2986
C	-2.4955	-0.1656	-2.6983
H	-3.3182	-0.0740	-3.4198
H	-1.6185	0.3450	-3.1265
C	-1.3875	-2.8109	2.8461

H	-0.6513	-3.4409	3.3716
C	-2.4857	-3.7151	2.2976
H	-3.0159	-4.1923	3.1329
H	-2.1053	-4.5163	1.6541
H	-3.2276	-3.1363	1.7288
C	-1.9995	-1.8259	3.8365
H	-2.8119	-1.2580	3.3649
H	-1.2814	-1.1033	4.2386
H	-2.4306	-2.3746	4.6847
C	1.2912	-1.7240	2.2131
H	1.8179	-1.2467	1.3703
C	1.3147	-0.7740	3.4042
H	0.8892	-1.2491	4.2984
H	0.7618	0.1568	3.2206
H	2.3520	-0.5056	3.6497
C	2.0210	-3.0181	2.5554
H	3.0463	-2.7838	2.8749
H	2.0969	-3.7076	1.7070
H	1.5395	-3.5524	3.3859
C	-4.6707	0.4894	-0.7807
H	-5.1612	1.2178	-1.4456
C	-5.1957	-0.8975	-1.1318
H	-4.7011	-1.6756	-0.5326
H	-5.0750	-1.1450	-2.1928
H	-6.2696	-0.9476	-0.9059
C	-5.0326	0.8178	0.6641
H	-6.1245	0.8069	0.7836
H	-4.6729	1.7992	0.9917
H	-4.6167	0.0654	1.3482
C	-2.6590	2.4776	-1.6023
H	-1.5910	2.5339	-1.8610
C	-3.4679	2.8694	-2.8338
H	-4.5492	2.8397	-2.6431
H	-3.2585	2.2362	-3.7037
H	-3.2227	3.9027	-3.1157
C	-2.9170	3.4480	-0.4574
H	-2.6253	4.4638	-0.7573
H	-2.3491	3.1931	0.4462
H	-3.9835	3.4841	-0.1963
N	0.4568	0.7544	-0.3360
C	1.4782	0.2406	-1.0297
C	0.5170	2.1424	-0.0594
C	0.4214	2.6225	1.2522
H	0.3229	1.9103	2.0676
C	0.4925	3.9841	1.5349
H	0.4264	4.3185	2.5691
C	0.6650	4.9101	0.5080
H	0.7272	5.9742	0.7268
C	0.7502	4.4504	-0.8070
H	0.8749	5.1578	-1.6256
C	0.6718	3.0895	-1.0858
H	0.7418	2.7481	-2.1180
N	2.6974	0.9341	-1.1569
H	3.2060	0.7102	-2.0050
C	3.4579	1.5914	-0.1874
C	4.4682	2.4652	-0.6138
C	3.2746	1.3868	1.1847
C	5.2702	3.1208	0.3138
H	4.6095	2.6292	-1.6819
C	4.0725	2.0583	2.1064
H	2.4949	0.7107	1.5240
C	5.0743	2.9293	1.6822
H	6.0478	3.7967	-0.0371
H	3.9053	1.8936	3.1701
H	5.6953	3.4514	2.4066
N	1.3554	-0.9041	-1.6933
C	2.4141	-1.7513	-1.9593
C	2.3288	-2.5775	-3.0992
C	3.5211	-1.9462	-1.1016
C	3.3015	-3.5312	-3.3794
H	1.4697	-2.4503	-3.7595
C	4.4911	-2.9012	-1.3901
H	3.6051	-1.3555	-0.1892
C	4.3966	-3.7006	-2.5305
H	3.2026	-4.1495	-4.2705
H	5.3283	-3.0290	-0.7050
H	5.1571	-4.4474	-2.7477

Adduct_Methyl_formanilide_ON

Gibbs energy: -1283523.9 kcal mol-1

Atom	X	Y	Z
Fe	0.7453	0.4610	0.2936
H	1.5355	1.2927	-0.6770
P	-0.9083	1.8291	-0.3453
P	2.5730	-0.8188	0.2447
O	1.8022	2.3053	2.2378
N	0.1643	-0.6467	-1.3943
H	-0.6070	-1.1715	-0.9472
C	1.3447	1.5272	1.4898
C	-1.5323	1.0553	-1.9119
H	-2.4106	0.4563	-1.6411
H	-1.8453	1.8065	-2.6485
C	-0.4452	0.1597	-2.4684
H	-0.8508	-0.5033	-3.2509
H	0.3555	0.7563	-2.9293
C	1.1506	-1.5756	-1.9739
H	1.7517	-1.0099	-2.6977
H	0.6338	-2.3672	-2.5391
C	2.0462	-2.1673	-0.9076
H	2.8898	-2.7102	-1.3544
H	1.4832	-2.8801	-0.2843
C	-0.4932	3.5704	-0.8840
H	-1.4550	3.9969	-1.2083
C	0.4580	3.6118	-2.0739
H	0.6266	4.6565	-2.3690
H	0.0686	3.0844	-2.9531
H	1.4357	3.1783	-1.8212

C	0.0665	4.4135	0.2545
H	1.0727	4.0739	0.5322
H	-0.5544	4.3889	1.1583
H	0.1495	5.4623	-0.0615
C	-2.4981	1.9887	0.6320
H	-2.9232	0.9816	0.5002
C	-2.2794	2.2034	2.1232
H	-1.7999	3.1671	2.3420
H	-1.6632	1.4075	2.5549
H	-3.2458	2.1968	2.6467
C	-3.4821	3.0040	0.0638
H	-4.4564	2.8915	0.5588
H	-3.6469	2.8795	-1.0142
H	-3.1480	4.0356	0.2401
C	4.1322	-0.0741	-0.4759
H	4.9350	-0.7889	-0.2358
C	4.0893	0.0922	-1.9898
H	3.2732	0.7623	-2.2965
H	3.9770	-0.8600	-2.5216
H	5.0287	0.5470	-2.3327
C	4.4547	1.2678	0.1754
H	5.4371	1.6196	-0.1674
H	4.4802	1.2260	1.2699
H	3.7124	2.0259	-0.1108
C	3.1951	-1.8134	1.6965
H	2.2747	-2.2997	2.0510
C	4.1994	-2.9031	1.3376
H	5.1500	-2.4867	0.9780
H	3.8245	-3.5991	0.5782
H	4.4299	-3.4944	2.2347
C	3.7307	-0.9425	2.8264
H	3.8896	-1.5539	3.7252
H	3.0421	-0.1322	3.0957
H	4.7002	-0.4974	2.5632
C	-2.6502	-1.7764	2.2988
H	-2.7037	-2.8717	2.3327
H	-2.4423	-1.4136	3.3104
H	-3.6373	-1.4199	1.9828
C	-1.6544	-1.3221	1.2442
O	-2.0644	-1.3813	0.0547
N	-0.4542	-0.8293	1.5849
C	-0.0149	-1.1210	2.8963
C	0.2350	-0.1226	3.8482
C	0.1887	-2.4553	3.2892
C	0.6577	-0.4443	5.1362
H	0.0838	0.9201	3.5834
C	0.6103	-2.7794	4.5755
H	0.0126	-3.2457	2.5579
C	0.8492	-1.7732	5.5116
H	0.8350	0.3556	5.8535
H	0.7565	-3.8242	4.8460
H	1.1809	-2.0211	6.5178

Concerted_proton_transfer_with_methanol

Gibbs energy:-229134.0 kcal mol-1

Atom	X	Y	Z
N	-0.8735	-0.2741	-0.0670
C	-0.9568	-0.7928	1.3116
H	-0.8068	-1.8758	1.2986
H	-0.1779	-0.3199	1.9145
H	-1.9428	-0.5581	1.7277
C	-1.9456	-0.8006	-0.9256
H	-1.7674	-0.4922	-1.9589
H	-1.9532	-1.8920	-0.8671
H	-2.9109	-0.4099	-0.5837
C	-0.8221	1.2516	-0.0867
H	-1.6852	1.6064	0.4979
O	0.3588	1.6780	0.4271
H	1.0887	1.0521	-0.0667
H	-0.9742	1.5124	-1.1498
O	1.6147	-0.0743	-0.7081
H	0.1185	-0.5003	-0.4505
C	2.5333	-0.7470	0.0791
H	3.5740	-0.6143	-0.2766
H	2.5286	-0.4120	1.1396
H	2.3559	-1.8415	0.1020

Protonation_with_formanilide

Gibbs energy: -408001.1 kcal mol-1

Atom	X	Y	Z
C	-0.3228	2.0265	-0.3709
H	0.5019	2.7594	-0.5024
H	-2.6666	1.4450	0.2868
H	-0.9859	-0.2804	-0.1095
O	-1.5004	2.4476	-0.4106
O	-3.2566	0.7168	0.6189
N	-1.8281	-1.0793	0.0180
C	-1.6454	-2.1390	-0.9847
H	-0.7309	-2.6965	-0.7632
H	-2.4989	-2.8284	-0.9643
H	-1.5635	-1.6866	-1.9784
C	-1.7487	-1.5977	1.3928
H	-2.5207	-2.3615	1.5504
H	-0.7585	-2.0365	1.5502
H	-1.8958	-0.7737	2.0948
N	0.0274	0.7553	-0.2158
C	1.3760	0.4183	-0.0505
C	2.2698	1.1921	0.7090
C	1.8478	-0.7755	-0.6198
C	3.5961	0.7955	0.8616
H	1.9139	2.0954	1.2017
C	3.1699	-1.1741	-0.4510
H	1.1608	-1.3775	-1.2146
C	4.0562	-0.3881	0.2862

H	4.2719	1.4114	1.4528
H	3.5129	-2.1022	-0.9051
H	5.0905	-0.6985	0.4169
C	-3.1128	-0.3461	-0.2326
H	-3.9352	-1.0608	-0.0805
H	-3.0818	-0.0508	-1.2941

Deprotonation_with_formanilide

Gibbs energy: -407997.6 kcal mol-1

Atom	X	Y	Z
C	-4.0474	0.8302	0.5051
C	-4.5309	-0.4463	0.2239
C	-3.6426	-1.4321	-0.2061
C	-2.2926	-1.1412	-0.3708
C	-1.8058	0.1443	-0.0995
C	-2.6940	1.1258	0.3605
H	-4.7259	1.6036	0.8605
H	-5.5872	-0.6739	0.3487
H	-4.0033	-2.4360	-0.4223
H	-1.5986	-1.9051	-0.7181
H	-2.3261	2.1141	0.6294
N	-0.4322	0.3807	-0.2651
H	0.3051	-0.5053	-0.1690
C	0.0596	1.5656	-0.6329
H	-0.6891	2.3445	-0.8754
O	1.2706	1.8263	-0.7342
N	3.1772	-0.0712	0.0951
C	3.9185	-0.8489	-0.9118
H	3.1989	-1.3737	-1.5434
H	4.5350	-0.1786	-1.5167
H	4.5558	-1.5750	-0.3951
C	4.0685	0.6237	1.0380
H	4.7804	1.2449	0.4879
H	3.4699	1.2548	1.7012
H	4.6130	-0.1203	1.6291
C	2.1320	-0.9819	0.8446
H	1.7293	-0.2764	1.6076
H	2.7782	-1.7240	1.3586
O	1.2483	-1.4790	0.0029
H	2.5695	0.6337	-0.3747

Protonation_with_trimethylphenol

Gibbs energy: -423304.7 kcal mol-1

Atom	X	Y	Z
N	-2.6512	-0.4613	0.3164
C	-2.3716	-0.3313	1.7578
H	-1.6910	-1.1325	2.0608
H	-1.8967	0.6353	1.9464
H	-3.3068	-0.4041	2.3264
C	-3.3085	-1.7357	-0.0094
H	-3.3559	-1.8526	-1.0963
H	-2.7302	-2.5598	0.4173
H	-4.3223	-1.7514	0.4095
C	-3.4438	0.6958	-0.2097
H	-4.3694	0.7809	0.3758
O	-2.7275	1.8679	-0.1029
H	-1.8554	1.7011	-0.5303
H	-3.6910	0.4353	-1.2510
O	-0.6572	0.3398	-0.9231
H	-1.6579	-0.3192	-0.2486
C	0.5976	0.1608	-0.5351
C	1.1567	-1.1363	-0.4510
C	1.4094	1.2728	-0.1979
C	2.4876	-1.2928	-0.0539
C	2.7326	1.0693	0.1920
C	3.3018	-0.2064	0.2714
H	2.9016	-2.3029	-0.0014
H	3.3432	1.9400	0.4458
C	0.3099	-2.3248	-0.7929
H	-0.4612	-2.5184	-0.0309
H	-0.2219	-2.1829	-1.7434
H	0.9169	-3.2345	-0.8712
C	0.8214	2.6494	-0.2537
H	0.3729	2.8628	-1.2335
H	0.0223	2.7813	0.4909
H	1.5826	3.4130	-0.0559
C	4.7394	-0.3896	0.6664
H	4.9999	0.2102	1.5484
H	4.9587	-1.4381	0.9018
H	5.4276	-0.0870	-0.1354

Deprotonation_with_trimethylphenol

Gibbs energy: -423300.4 kcal mol-1

Atom	X	Y	Z
N	-2.7744	-0.4932	0.3762
C	-2.1613	-0.5116	1.7185
H	-1.7370	-1.5000	1.9174
H	-1.3787	0.2500	1.7572
H	-2.9368	-0.2825	2.4567
C	-3.8868	-1.4496	0.2520
H	-4.2633	-1.4356	-0.7739
H	-3.5408	-2.4562	0.5037
H	-4.6832	-1.1535	0.9421
C	-3.2071	0.9847	-0.0274
H	-3.9844	1.2174	0.7302
O	-2.1678	1.7919	-0.0430
H	-1.1936	1.1486	-0.7622
H	-3.7068	0.7993	-1.0038
O	-0.5875	0.3852	-1.2420
H	-2.0378	-0.7135	-0.3128
C	0.6288	0.1882	-0.6971

C	1.1342	-1.1242	-0.6486
C	1.4062	1.2597	-0.2094
C	2.4044	-1.3473	-0.1103
C	2.6659	0.9864	0.3260
C	3.1904	-0.3078	0.3881
H	2.7872	-2.3697	-0.0809
H	3.2650	1.8203	0.6998
C	0.3076	-2.2604	-1.1707
H	-0.6087	-2.4091	-0.5785
H	-0.0171	-2.0890	-2.2047
H	0.8697	-3.2007	-1.1394
C	0.8936	2.6661	-0.2879
H	0.5726	2.9198	-1.3075
H	0.0182	2.8227	0.3557
H	1.6699	3.3792	0.0108
C	4.5532	-0.5573	0.9665
H	4.6185	-0.2243	2.0109
H	4.8086	-1.6231	0.9430
H	5.3346	-0.0180	0.4144
H	-1.3019	4.5373	-0.4749
H	-1.8323	3.2964	-1.6255
H	-2.7613	3.6011	-0.1430
C	-0.8174	2.9123	1.6731
H	-1.8229	2.8916	2.1183
H	-0.1828	2.2199	2.2385
H	-0.4159	3.9276	1.7974
C	-0.2175	-2.9554	1.9746
H	0.4913	-3.7359	2.2844
H	-0.1868	-2.1511	2.7210
H	-1.2269	-3.3909	1.9943
C	0.1339	-3.5691	-0.4339
H	0.3321	-3.2089	-1.4526
H	0.9131	-4.2986	-0.1740
H	-0.8198	-4.1136	-0.4577
C	-4.4336	-0.8882	-1.0031
H	-5.1826	-0.6055	-0.2501
H	-4.6955	-0.3503	-1.9241
H	-4.5580	-1.9599	-1.1993

Protonation_with_diisopropyl-methylphenol

Gibbs energy: -521860.5 kcal mol-1

Atom	X	Y	Z
N	2.8345	-0.0885	-0.5538
C	2.4906	0.2459	-1.9482
H	1.8673	-0.5548	-2.3580
H	1.9294	1.1837	-1.9666
H	3.4059	0.3475	-2.5437
C	3.5853	-1.3499	-0.4573
H	3.7226	-1.6128	0.5959
H	3.0245	-2.1434	-0.9597
H	4.5647	-1.2384	-0.9389
C	3.5638	1.0220	0.1377
H	4.4618	1.2703	-0.4433
O	2.7649	2.1404	0.2407
H	1.9189	1.8451	0.6486
H	3.8613	0.6142	1.1166
O	0.8001	0.3468	0.8125
H	1.8579	-0.1081	0.0434
C	-0.4136	0.0495	0.3656
C	-0.8232	-1.2983	0.2007
C	-1.3327	1.0868	0.0336
C	-2.1201	-1.5764	-0.2439
C	-2.6130	0.7531	-0.4036
C	-3.0372	-0.5730	-0.5481
H	-2.4316	-2.6181	-0.3522
H	-3.3181	1.5483	-0.6525
C	0.1129	-2.4274	0.5781
H	1.1281	-2.0100	0.6284
C	-0.8900	2.5259	0.1938
H	0.1296	2.5945	-0.2195
C	-1.7457	3.5368	-0.5580

Deprotonation_with_diisopropyl-methylphenol

Gibbs energy: -521859.5 kcal mol-1

Atom	X	Y	Z
N	0.8881	2.1045	0.7827
C	2.3216	2.0999	1.1301
H	2.4726	1.5343	2.0543
H	2.8763	1.6446	0.3059
H	2.6479	3.1361	1.2685
C	0.0603	2.7639	1.8075
H	-0.9930	2.6904	1.5226
H	0.2141	2.2771	2.7747
H	0.3527	3.8168	1.8729
C	0.6617	2.7297	-0.6683
H	1.0049	3.7737	-0.5137
O	1.3026	2.0495	-1.5903
H	0.5708	0.9534	-1.9134
H	-0.4491	2.7235	-0.7340
O	-0.0962	0.0951	-2.0146
H	0.5832	1.1246	0.6876
C	-0.2613	-0.4700	-0.8063
C	-1.5250	-0.4029	-0.1720
C	0.8197	-1.1095	-0.1526
C	-1.6759	-0.9588	1.0998
C	0.6170	-1.6442	1.1250
C	-0.6188	-1.5796	1.7716
H	-2.6472	-0.9061	1.5953
H	1.4460	-2.1339	1.6377
C	-2.6823	0.2328	-0.9094
H	-2.2573	1.0189	-1.5503
C	2.1429	-1.2472	-0.8783
H	2.3196	-0.3048	-1.4178

C	-3.7291	0.8652	-0.0008
H	-3.2872	1.5829	0.7036
H	-4.4742	1.4025	-0.6013
H	-4.2735	0.1122	0.5857
C	-3.3388	-0.7983	-1.8296
H	-2.6121	-1.2334	-2.5261
H	-3.7736	-1.6167	-1.2372
H	-4.1461	-0.3432	-2.4191
C	2.0452	-2.3677	-1.9160
H	1.2211	-2.1908	-2.6165
H	2.9747	-2.4503	-2.4952
H	1.8712	-3.3334	-1.4192
C	3.3373	-1.4914	0.0347
H	4.2657	-1.4634	-0.5497
H	3.4194	-0.7360	0.8280
H	3.2905	-2.4786	0.5153
C	-0.8231	-2.1907	3.1277
H	-1.4569	-1.5609	3.7646
H	-1.3168	-3.1697	3.0577
H	0.1298	-2.3451	3.6476

Protonation_with_tertbutyl-methylphenol

Gibbs energy: -571132.9 kcal mol-1

Atom	X	Y	Z
N	-3.0324	-0.1940	0.4585
C	-3.8570	0.9768	0.1064
H	-3.5806	1.8209	0.7439
H	-3.6911	1.2419	-0.9401
H	-4.9168	0.7358	0.2606
C	-3.2560	-0.5959	1.8571
H	-2.5802	-1.4156	2.1182
H	-3.0568	0.2561	2.5129
H	-4.2952	-0.9214	1.9932
C	-3.3067	-1.3368	-0.4655
H	-4.3887	-1.5251	-0.4832
O	-2.8834	-1.0363	-1.7450
H	-1.9211	-0.8646	-1.6779
H	-2.7898	-2.2102	-0.0385
O	-0.6969	-0.2983	-0.2790
H	-1.8664	-0.0309	0.2583
C	0.5823	0.0253	-0.1178
C	1.5554	-1.0195	-0.0100
C	1.0185	1.3839	-0.0810
C	2.9044	-0.6750	0.0915
C	2.3891	1.6485	0.0234
C	3.3509	0.6463	0.1017
H	3.6566	-1.4589	0.1679
H	2.7362	2.6801	0.0439
C	1.1376	-2.4977	0.0117
C	0.0185	2.5468	-0.1088
C	0.6998	3.9186	-0.1385
H	-0.0735	4.6984	-0.1641
H	1.3166	4.1029	0.7506
H	1.3292	4.0499	-1.0287
C	-0.8675	2.4888	-1.3614
H	-0.2538	2.6264	-2.2627
H	-1.3912	1.5350	-1.4624
H	-1.6123	3.2979	-1.3393
C	0.4506	-2.8922	-1.3022
H	0.1806	-3.9581	-1.2846
H	-0.4600	-2.3133	-1.4769
H	1.1238	-2.7317	-2.1558
C	2.3304	-3.4436	0.1768
H	2.8798	-3.2661	1.1110
H	1.9634	-4.4785	0.2059
H	3.0401	-3.3733	-0.6585
C	0.2026	-2.7608	1.1996
H	0.7283	-2.5894	2.1495
H	-0.6715	-2.1029	1.1698
H	-0.1439	-3.8047	1.1914
C	-0.8173	2.5145	1.1793
H	-1.2954	1.5446	1.3518
H	-0.1740	2.7128	2.0478
H	-1.5984	3.2887	1.1578
C	4.8162	0.9655	0.1869
H	5.3010	0.4415	1.0214
H	5.3537	0.6701	-0.7251
H	4.9832	2.0400	0.3297

Deprotonation_with_tertbutyl-methylphenol

Gibbs energy: -571129.5 kcal mol-1

Atom	X	Y	Z
N	0.3400	2.4782	0.4272
C	1.7196	2.9905	0.5454
H	2.1997	2.5648	1.4320
H	2.2695	2.7107	-0.3563
H	1.6770	4.0808	0.6319
C	-0.5416	2.9908	1.4927
H	-1.5146	2.4953	1.4266
H	-0.0918	2.7925	2.4701
H	-0.6647	4.0699	1.3547
C	-0.2403	2.7705	-1.0251
H	-0.0984	3.8679	-1.1049
O	0.3802	2.0598	-1.9427
H	0.1204	0.7524	-1.9203
H	-1.3183	2.5617	-0.8779
O	-0.0586	-0.3350	-1.8191
H	0.3726	1.4495	0.4879
C	-0.0855	-0.6393	-0.5103
C	-1.3323	-0.7015	0.1767
C	1.1227	-0.9143	0.1896
C	-1.3118	-0.8084	1.5703
C	1.0682	-1.0040	1.5881

C	-0.1255	-0.9057	2.3002
H	-2.2481	-0.8254	2.1261
H	1.9821	-1.1760	2.1543
C	-2.6592	-0.7648	-0.5966
C	2.4292	-1.2161	-0.5634
C	-3.8532	-0.9918	0.3337
H	-3.9964	-0.1629	1.0409
H	-4.7676	-1.0649	-0.2697
H	-3.7640	-1.9236	0.9079
C	-2.6021	-1.9601	-1.5600
H	-1.7925	-1.8489	-2.2889
H	-2.4448	-2.8963	-1.0062
H	-3.5514	-2.0501	-2.1071
C	2.1602	-2.3280	-1.5891
H	1.4165	-2.0182	-2.3301
H	3.0901	-2.5876	-2.1148
H	1.7943	-3.2356	-1.0884
C	3.5226	-1.7319	0.3763
H	4.4107	-1.9881	-0.2167
H	3.8330	-0.9792	1.1140
H	3.2154	-2.6374	0.9165
C	-2.9524	0.5150	-1.3873
H	-3.0807	1.3728	-0.7110
H	-2.1605	0.7449	-2.1061
H	-3.8942	0.3973	-1.9421
C	3.0001	0.0156	-1.2734
H	2.2832	0.4771	-1.9580
H	3.3116	0.7730	-0.5398
H	3.8944	-0.2687	-1.8467
C	-0.1472	-0.9415	3.8006
H	-0.2889	0.0614	4.2288
H	-0.9668	-1.5653	4.1790
H	0.7912	-1.3373	4.2068

Protonation_with_methylformanilide

Gibbs energy: -432644.4 kcal mol-1

Atom	X	Y	Z
C	-0.2360	2.0646	-0.6142
H	-2.5451	1.5950	0.2703
H	-1.0064	-0.2072	-0.1038
O	-1.4319	2.4665	-0.5890
O	-3.1569	0.9264	0.6925
N	-1.8386	-0.9572	0.1147
C	-1.7486	-2.0723	-0.8406
H	-0.8339	-2.6401	-0.6497
H	-2.6158	-2.7344	-0.7266
H	-1.7230	-1.6728	-1.8594
C	-1.6790	-1.4043	1.5085
H	-2.4638	-2.1280	1.7602
H	-0.6959	-1.8715	1.6202
H	-1.7463	-0.5377	2.1703
N	0.0762	0.7981	-0.3382
C	1.3816	0.3344	-0.1563
C	2.2935	0.9415	0.7250
C	1.7742	-0.8534	-0.7963
C	3.5569	0.3945	0.9308
H	1.9950	1.8422	1.2596
C	3.0356	-1.4017	-0.5812
H	1.0729	-1.3329	-1.4795
C	3.9385	-0.7797	0.2809
H	4.2463	0.8855	1.6157
H	3.3169	-2.3192	-1.0954
H	4.9247	-1.2071	0.4488
C	-3.1172	-0.1936	-0.0903
H	-3.9456	-0.8687	0.1697
H	-3.1537	0.0297	-1.1690
C	0.8080	3.0745	-1.0272
H	1.0138	3.7590	-0.1954
H	1.7540	2.6285	-1.3481
H	0.3943	3.6779	-1.8417

Deprotonation_with_methylformanilide

Gibbs energy: -432641.3 kcal mol-1

Atom	X	Y	Z
C	-3.9687	0.6571	0.8357
C	-4.4700	-0.5659	0.3926
C	-3.6316	-1.4334	-0.3073
C	-2.3136	-1.0764	-0.5744
C	-1.8082	0.1580	-0.1433
C	-2.6467	1.0141	0.5834
H	-4.6069	1.3362	1.3981
H	-5.5016	-0.8437	0.5978
H	-4.0068	-2.3949	-0.6530
H	-1.6573	-1.7485	-1.1252
H	-2.2544	1.9542	0.9663
N	-0.4541	0.4410	-0.3839
H	0.2923	-0.4513	-0.2664
C	0.0570	1.6119	-0.7992
O	1.2957	1.7884	-0.8528
N	3.1140	-0.0623	0.1531
C	3.8992	-0.8282	-0.8289
H	3.2083	-1.3381	-1.5034
H	4.5471	-0.1514	-1.3924
H	4.5086	-1.5660	-0.2951
C	3.9613	0.6133	1.1480
H	4.6966	1.2447	0.6423
H	3.3323	1.2318	1.7948
H	4.4786	-0.1413	1.7501
C	2.0305	-0.9723	0.8337
H	1.5980	-0.2794	1.5912
H	2.6386	-1.7351	1.3629
O	1.1801	-1.4408	-0.0600
H	2.5264	0.6495	-0.3393
C	-0.8368	2.7355	-1.2507

H	-1.8312	2.4059	-1.5644
H	-0.9563	3.4678	-0.4434
H	-0.3406	3.2471	-2.0808

Protonation_with_urea

Gibbs energy: -297859.8 kcal mol-1

Atom	X	Y	Z
C	2.0187	-0.1239	-0.0008
H	-0.0341	1.6447	0.2760
H	-0.3296	-0.2353	-0.4692
O	1.7821	-0.6573	1.1013
O	-0.9265	1.8127	0.6675
N	-1.3923	-0.3487	-0.1560
C	-2.1465	-1.0839	-1.1839
H	-1.8127	-2.1241	-1.1955
H	-3.2186	-1.0453	-0.9582
H	-1.9580	-0.6318	-2.1624
C	-1.4788	-0.9920	1.1689
H	-2.5222	-0.9828	1.5057
H	-1.1221	-2.0212	1.0852
H	-0.8395	-0.4527	1.8695
N	1.0615	0.4305	-0.7721
C	-1.8033	1.0941	-0.1108
H	-2.8151	1.1567	0.3098
H	-1.8208	1.4266	-1.1610
H	1.4275	0.7420	-1.6693
N	3.3335	-0.1355	-0.4789
H	3.5981	0.5710	-1.1537
H	4.0313	-0.3086	0.2335

Deprotonation_with_urea

Gibbs energy: -297869.7 kcal mol-1

Atom	X	Y	Z
N	-1.7447	1.0572	-0.1856
H	-0.6341	1.4945	0.0088
C	-2.0106	-0.2312	0.0481
O	-1.1178	-1.0967	0.2408
N	1.5086	-0.3520	0.0156
C	2.2400	-0.2462	1.2888
H	1.7379	0.4917	1.9180
H	2.2524	-1.2194	1.7868
H	3.2664	0.0777	1.0827
C	2.1496	-1.2880	-0.9211
H	2.2673	-2.2646	-0.4438
H	1.5230	-1.3913	-1.8118
H	3.1330	-0.8982	-1.2055
C	1.2978	1.0561	-0.6275
H	0.8112	0.7993	-1.5945
H	2.3299	1.4044	-0.8331
O	0.5894	1.8420	0.1686
H	0.5244	-0.6780	0.2003
H	-2.5500	1.6663	-0.2730
N	-3.3298	-0.6338	0.1097
H	-3.4862	-1.6293	0.0302
H	-4.0431	-0.0447	-0.2985

Protonation_with_triphenylguanidine

Gibbs energy: -719957.0 kcal mol-1

Atom	X	Y	Z
N	0.4226	-1.1158	-0.1442
C	-0.2002	-0.0075	0.2240
C	1.7459	-1.4246	0.1559
C	2.4577	-2.1930	-0.7835
H	1.9543	-2.4744	-1.7086
C	3.7786	-2.5666	-0.5616
H	4.3036	-3.1505	-1.3161
C	4.4307	-2.1940	0.6138
H	5.4658	-2.4796	0.7883
C	3.7285	-1.4555	1.5669
H	4.2165	-1.1664	2.4967
C	2.4058	-1.0810	1.3515
H	1.8839	-0.5034	2.1119
N	0.4711	1.1536	0.5926
H	-0.0646	1.8082	1.1521
C	1.6998	1.6363	0.1230
C	2.4188	2.5158	0.9412
C	2.2189	1.2845	-1.1281
C	3.6469	3.0179	0.5249
H	2.0108	2.7869	1.9148
C	3.4584	1.7767	-1.5268
H	1.6627	0.6136	-1.7795
C	4.1819	2.6417	-0.7068
H	4.1956	3.6966	1.1752
H	3.8574	1.4827	-2.4958
H	5.1500	3.0209	-1.0260
N	-1.5407	0.0012	0.2723
C	-2.2945	1.1691	0.1533
C	-3.4651	1.2884	0.9222
C	-2.0049	2.1926	-0.7709
C	-4.3097	2.3861	0.7822
H	-3.6943	0.5010	1.6410
C	-2.8473	3.2921	-0.8980
H	-1.1193	2.1096	-1.4007
C	-4.0051	3.4000	-0.1254
H	-5.2089	2.4525	1.3924
H	-2.6023	4.0693	-1.6202
H	-4.6619	4.2602	-0.2340
O	-1.1252	-2.9516	-1.3731
N	-2.8964	-2.2334	0.0276
C	-1.8847	-3.2988	-0.2901
H	-1.2911	-3.4232	0.6304

C	-3.8413	-2.0336	-1.0842
H	-4.5151	-1.2077	-0.8378
H	-3.2801	-1.7860	-1.9884
H	-4.4236	-2.9493	-1.2470
C	-3.5817	-2.5362	1.2929
H	-4.0578	-3.5229	1.2367
H	-2.8511	-2.5254	2.1083
H	-4.3465	-1.7781	1.4829
H	-0.4739	-2.2587	-1.0434
H	-2.4396	-4.2263	-0.4943
H	-2.2921	-1.2584	0.1601

Deprotonation_with_triphenylguanidine

Gibbs energy: -719954.2 kcal mol-1

Atom	X	Y	Z
N	-0.4398	-1.0789	0.0200
C	0.2090	0.0613	-0.2957
C	-1.7622	-1.4098	-0.2939
C	-2.4372	-2.2687	0.5868
H	-1.9146	-2.6237	1.4740
C	-3.7547	-2.6429	0.3454
H	-4.2597	-3.3039	1.0476
C	-4.4308	-2.1652	-0.7769
H	-5.4657	-2.4461	-0.9597
C	-3.7581	-1.3280	-1.6665
H	-4.2664	-0.9568	-2.5548
C	-2.4348	-0.9615	-1.4407
H	-1.9274	-0.3130	-2.1514
N	-0.4995	1.2176	-0.5662
H	0.0154	1.9213	-1.0843
C	-1.7224	1.6469	-0.0235
C	-2.4788	2.5674	-0.7574
C	-2.1950	1.1991	1.2144
C	-3.7017	3.0165	-0.2704
H	-2.1058	2.9134	-1.7210
C	-3.4306	1.6375	1.6818
H	-1.6093	0.4961	1.8030
C	-4.1925	2.5437	0.9460
H	-4.2806	3.7296	-0.8541
H	-3.7950	1.2696	2.6390
H	-5.1564	2.8821	1.3192
N	1.5242	0.0435	-0.3603
C	2.2935	1.2043	-0.2603
C	3.4152	1.3319	-1.0966
C	2.0756	2.1979	0.7138
C	4.2765	2.4196	-0.9800
H	3.5907	0.5619	-1.8485
C	2.9392	3.2828	0.8238
H	1.2321	2.1019	1.3971
C	4.0435	3.4050	-0.0214
H	5.1350	2.4975	-1.6448
H	2.7533	4.0367	1.5869
H	4.7169	4.2541	0.0718
O	0.9277	-2.8363	1.1863
N	3.0096	-2.2933	0.1527
C	1.7903	-3.2699	0.2853
H	1.4136	-3.3019	-0.7632
C	3.7066	-2.1336	1.4381
H	4.4657	-1.3503	1.3490
H	2.9715	-1.8585	2.1978
H	4.1824	-3.0834	1.7082
C	3.9113	-2.6870	-0.9389
H	4.2835	-3.7007	-0.7532
H	3.3606	-2.6653	-1.8844
H	4.7563	-1.9944	-0.9918
H	0.1823	-1.8825	0.5928
H	2.2694	-4.2445	0.5161
H	2.5361	-1.3827	-0.0872

Concerted_proton_transfer_with_tbd

Gibbs energy: -431707.7 kcal mol-1

Atom	X	Y	Z
C	1.2662	2.6848	0.3367
C	2.4377	1.8527	-0.1391
C	0.8451	-0.0118	-0.1718
C	0.0256	2.2373	-0.4103
H	3.5671	-0.6571	-1.1306
H	1.1254	2.5396	1.4171
H	3.3311	2.0458	0.4683
C	3.2557	-0.4942	-0.0842
H	-1.4808	0.4123	-0.1069
H	0.1109	2.5345	-1.4704
C	1.6446	-2.3540	-0.0983
C	2.8879	-1.8092	0.5696
H	1.2536	-3.2262	0.4390
H	3.7154	-2.5210	0.4764
N	0.6065	-1.3408	-0.1319
N	-0.1867	0.8046	-0.3041
N	2.1302	0.4318	-0.0284
H	4.0974	-0.0192	0.4346
H	2.7006	-1.6459	1.6398
H	1.8919	-2.6894	-1.1199
H	2.6915	2.1075	-1.1827
H	1.4688	3.7483	0.1645
H	-0.8699	2.7433	-0.0203
O	-1.9864	-2.0956	-0.4881
N	-2.6374	0.1164	0.1256
C	-2.5488	-1.3979	0.4709
H	-1.9928	-1.3671	1.4475
C	-3.4347	0.3271	-1.0789
H	-3.3614	1.3732	-1.4010
H	-3.0503	-0.3272	-1.8668
H	-4.4909	0.0819	-0.8896
C	-3.1245	0.8949	1.2601

H	-4.0851	0.4973	1.6208
H	-2.3922	0.8483	2.0753
H	-3.2675	1.9425	0.9724
H	-0.3784	-1.6527	-0.3373
H	-3.6108	-1.6663	0.7169

Direct_proton_transfer

Gibbs energy: -156539.6 kcal mol-1

Atom	X	Y	Z
N	-1.4727	0.5609	0.0691
C	-1.3171	1.9832	0.3802
H	-0.5239	2.4075	-0.2432
H	-2.2566	2.5028	0.1667
H	-1.0558	2.1214	1.4367
C	-0.2431	-0.2089	0.2680
H	-0.4185	-1.2488	-0.0251
H	0.5531	0.2092	-0.3557
H	0.0689	-0.1739	1.3193
C	-2.7521	-0.0930	0.5975
H	-3.2594	0.6270	1.2700
O	-3.3454	-0.3226	-0.6026
H	-2.1520	0.2773	-0.8957
H	-2.4685	-0.9871	1.1877

Urea

Gibbs energy: -141312.8 kcal mol-1

Atom	X	Y	Z
C	0.0143	0.1106	0.0157
N	-1.3129	-0.2249	-0.0210
N	0.8818	-0.9471	-0.0100
H	1.8560	-0.7374	0.1539
H	0.5720	-1.8873	0.1935
H	-1.6213	-1.1604	0.2060
H	-1.9683	0.5247	0.1490
O	0.3989	1.2794	0.0053

TBD

Gibbs energy: -275146.8 kcal mol-1

Atom	X	Y	Z
C	-2.9330	-1.4619	-0.0838
C	-1.5767	-1.3914	0.5837
C	-1.4625	0.9940	-0.0812
C	-3.6574	-0.1522	0.1377
H	0.6622	-0.0455	1.6313
H	-2.8097	-1.6395	-1.1611
H	-0.9733	-2.2751	0.3378
C	0.5687	-0.1835	0.5381
H	-3.2341	1.8543	-0.3633
H	-3.8931	-0.0349	1.2105
C	0.5479	2.2366	0.0709
C	1.2790	0.9323	-0.1971
H	0.9477	3.0335	-0.5721
H	2.3250	0.9946	0.1269
N	-0.8880	2.1537	-0.1368
N	-2.8185	0.9306	-0.3498
N	-0.8335	-0.2148	0.1472
H	1.0042	-1.1624	0.2976
H	1.2783	0.7130	-1.2745
H	0.7504	2.5596	1.1072
H	-1.6963	-1.3788	1.6834
H	-3.5092	-2.2954	0.3335
H	-4.6050	-0.1252	-0.4114

Formanilide

Gibbs energy: -251437.9 kcal mol-1

Atom	X	Y	Z
O	2.7688	0.9552	0.0001
N	1.4098	-0.9091	-0.0001
C	2.6023	-0.2542	-0.0001
H	3.4464	-0.9700	0.0004
C	0.1027	-0.3862	-0.0000
C	-0.9533	-1.3064	0.0000
H	-0.7325	-2.3734	0.0001
C	-2.2700	-0.8637	0.0000
H	-3.0781	-1.5922	0.0001
C	-2.5534	0.5020	-0.0000
H	-3.5839	0.8498	0.0000
C	-1.5011	1.4138	-0.0001
H	-1.7077	2.4822	-0.0001
C	-0.1748	0.9854	-0.0001
H	0.6386	1.7022	-0.0002
H	1.4775	-1.9218	0.0002

Methyl_tBuPhenol

Gibbs energy: -414572.7 kcal mol-1

Atom	X	Y	Z
H	1.0416	-0.9759	-1.9262
O	0.1582	-1.0799	-1.5561
C	0.2019	-1.0261	-0.1889
C	-1.0377	-1.1676	0.4774
C	1.4147	-0.8384	0.5074
C	-1.0200	-1.1141	1.8715
C	1.3463	-0.7964	1.9062
C	0.1522	-0.9307	2.6051
H	-1.9508	-1.2177	2.4254

H	2.2558	-0.6529	2.4846
C	-2.3539	-1.3690	-0.2869
C	2.7662	-0.6809	-0.2123
C	-3.5500	-1.4959	0.6598
H	-3.6977	-0.5951	1.2703
H	-4.4608	-1.6381	0.0636
H	-3.4620	-2.3601	1.3315
C	-2.3027	-2.6620	-1.1129
H	-1.5102	-2.6420	-1.8661
H	-2.1357	-3.5313	-0.4617
H	-3.2606	-2.8115	-1.6306
C	3.1111	-1.9425	-1.0231
H	2.4087	-2.1883	-1.8294
H	4.0973	-1.8249	-1.4913
H	3.1521	-2.8190	-0.3634
C	3.9198	-0.4929	0.7771
H	4.8561	-0.3863	0.2147
H	3.8005	0.4110	1.3877
H	4.0369	-1.3541	1.4472
C	-2.6345	-0.1657	-1.1980
H	-2.7061	0.7585	-0.6078
H	-1.8573	-0.0284	-1.9548
H	-3.5933	-0.3063	-1.7164
C	2.7721	0.5714	-1.1065
H	2.0338	0.5703	-1.9183
H	2.5774	1.4688	-0.5051
H	3.7571	0.6870	-1.5778
C	0.1138	-0.8896	4.1050
H	-0.6027	-0.1427	4.4703
H	-0.1921	-1.8559	4.5278
H	1.0959	-0.6423	4.5238

Methyl_iPrPhenol

Gibbs energy: -365299.1 kcal mol-1

Atom	X	Y	Z
H	0.8174	-2.4670	-0.5795
O	-0.0689	-2.1029	-0.4559
C	-0.0025	-0.7491	-0.2684
C	-1.2310	-0.0733	-0.1699
C	1.2224	-0.0714	-0.1779
C	-1.2026	1.3024	0.0492
C	1.1898	1.3100	0.0411
C	-0.0055	2.0155	0.1611
H	-2.1433	1.8483	0.1328
H	2.1287	1.8582	0.1199
C	-2.5256	-0.8535	-0.2504
H	-2.3597	-1.6887	-0.9458
C	2.5307	-0.8333	-0.2580
H	2.4139	-1.6539	-0.9889
C	-3.7033	-0.0387	-0.7704
H	-3.4767	0.4501	-1.7263
H	-4.5710	-0.6926	-0.9238
H	-4.0100	0.7384	-0.0570
C	-2.8655	-1.4492	1.1177
H	-2.0535	-2.0774	1.5028
H	-3.0473	-0.6464	1.8468
H	-3.7735	-2.0644	1.0628
C	2.8753	-1.4496	1.1009
H	2.0741	-2.0918	1.4878
H	3.7913	-2.0512	1.0385
H	3.0435	-0.6529	1.8387
C	3.7028	0.0014	-0.7598
H	4.5773	-0.6416	-0.9168
H	3.4750	0.5024	-1.7084
H	3.9938	0.7681	-0.0298
C	-0.0206	3.4984	0.3927
H	-0.5048	4.0316	-0.4360
H	-0.5744	3.7594	1.3038
H	0.9948	3.8980	0.4949

Methanol

Gibbs energy: -72581.8 kcal mol-1

Atom	X	Y	Z
C	-2.0810	1.5136	0.0099
H	-1.7085	0.4849	0.0245
H	-1.7204	1.9967	-0.9098
H	-3.1798	1.4810	-0.0159
O	-1.5941	2.1542	1.1744
H	-1.9124	3.0644	1.1779

Methyl_MePhenol

Gibbs energy: -266742.4 kcal mol-1

Atom	X	Y	Z
C	-3.1571	-7.4177	2.1101
C	-2.6443	-6.6646	3.1714
C	-2.0292	-5.4291	2.9772
C	-1.9302	-4.9396	1.6673
C	-2.4304	-5.6588	0.5768
C	-3.0392	-6.8936	0.8234
H	-2.7253	-7.0515	4.1893
H	-3.4323	-7.4578	-0.0240
C	-2.3145	-5.1118	-0.8151
H	-2.7565	-5.8030	-1.5399
H	-2.8347	-4.1496	-0.9303
H	-1.2683	-4.9562	-1.1165
C	-1.4853	-4.6306	4.1209
H	-0.4094	-4.4447	4.0090
H	-1.9641	-3.6454	4.1905
H	-1.6436	-5.1540	5.0698
C	-3.7977	-8.7520	2.3581
H	-3.0596	-9.4997	2.6782

H	-4.5559	-8.6956	3.1494
H	-4.2841	-9.1367	1.4546
O	-1.3233	-3.7249	1.5133
H	-1.3049	-3.4756	0.5798

Triphenylguanidine

Gibbs energy: -563394.2 kcal mol-1

Atom	X	Y	Z
N	-1.3129	0.0104	-0.3645
C	0.0480	-0.1707	-0.3400
C	-2.3398	-0.9234	-0.1651
C	-3.6201	-0.5547	-0.6037
H	-3.7573	0.4030	-1.1057
C	-4.7062	-1.3976	-0.4031
H	-5.6900	-1.0910	-0.7527
C	-4.5375	-2.6258	0.2351
H	-5.3861	-3.2882	0.3900
C	-3.2658	-2.9907	0.6706
H	-3.1161	-3.9447	1.1725
C	-2.1677	-2.1554	0.4780
H	-1.1823	-2.4553	0.8163
H	-1.6248	0.9095	-0.7143
N	0.7806	0.9975	-0.4401
H	1.7393	0.8694	-0.7452
C	0.4042	2.3253	-0.1684
C	1.0257	3.3454	-0.8994
C	-0.5097	2.6606	0.8386
C	0.7355	4.6782	-0.6305
H	1.7392	3.0804	-1.6787
C	-0.8084	3.9985	1.0839
H	-0.9717	1.8816	1.4406
C	-0.1909	5.0138	0.3561
H	1.2307	5.4589	-1.2042
H	-1.5201	4.2460	1.8689
H	-0.4240	6.0561	0.5604
N	0.5719	-1.3485	-0.2828
C	1.9422	-1.5479	-0.0985
C	2.6107	-2.4227	-0.9701
C	2.6649	-0.9967	0.9753
C	3.9581	-2.7193	-0.7894
H	2.0483	-2.8671	-1.7899
C	4.0110	-1.3036	1.1537
H	2.1627	-0.3361	1.6803
C	4.6690	-2.1618	0.2732
H	4.4542	-3.3975	-1.4816
H	4.5486	-0.8704	1.9955
H	5.7206	-2.3993	0.4184

Methyl_formanilide

Gibbs energy: -276084.4 kcal mol-1

Atom	X	Y	Z
C	2.1237	1.2954	0.0234
C	3.0507	0.2570	-0.0024
C	2.5929	-1.0605	-0.0228
C	1.2302	-1.3300	-0.0180
C	0.2988	-0.2826	0.0091
C	0.7532	1.0412	0.0296
H	2.4651	2.3287	0.0392
H	4.1173	0.4698	-0.0070
H	3.3008	-1.8865	-0.0437
H	0.8767	-2.3609	-0.0370
H	0.0385	1.8553	0.0491
N	-1.0604	-0.6429	0.0138
H	-1.2346	-1.6412	0.0292
C	-2.1733	0.1569	0.0020
O	-2.1323	1.3823	-0.0161
C	-3.4777	-0.5903	0.0313
H	-3.3766	-1.6628	-0.1601
H	-3.9414	-0.4525	1.0149
H	-4.1524	-0.1537	-0.7110

Fe_(PNP)

Gibbs energy: -1007434.6 kcal mol-1

Atom	X	Y	Z
Fe	0.0001	-0.0537	-0.1820
H	-0.0000	0.1977	1.2721
P	-2.2060	0.1336	-0.2029
P	2.2061	0.1339	-0.2026
O	0.0003	-2.7663	0.8435
N	0.0000	1.6018	-1.0640
C	0.0002	-1.6912	0.3680
C	-2.4598	1.6577	-1.2167
H	-2.6408	1.3184	-2.2460
H	-3.3362	2.2380	-0.8981
C	-1.1780	2.4638	-1.1544
H	-1.1040	3.1131	-2.0464
H	-1.2031	3.1552	-0.2872
C	1.1779	2.4640	-1.1540
H	1.2027	3.1553	-0.2866
H	1.1040	3.1135	-2.0458
C	2.4599	1.6583	-1.2161
H	3.3360	2.2386	-0.8972
H	2.6412	1.3192	-2.2454
C	-3.0718	0.4816	1.4092
H	-4.1364	0.6206	1.1639
C	-2.5502	1.7691	2.0375
H	-3.0554	1.9461	2.9967
H	-2.7280	2.6479	1.4060
H	-1.4710	1.7059	2.2368
C	-2.9243	-0.6841	2.3785
H	-1.8679	-0.8517	2.6298

H	-3.3268	-1.6234	1.9806
H	-3.4578	-0.4681	3.3141
C	-3.2817	-1.0918	-1.1233
H	-2.9528	-0.9223	-2.1617
C	-3.0100	-2.5543	-0.7989
H	-3.2566	-2.8060	0.2406
H	-1.9633	-2.8253	-0.9720
H	-3.6302	-3.1936	-1.4422
C	-4.7697	-0.7750	-1.0303
H	-5.3289	-1.3938	-1.7451
H	-4.9971	0.2747	-1.2560
H	-5.1646	-1.0006	-0.0304
C	3.0718	0.4816	1.4096
H	4.1364	0.6208	1.1644
C	2.5501	1.7690	2.0381
H	1.4708	1.7055	2.2375
H	2.7276	2.6479	1.4068
H	3.0552	1.9460	2.9974
C	2.9244	-0.6843	2.3787
H	3.4579	-0.4683	3.3143
H	3.3271	-1.6234	1.9806
H	1.8680	-0.8519	2.6300
C	3.2820	-1.0913	-1.1232
H	2.9531	-0.9216	-2.1616
C	4.7700	-0.7743	-1.0300
H	5.1649	-1.0002	-0.0302
H	4.9973	0.2754	-1.2555
H	5.3292	-1.3929	-1.7450
C	3.0103	-2.5538	-0.7991
H	3.6306	-3.1930	-1.4425
H	1.9637	-2.8248	-0.9723
H	3.2569	-2.8057	0.2404

FeH_(PNHP)

Gibbs energy: -1008179.8 kcal mol-1

Atom	X	Y	Z
Fe	-0.0000	-0.0365	-0.0464
H	-0.0000	0.8037	1.2789
P	-2.1878	0.1230	-0.1935
P	2.1878	0.1230	-0.1935
O	-0.0000	-2.5268	1.4037
N	-0.0000	1.7912	-1.0812
C	-0.0000	-1.5132	0.8093
C	-2.4361	1.7204	-1.1147
H	-2.5145	1.4742	-2.1841
H	-3.3628	2.2336	-0.8269
C	-1.2197	2.5919	-0.8758
H	-1.2182	3.4679	-1.5445
H	-1.1929	2.9602	0.1585
C	1.2197	2.5919	-0.8758
H	1.1929	2.9602	0.1585
H	1.2182	3.4679	-1.5445
C	2.4361	1.7204	-1.1147
H	3.3628	2.2336	-0.8269
H	2.5145	1.4742	-2.1841
C	-3.2841	0.3264	1.3061
H	-4.3112	0.4105	0.9172
C	-2.9605	1.5994	2.0776
H	-3.6237	1.6816	2.9496
H	-3.0979	2.5070	1.4771
H	-1.9254	1.5856	2.4445
C	-3.1902	-0.8815	2.2297
H	-2.1708	-0.9893	2.6241
H	-3.4607	-1.8223	1.7353
H	-3.8646	-0.7537	3.0874
C	-3.0886	-1.0865	-1.3000
H	-2.6500	-0.8351	-2.2799
C	-2.7425	-2.5416	-1.0122
H	-3.1183	-2.8717	-0.0350
H	-1.6595	-2.7109	-1.0331
H	-3.2002	-3.1905	-1.7715
C	-4.5962	-0.8788	-1.3727
H	-5.0194	-1.4863	-2.1842
H	-4.8725	0.1659	-1.5658
H	-5.0912	-1.1946	-0.4443
C	3.2841	0.3264	1.3061
H	4.3112	0.4104	0.9172
C	2.9606	1.5995	2.0775
H	1.9255	1.5858	2.4444
H	3.0981	2.5071	1.4769
H	3.6238	1.6817	2.9495
C	3.1901	-0.8815	2.2298
H	3.8645	-0.7536	3.0875
H	3.4605	-1.8223	1.7355
H	2.1707	-0.9891	2.6242
C	3.0886	-1.0865	-1.3000
H	2.6499	-0.8351	-2.2799
C	4.5962	-0.8788	-1.3727
H	5.0912	-1.1945	-0.4443
H	4.8725	0.1659	-1.5659
H	5.0194	-1.4863	-2.1843
C	2.7425	-2.5416	-1.0122
H	3.2003	-3.1905	-1.7715
H	1.6595	-2.7110	-1.0330
H	3.1184	-2.8717	-0.0350
H	-0.0000	1.4791	-2.0542
H	-0.0000	-0.7271	-1.4732

Concerted_eq_proton_transfer_with_tbd

Gibbs energy: -527431.3 kcal mol-1

Atom	X	Y	Z
C	1.8611	2.7599	0.2880
C	3.0594	2.0079	-0.2480
C	1.6430	0.0160	-0.1006

C	0.6101	2.1805	-0.3405
H	4.3932	-0.3715	-1.1830
H	1.8182	2.6502	1.3808
H	3.9787	2.3106	0.2689
C	4.0975	-0.2406	-0.1274
H	-0.7204	0.2188	-0.0299
H	0.5795	2.4510	-1.4108
C	2.6599	-2.2354	-0.0759
C	3.8835	-1.5860	0.5310
H	2.3896	-3.1537	0.4582
H	4.7666	-2.2175	0.3849
N	1.5290	-1.3281	-0.0097
N	0.5372	0.7362	-0.1875
N	2.8905	0.5750	-0.0399
H	4.9042	0.3131	0.3688
H	3.7403	-1.4501	1.6118
H	2.8718	-2.5201	-1.1207
H	3.2027	2.2236	-1.3212
H	1.9552	3.8282	0.0611
H	-0.2907	2.6179	0.1126
O	-0.9800	-2.3472	-0.3218
N	-1.8580	-0.1805	0.1217
C	-1.6158	-1.6510	0.5921
H	-1.0537	-1.4628	1.5475
C	-2.5135	-0.0866	-1.1928
H	-2.2918	0.9079	-1.6105
H	-2.0569	-0.8491	-1.8348
C	-2.5350	0.6661	1.1179
H	-2.1035	0.4521	2.1051
H	-2.3221	1.7179	0.8752
H	0.5743	-1.7365	-0.1830
H	-2.6185	-2.0414	0.8900
C	-4.0354	0.4488	1.1263
H	-4.2855	-0.5615	1.4937
H	-4.5173	1.1759	1.7889
C	-4.0094	-0.2814	-1.0870
H	-4.4872	-0.1042	-2.0563
H	-4.2451	-1.3149	-0.7772
O	-4.5829	0.6358	-0.1670

Concerted_ax_proton_transfer_with_tbd

Gibbs energy: -527430.8 kcal mol-1

Atom	X	Y	Z
C	1.2543	2.7836	0.3449
C	2.5815	2.2580	-0.1529
C	1.4922	0.0522	-0.1072
C	0.1490	2.0197	-0.3536
H	4.2400	0.1210	-1.2224
H	1.1798	2.6361	1.4315
H	3.4141	2.6681	0.4330
C	3.9525	0.1970	-0.1593
H	-0.8931	-0.1370	0.0156
H	0.1558	2.2730	-1.4292
C	2.8683	-2.0063	-0.1118
C	3.9725	-1.1682	0.4920
H	2.7462	-2.9530	0.4283
H	4.9456	-1.6464	0.3343
N	1.6054	-1.2928	-0.0627
N	0.2793	0.5831	-0.1717
N	2.6321	0.8060	-0.0342
H	4.6702	0.8720	0.3229
H	3.8215	-1.0624	1.5751
H	3.1272	-2.2612	-1.1535
H	2.7447	2.5573	-1.2027
H	1.1795	3.8587	0.1444
H	-0.8351	2.3272	0.0245
O	-0.6614	-2.6902	-0.4942
N	-1.9156	-0.7790	0.2058
C	-1.3753	-2.2148	0.4970
H	-0.8292	-2.0487	1.4656
C	-2.7357	-0.7880	-1.0148
H	-2.0891	-1.0712	-1.8527
H	-3.5190	-1.5571	-0.9075
C	-2.6826	-0.2717	1.3524
H	-3.4419	-1.0224	1.6263
H	-1.9966	-0.1507	2.2018
H	0.7368	-1.8472	-0.2876
H	-2.3067	-2.7863	0.7478
C	-3.3585	1.0453	1.0356
H	-4.0189	1.3353	1.8596
H	-2.6061	1.8440	0.9102
C	-3.3651	0.5665	-1.2397
H	-2.5842	1.3265	-1.4255
H	-4.0263	0.5402	-2.1119
O	-4.1563	0.9556	-0.1288

Direct_eq_proton_transfer

Gibbs energy: -252264.0 kcal mol-1

Atom	X	Y	Z
C	1.6400	-0.4264	-0.5957
H	1.6742	0.5107	-1.1869
C	-0.4602	-1.2922	0.5867
C	0.0235	1.0901	0.6869
C	-1.5714	-0.9748	-0.3913
H	-0.8504	-1.3020	1.6121
H	-0.0064	-2.2675	0.3748
C	-1.1072	1.3103	-0.2953
H	-0.3490	1.1682	1.7161
H	0.8246	1.8254	0.5471
H	-2.3924	-1.6906	-0.2825
H	-1.1963	-1.0371	-1.4290
H	-1.5862	2.2782	-0.1160
H	-0.7203	1.3048	-1.3305
O	-2.1053	0.3153	-0.1512
N	0.5940	-0.2610	0.5179

H	1.3161	-1.2511	-1.2619
O	2.7062	-0.6772	0.2042
H	1.6502	-0.4984	1.0573

Direct_ax_proton_transfer

Gibbs energy: -252264.8 kcal mol-1

Atom	X	Y	Z
C	-2.2667	0.0407	0.9629
H	-2.6517	-0.8654	0.4534
C	-0.1286	-1.1842	0.3048
C	-0.1286	1.2502	0.2765
C	1.3684	-1.1295	0.5212
H	-0.3604	-1.2536	-0.7677
H	-0.5673	-2.0478	0.8195
C	1.3684	1.2005	0.4940
H	-0.3604	1.2946	-0.7974
H	-0.5673	2.1255	0.7709
H	1.8525	-1.9961	0.0603
H	1.5910	-1.1434	1.6030
H	1.8526	2.0562	0.0132
H	1.5910	1.2395	1.5753
O	1.9285	0.0288	-0.0688
N	-0.7430	0.0395	0.8482
H	-2.6518	0.9350	0.4330
O	-2.3489	0.0561	2.3175
H	-1.0020	0.0530	2.0308

Protonation_eq_with_triphenylguanidine

Gibbs energy: -815679.4 kcal mol-1

Atom	X	Y	Z
N	0.6890	-1.0382	-0.0677
C	0.3964	0.2078	0.2729
C	1.8890	-1.6740	0.2348
C	2.3664	-2.6343	-0.6758
H	1.7988	-2.8090	-1.5901
C	3.5485	-3.3286	-0.4412
H	3.8967	-4.0555	-1.1735
C	4.2892	-3.0936	0.7172
H	5.2177	-3.6302	0.9000
C	3.8121	-2.1651	1.6432
H	4.3687	-1.9782	2.5607
C	2.6275	-1.4716	1.4166
H	2.2798	-0.7528	2.1560
N	1.3671	1.1598	0.5662
H	1.0500	1.9510	1.1156
C	2.6628	1.2755	0.0456
C	3.6226	1.9494	0.8101
C	3.0199	0.7611	-1.2058
C	4.9243	2.0876	0.3413
H	3.3384	2.3479	1.7838
C	4.3309	0.8863	-1.6566
H	2.2772	0.2523	-1.8168
C	5.2914	1.5448	-0.8898
H	5.6597	2.6100	0.9501
H	4.5999	0.4690	-2.6251
H	6.3135	1.6376	-1.2498
N	-0.8889	0.5783	0.3682
C	-1.2891	1.9146	0.2493
C	-2.2723	2.4072	1.1227
C	-0.8239	2.7666	-0.7708
C	-2.7722	3.6997	0.9868
H	-2.6324	1.7573	1.9201
C	-1.3196	4.0604	-0.8958
H	-0.0782	2.3985	-1.4753
C	-2.2976	4.5375	-0.0211
H	-3.5335	4.0557	1.6789
H	-0.9458	4.6996	-1.6941
H	-2.6855	5.5482	-0.1272
O	-1.2605	-2.3797	-1.3386
N	-2.7929	-1.1943	0.0185
C	-2.1218	-2.5097	-0.2840
H	-1.6161	-2.7908	0.6547
C	-3.5643	-0.6350	-1.1244
H	-3.7105	0.4323	-0.9132
H	-2.9500	-0.7311	-2.0250
C	-3.6347	-1.2390	1.2404
H	-3.0772	-1.7610	2.0267
H	-3.7895	-0.2003	1.5585
H	-0.4555	-1.8897	-0.9809
H	-2.8857	-3.2613	-0.5170
H	-1.9329	-0.4438	0.2128
C	-4.9007	-1.3239	-1.2814
H	-4.7716	-2.3770	-1.5865
H	-5.4829	-0.8220	-2.0602
C	-4.9702	-1.9017	0.9749
H	-5.6010	-1.8243	1.8658
H	-4.8442	-2.9737	0.7448
O	-5.6555	-1.2592	-0.0835

Protonation_ax_with_triphenylguanidine

Gibbs energy: -815682.4 kcal mol-1

Atom	X	Y	Z
N	0.8560	-1.1369	-0.0158
C	0.3385	0.0455	0.2858
C	2.1404	-1.5303	0.3393
C	2.8248	-2.4104	-0.5189
H	2.3372	-2.7181	-1.4442
C	4.1062	-2.8604	-0.2187
H	4.6135	-3.5301	-0.9114
C	4.7435	-2.4536	0.9536
H	5.7487	-2.7981	1.1866

C	4.0639	-1.6050	1.8287
H	4.5386	-1.2892	2.7567
C	2.7803	-1.1556	1.5365
H	2.2681	-0.4958	2.2350
N	1.1221	1.1725	0.5137
H	0.6759	1.9212	1.0324
C	2.3700	1.4920	-0.0381
C	3.1860	2.3937	0.6559
C	2.8136	0.9655	-1.2562
C	4.4304	2.7512	0.1481
H	2.8379	2.8011	1.6047
C	4.0694	1.3137	-1.7453
H	2.1820	0.2779	-1.8139
C	4.8868	2.2041	-1.0505
H	5.0523	3.4518	0.7019
H	4.4068	0.8873	-2.6881
H	5.8662	2.4718	-1.4404
N	-0.9901	0.1860	0.3804
C	-1.5892	1.4571	0.3057
C	-2.3890	1.9041	1.3660
C	-1.4935	2.2585	-0.8448
C	-3.0936	3.1030	1.2737
H	-2.4494	1.2921	2.2658
C	-2.1926	3.4583	-0.9313
H	-0.8732	1.9231	-1.6764
C	-3.0024	3.8844	0.1234
H	-3.7142	3.4282	2.1068
H	-2.1110	4.0624	-1.8333
H	-3.5538	4.8191	0.0486
O	-0.7772	-2.6445	-1.4927
N	-2.5854	-1.8242	-0.1934
C	-1.6575	-2.9678	-0.4994
H	-1.1623	-3.2059	0.4567
C	-3.3718	-1.4425	-1.3933
H	-2.6760	-1.0454	-2.1402
H	-3.8411	-2.3529	-1.7953
C	-3.4715	-2.1932	0.9356
H	-3.9422	-3.1589	0.6993
H	-2.8474	-2.3141	1.8298
H	-0.0664	-2.0802	-1.0523
H	-2.2842	-3.8183	-0.8058
H	-1.8821	-0.9283	0.1090
C	-4.4268	-0.4192	-1.0385
H	-5.0505	-0.2182	-1.9149
H	-3.9596	0.5321	-0.7261
C	-4.5309	-1.1380	1.1631
H	-4.0688	-0.1984	1.5116
H	-5.2294	-1.4797	1.9333
O	-5.2783	-0.8965	-0.0125

Deprotonation_eq_with_triphenylguanidine

Gibbs energy: -815677.8 kcal mol-1

Atom	X	Y	Z
N	-0.7123	-0.9722	-0.0947
C	-0.4311	0.3233	-0.3509
C	-1.8986	-1.6430	-0.4057
C	-2.2696	-2.7197	0.4140
H	-1.6359	-2.9736	1.2627
C	-3.4350	-3.4360	0.1624
H	-3.7060	-4.2626	0.8168
C	-4.2589	-3.0927	-0.9093
H	-5.1767	-3.6447	-1.0996
C	-3.8846	-2.0358	-1.7388
H	-4.5089	-1.7634	-2.5882
C	-2.7125	-1.3238	-1.5033
H	-2.4370	-0.5069	-2.1667
N	-1.4514	1.2482	-0.4752
H	-1.2026	2.0967	-0.9723
C	-2.7136	1.2599	0.1406
C	-3.7430	1.9695	-0.4879
C	-2.9682	0.6045	1.3497
C	-5.0144	2.0064	0.0745
H	-3.5391	2.4783	-1.4297
C	-4.2497	0.6292	1.8926
H	-2.1723	0.0632	1.8563
C	-5.2799	1.3249	1.2617
H	-5.8057	2.5594	-0.4275
H	-4.4391	0.1024	2.8259
H	-6.2779	1.3399	1.6935
N	0.8261	0.6828	-0.5033
C	1.2434	2.0125	-0.3907
C	2.1586	2.5046	-1.3357
C	0.8874	2.8464	0.6861
C	2.6860	3.7882	-1.2219
H	2.4427	1.8586	-2.1667
C	1.4167	4.1287	0.7930
H	0.2053	2.4745	1.4498
C	2.3164	4.6111	-0.1588
H	3.3902	4.1474	-1.9703
H	1.1303	4.7546	1.6366
H	2.7293	5.6133	-0.0676
O	1.1304	-2.3203	0.9485
N	2.9314	-1.1387	-0.0760
C	2.0567	-2.4468	0.0151
H	1.6801	-2.5161	-1.0311
C	3.4901	-0.7060	1.2315
H	3.7508	0.3564	1.1389
H	2.6950	-0.8183	1.9757
C	3.9818	-1.1794	-1.1236
H	3.5488	-1.6277	-2.0258
H	4.2642	-0.1429	-1.3480
H	0.1332	-1.5954	0.4189
H	2.7767	-3.2702	0.1774
H	2.2014	-0.4255	-0.3394
C	4.7115	-1.5204	1.5861
H	4.4425	-2.5753	1.7676
H	5.1626	-1.1280	2.5025

C	5.1907	-1.9596	-0.6501
H	5.9893	-1.8809	-1.3945
H	4.9485	-3.0293	-0.5299
O	5.6936	-1.4409	0.5661

Deprotonation_ax_with_triphenylguanidine

Gibbs energy: -815679.4 kcal mol-1

Atom	X	Y	Z
N	-0.8778	-1.0543	-0.0841
C	-0.3665	0.1644	-0.3595
C	-2.1673	-1.5057	-0.3795
C	-2.7218	-2.4785	0.4664
H	-2.1393	-2.8227	1.3198
C	-3.9994	-2.9766	0.2351
H	-4.4117	-3.7242	0.9104
C	-4.7548	-2.5140	-0.8423
H	-5.7594	-2.8931	-1.0162
C	-4.1998	-1.5637	-1.6990
H	-4.7700	-1.2023	-2.5532
C	-2.9161	-1.0714	-1.4839
H	-2.4998	-0.3351	-2.1682
N	-1.2004	1.2576	-0.5076
H	-0.7959	2.0389	-1.0126
C	-2.4468	1.5117	0.0882
C	-3.3197	2.3839	-0.5717
C	-2.8336	0.9411	1.3050
C	-4.5707	2.6650	-0.0339
H	-3.0114	2.8251	-1.5191
C	-4.0967	1.2119	1.8239
H	-2.1571	0.2766	1.8376
C	-4.9733	2.0694	1.1609
H	-5.2400	3.3423	-0.5607
H	-4.3926	0.7502	2.7639
H	-5.9578	2.2758	1.5744
N	0.9351	0.2940	-0.5053
C	1.5651	1.5399	-0.4079
C	2.4832	1.9077	-1.4035
C	1.4195	2.3834	0.7090
C	3.2350	3.0744	-1.2890
H	2.5974	1.2544	-2.2688
C	2.1723	3.5487	0.8179
H	0.7231	2.1067	1.5006
C	3.0864	3.9016	-0.1766
H	3.9420	3.3373	-2.0740
H	2.0500	4.1831	1.6941
H	3.6764	4.8107	-0.0829
O	0.6776	-2.6725	1.0387
N	2.7108	-1.8361	0.1093
C	1.6214	-2.9626	0.1628
H	1.2960	-3.0052	-0.9021
C	3.2935	-1.5815	1.4482
H	2.4778	-1.2762	2.1110
H	3.7103	-2.5318	1.8095
C	3.7633	-2.1214	-0.8921
H	4.1954	-3.1004	-0.6458
H	3.2876	-2.1794	-1.8785
H	-0.1650	-1.8035	0.4569
H	2.2121	-3.8745	0.3876
H	2.1490	-0.9924	-0.1812
C	4.3659	-0.5201	1.3530
H	4.8468	-0.3870	2.3269
H	3.9236	0.4488	1.0537
C	4.8258	-1.0434	-0.8640
H	4.4007	-0.0816	-1.2029
H	5.6447	-1.3107	-1.5389
O	5.3740	-0.8940	0.4307

Protonation_eq_with_Methyl_formanilide

Gibbs energy: -528366.5 kcal mol-1

Atom	X	Y	Z
C	1.2603	2.1456	-0.2310
H	-1.1221	2.7243	0.3380
H	-0.5154	0.4663	-0.1580
O	0.3876	3.0566	-0.1955
O	-2.0437	2.3966	0.5530
N	-1.6198	0.1681	-0.1173
C	-1.8431	-0.8609	-1.1658
H	-1.7447	-0.3816	-2.1470
H	-1.0406	-1.6014	-1.0579
C	-1.8728	-0.4064	1.2304
H	-1.8040	0.4037	1.9627
H	-1.0644	-1.1238	1.4236
N	0.9249	0.8556	-0.1963
C	1.8657	-0.1764	-0.0725
C	2.7636	-0.2532	1.0051
C	1.8559	-1.2283	-1.0018
C	3.6376	-1.3299	1.1281
H	2.7620	0.5395	1.7525
C	2.7253	-2.3080	-0.8715
H	1.1620	-1.1756	-1.8408
C	3.6246	-2.3651	0.1929
H	4.3286	-1.3647	1.9689
H	2.7037	-3.1074	-1.6102
H	4.3055	-3.2073	0.2951
C	-2.3593	1.4540	-0.3855
H	-3.4382	1.2615	-0.3686
H	-2.0625	1.7390	-1.4084
C	2.6973	2.5927	-0.3570
H	3.0782	2.8997	0.6248
H	3.3661	1.8249	-0.7574
H	2.7263	3.4761	-1.0024
C	-3.2165	-1.0987	1.2854
H	-4.0407	-0.3722	1.1743
H	-3.3370	-1.5923	2.2546

C	-3.1887	-1.5359	-1.0044
H	-3.2757	-2.3540	-1.7264
H	-4.0168	-0.8319	-1.1954
O	-3.3201	-2.0994	0.2873

Protonation_ax_with_Methyl_formanilide

Gibbs energy: -528370.3 kcal mol-1

Atom	X	Y	Z
C	0.3655	2.4131	0.1946
H	-2.1592	2.3701	0.2005
H	-0.9151	0.3052	-0.0577
O	-0.6940	3.0973	0.2008
O	-2.9976	1.8258	0.1241
N	-1.8995	-0.2295	-0.2971
C	-1.6402	-1.2452	-1.3460
H	-2.6087	-1.6158	-1.7112
H	-1.1135	-0.7517	-2.1725
C	-2.4646	-0.8544	0.9232
H	-3.4791	-1.2066	0.6854
H	-2.5292	-0.0858	1.6996
N	0.3511	1.0849	0.1019
C	1.5386	0.3314	0.0431
C	2.0414	-0.2956	1.1919
C	2.1814	0.0991	-1.1816
C	3.1510	-1.1347	1.1168
H	1.5432	-0.1171	2.1449
C	3.2919	-0.7384	-1.2547
H	1.7889	0.5794	-2.0784
C	3.7804	-1.3629	-0.1068
H	3.5255	-1.6144	2.0195
H	3.7771	-0.9074	-2.2146
H	4.6439	-2.0220	-0.1656
C	-2.7809	0.8686	-0.8254
H	-3.7329	0.4074	-1.1250
H	-2.2613	1.2486	-1.7214
C	1.6826	3.1466	0.2923
H	2.3272	2.7183	1.0690
H	2.2327	3.0760	-0.6545
H	1.5000	4.2011	0.5126
C	-1.5867	-2.0016	1.3679
H	-2.0426	-2.5057	2.2254
H	-0.5949	-1.6262	1.6776
C	-0.8117	-2.3818	-0.7856
H	0.1980	-2.0243	-0.5127
H	-0.7019	-3.1644	-1.5424
O	-1.4372	-2.9641	0.3411

Deprotonation_eq_with_Methyl_formanilide

Gibbs energy: -528364.2 kcal mol-1

Atom	X	Y	Z
C	-4.8396	0.0057	0.9649
C	-5.1942	-1.1855	0.3335
C	-4.2559	-1.8404	-0.4638
C	-2.9847	-1.3033	-0.6405
C	-2.6278	-0.0976	-0.0208
C	-3.5646	0.5417	0.8022
H	-5.5564	0.5182	1.6039
H	-6.1895	-1.6036	0.4678
H	-4.5158	-2.7751	-0.9572
H	-2.2512	-1.8094	-1.2663
H	-3.2869	1.4532	1.3276
N	-1.3129	0.3682	-0.1876
H	-0.4709	-0.4487	-0.1940
C	-0.9404	1.6333	-0.4367
O	0.2716	1.9514	-0.4675
N	2.3173	0.1722	0.0539
C	2.9944	-0.3161	-1.1766
H	3.2876	0.5650	-1.7601
H	2.2578	-0.8942	-1.7430
C	3.2821	0.8224	0.9783
H	3.5847	1.7722	0.5209
H	2.7617	1.0388	1.9188
C	1.3945	-0.9150	0.7277
H	0.9789	-0.3355	1.5833
H	2.0845	-1.6788	1.1304
O	0.5087	-1.3620	-0.1441
H	1.6022	0.8843	-0.2276
C	-1.9571	2.7052	-0.7220
H	-2.9062	2.3180	-1.1032
H	-2.1618	3.2806	0.1888
H	-1.5234	3.3964	-1.4505
C	4.4930	-0.0561	1.2102
H	4.2211	-0.9650	1.7730
H	5.2324	0.4934	1.8013
C	4.2082	-1.1443	-0.8263
H	4.7427	-1.4161	-1.7415
H	3.9156	-2.0789	-0.3171
O	5.1095	-0.4133	-0.0122

Deprotonation_ax_with_Methyl_formanilide

Gibbs energy: -528365.7 kcal mol-1

Atom	X	Y	Z
C	0.3655	2.4131	0.1946
H	-2.1592	2.3701	0.2005
H	-0.9151	0.3052	-0.0577
O	-0.6940	3.0973	0.2008
O	-2.9976	1.8258	0.1241
N	-1.8995	-0.2295	-0.2971
C	-1.6402	-1.2452	-1.3460

H	-2.6087	-1.6158	-1.7112
H	-1.1135	-0.7517	-2.1725
C	-2.4646	-0.8544	0.9232
H	-3.4791	-1.2066	0.6854
H	-2.5292	-0.0858	1.6996
N	0.3511	1.0849	0.1019
C	1.5386	0.3314	0.0431
C	2.0414	-0.2956	1.1919
C	2.1814	0.0991	-1.1816
C	3.1510	-1.1347	1.1168
H	1.5432	-0.1171	2.1449
C	3.2919	-0.7384	-1.2547
H	1.7889	0.5794	-2.0784
C	3.7804	-1.3629	-0.1068
H	3.5255	-1.6144	2.0195
H	3.7771	-0.9074	-2.2146
H	4.6439	-2.0220	-0.1656
C	-2.7809	0.8686	-0.8254
H	-3.7329	0.4074	-1.1250
H	-2.2613	1.2486	-1.7214
C	1.6826	3.1466	0.2923
H	2.3272	2.7183	1.0690
H	2.2327	3.0760	-0.6545
H	1.5000	4.2011	0.5126
C	-1.5867	-2.0016	1.3679
H	-2.0426	-2.5057	2.2254
H	-0.5949	-1.6262	1.6776
C	-0.8117	-2.3818	-0.7856
H	0.1980	-2.0243	-0.5127
H	-0.7019	-3.1644	-1.5424
O	-1.4372	-2.9641	0.3411

Concerted_ax_proton_transfer_with_methanol

Gibbs energy: -324860.4 kcal mol-1

Atom	X	Y	Z
N	-0.0733	0.1467	0.2992
C	0.3504	-0.9725	-0.5802
H	-0.4205	-1.1126	-1.3446
H	1.2907	-0.6778	-1.0657
C	0.8885	0.3332	1.4091
H	1.8408	0.6737	0.9800
H	0.4975	1.1098	2.0758
C	-0.3457	1.4246	-0.4885
H	0.5459	1.6190	-1.1048
O	-1.4666	1.2640	-1.2334
H	-2.1790	0.8315	-0.5263
H	-0.4238	2.2063	0.2901
O	-2.6301	0.1443	0.5784
H	-1.0793	-0.0670	0.6651
C	-3.3858	-0.9761	0.2765
H	-4.4527	-0.7327	0.1083
H	-3.0444	-1.5043	-0.6409
H	-3.3653	-1.7253	1.0912
C	1.0582	-0.9759	2.1492
H	1.8166	-0.8697	2.9305
H	0.1044	-1.2582	2.6311
C	0.5376	-2.2199	0.2528
H	-0.4285	-2.5343	0.6888
H	0.9095	-3.0367	-0.3728
O	1.4844	-2.0090	1.2829

Protonation_ax_with_formanilide

Gibbs energy: -503725.0 kcal mol-1

Atom	X	Y	Z
C	-0.3705	2.3515	0.1415
H	2.1310	2.4271	-0.1441
H	0.8975	0.3136	-0.0414
O	0.6262	3.1049	0.2049
O	2.9481	1.8609	-0.1858
N	1.9098	-0.2293	0.2197
C	1.6473	-1.2287	1.2823
H	2.6138	-1.5845	1.6687
H	1.1051	-0.7251	2.0933
C	2.4971	-0.8713	-0.9800
H	3.5107	-1.2123	-0.7213
H	2.5681	-0.1171	-1.7702
N	-0.3390	1.0557	-0.1478
C	-1.5340	0.3175	-0.0665
C	-1.9196	-0.4918	-1.1445
C	-2.3146	0.3024	1.0985
C	-3.0516	-1.2970	-1.0584
H	-1.3192	-0.4730	-2.0537
C	-3.4522	-0.4986	1.1780
H	-2.0058	0.9069	1.9512
C	-3.8239	-1.3058	0.1038
H	-3.3353	-1.9186	-1.9058
H	-4.0451	-0.4997	2.0909
H	-4.7069	-1.9376	0.1710
C	2.7880	0.8688	0.7441
H	3.7620	0.4218	0.9910
H	2.3032	1.2175	1.6706
C	1.6392	-2.0362	-1.4177
H	2.1165	-2.5527	-2.2561
H	0.6501	-1.6784	-1.7537
C	0.8370	-2.3835	0.7346
H	-0.1738	-2.0420	0.4460
H	0.7275	-3.1538	1.5040
O	1.4807	-2.9802	-0.3748
H	-1.3759	2.7917	0.3191

Deprotonation_ax_with_formanilide

Gibbs energy: -503722.9 kcal mol-1

Atom	X	Y	Z
C	-4.8588	0.5895	0.6111
C	-5.3701	-0.5815	0.0548
C	-4.4943	-1.5029	-0.5197
C	-3.1273	-1.2496	-0.5534
C	-2.6119	-0.0681	-0.0046
C	-3.4892	0.8437	0.5972
H	-5.5287	1.3080	1.0797
H	-6.4394	-0.7794	0.0771
H	-4.8784	-2.4248	-0.9522
H	-2.4420	-1.9610	-1.0116
H	-3.1005	1.7406	1.0756
N	-1.2225	0.1323	-0.0474
H	-0.5249	-0.7919	-0.0648
C	-0.6723	1.3403	-0.1752
O	0.5514	1.5638	-0.1711
N	2.3314	-0.5420	0.3475
C	3.0607	-1.1298	-0.8023
H	2.3224	-1.3965	-1.5640
H	3.5510	-2.0445	-0.4422
C	3.2754	-0.0659	1.3855
H	2.6978	0.4386	2.1689
H	3.7695	-0.9471	1.8147
C	1.2461	-1.5307	0.9079
H	0.8563	-0.9589	1.7822
H	1.8506	-2.3807	1.2865
O	0.3623	-1.8295	-0.0236
H	1.7564	0.2684	0.0214
C	4.2848	0.8751	0.7639
H	5.0285	1.1733	1.5090
H	3.7771	1.7881	0.4028
C	4.0754	-0.1373	-1.3213
H	3.5624	0.7515	-1.7313
H	4.6667	-0.5889	-2.1235
O	4.9765	0.2552	-0.3020
H	-1.3793	2.1812	-0.3117

TBD_assisted_protonation (diphenylformamide)

Gibbs energy: -672158.3 kcal mol-1

Atom	X	Y	Z
O	-0.1859	1.6767	2.4154
N	-1.2883	0.0088	0.0756
C	-0.8009	0.6217	2.4221
H	-1.8995	0.5811	2.5550
C	-1.7618	1.2324	-0.3859
C	-0.9607	1.9781	-1.2724
H	-0.0415	1.5313	-1.6509
C	-1.3319	3.2538	-1.6889
H	-0.6890	3.7980	-2.3794
C	-2.5171	3.8314	-1.2368
C	-3.3203	3.1094	-0.3515
H	-4.2434	3.5480	0.0254
C	-2.9521	1.8371	0.0710
H	-3.5826	1.3053	0.7823
H	-0.2824	-0.3577	2.4436
H	1.3065	1.0108	1.3361
H	-2.8095	4.8273	-1.5627
C	-2.0991	-1.0999	0.2023
C	-1.5660	-2.2398	0.8546
C	-3.4074	-1.2251	-0.3224
C	-2.2952	-3.4156	0.9817
H	-0.5509	-2.1894	1.2492
C	-4.1279	-2.4075	-0.1874
H	-3.8533	-0.3916	-0.8607
C	-3.5901	-3.5153	0.4690
H	-1.8438	-4.2669	1.4902
H	-5.1300	-2.4632	-0.6117
H	-4.1625	-4.4344	0.5735
C	2.4205	-1.5173	-2.4225
C	3.5936	-1.6266	-1.4712
C	2.2847	-0.2137	0.0262
C	1.1367	-1.5845	-1.6233
H	4.9708	-0.9929	1.0267
H	2.4777	-0.5672	-2.9711
H	4.5438	-1.4715	-1.9951
C	4.7306	-0.2345	0.2634
H	0.0868	-0.2872	-0.1766
H	0.9837	-2.6081	-1.2442
C	3.3770	1.1553	1.7835
C	4.6007	1.1353	0.8947
H	3.1559	2.1664	2.1406
H	5.4991	1.3618	1.4783
N	2.2239	0.6891	1.0286
N	1.1551	-0.6438	-0.5130
N	3.4995	-0.6019	-0.4333
H	5.5383	-0.2473	-0.4773
H	4.5055	1.8972	0.1093
H	3.5392	0.5195	2.6681
H	3.6296	-2.6283	-1.0123
H	2.4579	-2.3291	-3.1570
H	0.2641	-1.3436	-2.2456

FeN_assisted_CN_cleavage (diphenylformamide)

Gibbs energy: -1404446.6 kcal mol-1

Atom	X	Y	Z
Fe	-1.1424	0.2979	-0.0769
H	-2.0824	0.5816	-1.1746
P	-1.9425	-1.7882	-0.2338
P	-0.3470	2.3388	-0.5202
O	-3.2232	1.2107	1.7049

O	1.5460	-3.8287	0.5610
N	0.2469	-0.3518	-1.4663
H	0.9845	-0.7043	-0.8251
N	2.2314	-1.1873	0.5586
C	-2.3670	0.8377	1.0033
C	-0.7724	-2.5840	-1.4208
H	0.0174	-3.0603	-0.8161
H	-1.2578	-3.3653	-2.0203
C	-0.1789	-1.5023	-2.2952
H	0.6855	-1.8864	-2.8603
H	-0.9099	-1.1262	-3.0247
C	0.8492	0.6799	-2.3413
H	0.1421	0.8626	-3.1612
H	1.7762	0.2871	-2.7902
C	1.1195	1.9556	-1.5766
H	1.3880	2.7792	-2.2509
H	1.9638	1.8098	-0.8865
C	-3.6272	-2.0386	-0.9873
H	-3.7807	-3.1290	-0.9754
C	-3.6860	-1.5692	-2.4362
H	-4.6907	-1.7561	-2.8382
H	-2.9730	-2.0930	-3.0837
H	-3.4962	-0.4892	-2.5161
C	-4.7252	-1.3671	-0.1731
H	-4.6318	-0.2733	-0.2172
H	-4.7223	-1.6633	0.8824
H	-5.7081	-1.6287	-0.5868
C	-1.8284	-2.9269	1.2395
H	-0.7349	-3.0366	1.3360
C	-2.3644	-2.3227	2.5305
H	-3.4510	-2.1692	2.5002
H	-1.8949	-1.3595	2.7635
H	-2.1554	-3.0005	3.3691
C	-2.4110	-4.3110	0.9845
H	-2.1351	-4.9843	1.8070
H	-2.0360	-4.7608	0.0562
H	-3.5085	-4.2880	0.9382
C	-1.4391	3.4748	-1.5216
H	-0.9605	4.4658	-1.4688
C	-1.5263	3.0602	-2.9858
H	-1.9466	2.0493	-3.0900
H	-0.5576	3.0875	-3.4977
H	-2.1968	3.7469	-3.5196
C	-2.8427	3.5642	-0.9306
H	-3.4221	4.3270	-1.4675
H	-2.8524	3.8285	0.1326
H	-3.3712	2.6069	-1.0426
C	0.4047	3.4139	0.8053
H	1.0441	2.6995	1.3495
C	1.2822	4.5351	0.2609
H	0.7052	5.2573	-0.3326
H	2.1075	4.1670	-0.3591
H	1.7267	5.0898	1.0984
C	-0.6308	3.9660	1.7772
H	-0.1240	4.4078	2.6457
H	-1.3185	3.1979	2.1512
H	-1.2282	4.7620	1.3124
C	2.0323	-2.9797	1.3351
C	3.3347	-1.0565	-0.2735
C	4.0541	0.1442	-0.4733
H	3.8081	1.0277	0.1131
C	5.0636	0.2312	-1.4279
H	5.5871	1.1782	-1.5564
C	5.4090	-0.8675	-2.2140
H	6.2011	-0.7949	-2.9562
C	4.7119	-2.0628	-2.0248
H	4.9587	-2.9363	-2.6272
C	3.6955	-2.1602	-1.0822
H	3.1414	-3.0903	-0.9620
H	1.4207	-2.5765	2.1738
H	3.1191	-3.0037	1.5854
C	1.9808	-0.2860	1.5828
C	0.6328	-0.0333	1.9222
C	2.9678	0.2778	2.4191
C	0.2894	0.7296	3.0358
H	-0.1509	-0.5982	1.3785
C	2.6193	1.0596	3.5156
H	4.0173	0.0710	2.2176
C	1.2797	1.2955	3.8344
H	-0.7602	0.8811	3.2841
H	3.4059	1.4724	4.1456
H	1.0131	1.8981	4.7000

Diphenylformamide

Gibbs energy: -396295.4 kcal mol-1

Atom	X	Y	Z
O	-3.0514	-1.4263	0.0022
N	-2.4434	0.7949	0.0065
C	-3.3410	-0.2428	0.0082
H	-4.3865	0.1181	0.0224
C	-1.0342	0.5521	0.0797
C	-0.2015	1.0847	-0.9043
H	-0.6340	1.6610	-1.7205
C	1.1725	0.8751	-0.8318
H	1.8216	1.2918	-1.5989
C	0.8745	-0.3999	1.1947
H	1.2919	-0.9771	2.0170
C	-0.5001	-0.1862	1.1343
H	-1.1595	-0.5872	1.9004
C	1.7131	0.1302	0.2154
H	2.7868	-0.0354	0.2697
C	-2.9107	2.1403	-0.0939
C	-2.4185	3.1068	0.7861
C	-3.8514	2.4883	-1.0640
C	-2.8776	4.4163	0.6987
H	-1.6822	2.8258	1.5371
C	-4.3191	3.7996	-1.1328

H	-4.2025	1.7396	-1.7716
C	-3.8336	4.7660	-0.2558
H	-2.4934	5.1659	1.3869
H	-5.0542	4.0667	-1.8888
H	-4.1930	5.7906	-0.3183

Adduct Morpholine

Gibbs energy: -1187889.2 kcal mol-1

Atom	X	Y	Z
Fe	-0.8212	0.1595	-0.3075
H	-1.9842	0.5575	0.6107
P	-0.1626	2.2260	0.1551
P	-1.7559	-1.8596	-0.1164
O	-2.3435	0.9265	-2.6274
N	0.2155	-0.3581	1.4514
H	1.0841	-0.6933	1.0266
C	-1.7137	0.6149	-1.6873
C	0.9442	2.0072	1.6313
H	1.9715	1.9073	1.2544
H	0.9292	2.8799	2.2984
C	0.5199	0.7562	2.3748
H	1.2880	0.4456	3.1009
H	-0.4001	0.9489	2.9420
C	-0.3599	-1.4854	2.2122
H	-1.2242	-1.0942	2.7643
H	0.3664	-1.8477	2.9575
C	-0.7793	-2.5947	1.2751
H	-1.3199	-3.3868	1.8091
H	0.1087	-3.0511	0.8129
C	-1.4405	3.4601	0.7432
H	-0.8836	4.3944	0.9101
C	-2.0991	3.0756	2.0618
H	-2.8267	3.8491	2.3437
H	-1.3821	2.9904	2.8874
H	-2.6428	2.1246	1.9768
C	-2.5028	3.6975	-0.3229
H	-3.0894	2.7850	-0.4979
H	-2.0819	4.0141	-1.2850
H	-3.1997	4.4804	0.0060
C	0.9410	3.2301	-0.9826
H	1.8892	2.6753	-0.9166
C	0.4899	3.1861	-2.4366
H	-0.4493	3.7327	-2.5940
H	0.3448	2.1576	-2.7887
H	1.2493	3.6550	-3.0778
C	1.2054	4.6607	-0.5299
H	2.0088	5.0980	-1.1385
H	1.5187	4.7239	0.5204
H	0.3215	5.2995	-0.6603
C	-3.5528	-1.9698	0.4036
H	-3.8567	-3.0110	0.2096
C	-3.7737	-1.6811	1.8834
H	-3.4544	-0.6613	2.1406
H	-3.2493	-2.3847	2.5410
H	-4.8450	-1.7545	2.1157
C	-4.4248	-1.0374	-0.4323
H	-5.4839	-1.2024	-0.1915
H	-4.3029	-1.1798	-1.5118
H	-4.1901	0.0125	-0.2084
C	-1.6063	-3.2074	-1.4060
H	-0.5597	-3.1077	-1.7319
C	-1.8022	-4.6197	-0.8646
H	-2.8038	-4.7646	-0.4365
H	-1.0654	-4.8892	-0.0998
H	-1.6979	-5.3440	-1.6846
C	-2.5179	-2.9731	-2.6059
H	-2.2350	-3.6463	-3.4265
H	-2.4704	-1.9463	-2.9892
H	-3.5660	-3.1917	-2.3589
C	0.6688	-0.9337	-2.7096
C	2.1455	-0.0720	-1.1717
C	1.7403	-1.8792	-3.2307
H	0.7208	-0.0070	-3.3353
H	-0.3109	-1.3853	-2.9170
C	3.2292	-1.0256	-1.6513
H	2.2649	0.8646	-1.7724
H	2.3819	0.1946	-0.1271
H	1.6439	-2.0371	-4.3135
H	1.6452	-2.8609	-2.7251
H	4.2276	-0.5736	-1.5749
H	3.2100	-1.9447	-1.0321
O	3.0461	-1.3664	-3.0146
N	0.8270	-0.6513	-1.3000

Concerted proton transfer with morpholine

Gibbs energy: -337010.2 kcal mol-1

Atom	X	Y	Z
C	-1.3033	2.1522	0.3688
H	-0.9893	2.2817	1.4397
C	-1.7710	-0.0892	1.3446
C	-1.8932	0.2161	-1.0353
H	-2.8349	0.1602	1.5065
H	-1.2142	0.1779	2.2514
H	-2.9858	0.3578	-0.9610
H	-1.5201	0.8343	-1.8590
N	-1.2282	0.6170	0.1973
H	-2.4072	2.3722	0.3440
O	-0.5779	2.8068	-0.5206
H	0.9568	1.8752	-0.5260
C	1.8724	0.1637	-1.3988
C	2.1618	0.8935	0.9120
C	2.1783	-1.2443	-0.9374
H	2.7899	0.6662	-1.7340

H	1.1538	0.1571	-2.2263
C	2.4580	-0.5453	1.2744
H	3.0909	1.4353	0.6896
H	1.6460	1.4049	1.7338
H	2.6787	-1.8116	-1.7279
H	1.2377	-1.7677	-0.6796
H	3.1651	-0.5977	2.1078
H	1.5248	-1.0542	1.5809
O	3.0423	-1.2382	0.1854
N	1.2885	0.9099	-0.2732
H	0.1998	0.5398	-0.0047
H	-1.6936	-1.1738	1.1964
H	-1.6940	-0.8405	-1.2570

Morpholine

Gibbs energy: -180462.6 kcal mol-1

Atom	X	Y	Z
C	-3.1765	-2.8663	-0.8622
C	-4.1810	-2.0911	1.1666
C	-3.9554	-1.8114	-1.6185
H	-3.7631	-3.8062	-0.8633
H	-2.2244	-3.0597	-1.3713
C	-4.9369	-1.0540	0.3637
H	-4.8173	-2.9926	1.2658
H	-3.9794	-1.7053	2.1734
H	-4.2167	-2.1596	-2.6238
H	-3.3457	-0.8945	-1.7135
H	-5.9164	-0.8480	0.8090
H	-4.3602	-0.1116	0.3357
O	-5.1746	-1.5055	-0.9602
N	-2.9208	-2.3817	0.4904
H	-2.3920	-3.0717	1.0159

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