Supporting Information for "**Ligand Lone-Pair Influence on Hydrocarbon C-H Activation: A Computational Perspective**"

Daniel H. Ess,[‡] *T. Brent Gunnoe,*[*&] *Thomas R. Cundari,*[*%] *William A. Goddard III,*[◊] *and*

Roy A. Periana[#]

A contribution from the Center for Catalytic Hydrocarbon Functionalization.
[‡]Department of Chemistry and Biochemistry, Brigham Young University, Provo, Utah 84602; [&]Department of Chemistry, University of Virginia, Charlottesville, Virginia 22904; [%]Department of Chemistry, Center for Advanced Scientific Computing and Modeling (CASCaM); University of North Texas, Denton, Texas 76203; [◊]Materials and Process Simulation Center, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California 91125; [#]The Scripps Research Institute, Jupiter, Florida 33458, Department of Chemistry

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XYZ coordinates and absolute energies (au)

1Me-Py: B3LYP/LACVP** SCF = -1083.41444605318
Total internal energy, Utot (SCFE + ZPE + U): -1083.033507 hartrees
Total enthalpy, Htot (Utot + pV): -1083.032562 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1083.115186 hartrees

Ir1	0.0511392233	0.0673747121	0.0048323112
O2	0.0483548616	0.0632735373	2.0507828707
O3	2.0910542636	-0.1067639750	-0.1241590883
O4	0.3102138736	2.2578192065	0.0958897918
O5	0.0200066201	0.0835557531	-2.0475399773
C6	-0.1223339998	-1.9971330036	-0.0495057845
C7	1.1270157404	0.0116248432	2.7421789376
C8	2.4376767819	-0.0849093847	2.2515746237
C9	2.8465573704	-0.1309383679	0.9049229780
C10	0.4522846099	2.9404359626	-0.9628751877
C11	0.4201461833	2.4566732760	-2.2937714409
C12	0.2264443714	1.1442364580	-2.7446841558
H13	3.2258611264	-0.1197107494	2.9939814206
H14	0.5729932676	3.1981530170	-3.0691226247
H15	0.6890144729	-2.4637940190	0.5231734421
H16	-1.0741073551	-2.3445884125	0.3741134587
H17	-0.0498784644	-2.3440882206	-1.0879890201
C18	4.3245148785	-0.2140379632	0.5851924003
H19	4.6165287072	0.6580845496	-0.0096993903
H20	4.9445970256	-0.2566231509	1.4827821068
H21	4.5165461172	-1.1006504339	-0.0276316957
C22	0.8976381955	0.0705228484	4.2377412471
H23	0.4069608960	1.0157792279	4.4949075605
H24	0.2225269130	-0.7373257512	4.5382832377
H25	1.8272774155	-0.0104695731	4.8042496866
C26	0.6837473723	4.4269876635	-0.7464878497
H27	-0.1192671377	4.8329474288	-0.1225961878
H28	1.6200346088	4.5691700462	-0.1956157007
H29	0.7331158724	4.9914824309	-1.6802223953
C30	0.2561911726	0.8761023501	-4.2365684981
H31	0.3465917644	1.7915044685	-4.8245872306
H32	1.1019427944	0.2194017923	-4.4679202445
H33	-0.6533492878	0.3446206014	-4.5346348552
N34	-1.9729180154	0.3093019082	0.0485157031
C35	-2.7668871266	-0.2672669568	-0.8812536632
C36	-4.1433861094	-0.0831300449	-0.8919999819
C37	-4.7339114114	0.7152263346	0.0867683756
C38	-3.9121078563	1.3040058413	1.0471781370
C39	-2.5420433184	1.0824946100	1.0002045567
H40	-2.2538109961	-0.8659041312	-1.6233312446

H41	-4.7368088435	-0.5642107311	-1.6624127428
H42	-5.8077056250	0.8753388302	0.1003148466
H43	-4.3207087555	1.9344999844	1.8299784108
H44	-1.8572481931	1.5103345187	1.7210959796

1OH-Py: B3LYP/LACVP** SCF = -1119.32355046304

Total internal energy, Utot (SCFE + ZPE + U): -1118.965858 hartrees

Total enthalpy, Htot (Utot + pV): -1118.964913 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1119.046084 hartrees

Ir1	0.0524013895	0.1319909106	-0.0116591316
O2	0.0247344366	0.0759117181	2.0257290231
O3	2.0822628747	-0.1084993491	-0.1422558223
O4	0.3346423653	2.2115964645	0.1267733970
O5	0.0420154297	0.1319097992	-2.0575706940
O6	-0.2324426491	-1.8684888221	-0.0729494939
C7	1.0877033416	-0.0808814949	2.7196273661
C8	2.3999193339	-0.2186388868	2.2360087824
C9	2.8208562000	-0.2284041296	0.8962418988
C10	0.5107468980	2.9282140522	-0.9164846051
C11	0.4776394794	2.4929788658	-2.2554766222
C12	0.2605972304	1.1920678795	-2.7425642379
H13	3.1750213284	-0.3383489288	2.9832035320
H14	0.6487474912	3.2550685525	-3.0064291128
H15	0.3285024521	-2.1756763893	-0.7989527345
C16	4.2931604100	-0.3946195289	0.5849670958
H17	4.6388612292	0.4577475295	-0.0093527323
H18	4.9036427494	-0.4740918671	1.4865090338
H19	4.4371115890	-1.2926358228	-0.0250183268
C20	0.8422643701	-0.1058533293	4.2130647075
H21	0.3507907890	0.8241054765	4.5181291359
H22	0.1598076685	-0.9273624789	4.4540017743
H23	1.7643920667	-0.2269644403	4.7846240664
C24	0.7788509396	4.3921716289	-0.6299682920
H25	-0.0179776286	4.7943264340	0.0042129388
H26	1.7139432683	4.4857412674	-0.0669281409
H27	0.8510722390	4.9920088679	-1.5393835118
C28	0.2819293869	0.9542158546	-4.2379822043
H29	0.3920613141	1.8796150252	-4.8065401534
H30	1.1118515169	0.2831899024	-4.4848997598
H31	-0.6409464740	0.4504398066	-4.5423601277
N32	-1.9826637552	0.3419176902	0.0535603815
C33	-2.7588970493	-0.6058033361	-0.5142685872
C34	-4.1454638490	-0.5122622781	-0.4986646708
C35	-4.7518708435	0.5772829236	0.1248109269
C36	-3.9408733758	1.5401035867	0.7260986410
C37	-2.5613405275	1.3910301873	0.6736768426

H38	-2.2045345662	-1.4469034010	-0.9176074028
H39	-4.7349304828	-1.2931387030	-0.9677320063
H40	-5.8335331065	0.6724249452	0.1475983922
H41	-4.3652541745	2.4010882981	1.2317578075
H42	-1.8780468557	2.1084156013	1.1119534464

1NH2-Py: SCF = -1099.44798365850

Total internal energy, Utot (SCFE + ZPE + U): -1099.077973 hartrees

Total enthalpy, Htot (Utot + pV): -1099.077029 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1099.158597 hartrees

Ir1	0.0537944501	0.1059328368	0.0073645509
O2	0.0343792661	0.1161450436	2.0499535044
O3	2.0908591476	-0.0838529844	-0.1233718954
O4	0.3127610470	2.2343768521	0.0794125137
O5	0.0242477144	0.0601745379	-2.0417167543
N6	-0.0513834131	-1.9357812140	0.0273102927
C7	1.1085340119	0.0010527837	2.7418874889
C8	2.4159109848	-0.1293061422	2.2556977158
C9	2.8319050895	-0.1702839922	0.9115115841
C10	0.4456064267	2.9152598752	-0.9861535006
C11	0.4074808079	2.4279342958	-2.3129949564
C12	0.2196825228	1.1110001734	-2.7557462901
H13	3.1969169524	-0.2170609556	3.0012085493
H14	0.5516292977	3.1676320969	-3.0916278705
H15	-0.9762291576	-2.2273248684	0.3543112891
H16	-0.0141632091	-2.2421976308	-0.9486260689
C17	4.3059127053	-0.3277678984	0.6023787370
H18	4.6292501721	0.4827259406	-0.0587864673
H19	4.9241150945	-0.3265624677	1.5023450982
H20	4.4623580562	-1.2680136796	0.0630755709
C21	0.8727141140	0.0205101269	4.2372856079
H22	0.3390033715	0.9362271521	4.5131427109
H23	0.2343919629	-0.8245452171	4.5164882388
H24	1.8033379549	-0.0346046315	4.8052721282
C25	0.6717776849	4.3996609220	-0.7671660830
H26	-0.1194295953	4.7974904557	-0.1235261968
H27	1.6198740120	4.5462812804	-0.2380900511
H28	0.6960590399	4.9665764224	-1.7002062710
C29	0.2456714925	0.8277959657	-4.2437581001
H30	0.3192999145	1.7383645627	-4.8414114465
H31	1.1007985084	0.1822862705	-4.4724506975
H32	-0.6570770687	0.2793880567	-4.5314748205
N33	-1.9672256231	0.3351958808	0.0430911308
C34	-2.7490540194	-0.2952824328	-0.8630693649
C35	-4.1308521071	-0.1520634615	-0.8687462364
C36	-4.7378473286	0.6592052674	0.0884780298

C37	-3.9276857389	1.3020154172	1.0252235890
C38	-2.5527137118	1.1193462099	0.9766199147
H39	-2.2222277893	-0.9013303576	-1.5887987658
H40	-4.7149654157	-0.6738191558	-1.6195788384
H41	-5.8156790630	0.7887132675	0.1041106928
H42	-4.3505218191	1.9434953441	1.7912418257
H43	-1.8759217523	1.5861449083	1.6809161223

1Me: SCF = -835.05393517354

Total internal energy, Utot (SCFE + ZPE + U): -834.770225 hartrees

Total enthalpy, Htot (Utot + pV): -834.769281 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -834.840917 hartrees

Ir1	0.0982043335	0.0072686382	0.0018561995
O2	0.0293404884	-0.0308517072	2.0332938430
O3	2.0629637512	-0.0101473708	-0.1189892246
O4	0.2288497603	2.2000082497	0.0976099608
O5	-0.0132907468	0.0580871740	-2.0342975274
C6	-0.1206962144	-2.0397577857	-0.0698481894
C7	1.0807786291	-0.0152931082	2.7536056334
C8	2.4073320712	-0.0131444877	2.2680606329
C9	2.8137406285	-0.0052142552	0.9352168716
C10	0.3742302115	2.9025537777	-0.9484709296
C11	0.3705723513	2.4308661182	-2.2839476335
C12	0.1701386490	1.1223558699	-2.7379240823
H13	3.1960497051	-0.0044203687	3.0101557699
H14	0.5155110469	3.1790662934	-3.0541056875
H15	0.3975607495	-2.5522365868	0.7498284132
H16	-1.1947312509	-2.2763812979	0.0174482440
H17	0.2364935496	-2.4346819291	-1.0265747727
C18	4.2841586049	0.0163935031	0.5840325830
H19	4.5057206799	0.9057103015	-0.0147950942
H20	4.9123356456	0.0197068683	1.4762414743
H21	4.5311963398	-0.8573965768	-0.0271633375
C22	0.8304331223	0.0183507820	4.2431664839
H23	0.3442632402	0.9642617605	4.5060934710
H24	0.1434672365	-0.7872922762	4.5187270586
H25	1.7518585157	-0.0777477452	4.8202545630
C26	0.5567186731	4.3904628925	-0.7086003503
H27	-0.3060178443	4.7767144178	-0.1558801888
H28	1.4377709470	4.5488644169	-0.0774970157
H29	0.6729688277	4.9595675846	-1.6333591991
C30	0.1485751956	0.8560083288	-4.2281483082
H31	0.2874524508	1.7649365456	-4.8164778404
H32	0.9388060582	0.1405480669	-4.4791644547
H33	-0.8039900764	0.3917254383	-4.5035749631

1Me-CH_4: SCF = -875.58904508991

Total internal energy, Utot (SCFE + ZPE + U): -875.254491 hartrees

Total enthalpy, Htot (Utot + pV): -875.253546 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -875.331899 hartrees

Ir1	0.0527837972	0.0241193463	0.0112657721
O2	0.0236349505	-0.0041874903	2.0517967078
O3	2.0388580302	-0.0286844240	-0.1380133857
O4	0.2080455721	2.2236523153	0.0935255211
O5	0.0193640474	0.0540075824	-2.0383550220
C6	0.0117680993	-2.0563332054	-0.0509270155
C7	1.0958138879	-0.0245973569	2.7447646291
C8	2.4110821655	-0.0566159729	2.2401927391
C9	2.8037635005	-0.0504881872	0.8978642633
C10	0.4077739983	2.9072094618	-0.9586301582
C11	0.4457675598	2.4207983892	-2.2858958698
C12	0.2554928514	1.1062235084	-2.7361407917
H13	3.2087593674	-0.0745366614	2.9725728557
H14	0.6349022029	3.1576934446	-3.0574101642
H15	1.0382117740	-2.4395909401	-0.0084790198
H16	-0.5499479770	-2.4803342346	0.7908415525
H17	-0.4368666829	-2.3986178229	-0.9909511250
C18	-2.4918769746	0.4811669061	0.0453740472
H19	-2.8710323029	0.5722351716	-0.9717355944
H20	-3.2595781876	0.1133118600	0.7303942284
H21	-2.1082741314	1.4318689317	0.4064733530
H22	-1.7755956815	-0.4015591587	0.0430300544
C23	4.2740895140	-0.0629344220	0.5437325411
H24	4.5146537895	0.8247625503	-0.0504782822
H25	4.9095326275	-0.0823325876	1.4308053353
H26	4.4952646016	-0.9373001196	-0.0767525416
C27	0.8743592859	0.0010002597	4.2406048138
H28	0.3755364600	0.9360993416	4.5173586454
H29	0.2087082538	-0.8190214139	4.5273650066
H30	1.8083426972	-0.0814373616	4.7994431055
C31	0.6215372049	4.3931344941	-0.7297863308
H32	-0.2218522772	4.7991648520	-0.1620087652
H33	1.5180392638	4.5368887692	-0.1166735130
H34	0.7334522089	4.9552835023	-1.6593272420
C35	0.3256981695	0.8261322709	-4.2236584081
H36	0.4413979236	1.7357968623	-4.8159185222
H37	1.1721267719	0.1600544613	-4.4238217415
H38	-0.5791495241	0.2990222168	-4.5419796397

1Me-CH_4-TS: SCF = -875.57180785823

Total internal energy, Utot (SCFE + ZPE + U): -875.240098 hartrees

Total enthalpy, Htot (Utot + pV): -875.239154 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -875.314162 hartrees

Ir1	-0.0335729649	0.0125811670	-0.0048381856
O2	-0.0080770694	-0.0429722476	2.0435838842
O3	2.0633360333	0.0148992677	-0.1484136438
O4	0.3606870629	2.1537052352	0.1208961034
O5	-0.0623390565	0.0618277298	-2.0552338694
C6	0.1642583997	-2.0932472545	-0.1042716863
C7	1.0753340037	0.0084306702	2.7235690456
C8	2.3910313805	0.0494018791	2.2313514728
C9	2.8091126207	0.0530190878	0.8895725430
C10	0.5845706864	2.8430727673	-0.9267642724
C11	0.5405327164	2.3922598498	-2.2621140292
C12	0.2385742034	1.1060760035	-2.7362702828
H13	3.1760104970	0.0868228987	2.9766158067
H14	0.7634026412	3.1321291906	-3.0212275175
H15	1.2406463041	-2.2676198986	-0.1736360957
H16	-0.2330978126	-2.5852745631	0.7876655421
H17	-0.3174263517	-2.4967954858	-0.9983583937
C18	-2.1023524770	0.6983255066	0.1063619907
H19	-2.6300852696	0.5842349747	-0.8423829628
H20	-2.6922519103	0.2816979647	0.9256879366
H21	-1.9084205734	1.7516972835	0.3116469437
H22	-1.3830282628	-0.7696048348	0.0009055370
C23	4.2917959140	0.1032493413	0.5839821293
H24	4.5017621751	0.9764527711	-0.0424553506
H25	4.9053499292	0.1519886490	1.4855839337
H26	4.5732199517	-0.7822378606	0.0044699564
C27	0.8490342083	0.0326839950	4.2198940982
H28	0.3015336645	0.9431464554	4.4865956201
H29	0.2238547954	-0.8173442604	4.5100259718
H30	1.7838048683	0.0025408617	4.7825656736
C31	0.9254758938	4.2979434877	-0.6650988589
H32	0.1067430638	4.7683038375	-0.1106143484
H33	1.8145943658	4.3497643495	-0.0277934352
H34	1.1085551764	4.8618036466	-1.5819996917
C35	0.2568157758	0.8551511280	-4.2296778888
H36	0.4344809566	1.7662260663	-4.8038583795
H37	1.0425165920	0.1280227043	-4.4616916661
H38	-0.6945175422	0.4112111924	-4.5388092878

1OH: SCF = -870.97837607535

Total internal energy, Utot (SCFE + ZPE + U): -870.717073 hartrees

Total enthalpy, Htot (Utot + pV): -870.716129 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -870.784909 hartrees

Ir1	0.4057806525	0.1187621743	0.1879107897
O2	0.1330539744	-0.9630108126	1.7292410658

C3	1.2104259795	-1.7608866858	-1.9119192946
O4	1.3481441196	-1.4727811451	-0.6761077059
C5	-0.2211845187	2.8640131006	0.9971318116
O6	-0.5417081053	1.6344233908	1.1707163414
C7	1.7035628243	2.6208169937	-0.6195882637
C8	0.8076125564	3.3555329126	0.1754969885
H9	0.9369831267	4.4307660171	0.1663090904
O10	1.7386751368	1.3487162458	-0.7735559348
C11	-0.4185706750	0.0256903362	-2.6212267448
C12	0.3967509471	-1.0884550498	-2.8471667500
H13	0.3930212541	-1.4868032315	-3.8542123138
O14	-0.5706658761	0.6691016833	-1.5175558545
H15	-0.3498407998	-0.4500771728	2.4000065411
C16	2.7798728175	3.3501191660	-1.3935985351
H17	2.6896853578	3.1114552880	-2.4581404286
H18	2.7238492165	4.4319687353	-1.2610625773
H19	3.7638628284	2.9984683177	-1.0663903377
C20	-1.0717243918	3.8347481857	1.7842612351
H21	-0.7219245100	4.8643873897	1.6924377395
H22	-2.1065957825	3.7770012291	1.4295096484
H23	-1.0758991524	3.5459458231	2.8398604938
C24	-1.2522832355	0.5864331539	-3.7525616196
H25	-2.3100498915	0.5655624203	-3.4707094874
H26	-0.9835699462	1.6343571513	-3.9213092132
H27	-1.1171570232	0.0274340145	-4.6801580667
C28	2.0168480571	-2.9594531782	-2.3582980816
H29	1.7619325064	-3.8209251784	-1.7332562274
H30	1.8464482026	-3.2092792242	-3.4070117089
H31	3.0818454032	-2.7545866833	-2.2064854098

1OH-CH$_4$: SCF = -911.49174028100

Total internal energy, Utot (SCFE + ZPE + U): -911.180644 hartrees

Total enthalpy, Htot (Utot + pV): -911.179700 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -911.256887 hartrees

Ir1	0.3112940449	0.1120804997	0.1509879109
O2	1.2597883684	-0.3733570751	1.8558372842
C3	1.1829371022	-1.7404695303	-1.9620990342
O4	1.2638103753	-1.4741738442	-0.7124563613
C5	-0.2504619604	2.8524429748	1.0083120512
O6	-0.6587834850	1.6417016131	1.0886350942
C7	1.8270771895	2.5066547686	-0.3637629178
C8	0.9084449542	3.2917153687	0.3422591352
H9	1.1162928399	4.3537960757	0.3813686755
O10	1.7803629892	1.2332792145	-0.5522778961
C11	-0.5063910812	-0.0238175933	-2.7163734264
C12	0.3842476910	-1.0926574692	-2.9216219052

H13	0.4567768246	-1.4691167166	-3.9347525841
O14	-0.7404482655	0.5732159770	-1.6097029475
C15	-1.7238646220	-1.4953167906	0.8729562395
H16	-0.7376642543	-1.2151897369	1.3157615344
H17	1.0426764313	0.3149153231	2.5012714352
H18	-2.0430086956	-0.9218731541	0.0018635962
H19	-1.6478269317	-2.5516421962	0.6123310374
H20	-2.4386065908	-1.3278562766	1.6816120404
C21	3.0346991117	3.1464378969	-1.0086010562
H22	3.0383181339	2.9250155689	-2.0807464412
H23	3.0492586779	4.2280541054	-0.8646991504
H24	3.9468065057	2.7143474088	-0.5846747490
C25	-1.1349230865	3.8562486941	1.7108927018
H26	-0.7220186698	4.8660438160	1.6798295048
H27	-2.1231241502	3.8600301914	1.2383323715
H28	-1.2766129055	3.5555135642	2.7537119342
C29	-1.2997582039	0.5105270595	-3.8910667222
H30	-2.3700226515	0.4477112515	-3.6681660029
H31	-1.0645326347	1.5705144035	-4.0352609805
H32	-1.0943336749	-0.0301831354	-4.8169558861
C33	2.0644053037	-2.8932300107	-2.3910535435
H34	1.8199065461	-3.7804302551	-1.7983582381
H35	1.9587902116	-3.1271169427	-3.4520492859
H36	3.1091666567	-2.6439712539	-2.1782916052

1OH-CH_4-TS: SCF = -911.47509302615

Total internal energy, Utot (SCFE + ZPE + U): -911.168792 hartrees

Total enthalpy, Htot (Utot + pV): -911.167848 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -911.241343 hartrees

Ir1	0.2048112456	0.0675741639	0.0978802733
O2	0.9292190391	-0.6062277225	1.9391235594
C3	1.1002111010	-1.7541484519	-2.0209737467
O4	1.1642109065	-1.5127980584	-0.7668655161
C5	-0.3304804451	2.8342901798	0.9290851476
O6	-0.7397031945	1.6217330306	1.0349900748
C7	1.7810971153	2.4975986170	-0.4066352677
C8	0.8278852954	3.2782139292	0.2741280531
H9	1.0150786053	4.3446431439	0.3025883161
O10	1.7544986513	1.2306301188	-0.5743163966
C11	-0.5035763926	0.0433894495	-2.7608041706
C12	0.3380959502	-1.0581700008	-2.9779449784
H13	0.4078186057	-1.4153515594	-3.9981346216
O14	-0.7306571088	0.6289790856	-1.6429426958
C15	-1.4331394307	-1.3242005837	0.9358688144
H16	-0.2926258031	-1.0436153862	1.5627220706
H17	0.7622246503	0.1107092176	2.5705306560

H18	-1.9393150247	-1.0845651250	-0.0033008652
H19	-1.2994338073	-2.4098667431	0.9600134175
H20	-2.0950022351	-0.9782303969	1.7357682241
C21	2.9905947874	3.1702455410	-1.0189642179
H22	3.0243699208	2.9518633898	-2.0912953744
H23	2.9845568891	4.2518369418	-0.8721217522
H24	3.9006023989	2.7522696321	-0.5762690813
C25	-1.2351818917	3.8414202122	1.6033807961
H26	-0.8170363336	4.8496521210	1.5922225076
H27	-2.2050430808	3.8518605771	1.0936577853
H28	-1.4188606219	3.5368311674	2.6384708053
C29	-1.2524827404	0.6482324124	-3.9290390958
H30	-2.3277612008	0.6316151215	-3.7234665437
H31	-0.9631662224	1.6985193937	-4.0413903780
H32	-1.0582855293	0.1220146642	-4.8654344125
C33	1.9493232754	-2.9262747697	-2.4611580707
H34	1.6512466247	-3.8220697321	-1.9070863429
H35	1.8662645637	-3.1212439386	-3.5319144348
H36	2.9962746069	-2.7266505420	-2.2109879628

1OH-CH_4-Product: SCF = -911.52008345094

Total internal energy, Utot (SCFE + ZPE + U): -911.207838 hartrees

Total enthalpy, Htot (Utot + pV): -911.206893 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -911.283148 hartrees

Ir1	0.0651484011	0.0051594145	0.0363719761
O2	0.9478039932	-0.4679901535	1.9618570689
C3	0.9223260183	-1.8716759050	-2.0461764501
O4	1.0120245433	-1.5947007565	-0.8008040237
C5	-0.4090160346	2.7958396100	0.9420632007
O6	-0.8247825021	1.5750175495	1.0239583734
C7	1.7467263277	2.5293448508	-0.3645632416
C8	0.7430339622	3.2723883813	0.3129471530
H9	0.8975443967	4.3438134463	0.3628634952
O10	1.7643361542	1.2775023287	-0.5419510446
C11	-0.6321029238	-0.0372069131	-2.7855023865
C12	0.1601455388	-1.1740816752	-3.0007321219
H13	0.1948752411	-1.5506946453	-4.0158105818
O14	-0.8138651924	0.5784959881	-1.6739989962
C15	-1.5525280963	-1.1872890544	0.5323804862
H16	0.6215202477	-1.3545168802	2.1847697260
H17	0.4723385905	0.1449556716	2.5476986213
H18	-1.8946472266	-1.7758958412	-0.3276253444
H19	-1.3183792581	-1.9106488026	1.3346341743
H20	-2.3841259376	-0.5629544298	0.8795949076
C21	2.9343817920	3.2835352005	-0.9374833082
H22	2.9763145919	3.1178734438	-2.0193580488

H23	2.8921889924	4.3573681876	-0.7427652574
H24	3.8594635504	2.8773380516	-0.5156125232
C25	-1.3284467985	3.7805413900	1.6348766602
H26	-0.9300449151	4.7969353494	1.6331111791
H27	-2.3023880158	3.7779551647	1.1331764740
H28	-1.5008965131	3.4633474678	2.6686557636
C29	-1.3782282004	0.5859037014	-3.9449242654
H30	-2.4498088811	0.6086505206	-3.7213189109
H31	-1.0531337591	1.6237029584	-4.0735802592
H32	-1.2183353968	0.0433637049	-4.8785092535
C33	1.7408794403	-3.0688707110	-2.4764908581
H34	1.4568489417	-3.9428861183	-1.8814784369
H35	1.6128509365	-3.2998421233	-3.5357162672
H36	2.8003974610	-2.8730508469	-2.2796626032

1OMe: SCF = -910.28036614018

Total internal energy, Utot (SCFE + ZPE + U): -909.989654 hartrees

Total enthalpy, Htot (Utot + pV): -909.988710 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -910.061226 hartrees

Ir1	0.5071553092	0.1773259189	0.2305509803
O2	0.5255685952	-0.8880592292	1.8014619004
C3	1.2487245129	-1.7437679708	-1.8501426715
O4	1.4718101347	-1.3999454204	-0.6410034584
C5	-0.2553003285	2.9537980381	0.8371412126
O6	-0.4650940836	1.7293000647	1.1495934549
C7	1.5587294797	2.6885551622	-0.8923363549
C8	0.6746270096	3.4368235412	-0.1000393705
H9	0.7214183076	4.5125442557	-0.2169395587
O10	1.6668242430	1.4116903737	-0.9320161843
C11	-0.5691092836	-0.1106869929	-2.4792888034
C12	0.3082092649	-1.1721210772	-2.7320013554
H13	0.2475810600	-1.6155058223	-3.7182761424
O14	-0.6730962089	0.5737681383	-1.3962733349
C15	2.5270624288	3.4042441559	-1.8088332736
H16	2.3928496478	3.0467060795	-2.8346760395
H17	2.3956944189	4.4875507347	-1.7848265304
H18	3.5534539563	3.1613219921	-1.5141482759
C19	-1.1244799774	3.9345518059	1.5921216097
H20	-0.8777418760	4.9726272631	1.3625405332
H21	-2.1750512068	3.7533499561	1.3401593797
H22	-1.0172329607	3.7665662979	2.6684757692
C23	-1.5409663325	0.3258591361	-3.5544955260
H24	-2.5666208503	0.2043279230	-3.1904779391
H25	-1.3981690341	1.3902788702	-3.7669304741
H26	-1.4195515361	-0.2447644331	-4.4769335503
C27	2.1030433478	-2.8969052698	-2.3285443453

H28	1.9799741947	-3.7464388444	-1.6496728791
H29	1.8547025505	-3.2065170142	-3.3453387305
H30	3.1575595710	-2.6037766322	-2.2908160225
C31	-0.0166689019	-0.5229652006	3.0601020587
H32	-0.4617184392	0.4766460002	3.0549507902
H33	-0.7819678482	-1.2598850240	3.3362797992
H34	0.7841349439	-0.5635626101	3.8095196437

1OMe-CH_4: SCF = -950.79407107182

Total internal energy, Utot (SCFE + ZPE + U): -950.453528 hartrees

Total enthalpy, Htot (Utot + pV): -950.452584 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -950.533641 hartrees

Ir1	0.2827214690	0.1029216635	0.1722299631
O2	1.1507244023	-0.5015135125	1.8791697032
C3	1.2232421051	-1.7163245704	-1.9340532736
O4	1.2477669741	-1.4878837801	-0.6745244057
C5	-0.3433348440	2.8639095626	0.9040193881
O6	-0.7297677310	1.6522976892	1.0302204984
C7	1.7927205843	2.4979254138	-0.3706488415
C8	0.8307556624	3.2957285866	0.2541214175
H9	1.0146413401	4.3629423598	0.2463284537
O10	1.7821474066	1.2126498043	-0.4906091744
C11	-0.4122915280	0.0403074366	-2.7246107716
C12	0.4791513378	-1.0309340272	-2.9122685125
H13	0.5977523751	-1.3812338820	-3.9304604668
O14	-0.6983510880	0.6128184468	-1.6167851847
C15	-1.8541342993	-1.4577740446	0.8060430632
H16	-0.8587290257	-1.2363951833	1.2568070040
H17	-2.1118683618	-0.8827052998	-0.0836427378
H18	-1.8417677298	-2.5221130278	0.5663638012
H19	-2.5733334364	-1.2297828722	1.5951149256
C20	3.0164253623	3.1289711763	-0.9935145712
H21	3.0798998014	2.8451779845	-2.0489138241
H22	2.9985186535	4.2172106385	-0.9141162233
H23	3.9167252017	2.7479106496	-0.5004096822
C24	-1.2623435947	3.8811898822	1.5391447995
H25	-0.9017390126	4.9033358276	1.4110593940
H26	-2.2607479658	3.7941550432	1.0981130784
H27	-1.3606955204	3.6662269448	2.6083698900
C28	-1.1416300177	0.6096596433	-3.9242516680
H29	-2.2223567678	0.5421151676	-3.7614348807
H30	-0.8990753492	1.6729978411	-4.0243754361
H31	-0.8869533032	0.0958276330	-4.8532052962
C32	2.1097196407	-2.8680972206	-2.3561597698
H33	1.8272414565	-3.7690643706	-1.8024108665
H34	2.0507634268	-3.0691832286	-3.4274645923

H35	3.1465148511	-2.6391271079	-2.0884559787
C36	1.2811391562	0.4184323330	2.9256107689
H37	0.3135793953	0.7930161683	3.3050736101
H38	1.7919518634	-0.0866557370	3.7590174677
H39	1.8913501855	1.2998040971	2.6574603683

1OMe-CH$_4$-TS: SCF = -950.77593567847

Total internal energy, Utot (SCFE + ZPE + U): -950.440019 hartrees

Total enthalpy, Htot (Utot + pV): -950.439075 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -950.516295 hartrees

Ir1	0.1975874666	0.0764242838	0.1094862759
O2	0.9246056500	-0.6644048722	1.9226034224
C3	1.1077758545	-1.7577961496	-1.9865636956
O4	1.1701500314	-1.5078469574	-0.7340823048
C5	-0.3863443436	2.8598075923	0.8466939205
O6	-0.7882965566	1.6494934401	0.9742130774
C7	1.7631554661	2.5081162184	-0.4234686424
C8	0.7897517385	3.2965205314	0.2150874121
H9	0.9659311678	4.3652330500	0.2179935630
O10	1.7535714845	1.2353133231	-0.5547506906
C11	-0.4910507470	0.0377136606	-2.7510007778
C12	0.3491209065	-1.0683354552	-2.9514990521
H13	0.4223853926	-1.4353283653	-3.9679514513
O14	-0.7240862359	0.6368393547	-1.6415854926
C15	-1.4489607793	-1.3176666713	0.9212309711
H16	-0.2948234155	-1.0737224407	1.5414689749
H17	-2.0052979529	-0.9753910683	0.0451767203
H18	-1.3313516381	-2.4012744253	0.8364660691
H19	-2.0622616098	-1.0446647043	1.7865082595
C20	2.9765413032	3.1754693143	-1.0341543898
H21	3.0345166134	2.9215815947	-2.0975722217
H22	2.9536440498	4.2612556516	-0.9244427183
H23	3.8833904136	2.7856328912	-0.5602578042
C24	-1.3186008218	3.8785664818	1.4640181688
H25	-0.9158083475	4.8921375044	1.4203793043
H26	-2.2790245098	3.8537279474	0.9376058554
H27	-1.5158598513	3.6115832688	2.5070294235
C28	-1.2312983298	0.6305382784	-3.9311153419
H29	-2.3081776617	0.6151850879	-3.7337243865
H30	-0.9416692753	1.6797793124	-4.0518808037
H31	-1.0299072399	0.0949925180	-4.8607216466
C32	1.9571947137	-2.9335518625	-2.4172928047
H33	1.6607609466	-3.8244164432	-1.8544225753
H34	1.8725617297	-3.1384903713	-3.4860996753
H35	3.0045535968	-2.7307975756	-2.1711031567
C36	0.9050741718	0.2008058263	3.0461329767

H37	-0.1001906872	0.5948415498	3.2529076558
H38	1.2473659566	-0.3683107016	3.9200823871
H39	1.5814027096	1.0530638086	2.8977296511

1OMe-CH_4-Product: SCF = -950.82211161965

Total internal energy, Utot (SCFE + ZPE + U): -950.480694 hartrees

Total enthalpy, Htot (Utot + pV): -950.479750 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -950.556728 hartrees

Ir1	0.0290251877	-0.0077448535	0.0707632867
O2	0.8313701499	-0.6722388200	1.9544487616
C3	0.9562142959	-1.8449117717	-2.0079065671
O4	0.9917650484	-1.6029790698	-0.7536764780
C5	-0.5415897900	2.8076891096	0.8174128612
O6	-0.9248839512	1.5883862554	0.9565861558
C7	1.7199054044	2.5219831780	-0.2881068087
C8	0.6492751702	3.2781870542	0.2477743161
H9	0.7697602725	4.3549698939	0.2294587650
O10	1.7865664709	1.2575926768	-0.3689116839
C11	-0.5167223050	0.0445113841	-2.7832808312
C12	0.2597116583	-1.1053130131	-2.9831423057
H13	0.3380837456	-1.4599411868	-4.0037746329
O14	-0.7457274991	0.6385017053	-1.6682234891
C15	-1.6401182191	-1.1719870877	0.4439037208
H16	0.0979016303	-1.1284487773	2.3941953511
H17	-1.9384222945	-1.7400939795	-0.4462052227
H18	-1.4721323596	-1.9154765940	1.2445096255
H19	-2.4782366519	-0.5331695946	0.7460773635
C20	2.9308077419	3.2678514227	-0.8223136050
H21	3.0155358055	3.0870780970	-1.8997342924
H22	2.8795656499	4.3448264490	-0.6478764990
H23	3.8393564197	2.8686783337	-0.3601951902
C24	-1.5371415442	3.8109645276	1.3646340939
H25	-1.1647943987	4.8364572255	1.3236139105
H26	-2.4661253086	3.7453872543	0.7876541323
H27	-1.7860407345	3.5583117328	2.4004697134
C28	-1.1852178402	0.7105924806	-3.9664155658
H29	-2.2699029678	0.7224428386	-3.8163386773
H30	-0.8573373492	1.7532262441	-4.0324464016
H31	-0.9606277001	0.2045656044	-4.9072461109
C32	1.7658049468	-3.0516321781	-2.4309659358
H33	1.4315867647	-3.9326058899	-1.8736796501
H34	1.6837289539	-3.2518858630	-3.5010592720
H35	2.8190018095	-2.8889187912	-2.1782561632
C36	1.3958106265	0.3210805739	2.8365828293
H37	0.6509475035	1.0758635536	3.0998771798
H38	1.7833344490	-0.1746037538	3.7313672019

H39	2.2103569964	0.7826597715	2.2809834489

1NH$_2$: SCF = -851.12551317314
Total internal energy, Utot (SCFE + ZPE + U): -850.851733 hartrees
Total enthalpy, Htot (Utot + pV): -850.850789 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -850.919696 hartrees

Ir1	0.1578451083	0.4246334650	0.3282328727
N2	0.3412393901	0.1251077645	2.1678076981
C3	2.8794252848	0.4614474323	-0.7723897319
O4	2.1671254671	0.7968682752	0.2382906491
C5	-2.7253706609	0.6554107640	-0.1751909674
O6	-1.8416103617	0.0369112351	0.5160547800
C7	-1.2830425061	2.2645066761	-1.4818156215
C8	-2.5085308412	1.6898680252	-1.1013881294
H9	-3.3933116001	2.0987824297	-1.5739331503
O10	-0.1176173729	1.9352478970	-1.0710692435
C11	1.1623637137	-0.6997975981	-2.2144761159
C12	2.4546346601	-0.2313188367	-1.9189794284
H13	3.2174201814	-0.4384266419	-2.6596817346
O14	0.1100520415	-0.5580796394	-1.5019384356
H15	-0.4353465689	-0.1254791921	2.7743639090
C16	-1.2795552232	3.4069647115	-2.4763197999
H17	-0.6629149068	3.1371261160	-3.3398869105
H18	-2.2838334159	3.6635538972	-2.8188020766
H19	-0.8212376886	4.2885146895	-2.0160250989
C20	-4.1385677801	0.1763636922	0.0774877589
H21	-4.8836383370	0.7838562424	-0.4394635317
H22	-4.2324544933	-0.8623307936	-0.2581448068
H23	-4.3433407513	0.1878984900	1.1524588626
C24	0.9319299636	-1.4735684097	-3.4961165221
H25	0.5877757445	-2.4846260612	-3.2533693345
H26	0.1368683782	-0.9928934697	-4.0750230448
H27	1.8328465735	-1.5416069811	-4.1088823228
C28	4.3289763459	0.8816206481	-0.6596429069
H29	4.7438258773	0.5182957794	0.2857808813
H30	4.9365165916	0.5106188758	-1.4870596010
H31	4.3866077743	1.9754107444	-0.6383668466
H32	1.2266152471	0.1979724821	2.6623187862

1NH$_2$-CH$_4$-TS: SCF = -891.61103176221
Total internal energy, Utot (SCFE + ZPE + U): -891.292227 hartrees
Total enthalpy, Htot (Utot + pV): -891.291283 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -891.365172 hartrees

Ir1	-0.0038091675	-0.0062799666	0.0061972662
N2	-0.0005172658	0.0399722356	2.0752843821
C3	2.7720146703	0.0083354506	-0.9598758293

O4	2.0392514314	0.0354411333	0.0927264039
C5	-2.7507453913	0.9634242397	-0.3525386399
O6	-2.0482966277	-0.0567380111	-0.0268481402
C7	-0.9415296106	2.6897891837	-0.6707259209
C8	-2.2766505471	2.2525326038	-0.6505170413
H9	-3.0271092663	2.9942418486	-0.8953812369
O10	0.1011303979	1.9885830267	-0.4261760577
C11	1.0296794014	-0.2672244835	-2.7715413988
C12	2.3477241183	-0.1301122637	-2.2904978102
H13	3.1307567882	-0.1336245611	-3.0390749072
O14	-0.0394092153	-0.2858548675	-2.0757246695
C15	-0.0321578746	-2.2609677559	0.6014272134
H16	-0.0175801052	-1.2658736418	1.4449533267
H17	-0.8213728667	0.4939515049	2.4646952784
H18	-0.0829149115	-2.3740578737	-0.4848687335
H19	0.8778933557	-2.7607352628	0.9444639096
H20	-0.9334745354	-2.7319152590	1.0048691968
C21	-0.6381672062	4.1336723607	-1.0097585904
H22	0.0095237946	4.1714651020	-1.8919842361
H23	-1.5420080991	4.7139845984	-1.2043377788
H24	-0.0853276132	4.5948769206	-0.1848544615
C25	-4.2377709721	0.6900054236	-0.4081422698
H26	-4.8210770870	1.5965427115	-0.5797278704
H27	-4.4429914357	-0.0224797467	-1.2146851477
H28	-4.5612455501	0.2213314113	0.5263087542
C29	0.8072233834	-0.4127080345	-4.2636512101
H30	0.2612023266	-1.3405211434	-4.4632597279
H31	0.1787617586	0.4116109830	-4.6174886050
H32	1.7410112365	-0.4174844953	-4.8293019716
C33	4.2515474235	0.1406825881	-0.6680628279
H34	4.5614919434	-0.6506991193	0.0221362527
H35	4.8608279075	0.0869831880	-1.5721339234
H36	4.4373706797	1.0967391331	-0.1672171584
H37	0.8473437052	0.4790647049	2.4218394583

1NH$_2$-CH$_4$-Product: SCF = -891.68221255816

Total internal energy, Utot (SCFE + ZPE + U): -891.355929 hartrees

Total enthalpy, Htot (Utot + pV): -891.354985 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -891.431507 hartrees

Ir1	0.0139247552	-0.1708638319	-0.0736180042
N2	0.0937399081	0.0912683763	2.0129831935
C3	2.7862558697	-0.2240603109	-1.0153442471
O4	2.0524807098	-0.1435988914	0.0339361835
C5	-2.7617704290	0.8169842083	-0.4317044536
O6	-2.0425188013	-0.1968051816	-0.1121353332
C7	-1.0316777182	2.6617454081	-0.6146267289

C8	-2.3433955838	2.1350799061	-0.6705780133
H9	-3.1273876206	2.8371203293	-0.9294107716
O10	0.0302110788	2.0242032963	-0.3358934706
C11	1.0149569759	-0.4258819780	-2.8055474640
C12	2.3428578950	-0.3636786303	-2.3394919649
H13	3.1155492857	-0.4192088621	-3.0968715160
O14	-0.0499026569	-0.3765419810	-2.1010201646
C15	0.0017659180	-2.2298700403	0.1591832549
H16	-0.4423170320	-0.6137383499	2.5166317844
H17	-0.2396210679	1.0145248717	2.2876974638
H18	0.5050654541	-2.7207651286	-0.6835808751
H19	0.5124734485	-2.5557701519	1.0787695685
H20	-1.0337893747	-2.5904979852	0.1927925031
C21	-0.8375630633	4.1387377264	-0.9146867437
H22	-0.2510122386	4.2427706385	-1.8345011776
H23	-1.7803149328	4.6768397765	-1.0359341557
H24	-0.2559700609	4.6027407412	-0.1117418722
C25	-4.2370772023	0.4879799265	-0.5515006055
H26	-4.8528819371	1.3755067701	-0.7104579371
H27	-4.3836194948	-0.2007735962	-1.3909118986
H28	-4.5750555875	-0.0307041777	0.3511219816
C29	0.7619042228	-0.5578504584	-4.2929879933
H30	0.1604801163	-1.4526647000	-4.4832444939
H31	0.1792462947	0.3017344212	-4.6411043333
H32	1.6867666547	-0.6181149315	-4.8699539679
C33	4.2719565764	-0.1469559088	-0.7353943316
H34	4.5545553559	-0.9282835547	-0.0221976174
H35	4.8710699507	-0.2575883388	-1.6411937392
H36	4.5063306587	0.8173207647	-0.2710707570
H37	1.0739037908	0.0130281721	2.2879721601

1NMe$_2$: SCF = -929.74422437874

Total internal energy, Utot (SCFE + ZPE + U): -929.411229 hartrees

Total enthalpy, Htot (Utot + pV): -929.410284 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -929.485033 hartrees

Ir1	0.7746107828	0.0918296395	0.2806352496
N2	1.2686363529	-0.7873340407	1.8817727800
C3	1.5841586197	-1.5804629074	-2.0125310689
O4	1.9186985495	-1.2014493830	-0.8335126204
C5	-0.5248480915	2.6512539232	0.9689496361
O6	-0.3903653044	1.4257707213	1.3232166967
C7	1.0319936564	2.7604397094	-1.0120870043
C8	0.1189721736	3.3069308845	-0.0915357819
H9	-0.1106713738	4.3586721149	-0.2120731182
O10	1.4220967081	1.5468824704	-1.0742494887
C11	-0.6651595007	-0.4672451101	-2.2646365811

C12	0.4010217927	-1.2746037672	-2.7024039684
H13	0.2938146023	-1.7178603925	-3.6850003434
O14	-0.7374567450	0.1725165903	-1.1626017897
C15	1.6552116351	3.6628472101	-2.0578771864
H16	1.4740459818	3.2465338173	-3.0539829557
H17	1.2640845601	4.6813396190	-2.0166357526
H18	2.7405463788	3.6916080665	-1.9132131128
C19	-1.4929528290	3.4283819266	1.8353538684
H20	-1.5573779674	4.4795071893	1.5480796289
H21	-2.4879044049	2.9766082924	1.7605620515
H22	-1.1853247895	3.3606541963	2.8840277782
C23	-1.8845502950	-0.3097508379	-3.1503797592
H24	-2.7632497917	-0.7108287100	-2.6338892616
H25	-2.0722981964	0.7541554168	-3.3270304233
H26	-1.7724329487	-0.8198220972	-4.1091956558
C27	2.6176722601	-2.4634434725	-2.6788711303
H28	2.8226804125	-3.3330867239	-2.0457917778
H29	2.2994782325	-2.8058531629	-3.6652946560
H30	3.5564592546	-1.9083253645	-2.7791240226
C31	0.8221522510	-0.3961289594	3.2184964149
H32	0.1380335011	0.4469617172	3.1583214404
H33	0.3152026043	-1.2412051387	3.7059646352
H34	1.6871706096	-0.1229645544	3.8399091831
C35	2.1510174922	-1.9514597510	1.9547016195
H36	3.0094106116	-1.7300334900	2.6050708976
H37	1.6134162531	-2.8053407579	2.3915523617
H38	2.5105662492	-2.2175830841	0.9635439965

1NMe$_2$-CH$_4$-TS: SCF = -970.22321321579

Total internal energy, Utot (SCFE + ZPE + U): -969.845275 hartrees

Total enthalpy, Htot (Utot + pV): -969.844331 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -969.924337 hartrees

Ir1	-0.0059692593	-0.0139022298	0.0060316013
N2	-0.0005340496	0.0324467132	2.0978214845
C3	2.7466848750	0.0030579863	-1.0722166061
O4	2.0493891915	0.0222880679	0.0039606540
C5	-2.7505397970	0.9213381340	-0.4530381961
O6	-2.0512243371	-0.0830143800	-0.0748754585
C7	-0.9507704497	2.6624491247	-0.7299727151
C8	-2.2803243586	2.2113286852	-0.7524993159
H9	-3.0284386971	2.9393717371	-1.0413695510
O10	0.0886496747	1.9736277542	-0.4383883346
C11	0.9514420055	-0.2828345687	-2.8210455055
C12	2.2841434874	-0.1353183758	-2.3891490929
H13	3.0423451920	-0.1315924547	-3.1627906029
O14	-0.0880068983	-0.3071140843	-2.0826087012

C15	-0.0010942809	-2.2850637343	0.5841044479
H16	0.0304696010	-1.2918930482	1.4077442381
H17	-0.0954469887	-2.3914786643	-0.4994587052
H18	0.9279397637	-2.7745275257	0.8883184004
H19	-0.8775472904	-2.7712963847	1.0225027199
C20	-0.6463258426	4.1033897712	-1.0792237487
H21	0.0360661829	4.1346996264	-1.9351712511
H22	-1.5469311245	4.6719313469	-1.3183910381
H23	-0.1318465810	4.5822544895	-0.2395748222
C24	-4.2307200935	0.6288289722	-0.5617112170
H25	-4.8071985214	1.5070420879	-0.8580708281
H26	-4.3886674915	-0.1680120334	-1.2961437311
H27	-4.6041219869	0.2607520830	0.3995215996
C28	0.6735341060	-0.4344606133	-4.3032398057
H29	0.1394375703	-1.3736698466	-4.4808926834
H30	0.0153686104	0.3764252398	-4.6331522310
H31	1.5847095883	-0.4217931327	-4.9046074830
C32	4.2341761684	0.1459382813	-0.8273109079
H33	4.5710392601	-0.6403865260	-0.1440161073
H34	4.8151850283	0.0925797063	-1.7498756837
H35	4.4289904434	1.1053909312	-0.3363901388
C36	-1.2423408840	0.4471004541	2.7327705112
H37	-2.0807867270	-0.1247388545	2.3287612815
H38	-1.1886696536	0.2587871975	3.8157260400
H39	-1.4627562190	1.5203011112	2.5943801541
C40	1.1638707525	0.6438574083	2.7231813992
H41	1.1720302178	1.7423483560	2.6155372486
H42	1.1742810154	0.4131291921	3.7991674418
H43	2.0795860785	0.2580979530	2.2752143105

1NMe$_2$-CH$_4$-Product: SCF = -970.29720867880

Total internal energy, Utot (SCFE + ZPE + U): -969.911421 hartrees

Total enthalpy, Htot (Utot + pV): -969.910477 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -969.991286 hartrees

Ir1	0.0181087116	-0.2356259981	-0.1035993969
N2	0.1072156089	-0.0690247135	2.0201360992
C3	2.7682778463	-0.3545630590	-1.1340711853
O4	2.0662245208	-0.2724736959	-0.0635626964
C5	-2.7361924267	0.7952159820	-0.5058280967
O6	-2.0394844177	-0.2254536609	-0.1586226313
C7	-0.9729927280	2.6102290421	-0.6842232931
C8	-2.2933616832	2.1044513427	-0.7480602868
H9	-3.0615468280	2.8151677044	-1.0296392407
O10	0.0741727224	1.9591245268	-0.3858830973
C11	0.9494981631	-0.4584013192	-2.8795735061
C12	2.2904480749	-0.4481272885	-2.4496533728

H13	3.0421030364	-0.5111405243	-3.2272884415
O14	-0.0910580457	-0.3962300398	-2.1423390430
C15	-0.0327904056	-2.2979437653	0.0817265089
H16	0.5121914866	-0.9631494659	2.3009384832
H17	0.5128108922	-2.7746106816	-0.7430344936
H18	0.4230081609	-2.6639545086	1.0175894841
H19	-1.0720097156	-2.6481636232	0.0502648115
C20	-0.7514325380	4.0798466583	-1.0017139102
H21	-0.1199446174	4.1623649370	-1.8932218168
H22	-1.6824711395	4.6234015055	-1.1767972535
H23	-0.2058441828	4.5547538218	-0.1797687291
C24	-4.2131816100	0.4868294200	-0.6559726429
H25	-4.8114294205	1.3812289016	-0.8411248216
H26	-4.3507140425	-0.2110605880	-1.4892422178
H27	-4.5804679676	-0.0142266881	0.2453143166
C28	0.6520020461	-0.5474110606	-4.3621895692
H29	0.0233033454	-1.4222556852	-4.5572846267
H30	0.0820077249	0.3347414489	-4.6728237585
H31	1.5587545789	-0.6161209478	-4.9664514938
C32	4.2628756919	-0.3362111208	-0.8908114005
H33	4.5342944989	-1.1407134887	-0.1993567763
H34	4.8349710827	-0.4508381430	-1.8134981273
H35	4.5441750151	0.6099203921	-0.4152482634
C36	-1.2137553835	0.0442110626	2.6835602967
H37	-1.8514213439	-0.7740255046	2.3503872141
H38	-1.1029548425	0.0223825097	3.7747644697
H39	-1.6751682171	0.9879325911	2.3865261476
C40	1.0334001373	1.0013714879	2.4709317973
H41	0.6539079406	1.9595804760	2.1145530429
H42	1.1124287397	1.0112288266	3.5651132322
H43	2.0088067651	0.8254551697	2.0195507932

2Me: SCF =-949.58238943029

Total internal energy, Utot (SCFE + ZPE + U): -949.317278 hartrees

Total enthalpy, Htot (Utot + pV): -949.316334 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -949.381300 hartrees

Ru1	0.7075284425	-0.1260602295	0.2851510465
N2	0.7043478768	-0.5398759506	-1.8500522001
C3	0.7466598442	0.1885743274	2.1253569408
C4	1.1531247140	-2.1586982406	0.6305786152
N5	0.1188141816	1.9654589088	-0.3673184114
N6	2.6258826322	0.4933047268	0.0518101991
N7	2.9557944884	1.2364177466	-1.0390221597
N8	1.2636538483	0.3730757113	-2.6842510874
N9	0.8066544162	2.4937475162	-1.4114751310
B10	1.9008258016	1.6575817417	-2.1024036649

H11	2.4326831074	2.2908186082	-2.9714646772
O12	0.8084391823	0.3583724935	3.2719833681
H13	1.7494119328	-2.3787289160	1.5220735386
H14	1.6657510861	-2.5838765507	-0.2385521398
H15	0.1875826434	-2.6830902421	0.7488272350
C16	4.2815379165	1.4991178896	-1.0039154158
H17	4.7395311268	2.0783614074	-1.7917837256
C18	4.8230660930	0.9192907489	0.1330883161
H19	5.8518014701	0.9418880868	0.4580498169
C20	0.2320866545	-1.5332225257	-2.6126071639
H21	-0.2451498890	-2.3878188289	-2.1540616607
C22	0.4777043527	-1.2628372727	-3.9669024842
H23	0.2189147179	-1.8693946052	-4.8212523225
C24	0.3553401073	3.7407097692	-1.6799978444
H25	0.7866193794	4.3204732514	-2.4831230267
C26	-0.6580178818	4.0390713838	-0.7825961774
H27	-1.2315795597	4.9511123032	-0.7159327222
C28	3.7408821967	0.2942233615	0.7669601282
H29	3.7028646154	-0.2812497652	1.6791975480
C30	1.1388742721	-0.0428790939	-3.9634940055
H31	1.5308534907	0.5535515253	-4.7742840390
C32	-0.7639323890	2.8911801500	0.0204321921
H33	-1.4249675217	2.6943356064	0.8532518780

2Me pyridine complex: SCF = -1197.92003185067

Total internal energy, Utot (SCFE + ZPE + U): -1197.557977 hartrees

Total enthalpy, Htot (Utot + pV): -1197.557033 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1197.634760 hartrees

Ru1	0.6717466564	-0.0742191509	0.2935362189
N2	0.1105434000	2.0369425119	0.6061227573
C3	1.2140818424	-1.8135788953	-0.0271280353
C4	0.6491917323	0.3088355029	-1.8034181745
N5	0.7294853516	-0.1394549880	2.5681192831
N6	2.6624546700	0.6353945988	0.4314525724
N7	2.9791456212	1.5424198570	1.3934217166
N8	0.7769240749	2.7444017415	1.5548976676
N9	1.3279772730	0.9057831159	3.1953806774
B10	1.9112034867	2.0813788242	2.3766977996
H11	2.4060284337	2.8885562511	3.1155874182
O12	1.5532545533	-2.9004069382	-0.2719748939
H13	1.3168252312	1.1539843543	-2.0054347569
H14	-0.3618145023	0.5973055284	-2.1245674222
H15	0.9686038738	-0.5265442235	-2.4391644688
C16	4.2901220274	1.8624812016	1.2967428363
H17	4.7289036916	2.5756433501	1.9788837132
C18	4.8436282325	1.1445854461	0.2484775431

H19	5.8662208306	1.1640539350	-0.0962673457
C20	-0.7691922749	2.8721902947	0.0414169035
H21	-1.4052580387	2.5245957513	-0.7599864826
C22	-0.6825267137	4.1429361618	0.6308404859
H23	-1.2552435771	5.0260972845	0.3915557039
C24	1.3316668644	0.7018023148	4.5328175002
H25	1.7718873761	1.4301203728	5.1982333966
C26	0.7161683844	-0.5132348677	4.7912299503
H27	0.5545782258	-0.9789371912	5.7517015189
C28	3.7778965168	0.3893317894	-0.2642206596
H29	3.7546651685	-0.3065652740	-1.0899601875
C30	0.3163175667	4.0146322571	1.5851288660
H31	0.7332676307	4.7321379848	2.2766483080
C32	0.3594809630	-1.0006388786	3.5229850579
H33	-0.1350805330	-1.9241814469	3.2548441623
N34	-1.3928169913	-0.6077627344	0.2185589881
C35	-1.9010941886	-1.3966542026	-0.7528179459
C36	-3.2462861943	-1.7419863974	-0.8127841187
C37	-4.1181489905	-1.2525277500	0.1589232486
C38	-3.5996163361	-0.4327190390	1.1599437412
C39	-2.2408207359	-0.1365807164	1.1583932080
H40	-1.1942253708	-1.7460007261	-1.4950599563
H41	-3.5959459528	-2.3842559096	-1.6143906306
H42	-5.1741533446	-1.5045291027	0.1371876514
H43	-4.2326316971	-0.0243866235	1.9409948308
H44	-1.7933063101	0.4855591364	1.9232005582

2Me-CH$_4$: SCF = -990.11261390868

Total internal energy, Utot (SCFE + ZPE + U): -989.796467 hartrees

Total enthalpy, Htot (Utot + pV): -989.795523 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -989.867979 hartrees

Ru1	0.6998590939	-0.1231449330	0.2967158100
N2	0.7050646486	-0.5552282473	-1.8490881746
C3	0.7504127172	0.2209710008	2.1273437735
C4	1.3293275950	-2.1217530110	0.6897301082
N5	0.1202322374	1.9700848482	-0.3886194651
N6	2.6445954674	0.4943326533	0.0457188498
N7	2.9703530088	1.2286444340	-1.0522119549
N8	1.2784208089	0.3453574945	-2.6866344497
N9	0.8170476111	2.4791776659	-1.4361305519
B10	1.9146439429	1.6336923947	-2.1160542361
H11	2.4425081372	2.2608608634	-2.9923486395
O12	0.8064610952	0.4115720027	3.2712943523
H13	2.3571706905	-2.1494294296	1.0683105228
H14	1.3093876000	-2.6884132858	-0.2482014724
H15	0.6989647802	-2.6453868404	1.4205714165

C16	4.2914414352	1.5142033377	-1.0166824301
H17	4.7425092464	2.0915127210	-1.8099330438
C18	4.8371183787	0.9587220868	0.1297089595
H19	5.8636429167	1.0028386662	0.4593995662
C20	0.2377744598	-1.5530066997	-2.6079448749
H21	-0.2542777713	-2.3989261069	-2.1496261008
C22	0.5037832740	-1.3001267418	-3.9620455921
H23	0.2536678728	-1.9153584670	-4.8127552225
C24	0.3931312982	3.7348839897	-1.7079375739
H25	0.8360546363	4.3019093050	-2.5137382035
C26	-0.6122705285	4.0592853924	-0.8108225176
H27	-1.1655981987	4.9839102500	-0.7467538446
C28	3.7604597659	0.3262455938	0.7665218820
H29	3.7300892034	-0.2318053959	1.6898977226
C30	1.1696432422	-0.0833968910	-3.9632105101
H31	1.5737870331	0.5037520659	-4.7747398439
C32	-0.7410465205	2.9173964358	-0.0028476810
H33	-1.4028796584	2.7401523920	0.8338905164
H34	-0.9760660406	-1.2166865622	0.5581509363
C35	-1.9667353930	-0.7577345990	0.3296268370
H36	-1.9132894915	0.2243764485	-0.1366834712
H37	-2.4533913148	-1.4564989629	-0.3541199650
H38	-2.5110707699	-0.6977656112	1.2728553307

2Me-CH$_4$-TS: SCF = -990.07929754306

Total internal energy, Utot (SCFE + ZPE + U): -989.766443 hartrees

Total enthalpy, Htot (Utot + pV): -989.765499 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -989.835320 hartrees

Ru1	0.5734373866	-0.1682832640	0.2615580443
N2	0.6795555036	-0.5356943929	-1.8893128535
C3	0.4729605839	0.1342221625	2.1005195636
C4	1.4340486312	-2.1546376727	0.6370476941
N5	0.2113548982	1.9527013647	-0.3275095585
N6	2.6832759634	0.5258017046	0.0468127451
N7	3.0322936775	1.2239764990	-1.0635549970
N8	1.3171165608	0.3517098284	-2.6942474452
N9	0.8848060637	2.4636173659	-1.3890833027
B10	1.9668512354	1.6264156834	-2.1113496919
H11	2.4712005052	2.2694802172	-2.9899445030
O12	0.4011601772	0.3066042070	3.2433632382
H13	2.4711584701	-1.9266355593	0.8871952521
H14	1.4159730897	-2.7416613106	-0.2839838992
H15	1.0029615926	-2.7477103292	1.4475051032
C16	4.3432150929	1.5484005329	-1.0050432121
H17	4.8022739990	2.1143719467	-1.8023680214
C18	4.8686204500	1.0452919936	0.1751954916

H19	5.8838826434	1.1262505959	0.5322895371
C20	0.2254600520	-1.5193299954	-2.6739424251
H21	-0.3212783786	-2.3468860765	-2.2449026609
C22	0.5686339240	-1.2735845471	-4.0115005285
H23	0.3444706709	-1.8798689336	-4.8756846808
C24	0.5137775004	3.7478190343	-1.5898121863
H25	0.9503362718	4.3241137845	-2.3923276631
C26	-0.4318861839	4.0866654639	-0.6343271001
H27	-0.9338943913	5.0339419904	-0.5097537820
C28	3.7829380187	0.4147965169	0.8008622270
H29	3.7431930422	-0.1059058268	1.7470983524
C30	1.2616471167	-0.0732899569	-3.9757664226
H31	1.7162526734	0.5077900783	-4.7645737539
C32	-0.5829371671	2.9238840423	0.1356934547
H33	-1.2177252710	2.7452332407	0.9920728852
H34	-0.2211555638	-1.4958042714	0.4143088428
C35	-1.6116813487	-0.3951046425	0.1797563587
H36	-1.9059796037	-0.8656587956	-0.7612515183
H37	-2.0913688449	-0.9231360046	1.0075905866
H38	-1.9596927979	0.6387660497	0.1768524298

2OH: SCF = -985.50748137884

Total internal energy, Utot (SCFE + ZPE + U): -985.265057 hartrees

Total enthalpy, Htot (Utot + pV): -985.264113 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -985.327714 hartrees

Ru1	0.1173757300	-0.2051196606	0.0166627857
N2	0.0792744628	-0.1351133002	2.1952738205
C3	0.1372926829	-0.2099840025	-1.8630252641
N4	2.1307550580	-0.6148215634	0.1532191391
N5	0.8208409367	1.8284603600	0.1504756772
N6	1.7148943816	2.1617433607	1.1169376551
N7	1.1280339335	0.4320991264	2.8437948194
N8	2.8932572571	-0.0313852807	1.1133942923
B9	2.2901287163	1.0598745750	2.0315562216
H10	3.1254611179	1.5015409808	2.7692640769
O11	0.1982538658	-0.1731133004	-3.0178888238
O12	-1.1647903561	-1.6972514283	0.0518747479
H13	-1.2375020398	-2.0428166568	0.9525440758
C14	1.9471823780	3.4933546697	1.0829327821
H15	2.6348552377	3.9469436529	1.7815004725
C16	1.1836521509	4.0447568411	0.0656478675
H17	1.1344764455	5.0806709225	-0.2329052794
C18	-0.7955650651	-0.5282800327	3.1302699078
H19	-1.7291740453	-0.9912008690	2.8423047203
C20	-0.3097329163	-0.2194396818	4.4088118488
H21	-0.7817083191	-0.4088782855	5.3606096033

C22	4.1357622955	-0.5612477214	1.0753485462
H23	4.8926281552	-0.2246121142	1.7682052177
C24	4.1822416615	-1.5098789155	0.0644125667
H25	5.0247719397	-2.1152081291	-0.2324278413
C26	0.4933467203	2.9567424675	-0.4904211048
H27	-0.2129937352	2.9300275849	-1.3075912519
C28	0.9142549423	0.3915332626	4.1770646189
H29	1.6429796202	0.8005298403	4.8614625710
C30	2.8945857374	-1.5097283445	-0.4884632686
H31	2.4804233254	-2.0958408228	-1.2950623471

2OH pyridine complex: SCF = -1233.84115464281

Total internal energy, Utot (SCFE + ZPE + U): -1233.502432 hartrees

Total enthalpy, Htot (Utot + pV): -1233.501488 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1233.578356 hartrees

Ru1	0.6719100153	-0.1019216640	0.3927740309
N2	0.1000762264	1.9959750020	0.5801146461
C3	1.2279487010	-1.8746412149	0.2278926439
O4	0.5876117978	0.0734294155	-1.6625699651
N5	0.7828146156	-0.1046121155	2.5686572317
N6	2.6395136473	0.6481722435	0.4288068875
N7	2.9690652092	1.6042511924	1.3368906742
N8	0.7489278061	2.7623065315	1.4924556185
N9	1.3559210028	0.9727222996	3.1665616049
B10	1.9058812982	2.1496267458	2.3225533744
H11	2.3888879365	2.9812316235	3.0404731429
O12	1.5837963787	-2.9731837665	0.1197971457
H13	0.8439944452	0.9867805562	-1.8449782071
C14	4.2526791209	1.9841154823	1.1403337443
H15	4.6995903122	2.7426780820	1.7660049156
C16	4.7702625296	1.2560764431	0.0800885056
H17	5.7658997503	1.3125539386	-0.3327663953
C18	-0.7936592679	2.7786999429	-0.0339003886
H19	-1.4170523487	2.3690282159	-0.8158616589
C20	-0.7328573877	4.0803234678	0.4890383178
H21	-1.3234146225	4.9378053128	0.2042216281
C22	1.4046130230	0.7811328829	4.5048564463
H23	1.8312918769	1.5350594152	5.1498869236
C24	0.8495421010	-0.4558490683	4.7925608065
H25	0.7347430106	-0.9177580147	5.7613382438
C26	3.7133628708	0.4310726129	-0.3366903878
H27	3.6616835351	-0.2907940708	-1.1383608236
C28	0.2626566768	4.0228270699	1.4541447809
H29	0.6596650516	4.7841527341	2.1096883925
C30	0.4798638125	-0.9743734973	3.5416856300
H31	0.0224608199	-1.9226291989	3.2963159558

N32	-1.4123114214	-0.6259755898	0.2662599193
C33	-1.9058167804	-0.9792974685	-0.9394606618
C34	-3.2473843559	-1.3053914829	-1.1158012208
C35	-4.1129038441	-1.2546749918	-0.0243865558
C36	-3.6019423519	-0.8698147762	1.2146981331
C37	-2.2487623766	-0.5649002370	1.3194249266
H38	-1.1778099465	-0.9267703720	-1.7462964872
H39	-3.6005655861	-1.5883429361	-2.1021752360
H40	-5.1642989796	-1.5036720116	-0.1366731661
H41	-4.2360618893	-0.8028187955	2.0926761276
H42	-1.8055963888	-0.2616074885	2.2605304808

2OH-CH$_4$: SCF = -1026.03136659356

Total internal energy, Utot (SCFE + ZPE + U): -1025.738713 hartrees

Total enthalpy, Htot (Utot + pV): -1025.737769 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1025.808888 hartrees

Ru1	0.0743426173	-0.1241473116	0.0107615428
N2	0.0633934817	-0.1158334332	2.1757773938
C3	0.1445084827	-0.1676132454	-1.8657191050
N4	2.0274143672	-0.6831605186	0.1851299741
N5	0.7696513656	1.9370901477	0.1625613554
N6	1.7180580497	2.2030923191	1.0985548720
N7	1.1019522581	0.4702848456	2.8223666386
N8	2.8275721914	-0.0541847086	1.0861518790
B9	2.2669011272	1.0719995787	1.9959131682
H10	3.1268091657	1.4878166740	2.7207456230
O11	0.2109639286	-0.2011031288	-3.0200671191
O12	-0.6274958849	-2.0399553636	0.0581910577
H13	-0.3290477612	-2.4010649134	0.9037621146
C14	2.0392864069	3.5166485790	1.0626851128
H15	2.7813076935	3.9171754421	1.7376422386
C16	1.2814175234	4.1265525991	0.0756108004
H17	1.2931743219	5.1654294367	-0.2165797185
C18	-0.7714985809	-0.5902667822	3.1083776729
H19	-1.6691009244	-1.1130953965	2.8102987837
C20	-0.2732283665	-0.3024885397	4.3881430797
H21	-0.7138070925	-0.5506563328	5.3415971418
C22	4.0469416612	-0.6381382390	1.0706294612
H23	4.8290282032	-0.2802302415	1.7236956960
C24	4.0370702328	-1.6650805432	0.1387742442
H25	4.8502031270	-2.3253156599	-0.1207944946
C26	0.5015806599	3.0904277003	-0.4611692763
H27	-0.2265131577	3.1188163532	-1.2595170448
C28	0.9188346567	0.3698122238	4.1571481736
H29	1.6472416422	0.7773370558	4.8428672659
C30	2.7389117065	-1.6586697836	-0.3917894635

H31	2.2789626814	-2.2928364722	-1.1343877827
C32	-2.6863429960	0.3032720079	-0.0105973489
H33	-2.4568776833	-0.7648119562	0.0292896207
H34	-1.7680914301	0.9328078044	-0.0162632462
H35	-3.2519695972	0.6086965536	0.8729137509
H36	-3.2380648442	0.5415432054	-0.9221614983

2OH-CH_4-TS: SCF = -1026.00769268505

Total internal energy, Utot (SCFE + ZPE + U): -1025.719861 hartrees

Total enthalpy, Htot (Utot + pV): -1025.718917 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1025.786294 hartrees

Ru1	0.0018660000	0.0006350000	0.0002040000
N2	-0.0031960000	-0.0023360000	2.1835400000
C3	0.0629410000	0.0140050000	-1.8687930000
N4	2.0271250000	-0.5964110000	0.1828770000
N5	0.7351790000	1.9865860000	0.1598990000
N6	1.6868860000	2.2551270000	1.0918160000
N7	1.0672590000	0.5358020000	2.8207830000
N8	2.8193580000	0.0140000000	1.1013560000
B9	2.2403500000	1.1310480000	2.0001030000
H10	3.0847680000	1.5627510000	2.7341260000
O11	0.1206370000	0.0286400000	-3.0246820000
O12	-0.9872400000	-1.8976640000	-0.0057400000
H13	-0.8857550000	-2.2450390000	0.8918960000
C14	2.0086450000	3.5675700000	1.0436550000
H15	2.7524910000	3.9719540000	1.7141870000
C16	1.2497730000	4.1715900000	0.0534700000
H17	1.2630420000	5.2080540000	-0.2468540000
C18	-0.8438290000	-0.4409610000	3.1297450000
H19	-1.7808550000	-0.9035600000	2.8537560000
C20	-0.3149950000	-0.1870280000	4.4036430000
H21	-0.7541170000	-0.4188540000	5.3617950000
C22	4.0465700000	-0.5538330000	1.0850080000
H23	4.8198810000	-0.2035470000	1.7527780000
C24	4.0543060000	-1.5572000000	0.1280830000
H25	4.8761740000	-2.2022790000	-0.1424310000
C26	0.4657080000	3.1347510000	-0.4738670000
H27	-0.2652190000	3.1568290000	-1.2693430000
C28	0.8998330000	0.4358310000	4.1573670000
H29	1.6525800000	0.8144080000	4.8332040000
C30	2.7587700000	-1.5453320000	-0.4113840000
H31	2.3206560000	-2.1610680000	-1.1834990000
C32	-2.3326600000	0.3811870000	0.0270720000
H33	-1.7435660000	-0.8632810000	0.0413740000
H34	-2.0109500000	1.4271130000	0.0117860000
H35	-2.9227070000	0.2627020000	0.9430440000

H36	-2.9715860000	0.2301780000	-0.8481880000

2OH-CH_4-Product: SCF = -1026.03893593198

Total internal energy, Utot (SCFE + ZPE + U): -1025.745686 hartrees

Total enthalpy, Htot (Utot + pV): -1025.744742 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1025.814486 hartrees

Ru1	-0.1035131837	0.1086167984	-0.0239084110
N2	-0.0877650203	0.0515815773	2.1800681293
C3	-0.1356661331	0.1963161838	-1.8760858802
N4	2.0294196379	-0.6161619364	0.1963459174
N5	0.6651533838	2.0280700284	0.1648079761
N6	1.6340297779	2.2578084497	1.0928345708
N7	1.0066050171	0.5344328810	2.8180164840
N8	2.7947382465	0.0132199798	1.1246814430
B9	2.1860205682	1.1281043914	1.9998316232
H10	3.0149134870	1.5728588932	2.7454614401
O11	-0.1760468857	0.2754141924	-3.0353374214
O12	-0.9078394424	-1.9674495214	0.0454824951
H13	-0.7047385828	-2.2726915359	0.9420258244
C14	1.9763384274	3.5669274097	1.0649687803
H15	2.7326844982	3.9453252657	1.7364426358
C16	1.2179085279	4.2033306040	0.0959708071
H17	1.2449093283	5.2455093277	-0.1829249087
C18	-0.9409238125	-0.3622679077	3.1275009926
H19	-1.9097171814	-0.7570107095	2.8527193882
C20	-0.3925736101	-0.1546447714	4.4019096274
H21	-0.8352892505	-0.3792555928	5.3602625456
C22	4.0446054514	-0.5057653577	1.1224478123
H23	4.7978670670	-0.1275021478	1.7981020653
C24	4.0996447961	-1.5042674878	0.1627525342
H25	4.9478772040	-2.1173228389	-0.1018263292
C26	0.4074958140	3.1922701629	-0.4418055349
H27	-0.3384933304	3.2408816516	-1.2208648400
C28	0.8448210220	0.4225935180	4.1544922332
H29	1.6150145773	0.7646149698	4.8301233753
C30	2.8080767244	-1.5311475481	-0.3902963415
H31	2.4089179175	-2.1537884643	-1.1790118715
C32	-2.1151159237	0.7874956222	0.0361993385
H33	-1.8681259761	-1.8295489511	0.0175991520
H34	-2.3401507975	1.5883380934	-0.6772342076
H35	-2.3360292006	1.1672346575	1.0407077058
H36	-2.8417051961	-0.0195867282	-0.1799396879

2OMe: SCF = -1024.81542001027

Total internal energy, Utot (SCFE + ZPE + U): -1024.543357 hartrees

Total enthalpy, Htot (Utot + pV): -1024.542413 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1024.610620 hartrees

Ru1	0.4571195621	-0.5659569421	0.0315943333
N2	0.1453036257	-0.0370064307	2.1189524539
C3	0.7628898641	-0.9920975795	-1.7676608170
N4	2.5176360672	-0.5932242584	0.5115064925
N5	0.8992191759	1.4770670050	-0.2562459841
N6	1.5712672823	2.1818022112	0.6896704318
N7	0.9815128558	0.8401088428	2.7288596872
N8	3.0365935163	0.3053336335	1.3867254810
B9	2.1495520821	1.4526988762	1.9276027188
H10	2.7887927045	2.2051981976	2.6077943052
O11	0.9975291268	-1.2196637634	-2.8804112957
O12	-1.1277743023	-1.6573624310	0.2910027234
C13	1.6128951122	3.4840779587	0.3333965284
H14	2.1084020432	4.2067653222	0.9648085036
C15	0.9518504749	3.6320119225	-0.8771950935
H16	0.8044592755	4.5403839207	-1.4408077530
C17	-0.7726813207	-0.4080603455	3.0142660756
H18	-1.5375373562	-1.1098021295	2.7158761278
C19	-0.5341047076	0.2378352294	4.2377597537
H20	-1.0967197015	0.1491486248	5.1546427192
C21	4.3297845647	0.0003131187	1.6302526714
H22	4.9149487345	0.6055528321	2.3068487930
C23	4.6635580836	-1.1261464563	0.8927893114
H24	5.6168713893	-1.6304043118	0.8551336134
C25	0.5200005660	2.3399841665	-1.2070313612
H26	-0.0373760641	1.9914918189	-2.0640170832
C27	0.5890427171	1.0205326235	4.0099587530
H28	1.1337065576	1.6882255265	4.6616611695
C29	3.4888596549	-1.4623342203	0.2056745866
H30	3.2937864585	-2.2734092067	-0.4804257472
C31	-1.8497228247	-2.4870475482	-0.5843081267
H32	-1.9243481245	-3.4990559680	-0.1585424691
H33	-2.8735566243	-2.1014048915	-0.7039766943
H34	-1.3976820286	-2.5696147101	-1.5825659418

2OMe-CH$_4$-TS: SCF = -1065.30888724796

Total internal energy, Utot (SCFE + ZPE + U): -1064.991395 hartrees

Total enthalpy, Htot (Utot + pV): -1064.990451 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1065.061831 hartrees

Ru1	0.0069797831	0.0391967347	-0.0419926673
N2	-0.0142145038	-0.0522932851	2.1221545432
C3	0.0955850580	0.1514784775	-1.9085596997
N4	2.0289154937	-0.5912343110	0.1584917961
N5	0.7789213255	2.0067942212	0.1815821141
N6	1.7087620504	2.2409378169	1.1428683490

N7	1.0261879157	0.4839534466	2.8091627803
N8	2.8036745944	-0.0148262002	1.1137178356
B9	2.2209088164	1.0850027339	2.0365316320
H10	3.0594709619	1.4836094697	2.7957361942
O11	0.1771128818	0.2548649699	-3.0603662721
O12	-1.0793778690	-1.7986274996	0.0764626797
C13	2.0472933345	3.5491539072	1.1350807449
H14	2.7769413312	3.9280415729	1.8354951599
C15	1.3210766910	4.1868487338	0.1408304074
H16	1.3539671989	5.2302073885	-0.1329655665
C17	-0.8513056389	-0.5854669076	3.0172953181
H18	-1.7442575480	-1.0916790471	2.6823637393
C19	-0.3550542763	-0.3880047352	4.3152551758
H20	-0.7998645692	-0.6984926832	5.2483122489
C21	4.0307720218	-0.5815659963	1.1011508341
H22	4.7899088386	-0.2559553807	1.7970534394
C23	4.0592507364	-1.5498930920	0.1092432284
H24	4.8862267265	-2.1860730177	-0.1666161081
C25	0.5390103745	3.1731694934	-0.4314375984
H26	-0.1698842008	3.2231363464	-1.2453260056
C27	0.8407921590	0.2912149321	4.1340917377
H28	1.5705059298	0.6469660965	4.8467320616
C29	2.7752712293	-1.5167501130	-0.4548404469
H30	2.3575600293	-2.1041778547	-1.2594214466
C31	-2.3050311082	0.5312134433	-0.0442963792
H32	-1.7705190947	-0.7364707824	-0.0174516902
H33	-1.9520513470	1.5655257840	-0.0139627560
H34	-2.9156907874	0.3947714575	0.8554226810
H35	-2.9301963795	0.4314972396	-0.9373657840
C36	-1.1863341523	-2.6529060555	-1.0436894768
H37	-1.5865175833	-2.1342773414	-1.9292340590
H38	-0.2091592235	-3.0761084186	-1.3127144211
H39	-1.8610330293	-3.4860360628	-0.8031806130

2OMe-CH_4-Product: SCF = -1065.34036953270
Total internal energy, Utot (SCFE + ZPE + U): -1065.016735 hartrees
Total enthalpy, Htot (Utot + pV): -1065.015791 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1065.089070 hartrees

Ru1	-0.1383537488	0.2010928369	-0.0686787380
N2	-0.1061778104	0.0115388673	2.1191989403
C3	-0.1685673954	0.4087264287	-1.9099748089
N4	1.9869319325	-0.6268446330	0.0938510690
N5	0.7570598399	2.0595067930	0.2170960207
N6	1.7254208645	2.1954884727	1.1619814109
N7	0.9974827699	0.4223683949	2.7917731089
N8	2.7636768992	-0.0991648853	1.0741653660

B9	2.2056303553	0.9942190601	2.0156175634
H10	3.0577213713	1.3541081744	2.7810465618
O11	-0.2071030619	0.5585978852	-3.0646066859
O12	-1.1970228045	-1.7422636976	-0.0754013298
C13	2.1405572035	3.4822966309	1.1951401138
H14	2.9086939782	3.7879118371	1.8899467925
C15	1.4297544769	4.2019751956	0.2479423483
H16	1.5174736803	5.2522991476	0.0158828224
C17	-0.9648392957	-0.4636380464	3.0274071159
H18	-1.9249934597	-0.8468555032	2.7140460747
C19	-0.4153160714	-0.3632863216	4.3151639318
H20	-0.8624242757	-0.6581658794	5.2523035779
C21	4.0025196617	-0.6408321795	1.0272939766
H22	4.7610831364	-0.3373928038	1.7339912834
C23	4.0418711526	-1.5512113774	-0.0167508986
H24	4.8783372246	-2.1556916236	-0.3333457915
C25	0.5716807906	3.2618646308	-0.3411441852
H26	-0.1597965632	3.3861453704	-1.1254370237
C27	0.8334513119	0.2067660815	4.1158894404
H28	1.6118392550	0.4740579482	4.8155247456
C29	2.7525158407	-1.4995255031	-0.5715634096
H30	2.3517187744	-2.0347927572	-1.4211769310
C31	-2.0932938281	1.0207057978	0.0377046497
H32	-2.0805250040	-1.5044703435	-0.3914604854
H33	-2.1756892004	2.0011287741	-0.4445709834
H34	-2.3708757040	1.1434542416	1.0907031557
H35	-2.8614853066	0.3835723409	-0.4388689967
C36	-0.7070154342	-2.8809985427	-0.7997237692
H37	-0.6161857661	-2.6650151298	-1.8699138469
H38	0.2763413189	-3.1067933354	-0.3891151004
H39	-1.3731092724	-3.7361587231	-0.6441477453

2NH$_2$: SCF = -965.64514867926

Total internal energy, Utot (SCFE + ZPE + U): -965.391074 hartrees

Total enthalpy, Htot (Utot + pV): -965.390129 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -965.451866 hartrees

Ru1	-0.1675782291	0.3293753977	-0.0618521593
N2	-0.1321638051	0.2557039483	2.1536789889
C3	-0.2440035041	0.3730600275	-1.9233812470
N4	-1.7734412611	1.7104457478	0.1725261688
N5	-1.7899643781	-1.0612908509	0.1093231332
N6	-2.7126206429	-0.9371529616	1.0963763527
N7	-1.3204563630	0.2548650735	2.8135831495
N8	-2.6948345523	1.5511318258	1.1556109673
B9	-2.6600187958	0.2852857446	2.0381037832
H10	-3.5820875863	0.2747437962	2.8053810606

O11	-0.3420131579	0.3978490172	-3.0795922473
N12	1.7645041432	0.3825886501	-0.0764507708
H13	2.3750342473	0.4380699088	-0.8844102185
C14	-3.5508866746	-1.9968586408	1.0698473021
H15	-4.3552820149	-2.0757061590	1.7863646750
C16	-3.1664144048	-2.8343474158	0.0334018887
H17	-3.6242128280	-3.7648410092	-0.2654182594
C18	0.8242256111	0.1921472774	3.0863354473
H19	1.8674835026	0.1729363005	2.8061388151
C20	0.2613196061	0.1512068521	4.3697065665
H21	0.7741749622	0.0982183520	5.3178476670
C22	-3.5254547746	2.6168925238	1.1745016679
H23	-4.3283400727	2.6712612594	1.8949073869
C24	-3.1366039210	3.4945354959	0.1733895477
H25	-3.5879475045	4.4401230754	-0.0850610283
C26	-2.0529975248	-2.2022083738	-0.5397370744
H27	-1.4342498001	-2.5054938832	-1.3714758401
C28	-1.1063256978	0.1924092379	4.1459318114
H29	-1.9386985661	0.1805528467	4.8341547059
C30	-2.0289776313	2.8795680687	-0.4281108281
H31	-1.4087049435	3.2130793227	-1.2469704972
H32	2.3279874223	0.4102346712	0.7676377521

2NH$_2$ pyridine complex: SCF = -1213.95689375115

Total internal energy, Utot (SCFE + ZPE + U): -1213.605904 hartrees

Total enthalpy, Htot (Utot + pV): -1213.604960 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1213.682392 hartrees

Ru1	0.6828573208	-0.0927404305	0.3284187020
N2	0.0857265544	2.0085059620	0.6220931889
C3	1.2560006283	-1.8419844354	0.0925840394
N4	0.7561332382	0.2461133229	-1.7459001817
N5	0.7456768279	-0.1533554656	2.5432882828
N6	2.6489169472	0.6644773434	0.4322392275
N7	2.9703366111	1.5655475866	1.3976813622
N8	0.7515782873	2.7301838904	1.5597566604
N9	1.3255123053	0.8920874152	3.1868769529
B10	1.8992522246	2.0836101637	2.3813901005
H11	2.3741004290	2.8941887904	3.1289087025
O12	1.6188135307	-2.9334843379	-0.0767463901
H13	-0.0744951909	0.7944889346	-1.9867004821
H14	0.6236584619	-0.6216160083	-2.2717450897
C15	4.2550268325	1.9583077098	1.2321892364
H16	4.6951901306	2.6812880071	1.9031412189
C17	4.7807177969	1.2928794312	0.1362486175
H18	5.7787777200	1.3747418823	-0.2664405216
C19	-0.8048943589	2.8302303552	0.0550509860

H20	-1.4484751567	2.4701425676	-0.7351589627
C21	-0.7244590801	4.1076518253	0.6302381639
H22	-1.3058261634	4.9836262880	0.3858098446
C23	1.3184372190	0.6716312429	4.5207523722
H24	1.7417752324	1.3984441630	5.1984744968
C25	0.7166782856	-0.5548010514	4.7592763991
H26	0.5526183585	-1.0339060337	5.7125409323
C27	3.7261151662	0.4956614880	-0.3368978059
H28	3.6743724328	-0.1618505042	-1.1910341753
C29	0.2805990919	3.9964467770	1.5799288109
H30	0.6949386961	4.7239960809	2.2623742606
C31	0.3779044469	-1.0329254662	3.4836228486
H32	-0.1024970612	-1.9586675055	3.1989299097
N33	-1.3869562539	-0.6292832042	0.2338244615
C34	-1.8939194746	-1.3359420038	-0.7985200922
C35	-3.2443343611	-1.6513905667	-0.9007606185
C36	-4.1202017703	-1.2169813117	0.0928343069
C37	-3.6019260662	-0.4807376698	1.1573486391
C38	-2.2381963136	-0.2102851191	1.1941395927
H39	-1.1817498428	-1.6294876480	-1.5592504237
H40	-3.5947081009	-2.2268194951	-1.7513765508
H41	-5.1801324971	-1.4470810102	0.0395939819
H42	-4.2393635901	-0.1163456519	1.9562267890
H43	-1.7909356096	0.3508120300	2.0049980106

2NH$_2$-CH$_4$-TS: SCF = -1006.13607533144

Total internal energy, Utot (SCFE + ZPE + U): -1005.835864 hartrees

Total enthalpy, Htot (Utot + pV): -1005.834919 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1005.902783 hartrees

Ru1	-0.0978851763	-0.0049116647	-0.0742377488
N2	-0.0533106974	0.0022450688	2.1070582135
C3	-0.1786417383	0.0222011702	-1.9368609319
N4	-1.5415864588	1.5290663753	0.1347517582
N5	-1.7627056069	-1.3747597923	0.1484218467
N6	-2.6921498644	-1.1071440501	1.1018861986
N7	-1.2314798984	0.0716264126	2.7764017217
N8	-2.5120686684	1.4005347040	1.0763361511
B9	-2.5630263375	0.1509600999	1.9901460511
H10	-3.4906293625	0.2261350094	2.7471759402
O11	-0.2336739214	0.0586831256	-3.0952754449
N12	1.7006509376	1.1226991993	-0.0266431651
H13	1.9103105403	1.6788052535	-0.8484153379
C14	-3.6395504985	-2.0723545810	1.0985051449
H15	-4.4655460958	-2.0302935498	1.7931518176
C16	-3.3222951155	-2.9954148585	0.1145401728
H17	-3.8690691937	-3.8861183614	-0.1547695944

C18	0.9195667895	-0.0403941123	3.0243271511
H19	1.9532687900	-0.0998912675	2.7145465442
C20	0.3703864958	0.0011948328	4.3147681120
H21	0.8935131566	-0.0196374303	5.2585646228
C22	-3.3000720431	2.4992316256	1.0634990674
H23	-4.1302228500	2.5832074623	1.7492666956
C24	-2.8343553449	3.3648597640	0.0856224370
H25	-3.2376515871	4.3278168016	-0.1879780976
C26	-2.1344904115	-2.5096048416	-0.4539105138
H27	-1.5392188021	-2.9155754699	-1.2595616459
C28	-0.9994505354	0.0720808651	4.1074206030
H29	-1.8212836854	0.1219044507	4.8066139957
C30	-1.7256929611	2.7083870969	-0.4695809085
H31	-1.0630044147	3.0185522114	-1.2642758313
H32	1.7404941205	1.7096341303	0.8007358513
C33	1.6923713303	-1.5893927296	-0.0739978886
H34	1.8416196596	-0.2532013763	-0.0373840135
H35	0.8403192771	-2.2757307835	-0.0694177610
H36	2.2701657913	-1.8117002116	0.8298965460
H37	2.2887536754	-1.8118637042	-0.9639339126

2NH_2-CH_4-Product: SCF = -1006.19150218919

Total internal energy, Utot (SCFE + ZPE + U): -1005.884278 hartrees

Total enthalpy, Htot (Utot + pV): -1005.883334 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1005.953282 hartrees

Ru1	-0.0514207504	-0.2086039647	-0.0925526433
N2	-0.0170140670	-0.1443553448	2.1149679874
C3	-0.0804807957	-0.3310081064	-1.9374529651
N4	-1.5392399785	1.4997947005	0.1353336189
N5	-1.7178419721	-1.4786129099	0.1554241994
N6	-2.6523726476	-1.1643426552	1.0932451167
N7	-1.1922298480	0.0053829556	2.7739457900
N8	-2.4913681066	1.3577326402	1.0919085848
B9	-2.5222239691	0.0957140184	1.9827697750
H10	-3.4472058626	0.1537829576	2.7463737368
O11	-0.0778489175	-0.4357193435	-3.0981817739
N12	1.6630690488	1.1372724977	-0.0739417607
H13	1.5422133205	1.9654753528	-0.6521315367
C14	-3.6207553213	-2.1101153898	1.0975692236
H15	-4.4521846408	-2.0352792919	1.7827139320
C16	-3.3141310628	-3.0608110816	0.1378889206
H17	-3.8777199341	-3.9449805794	-0.1180484363
C18	0.9421770087	-0.2301189778	3.0450864930
H19	1.9707684319	-0.3903322409	2.7518281090
C20	0.3880683514	-0.1273661074	4.3304173164
H21	0.9002225055	-0.1656021428	5.2797972080

C22	-3.3157708442	2.4306920333	1.0895945447
H23	-4.1396656068	2.4914482422	1.7856096735
C24	-2.8926357751	3.3037828349	0.1000045431
H25	-3.3303387085	4.2518752796	-0.1736236456
C26	-2.1076211688	-2.6174255294	-0.4257948601
H27	-1.5071506155	-3.0551566275	-1.2094997011
C28	-0.9733828512	0.0166229865	4.1073795680
H29	-1.7981470251	0.1193998199	4.7972641505
C30	-1.7764520139	2.6687701756	-0.4698505179
H31	-1.1514530835	2.9911621506	-1.2918329540
H32	1.8170629995	1.4521972190	0.8823718239
C33	1.3135203453	-1.8380749009	-0.0514272052
H34	2.5029474226	0.6521499220	-0.3861772462
H35	0.9419321921	-2.7195636503	-0.5872722067
H36	1.4799463653	-2.1381368180	0.9904169100
H37	2.2943411609	-1.5952884954	-0.4929430238

2NMe$_2$: SCF = -1044.25249042378

Total internal energy, Utot (SCFE + ZPE + U): -1043.938419 hartrees

Total enthalpy, Htot (Utot + pV): -1043.937475 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1044.007629 hartrees

Ru1	-0.1644439540	0.4717918377	-0.0405681023
N2	-0.1279656031	0.2639433824	2.1928535808
C3	-0.3648893279	0.3691923432	-1.8853827971
N4	-1.8827304269	1.6658162633	0.1867624240
N5	-1.6431999704	-1.1406601142	0.1935220408
N6	-2.6233899768	-1.0518249368	1.1268579588
N7	-1.3202416121	0.1981212622	2.8467260027
N8	-2.7719637706	1.4391591343	1.1857702199
B9	-2.6566925951	0.1749580699	2.0639221138
H10	-3.5816292160	0.1094468799	2.8252879546
O11	-0.5867071105	0.2443405705	-3.0191921351
N12	1.6515519927	1.2230677166	-0.1452853142
C13	-3.3960423155	-2.1606110332	1.0870564257
H14	-4.2277771468	-2.2741758086	1.7669120290
C15	-2.9101146921	-2.9955783360	0.0925444011
H16	-3.2948017418	-3.9591683330	-0.2047870038
C17	0.8188604567	-0.0311060111	3.0945424467
H18	1.8577513127	-0.0552781463	2.8023114006
C19	0.2460968181	-0.2762044894	4.3507621435
H20	0.7500803665	-0.5265505370	5.2717810407
C21	-3.6852722950	2.4346174320	1.2093236685
H22	-4.4799815612	2.4282782397	1.9405970232
C23	-3.3841266041	3.3334365205	0.1966655084
H24	-3.9147385933	4.2371809052	-0.0607899246
C25	-1.8072535126	-2.3083382163	-0.4383278842

H26	-1.1326680096	-2.5927913262	-1.2329920441
C27	-1.1154132594	-0.1256285917	4.1431904110
H28	-1.9518835761	-0.2298715249	4.8186701510
C29	-2.2406472064	2.8061393176	-0.4189748643
H30	-1.6620385096	3.1806870246	-1.2502957568
C31	2.4042567562	1.4686212904	-1.3728127551
H32	2.3906387737	2.5377658036	-1.6470352902
H33	3.4602472914	1.1873900127	-1.2354728063
H34	2.0135738917	0.8892912879	-2.2078762960
C35	2.2877371877	1.9727712494	0.9337041946
H36	2.4444811577	3.0218453324	0.6311589206
H37	1.6756783991	1.9757286733	1.8323845031
H38	3.2805291174	1.5606757150	1.1785797973

2NMe$_2$-CH$_4$-TS: SCF = -1084.74398239243

Total internal energy, Utot (SCFE + ZPE + U): -1084.384587 hartrees

Total enthalpy, Htot (Utot + pV): -1084.383642 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1084.457455 hartrees

Ru1	-0.0823578609	0.0556351066	-0.0506726163
N2	-0.0628986564	-0.0386420879	2.1566191760
C3	-0.2556997607	0.0192109071	-1.9036370998
N4	-1.5586135653	1.5504247101	0.1674765058
N5	-1.7167182175	-1.3680074771	0.1731896130
N6	-2.6842956490	-1.1094546090	1.0892185825
N7	-1.2563144222	0.0242555423	2.8018898879
N8	-2.5215167911	1.4009214621	1.1132781173
B9	-2.5745781710	0.1345815299	1.9999831050
H10	-3.5120247195	0.1921837211	2.7464471513
O11	-0.4198860465	-0.0353945820	-3.0507072004
N12	1.6943112184	1.2657665795	-0.1050815134
C13	-3.6217252326	-2.0832540072	1.0503469899
H14	-4.4722333936	-2.0510058443	1.7154100278
C15	-3.2591802334	-3.0024107987	0.0782099198
H16	-3.7867633974	-3.8981743056	-0.2118358076
C17	0.8737652774	-0.2428389813	3.0907942102
H18	1.9132019541	-0.3235118283	2.8079626116
C19	0.2884224512	-0.3101782424	4.3635109346
H20	0.7806392440	-0.4605860198	5.3122648106
C21	-3.3227461874	2.4899015179	1.1157987348
H22	-4.1504837273	2.5561662469	1.8063493563
C23	-2.8735368400	3.3706355105	0.1439084179
H24	-3.2893016881	4.3319570849	-0.1162943807
C25	-2.0552861366	-2.5051552999	-0.4445640057
H26	-1.4279195008	-2.9038502723	-1.2293985597
C27	-1.0676329049	-0.1378654921	4.1299375447
H28	-1.9080263188	-0.1209978705	4.8082640756

C29	-1.7610495819	2.7333612644	-0.4251608404
H30	-1.1044164238	3.0604354030	-1.2179245002
C31	1.7786064768	-1.4560223637	-0.0408285432
H32	1.8622410555	-0.1254687265	0.0306555127
H33	0.9532748643	-2.1739171386	-0.0712401506
H34	2.3469438575	-1.6843738857	0.8667427490
H35	2.3995857209	-1.6347963545	-0.9234958238
C36	1.8078957952	2.3172983987	0.8947071826
H37	1.1690813532	3.1869734040	0.6645173075
H38	1.5193405523	1.9542948925	1.8809004658
H39	2.8458496339	2.6837133537	0.9550782944
C40	2.1694936239	1.7320460981	-1.3983630381
H41	3.1765926234	2.1703178569	-1.3055836265
H42	2.2351122108	0.8987593347	-2.1053345841
H43	1.5227931122	2.5051126480	-1.8500445083

2NMe$_2$-CH$_4$-Product: SCF = -1084.80151026825

Total internal energy, Utot (SCFE + ZPE + U): -1084.434671 hartrees

Total enthalpy, Htot (Utot + pV): -1084.433727 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1084.509330 hartrees

Ru1	-0.0383586959	-0.1620421480	-0.0601503389
N2	0.0044073753	-0.2400234753	2.1621229912
C3	-0.1411127242	-0.2009645268	-1.9022260367
N4	-1.5614894979	1.5100124142	0.2573596578
N5	-1.7031493472	-1.4536788232	0.1373996765
N6	-2.6333688248	-1.2068460687	1.0978925625
N7	-1.1728322487	-0.1214050697	2.8264926502
N8	-2.5004880066	1.3070518492	1.2164469824
B9	-2.5069226729	0.0065895101	2.0492532772
H10	-3.4263773598	0.0185835439	2.8216565724
O11	-0.2117408273	-0.2648867582	-3.0641411482
N12	1.7704342100	1.1351000130	-0.0065655338
C13	-3.5860095648	-2.1670210224	1.0610041599
H14	-4.4115489184	-2.1428232025	1.7569159235
C15	-3.2736495706	-3.0596686930	0.0486079092
H16	-3.8257705831	-3.9378302324	-0.2497504123
C17	0.9540926531	-0.4180747113	3.0889875361
H18	1.9844790702	-0.5614709907	2.7938845901
C19	0.3943020288	-0.4089697203	4.3753915196
H20	0.9004011180	-0.5298886271	5.3210400818
C21	-3.3849035642	2.3314628924	1.2259407856
H22	-4.2077131248	2.3395964777	1.9259245054
C23	-3.0159717571	3.2347933964	0.2423108226
H24	-3.5059723974	4.1602311099	-0.0196628168
C25	-2.0801846281	-2.5665105333	-0.5011708926
H26	-1.4823954531	-2.9509930314	-1.3142734098

C27	-0.9626424836	-0.2225629434	4.1573201662
H28	-1.7902221108	-0.1619136867	4.8486969207
C29	-1.8695283050	2.6675853338	-0.3381855590
H30	-1.2652607262	3.0322185427	-1.1573680675
C31	1.3216805876	-1.7977023545	-0.1182245654
H32	2.4112079434	0.5142927136	0.4857990450
H33	0.8950505626	-2.6799019170	-0.6096060816
H34	1.5718043791	-2.0947512597	0.9083361521
H35	2.2632794038	-1.5708948061	-0.6426910919
C36	1.6231358546	2.3660272607	0.8007546587
H37	0.9025729590	3.0265852857	0.3164928842
H38	1.2411833513	2.1075683930	1.7879523743
H39	2.5816272047	2.8941124359	0.9012133887
C40	2.3926390968	1.4366775848	-1.3140820182
H41	3.3374426899	1.9843779187	-1.1924355126
H42	2.5799482962	0.5059140505	-1.8503304823
H43	1.7057608496	2.0472963981	-1.9044139836

TpRu(PMe$_3$)Me: SCF = -1297.35628243789

Total internal energy, Utot (SCFE + ZPE + U): -1296.979663 hartrees

Total enthalpy, Htot (Utot + pV): -1296.978718 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1297.055012 hartrees

Ru1	0.7256957533	-0.1313896115	0.2685650505
N2	0.7340297516	-0.5121728850	-1.8574757122
C3	1.1686985564	-2.1650201224	0.6112150666
N4	0.1356883960	1.9842951951	-0.3501690962
N5	2.6604372400	0.4556851999	0.0437536442
N6	2.9937650417	1.2416176787	-1.0167213969
N7	1.3017959167	0.4112848187	-2.6748198483
N8	0.8441709743	2.5171466605	-1.3777110316
B9	1.9421622136	1.6814749875	-2.0690788739
H10	2.4762637606	2.3291977586	-2.9281934802
H11	1.8963984273	-2.3831752632	1.4045278674
H12	1.5453363857	-2.6364405830	-0.3060650647
H13	0.2365085976	-2.6945094510	0.8898060507
C14	4.3290009208	1.4642135113	-1.0073453137
H15	4.7840882375	2.0670564648	-1.7790097207
C16	4.8799500601	0.8106841950	0.0824472717
H17	5.9173664797	0.7825170852	0.3789044089
C18	0.2625891896	-1.4890782114	-2.6397347612
H19	-0.2204801628	-2.3490978268	-2.1979601878
C20	0.5180754641	-1.1982555896	-3.9901494985
H21	0.2622161056	-1.7903227494	-4.8557705870
C22	0.3779585313	3.7519520957	-1.6786915942
H23	0.8224697052	4.3280774870	-2.4771913151
C24	-0.6708991648	4.0411822804	-0.8209578274

H25	-1.2664923413	4.9410073673	-0.7868050443
C26	3.7919127388	0.1848352661	0.7099602535
H27	3.7654357830	-0.4526321761	1.5799257039
C28	1.1840463915	0.0172370753	-3.9636825195
H29	1.5831808701	0.6260916019	-4.7618274391
C30	-0.7804106155	2.8984420914	-0.0099193810
H31	-1.4764942963	2.6968488060	0.7928342474
P32	0.6483834404	0.3242400963	2.5385981595
C33	1.3218888471	1.9687931627	3.0619800469
H34	1.2020958239	2.1384277590	4.1372208170
H35	2.3839952381	2.0156259360	2.8058991616
H36	0.8101902362	2.7593388703	2.5075632799
C37	-1.0686075600	0.3768363088	3.2525331570
H38	-1.0586105870	0.6250757102	4.3193621391
H39	-1.6695243586	1.1219712507	2.7236659353
H40	-1.5463844816	-0.5992174584	3.1229496659
C41	1.4690193026	-0.8057724541	3.7601709895
H42	1.2965456891	-0.4723734625	4.7886384948
H43	1.0799597122	-1.8195362469	3.6381123505
H44	2.5465589525	-0.8362950538	3.5776528108

TpRu(PMe$_3$)Me-CH$_4$complex: SCF =-1337.88479036668

Total internal energy, Utot (SCFE + ZPE + U): -1337.457188 hartrees

Total enthalpy, Htot (Utot + pV): -1337.456244 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1337.539171 hartrees

Ru1	0.6741408961	-0.1443847233	0.2565460029
N2	0.7440371881	-0.5150900439	-1.8809916090
C3	1.2659286510	-2.1589593391	0.6264062424
N4	0.1048678610	1.9786550062	-0.3632655558
N5	2.6445498230	0.4371966198	0.0621999160
N6	2.9867077966	1.2410932929	-0.9821960625
N7	1.3279978094	0.4187964346	-2.6747908956
N8	0.8391984200	2.5161647902	-1.3694846039
B9	1.9505925457	1.6849067852	-2.0463548317
H10	2.4964537096	2.3421315699	-2.8909969432
H11	2.2369718025	-2.2294352644	1.1354733211
H12	1.3762270903	-2.6915691839	-0.3282317923
H13	0.5532072317	-2.7369293572	1.2375417904
C14	4.3193286561	1.4754547711	-0.9546343786
H15	4.7782311017	2.0919610930	-1.7132045350
C16	4.8628512792	0.8124757661	0.1328282773
H17	5.8966503295	0.7891973570	0.4421677498
C18	0.3152442212	-1.4943123514	-2.6842185076
H19	-0.1737789418	-2.3620425416	-2.2653487497
C20	0.6160561648	-1.1954768496	-4.0237226924
H21	0.3995024382	-1.7876461599	-4.8999785826

C22	0.4004512872	3.7642278097	-1.6557678255
H23	0.8694903783	4.3463062657	-2.4356594639
C24	-0.6573522121	4.0579799942	-0.8106116390
H25	-1.2366810038	4.9681263869	-0.7700409631
C26	3.7712885163	0.1700421071	0.7372276711
H27	3.7439482984	-0.4758286431	1.6007490513
C28	1.2633416227	0.0286135609	-3.9686928540
H29	1.6826706238	0.6466900080	-4.7491331898
C30	-0.8003925348	2.9038809320	-0.0212336707
H31	-1.5109281591	2.7025158886	0.7689674981
H32	-1.0281748923	-1.2396732076	0.4430522861
C33	-1.9938805897	-0.8198974622	0.0790661705
H34	-2.3209396320	-1.4683490614	-0.7358016236
H35	-2.6952644204	-0.8732287231	0.9138653162
H36	-1.9223536578	0.2044011865	-0.2829754939
P37	0.6358391378	0.3283097929	2.5264145907
C38	1.4098843182	1.9408747312	3.0133751006
H39	1.3442978137	2.1158978081	4.0924975676
H40	2.4603232488	1.9421583252	2.7107830058
H41	0.9077798875	2.7531251958	2.4814467835
C42	-1.0360706679	0.4845437115	3.3258036520
H43	-0.9521365485	0.7691981496	4.3801045124
H44	-1.6312171191	1.2391624087	2.8041120586
H45	-1.5648511960	-0.4706740463	3.2603837315
C46	1.4450040620	-0.8377295666	3.7217274249
H47	1.3127897744	-0.5035226291	4.7558844473
H48	1.0146338800	-1.8352562568	3.6044160997
H49	2.5148246617	-0.9100549902	3.5104736539

TpRu(PMe$_3$)Me-CH$_4$TS: SCF = -1337.85585763278

Total internal energy, Utot (SCFE + ZPE + U): -1337.430917 hartrees

Total enthalpy, Htot (Utot + pV): -1337.429973 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1337.509528 hartrees

Ru1	0.5994396359	-0.1083381997	0.2924791127
N2	0.6642360853	-0.5398282779	-1.8298965138
C3	1.5486438234	-2.0519190240	0.6861068781
N4	0.2430998586	2.0216102976	-0.3780343776
N5	2.7727991085	0.5764641786	-0.0114186607
N6	3.0668133936	1.2283622553	-1.1655994920
N7	1.2890664053	0.2985395736	-2.6934132894
N8	0.9121840209	2.4664858129	-1.4734898466
B9	1.9646048157	1.5883814370	-2.1845114464
H10	2.4419934280	2.1902491994	-3.1082044275
H11	2.5442928322	-1.7827047572	1.0462136058
H12	1.6591545549	-2.5785501824	-0.2654770245
H13	1.1080106550	-2.7464788083	1.4088457036

C14	4.3915001924	1.4884087644	-1.2313651999
H15	4.8049327084	2.0084068798	-2.0831096605
C16	4.9917302504	0.9888908636	-0.0871576593
H17	6.0366716820	1.0264885028	0.1810384097
C18	0.1712352841	-1.5493331775	-2.5553309017
H19	-0.3751652712	-2.3461261491	-2.0714123439
C20	0.4768888621	-1.3699041716	-3.9141403511
H21	0.2166485704	-2.0108995300	-4.7427238503
C22	0.5071866458	3.7162111400	-1.7903490576
H23	0.9372822144	4.2318436580	-2.6364095569
C24	-0.4612817420	4.1063864748	-0.8797227848
H25	-0.9952422026	5.0438126476	-0.8429448977
C26	3.9322727086	0.4276432819	0.6420390105
H27	3.9603719893	-0.0752351257	1.5965012361
C28	1.1879631981	-0.1814110597	-3.9543495316
H29	1.6270377737	0.3569608374	-4.7814523892
C30	-0.5889815161	3.0066678767	-0.0184817573
H31	-1.2459774779	2.8840194396	0.8281268339
H32	-0.0878842647	-1.4847469528	0.4664403934
C33	-1.5682483048	-0.2489290653	0.2322076861
H34	-1.8708429635	-0.6349398700	-0.7462731768
H35	-2.0659567182	-0.8555005247	0.9966695773
H36	-1.9454641436	0.7738010885	0.3180024269
P37	0.4416692949	0.2312054748	2.5911940236
C38	-0.5117596547	1.6943602343	3.2146735887
H39	-0.5449588595	1.7055338232	4.3090252874
H40	-0.0446236174	2.6177918321	2.8637212786
H41	-1.5355508162	1.6534749591	2.8327117461
C42	-0.3915818605	-1.1307536285	3.5320628408
H43	-0.4383883585	-0.9033529146	4.6020154471
H44	-1.4066251245	-1.2697930973	3.1520042270
H45	0.1566082572	-2.0652342975	3.3904893959
C46	2.0016957354	0.4164080314	3.5778356246
H47	1.7825544284	0.5754550291	4.6388423758
H48	2.6081276177	-0.4884008840	3.4786342371
H49	2.5795978879	1.2637213828	3.2004005666

TpRu(PMe$_3$)OH: SCF =-1333.29137574183

Total internal energy, Utot (SCFE + ZPE + U): -1332.937217 hartrees

Total enthalpy, Htot (Utot + pV): -1332.936273 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1333.011473 hartrees

Ru1	0.1542475632	-0.1400483066	-0.0144122417
N2	0.0354280524	-0.1483216764	2.1511464846
N3	2.1447240694	-0.6268671553	0.1846078403
N4	0.8975927950	1.8771792780	0.2056476449
N5	1.7682398795	2.1476942996	1.2129363074

N6	1.0656404106	0.3800278853	2.8584455178
N7	2.8852931100	-0.0794866601	1.1847347787
B8	2.2724567314	0.9979977844	2.1100321296
H9	3.0909999756	1.3945571449	2.8933436055
O10	-1.1284704684	-1.6633917916	-0.1471821077
H11	-1.2551577240	-2.0686653738	0.7212379437
C12	2.0345587187	3.4740468612	1.2529261565
H13	2.7094047074	3.8755768609	1.9945867692
C14	1.3175443860	4.0922666792	0.2414750491
H15	1.2995884857	5.1426465092	-0.0068282868
C16	-0.8804535467	-0.5554317328	3.0380203879
H17	-1.8060823466	-0.9976149222	2.6964917690
C18	-0.4411422519	-0.2933364680	4.3460545588
H19	-0.9538790579	-0.5033406338	5.2724371547
C20	4.1118519680	-0.6499478717	1.2048501783
H21	4.8441816491	-0.3414657161	1.9360542274
C22	4.1748333360	-1.5939529403	0.1925017106
H23	5.0087418598	-2.2281958867	-0.0667180497
C24	0.6196354031	3.0465262146	-0.3847315592
H25	-0.0714365161	3.0836225121	-1.2143725734
C26	0.8000279024	0.3025955238	4.1825874309
H27	1.5081544271	0.6784543517	4.9066337316
C28	2.9128946367	-1.5465125281	-0.4186511515
H29	2.5179823835	-2.1282878758	-1.2371921197
P30	0.1106864627	-0.1719917114	-2.3371021244
C31	-0.0121090579	-1.8661955616	-3.0628219705
H32	-0.3011744742	-1.8460312433	-4.1185143929
H33	0.9463903360	-2.3847908103	-2.9694826093
H34	-0.7519820710	-2.4062887010	-2.4665456083
C35	1.4970429126	0.6100807970	-3.2798665849
H36	1.5714691590	1.6658197877	-3.0052373266
H37	2.4380214271	0.1272337425	-3.0024819411
H38	1.3539421547	0.5267818079	-4.3622387522
C39	-1.3826626102	0.6416765175	-3.0743808902
H40	-1.4030993558	1.7029820711	-2.8117117021
H41	-1.4013467854	0.5448147088	-4.1653196415
H42	-2.2757242060	0.1697049026	-2.6554217034

TpRu(PMe$_3$)OH-CH$_4$complex SCF = -1373.81514371714

Total internal energy, Utot (SCFE + ZPE + U): -1373.410614 hartrees

Total enthalpy, Htot (Utot + pV): -1373.409669 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1373.491463 hartrees

Ru1	0.0718185113	-0.0722782310	0.0051173476
N2	0.0457106446	-0.1184880861	2.1659149473
N3	2.0082175548	-0.7108906526	0.1948073549
N4	0.8167668701	1.9633321806	0.1970691246

N5	1.7668221377	2.1861388631	1.1422287304
N6	1.0967900136	0.4309191440	2.8258509959
N7	2.8239507695	-0.0991314722	1.0953104060
B8	2.2786015990	1.0222048752	2.0174493352
H9	3.1424377705	1.4051266196	2.7582070377
O10	-0.7099980367	-1.9772465726	-0.0868372788
H11	-0.4961486557	-2.4006626753	0.7549388100
C12	2.1006349150	3.4978531624	1.1650872028
H13	2.8451819974	3.8615288693	1.8579533661
C14	1.3469733226	4.1565692130	0.2074938310
H15	1.3649454856	5.2077817015	-0.0372470510
C16	-0.7899805401	-0.6054759550	3.0903113992
H17	-1.7004912466	-1.1008030428	2.7845450319
C18	-0.2797834230	-0.3660444576	4.3773951859
H19	-0.7198645297	-0.6353956938	5.3256042903
C20	4.0173736081	-0.7367677438	1.1240750142
H21	4.7997787706	-0.3975395899	1.7867035141
C22	3.9784401628	-1.7889293986	0.2234085254
H23	4.7637650067	-2.4954562244	0.0017540851
C24	0.5572182699	3.1490499399	-0.3711422391
H25	-0.1800222099	3.2230045557	-1.1582003764
C26	0.9213586212	0.2918327989	4.1601023213
H27	1.6610632417	0.6665507030	4.8525781249
C28	2.6892764195	-1.7384071567	-0.3302487696
H29	2.2113247672	-2.3875961111	-1.0466851868
C30	-2.6596678685	0.4755484101	0.1511268114
H31	-2.4830268844	-0.6016779335	0.0876164593
H32	-1.7220880825	1.0557668546	0.0018966071
H33	-3.0423346890	0.7450641905	1.1377553482
H34	-3.3547555136	0.8002804838	-0.6269609805
P35	0.1328650463	-0.1345386641	-2.3242521001
C36	0.1024726726	-1.8437502688	-3.0277032665
H37	-0.2699429212	-1.8594014000	-4.0565183003
H38	1.1116180636	-2.2653172397	-3.0177390544
H39	-0.5238065872	-2.4438405702	-2.3619230132
C40	1.5905053242	0.6499756656	-3.1510921937
H41	1.6232954569	1.7135010718	-2.8993127281
H42	2.5050847352	0.1872317209	-2.7702810475
H43	1.5537873898	0.5352302686	-4.2394681943
C44	-1.2832280317	0.6619608390	-3.2197252637
H45	-1.3552877602	1.7190644328	-2.9483005193
H46	-1.1648631506	0.5818220611	-4.3055211760
H47	-2.2147507650	0.1696844367	-2.9272720934

TpRu(PMe$_3$)OH-CH$_4$TS SCF = -1373.78783375773
Total internal energy, Utot (SCFE + ZPE + U): -1373.388305 hartrees

Total enthalpy, Htot (Utot + pV): -1373.387361 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1373.466050 hartrees

Ru1	0.0011121843	0.0233718090	0.0109444926
N2	0.0134849702	0.0021670752	2.1874918591
N3	2.0261885665	-0.6118552980	0.1818304369
N4	0.7293551093	2.0109985864	0.1856085085
N5	1.7083812124	2.2594804241	1.0955647374
N6	1.0934643805	0.5320362113	2.8166400919
N7	2.8305855786	0.0063601357	1.0850341711
B8	2.2598101182	1.1240667987	1.9875561583
H9	3.1140197621	1.5478333035	2.7172033899
O10	-1.0222605325	-1.8862876874	-0.0499384148
H11	-0.9325354192	-2.2561771522	0.8393619605
C12	2.0162950752	3.5773213596	1.0926930236
H13	2.7754306436	3.9624144378	1.7573925976
C14	1.2177365243	4.2119886187	0.1559435381
H15	1.2068695797	5.2607241410	-0.0992234021
C16	-0.8206604166	-0.4282226054	3.1420725330
H17	-1.7649630890	-0.8804240032	2.8742658899
C18	-0.2788608931	-0.1769718535	4.4132968408
H19	-0.7122718653	-0.4039529942	5.3754511897
C20	4.0401796869	-0.5997514923	1.1132491545
H21	4.8130862699	-0.2476229564	1.7804846522
C22	4.0283316722	-1.6426997364	0.2012269648
H23	4.8311404703	-2.3267611674	-0.0281932374
C24	0.4251453041	3.1860353504	-0.3836460940
H25	-0.3452266548	3.2391004313	-1.1386773168
C26	0.9375964456	0.4357134478	4.1567908286
H27	1.6992234684	0.8101042619	4.8250605060
C28	2.7383721953	-1.6120342499	-0.3534084106
H29	2.2897379370	-2.2599897922	-1.0917002824
C30	-2.3468924881	0.4033888953	0.0884121950
H31	-1.7411168804	-0.8708711860	0.0386900981
H32	-2.0221566844	1.4475407853	0.0291495249
H33	-2.8786851059	0.3061131317	1.0423602130
H34	-3.0591211779	0.2493499982	-0.7306939371
P35	0.0628119569	0.0169908081	-2.3094856738
C36	-0.1324420516	-1.6475071850	-3.0920631193
H37	-0.2094836244	-1.5765498200	-4.1818094643
H38	0.7238629131	-2.2767531709	-2.8366370245
H39	-1.0229503874	-2.1240498165	-2.6772110473
C40	1.6194979948	0.6525101275	-3.0840883670
H41	1.7632711007	1.6965450130	-2.7923960731
H42	2.4714905083	0.0795033453	-2.7101461310
H43	1.5869259132	0.5835249842	-4.1764578000
C44	-1.2180487621	0.9904113322	-3.2321128560

H45	-1.1472148331	2.0494411916	-2.9701472307
H46	-1.0886426068	0.8874500322	-4.3144760334
H47	-2.2148613495	0.6389598351	-2.9554966960

TpRu(PMe$_3$)OMe: SCF = -1372.59048382396

Total internal energy, Utot (SCFE + ZPE + U): -1372.206900 hartrees

Total enthalpy, Htot (Utot + pV): -1372.205955 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1372.285668 hartrees

Ru1	0.1110932001	-0.0243781843	0.0324094354
N2	0.0363390585	0.0740340770	2.2070781809
N3	2.0768367456	-0.5924258889	0.2265149176
N4	0.8868951403	1.9886659143	0.1989787920
N5	1.8290458329	2.2593823916	1.1380616530
N6	1.1047918219	0.5971562091	2.8631392480
N7	2.8631094830	-0.0173454545	1.1745597198
B8	2.3180054523	1.1240201628	2.0627599765
H9	3.1730628269	1.5190453672	2.8071492590
O10	-1.1565068059	-1.5725202557	-0.1650013482
C11	2.1174528664	3.5816842515	1.1396398727
H12	2.8470498301	3.9828866298	1.8277801619
C13	1.3424678902	4.1970843742	0.1696592540
H14	1.3246270295	5.2437578878	-0.0940202759
C15	-0.8988713797	-0.1803537806	3.1289657826
H16	-1.8479110180	-0.6026124561	2.8324538711
C17	-0.4354706530	0.1735606093	4.4067186106
H18	-0.9549124190	0.0823595288	5.3486459154
C19	4.0605085145	-0.6458147974	1.2127027482
H20	4.8204052422	-0.3271827265	1.9107221263
C21	4.0579080719	-1.6560656456	0.2645654259
H22	4.8550286173	-2.3464895383	0.0347492718
C23	0.5855288431	3.1543172720	-0.3895902348
H24	-0.1594027637	3.1901955687	-1.1716744430
C25	0.8421016584	0.6644300959	4.1887902432
H26	1.5795994035	1.0558107308	4.8743531330
C27	2.7879645345	-1.5861912687	-0.3273838304
H28	2.3474213814	-2.2024931139	-1.0954893461
P29	0.0598847525	-0.0758419053	-2.2986544675
C30	0.0983959684	-1.7590602586	-3.0598414065
H31	-0.2014980535	-1.7407054695	-4.1125310051
H32	1.1037120142	-2.1837549399	-2.9904843358
H33	-0.5873714095	-2.3773602285	-2.4760414260
C34	1.3447645420	0.8471513862	-3.2556773401
H35	1.3392555789	1.8992830621	-2.9598968918
H36	2.3299562163	0.4384985374	-3.0132279612
H37	1.1811004372	0.7731308784	-4.3357139251
C38	-1.5301353280	0.5824926566	-2.9822905690

H39	-1.6552047152	1.6330196155	-2.7051480924
H40	-1.5759429638	0.4929238202	-4.0729430429
H41	-2.3486447050	0.0102090582	-2.5367425931
C42	-1.3243257625	-2.6577868117	0.6980391571
H43	-1.0292452677	-2.4538693629	1.7388510873
H44	-2.3815140820	-2.9746189985	0.7104423807
H45	-0.7352414340	-3.5325223180	0.3641881767

TpRu(PMe$_3$)OMe-CH$_4$TS SCF = -1413.08570396539

Total internal energy, Utot (SCFE + ZPE + U): -1412.656531 hartrees

Total enthalpy, Htot (Utot + pV): -1412.655587 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1412.738686 hartrees

Ru1	0.0036748567	0.0006414098	0.0529582898
N2	0.0531438325	0.0824446833	2.2546007191
N3	2.0231731810	-0.6479401471	0.2007234600
N4	0.7291962649	1.9913080453	0.1954320598
N5	1.7619745912	2.2530786865	1.0384595023
N6	1.1746425558	0.6014779956	2.8239761922
N7	2.8590043691	-0.0157016973	1.0628026055
B8	2.3295262053	1.1354324555	1.9448803744
H9	3.2120290236	1.5690937990	2.6341918148
O10	-1.0279324247	-1.9043135158	-0.1402863812
C11	2.0638097217	3.5714922438	1.0015791331
H12	2.8591192267	3.9674040239	1.6158153592
C13	1.2070996050	4.1925254207	0.1074043430
H14	1.1762260666	5.2380915218	-0.1590266024
C15	-0.7965844850	-0.1801341998	3.2544360377
H16	-1.7713189227	-0.5927429625	3.0431885258
C17	-0.2256937553	0.1619382207	4.4907640617
H18	-0.6626271010	0.0625832019	5.4728271562
C19	4.0612417552	-0.6363931545	1.0767547069
H20	4.8561733269	-0.2751342103	1.7125176748
C21	4.0114517572	-1.7052863916	0.1963500026
H22	4.7989878282	-2.4067192252	-0.0337694219
C23	0.3858792244	3.1581247810	-0.3691684918
H24	-0.4301338405	3.1991675604	-1.0754358834
C25	1.0266940934	0.6576890062	4.1673586564
H26	1.8193845907	1.0473601266	4.7892676879
C27	2.7076709410	-1.6731599709	-0.3246345647
H28	2.2299071587	-2.3357742491	-1.0308984480
C29	-2.3478422196	0.3651848670	0.1389302547
H30	-1.7421029199	-0.9058872089	0.0015445480
H31	-2.0244406003	1.4085885375	0.2156101762
H32	-2.9125301099	0.1599367989	1.0566405832
H33	-3.0332126235	0.3082832780	-0.7142267687
P34	0.0741900529	0.0129006249	-2.2705047555

C35	-0.0444260429	-1.6412248403	-3.0893339472
H36	-0.1472983743	-1.5478334527	-4.1751554671
H37	0.8518267319	-2.2264281578	-2.8683608037
H38	-0.8991899024	-2.1715086215	-2.6653191585
C39	1.6121497110	0.7244382121	-3.0148194082
H40	1.7131352574	1.7679603857	-2.7047630320
H41	2.4801243927	0.1759302795	-2.6404624053
H42	1.5943133168	0.6723429437	-4.1084488170
C43	-1.2394775452	0.9474080179	-3.1858446576
H44	-1.2325085795	1.9990988617	-2.8882220724
H45	-1.0843452246	0.8868506747	-4.2680523272
H46	-2.2200713459	0.5323077997	-2.9413432308
C47	-1.0645444909	-2.8207578651	0.9346038618
H48	-1.6725361439	-2.4576048162	1.7756158280
H49	-1.5061201866	-3.7673248517	0.5908217604
H50	-0.0569548196	-3.0293428555	1.3173181415

TpRu(PMe$_3$)NH$_2$: SCF = -1313.41982171653

Total internal energy, Utot (SCFE + ZPE + U): -1313.053298 hartrees

Total enthalpy, Htot (Utot + pV): -1313.052354 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1313.128256 hartrees

Ru1	-0.2140894063	0.2301653517	-0.0780966609
N2	-0.1870190147	0.1420614225	2.1180236526
N3	-1.7125194145	1.7142773484	0.1317638300
N4	-1.9271619480	-1.0916361449	0.1137268497
N5	-2.8423940507	-0.8706950178	1.0922609607
N6	-1.3654602261	0.2448716946	2.7856453880
N7	-2.6470513644	1.6176144415	1.1123006586
B8	-2.6982018068	0.3633048448	2.0088724730
H9	-3.6193678622	0.4318341595	2.7764459269
N10	1.7342747120	0.3549603347	-0.0821895543
H11	2.3713017482	0.4903490103	-0.8628808856
C12	-3.7271408349	-1.8929948591	1.1394674803
H13	-4.5275341682	-1.8914535442	1.8647943332
C14	-3.3849737641	-2.8110239923	0.1593634063
H15	-3.8816591232	-3.7401299981	-0.0756976728
C16	0.7624988129	-0.0384860052	3.0409714938
H17	1.7936975117	-0.1685173113	2.7455709733
C18	0.2042137714	-0.0479214275	4.3293656500
H19	0.7140991689	-0.1725316518	5.2727017264
C20	-3.3805813791	2.7529099126	1.1635602177
H21	-4.1724576652	2.8592229362	1.8902075709
C22	-2.9157606906	3.6181079421	0.1860673431
H23	-3.2783230146	4.6083079719	-0.0443010109
C24	-2.2460018334	-2.2634930262	-0.4526127489
H25	-1.6382516832	-2.6603003547	-1.2523820199

C26	-1.1530256007	0.1328460016	4.1171251628
H27	-1.9797795784	0.1868897188	4.8102652768
C28	-1.8656466326	2.9216123248	-0.4316413841
H29	-1.2087180232	3.2322787751	-1.2298298981
H30	2.2648131479	0.4924550174	0.7744818478
P31	-0.2224553961	0.2445292336	-2.3805161696
C32	0.5697512568	-1.2185000482	-3.2033726791
H33	1.5968417300	-1.3156465217	-2.8408780917
H34	0.0343779582	-2.1310803396	-2.9283008302
H35	0.5768207882	-1.1246461396	-4.2949623561
C36	-1.8726333761	0.3102548500	-3.2168513921
H37	-1.7792810302	0.2997315912	-4.3078198771
H38	-2.4725128858	-0.5447950941	-2.8949599916
H39	-2.3954527697	1.2185954349	-2.9059367384
C40	0.6799570101	1.6266255674	-3.2333857338
H41	1.7128275825	1.6647367270	-2.8763793272
H42	0.6826185188	1.5018173694	-4.3216394858
H43	0.2094411149	2.5827328460	-2.9889751917

TpRu(PMe$_3$)NH$_2$-CH$_4$TS SCF = -1353.91019822870

Total internal energy, Utot (SCFE + ZPE + U): -1353.498438 hartrees

Total enthalpy, Htot (Utot + pV): -1353.497494 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1353.576227 hartrees

Ru1	-0.0797131118	0.0124791036	-0.0527376185
N2	-0.0786792914	0.0145992646	2.1144424570
N3	-1.5385560318	1.5425508223	0.1389110407
N4	-1.7102484325	-1.4104702430	0.1419359919
N5	-2.6777980221	-1.1387057293	1.0563539359
N6	-1.2729980444	0.0630814206	2.7579354910
N7	-2.5405541878	1.3804446528	1.0419157374
B8	-2.5866396455	0.1231829515	1.9429656480
H9	-3.5323312775	0.1786862116	2.6812526129
N10	1.6953274769	1.1874210061	0.0137957628
H11	1.9231401747	1.7807509094	-0.7760032221
C12	-3.5835696811	-2.1439386580	1.0859504262
H13	-4.4249369151	-2.1027110400	1.7619677850
C14	-3.2018285851	-3.1035422113	0.1630347540
H15	-3.6997696134	-4.0332729358	-0.0670666827
C16	0.8709938598	-0.0227990545	3.0549304380
H17	1.9122431087	-0.0693466662	2.7696438617
C18	0.2910272656	0.0007719500	4.3343548294
H19	0.7926737212	-0.0216342415	5.2899853322
C20	-3.3140854086	2.4903175711	1.0740724987
H21	-4.1602431418	2.5470217023	1.7428648007
C22	-2.8069292187	3.4046318411	0.1650467386
H23	-3.1859810128	4.3898844911	-0.0602963873

C24	-2.0191201439	-2.5957245425	-0.3993986121
H25	-1.3776398038	-3.0317692085	-1.1515429400
C26	-1.0731661343	0.0550966188	4.0961169732
H27	-1.9123346087	0.0874598669	4.7755830746
C28	-1.6882698873	2.7634576021	-0.3916579628
H29	-0.9877684088	3.1206866321	-1.1319063075
H30	1.7540048348	1.7309479789	0.8694616643
C31	1.7723321400	-1.5204152865	0.0004477001
H32	1.8785544250	-0.1576909616	-0.0007035452
H33	0.9349316601	-2.2250646366	-0.0421723923
H34	2.2967610543	-1.7241387496	0.9413370082
H35	2.4375645758	-1.7557194211	-0.8383367039
P36	-0.1943521644	0.0252148855	-2.3692922054
C37	0.4350236518	-1.4582443888	-3.2902999989
H38	1.4908966153	-1.6135632635	-3.0553911930
H39	-0.1138480491	-2.3510312104	-2.9800423029
H40	0.3220586858	-1.3344769538	-4.3724537366
C41	-1.9017068977	0.1832244988	-3.0693840492
H42	-1.8958250260	0.1778940720	-4.1644414445
H43	-2.5104573885	-0.6489071094	-2.7059935515
H44	-2.3558409597	1.1109430598	-2.7125862253
C45	0.7071254977	1.3665525847	-3.2854529125
H46	1.7813054882	1.2797068148	-3.0971820408
H47	0.5347405445	1.2989752388	-4.3644868811
H48	0.3774986106	2.3492489365	-2.9377110196

TpRu(PMe$_3$)NMe$_2$: SCF = -1392.02109274647

Total internal energy, Utot (SCFE + ZPE + U): -1391.595307 hartrees

Total enthalpy, Htot (Utot + pV): -1391.594363 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1391.674707 hartrees

Ru1	-0.1777563350	0.3350915988	-0.0705755778
N2	-0.2450908142	0.1200777103	2.1254239876
N3	-1.7015059448	1.7672292515	0.1103799071
N4	-1.8343060869	-1.1120218546	0.1227378291
N5	-2.8425261175	-0.8710868663	0.9990444506
N6	-1.4500866489	0.2142553944	2.7502391486
N7	-2.6723131448	1.6306586886	1.0504715667
B8	-2.7509221095	0.3626424979	1.9235004509
H9	-3.7035950839	0.4188222488	2.6525272912
N10	1.7296308980	0.9256902413	-0.0181266889
C11	-3.6988120606	-1.9185924626	1.0242045445
H12	-4.5586232537	-1.9089457074	1.6779957953
C13	-3.2425792059	-2.8746933395	0.1310892990
H14	-3.6880574528	-3.8312738691	-0.0967103761
C15	0.6368009840	-0.2823960170	3.0493096214
H16	1.6704700080	-0.4340369809	2.7767399259

C17	0.0079356481	-0.4409871465	4.2946830807
H18	0.4553902785	-0.7438826675	5.2292922480
C19	-3.4178725761	2.7583341296	1.1069247951
H20	-4.2385044919	2.8348316143	1.8047639075
C21	-2.9232734561	3.6580117087	0.1765946339
H22	-3.2862120608	4.6518483834	-0.0369146715
C23	-2.0660667756	-2.3220162982	-0.4014420713
H24	-1.3780218564	-2.7405866129	-1.1216224673
C25	-1.3182779138	-0.1209194289	4.0551278220
H26	-2.1765002891	-0.1117206370	4.7111142742
C27	-1.8421620994	2.9918010070	-0.4201883866
H28	-1.1541822604	3.3328317896	-1.1785570165
P29	-0.3911228665	0.2893035429	-2.3977112000
C30	0.3665894775	-1.1418666909	-3.3137970584
H31	1.4494134315	-1.1597802125	-3.1657220212
H32	-0.0391107566	-2.0794004423	-2.9248776319
H33	0.1565513869	-1.0851805050	-4.3875779946
C34	-2.1521167778	0.1673373899	-2.9650477763
H35	-2.2147792315	0.1371711306	-4.0577382896
H36	-2.6148335116	-0.7297956562	-2.5496998917
H37	-2.7054867111	1.0343014605	-2.5953018097
C38	0.1703862850	1.7059325489	-3.4672681726
H39	1.2374654211	1.8912262187	-3.3360872748
H40	-0.0309666972	1.4995875163	-4.5239936200
H41	-0.3700711139	2.6129005916	-3.1837322246
C42	2.6548618154	1.0381234110	-1.1327339724
H43	3.6671468565	0.7214786053	-0.8286010571
H44	2.3632116309	0.4000012047	-1.9668142342
H45	2.7547249757	2.0778066047	-1.5019947773
C46	2.2726707890	1.7247447302	1.0756279972
H47	2.4763540478	2.7588477427	0.7408786382
H48	1.5790550458	1.7812108577	1.9114162259
H49	3.2336553388	1.3216605879	1.4418970524

TpRu(PMe$_3$)NMe$_2$-CH$_4$TS SCF = -1432.51321089463

Total internal energy, Utot (SCFE + ZPE + U): -1432.041939 hartrees

Total enthalpy, Htot (Utot + pV): -1432.040995 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1432.125426 hartrees

Ru1	-0.0503851397	0.0714294821	-0.0463178442
N2	-0.1201026134	-0.0438147224	2.1455099748
N3	-1.5143547220	1.5962758079	0.1354385292
N4	-1.6550386157	-1.3840436721	0.1404277287
N5	-2.6821620808	-1.1048352307	0.9839063626
N6	-1.3381485315	0.0379746504	2.7425321576
N7	-2.5367386527	1.4208572941	1.0133341593
B8	-2.6203343905	0.1496471625	1.8853446347

H9	-3.5900098279	0.2001298393	2.5920720708
N10	1.7749943029	1.2486278680	0.0758878017
C11	-3.5483790605	-2.1438691821	1.0195337049
H12	-4.4245725841	-2.1045920510	1.6498770216
C13	-3.0804813438	-3.1328156955	0.1699155719
H14	-3.5311110708	-4.0910600199	-0.0395674025
C15	0.7724022912	-0.2612042297	3.1179952690
H16	1.8213485915	-0.3530180764	2.8780280495
C17	0.1338700740	-0.3193063809	4.3670438777
H18	0.5849278558	-0.4768770860	5.3350120207
C19	-3.2986471923	2.5383844869	1.0597528455
H20	-4.1579006071	2.5864790539	1.7122800017
C21	-2.7637049927	3.4705001625	0.1858868883
H22	-3.1268948118	4.4660450276	-0.0193021747
C23	-1.8866393106	-2.6080161608	-0.3518236934
H24	-1.1934787853	-3.0521089277	-1.0520833355
C25	-1.2077003797	-0.1272494191	4.0788888707
H26	-2.0758356758	-0.0993887234	4.7211040063
C27	-1.6409756310	2.8325765729	-0.3658173135
H28	-0.9172093303	3.2027433691	-1.0761881061
C29	1.7933987455	-1.4712930728	0.0573864859
H30	1.8692544605	-0.1252533649	0.2002055540
H31	0.9755426269	-2.1832616308	-0.0873143260
H32	2.2667050001	-1.7465125936	1.0066895250
H33	2.5094705193	-1.6253910301	-0.7570805986
P34	-0.2931219850	0.0280783416	-2.3791204748
C35	0.5782136341	-1.3287658402	-3.2993130403
H36	1.6600082390	-1.1997085814	-3.2079089687
H37	0.3198708268	-2.2983515756	-2.8656717467
H38	0.3077419408	-1.3303617497	-4.3604705244
C39	-2.0525641512	-0.2347447274	-2.9059066267
H40	-2.1400553919	-0.2533138145	-3.9970210853
H41	-2.4371961121	-1.1694627022	-2.4956575001
H42	-2.6613654619	0.5827115259	-2.5101530225
C43	0.1076325066	1.4713021108	-3.4824485462
H44	1.1711431605	1.7079237192	-3.4485188464
H45	-0.1757440277	1.2454180144	-4.5157486341
H46	-0.4521237875	2.3512220666	-3.1553493867
C47	1.8383911660	2.2873790996	1.0920686869
H48	1.3791538874	3.2320684305	0.7486485252
H49	1.3162355620	1.9849591803	1.9987644699
H50	2.8842015091	2.5217737489	1.3594079362
C51	2.5361802344	1.6516800775	-1.0875206976
H52	3.5701439116	1.9239112411	-0.8100084467
H53	2.6012305023	0.8273483730	-1.8060409699
H54	2.1117798011	2.5292835955	-1.6086358345

3Me: SCF = -839.86962106446

Total internal energy, Utot (SCFE + ZPE + U): -839.586031 hartrees

Total enthalpy, Htot (Utot + pV): -839.585087 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -839.656034 hartrees

Rh1	0.1436235147	0.0687631813	0.0087710680
O2	0.0517642964	0.0269971922	2.0353296145
O3	2.1062268759	-0.0941179045	-0.0836056924
O4	0.1196995744	2.2714620520	0.0364515819
O5	0.0077240635	0.0862131129	-2.0202533826
C6	-0.0159119068	-1.9657691360	-0.0312170899
C7	1.0854545551	-0.0708191829	2.7687718531
C8	2.4156192261	-0.1770657874	2.3057418854
C9	2.8360940286	-0.1767272718	0.9739082256
C10	0.2425408087	2.9619108069	-1.0161094402
C11	0.2834690534	2.4625751062	-2.3432190114
C12	0.1458460091	1.1331712797	-2.7556171826
H13	3.1905905677	-0.2552377120	3.0578515939
H14	0.3993256449	3.1961199021	-3.1321701518
H15	0.6296857784	-2.4303342196	0.7199349469
H16	-1.0658277143	-2.2013652099	0.1899946653
H17	0.2482194877	-2.3108005584	-1.0334250775
C18	4.3116754921	-0.2765705354	0.6496131669
H19	4.6174225862	0.6003198780	0.0701930895
H20	4.9230552816	-0.3430499516	1.5510109920
H21	4.4900988721	-1.1577148344	0.0253350799
C22	0.8157437901	-0.0532477890	4.2573565126
H23	0.3947938613	0.9192813534	4.5342954696
H24	0.0663582089	-0.8123274933	4.5012082559
H25	1.7176792644	-0.2310341725	4.8457104614
C26	0.3362254387	4.4645287455	-0.8095754230
H27	-0.5657349943	4.8143784180	-0.2963608373
H28	1.1840263176	4.6844384782	-0.1523269482
H29	0.4532757590	5.0181494835	-1.7437633961
C30	0.1396178078	0.8213082940	-4.2392820966
H31	0.2368372774	1.7174427738	-4.8552271726
H32	0.9619157115	0.1351310526	-4.4679742038
H33	-0.7908142614	0.3058266267	-4.4994198885

3Me pyridine complex: SCF = -1088.21304601441

Total internal energy, Utot (SCFE + ZPE + U): -1087.832351 hartrees

Total enthalpy, Htot (Utot + pV): -1087.831407 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1087.914380 hartrees

Rh1	0.0680230687	0.1077019004	0.0134926264
O2	0.0582688048	0.0932783612	2.0593648659
O3	2.0998878487	-0.0738342132	-0.1030862589

O4	0.2763932475	2.3263984688	0.0372448442
O5	0.0144584910	0.0969710238	-2.0391988279
C6	-0.0900258457	-1.9355052038	-0.0036220657
C7	1.1260389388	-0.0184457622	2.7548393229
C8	2.4368396722	-0.1480811043	2.2724691444
C9	2.8471459136	-0.1571535598	0.9234874458
C10	0.4265727298	2.9815820040	-1.0302699476
C11	0.4151672680	2.4623277414	-2.3530302862
C12	0.2239899858	1.1384076872	-2.7630039943
H13	3.2192040427	-0.2357854103	3.0164074423
H14	0.5713404572	3.1821143770	-3.1479697380
H15	0.7667607931	-2.3606046337	0.5275752461
H16	-1.0160815551	-2.2567579647	0.4849413223
H17	-0.0758507278	-2.2601602258	-1.0485294647
C18	4.3259627823	-0.2730720563	0.6084160693
H19	4.6454505098	0.6110816882	0.0468263695
H20	4.9399312373	-0.3674952011	1.5062621822
H21	4.4925329851	-1.1420065435	-0.0363122249
C22	0.8902488901	0.0016046004	4.2524102408
H23	0.4237054711	0.9518822765	4.5340316867
H24	0.1905284898	-0.7961423590	4.5226227620
H25	1.8130843172	-0.1228588440	4.8221788224
C26	0.6429374299	4.4787534216	-0.8575462927
H27	-0.1690583144	4.8939566825	-0.2517694721
H28	1.5731956192	4.6441259680	-0.3030631197
H29	0.6954566587	5.0173615201	-1.8064966364
C30	0.2538738301	0.8297760159	-4.2496839351
H31	0.3701739843	1.7260734466	-4.8623262648
H32	1.0821356104	0.1440157992	-4.4583474975
H33	-0.6688708049	0.3149116444	-4.5377228822
N34	-1.9946033631	0.3177998209	0.0538523775
C35	-2.7642648736	-0.1908451410	-0.9265958891
C36	-4.1455249154	-0.0296949062	-0.9349350903
C37	-4.7506257008	0.6794427591	0.1019908051
C38	-3.9472828152	1.2032367980	1.1138961213
C39	-2.5719195009	1.0030512170	1.0583962816
H40	-2.2325327527	-0.7145704828	-1.7123347209
H41	-4.7288369910	-0.4547384810	-1.7449770531
H42	-5.8271864073	0.8217224850	0.1205296864
H43	-4.3726561436	1.7631968148	1.9400432487
H44	-1.8960273567	1.3736011636	1.8191927103

3Me-CH$_4$: SCF = -880.39848027994
Total internal energy, Utot (SCFE + ZPE + U): -880.064085 hartrees
Total enthalpy, Htot (Utot + pV): -880.063140 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -880.142315 hartrees

Rh1	0.0988691154	0.0451847766	0.0043565471
O2	0.0314743270	-0.0086394583	2.0374322103
O3	2.0745144307	-0.0480030439	-0.1059809907
O4	0.1825320214	2.2607663104	0.0508384343
O5	0.0440752669	0.0655289184	-2.0372758031
C6	0.0269020097	-2.0082701957	-0.0405936625
C7	1.0815612897	-0.0675829536	2.7540512867
C8	2.4080636721	-0.1180315877	2.2783206659
C9	2.8177481719	-0.0986357953	0.9407641646
C10	0.3582174112	2.9388688396	-1.0028623542
C11	0.4101463011	2.4371708231	-2.3277755075
C12	0.2466871300	1.1130164614	-2.7525022375
H13	3.1921823984	-0.1655434910	3.0235514620
H14	0.5729683793	3.1677989828	-3.1111286953
H15	1.0189260325	-2.4029484696	0.1950398382
H16	-0.6981754835	-2.3696466238	0.6962655057
H17	-0.2601883811	-2.3066882530	-1.0524421121
C18	-2.6093295083	0.4532205436	0.1258706916
H19	-3.2418875971	0.5498451292	-0.7580919655
H20	-3.1851854674	0.1365355002	0.9969314039
H21	-2.1164793353	1.4022263278	0.3350036804
H22	-1.9068538233	-0.3789159761	-0.0940203288
C23	4.2947930893	-0.1364006155	0.6098929045
H24	4.5611987065	0.7567989834	0.0358127837
H25	4.9148204942	-0.1853957288	1.5066274284
H26	4.5051298670	-1.0039861641	-0.0234511120
C27	0.8282857325	-0.0725974059	4.2464877551
H28	0.3234958886	0.8572689099	4.5289958900
H29	0.1542648896	-0.8972755301	4.4987833409
H30	1.7488561684	-0.1692044082	4.8249339285
C31	0.5170233023	4.4372177077	-0.7976924744
H32	-0.3609533638	4.8246230333	-0.2701370797
H33	1.3836407068	4.6209762991	-0.1534964164
H34	0.6443704733	4.9863292313	-1.7332122615
C35	0.2947768064	0.8132457482	-4.2388273501
H36	0.4392489956	1.7113788526	-4.8425299616
H37	1.1103286123	0.1100824408	-4.4380462491
H38	-0.6351164164	0.3213220081	-4.5425905108

3Me-CH$_4$-TS: SCF = -880.36047455400
Total internal energy, Utot (SCFE + ZPE + U): -880.030565 hartrees
Total enthalpy, Htot (Utot + pV): -880.029620 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -880.105908 hartrees

Rh1	0.0425184864	0.0924325515	-0.0125778993
O2	0.0273476137	0.0615886821	2.0306056864
O3	2.1403945404	-0.0623840030	-0.1115858709

O4	0.3459671462	2.1738586146	0.0889036450
O5	0.0120453604	0.0864245880	-2.0558613957
C6	-0.2791331315	-2.0785230677	-0.0515211187
C7	1.0999325250	0.0453439044	2.7302822103
C8	2.4234160089	-0.0200918721	2.2707485222
C9	2.8658307600	-0.0776104658	0.9314464559
C10	0.4982023202	2.8849191690	-0.9531985062
C11	0.4654952754	2.4408058914	-2.2928196000
C12	0.2384331571	1.1360171867	-2.7539165076
H13	3.1931533887	-0.0348114158	3.0325776448
H14	0.6261240236	3.1947614818	-3.0536336907
H15	0.7132469318	-2.2795097205	-0.4528761847
H16	-0.3834775880	-2.4718968965	0.9602827149
H17	-1.0143822780	-2.5317675968	-0.7244846061
C18	-2.1472128717	0.2490931258	0.0239780636
H19	-2.5549629063	0.2328078384	-0.9875012020
H20	-2.7487135079	-0.3696802859	0.6978817659
H21	-2.1271508539	1.2618009341	0.4244656304
H22	-1.2249120176	-0.9241243608	-0.0143402096
C23	4.3566650854	-0.1692792665	0.6629957332
H24	4.6694729733	0.6978604077	0.0717880265
H25	4.9488679494	-0.2100551930	1.5793635334
H26	4.5619578350	-1.0599375347	0.0604491434
C27	0.8449221206	0.1004830800	4.2239430196
H28	0.3220717032	1.0319829431	4.4652031651
H29	0.1853970226	-0.7241417445	4.5131067385
H30	1.7662544168	0.0461901221	4.8068398850
C31	0.7360398065	4.3593171290	-0.6830529488
H32	-0.0907866136	4.7558534697	-0.0850160734
H33	1.6474205430	4.4729253006	-0.0865330442
H34	0.8321728367	4.9462185958	-1.5987059091
C35	0.2452462646	0.8754382444	-4.2474195223
H36	0.3906286290	1.7874513225	-4.8293689707
H37	1.0461137334	0.1672262413	-4.4849069764
H38	-0.6989237695	0.4057349466	-4.5412561899

3OH: SCF = -875.78019641197

Total internal energy, Utot (SCFE + ZPE + U): -875.519420 hartrees

Total enthalpy, Htot (Utot + pV): -875.518476 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -875.587585 hartrees

Rh1	0.4991888448	0.1640582389	0.1554090471
O2	-0.5139585973	-1.1323167019	1.1825114223
C3	1.2267064868	-1.7954239274	-1.8736962795
O4	1.4857204880	-1.3932698268	-0.6987465538
C5	-0.1641489040	2.8863137564	1.0203380802
O6	-0.4481028562	1.6439092319	1.1706993030

C7	1.8093680399	2.7358011579	-0.5443178840
C8	0.8558107179	3.4333088930	0.2298295308
H9	0.9377472328	4.5132066625	0.2346443375
O10	1.8904562669	1.4756087563	-0.6959517249
C11	-0.5444412624	-0.1312833443	-2.4971041858
C12	0.2796352844	-1.2239521212	-2.7557303449
H13	0.1775119548	-1.6865481611	-3.7291511789
O14	-0.6107176514	0.5750810642	-1.4188910374
H15	-1.2144309336	-0.6358810574	1.6348377070
C16	2.8745799127	3.5273309493	-1.2770375240
H17	2.8201790598	3.3017684538	-2.3470277485
H18	2.7748371449	4.6044445336	-1.1302440346
H19	3.8627552924	3.2069713899	-0.9309299843
C20	-1.0578939834	3.8110451137	1.8194454197
H21	-0.7966735167	4.8622059503	1.6850984339
H22	-2.0990231101	3.6563852589	1.5176228299
H23	-0.9885363691	3.5556743644	2.8818932630
C24	-1.5120847562	0.3538018798	-3.5555195626
H25	-2.5347424883	0.2943605678	-3.1697677362
H26	-1.3093111167	1.4051900323	-3.7823237396
H27	-1.4383838193	-0.2337891551	-4.4718985356
C28	2.0225034180	-3.0011569988	-2.3221407668
H29	1.7662476988	-3.8540054683	-1.6848889683
H30	1.8315941205	-3.2623376515	-3.3644883101
H31	3.0895711788	-2.8020998782	-2.1850937119

3OH pyridine complex: SCF = -1124.12304418162

Total internal energy, Utot (SCFE + ZPE + U): -1123.765582 hartrees

Total enthalpy, Htot (Utot + pV): -1123.764638 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1123.845809 hartrees

Rh1	0.0696474365	0.1769574768	-0.0125199682
O2	0.0303642510	0.1170296480	2.0200879116
O3	2.0865579152	-0.0580455163	-0.1357199248
O4	0.3105460628	2.2728923847	0.0954731419
O5	0.0397083846	0.1764814178	-2.0574095655
O6	-0.1865587707	-1.8018123292	-0.0600251956
C7	1.0786417569	-0.0988966415	2.7134228043
C8	2.3906727970	-0.2674894118	2.2372814089
C9	2.8136697180	-0.2384509693	0.8984198858
C10	0.4913441101	2.9795624414	-0.9490705684
C11	0.4757491437	2.5337845752	-2.2860585638
C12	0.2591176013	1.2253029585	-2.7530471296
H13	3.1570525327	-0.4389501075	2.9830631288
H14	0.6479599907	3.2875966877	-3.0447899201
H15	0.3752702767	-2.0802811358	-0.7981567462
C16	4.2840832944	-0.4345135863	0.5869501358

H17	4.6543920761	0.4273742491	0.0223261234
H18	4.8882976567	-0.5611959660	1.4873126107
H19	4.4037659774	-1.3154576631	-0.0523648710
C20	0.8231756799	-0.1660271923	4.2058557964
H21	0.3358316369	0.7577727926	4.5341595823
H22	0.1326251670	-0.9897281764	4.4145406413
H23	1.7398995801	-0.3127653180	4.7802475825
C24	0.7414665679	4.4517718060	-0.6779953433
H25	-0.0737029729	4.8545179549	-0.0678488918
H26	1.6616454338	4.5581727015	-0.0934219572
H27	0.8304301158	5.0407925352	-1.5930613511
C28	0.2762029748	0.9711625436	-4.2480587432
H29	0.4009624059	1.8878567852	-4.8276455830
H30	1.0940257033	0.2827978735	-4.4864872996
H31	-0.6556993752	0.4795396237	-4.5448898076
N32	-1.9960277310	0.3681260520	0.0500255099
C33	-2.7517801199	-0.6325600838	-0.4361139707
C34	-4.1415183128	-0.5654849964	-0.4120832666
C35	-4.7587104102	0.5575144592	0.1365650210
C36	-3.9624009945	1.5806295397	0.6515012222
C37	-2.5791933127	1.4517596702	0.5911306890
H38	-2.1799736350	-1.4872144912	-0.7864170217
H39	-4.7228069790	-1.3890953405	-0.8132479405
H40	-5.8419047117	0.6329731266	0.1684872114
H41	-4.3998627371	2.4685121264	1.0957379309
H42	-1.9022986706	2.2114335149	0.9651214600

3OH-CH_4: SCF = -916.30312972856

Total internal energy, Utot (SCFE + ZPE + U): -915.992021 hartrees

Total enthalpy, Htot (Utot + pV): -915.991077 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -916.069180 hartrees

Rh1	0.3112935806	0.1389642988	0.1096147095
O2	1.2255143848	-0.3120984959	1.8020693058
C3	1.1600264628	-1.7539802223	-1.9706616338
O4	1.2329469570	-1.4647449684	-0.7275498404
C5	-0.2404056598	2.8541714638	1.0335411681
O6	-0.6649170499	1.6518090874	1.0564210832
C7	1.8485158600	2.5204837442	-0.3122155474
C8	0.9391658384	3.3022087483	0.4082270326
H9	1.1684483898	4.3568477142	0.4930496648
O10	1.7821790540	1.2605812194	-0.5538443571
C11	-0.5153845402	-0.0483880731	-2.7557160717
C12	0.3797395972	-1.1174809448	-2.9510739187
H13	0.4577910765	-1.5087684474	-3.9579275322
O14	-0.7503570210	0.5526732214	-1.6561767440
C15	-1.6685604250	-1.6572030232	1.1263397285

H16	-0.7710716161	-1.5150236551	1.7351802034
H17	0.9333508040	0.3564459799	2.4405241194
H18	-1.6761025862	-1.0167725498	0.2282234204
H19	-1.7168739986	-2.6947753330	0.7897514578
H20	-2.5538246576	-1.3925623791	1.7089392969
C21	3.0847538552	3.1592565512	-0.9066786284
H22	3.1406794320	2.9248877315	-1.9738694974
H23	3.0894322946	4.2419801512	-0.7712303840
H24	3.9741763792	2.7326770317	-0.4316513588
C25	-1.1234592400	3.8480388876	1.7550978092
H26	-0.6785411612	4.8435763107	1.7999527752
H27	-2.0878985432	3.9105147466	1.2396584954
H28	-1.3216148353	3.4911919484	2.7703011604
C29	-1.3111091232	0.4683649879	-3.9382384444
H30	-2.3805452749	0.3954278567	-3.7150197363
H31	-1.0861162548	1.5295188535	-4.0886175716
H32	-1.0983185711	-0.0776974111	-4.8593720395
C33	2.0277446378	-2.9308503923	-2.3668311298
H34	1.7418169739	-3.8071325791	-1.7762475982
H35	1.9479894174	-3.1696611501	-3.4290035225
H36	3.0705076542	-2.7052294378	-2.1216749994

3OH-CH$_4$-TS: SCF = -916.28186573591

Total internal energy, Utot (SCFE + ZPE + U): -915.975660 hartrees

Total enthalpy, Htot (Utot + pV): -915.974716 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -916.047894 hartrees

Rh1	0.2057532452	0.0784796272	0.0802380028
O2	0.9335416647	-0.5596727839	1.9086890192
C3	1.0946671582	-1.7505866425	-2.0251066298
O4	1.1431736429	-1.5105398602	-0.7730943954
C5	-0.3141384731	2.8373529137	0.9335939211
O6	-0.7243121405	1.6267418873	1.0297638332
C7	1.7984712612	2.5037357532	-0.3905833368
C8	0.8445899209	3.2893458938	0.2863801223
H9	1.0351926341	4.3546679393	0.3242793807
O10	1.7644312893	1.2430476681	-0.5684194938
C11	-0.5165804391	0.0284135844	-2.7715239291
C12	0.3432935549	-1.0587264578	-2.9933716468
H13	0.4256520122	-1.4124020764	-4.0135466115
O14	-0.7561113757	0.6018577592	-1.6537703319
C15	-1.4074540505	-1.3209714618	0.9348272908
H16	-0.2635954355	-1.0233625438	1.5535375155
H17	0.7306296801	0.1657085017	2.5202708545
H18	-1.8875471938	-1.0896490711	-0.0195191045
H19	-1.2637439234	-2.4048935112	0.9726701411
H20	-2.0805154928	-0.9657230649	1.7208260845

C21	3.0190227898	3.1779592082	-0.9842027124
H22	3.0637701064	2.9652783090	-2.0571017098
H23	3.0151662235	4.2586682638	-0.8303172780
H24	3.9208125873	2.7523749446	-0.5323197804
C25	-1.2179039774	3.8421486589	1.6172169239
H26	-0.8066719746	4.8529890175	1.5983861937
H27	-2.1933303921	3.8432903976	1.1189409974
H28	-1.3864313440	3.5381292375	2.6550078704
C29	-1.2718712680	0.6245901538	-3.9419558580
H30	-2.3465019574	0.5959126796	-3.7350879289
H31	-0.9931485311	1.6778775822	-4.0522422588
H32	-1.0710771309	0.1005548118	-4.8782332848
C33	1.9522413015	-2.9223147994	-2.4559790627
H34	1.6553457093	-3.8153149176	-1.8970153002
H35	1.8758805966	-3.1236311767	-3.5260824092
H36	2.9962568805	-2.7144298648	-2.2003861169

3OH-CH_4-Product: SCF = -916.32718741149

Total internal energy, Utot (SCFE + ZPE + U): -916.015198 hartrees

Total enthalpy, Htot (Utot + pV): -916.014254 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -916.090892 hartrees

Rh1	0.0769413204	0.0145773169	0.0149790285
O2	0.9589614510	-0.4272097825	1.9478675878
C3	0.8921859625	-1.9038696578	-2.0360852295
O4	1.0032132741	-1.5999540291	-0.8026271983
C5	-0.4061754849	2.7933560076	0.9587265999
O6	-0.8051616968	1.5668475050	1.0316799960
C7	1.7643780627	2.5604868626	-0.3244523044
C8	0.7412112410	3.2926989422	0.3438228728
H9	0.8831110053	4.3652411880	0.4057022713
O10	1.7899672542	1.3160605831	-0.5149502291
C11	-0.6610963077	-0.0775220452	-2.7879338077
C12	0.1199294308	-1.2249741495	-2.9967410047
H13	0.1355680548	-1.6234802299	-4.0036484664
O14	-0.8209132769	0.5600380364	-1.6900492428
C15	-1.5320376806	-1.1637777089	0.4786831395
H16	0.6940896215	-1.3311209472	2.1736656516
H17	0.4160942250	0.1597256653	2.5004533632
H18	-1.9041352640	-1.6549420055	-0.4251429416
H19	-1.2548798021	-1.9418395698	1.2052855985
H20	-2.3097309114	-0.5215689470	0.9018451466
C21	2.9594441368	3.3349880044	-0.8599049530
H22	3.0287511680	3.1825783359	-1.9422314976
H23	2.9045843042	4.4060474339	-0.6526961102
H24	3.8765086140	2.9297047775	-0.4200797163
C25	-1.3419143264	3.7606494235	1.6583899932

H26	-0.9661785172	4.7857347563	1.6523246972
H27	-2.3202353930	3.7344999149	1.1662715453
H28	-1.4964757150	3.4408116758	2.6944105811
C29	-1.4219100463	0.5241955434	-3.9512088350
H30	-2.4891000186	0.5581935150	-3.7095368865
H31	-1.0919760036	1.5568209362	-4.1047157406
H32	-1.2796183991	-0.0389443150	-4.8753755914
C33	1.6939568383	-3.1189536041	-2.4539525169
H34	1.4067824919	-3.9768036133	-1.8373419766
H35	1.5524214461	-3.3699102058	-3.5068410781
H36	2.7567311631	-2.9291504336	-2.2705123707

3NH$_2$: SCF = -855.91830324144

Total internal energy, Utot (SCFE + ZPE + U): -855.645265 hartrees

Total enthalpy, Htot (Utot + pV): -855.644321 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -855.714409 hartrees

Rh1	0.1540160195	0.4309913151	0.2896712951
N2	0.3394123156	0.1300693401	2.1431067012
C3	2.9010723701	0.4477984166	-0.7522298381
O4	2.1676638110	0.8028571288	0.2307489372
C5	-2.7421114688	0.6598451324	-0.1485601227
O6	-1.8437366202	0.0331295812	0.5073730484
C7	-1.3270470675	2.2873593318	-1.4515509475
C8	-2.5479877125	1.7034020707	-1.0713454113
H9	-3.4401928426	2.1181774720	-1.5239743228
O10	-0.1585448767	1.9632886252	-1.0535291382
C11	1.2103296982	-0.7299092050	-2.2024844515
C12	2.4990305410	-0.2549575537	-1.9022669917
H13	3.2727662626	-0.4740871758	-2.6276922193
O14	0.1523846541	-0.5878817195	-1.5029747193
H15	-0.4329417562	-0.1391338388	2.7474659331
C16	-1.3382489269	3.4431696685	-2.4332121130
H17	-0.7328631332	3.1826994370	-3.3074070243
H18	-2.3472743657	3.7028575026	-2.7590656227
H19	-0.8734831347	4.3183948370	-1.9677846034
C20	-4.1537427165	0.1899248259	0.1400653339
H21	-4.9077829077	0.7873019696	-0.3758599668
H22	-4.2542771336	-0.8562941046	-0.1682904900
H23	-4.3367688417	0.2277889974	1.2185121789
C24	0.9955109841	-1.5172287164	-3.4806819626
H25	0.6252973277	-2.5172680407	-3.2320936546
H26	0.2237661044	-1.0278386840	-4.0833213278
H27	1.9090682419	-1.6097685883	-4.0711339550
C28	4.3555716003	0.8488980779	-0.6095358858
H29	4.7457800921	0.4715054739	0.3409298198
H30	4.9750211050	0.4767948011	-1.4277242346

H31	4.4253898500	1.9414754235	-0.5764944858
H32	1.2215895918	0.2222538177	2.6406182577

3NH_2 pyridine complex: SCF = -1104.24631395826

Total internal energy, Utot (SCFE + ZPE + U): -1103.876519 hartrees

Total enthalpy, Htot (Utot + pV): -1103.875575 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1103.957451 hartrees

Rh1	0.0748594255	0.1566600590	0.0154749101
O2	0.0480363248	0.1821186422	2.0543620982
O3	2.0995730128	-0.0245177637	-0.1062320160
O4	0.2740788295	2.3091175481	0.0210297440
O5	0.0220862097	0.0795864566	-2.0326933527
N6	-0.0077840087	-1.8705528897	0.0753666476
C7	1.1066990101	-0.0037973887	2.7487895288
C8	2.4114683575	-0.1781760581	2.2700884310
C9	2.8284917615	-0.1818862515	0.9249091313
C10	0.4193340060	2.9603175286	-1.0540790636
C11	0.4101756283	2.4374358548	-2.3721507520
C12	0.2268101842	1.1085713420	-2.7735492733
H13	3.1832234242	-0.3281305754	3.0150977649
H14	0.5634053400	3.1546546956	-3.1697773251
H15	-0.9757430838	-2.1231800686	0.2989756826
H16	0.0929141654	-2.1427686074	-0.9078614272
C17	4.2981667429	-0.3882409017	0.6159651528
H18	4.6496881139	0.4143227807	-0.0397716311
H19	4.9151533763	-0.4173007821	1.5163149564
H20	4.4187233924	-1.3302636773	0.0703294117
C21	0.8618092053	-0.0245232396	4.2445163762
H22	0.3348552070	0.8876760719	4.5429009093
H23	0.2129271553	-0.8717795875	4.4917721064
H24	1.7874615399	-0.1076467395	4.8172955226
C25	0.6268049560	4.4558449666	-0.8790840697
H26	-0.1773572960	4.8626851699	-0.2577934456
H27	1.5656978019	4.6261876196	-0.3409488087
H28	0.6588436270	4.9958468018	-1.8278562377
C29	0.2599901970	0.7833755640	-4.2552438672
H30	0.3697414339	1.6735874873	-4.8776534830
H31	1.0943205557	0.1023091178	-4.4548816949
H32	-0.6583475375	0.2577865311	-4.5376464839
N33	-1.9903851745	0.3464201298	0.0533973588
C34	-2.7522663710	-0.2196133633	-0.9017862677
C35	-4.1382934605	-0.1028156927	-0.9001544419
C36	-4.7549347487	0.6205536834	0.1198928841
C37	-3.9590122144	1.2037465519	1.1052252997
C38	-2.5786987420	1.0453937054	1.0420446188
H39	-2.2118986858	-0.7526411695	-1.6749888099

H40	-4.7162645351	-0.5726350727	-1.6889958152
H41	-5.8352874412	0.7285772104	0.1460214539
H42	-4.3947435426	1.7754492177	1.9177967263
H43	-1.9074197631	1.4584257326	1.7849168312

3NH$_2$-CH$_4$-TS: SCF = -896.41640369438

Total internal energy, Utot (SCFE + ZPE + U): -896.097802 hartrees

Total enthalpy, Htot (Utot + pV): -896.096858 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -896.170538 hartrees

Rh1	-0.0047295133	0.0001292919	-0.0114732351
N2	-0.0131173689	0.0489348868	2.0403449844
C3	2.7741062213	-0.0091018499	-0.9588575817
O4	2.0322165816	0.0177812408	0.0847892771
C5	-2.7533602212	0.9698775699	-0.3300905351
O6	-2.0446526723	-0.0468689361	-0.0186379729
C7	-0.9567962006	2.7047631510	-0.6369667657
C8	-2.2927964689	2.2645803846	-0.6231528098
H9	-3.0480321334	3.0045418226	-0.8575296655
O10	0.0847338714	2.0065673543	-0.4024324636
C11	1.0501331366	-0.2942718751	-2.7803169432
C12	2.3670403834	-0.1457105914	-2.2943368083
H13	3.1565246382	-0.1505181647	-3.0358756440
O14	-0.0188064830	-0.3100425525	-2.0915941598
C15	-0.0243879108	-2.2395490778	0.5961647404
H16	-0.0137768217	-1.2287614537	1.4394258899
H17	-0.8489602819	0.5142145422	2.3806631394
H18	-0.0727665609	-2.3406622795	-0.4908238024
H19	0.8898141668	-2.7302181989	0.9413196968
H20	-0.9241600376	-2.7123554922	1.0012164225
C21	-0.6643067098	4.1579922243	-0.9542576683
H22	-0.0183682017	4.2117281944	-1.8367204417
H23	-1.5720256120	4.7359634293	-1.1378277604
H24	-0.1120794270	4.6076115265	-0.1227533700
C25	-4.2417457926	0.6905616802	-0.3718727287
H26	-4.8307533161	1.5936645296	-0.5421802718
H27	-4.4486702250	-0.0266973029	-1.1734680739
H28	-4.5537859302	0.2238381287	0.5674199464
C29	0.8413300872	-0.4593650915	-4.2740651661
H30	0.2941082253	-1.3884822159	-4.4632349397
H31	0.2171416718	0.3616201805	-4.6426234900
H32	1.7795345640	-0.4740393089	-4.8323010952
C33	4.2528177623	0.1183140198	-0.6514923443
H34	4.5515479979	-0.6761474201	0.0400128121
H35	4.8716255612	0.0651861396	-1.5491472500
H36	4.4346235804	1.0724433921	-0.1456875655
H37	0.8271856289	0.5310796483	2.3451614904

3NH$_2$-CH$_4$-Product: SCF = -896.48477037292

Total internal energy, Utot (SCFE + ZPE + U): -896.158918 hartrees

Total enthalpy, Htot (Utot + pV): -896.157974 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -896.234308 hartrees

Rh1	0.0243424645	-0.1549740123	-0.0983516279
N2	0.0576921364	0.1308708124	1.9869528434
C3	2.8011245831	-0.2731414347	-1.0207410207
O4	2.0601847803	-0.1520737498	0.0145483550
C5	-2.7702067683	0.8098688235	-0.4032563481
O6	-2.0306237293	-0.1914663302	-0.0955293407
C7	-1.0818247780	2.6909892173	-0.5609786298
C8	-2.3851126758	2.1377125609	-0.6344695562
H9	-3.1846964077	2.8252621941	-0.8842371500
O10	-0.0144765049	2.0702946237	-0.2864473382
C11	1.0441823744	-0.4636197728	-2.8182144540
C12	2.3729737476	-0.4263971917	-2.3487954793
H13	3.1502023994	-0.5156664470	-3.0979336253
O14	-0.0187117906	-0.3806659591	-2.1211223238
C15	0.0316076133	-2.1890758160	0.1329204279
H16	-0.6410456738	-0.4247341509	2.4748137896
H17	-0.1061783120	1.1184783397	2.1736426410
H18	0.5479355498	-2.6498822185	-0.7147918205
H19	0.5451812406	-2.4766747169	1.0592899985
H20	-1.0093244482	-2.5250164388	0.1584789340
C21	-0.9238990560	4.1801190099	-0.8320619420
H22	-0.3421185087	4.3146770406	-1.7508783720
H23	-1.8784445860	4.7002240457	-0.9402166471
H24	-0.3498119468	4.6392026843	-0.0210057163
C25	-4.2426272920	0.4541316739	-0.5099328107
H26	-4.8738911893	1.3264792521	-0.6912009627
H27	-4.3795140801	-0.2620215894	-1.3274924375
H28	-4.5687760919	-0.0429768755	0.4094482245
C29	0.7978282293	-0.6125691213	-4.3069315591
H30	0.1800292715	-1.4984632913	-4.4859543705
H31	0.2324065688	0.2530265745	-4.6676378499
H32	1.7241614191	-0.6981142021	-4.8783242426
C33	4.2872118439	-0.2344302267	-0.7251825149
H34	4.5385355488	-1.0234498204	-0.0086265927
H35	4.8947348893	-0.3605973581	-1.6232980026
H36	4.5386611548	0.7227245112	-0.2558470081
H37	0.9857437665	-0.1146523234	2.3269752874

4Me: SCF = -946.75565507485

Total internal energy, Utot (SCFE + ZPE + U): -946.490539 hartrees

Total enthalpy, Htot (Utot + pV): -946.489594 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -946.554269 hartrees

Os1	0.7689844111	-0.1534624176	0.2907054633
N2	0.7387099702	-0.5518371457	-1.8530270044
C3	0.7877452662	0.1860199244	2.1133759360
C4	0.6156183142	-2.2223925871	0.6177542338
N5	0.1936212721	1.8939574829	-0.3214521243
N6	2.6290487300	0.6372976772	0.0063668876
N7	2.9431305987	1.3377155231	-1.1194574830
N8	1.2567988992	0.3688077192	-2.7105185099
N9	0.7503177405	2.4611041924	-1.4224783686
B10	1.8559345023	1.6880665268	-2.1645543566
H11	2.3220407776	2.3386515566	-3.0568042881
O12	0.8202314502	0.4070720716	3.2604893932
H13	0.9391495817	-2.6274567909	1.5797599167
H14	1.0158098744	-2.8488279189	-0.1859358720
H15	-0.4947883434	-2.3456967276	0.5950109778
C16	4.2539484364	1.6639982561	-1.0836884153
H17	4.6965378428	2.2191094353	-1.8972102876
C18	4.8029249115	1.1731651442	0.0911485733
H19	5.8242260276	1.2609846293	0.4278681918
C20	0.2582994111	-1.5558080074	-2.5994872971
H21	-0.2005621533	-2.4104695972	-2.1250758522
C22	0.4636208773	-1.2897631971	-3.9588635096
H23	0.1897000558	-1.9053788153	-4.8016531301
C24	0.1926554251	3.6719618352	-1.6470820329
H25	0.5088847153	4.2753672575	-2.4853425721
C26	-0.7557504847	3.9030059511	-0.6624437311
H27	-1.3816850019	4.7740494550	-0.5431665622
C28	3.7441058127	0.5337849726	0.7461351405
H29	3.7171885532	0.0076589189	1.6878573107
C30	1.1030708857	-0.0584274444	-3.9812074599
H31	1.4586824282	0.5412865063	-4.8060935337
C32	-0.7161687044	2.7564574653	0.1458811471
H33	-1.2854287912	2.5126865879	1.0312665606

4Me pyridine complex: SCF = -1195.09472865019

Total internal energy, Utot (SCFE + ZPE + U): -1194.732004 hartrees

Total enthalpy, Htot (Utot + pV): -1194.731060 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1194.808057 hartrees

Os1	0.6559608813	-0.1108935979	0.3534912469
N2	0.1490147359	2.0661306080	0.4513836398
C3	1.1797820491	-1.8769593577	0.2866675034
C4	0.7028476949	0.0278298912	-1.7813242531
N5	0.6960648680	0.0841101394	2.6049447505
N6	2.6471057786	0.5760482232	0.4598654911
N7	3.0005607070	1.5734077202	1.3150224462

N8	0.8404376217	2.8442603783	1.3272073034
N9	1.3176807522	1.1697900869	3.1375833287
B10	1.9450378876	2.2412953740	2.2223986828
H11	2.4538134528	3.1037705813	2.8842079144
O12	1.5122596130	-3.0006000881	0.2375874039
H13	1.7094055426	-0.1314793419	-2.1900721579
H14	0.4001340014	1.0328833473	-2.1128237398
H15	0.0462785721	-0.6950800011	-2.2870940865
C16	4.3283035748	1.8096432856	1.2085413096
H17	4.7950179028	2.5753492227	1.8101871707
C18	4.8555828992	0.9418536467	0.2663682224
H19	5.8824525715	0.8633273978	-0.0561183129
C20	-0.6874257980	2.8837067480	-0.2025920819
H21	-1.3414182714	2.5045803128	-0.9712437777
C22	-0.5478111266	4.2017566262	0.2513355435
H23	-1.0822965022	5.0773517227	-0.0836925231
C24	1.3108956162	1.0942682751	4.4875710280
H25	1.7631052307	1.8747168314	5.0816634368
C26	0.6711581208	-0.0774620254	4.8558598615
H27	0.4962078492	-0.4494142963	5.8538744320
C28	3.7594601234	0.1866458121	-0.1754868075
H29	3.7125683598	-0.6085181622	-0.9039005123
C30	0.4379752583	4.1280688903	1.2226578640
H31	0.8842679164	4.8917955823	1.8422541066
C32	0.3098359677	-0.6742208376	3.6387865328
H33	-0.1949033787	-1.6137623049	3.4731297639
N34	-1.3909397855	-0.7025936985	0.2227979072
C35	-2.2293384258	-0.1625187261	-0.6912432705
C36	-3.5698924118	-0.5147328080	-0.7978379480
C37	-4.0909996498	-1.4870649652	0.0508845982
C38	-3.2265666175	-2.0798775411	0.9705076185
C39	-1.9030747114	-1.6673119074	1.0248592076
H40	-1.7850247942	0.5484637844	-1.3721007385
H41	-4.1843534016	-0.0333629904	-1.5516036916
H42	-5.1331748699	-1.7846142943	-0.0103092561
H43	-3.5655881917	-2.8591421065	1.6450444869
H44	-1.2068688457	-2.1197246667	1.7168959774

4Me-CH$_4$: SCF = -987.28646213055
Total internal energy, Utot (SCFE + ZPE + U): -986.970132 hartrees
Total enthalpy, Htot (Utot + pV): -986.969188 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -987.040637 hartrees

Os1	0.6912809716	-0.1133560079	0.2934045955
N2	0.7095226118	-0.5475098558	-1.8477076956
C3	0.7078363989	0.2460496077	2.1134374716
C4	1.3359803685	-2.1361672305	0.6597487808

N5	0.1424124415	1.9360059409	-0.3931439827
N6	2.6315527908	0.5020991467	0.0401158632
N7	2.9820533847	1.2236440971	-1.0624594863
N8	1.2941864392	0.3390781216	-2.6948827765
N9	0.8307761011	2.4630685085	-1.4397743817
B10	1.9333228261	1.6289493744	-2.1278814050
H11	2.4558307740	2.2591927027	-3.0040557331
O12	0.7300141793	0.4536976720	3.2641863473
H13	2.4006254903	-2.1726496057	0.9263852405
H14	1.2257175979	-2.7516973598	-0.2437942237
H15	0.7964846378	-2.6508003909	1.4663159335
C16	4.3063360297	1.4933282489	-1.0109006084
H17	4.7759370299	2.0574914489	-1.8027674528
C18	4.8279364664	0.9425504966	0.1484264376
H19	5.8498230279	0.9783766571	0.4931602603
C20	0.2439763713	-1.5568403335	-2.5945503004
H21	-0.2525674034	-2.3938202595	-2.1258217525
C22	0.5231965493	-1.3251253472	-3.9483565859
H23	0.2780988997	-1.9531182100	-4.7909934677
C24	0.4032669660	3.7228902389	-1.6828896357
H25	0.8388253622	4.3048555124	-2.4818422384
C26	-0.5931669436	4.0302317645	-0.7698905832
H27	-1.1443699613	4.9540977041	-0.6827543267
C28	3.7368271086	0.3276408604	0.7771370484
H29	3.6839534050	-0.2191671808	1.7059331202
C30	1.1942167857	-0.1107409920	-3.9637084084
H31	1.6080133940	0.4613552144	-4.7810186561
C32	-0.7168099791	2.8759240282	0.0191708498
H33	-1.3650143123	2.6832846503	0.8623997504
H34	-0.8799062003	-1.1892711385	0.5347788062
C35	-1.8965361693	-0.7277135637	0.3239682422
H36	-1.9188051618	0.2160030141	-0.2144017294
H37	-2.3808601485	-1.4992261485	-0.2795559771
H38	-2.3878021260	-0.6267299967	1.2915604427

4Me-CH$_4$-TS: SCF = -987.27540507873

Total internal energy, Utot (SCFE + ZPE + U): -986.961822 hartrees

Total enthalpy, Htot (Utot + pV): -986.960878 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -987.029636 hartrees

Os1	0.3434995658	-0.0206784159	0.2274017844
N2	0.4538115271	-0.4097292322	-1.9159699706
C3	0.2122487051	0.3060990884	2.0501006190
C4	1.2835844958	-2.0645955163	0.5900494703
N5	0.0102762768	2.0250154293	-0.3510675866
N6	2.4712620830	0.6251540071	-0.0120589032
N7	2.8285249400	1.3203896825	-1.1232053829

N8	1.1012217692	0.4570387535	-2.7374111722
N9	0.6762404828	2.5514379521	-1.4144621478
B10	1.7563966026	1.7294478761	-2.1590696897
H11	2.2470212876	2.3826739623	-3.0368641263
O12	0.1089175094	0.5002019184	3.1964802830
H13	2.2119812874	-1.7669681555	1.0779358024
H14	1.5077208832	-2.4989876188	-0.3854778272
H15	0.8246655543	-2.8334166665	1.2205359149
C16	4.1417928302	1.6339655010	-1.0624176774
H17	4.6072201020	2.1958647589	-1.8588398326
C18	4.6597496696	1.1280587930	0.1196909361
H19	5.6742794854	1.2026047539	0.4802395282
C20	-0.0137182511	-1.4031950168	-2.6818569381
H21	-0.5754990618	-2.2113697330	-2.2365225305
C22	0.3335778829	-1.1850696655	-4.0223516937
H23	0.1010243509	-1.8041970598	-4.8750418055
C24	0.2946130439	3.8350163014	-1.5914442544
H25	0.7227871528	4.4255033935	-2.3879008776
C26	-0.6452063061	4.1553702326	-0.6234776452
H27	-1.1506327980	5.0982171252	-0.4819242730
C28	3.5677633083	0.5091349635	0.7458435502
H29	3.5195392194	0.0024388766	1.6991250162
C30	1.0391569792	0.0089466636	-4.0100657305
H31	1.4983956857	0.5704633060	-4.8101920951
C32	-0.7873094007	2.9847962458	0.1331205512
H33	-1.4125356048	2.7861005821	0.9908350236
H34	-0.1184780070	-1.5547224308	0.4436999363
C35	-1.8168663216	-0.2448301860	0.1046786200
H36	-2.0963021091	-0.7652286224	-0.8187508267
H37	-2.2712435448	-0.7875175154	0.9396659414
H38	-2.2797583129	0.7469556255	0.0675863359

4OH: SCF = -982.69182752974

Total internal energy, Utot (SCFE + ZPE + U): -982.448902 hartrees

Total enthalpy, Htot (Utot + pV): -982.447958 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -982.511985 hartrees

Os1	0.1206078275	-0.2227661868	0.0076397676
N2	0.1087686392	-0.1852154892	2.2119848989
C3	0.1720481222	-0.2259210384	-1.8464290891
N4	2.1860941451	-0.5794949267	0.1830472470
N5	0.8367576909	1.7498182013	0.1360838191
N6	1.6975584300	2.1411390924	1.1134741544
N7	1.1381390301	0.4257424296	2.8579490701
N8	2.9357057295	-0.0003020160	1.1582059367
B9	2.2950732159	1.0771619838	2.0561672360
H10	3.0987833525	1.5576412766	2.8034485085

O11	0.2636923131	-0.1904854089	-3.0088225133
O12	-1.5591276042	-1.1919588973	0.0245843487
H13	-1.8932701613	-1.3681989414	0.9142292718
C14	1.8755141653	3.4791162362	1.0461026820
H15	2.5276929186	3.9788498121	1.7466929250
C16	1.1165788981	3.9708063911	-0.0050708026
H17	1.0338755792	4.9947174295	-0.3350795556
C18	-0.7237812510	-0.6408611286	3.1587177672
H19	-1.6292155911	-1.1703973230	2.8983488354
C20	-0.2364619870	-0.3272452810	4.4326405161
H21	-0.6825755027	-0.5593395077	5.3872694170
C22	4.1854231125	-0.5135777186	1.1292645925
H23	4.9302953911	-0.1767336947	1.8347754075
C24	4.2533215189	-1.4469933832	0.1058741325
H25	5.1058169283	-2.0380826602	-0.1910498637
C26	0.4802170296	2.8469940307	-0.5468912707
H27	-0.2086036997	2.7653076330	-1.3741557368
C28	0.9494019952	0.3511191598	4.1915212710
H29	1.6689856561	0.7848505232	4.8700371578
C30	2.9719635579	-1.4548906712	-0.4600542914
H31	2.5733615828	-2.0355332631	-1.2785902840

4OH pyridine complex: SCF = -1231.02380973133

Total internal energy, Utot (SCFE + ZPE + U): -1230.684737 hartrees

Total enthalpy, Htot (Utot + pV): -1230.683793 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1230.759640 hartrees

Os1	0.6780459224	-0.0993334280	0.3620216151
N2	0.0995727432	1.9907184339	0.6265552213
C3	1.2313623186	-1.8517273088	0.1386459060
O4	0.3674473945	0.2967775116	-1.6404640209
N5	0.8261238467	-0.1511015259	2.4965774980
N6	2.6306097391	0.6758494183	0.4073197690
N7	2.9559810316	1.6242728013	1.3300259731
N8	0.7294128954	2.7520135689	1.5570859126
N9	1.3766362622	0.9108157872	3.1479378374
B10	1.9010460796	2.1292109602	2.3503439459
H11	2.3900167130	2.9356989721	3.0913063998
O12	1.5866988423	-2.9587154342	-0.0062549991
H13	1.2124575986	0.5032933705	-2.0577553463
C14	4.2437368700	1.9972715183	1.1533682947
H15	4.6865348160	2.7467060890	1.7924016545
C16	4.7735213241	1.2742808343	0.0961677541
H17	5.7755705013	1.3260884429	-0.3010679480
C18	-0.7561243334	2.7784718216	-0.0296384282
H19	-1.3303313459	2.3688886526	-0.8473196215
C20	-0.6980048768	4.0805149012	0.4917141491

H21	-1.2659808274	4.9437695196	0.1798355143
C22	1.4025562978	0.6643252018	4.4774901897
H23	1.8081227553	1.3961126123	5.1602233917
C24	0.8568001923	-0.5894299843	4.7037148188
H25	0.7322228259	-1.0928761501	5.6501647597
C26	3.7207115823	0.4569974373	-0.3393831763
H27	3.6915532593	-0.2762956454	-1.1322293803
C28	0.2634377679	4.0188063313	1.4910099272
H29	0.6514935164	4.7809872871	2.1508417084
C30	0.5134261319	-1.0626665146	3.4287044306
H31	0.0753233508	-2.0048274596	3.1325034892
N32	-1.3763319084	-0.6230545706	0.2674243149
C33	-1.8593169966	-1.1554734547	-0.8790113581
C34	-3.1973918011	-1.5006907258	-1.0247953430
C35	-4.0815219560	-1.2807331289	0.0300146694
C36	-3.5865737274	-0.7097354924	1.2020842344
C37	-2.2352871055	-0.3969058990	1.2849030251
H38	-1.1303946804	-1.2344108438	-1.6780860824
H39	-3.5338676373	-1.9296739948	-1.9630390808
H40	-5.1316895345	-1.5423426747	-0.0599358808
H41	-4.2332592830	-0.5077882875	2.0495297681
H42	-1.8045425034	0.0396382397	2.1776681063

4OH-CH$_4$: SCF = -1023.20545778309

Total internal energy, Utot (SCFE + ZPE + U): -1022.912732 hartrees

Total enthalpy, Htot (Utot + pV): -1022.911787 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1022.982472 hartrees

Os1	0.0595014401	-0.1014158127	0.0084804107
N2	0.0595145892	-0.0946865985	2.1763235576
C3	0.1252438853	-0.1453782230	-1.8508730583
N4	2.0086376858	-0.6764264065	0.2046338907
N5	0.7884569122	1.9130638923	0.1537579489
N6	1.7272067502	2.1966163509	1.0979538759
N7	1.0871594153	0.4946677963	2.8393103618
N8	2.8142236348	-0.0622624743	1.1167755352
B9	2.2628999535	1.0778618722	2.0159751104
H10	3.1232066599	1.4946873338	2.7386711627
O11	0.1903942487	-0.1705782071	-3.0157804525
O12	-0.7177687353	-1.9981709774	0.1910276366
H13	-0.1834570116	-2.4713114714	0.8413514708
C14	2.0517072919	3.5087824217	1.0361929426
H15	2.7845458092	3.9224737370	1.7128140106
C16	1.3093779273	4.0972271497	0.0253045649
H17	1.3278448685	5.1288305431	-0.2910339783
C18	-0.7643531026	-0.6190445855	3.0908855698
H19	-1.6391735974	-1.1639631013	2.7677120575

C20	-0.2723513950	-0.3574245515	4.3776828559
H21	-0.7087148135	-0.6429332181	5.3225099825
C22	4.0366330826	-0.6382420030	1.0791928252
H23	4.8206963554	-0.2908519559	1.7353001869
C24	4.0270430628	-1.6431170916	0.1239511611
H25	4.8421638532	-2.2921416141	-0.1564293677
C26	0.5331100257	3.0538908324	-0.5001341422
H27	-0.1816567903	3.0636224613	-1.3103530520
C28	0.9062508556	0.3464762895	4.1694296915
H29	1.6258090995	0.7468735453	4.8684607224
C30	2.7271341875	-1.6330743837	-0.3995449706
H31	2.2715449352	-2.2445856663	-1.1637070733
C32	-2.6055998819	0.2907609448	0.0113384828
H33	-2.4611306333	-0.7857589954	0.1141007116
H34	-1.6478339920	0.8898627669	-0.0732555306
H35	-3.1052243743	0.7041335640	0.8898585273
H36	-3.1561315910	0.5238296072	-0.9017997970

4OH-CH$_4$-TS: SCF = -1023.18202857989

Total internal energy, Utot (SCFE + ZPE + U): -1022.894006 hartrees

Total enthalpy, Htot (Utot + pV): -1022.893062 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1022.960337 hartrees

Os1	0.0126732265	0.0025314952	-0.0036774864
N2	0.0030704705	-0.0003589852	2.1767738001
C3	0.0696602649	0.0172463008	-1.8608823890
N4	2.0189088354	-0.5832629814	0.1913598622
N5	0.7482019629	1.9639824564	0.1640273593
N6	1.6880054941	2.2500713828	1.1077482321
N7	1.0661175780	0.5333819043	2.8315997202
N8	2.8186850058	0.0154564349	1.1158001355
B9	2.2442218671	1.1310013462	2.0172120078
H10	3.0859061148	1.5612641589	2.7539906083
O11	0.1227166715	0.0410977799	-3.0261573607
O12	-0.9983920494	-1.8995677848	0.0463891571
H13	-0.8878117431	-2.2567683030	0.9388612284
C14	1.9997648846	3.5651001831	1.0490015364
H15	2.7302519965	3.9829003704	1.7256674681
C16	1.2510414666	4.1509498590	0.0412157806
H17	1.2609255638	5.1836446852	-0.2717306748
C18	-0.8542745174	-0.4404434524	3.1089103238
H19	-1.7880316691	-0.8993716608	2.8171596580
C20	-0.3436249926	-0.1913322853	4.3893731638
H21	-0.7983419852	-0.4253142032	5.3395570694
C22	4.0477110522	-0.5476458926	1.0762601035
H23	4.8255241978	-0.2077991767	1.7438820599
C24	4.0500113121	-1.5316182849	0.0998505108

H25	4.8714494092	-2.1679156465	-0.1914178877
C26	0.4806969831	3.1047976885	-0.4863011067
H27	-0.2361416834	3.1100638664	-1.2942768130
C28	0.8770417539	0.4295946714	4.1636710745
H29	1.6200452647	0.8043299237	4.8521115310
C30	2.7507648199	-1.5177677420	-0.4277496848
H31	2.3068719965	-2.1176887656	-1.2084788436
C32	-2.3279924739	0.3963761619	0.0466518947
H33	-1.7527196357	-0.8459199666	0.0823859436
H34	-2.0266303749	1.4447047030	-0.0389788956
H35	-2.8972049358	0.3229887225	0.9801182007
H36	-2.9845018340	0.1924751076	-0.8046679856

4OH-CH$_4$-Product: SCF = -1023.21513246040

Total internal energy, Utot (SCFE + ZPE + U): -1022.921552 hartrees

Total enthalpy, Htot (Utot + pV): -1022.920607 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1022.989705 hartrees

Os1	-0.0907006802	0.1084081989	-0.0221991778
N2	-0.0821219052	0.0612489602	2.1670523986
C3	-0.1080140490	0.1744372685	-1.8706035308
N4	2.0022532686	-0.5796024027	0.2020574963
N5	0.6793029641	2.0134852535	0.1753286111
N6	1.6408669808	2.2603327698	1.1121390122
N7	1.0031629863	0.5381720140	2.8274556478
N8	2.7855155386	0.0212139716	1.1365751935
B9	2.1902695478	1.1346106919	2.0204090651
H10	3.0184727092	1.5714827799	2.7700911754
O11	-0.1388580422	0.2368817839	-3.0398231572
O12	-0.9257598604	-1.9531454026	0.0520841258
H13	-0.7661288161	-2.2935845323	0.9449890912
C14	1.9724079185	3.5725433352	1.0750004287
H15	2.7181303475	3.9638921601	1.7507530290
C16	1.2190535887	4.1917441820	0.0918485967
H17	1.2412150737	5.2310060067	-0.1979996819
C18	-0.9594693230	-0.3475375322	3.0956367195
H19	-1.9264224983	-0.7296219119	2.7986811127
C20	-0.4350890729	-0.1434285588	4.3793695005
H21	-0.8999520738	-0.3647289466	5.3278044378
C22	4.0283915327	-0.5124179339	1.1061554785
H23	4.7938936034	-0.1589508684	1.7812573920
C24	4.0595841788	-1.4881182670	0.1223389252
H25	4.8974044347	-2.1038706726	-0.1675065319
C26	0.4197342497	3.1717716167	-0.4444591983
H27	-0.3180695873	3.2049596561	-1.2315739212
C28	0.8111774434	0.4267139464	4.1586695923
H29	1.5679484321	0.7652930616	4.8507789901

C30	2.7626664017	-1.4899431067	-0.4164961365
H31	2.3451718642	-2.0863414170	-1.2152936569
C32	-2.1367139108	0.7393988283	0.0683898810
H33	-1.8839623547	-1.7980497576	-0.0154702650
H34	-2.4250339082	1.4708508945	-0.6963177613
H35	-2.3671577731	1.1921403384	1.0424920985
H36	-2.8630476323	-0.0943276415	-0.0564298495

4NH_2: SCF = -962.83397180118

Total internal energy, Utot (SCFE + ZPE + U): -962.578216 hartrees

Total enthalpy, Htot (Utot + pV): -962.577271 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -962.641094 hartrees

Os1	-0.1628553488	0.3297641813	-0.0602160385
N2	-0.1358662569	0.2619311468	2.1488694941
C3	-0.2423928361	0.3752239700	-1.9071315869
N4	-1.7870978492	1.6855821893	0.1821382490
N5	-1.7911673784	-1.0358928070	0.1127531252
N6	-2.7127566243	-0.9365772500	1.1070198947
N7	-1.3187552521	0.2526268167	2.8211126462
N8	-2.7062487582	1.5408693336	1.1729746198
B9	-2.6666706876	0.2778869279	2.0558854315
H10	-3.5820575561	0.2600803753	2.8296868591
O11	-0.3337752220	0.4011792861	-3.0729182996
N12	1.7607080237	0.3407946887	-0.0443945024
H13	2.3620992927	0.3664273617	-0.8593618113
C14	-3.5545173813	-1.9923058879	1.0506488894
H15	-4.3562142628	-2.0906541155	1.7675576796
C16	-3.1754048478	-2.7987707353	-0.0119479364
H17	-3.6359001623	-3.7187846622	-0.3374341319
C18	0.8316371131	0.2149351469	3.0741986754
H19	1.8724736630	0.2082732552	2.7870844632
C20	0.2807156664	0.1750613312	4.3604158676
H21	0.8035109393	0.1334319775	5.3034747716
C22	-3.5414502995	2.6033092138	1.1737981717
H23	-4.3405738365	2.6694396500	1.8972470869
C24	-3.1603796702	3.4614153673	0.1529829684
H25	-3.6160143982	4.3997987494	-0.1232821486
C26	-2.0614149786	-2.1567759212	-0.5693072882
H27	-1.4434333291	-2.4357557601	-1.4094852277
C28	-1.0899247399	0.2001940434	4.1496897456
H29	-1.9156311713	0.1846010860	4.8456767025
C30	-2.0521768363	2.8421836245	-0.4404726186
H31	-1.4348737627	3.1601789805	-1.2673807624
H32	2.3282475669	0.3311293470	0.7960708021

4NH_2 pyridine complex:SCF = -1211.14651881927

Total internal energy, Utot (SCFE + ZPE + U): -1210.794972 hartrees

Total enthalpy, Htot (Utot + pV): -1210.794028 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1210.870027 hartrees

Os1	0.6747803030	-0.1006828930	0.3497261783
N2	0.1122976253	1.9868895573	0.6034811716
C3	1.1866177676	-1.8666508612	0.1123553203
N4	0.5081973806	0.2218811020	-1.7362558188
N5	0.7792553482	-0.1281282666	2.5177070191
N6	2.6464881016	0.6178672199	0.4295464689
N7	2.9810515601	1.5711736330	1.3440684463
N8	0.7719827188	2.7473042871	1.5149705716
N9	1.3600779611	0.9275559758	3.1528370951
B10	1.9235696017	2.1139714285	2.3363004587
H11	2.4138478132	2.9296500783	3.0665461689
O12	1.5097035676	-2.9797343345	-0.0551377644
H13	1.2543178093	-0.2658111465	-2.2347458621
H14	0.7212891187	1.2071031356	-1.9071872333
C15	4.2823296991	1.9056859596	1.1880533669
H16	4.7333300294	2.6523258243	1.8246203872
C17	4.8107695920	1.1521385137	0.1519434926
H18	5.8211933986	1.1696105828	-0.2267115018
C19	-0.7863293206	2.7745956043	0.0003150116
H20	-1.4165166143	2.3682452245	-0.7778312033
C21	-0.7163066430	4.0716957889	0.5293783953
H22	-1.3074102665	4.9313686064	0.2530442230
C23	1.3921057020	0.6965861625	4.4857155599
H24	1.8191038704	1.4270869613	5.1568161164
C25	0.8204031995	-0.5415970009	4.7307600753
H26	0.6903979345	-1.0298513904	5.6845289405
C27	3.7428300670	0.3601613499	-0.2940061155
H28	3.7061648067	-0.3771181799	-1.0819548511
C29	0.2877614639	4.0076809959	1.4857958851
H30	0.6922567065	4.7648521306	2.1412931896
C31	0.4541347968	-1.0203236797	3.4633761478
H32	-0.0152056620	-1.9525739570	3.1836194836
N33	-1.3982487063	-0.5831901348	0.2600201917
C34	-1.9077770454	-1.1516900536	-0.8575281465
C35	-3.2487650538	-1.5042233279	-0.9610396748
C36	-4.1118031699	-1.2473439676	0.1025494987
C37	-3.5925235340	-0.6301572866	1.2406329168
C38	-2.2394456041	-0.3182991658	1.2833089673
H39	-1.1996901989	-1.2430641472	-1.6736006949
H40	-3.6046758161	-1.9682173096	-1.8753404034
H41	-5.1627124217	-1.5156205495	0.0458427967
H42	-4.2202319651	-0.3947230141	2.0938654032
H43	-1.7915078842	0.1459239643	2.1532868468

4NH$_2$-CH$_4$-TS: SCF = -1003.31262840589

Total internal energy, Utot (SCFE + ZPE + U): -1003.012144 hartrees

Total enthalpy, Htot (Utot + pV): -1003.011200 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1003.078974 hartrees

Os1	-0.1110898140	-0.0015910331	-0.0773720692
N2	-0.0592133275	0.0053422607	2.1009049990
C3	-0.1877334797	0.0147322812	-1.9316131320
N4	-1.5472946043	1.5099155324	0.1414768464
N5	-1.7564022346	-1.3516526698	0.1529949811
N6	-2.6878610944	-1.1039541035	1.1143026153
N7	-1.2293176353	0.0724895291	2.7866824811
N8	-2.5155248631	1.3968438633	1.0920776860
B9	-2.5659100999	0.1505113231	2.0069072321
H10	-3.4907140608	0.2216469007	2.7666636275
O11	-0.2367062666	0.0371309835	-3.0996924143
N12	1.7061238361	1.1246892165	0.0013353695
H13	1.9393509641	1.6713794952	-0.8201710998
C14	-3.6301137381	-2.0743097219	1.0940887359
H15	-4.4545449849	-2.0496366135	1.7912251891
C16	-3.3103570723	-2.9761632868	0.0920196731
H17	-3.8540323576	-3.8636023329	-0.1935458137
C18	0.9280561661	-0.0399776622	3.0051495441
H19	1.9568562271	-0.0971625073	2.6800454891
C20	0.3953191918	-0.0027547669	4.3009182960
H21	0.9315395759	-0.0260679205	5.2370999430
C22	-3.3042235995	2.4950163034	1.0623331665
H23	-4.1302509348	2.5915315213	1.7511765129
C24	-2.8446142019	3.3410447392	0.0654152668
H25	-3.2503432453	4.2979764828	-0.2248461628
C26	-2.1258018608	-2.4779301921	-0.4705644356
H27	-1.5311135790	-2.8629151181	-1.2862750030
C28	-0.9778419359	0.0682924493	4.1128466959
H29	-1.7896550086	0.1158905875	4.8236096928
C30	-1.7375667452	2.6785620932	-0.4839805090
H31	-1.0801102430	2.9711645289	-1.2890520402
H32	1.7760370439	1.7144071505	0.8250007685
C33	1.6783032398	-1.6039439386	-0.0562921229
H34	1.8310174918	-0.2769715786	-0.0139393218
H35	0.8415405652	-2.3073905228	-0.0944379345
H36	2.2333915740	-1.8363910382	0.8590662925
H37	2.3030385619	-1.8009454980	-0.9325740164

4NH$_2$-CH$_4$-Product: SCF = -1003.37151987652

Total internal energy, Utot (SCFE + ZPE + U): -1003.063855 hartrees

Total enthalpy, Htot (Utot + pV): -1003.062910 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1003.132209 hartrees

Os1	-0.0619506915	-0.2020499780	-0.0891917543
N2	-0.0199905561	-0.1457382014	2.1052615589
C3	-0.0985467676	-0.2876524758	-1.9332837447
N4	-1.5289575077	1.4547932384	0.1474527459
N5	-1.7162027838	-1.4629668935	0.1632954470
N6	-2.6524405889	-1.1710768684	1.1112666254
N7	-1.1862055978	-0.0035655466	2.7847239237
N8	-2.4853535641	1.3399039849	1.1062874735
B9	-2.5244097820	0.0840521465	2.0045836490
H10	-3.4452644112	0.1458290925	2.7715056548
O11	-0.1017078098	-0.3550986779	-3.1053784635
N12	1.6715937429	1.1153858492	-0.0668643605
H13	1.5806109733	1.9266714531	-0.6749180046
C14	-3.6164753389	-2.1214925558	1.0971263774
H15	-4.4473585914	-2.0642618437	1.7844865245
C16	-3.3071697205	-3.0493337057	0.1167641576
H17	-3.8686378934	-3.9291409013	-0.1577902841
C18	0.9570101812	-0.2363294206	3.0183624788
H19	1.9794019999	-0.3955150569	2.7053951918
C20	0.4227069482	-0.1421823515	4.3113083856
H21	0.9508922060	-0.1847456144	5.2514526498
C22	-3.3047045591	2.4160157293	1.0720456893
H23	-4.1302392334	2.4985846035	1.7636060964
C24	-2.8751861693	3.2597863415	0.0601552033
H25	-3.3088943030	4.2011702634	-0.2412802565
C26	-2.1032259647	-2.5927170557	-0.4406573994
H27	-1.5021542648	-3.0085110304	-1.2351795212
C28	-0.9433136922	-0.0004539140	4.1127023338
H29	-1.7563872031	0.0960215237	4.8170456007
C30	-1.7599541680	2.6084514241	-0.4907535207
H31	-1.1332362059	2.9020177364	-1.3213713265
H32	1.8410452949	1.4636176355	0.8763634249
C33	1.3312628447	-1.8294599509	-0.0238042897
H34	2.5000802951	0.5957936897	-0.3606550887
H35	1.0063356762	-2.7062737699	-0.5993915622
H36	1.4795054285	-2.1779791404	1.0082523000
H37	2.3336127277	-1.5774728328	-0.4181724186

5Me: SCF = -824.01828909448

Total internal energy, Utot (SCFE + ZPE + U): -823.735096 hartrees

Total enthalpy, Htot (Utot + pV): -823.734152 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -823.804447 hartrees

Ru1	0.4001709280	0.2117662176	0.0170535530
O2	0.2547035034	0.1799296417	2.0614119427
O3	2.2340475857	-0.3205595426	0.0339704917

O4	-0.2827772005	1.9923180955	-0.0810486144
O5	0.5327095229	0.1205146082	-2.0589683231
C6	-0.9385524065	-1.3079125226	-0.1532262183
C7	1.2259184161	-0.0048148289	2.8561350106
C8	2.5637880651	-0.2701902567	2.4286385485
C9	2.9901316406	-0.4171113774	1.1289253175
C10	-0.4432629066	2.7415189801	-1.1767307317
C11	-0.1883709640	2.3512659522	-2.4654631735
C12	0.2785575280	1.0573769343	-2.8667324187
H13	3.3096911923	-0.3924630566	3.2049366718
H14	-0.3626836860	3.0797770742	-3.2482075811
H15	-0.6727856310	-2.0464680802	0.6094362298
H16	-1.8810853893	-0.8165781850	0.1262841927
H17	-0.9464501403	-1.7025520562	-1.1677092208
C18	4.4177704423	-0.7316825360	0.7833152587
H19	4.8261715798	0.0639757275	0.1511539496
H20	5.0331604079	-0.8363664074	1.6774874641
H21	4.4601760236	-1.6592103064	0.2028588738
C22	0.9227505456	0.0521376892	4.3278448283
H23	1.4995439534	0.8583144515	4.7953827351
H24	-0.1410160203	0.2268525862	4.4887185223
H25	1.2218880042	-0.8823786722	4.8146860158
C26	-0.9518444647	4.1112549840	-0.8297749020
H27	-1.8980384148	4.0267301148	-0.2850540584
H28	-0.2391543635	4.6108997144	-0.1651001665
H29	-1.1022234426	4.7183983442	-1.7231997067
C30	0.4760277864	0.7744264974	-4.3304489258
H31	1.1896175375	1.4881071447	-4.7570725768
H32	0.8434657475	-0.2416473593	-4.4735638674
H33	-0.4693415267	0.9041843377	-4.8692526281

5Me pyridine complex: SCF = -1072.35147661398

Total internal energy, Utot (SCFE + ZPE + U): -1071.970700 hartrees

Total enthalpy, Htot (Utot + pV): -1071.969756 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1072.052205 hartrees

Ru1	0.1172484897	0.0965214512	0.0461183218
O2	0.1534187532	0.0205535859	2.0468948829
O3	2.1213967205	-0.0628755269	-0.0604855336
O4	-0.0738362796	2.0622144658	-0.2138601620
O5	0.1857465217	0.0042480316	-2.0800303090
C6	-0.4624030303	-1.8509837867	-0.3497360848
C7	1.2221062177	-0.0276008829	2.7808695033
C8	2.5336733803	-0.0714692146	2.2954539456
C9	2.9273655637	-0.0869759292	0.9435224832
C10	0.2254083736	2.7954426323	-1.2488664534
C11	0.4956140960	2.3247203916	-2.5197429516

C12	0.4382747770	0.9569336485	-2.8823807315
H13	3.3246891649	-0.1053583849	3.0340287575
H14	0.7137170760	3.0500197891	-3.2927096130
H15	0.3478148159	-2.2544546846	0.2827835305
H16	-1.4407802349	-2.1234658058	0.0383157632
H17	-0.3096330199	-2.1065744747	-1.3946816759
C18	4.3873240461	-0.1471856510	0.5780484407
H19	4.6463459895	0.7279713346	-0.0271844308
H20	5.0334501231	-0.1803971755	1.4560988839
H21	4.5720083056	-1.0316548711	-0.0403186649
C22	0.9523087287	-0.0428596493	4.2626059405
H23	0.4206872026	0.8718855040	4.5465637460
H24	0.2994621046	-0.8869700479	4.5078530163
H25	1.8693622038	-0.1170989048	4.8481498777
C26	0.2182564730	4.2708217017	-0.9378669089
H27	-0.7859609094	4.5760033740	-0.6255660501
H28	0.8959109392	4.4761714461	-0.1032663948
H29	0.5205845740	4.8612663255	-1.8039021466
C30	0.6923839587	0.5537795413	-4.3132188387
H31	0.5607429233	1.3859166688	-5.0068072719
H32	1.7246027154	0.1926099380	-4.3978579130
H33	0.0345086283	-0.2732432716	-4.5904573326
N34	-2.0303211125	0.3477014526	0.1722344057
C35	-2.8039509698	0.1773143280	-0.9174579214
C36	-4.1689200596	0.4356779717	-0.9021057335
C37	-4.7568115052	0.8860822497	0.2799466991
C38	-3.9521585075	1.0622522549	1.4043072807
C39	-2.5917138229	0.7860879206	1.3138959302
H40	-2.2991185309	-0.1738882250	-1.8102925860
H41	-4.7531713322	0.2839980356	-1.8032140289
H42	-5.8211321943	1.0955010162	0.3227323934
H43	-4.3651150928	1.4100433562	2.3448966618
H44	-1.9233351301	0.9017948271	2.1578742056

5Me-CH$_4$: SCF = -864.51361422926

Total internal energy, Utot (SCFE + ZPE + U): -864.180209 hartrees

Total enthalpy, Htot (Utot + pV): -864.179265 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -864.258572 hartrees

Ru1	-0.2233038364	0.2930374116	0.0907837112
O2	0.2175207164	-0.2431199332	1.8771507936
O3	2.0368913177	0.0259095961	-0.2206405604
O4	0.1588027066	2.2381917684	0.1255261365
O5	-0.1594703541	0.2090246123	-1.8591946687
C6	-0.5344875225	-2.5126787056	-0.1889556622
C7	1.2871565619	0.0390507614	2.6098546803
C8	2.5314568096	0.2913660163	2.0896806235

C9	2.8808027674	0.1930563513	0.6902406654
C10	0.6663590646	2.8796778845	-0.8656254575
C11	0.8652667790	2.3451531029	-2.1587592764
C12	0.4523084964	1.0880328765	-2.6035498266
H13	3.3401484561	0.4384469005	2.7961551540
H14	1.3084168371	3.0052066679	-2.8939269613
H15	0.5214629233	-2.3350047708	-0.3882989018
H16	-0.6526039574	-3.1241952136	0.7061088063
H17	-0.9979686393	-2.9794911246	-1.0592692152
C18	-2.2369829384	0.7123032794	0.1886137315
H19	-2.4578730744	1.5105227768	-0.5260525868
H20	-2.8523103599	-0.1648655489	-0.0192834857
H21	-2.3969225881	1.0930144641	1.2043707944
H22	-1.1229425202	-1.5863002883	-0.0091816951
C23	4.3426268447	0.2538603513	0.3248370613
H24	4.4609970096	0.2827985823	-0.7585005580
H25	4.8163727389	1.1316392170	0.7775389000
H26	4.8616029986	-0.6274551969	0.7200640951
C27	1.0139855515	-0.0398320873	4.0858950764
H28	0.2187800649	0.6633450039	4.3543592131
H29	0.6621634153	-1.0445422236	4.3432189203
H30	1.9090007481	0.1883841350	4.6661438332
C31	0.9896753165	4.3205889513	-0.5769265801
H32	0.0566143111	4.8898431263	-0.4938179313
H33	1.5063370949	4.4010356597	0.3830501673
H34	1.6000314668	4.7637209582	-1.3647201498
C35	0.6465790380	0.6590357310	-4.0291993367
H36	1.1230427718	1.4342160194	-4.6301964036
H37	1.2626344125	-0.2465454608	-4.0500697357
H38	-0.3213199542	0.4009730709	-4.4711739161

5Me-CH$_4$-TS: SCF = -864.47838003318

Total internal energy, Utot (SCFE + ZPE + U): -864.148902 hartrees

Total enthalpy, Htot (Utot + pV): -864.147958 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -864.224511 hartrees

Ru1	0.0142015025	0.1627311376	0.0727107332
O2	0.1867286943	-0.1952848558	2.0056282983
O3	2.0910333836	0.0680983967	-0.0977905412
O4	0.0250958381	2.1424049425	-0.1095530342
O5	-0.0000394116	0.1110301809	-1.9893452838
C6	-0.7442974283	-1.9522701588	-0.2863258287
C7	1.2666644017	-0.1160678675	2.7348648063
C8	2.5539425489	0.0782121348	2.2374218880
C9	2.9239555189	0.1232901087	0.8656184406
C10	0.4815031906	2.8454359304	-1.1064728088
C11	0.7787104494	2.3295273875	-2.3604749952

C12	0.4736746280	1.0049797217	-2.7643930188
H13	3.3575630905	0.1072800272	2.9631936043
H14	1.1271370842	3.0197552482	-3.1180239506
H15	0.1625608162	-2.3363329227	0.1849979634
H16	-1.6085035925	-2.4310860814	0.1849614601
H17	-0.7352793169	-2.0820087129	-1.3645615296
C18	-2.2096551203	0.4423134741	0.3682535868
H19	-2.9170151669	0.0840663892	-0.3848631310
H20	-2.4910887875	0.1129672918	1.3695598816
H21	-2.1562470811	1.5274955915	0.3220208283
H22	-1.4028278122	-0.7850106041	0.0131598226
C23	4.3806577037	0.1797785172	0.4865346584
H24	4.5150432060	0.8514101167	-0.3649146289
H25	5.0120635676	0.5005263800	1.3166887037
H26	4.7067081510	-0.8183592344	0.1698210423
C27	1.0194720538	-0.2996200156	4.2069762235
H28	0.2979515317	0.4478849972	4.5524491297
H29	0.5729762049	-1.2842706893	4.3824816643
H30	1.9367916877	-0.2130093677	4.7904594811
C31	0.5940561914	4.3165672799	-0.8086447892
H32	-0.4071685906	4.7350109335	-0.6578087957
H33	1.1529151148	4.4668730899	0.1196886784
H34	1.0849581355	4.8518885407	-1.6225234716
C35	0.6649285545	0.5859375395	-4.1971571438
H36	0.8403324762	1.4359223639	-4.8576238871
H37	1.5261331598	-0.0903073443	-4.2549743470
H38	-0.2102507759	0.0264090097	-4.5379567044

5OH: SCF = -859.93686413547

Total internal energy, Utot (SCFE + ZPE + U): -859.675859 hartrees

Total enthalpy, Htot (Utot + pV): -859.674915 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -859.742715 hartrees

Ru1	0.4826588878	0.3070268002	-0.1129479778
O2	0.1872248603	-0.7019945071	1.4020435984
C3	1.2042448821	-1.8637629450	-1.9944007118
O4	1.5567290076	-1.2111685870	-0.9688518613
C5	-0.2349463359	2.9695068556	1.0535451533
O6	-0.6130855664	1.7734586562	0.8714269200
C7	2.0254107611	2.7720639469	0.0039156360
C8	1.0279771160	3.4845391431	0.6219860526
H9	1.2248103212	4.5300807409	0.8263726844
O10	1.9803619407	1.4772726779	-0.3255215831
C11	-0.9150443267	-0.6214078034	-2.4684683099
C12	0.0083838500	-1.5998928338	-2.7375837640
H13	-0.1824719338	-2.2316162087	-3.5967701738
O14	-0.8656493960	0.2564639915	-1.4583905718

H15	-0.4024321881	-0.2142125772	2.0128675067
C16	3.3403788596	3.3856962227	-0.3767742698
H17	3.5130613149	3.2513774954	-1.4497138834
H18	3.3729469272	4.4479489050	-0.1324279620
H19	4.1499486264	2.8663918129	0.1475638627
C20	-1.1860430876	3.8820730204	1.7747951653
H21	-0.7079336285	4.2968335460	2.6689797787
H22	-1.4468071316	4.7283870945	1.1288686357
H23	-2.0924121445	3.3453172137	2.0542507308
C24	-2.1406095661	-0.4112087652	-3.3096072397
H25	-3.0359066514	-0.5395857149	-2.6918347410
H26	-2.1549080612	0.6147013116	-3.6921507755
H27	-2.1750493586	-1.1102917314	-4.1458627462
C28	2.1105279575	-2.9786656201	-2.4329065515
H29	1.6043243467	-3.9393618558	-2.2780240429
H30	2.3323981874	-2.8977876464	-3.5015793400
H31	3.0342829450	-2.9642402518	-1.8549031096

5OH pyridine complex: SCF = -1108.27880162451

Total internal energy, Utot (SCFE + ZPE + U): -1107.921015 hartrees

Total enthalpy, Htot (Utot + pV): -1107.920071 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1108.001575 hartrees

Ru1	-0.0068087264	0.1110618920	-0.0560842249
O2	0.0471256418	0.1442548379	1.9169651218
O3	2.0347726950	-0.1013992922	-0.2068510788
O4	0.1450058480	2.1354505404	0.0025213220
O5	-0.0897923938	0.3726305894	-2.0692920986
O6	-0.2583895431	-1.7455658130	-0.2740434405
C7	1.1330637998	0.1299058468	2.6367353830
C8	2.4339830508	0.0239394362	2.1474687538
C9	2.8304293877	-0.1039999991	0.7909700365
C10	0.7854902636	2.8612155206	-0.8531860479
C11	1.0728185269	2.4418368902	-2.1569459533
C12	0.5490591796	1.2649935799	-2.7309351772
H13	3.2275678255	0.0157954626	2.8843294313
H14	1.5577021375	3.1483493192	-2.8185032693
H15	0.5169333301	-2.1445825704	-0.7089036323
C16	4.2884688696	-0.2884411719	0.4569452634
H17	4.5371126258	0.2814610815	-0.4416341078
H18	4.9406622089	0.0097448560	1.2791728301
H19	4.4748392093	-1.3464047414	0.2360603058
C20	0.8731276680	0.2346111026	4.1159256142
H21	0.3340662580	1.1641427780	4.3274681579
H22	0.2272372489	-0.5918318479	4.4302634260
H23	1.7947529952	0.2125038317	4.6987514095
C24	1.1340985212	4.2478970204	-0.3847652924

H25	0.2137727744	4.8049803610	-0.1774124719
H26	1.6941414591	4.1888993182	0.5539308710
H27	1.7211332148	4.7941119648	-1.1244442723
C28	0.6287391168	1.0285181548	-4.2147239181
H29	1.2084389955	1.8006485428	-4.7219920456
H30	1.0788929937	0.0491969123	-4.4048105774
H31	-0.3831225019	1.0056537519	-4.6335592948
N32	-2.1102121941	0.2629171763	0.1226356119
C33	-2.9242779197	-0.6186081572	-0.4903779979
C34	-4.3055825058	-0.5556183559	-0.3500568349
C35	-4.8613055536	0.4432352089	0.4484777600
C36	-4.0118325086	1.3513112798	1.0800276811
C37	-2.6401967032	1.2321406259	0.8943162995
H38	-2.4389323974	-1.3875308951	-1.0782409845
H39	-4.9271317966	-1.2848424532	-0.8578903073
H40	-5.9369659401	0.5121569960	0.5776956884
H41	-4.3996298066	2.1439097697	1.7104836069
H42	-1.9369132116	1.9137788708	1.3563521254

5OH-CH$_4$: SCF = -900.44489993523

Total internal energy, Utot (SCFE + ZPE + U): -900.133916 hartrees

Total enthalpy, Htot (Utot + pV): -900.132971 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -900.210626 hartrees

Ru1	0.2675801346	0.0579255505	0.1611046687
O2	1.3660112280	-0.2836810641	1.6549251079
C3	1.2806009093	-1.6196909600	-2.0545604909
O4	1.0403162678	-1.5544191354	-0.7989881916
C5	-0.2841944125	2.8325527686	0.8738209485
O6	-0.6772843130	1.5989985990	0.9686818055
C7	1.8110648082	2.4325356073	-0.4503136186
C8	0.8846955168	3.2488664596	0.2291837731
H9	1.1048176443	4.3085539131	0.2533674333
O10	1.7213037661	1.1587508281	-0.6079992518
C11	-0.4233347498	0.0559343192	-2.7094883847
C12	0.6592020870	-0.7777506409	-3.0075043212
H13	0.8933723957	-0.9467810571	-4.0510642326
O14	-0.8390556163	0.2625327000	-1.4991654915
C15	-1.8731246838	-1.3506049963	1.4052673791
H16	-1.0128747827	-1.5774342676	0.7406292426
H17	0.8691708336	-0.5574158072	2.4472686101
H18	-2.7480200129	-1.7473909504	0.8877212707
H19	-1.6974437603	-1.8891629270	2.3381663245
H20	-2.0237634998	-0.2895310926	1.6027908341
C21	3.0512153749	3.0317979508	-1.0580060610
H22	3.2668238200	2.5546216206	-2.0167849542
H23	2.9566864481	4.1103550787	-1.1902142618

H24	3.9001174595	2.8334139801	-0.3928449756
C25	-1.2006256770	3.8258812758	1.5318827030
H26	-0.8289636936	4.8472944478	1.4449030068
H27	-2.1936762345	3.7616428507	1.0744468522
H28	-1.3156503102	3.5715915466	2.5906161116
C29	-1.2459705441	0.6993844439	-3.7892331860
H30	-2.2698508199	0.3124775331	-3.7452763813
H31	-1.3026791396	1.7786685267	-3.6144607388
H32	-0.8343666404	0.5131247095	-4.7820197462
C33	2.1960281713	-2.7315263827	-2.4815996219
H34	1.7290873414	-3.6946517158	-2.2469752275
H35	2.4169249905	-2.6925035487	-3.5489230604
H36	3.1258853951	-2.6761374562	-1.9076340005

5OH-CH_4-TS: SCF = -900.39496069689

Total internal energy, Utot (SCFE + ZPE + U): -900.089757 hartrees

Total enthalpy, Htot (Utot + pV): -900.088813 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -900.162367 hartrees

Ru1	0.1562543848	0.0172890015	0.1494290728
O2	0.9839638466	-0.7957964071	1.8481345996
C3	1.1689841560	-1.5979677403	-2.0469317928
O4	0.8734613320	-1.5697386825	-0.7942281590
C5	-0.2825619111	2.8344131027	0.8376036441
O6	-0.5083187599	1.5969351731	1.1457811395
C7	1.7407442881	2.4122683326	-0.5818051051
C8	0.7411790703	3.2497374894	-0.0281616720
H9	0.8714716137	4.3176019926	-0.1551523260
O10	1.7269253264	1.1351320911	-0.4912783280
C11	-0.4128667152	0.2254020587	-2.7230347419
C12	0.6185834041	-0.7025603116	-2.9891616682
H13	0.8728481191	-0.8689516754	-4.0294385384
O14	-0.8318279726	0.4990360314	-1.5376400965
C15	-1.5366437957	-1.2124304714	1.0932599575
H16	-0.3069753270	-1.1391345589	1.5830113410
H17	0.8793262332	-0.1876640640	2.5983977312
H18	-1.8913728867	-1.5460279059	0.1163533828
H19	-1.5280102626	-2.1240343185	1.7123138783
H20	-2.2145315905	-0.4818596428	1.5332215741
C21	2.9455324456	3.0064534952	-1.2583474387
H22	3.1502636638	2.4685040081	-2.1883452727
H23	2.8183993168	4.0701371545	-1.4652499144
H24	3.8198458307	2.8752173768	-0.6101080248
C25	-1.1652651149	3.8313989043	1.5335616959
H26	-0.9305408357	4.8579943650	1.2497639527
H27	-2.2120549849	3.6187188510	1.2923648692
H28	-1.0561298028	3.7225676962	2.6178491532

C29	-1.1504716719	0.9007126346	-3.8457259607
H30	-2.1783062046	0.5218629548	-3.8812282161
H31	-1.2098779368	1.9760129594	-3.6536346932
H32	-0.6763570045	0.7255457967	-4.8127444487
C33	2.0771972223	-2.7155532020	-2.4702984918
H34	1.5904025862	-3.6755336534	-2.2655714476
H35	2.3322802355	-2.6612174343	-3.5291437169
H36	2.9904871448	-2.6851784546	-1.8678291035

5NH$_2$: SCF = -840.08950057656

Total internal energy, Utot (SCFE + ZPE + U): -839.816105 hartrees

Total enthalpy, Htot (Utot + pV): -839.815161 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -839.883535 hartrees

Ru1	0.1148688016	0.4962113823	-0.1017267889
N2	0.2957758156	0.2012214435	1.6918238488
C3	3.0097264056	0.4191885515	-0.8064268462
O4	2.1074498221	1.0415361021	-0.1673269522
C5	-2.8579012262	0.6984904225	-0.1709850609
O6	-1.8689576024	-0.0634802545	0.0546764736
C7	-1.5830862464	2.7617309204	-0.7881036984
C8	-2.7495933022	2.0629648204	-0.5773658206
H9	-3.6776239089	2.5973178257	-0.7415103640
O10	-0.3471907346	2.2913981522	-0.6395892932
C11	1.5748453066	-1.3848011724	-1.7804128699
C12	2.7822437017	-0.7528982053	-1.5891605074
H13	3.6437559607	-1.1806460943	-2.0875865449
O14	0.4065753778	-1.0226556438	-1.2567801978
H15	-0.4707772860	-0.1693049639	2.2502938263
C16	-1.5810823030	4.1970398680	-1.2300088590
H17	-1.0323271385	4.2892464168	-2.1733337739
H18	-2.5935399615	4.5806008019	-1.3608949774
H19	-1.0527278148	4.8068194605	-0.4894228481
C20	-4.2254791699	0.0946416037	-0.0031329818
H21	-4.8287425018	0.6995592009	0.6819011218
H22	-4.7456795025	0.0852596190	-0.9679148772
H23	-4.1463667829	-0.9252634797	0.3730415317
C24	1.4421299983	-2.6079190783	-2.6415215224
H25	1.0478380296	-3.4357197231	-2.0425619045
H26	0.7190022561	-2.4163516622	-3.4414232782
H27	2.3977017335	-2.8990245863	-3.0790826476
C28	4.3996798264	0.9896432255	-0.7338406279
H29	4.4478992518	1.7764964495	0.0189369628
H30	5.1295828081	0.2064327696	-0.5076063741
H31	4.6700589826	1.4125267751	-1.7089281442
H32	1.1656958551	0.4048392974	2.1802453614

5NH$_2$ pyridine complex: SCF = -1088.42590149000

Total internal energy, Utot (SCFE + ZPE + U): -1088.055436 hartrees

Total enthalpy, Htot (Utot + pV): -1088.054492 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1088.136370 hartrees

Ru1	-0.0218797549	0.0574679329	-0.0203554081
O2	0.0727165508	0.2546065326	1.9679825012
O3	2.0231825886	-0.1180433601	-0.2156863536
O4	0.1655256084	2.1128144289	-0.0104967904
O5	-0.1438892168	0.2836436420	-2.0419957708
N6	-0.1764272532	-1.8028012384	-0.0824017937
C7	1.1844581201	0.2825442808	2.6428688693
C8	2.4688402422	0.1317044221	2.1244195754
C9	2.8337924397	-0.0535961568	0.7674270710
C10	0.7464974140	2.8212543825	-0.9090839079
C11	0.9769120818	2.3781934453	-2.2222292841
C12	0.4574236865	1.1847412864	-2.7403273939
H13	3.2813873067	0.1732227160	2.8386230811
H14	1.4298347262	3.0717218959	-2.9189691953
H15	-1.0033720354	-2.3336978507	0.1884536552
H16	0.5635085713	-2.3916116676	-0.4642644303
C17	4.2916873371	-0.1878019599	0.4020472797
H18	4.5536824940	0.5835087445	-0.3294471000
H19	4.9486279371	-0.1017589739	1.2682976393
H20	4.4585561393	-1.1566440680	-0.0802233588
C21	0.9810016031	0.5093151569	4.1192234191
H22	0.5231420976	1.4923075984	4.2759882602
H23	0.2869428175	-0.2391451213	4.5144999530
H24	1.9175590523	0.4612741929	4.6760414159
C25	1.1082828695	4.2242527155	-0.4967043602
H26	0.1951477437	4.7765321664	-0.2493790246
H27	1.7206280536	4.1926389391	0.4100343386
H28	1.6466839567	4.7592800407	-1.2803763825
C29	0.5005924223	0.9025019165	-4.2193878815
H30	0.9826528881	1.7073028434	-4.7757589861
H31	1.0413206166	-0.0333303302	-4.3953138480
H32	-0.5178162797	0.7636749351	-4.5971475289
N33	-2.1390019156	0.2446607013	0.1240085796
C34	-2.9260869634	-0.1536408935	-0.8971876244
C35	-4.3091543551	-0.0290867570	-0.8520978650
C36	-4.9012459270	0.5330761968	0.2789464979
C37	-4.0831900417	0.9523415066	1.3270238370
C38	-2.7065758265	0.7928446458	1.2171908454
H39	-2.4153923008	-0.5596503938	-1.7627538896
H40	-4.9043550017	-0.3651343626	-1.6941210111
H41	-5.9792898577	0.6447540171	0.3403221571
H42	-4.4986250369	1.3987298617	2.2239042510

H43	-2.0257417356	1.0910525520	2.0044031851

5NH$_2$-CH$_4$-TS: SCF = -880.54240474085

Total internal energy, Utot (SCFE + ZPE + U): -880.223189 hartrees

Total enthalpy, Htot (Utot + pV): -880.222245 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -880.296089 hartrees

Ru1	0.3096472776	0.0865912283	0.1818829972
N2	0.6232694611	-0.8892470374	1.8628518273
C3	1.1864912000	-1.7471472031	-1.9784368644
O4	1.2701048329	-1.4995543391	-0.7329961316
C5	-0.3053731514	2.8764906742	0.9668512439
O6	-0.5524004334	1.6528320726	1.2038104761
C7	1.6403855904	2.5588521756	-0.5902589365
C8	0.7120284154	3.3390656349	0.0802928163
H9	0.8049469294	4.4130424430	-0.0297112567
O10	1.6786082369	1.2462155786	-0.5842257110
C11	-0.5530921466	-0.0443612465	-2.6246548143
C12	0.3344281019	-1.0762971465	-2.8985720434
H13	0.3692221512	-1.4257302892	-3.9231324666
O14	-0.7513874144	0.5184500727	-1.4642063523
C15	-1.6546716860	-1.2367655321	0.4140078137
H16	-0.5037021993	-1.2227773350	1.3170141438
H17	0.3385518156	-0.5557032493	2.7809395255
H18	-1.5872380253	-1.8195432368	-0.5005940924
H19	-1.9635164164	-1.8956769757	1.2383722366
H20	-2.3421975538	-0.3982877488	0.3521422359
C21	2.7415808944	3.1777368391	-1.4064643012
H22	2.6717335317	2.8284106946	-2.4418883598
H23	2.7001519877	4.2674891047	-1.3876673547
H24	3.7117473560	2.8484376176	-1.0197858257
C25	-1.1416389332	3.8879996797	1.7044531133
H26	-0.5172767099	4.6724879937	2.1417301066
H27	-1.8280135298	4.3721359049	0.9990357090
H28	-1.7256593903	3.3989938564	2.4843703968
C29	-1.4241672855	0.5309111992	-3.7125666105
H30	-2.4778213419	0.3803877681	-3.4548095817
H31	-1.2606282794	1.6110771976	-3.7822287580
H32	-1.2218721709	0.0726419473	-4.6813632353
C33	2.0875261604	-2.8411155048	-2.4909485391
H34	2.4562731256	-3.4465352928	-1.6623021209
H35	1.5718065983	-3.4731436604	-3.2186433491
H36	2.9474911091	-2.3881078526	-2.9994581282
H37	1.2024614178	-1.7267735251	1.8715150182

6Me: SCF = -960.18068895670

Total internal energy, Utot (SCFE + ZPE + U): -959.913775 hartrees

Total enthalpy, Htot (Utot + pV): -959.912830 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -959.977210 hartrees

Ir1	0.7236633514	-0.1120410314	0.2407989926
N2	0.7214690322	-0.5291369237	-1.7913006475
C3	0.7057992503	0.2343974781	2.1069313262
C4	1.1344625307	-2.1384263726	0.6133809878
N5	0.1469362476	1.9342653970	-0.3474013459
N6	2.6102633624	0.4772201837	0.0463299411
N7	2.9481200769	1.2416855035	-1.0281107138
N8	1.2594796510	0.3745330966	-2.6557178002
N9	0.8081272884	2.4940759489	-1.3948610595
B10	1.8967613992	1.6755800439	-2.1046766716
H11	2.4305250072	2.2970483031	-2.9709324131
O12	0.7152792225	0.4288975840	3.2340503975
H13	1.6595372763	-2.3343309663	1.5501248568
H14	1.7081852686	-2.5644373491	-0.2112851012
H15	0.1569066146	-2.6448844863	0.6662497121
C16	4.2714145896	1.4861384918	-0.9571976622
H17	4.7519352195	2.0779431572	-1.7223573940
C18	4.7918046902	0.8754504465	0.1782088194
H19	5.8155580710	0.8828331600	0.5188458622
C20	0.2546304182	-1.5647717880	-2.5150756293
H21	-0.2060816976	-2.4129668184	-2.0299746223
C22	0.4775740837	-1.3214982467	-3.8696015306
H23	0.2141776002	-1.9544112373	-4.7025731256
C24	0.3314592049	3.7390045049	-1.6132008133
H25	0.7331369624	4.3506955118	-2.4079095857
C26	-0.6658802487	3.9981393002	-0.6838644803
H27	-1.2498673299	4.8995636288	-0.5812678383
C28	3.7088156720	0.2427026937	0.7864380753
H29	3.6584228933	-0.3550433716	1.6836235356
C30	1.1217497159	-0.0892538453	-3.9126478390
H31	1.4931885533	0.4824251811	-4.7505658849
C32	-0.7430280297	2.8369184709	0.0927561920
H33	-1.3857183066	2.6146143566	0.9332805222

6Me pyridine complex: SCF = -1208.55888180902
Total internal energy, Utot (SCFE + ZPE + U): -1208.193963 hartrees
Total enthalpy, Htot (Utot + pV): -1208.193019 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1208.268829 hartrees

Ir1	0.6740411375	-0.0456836902	0.3006808329
N2	0.1366865658	1.9752284353	0.5856615483
C3	1.2232598001	-1.8142057584	0.0237875528
C4	0.6727725153	0.3299882993	-1.7859991644
N5	0.7173144142	-0.1605927906	2.5167310989

N6	2.6295215454	0.6288330380	0.4252378140
N7	2.9674878045	1.5097913038	1.4060875650
N8	0.7736189613	2.6976497860	1.5481714003
N9	1.3141132139	0.8627848370	3.1831936359
B10	1.9025074622	2.0533799896	2.3953844536
H11	2.3867309121	2.8565245669	3.1344627096
O12	1.5693090036	-2.8926069095	-0.1646319988
H13	1.2545459920	1.2373199803	-1.9606816820
H14	-0.3494512836	0.4970961812	-2.1386961646
H15	1.1098162728	-0.4794779522	-2.3767262507
C16	4.2823979151	1.7929744419	1.3003611152
H17	4.7477122221	2.4822015046	1.9893974893
C18	4.8118647507	1.0797318110	0.2337930211
H19	5.8321772408	1.0801985469	-0.1167413219
C20	-0.7314492698	2.7937223210	-0.0299478496
H21	-1.3396365174	2.4331210664	-0.8463491554
C22	-0.6657171290	4.0659475148	0.5431120746
H23	-1.2342550563	4.9413498507	0.2703568932
C24	1.3286974625	0.5904677097	4.5055937134
H25	1.7641572082	1.2889103316	5.2051880060
C26	0.7263906879	-0.6431717593	4.7094908788
H27	0.5758042566	-1.1540005175	5.6479633257
C28	3.7335622589	0.3621462306	-0.2891719422
H29	3.6945657355	-0.3153371431	-1.1294410765
C30	0.3026181548	3.9603458862	1.5338819950
H31	0.6897983203	4.6954246750	2.2240454100
C32	0.3636517073	-1.0775094048	3.4294609087
H33	-0.1278623255	-1.9919057656	3.1274621758
N34	-1.3715963711	-0.5792901753	0.2345575462
C35	-1.8714300039	-1.3823958382	-0.7318551707
C36	-3.2094011968	-1.7498957045	-0.7698801899
C37	-4.0742959356	-1.2710707125	0.2134522115
C38	-3.5601445109	-0.4374728284	1.2048726423
C39	-2.2093772789	-0.1144572299	1.1879389661
H40	-1.1731386492	-1.7278268675	-1.4837192306
H41	-3.5579642731	-2.4027071077	-1.5624990678
H42	-5.1249887970	-1.5429789380	0.2075004405
H43	-4.1905570761	-0.0378847889	1.9915326409
H44	-1.7668042389	0.5198202338	1.9443208777

6Me-CH$_4$: SCF = -1000.72027078318
Total internal energy, Utot (SCFE + ZPE + U): -1000.402207 hartrees
Total enthalpy, Htot (Utot + pV): -1000.401263 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1000.473060 hartrees

Ir1	0.7070372269	-0.1265097051	0.2524991118
N2	0.7202789325	-0.5477652572	-1.8029132466

C3	0.7230645027	0.2461237042	2.1042397168
C4	1.3474431748	-2.1146462727	0.6613364156
N5	0.1265737106	1.9234088612	-0.3718417853
N6	2.6200204438	0.4882242070	0.0424842242
N7	2.9608749476	1.2395315116	-1.0399274622
N8	1.2806776953	0.3485339489	-2.6594773561
N9	0.8120068510	2.4726723645	-1.4096343543
B10	1.9094640066	1.6519494665	-2.1125522072
H11	2.4316691980	2.2767906496	-2.9842311254
O12	0.7432369691	0.4629108843	3.2280149650
H13	2.3942431266	-2.1181221009	0.9708157520
H14	1.2635249979	-2.7066377805	-0.2516592881
H15	0.7539039454	-2.5854438091	1.4499236899
C16	4.2735518261	1.5322225642	-0.9551598079
H17	4.7467215970	2.1239125004	-1.7249264579
C18	4.7925458529	0.9661024369	0.2025009207
H19	5.8087558200	1.0158657381	0.5615975301
C20	0.2526137974	-1.5735757377	-2.5351584706
H21	-0.2305866109	-2.4162836900	-2.0627067053
C22	0.5076776364	-1.3389872411	-3.8872085035
H23	0.2565114617	-1.9729347407	-4.7232273196
C24	0.3820748123	3.7364392203	-1.6138366517
H25	0.8078639500	4.3412216317	-2.4012053786
C26	-0.6088116965	4.0212540622	-0.6853360948
H27	-1.1607060327	4.9417692332	-0.5739202881
C28	3.7155014108	0.3155244096	0.8036284588
H29	3.6726682345	-0.2533672697	1.7200105426
C30	1.1626992871	-0.1140107878	-3.9195427708
H31	1.5523935758	0.4564064169	-4.7498865256
C32	-0.7303585445	2.8534630290	0.0758666902
H33	-1.3832470817	2.6459850814	0.9122336528
H34	-0.8841122107	-1.1384727565	0.4430053386
C35	-1.8900104191	-0.6224570934	0.2891363114
H36	-1.9233462161	0.1363582170	-0.4870281516
H37	-2.4706546782	-1.4957783022	-0.0216168570
H38	-2.2446965597	-0.2453198905	1.2462662939

6Me-CH$_4$-TS: SCF = -1000.69162701240

Total internal energy, Utot (SCFE + ZPE + U): -1000.375993 hartrees

Total enthalpy, Htot (Utot + pV): -1000.375049 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1000.444362 hartrees

Ir1	0.5827440594	-0.1611580881	0.2191611666
N2	0.6757549944	-0.5409837536	-1.8391818464
C3	0.4846638171	0.1588504950	2.0822044035
C4	1.5002270383	-2.1307191969	0.6150261643
N5	0.2271496718	1.9168323797	-0.3135864915

N6	2.6373250146	0.5286021651	0.0507491338
N7	3.0139818141	1.2144011380	-1.0609756940
N8	1.3023884072	0.3327473806	-2.6716330911
N9	0.8804426134	2.4451001468	-1.3823075635
B10	1.9603997303	1.6179468209	-2.1206133795
H11	2.4576728552	2.2500451577	-3.0016296580
O12	0.4173725476	0.3392932622	3.2087035075
H13	2.5190691081	-1.8751617605	0.8957056968
H14	1.5043805068	-2.6975271575	-0.3143791493
H15	1.0310675834	-2.7074347976	1.4118302619
C16	4.3152566538	1.5515463684	-0.9521785628
H17	4.8019730008	2.1111665235	-1.7375609891
C18	4.8019957344	1.0717772205	0.2564422507
H19	5.8021024512	1.1703318884	0.6492057167
C20	0.2066347469	-1.5532701556	-2.5900485133
H21	-0.3324849474	-2.3738892457	-2.1390636604
C22	0.5324365827	-1.3350188379	-3.9289330351
H23	0.2980164888	-1.9631176983	-4.7741343881
C24	0.5245389707	3.7383500488	-1.5225603721
H25	0.9452154718	4.3376427562	-2.3167781932
C26	-0.3856571537	4.0623077961	-0.5253262022
H27	-0.8650769281	5.0138019515	-0.3550773729
C28	3.7099348855	0.4399133225	0.8550963048
H29	3.6493850838	-0.0620970002	1.8103496802
C30	1.2251010210	-0.1309226793	-3.9344425381
H31	1.6670709747	0.4260861053	-4.7474586288
C32	-0.5383134464	2.8871935608	0.2136028589
H33	-1.1507553089	2.7015717418	1.0846216132
H34	-0.2146273665	-1.5046110769	0.3513339366
C35	-1.6187078192	-0.3364196036	0.1419963237
H36	-1.8950274537	-0.7463261975	-0.8279172534
H37	-2.0645363995	-0.9221819837	0.9455516887
H38	-1.9479093519	0.6974330831	0.2123799018

6OH: SCF = -996.09666882871

Total internal energy, Utot (SCFE + ZPE + U): -995.852759 hartrees

Total enthalpy, Htot (Utot + pV): -995.851815 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -995.916305 hartrees

Ir1	0.1192216991	-0.1361580235	0.0449585486
N2	0.0926687606	-0.1361621340	2.1450070614
C3	0.1414805763	-0.1624291207	-1.8614622185
N4	2.1360001418	-0.5805549760	0.1815367712
N5	0.8776088595	1.7751786471	0.1290397242
N6	1.7569782622	2.1476504169	1.0931264496
N7	1.1266584601	0.4461960713	2.8173721107
N8	2.9197428106	-0.0251005636	1.1405532080

B9	2.3196115962	1.0716690472	2.0495732617
H10	3.1273183379	1.5220040682	2.8006347241
O11	0.1889754679	-0.1634909935	-3.0012257350
O12	-1.6082647386	-0.9556931900	-0.0363424091
H13	-2.0419797940	-1.1026435048	0.8173732994
C14	1.9526196336	3.4781963859	1.0053281101
H15	2.6254030321	3.9763536573	1.6878885993
C16	1.1816655135	3.9773347343	-0.0378842869
H17	1.1126566793	5.0002680675	-0.3740226286
C18	-0.7538541811	-0.6333465463	3.0659700245
H19	-1.6554794327	-1.1592266910	2.7872553989
C20	-0.2718924005	-0.3683668608	4.3461826931
H21	-0.7246452131	-0.6378062203	5.2875627784
C22	4.1354021151	-0.6053004803	1.0941084411
H23	4.9121215326	-0.2996618397	1.7796892174
C24	4.1379681678	-1.5593982518	0.0837828281
H25	4.9547511411	-2.1970550005	-0.2166321142
C26	0.5145844979	2.8700177399	-0.5630909365
H27	-0.1931707905	2.8053575963	-1.3765929864
C28	0.9208212656	0.3147520433	4.1416426706
H29	1.6348305091	0.7131282290	4.8475366335
C30	2.8552470233	-1.5147098649	-0.4646830729
H31	2.4221626425	-2.0938899947	-1.2671079895

6OH pyridine complex: SCF = -1244.46431708870

Total internal energy, Utot (SCFE + ZPE + U): -1244.123341 hartrees

Total enthalpy, Htot (Utot + pV): -1244.122396 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1244.197595 hartrees

Ir1	0.6725918730	-0.0594388370	0.3722685971
N2	0.1083722939	1.9405818119	0.5981572865
C3	1.2442554260	-1.8417698805	0.1390086386
O4	0.4749674322	0.2062677847	-1.6268778380
N5	0.7949222919	-0.1543610790	2.4913332642
N6	2.6118691694	0.6648905506	0.4076056171
N7	2.9539808298	1.5930874927	1.3415571381
N8	0.7303956084	2.7154807908	1.5267351083
N9	1.3596149924	0.8966778881	3.1451495997
B10	1.8948290014	2.1160626274	2.3522454169
H11	2.3707408658	2.9275282989	3.0861972283
O12	1.6061371363	-2.9184004245	-0.0059944027
H13	1.1737052263	0.8069661507	-1.9193616144
C14	4.2462328526	1.9343210879	1.1586649975
H15	4.7131450504	2.6652336953	1.8023137268
C16	4.7550602580	1.2123016160	0.0869752977
H17	5.7556792050	1.2486216131	-0.3148856202
C18	-0.7578487522	2.7092312349	-0.0764026631

H19	-1.3353291768	2.2883531819	-0.8858933650
C20	-0.7129167836	4.0106680828	0.4330778881
H21	-1.2895371242	4.8635219192	0.1100496506
C22	1.3960271772	0.6266317700	4.4665110909
H23	1.8117768976	1.3433857492	5.1593560459
C24	0.8447413235	-0.6294456561	4.6811028820
H25	0.7248652966	-1.1432910812	5.6222799360
C26	3.6893988724	0.4249217652	-0.3565826162
H27	3.6409379239	-0.2877016530	-1.1676242915
C28	0.2445210916	3.9712524001	1.4396747370
H29	0.6144562996	4.7478866494	2.0930192212
C30	0.4861910976	-1.0849572562	3.4091207633
H31	0.0303911411	-2.0194911232	3.1136947943
N32	-1.3680412933	-0.6031152491	0.2697977474
C33	-1.8502036302	-1.1238869567	-0.8801664217
C34	-3.1863992941	-1.4804214901	-1.0110522219
C35	-4.0545097655	-1.2838463104	0.0616183502
C36	-3.5525650075	-0.7259665981	1.2373101779
C37	-2.2055145140	-0.3976407449	1.3081088758
H38	-1.1386000086	-1.2087012774	-1.6928534047
H39	-3.5316369330	-1.9023546269	-1.9485091809
H40	-5.1027213157	-1.5545211330	-0.0180669549
H41	-4.1906050407	-0.5426014880	2.0947314910
H42	-1.7707449576	0.0381442066	2.1982619971

6OH-CH$_4$: SCF = -1036.62235944680

Total internal energy, Utot (SCFE + ZPE + U): -1036.328511 hartrees

Total enthalpy, Htot (Utot + pV): -1036.327567 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1036.397402 hartrees

Ir1	0.0772364778	-0.1015394007	0.0594319963
N2	0.0665821665	-0.1077497206	2.1363725224
C3	0.1225211954	-0.1502180231	-1.8463287025
N4	1.9878596507	-0.6926841962	0.2123503292
N5	0.7535964093	1.9099277953	0.1747678535
N6	1.7171975786	2.2000588307	1.0898385138
N7	1.0951726773	0.4782953333	2.8066544449
N8	2.8151121603	-0.0542973239	1.0835530358
B9	2.2734665008	1.0845551357	2.0006244192
H10	3.1311714860	1.4932774077	2.7201022475
O11	0.1622926275	-0.1876767016	-2.9862141859
O12	-0.5896220535	-2.0068738263	0.0705437347
H13	-0.2105380638	-2.4465517310	0.8445704570
C14	2.0191404898	3.5132944000	1.0100499062
H15	2.7668447334	3.9433258778	1.6602074801
C16	1.2365657060	4.0911363758	0.0198601699
H17	1.2318297163	5.1224602287	-0.2972120593

C18	-0.7844063087	-0.6199731341	3.0418228853
H19	-1.6701880407	-1.1496346854	2.7223986691
C20	-0.3056446057	-0.3522504082	4.3258789853
H21	-0.7591775159	-0.6262150320	5.2657822519
C22	4.0199911314	-0.6571524166	1.0306761447
H23	4.8300313694	-0.3048025180	1.6523208825
C24	3.9684158423	-1.6985417514	0.1110956976
H25	4.7654187927	-2.3716603266	-0.1645149061
C26	0.4577394415	3.0439156112	-0.4801155183
H27	-0.2854524074	3.0521170647	-1.2650559042
C28	0.8849588444	0.3391599412	4.1308562494
H29	1.5937991107	0.7369149158	4.8424258299
C30	2.6623758993	-1.6923691797	-0.3809525473
H31	2.1747774777	-2.3356561696	-1.0982607211
C32	-2.5830805421	0.2732427371	-0.0153935273
H33	-2.4695874672	-0.8101732639	-0.0070330276
H34	-1.6155754587	0.8651748729	0.0681205685
H35	-3.1401872004	0.6166602771	0.8583124696
H36	-3.0362939999	0.6175758847	-0.9457377874

6OH-CH$_4$-TS: SCF = -1036.60318820908

Total internal energy, Utot (SCFE + ZPE + U): -1036.313765 hartrees

Total enthalpy, Htot (Utot + pV): -1036.312821 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1036.379874 hartrees

Ir1	0.0165106315	-0.0022652949	0.0388832637
N2	0.0095302315	0.0178123199	2.1349682594
C3	0.0762854692	-0.0301233888	-1.8553996831
N4	1.9956174261	-0.5944927658	0.1965504228
N5	0.7167460290	1.9541155296	0.1495881595
N6	1.6846905803	2.2586313978	1.0553931168
N7	1.0720636128	0.5597302861	2.7889789683
N8	2.8168632221	0.0292475936	1.0817284583
B9	2.2565212084	1.1574239537	1.9810437253
H10	3.0956260867	1.5934556904	2.7069473701
O11	0.1234624791	-0.0430210496	-2.9964308075
O12	-0.9362502303	-1.8611052654	0.0265708418
H13	-0.7795847333	-2.2861967466	0.8836514159
C14	1.9646150617	3.5752430185	0.9672785561
H15	2.7115583487	4.0184446102	1.6093560224
C16	1.1646459708	4.1385270570	-0.0180074351
H17	1.1432241494	5.1683375360	-0.3391395046
C18	-0.8597157089	-0.4241108443	3.0614839295
H19	-1.7899308475	-0.8922899270	2.7722587391
C20	-0.3552569578	-0.1653837159	4.3365316042
H21	-0.8146048887	-0.3963393760	5.2850223293
C22	4.0331321594	-0.5513002119	1.0247521805

H23	4.8348334664	-0.2016282158	1.6586291135
C24	3.9997473997	-1.5703679055	0.0814343011
H25	4.8069357066	-2.2257668116	-0.2066964566
C26	0.3941872226	3.0805988454	-0.5061109022
H27	-0.3595051197	3.0742091727	-1.2802751397
C28	0.8674295358	0.4583333248	4.1166968654
H29	1.6015463942	0.8361471544	4.8132020384
C30	2.6939423634	-1.5641372448	-0.4152606416
H31	2.2286959130	-2.1939117347	-1.1599488345
C32	-2.2454407262	0.5047920265	0.0432945281
H33	-1.7595251425	-0.7118851759	0.1002971193
H34	-2.1744074414	1.2731398324	0.8109886980
H35	-3.1247453250	-0.1018412930	0.3269676709
H36	-2.4688458707	0.9168819892	-0.9383393022

6OH-Product: SCF = -1036.65979937017

Total internal energy, Utot (SCFE + ZPE + U): -1036.363968 hartrees

Total enthalpy, Htot (Utot + pV): -1036.363024 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1036.432056 hartrees

Ir1	-0.1204894990	0.1561500073	0.0397192701
N2	-0.1076088412	0.1580629860	2.1430981537
C3	-0.1408698213	0.1865313451	-1.8429987363
N4	1.9578649627	-0.5657704821	0.2146670881
N5	0.6096432733	2.0427876203	0.1591765448
N6	1.6163472546	2.3017489718	1.0396254236
N7	0.9888340727	0.6332335348	2.7923813778
N8	2.7627957643	0.0639933312	1.1108760214
B9	2.1853173440	1.1986905177	1.9786802544
H10	3.0141557896	1.6569785111	2.7043268777
O11	-0.1641806328	0.2234778301	-2.9876150578
O12	-0.8304165461	-1.8979811090	0.0795574570
H13	-0.4709865466	-2.3688727642	0.8482636330
C14	1.9377854886	3.6085273956	0.9461808868
H15	2.7169944284	4.0212153978	1.5697998930
C16	1.1318048406	4.2063105519	-0.0133829849
H17	1.1386052256	5.2380413566	-0.3287456422
C18	-1.0047333827	-0.2100167779	3.0747863840
H19	-1.9748581539	-0.5898175458	2.7877888984
C20	-0.4797159591	0.0174251824	4.3480842979
H21	-0.9524209269	-0.1725039322	5.2991317123
C22	4.0028993913	-0.4673101932	1.0511407805
H23	4.7906646160	-0.0976324311	1.6912632745
C24	4.0083762931	-1.4685098492	0.0903136713
H25	4.8397125115	-2.0883290205	-0.2080961423
C26	0.3070846583	3.1826638861	-0.4829252456
H27	-0.4726146931	3.2055891046	-1.2294926732

C28	0.7810451647	0.5574909223	4.1213222510
H29	1.5384621743	0.8950215258	4.8135149140
C30	2.7015792997	-1.4901118162	-0.4108838806
H31	2.2713653532	-2.1120061398	-1.1838241057
C32	-2.1152218994	0.8579190603	0.0979421171
H33	-1.7982673136	-1.9596087317	0.1237350999
H34	-2.2274986569	1.5070084770	0.9685845174
H35	-2.8193174306	0.0198583933	0.1990714231
H36	-2.4071602933	1.4187572088	-0.7926837309

6NH$_2$: SCF = -976.25200259009

Total internal energy, Utot (SCFE + ZPE + U): -975.994947 hartrees

Total enthalpy, Htot (Utot + pV): -975.994003 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -976.057527 hartrees

Ir1	-0.1827442545	0.3296332908	-0.0228895447
N2	-0.1339532633	0.2572004152	2.0937464674
C3	-0.2740678447	0.3729407296	-1.9100641792
N4	-1.7675040824	1.6794250593	0.1712551433
N5	-1.7759735172	-1.0297031984	0.1097099213
N6	-2.7172241963	-0.9281333573	1.0818935907
N7	-1.3155269913	0.2576348793	2.7765262497
N8	-2.7057123410	1.5424040099	1.1414642123
B9	-2.6770931871	0.2851047836	2.0360418013
H10	-3.5832360615	0.2717131036	2.8107368017
O11	-0.3713831225	0.3952021656	-3.0496847989
N12	1.7111067367	0.3729573695	-0.0617153168
H13	2.2923389557	0.4151297433	-0.8931894142
C14	-3.5327365830	-1.9991550140	1.0125497748
H15	-4.3537743115	-2.1058357770	1.7062751819
C16	-3.1099791350	-2.8156434437	-0.0290234950
H17	-3.5464401418	-3.7476586940	-0.3528423437
C18	0.8508411808	0.1914179066	3.0071477458
H19	1.8915073902	0.1676927655	2.7212042960
C20	0.3110783374	0.1526294161	4.2916125796
H21	0.8442327922	0.0986294895	5.2278626902
C22	-3.5144304610	2.6203642437	1.1197447296
H23	-4.3327352402	2.7027167130	1.8199460060
C24	-3.0895010447	3.4777528497	0.1121979412
H25	-3.5206206292	4.4255687798	-0.1702749944
C26	-1.9965479497	-2.1684544206	-0.5685410018
H27	-1.3551553122	-2.4589118541	-1.3877823597
C28	-1.0634706954	0.1955137073	4.0977768448
H29	-1.8769757127	0.1842461684	4.8081848770
C30	-1.9822809249	2.8473642590	-0.4582343274
H31	-1.3412299341	3.1679757794	-1.2663196773
H32	2.2901525466	0.3900040730	0.7714147402

6NH$_2$ pyridine complex: SCF = -1224.59455400114

Total internal energy, Utot (SCFE + ZPE + U): -1224.240739 hartrees

Total enthalpy, Htot (Utot + pV): -1224.239795 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1224.315014 hartrees

Ir1	0.6778268086	-0.0633852292	0.3542991765
N2	0.0930882287	1.9362998261	0.5785273889
C3	1.2274306364	-1.8521596703	0.1520829786
N4	0.5616453841	0.1963494882	-1.7038437998
N5	0.7627549695	-0.1289209190	2.5190583095
N6	2.6223788086	0.6432044075	0.4302497592
N7	2.9472118783	1.5876062020	1.3541107194
N8	0.7209405503	2.7158366287	1.4991959121
N9	1.3382629733	0.9263405141	3.1562067426
B10	1.8792608740	2.1264965655	2.3426325419
H11	2.3489531609	2.9540671974	3.0630248967
O12	1.5638992336	-2.9411169116	0.0282666600
H13	1.3438478210	-0.2776477079	-2.1578743766
H14	0.7544793864	1.1852945516	-1.8720578325
C15	4.2485407324	1.9109280877	1.2062594337
H16	4.7023168615	2.6508987691	1.8488340732
C17	4.7823448518	1.1604798307	0.1673681968
H18	5.7951670923	1.1764963848	-0.2039042508
C19	-0.8239860722	2.6914933968	-0.0464770033
H20	-1.4351780307	2.2680441862	-0.8303104439
C21	-0.7956080686	3.9862248466	0.4785930136
H22	-1.4076858600	4.8266292368	0.1902672938
C23	1.4025438848	0.6664329861	4.4791111994
H24	1.8287701813	1.3894919529	5.1589777573
C25	0.8579754987	-0.5888343394	4.7130742382
H26	0.7555614641	-1.0955446179	5.6601932074
C27	3.7210061104	0.3775230467	-0.2928953176
H28	3.6953951023	-0.3507234460	-1.0900771102
C29	0.1967422249	3.9571755214	1.4511151225
H30	0.5647813675	4.7320137394	2.1074999131
C31	0.4758499497	-1.0526111085	3.4502608344
H32	0.0130490907	-1.9891042041	3.1713662896
N33	-1.3810952747	-0.6025105458	0.2619019882
C34	-1.8919146028	-1.1274650855	-0.8724683370
C35	-3.2250252283	-1.5101810398	-0.9617282424
C36	-4.0624813690	-1.3339897528	0.1379472973
C37	-3.5333743146	-0.7675652899	1.2977403832
C38	-2.1907772147	-0.4161478465	1.3264924572
H39	-1.2025495535	-1.1710125709	-1.7081744323
H40	-3.5922318339	-1.9352385721	-1.8894538442
H41	-5.1071831171	-1.6254386021	0.0918715729

H42	-4.1466157689	-0.5967262508	2.1756744735
H43	-1.7370473867	0.0228858323	2.2049802446

6NH$_2$-CH$_4$-TS: SCF = -1016.74137353798

Total internal energy, Utot (SCFE + ZPE + U): -1016.439076 hartrees

Total enthalpy, Htot (Utot + pV): -1016.438132 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -1016.505694 hartrees

Ir1	-0.1088004163	0.0091168754	-0.0384280781
N2	-0.0658779200	0.0075046001	2.0584012701
C3	-0.1920269682	0.0329795697	-1.9257245706
N4	-1.5216746059	1.5083609659	0.1400221353
N5	-1.7252453895	-1.3588607949	0.1356719033
N6	-2.6861243286	-1.1156360226	1.0665038606
N7	-1.2397079154	0.0557166993	2.7436032408
N8	-2.5183226912	1.3816126522	1.0558775471
B9	-2.5837091398	0.1317908582	1.9724797083
H10	-3.5070078486	0.2001730199	2.7241939538
O11	-0.2510667077	0.0505130460	-3.0684209246
N12	1.6587739937	1.1374761632	0.0268558852
H13	1.8523842979	1.6793958654	-0.8098703429
C14	-3.6076181995	-2.1000009386	1.0167160892
H15	-4.4564526675	-2.0887041981	1.6846965699
C16	-3.2405298354	-3.0042935832	0.0296662833
H17	-3.7612763592	-3.9017721534	-0.2662736710
C18	0.9333091104	-0.0376000838	2.9564702652
H19	1.9638579234	-0.0761924461	2.6333893911
C20	0.4012079156	-0.0196785265	4.2469430179
H21	0.9404731533	-0.0468763590	5.1810742720
C22	-3.2868010160	2.4889056467	1.0129236026
H23	-4.1367541514	2.5876146288	1.6719662455
C24	-2.7820033223	3.3502606085	0.0468529689
H25	-3.1665950424	4.3171900528	-0.2382943895
C26	-2.0499110915	-2.4963634578	-0.4980009386
H27	-1.4243545508	-2.8867670778	-1.2880083070
C28	-0.9754176107	0.0410084006	4.0649893420
H29	-1.7809833532	0.0746586399	4.7837559392
C30	-1.6677787054	2.6918512866	-0.4773593471
H31	-0.9800361768	3.0011911621	-1.2508475249
H32	1.6420049910	1.7650772673	0.8261491205
C33	1.5436950195	-1.6509819027	-0.0464443351
H34	1.7545499237	-0.3787549489	0.0144890825
H35	0.9893726385	-2.2648485883	0.6611542400
H36	2.5802475204	-1.6402865338	0.3303863666
H37	1.5650685479	-2.0855360519	-1.0436169788

6NH$_2$-Product: SCF = -1016.82414350042

Total internal energy, Utot (SCFE + ZPE + U): -1016.513951 hartrees
Total enthalpy, Htot (Utot + pV): -1016.513007 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1016.582326 hartrees

Ir1	-0.0692906092	-0.2407555230	-0.0418350290
N2	-0.0472129543	-0.2248386829	2.0670887724
C3	-0.1008390695	-0.3262747308	-1.9154406399
N4	-1.5202438243	1.4261074089	0.1281294838
N5	-1.6804672348	-1.5122714072	0.1441065588
N6	-2.6568597656	-1.2047088001	1.0428222198
N7	-1.2182648868	-0.0629125017	2.7383052615
N8	-2.4977090826	1.3059282178	1.0638599696
B9	-2.5548688986	0.0483522274	1.9551054014
H10	-3.4814036548	0.0957597004	2.7060594287
O11	-0.1156628524	-0.4047804432	-3.0602023685
N12	1.5804560574	1.1301714903	0.0024645317
H13	1.3807074015	2.0064578821	-0.4795934085
C14	-3.6075059110	-2.1610619824	0.9907737659
H15	-4.4719364744	-2.1040602229	1.6358044812
C16	-3.2463814307	-3.1047363133	0.0390721999
H17	-3.7892841430	-3.9922233997	-0.2466749848
C18	0.9268985626	-0.3801135876	2.9812639667
H19	1.9469598025	-0.5657553486	2.6753991783
C20	0.3838001475	-0.3034245520	4.2653476835
H21	0.9033483314	-0.3906953071	5.2068991539
C22	-3.3137712601	2.3801007856	1.0044740805
H23	-4.1577049244	2.4660591671	1.6732402828
C24	-2.8594798963	3.2252423000	0.0022975578
H25	-3.2862391934	4.1663116868	-0.3083341331
C26	-2.0242831841	-2.6563041951	-0.4672455679
H27	-1.3857144569	-3.0911677974	-1.2218444402
C28	-0.9774045086	-0.1088703771	4.0634012034
H29	-1.7878443299	-0.0068485623	4.7702193813
C30	-1.7342075219	2.5794884448	-0.5223350367
H31	-1.0922163661	2.8830420617	-1.3383476272
H32	1.7791269208	1.3688923650	0.9750775610
C33	1.2757765877	-1.8782574094	0.0158070694
H34	2.4321962168	0.7384866882	-0.4003134163
H35	1.0275900046	-2.4865432287	0.8877814656
H36	2.3147196674	-1.5394784948	0.1105855448
H37	1.2161213058	-2.5115598184	-0.8723699680