

Supporting Information for

The Effect of Co-adsorbed Solvent Molecules on H₂ Binding to Metal Alkoxides

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S1. Comparison between MP2/6-311++G(d,p) and M06/6-311+G(d,p)

Binding energies of solvent molecules onto Zn alkoxide were calculated at the MP2/6-311+G(d,p) and M06/6-311++G(d,p) levels of theory. Table S1 shows the results. The resulting binding energies are in reasonable agreement, with the biggest difference obtained for the binding energy of chloroform.

Table S1. Solvent binding energies onto Zn alkoxide calculated with MP2 and M06.

Solvent	MP2 (kJ/mol)	M06 (kJ/mol)
CHCl ₃	-85.3	-73.8
DMF	-161.4	-166.8
Ethanol	-133.7	-134.8
Methanol	-123.8	-127.4
H ₂ O	-108.7	-110.3

S2. Solvent Release Temperatures

Table S2. Temperature (K) to drive solvent off of metal alkoxides

	Li	Mg	Zn	Cu	Ni
CHCl ₃	253	482	447	518	597
DMF	866	1339	1177	756	1005
Ethanol	480	1030	840	575	833
Methanol	567	957	862	623	809
H ₂ O	509	1050	833	596	826

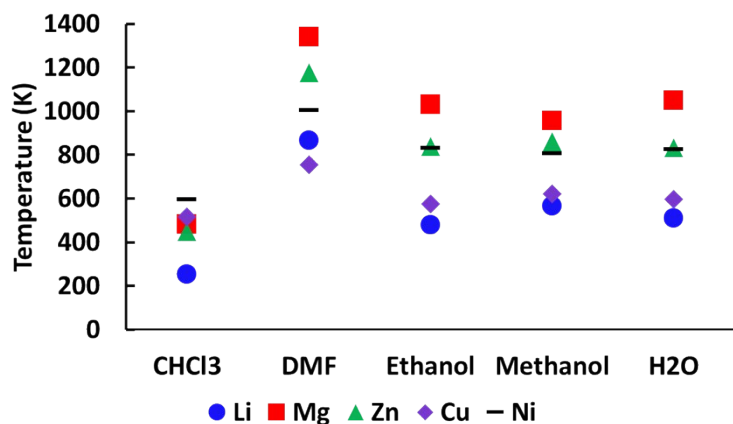


Figure S1. Solvent release temperature of solvent molecule from metal alkoxides.

S3. Hydrogen Binding Energies onto Solvent-Metal Alkoxide Complexes

Hydrogen binding energies onto solvent-metal alkoxide complexes are reported in Table S3. Calculations involving Li, Mg, and Zn were performed at the MP2 level of theory, while calculations for Cu and Ni were performed using M06.

Table S3. Hydrogen binding energies (kJ/mol) onto solvent-metal alkoxide complexes

	Li	Mg	Zn	Cu	Ni
CHCl ₃	-9.5	-16.2	-5.2	-10.3	-9.4
DMF	-19.2	-8.1	-1.9	-10.5	-64.5
Ethanol	-7.2	-8.4	-5.9	-8.2	-68.5
Methanol	-7.4	-11.1	-5.3	-7.9	-71.8
H ₂ O	-8.9	-13.9	-6.7	-6.0	-71.1

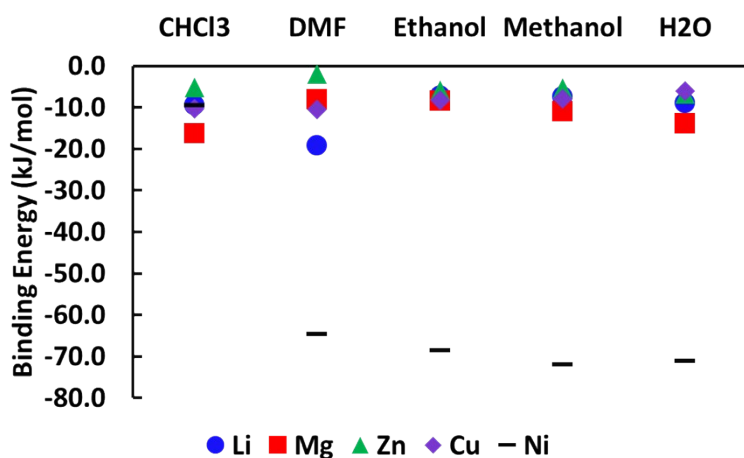


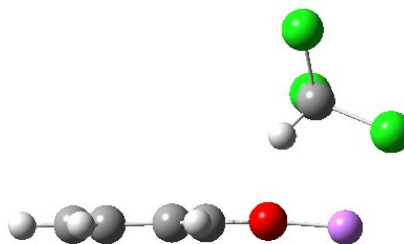
Figure S2. Hydrogen binding energy onto solvent-metal alkoxide complexes.

S4. Optimized configurations

Solvent onto metal alkoxide

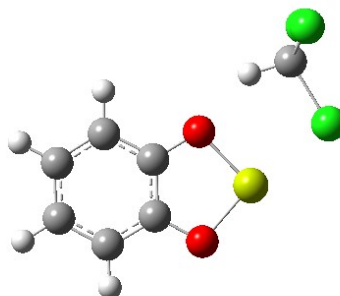
CHCl₃_Li

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C 8.2308980000 0.2783770000 -1.3522260000
C 9.1238550000 1.3165840000 -1.0018010000
C 8.5739780000 2.5961940000 -0.7562960000
C 7.2020660000 2.8327310000 -0.8926740000
C 6.3314380000 1.7933360000 -1.2430320000
H 6.1994320000 -0.2994650000 -1.7644110000
H 8.6401080000 -0.7125860000 -1.5373690000
H 9.2510290000 3.4071090000 -0.4935430000
H 6.8105360000 3.8297830000 -0.7025350000
H 5.2661650000 1.9779810000 -1.3488460000
O 10.4254290000 1.0959390000 -0.8659840000
Li 12.0376280000 0.6884740000 -0.9147790000
C 11.3273090000 1.6230810000 2.0168000000
H 10.6568880000 1.5777740000 1.1588040000
Cl 10.7672790000 0.5284730000 3.2663160000
Cl 12.9282260000 1.0714030000 1.3833160000
Cl 11.4486260000 3.2776150000 2.5873740000
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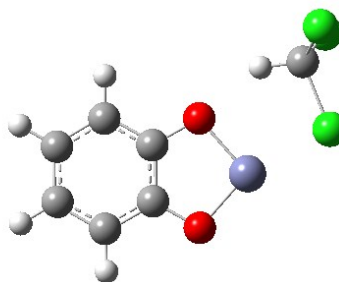
CHCl₃_Mg

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C 8.5635870000 0.4626130000 -1.0797740000
C 9.0069320000 1.7008410000 -0.5071990000
C 8.2352460000 2.8561560000 -0.6799180000
C 7.0058890000 2.8020820000 -1.3498920000
C 6.5670910000 1.5937860000 -1.9052720000
H 7.0062330000 -0.5192000000 -2.1655420000
H 8.5975710000 3.7834640000 -0.2418490000
H 6.4174400000 3.7079040000 -1.4709630000
H 5.6152750000 1.5451550000 -2.4280960000
O 10.2010300000 1.7327880000 0.1632730000
O 9.3175350000 -0.6675990000 -0.9419040000
Mg 10.8020180000 -0.0602820000 0.0402030000
C 12.6792570000 2.1092490000 1.6758150000
H 11.7246310000 2.3450630000 1.1972630000
Cl 12.5814560000 2.3597720000 3.3981020000
Cl 12.9302700000 0.3019870000 1.3502020000
Cl 13.9777020000 2.9992630000 0.9270980000
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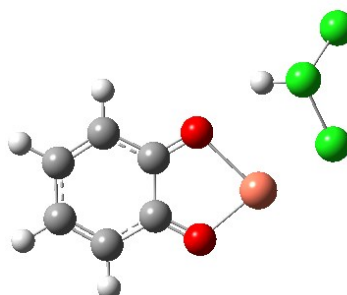
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C	7.1039760000	0.4362150000	-2.1200220000
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C	7.8324690000	2.4934420000	-0.3555290000
C	6.9093700000	2.7400970000	-1.3790430000
C	6.5640720000	1.7188410000	-2.2741710000
H	6.8487970000	-0.3716630000	-2.8010130000
H	8.1165010000	3.2715500000	0.3487520000
H	6.4901850000	3.7358370000	-1.4965200000
H	5.8491790000	1.9080880000	-3.0704900000
O	9.2697150000	0.9456720000	0.8171890000
O	8.5734730000	-1.0771890000	-0.9607400000
Zn	9.6523040000	-0.8575390000	0.5047070000
C	11.1931930000	0.2890360000	3.0246180000
H	10.5026080000	0.8781710000	2.4191780000
Cl	10.6126590000	0.1685160000	4.6638940000
Cl	11.1749720000	-1.3935150000	2.2580630000
Cl	12.8048760000	0.9438080000	2.9141670000



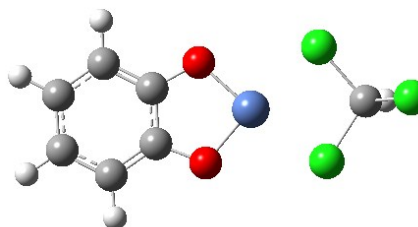
CHCl₃_Cu

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C	8.4590080000	1.2833110000	-0.1187620000
C	7.8318400000	2.5497590000	-0.2794910000
C	6.8710920000	2.7348120000	-1.2323340000
C	6.4706490000	1.6709190000	-2.0861510000
H	6.7415450000	-0.3916310000	-2.6239590000
H	8.1468250000	3.3527460000	0.3799430000
H	6.4007430000	3.7071890000	-1.3454240000
H	5.7038390000	1.8537350000	-2.8330020000
O	9.3552150000	1.0581740000	0.7473410000
O	8.5863010000	-0.9655670000	-0.8855000000
Cu	9.9222880000	-0.9987870000	0.5002890000
C	11.2782470000	0.2565110000	2.8920550000
H	10.8833390000	0.9489610000	2.1467920000
Cl	10.0751760000	0.0095890000	4.1399290000
Cl	11.5501080000	-1.3284480000	1.9706930000
Cl	12.8152550000	0.8148430000	3.5227440000



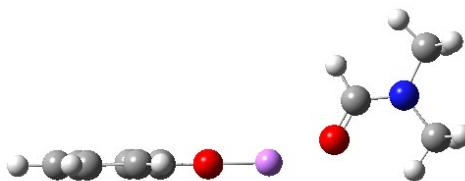
CHCl₃_Ni

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C	9.4237160000	1.8306430000	-1.4279630000
C	8.4511030000	2.7993750000	-1.5998760000
C	7.1119870000	2.4317620000	-1.4721440000
C	6.7632380000	1.1206070000	-1.1778410000
H	7.4923210000	-0.8849040000	-0.7751890000
H	8.7435760000	3.8199910000	-1.8284030000
H	6.3378830000	3.1818060000	-1.6039950000
H	5.7167220000	0.8475280000	-1.0809100000
O	10.7560510000	2.0591050000	-1.5246850000
O	10.1180910000	-0.3379050000	-0.9879690000
Ni	11.6382140000	0.5481460000	-1.2252540000
C	14.4398340000	-0.2237690000	-1.3432870000
H	14.7700690000	-0.5298020000	-2.3334750000
Cl	13.7783970000	1.4481040000	-1.4828840000
Cl	13.0520630000	-1.2781990000	-0.8822630000
Cl	15.7540560000	-0.3255600000	-0.2097370000



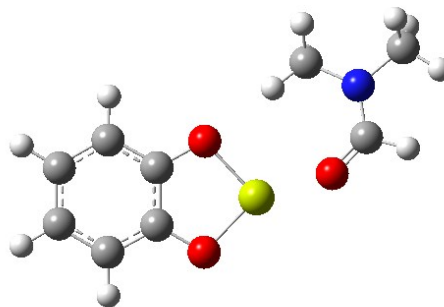
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C	7.5040520000	0.6903330000	-0.8430670000
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C	8.9026330000	2.5760250000	-2.3481230000
C	7.5440510000	2.7624480000	-2.0749590000
C	6.8348880000	1.8325590000	-1.3027950000
H	6.9715240000	-0.0466900000	-0.2445470000
H	9.3795580000	-0.3866310000	-0.7537990000
H	9.4508180000	3.3012760000	-2.9464340000
H	7.0429590000	3.6550610000	-2.4453140000
H	5.7788620000	1.9781650000	-1.0921460000
O	10.8715380000	1.2401000000	-2.1687040000
Li	12.5000590000	1.0103330000	-2.4827760000
N	16.5902150000	1.4338500000	-1.7785200000
C	17.5319300000	2.0383920000	-0.8487510000
H	16.9854370000	2.5625080000	-0.0630340000
H	18.1576660000	1.2653060000	-0.3932890000
H	18.1723250000	2.7522810000	-1.3749710000
C	17.1423600000	0.6875730000	-2.9008600000
H	17.7519490000	-0.1405680000	-2.5280930000
H	16.3214490000	0.2990300000	-3.5013230000
H	17.7662360000	1.3474880000	-3.5105000000
C	15.2656490000	1.5574740000	-1.6102160000
H	14.9914280000	2.1458960000	-0.7228980000
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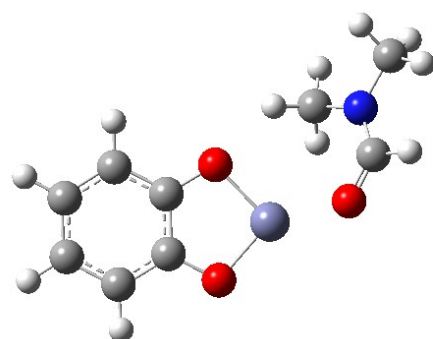
DMF_Mg

C	7.7350940000	0.5942900000	-2.3394320000
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C	8.8352890000	1.4268810000	-0.3208120000
C	7.5732110000	1.6789370000	0.2349970000
C	6.3998850000	1.3636640000	-0.4652800000
C	6.4817940000	0.8497500000	-1.7652440000
H	7.8213430000	0.1932700000	-3.3469200000
H	7.5334810000	2.0803880000	1.2456610000
H	5.4310050000	1.5628700000	-0.0134820000
H	5.5766180000	0.6039450000	-2.3155220000
O	9.9839710000	1.7063980000	0.3546430000
O	10.1388210000	0.6844220000	-2.2177060000
Mg	11.3632860000	1.2118840000	-0.8692250000
N	13.7252310000	2.3795560000	1.8399680000
C	14.7850220000	2.7278380000	2.7829980000
H	15.7435350000	2.3563130000	2.4182580000
H	14.8359590000	3.8146280000	2.8878930000
H	14.5700430000	2.2815030000	3.7566900000
C	12.3808630000	2.8796500000	2.1514550000
H	12.3027290000	3.9291380000	1.8533140000
H	11.6018570000	2.3025920000	1.6500670000
H	12.2400320000	2.8019840000	3.2308780000
C	14.0158210000	1.7350160000	0.7182620000
H	15.0693470000	1.4519110000	0.6177600000
O	13.2124570000	1.4370090000	-0.1932580000



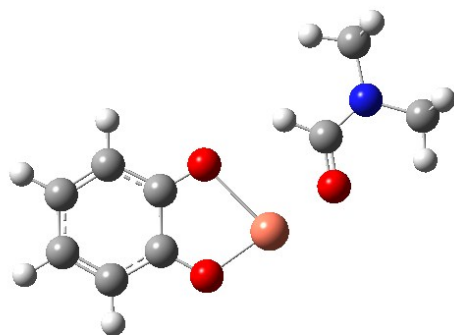
DMF_Zn

C	7.8656720000	0.7691330000	-2.2906060000
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C	7.7126020000	1.4748670000	0.4192720000
C	6.5410870000	1.2195640000	-0.3064180000
C	6.6170150000	0.8941930000	-1.6670980000
H	7.9478660000	0.5137930000	-3.3443990000
H	7.6758160000	1.7286740000	1.4764500000
H	5.5738820000	1.3143780000	0.1809070000
H	5.7106180000	0.6963200000	-2.2338080000
O	10.1237300000	1.5839030000	0.4949550000
O	10.2657530000	0.9252730000	-2.1787200000
Zn	11.4560400000	1.2874850000	-0.8088640000
N	13.5641360000	2.4483560000	1.7519880000
C	14.2546160000	2.4722320000	3.0388110000
H	15.0536710000	1.7296050000	3.0399790000
H	14.6803720000	3.4637450000	3.2091090000
H	13.5460140000	2.2378400000	3.8367900000
C	12.4370410000	3.3696770000	1.5595120000
H	12.5049030000	3.8126810000	0.5638160000
H	11.4781330000	2.8503770000	1.6584580000
H	12.5244060000	4.1607070000	2.3046610000
C	13.9085230000	1.5766790000	0.8169410000
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O	13.3419880000	1.4211330000	-0.2941180000



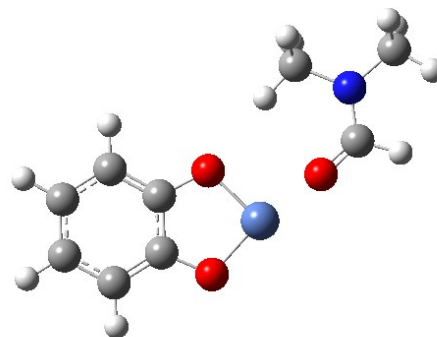
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C	6.7210760000	2.5162340000	-1.5887600000
C	6.8214940000	1.9180300000	-2.8149140000
C	7.7320990000	0.8505670000	-3.0334440000
H	9.2327530000	-0.4204750000	-2.1763170000
H	6.0295970000	3.3332050000	-1.4054500000
H	6.1986370000	2.2597800000	-3.6365120000
H	7.7882080000	0.3964920000	-4.0187700000
O	7.4373970000	2.6363750000	0.6459990000
O	9.2000540000	0.5801670000	0.2340460000
Cu	8.5805760000	1.9339320000	1.9801680000
N	11.3585160000	-0.2814600000	3.8180800000
C	12.2149400000	-1.3521550000	3.3566350000
H	12.0262010000	-1.5496920000	2.2998740000
H	13.2683030000	-1.0790440000	3.4826880000
H	12.0224130000	-2.2672610000	3.9272760000
C	11.4837900000	0.1138810000	5.2064440000
H	12.5037770000	0.4584230000	5.4075870000
H	10.7806420000	0.9192730000	5.4138670000
H	11.2672250000	-0.7382340000	5.8593870000
C	10.4926360000	0.3144720000	2.9985230000
H	10.4827750000	-0.0659870000	1.9653980000
O	9.7417290000	1.2336490000	3.3516640000



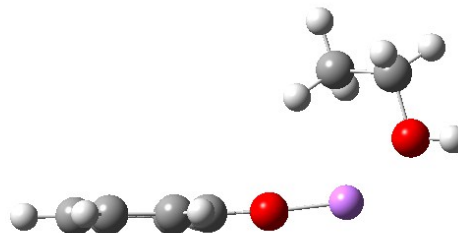
DMF_Ni

C	7.0590430000	0.3892480000	-0.6288640000
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C	8.5703910000	2.2016800000	-1.1752510000
C	7.7848770000	2.5551710000	-2.2602070000
C	6.6274850000	1.8224360000	-2.5234230000
C	6.2658450000	0.7542310000	-1.7159770000
H	6.7961440000	-0.4492070000	0.0103090000
H	8.0786170000	3.3985640000	-2.8782490000
H	6.0029240000	2.0969770000	-3.3687010000
H	5.3607480000	0.1934950000	-1.9308440000
O	9.6939880000	2.8543450000	-0.7977820000
O	9.0776840000	0.8235620000	0.6263660000
Ni	10.4229010000	1.9868710000	0.5645750000
N	11.5595350000	-0.2323510000	3.6291410000
C	12.2928520000	-0.8254120000	4.7254130000
H	13.2536840000	-0.3219970000	4.8608980000
H	11.7195460000	-0.7453460000	5.6560250000
H	12.4763870000	-1.8877550000	4.5233910000
C	10.2750350000	-0.8306630000	3.2864480000
H	9.6016790000	-0.7640210000	4.1478300000
H	9.8303250000	-0.3105840000	2.4315340000
H	10.4220950000	-1.8887800000	3.0378760000
C	12.0451160000	0.7868960000	2.9270480000
H	13.0334570000	1.1431440000	3.2652350000
O	11.4549080000	1.3058910000	1.9919970000



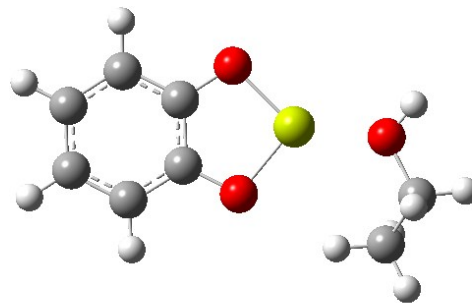
Ethanol_Li

C	7.2823930000	0.2887240000	-2.3713260000
C	8.6293230000	0.4218290000	-2.0206690000
C	9.0577400000	1.4042380000	-1.0938900000
C	8.0652970000	2.2709290000	-0.5720460000
C	6.7189440000	2.1343090000	-0.9248530000
C	6.3156700000	1.1528280000	-1.8397320000
H	6.9900730000	-0.4799320000	-3.0842960000
H	9.3792150000	-0.2463790000	-2.4394470000
H	8.3770140000	3.0403580000	0.1319010000
H	5.9843000000	2.8166550000	-0.5013600000
H	5.2695240000	1.0485460000	-2.1140310000
O	10.3219050000	1.5142860000	-0.7411990000
Li	11.8732630000	1.6158400000	-0.1380210000
C	11.0485610000	0.6060000000	2.6360180000
H	10.5854160000	-0.0379100000	3.3884480000
H	10.4209860000	0.5955400000	1.7400990000
H	11.0887650000	1.6243480000	3.0299240000
C	12.4410350000	0.0981020000	2.3306570000
H	13.0806370000	0.1533960000	3.2163340000
H	12.4136940000	-0.9357320000	1.9738990000
O	13.0172490000	0.9349180000	1.2930880000
H	13.9672830000	0.7950440000	1.2892700000



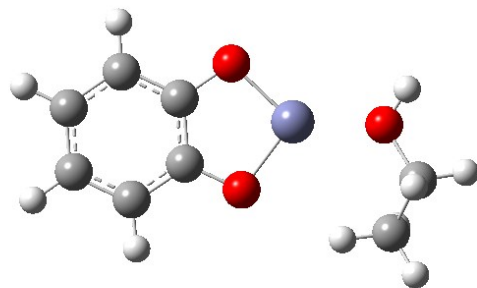
Ethanol_Mg

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C 7.6813430000 0.4997530000 -0.7903370000
C 8.8827720000 1.1802520000 -0.5474020000
C 8.9726140000 2.5769620000 -0.8760800000
C 7.8808130000 3.1994040000 -1.4981480000
C 6.6895850000 2.5003360000 -1.7362520000
C 6.5997900000 1.1417960000 -1.4090030000
H 7.6338230000 -0.5544430000 -0.5260220000
H 7.9740900000 4.2544290000 -1.7458420000
H 5.8544940000 3.0057950000 -2.2152240000
H 5.6792430000 0.5927680000 -1.5918250000
O 10.1228360000 3.2634450000 -0.6203060000
O 9.9480520000 0.5542490000 0.0307350000
Mg 11.2262110000 1.9451450000 0.1638570000
C 12.9406310000 -0.6885850000 0.9917920000
H 13.2360160000 -1.6132560000 1.4946540000
H 13.3664980000 -0.6968370000 -0.0143440000
H 11.8478040000 -0.6773560000 0.9207450000
C 13.4653440000 0.4849330000 1.7867630000
H 13.0806190000 0.4872760000 2.8088520000
H 14.5569590000 0.5005830000 1.8059740000
O 13.0215550000 1.7248360000 1.1385460000
H 13.5927320000 2.4477560000 1.4149810000
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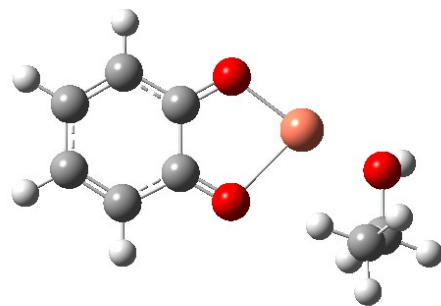
Ethanol_Zn

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C 8.4807320000 -0.1498480000 -1.6214500000
C 9.7840390000 0.3522630000 -1.5142000000
C 9.9800840000 1.7418950000 -1.2350430000
C 8.8669390000 2.5861810000 -1.1338640000
C 7.5698970000 2.0684840000 -1.2455090000
C 7.3775800000 0.7068820000 -1.5151570000
H 8.3550750000 -1.2100300000 -1.8281800000
H 9.0394820000 3.6397250000 -0.9277540000
H 6.7155960000 2.7354030000 -1.1611020000
H 6.3722710000 0.3030220000 -1.6038600000
O 11.2498010000 2.2318600000 -1.1066630000
O 10.8729460000 -0.4630130000 -1.6359600000
Zn 12.2848370000 0.7200450000 -1.3649750000
C 13.8645750000 -1.9921650000 -2.2469070000
H 14.1816250000 -3.0375740000 -2.1992980000
H 14.0363220000 -1.6244920000 -3.2608230000
H 12.7938360000 -1.9501670000 -2.0239990000
C 14.6690220000 -1.1948800000 -1.2474650000
H 14.5264230000 -1.5597850000 -0.2275390000
H 15.7331270000 -1.1967390000 -1.4935900000
O 14.2181750000 0.1980810000 -1.3007280000
H 14.8728470000 0.7737810000 -0.8930190000
```



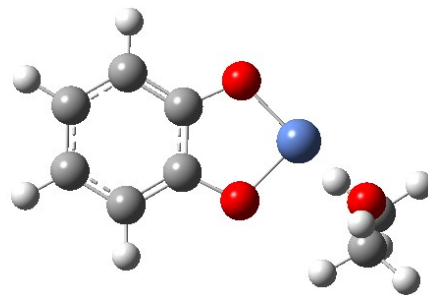
Ethanol_Cu

```
C 7.2523670000 0.0037110000 -1.1355560000
C 8.4339380000 0.3631960000 -0.4200450000
C 8.9803100000 1.7232400000 -0.6284870000
C 8.3099840000 2.5979070000 -1.5198830000
C 7.1798790000 2.1920880000 -2.1755010000
C 6.6494420000 0.8882850000 -1.9822390000
H 6.8593520000 -0.9960920000 -0.9762860000
H 8.7275770000 3.5907150000 -1.6580200000
H 6.6764020000 2.8720750000 -2.8565090000
H 5.7506810000 0.5993870000 -2.5195670000
O 10.0355020000 2.0736980000 -0.0036040000
O 9.0239000000 -0.4170970000 0.3745920000
Cu 10.7574260000 0.7183790000 1.1330260000
C 9.8618560000 -1.3403760000 3.4483560000
H 9.3595370000 -2.2604610000 3.7594320000
H 9.1740740000 -0.7869340000 2.8007730000
H 10.0839260000 -0.7466300000 4.3395360000
C 11.1198890000 -1.6763240000 2.7028480000
H 11.8144850000 -2.2563520000 3.3211030000
H 10.8978440000 -2.2340530000 1.7857090000
O 11.7774030000 -0.4338690000 2.3466810000
H 12.6805430000 -0.6051360000 2.0665640000
```



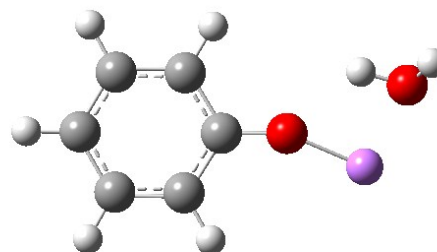
Ethanol_Ni

```
C 8.0068190000 0.0631230000 -1.6672620000
C 9.3610860000 0.0272860000 -1.9533600000
C 10.2229300000 0.9787170000 -1.4029640000
C 9.7461510000 1.9806900000 -0.5786080000
C 8.3812980000 2.0178740000 -0.2941060000
C 7.5226610000 1.0685740000 -0.8320210000
H 7.3492240000 -0.6854380000 -2.0990430000
H 10.4344570000 2.7133770000 -0.1671470000
H 7.9918230000 2.7967690000 0.3544540000
H 6.4619190000 1.1081290000 -0.6032780000
O 11.5350400000 0.8276640000 -1.7361040000
O 9.9532420000 -0.8842470000 -2.7550980000
Ni 11.6842450000 -0.5516930000 -2.8515460000
C 14.2089540000 -1.7083270000 -1.2547360000
H 14.8165300000 -1.7917240000 -0.3500140000
H 14.5329270000 -2.4804490000 -1.9585430000
H 13.1665360000 -1.8939040000 -0.9736270000
C 14.3630940000 -0.3385020000 -1.8455480000
H 13.9797240000 0.4377110000 -1.1753100000
H 15.4039400000 -0.1237580000 -2.1089940000
O 13.5886320000 -0.2846750000 -3.0780760000
H 13.6950840000 0.5921580000 -3.4661480000
```



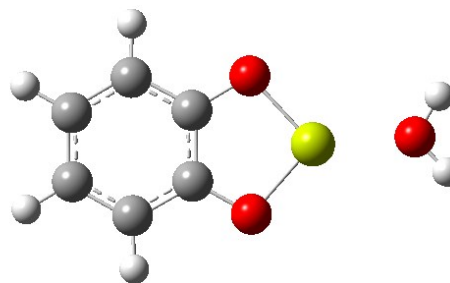
H₂O_Li

```
C 6.7276710000 0.3316790000 -1.5572100000
C 8.1084150000 0.2563350000 -1.3483620000
C 8.8803860000 1.4145610000 -1.0936140000
C 8.1866270000 2.6446400000 -1.0106690000
C 6.8060570000 2.7178290000 -1.2188480000
C 6.0599530000 1.5600660000 -1.4745980000
H 6.1671650000 -0.5796650000 -1.7554140000
H 8.6197760000 -0.7031790000 -1.4061230000
H 8.7626030000 3.5467130000 -0.8135990000
H 6.3070130000 3.6825190000 -1.1537060000
H 4.9872040000 1.6178780000 -1.6359530000
O 10.1911880000 1.3539380000 -0.9094310000
Li 11.7526280000 0.6648900000 -1.0694800000
H 13.0337980000 2.4936980000 0.6352600000
H 11.6563390000 2.4513920000 -0.0879000000
O 12.5887310000 2.1707260000 -0.1484430000
```



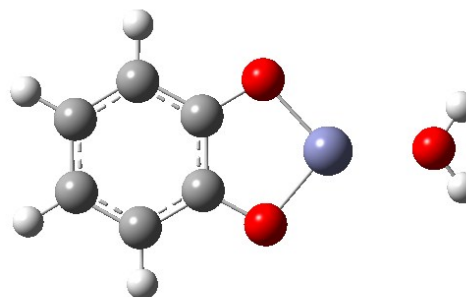
H₂O_Mg

```
C 7.0826870000 0.3529050000 -1.3524490000
C 8.3904870000 0.7479110000 -1.0373200000
C 8.6877500000 2.1503270000 -0.9270970000
C 7.6789240000 3.0827530000 -1.2072160000
C 6.3782660000 2.6671690000 -1.5225000000
C 6.0872780000 1.3012280000 -1.6239650000
H 6.8798170000 -0.7133330000 -1.4233760000
H 7.9289770000 4.1380920000 -1.1247100000
H 5.6107700000 3.4088200000 -1.7300000000
H 5.0808290000 0.9711930000 -1.8695400000
O 9.9488760000 2.5554250000 -0.5957600000
O 9.3655020000 -0.1774920000 -0.7960560000
Mg 10.8507230000 0.9113780000 -0.3900650000
H 13.2845790000 -0.2608730000 0.2641990000
H 13.4713350000 1.2672550000 0.3440640000
O 12.8298180000 0.5780520000 0.1469910000
```



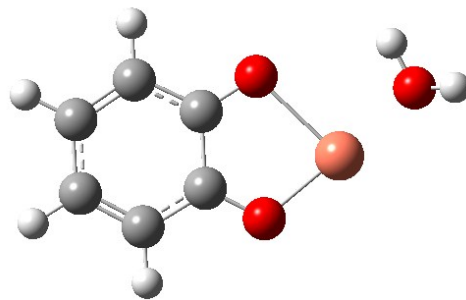
H₂O_Zn

```
C 7.0995540000 0.3506190000 -1.4176290000
C 8.3914990000 0.7570550000 -1.0604730000
C 8.6766160000 2.1527320000 -0.9259710000
C 7.6745660000 3.0891800000 -1.2102920000
C 6.3883220000 2.6664710000 -1.5695100000
C 6.1080910000 1.2994530000 -1.6976160000
H 6.9042260000 -0.7152340000 -1.5069450000
H 7.9147820000 4.1444960000 -1.1065230000
H 5.6202190000 3.4049450000 -1.7845110000
H 5.1110050000 0.9686870000 -1.9768780000
O 9.9307010000 2.5544040000 -0.5538900000
O 9.3731460000 -0.1612010000 -0.8033090000
Zn 10.7958810000 0.9314550000 -0.3478000000
H 13.1249740000 -0.3743710000 0.0789710000
H 13.4301560000 1.1414640000 0.2198570000
O 12.7218980000 0.4954140000 0.1488200000
```



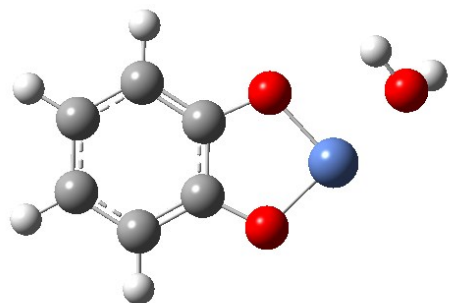
H₂O_Cu

C	7.4381840000	0.3622560000	-1.2664050000
C	8.8539060000	0.3718370000	-1.3196680000
C	9.5565010000	1.6770630000	-1.3511200000
C	8.7577840000	2.8599230000	-1.3182700000
C	7.3962590000	2.7891860000	-1.2666270000
C	6.7316050000	1.5334230000	-1.2415470000
H	6.9451350000	-0.6050100000	-1.2474150000
H	9.2811210000	3.8112880000	-1.3394730000
H	6.8052610000	3.7002330000	-1.2450850000
H	5.6465750000	1.5091990000	-1.2021720000
O	10.8157030000	1.7016100000	-1.4051150000
O	9.5285270000	-0.7134860000	-1.3407930000
Cu	11.4014950000	-0.4321650000	-1.4385300000
H	13.9414610000	-0.4440070000	-0.9159970000
H	13.3875720000	0.8946660000	-1.4802280000
O	13.3321090000	-0.0662410000	-1.5557760000



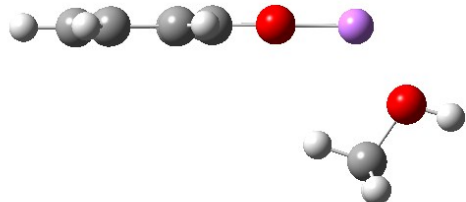
H₂O_Ni

C	7.3312800000	0.3799720000	-1.2270710000
C	8.5821050000	0.6806110000	-0.7152550000
C	8.9888890000	2.0099910000	-0.5880360000
C	8.1655590000	3.0503020000	-0.9741620000
C	6.9064830000	2.7461910000	-1.4906810000
C	6.4957510000	1.4258630000	-1.6147380000
H	7.0267060000	-0.6581520000	-1.3191890000
H	8.5062320000	4.0760690000	-0.8675920000
H	6.2451030000	3.5515020000	-1.7951520000
H	5.5135230000	1.2015120000	-2.0195250000
O	10.2363260000	2.1816300000	-0.0628070000
O	9.4868700000	-0.2396030000	-0.3109990000
Ni	10.9358100000	0.5772150000	0.2659830000
H	13.2615680000	1.5743680000	0.3771810000
H	12.1289520000	2.3917290000	1.0417660000
O	12.5080410000	1.5005780000	0.9726580000



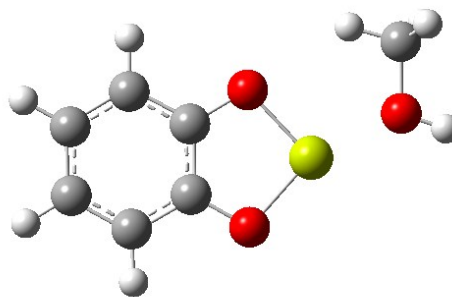
Methanol_Li

C	7.9348890000	0.3094660000	-2.0929930000
C	9.1414790000	0.6392760000	-2.7181110000
C	9.8780010000	1.7899500000	-2.3421770000
C	9.3571710000	2.5661530000	-1.2772450000
C	8.1502130000	2.2330650000	-0.6545770000
C	7.4365180000	1.0913900000	-1.0425160000
H	7.3934670000	-0.5788170000	-2.4129830000
H	9.5259460000	0.0306670000	-3.5343300000
H	9.9091430000	3.4539090000	-0.9745100000
H	7.7780380000	2.8567410000	0.1560350000
H	6.4982240000	0.8345820000	-0.5586280000
O	11.0108090000	2.1068980000	-2.9356200000
Li	12.4697000000	2.4811600000	-3.6545150000
C	14.0652210000	0.9740540000	-1.8797370000
H	13.0013470000	0.9236150000	-1.6524710000
H	14.6052470000	1.4036600000	-1.0334590000
H	14.4445400000	-0.0253140000	-2.1027830000
O	14.1880160000	1.8272070000	-3.0382940000
H	15.1155710000	1.8967410000	-3.2706520000



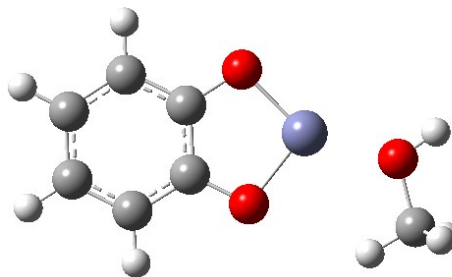
Methanol_Mg

```
C 6.9932800000 0.2691110000 -1.1111720000
C 8.2867160000 0.5626520000 -0.6565690000
C 8.8273130000 1.8735560000 -0.8934390000
C 8.0752220000 2.7956650000 -1.6346240000
C 6.7853370000 2.4812130000 -2.0836730000
C 6.2558260000 1.2068060000 -1.8467440000
H 6.6016040000 -0.7261150000 -0.9134210000
H 8.5075650000 3.7786520000 -1.8085890000
H 6.2185550000 3.2141770000 -2.6526310000
H 5.2564970000 0.9547050000 -2.1931010000
O 10.0737770000 2.1805430000 -0.4320720000
O 9.0128140000 -0.3610560000 0.0384690000
Mg 10.6043000000 0.5766290000 0.4245120000
C 13.0427910000 2.2229250000 0.9377530000
H 12.2892810000 2.7742590000 0.3757760000
H 13.9577880000 2.1243220000 0.3541250000
H 13.2382690000 2.7097640000 1.8930390000
O 12.4798280000 0.8978450000 1.1784880000
H 13.1070750000 0.3660500000 1.6739230000
```



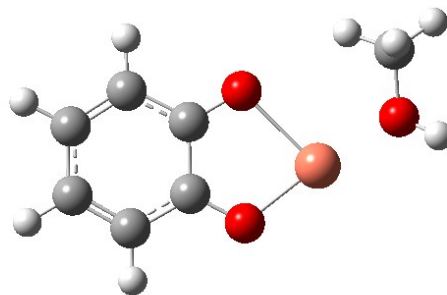
Methanol_Zn

```
C 8.0624240000 0.1213020000 -1.5539010000
C 9.3487060000 0.6768050000 -1.5587670000
C 9.5058700000 2.0746110000 -1.2953190000
C 8.3717840000 2.8714670000 -1.0971130000
C 7.0930450000 2.2995870000 -1.0980950000
C 6.9370200000 0.9304730000 -1.3519430000
H 7.9641170000 -0.9437330000 -1.7502210000
H 8.5173630000 3.9316990000 -0.9050500000
H 6.2218450000 2.9300040000 -0.9395780000
H 5.9459070000 0.4839540000 -1.3546380000
O 10.7603400000 2.6257700000 -1.2757210000
O 10.4552720000 -0.0926320000 -1.7743650000
Zn 11.8266670000 1.1636500000 -1.6228890000
C 13.7683690000 -1.0416690000 -2.2100420000
H 12.7558000000 -1.4414500000 -2.2061240000
H 14.3703770000 -1.5273860000 -1.4419370000
H 14.2188430000 -1.1625940000 -3.1953150000
O 13.6426710000 0.3723190000 -1.9044210000
H 14.5029890000 0.7992530000 -1.8915690000
```



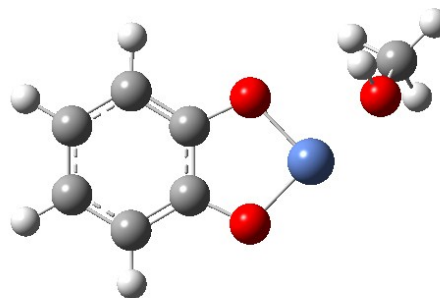
Methanol_Cu

```
C 0.0000000000 0.0000000000 0.0000000000
C 0.0000000000 0.0000000000 1.4173400000
C 1.2983010000 0.0000000000 2.1297420000
C 2.4885700000 0.0010750000 1.3417940000
C 2.4273430000 -0.0002560000 -0.0216640000
C 1.1772920000 -0.0008290000 -0.6966790000
H -0.9629620000 0.0000170000 -0.5017790000
H 3.4358540000 0.0011690000 1.8728860000
H 3.3429050000 -0.0011320000 -0.6061500000
H 1.1626160000 -0.0016860000 -1.7827250000
O 1.3056450000 -0.0005920000 3.3901570000
O -1.0831800000 0.0002710000 2.0915650000
Cu -0.8092380000 -0.0233340000 3.9790060000
C 0.4836700000 0.2598500000 6.5395960000
H 1.2589120000 -0.1138200000 5.8709930000
H 0.5613860000 -0.2244430000 7.5165690000
H 0.5952970000 1.3430810000 6.6407210000
O -0.7729350000 -0.0690670000 5.9292940000
H -1.5075850000 0.2692890000 6.4460030000
```



Methanol_Ni

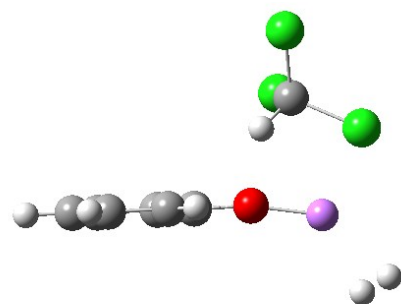
```
C 7.6024060000 0.1649070000 -1.0629370000
C 8.9848960000 0.1136730000 -1.1186260000
C 9.7201890000 1.2606180000 -1.4251210000
C 9.0919160000 2.4674750000 -1.6686030000
C 7.6995890000 2.5184480000 -1.6095040000
C 6.9646030000 1.3789940000 -1.3109780000
H 7.0432600000 -0.7354150000 -0.8263610000
H 9.6854040000 3.3472780000 -1.8998120000
H 7.1909100000 3.4588730000 -1.7987460000
H 5.8809190000 1.4310660000 -1.2680150000
O 11.0715770000 1.0858110000 -1.4646950000
O 9.7214640000 -0.9960790000 -0.8900740000
Ni 11.4331690000 -0.6095100000 -1.0590300000
C 13.8057230000 -0.0683740000 -2.5396940000
H 13.6629860000 -1.0130410000 -3.0635880000
H 14.8693420000 0.1790100000 -2.5218420000
H 13.2260640000 0.7189600000 -3.0274720000
O 13.3363190000 -0.2641420000 -1.1917870000
H 13.4436420000 0.5654420000 -0.7086680000
```



Hydrogen onto metal alkoxide/solvent complex

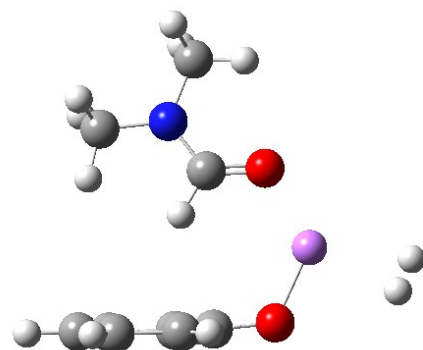
H₂_CHCl₃_Li

```
C 7.5590990000 0.1132340000 -1.7147980000
C 8.9041140000 0.0946280000 -1.3332540000
C 9.5697670000 1.2791020000 -0.9425430000
C 8.8125680000 2.4733630000 -0.9124710000
C 7.4668210000 2.4873420000 -1.2936450000
C 6.8236720000 1.3052830000 -1.6814820000
H 7.0764200000 -0.8146950000 -2.0142440000
H 9.4722360000 -0.8331400000 -1.3515200000
H 9.3130230000 3.3941880000 -0.6181350000
H 6.9133950000 3.4235620000 -1.2647780000
H 5.7783350000 1.3171190000 -1.9768730000
O 10.8450150000 1.2691960000 -0.5760090000
Li 12.5042420000 1.1477630000 -0.4313210000
C 11.2796400000 2.1439240000 2.3118710000
H 10.7410890000 1.9041880000 1.3945890000
Cl 10.7468540000 1.0909770000 3.6089790000
Cl 13.0148020000 1.8207190000 1.9258650000
Cl 11.0591710000 3.8408880000 2.7011880000
H 14.3032690000 0.7975210000 -1.5769600000
H 13.7669270000 0.7581940000 -2.0889390000
```



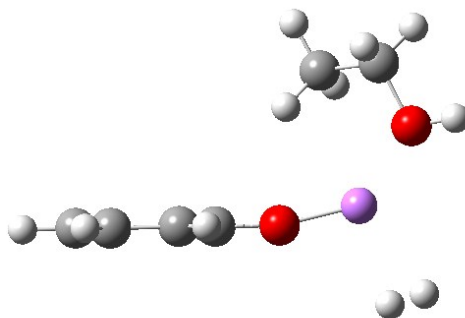
H₂_DMF_Li

```
C -0.0326960000 0.9079970000 2.1905610000
C 0.3910700000 -0.3370890000 2.6748290000
C 1.7354550000 -0.5617000000 3.0791880000
C 2.6292840000 0.5363080000 2.9322910000
C 2.2117600000 1.7657300000 2.4318960000
C 0.8665360000 1.9801740000 2.0943670000
H -1.0810710000 1.0481400000 1.9108000000
H -0.3054630000 -1.1705980000 2.7455670000
H 3.6599540000 0.3933600000 3.2118530000
H 2.9319930000 2.5773160000 2.3362800000
H 0.5380950000 2.9479050000 1.7105360000
O 2.1096490000 -1.7022740000 3.6208260000
Li 2.1134430000 -1.9039470000 5.3637650000
N 1.1493800000 1.6552490000 6.9649050000
C 0.7848940000 2.9287680000 6.3562870000
H 0.7044190000 2.8035220000 5.2730520000
H -0.1755410000 3.2762280000 6.7553720000
H 1.5551530000 3.6741040000 6.5745920000
C 1.3668580000 1.6258160000 8.4060970000
H 0.4719710000 2.0030110000 8.9146930000
H 1.5614560000 0.5965420000 8.7045470000
H 2.2256620000 2.2538720000 8.6709880000
C 1.3204760000 0.5583970000 6.2130140000
H 1.1242150000 0.7239730000 5.1415350000
O 1.6725590000 -0.5509850000 6.6627760000
H 2.5926560000 -3.9261150000 5.0609530000
H 2.5876630000 -3.9932590000 5.8008020000
```



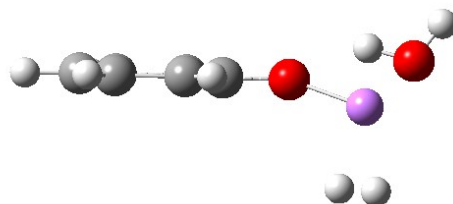
H₂Ethanol_Li

C	7.5603900000	-0.0078690000	-2.4948060000
C	8.8364310000	0.1209290000	-1.9382900000
C	9.1464310000	1.1661850000	-1.0321690000
C	8.0912650000	2.0484300000	-0.6871280000
C	6.8159350000	1.9160330000	-1.2460560000
C	6.5317130000	0.8754510000	-2.1399280000
H	7.3621780000	-0.8194350000	-3.1924960000
H	9.6335700000	-0.5658000000	-2.2162270000
H	8.3100620000	2.8625000000	0.0017590000
H	6.0334200000	2.6173680000	-0.9622540000
H	5.5411610000	0.7746530000	-2.5748380000
O	10.3504030000	1.2976970000	-0.5168370000
Li	11.6996530000	1.3580150000	0.4813570000
C	9.9293820000	0.5733780000	2.9071520000
H	9.1896880000	0.0039300000	3.4764440000
H	9.5971570000	0.6262160000	1.8665670000
H	9.9793080000	1.5844420000	3.3185870000
C	11.2755020000	-0.1097500000	3.0125600000
H	11.6233120000	-0.1307600000	4.0496120000
H	11.2274260000	-1.1341060000	2.6314440000
O	12.2367790000	0.6381620000	2.2207290000
H	13.1175410000	0.3939340000	2.5150650000
H	12.8356390000	2.4663110000	-0.9349360000
H	13.4047350000	2.4788220000	-0.4574780000



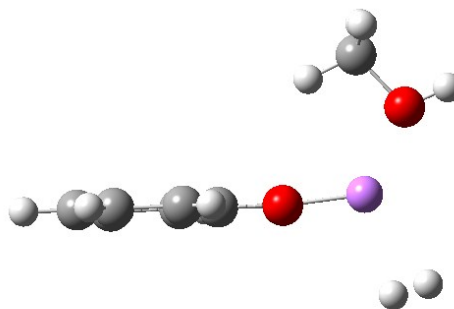
H₂H₂O_Li

C	7.4203860000	0.4787350000	-1.8213580000
C	8.7886310000	0.6118700000	-1.5632830000
C	9.2936390000	1.6874220000	-0.7940340000
C	8.3481340000	2.5886560000	-0.2500520000
C	6.9808730000	2.4529990000	-0.5082760000
C	6.5013740000	1.3859580000	-1.2794010000
H	7.0688730000	-0.3586630000	-2.4207770000
H	9.4964990000	-0.1061020000	-1.9747300000
H	8.7172400000	3.4189970000	0.3486150000
H	6.2833030000	3.1694490000	-0.0792370000
H	5.4385400000	1.2812460000	-1.4784490000
O	10.5903460000	1.8293890000	-0.5616830000
Li	12.2411850000	1.7494000000	-1.0491380000
H	13.2400440000	2.3390560000	1.5021020000
H	11.8524810000	2.4764720000	0.8137100000
O	12.8162270000	2.5144530000	0.6616300000
H	12.9126450000	1.5780720000	-3.1244950000
H	12.1703510000	1.5808110000	-3.1529330000



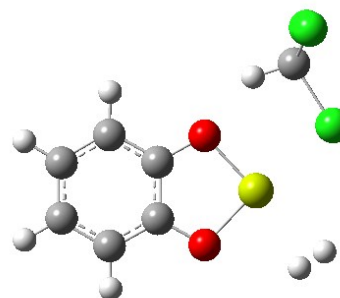
H₂_Methanol_Li

```
C 8.2347880000 0.5867860000 -1.9940230000
C 9.4278710000 1.0110900000 -2.5873640000
C 10.1496810000 2.1229410000 -2.0848760000
C 9.6285320000 2.7552730000 -0.9280890000
C 8.4351730000 2.3278340000 -0.3377170000
C 7.7363740000 1.2274800000 -0.8519130000
H 7.7047440000 -0.2666800000 -2.4127420000
H 9.8113860000 0.5125870000 -3.4756530000
H 10.1684560000 3.6109480000 -0.5270450000
H 8.0626660000 2.8429410000 0.5457820000
H 6.8085560000 0.8975070000 -0.3928320000
O 11.2665550000 2.5313900000 -2.6495040000
Li 12.7749320000 2.9278390000 -3.2652360000
C 14.1522480000 1.0642910000 -1.6436110000
H 13.0751310000 1.0611240000 -1.4833110000
H 14.6644750000 1.3290200000 -0.7161810000
H 14.4789530000 0.0809840000 -1.9885250000
O 14.4040650000 2.0607450000 -2.6577990000
H 15.3472050000 2.0928010000 -2.8270210000
H 12.1557830000 4.4117000000 -4.6507390000
H 12.8686320000 4.4976080000 -4.8407670000
```



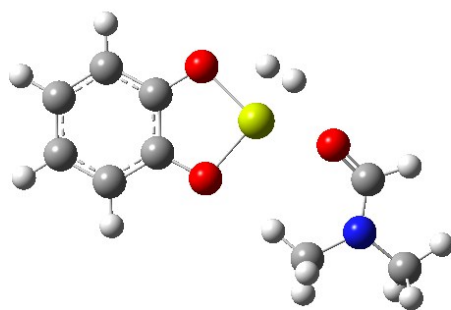
H₂_CHCl₃_Mg

```
C 7.0950300000 0.5038200000 -0.8043870000
C 8.3361830000 0.5928310000 -0.1589080000
C 9.0403470000 1.8414880000 -0.1818390000
C 8.5101660000 2.9199350000 -0.8999990000
C 7.2691190000 2.8095840000 -1.5418250000
C 6.5756000000 1.5932380000 -1.5162870000
H 6.5714250000 -0.4486970000 -0.7706080000
H 9.0667320000 3.8545120000 -0.9084780000
H 6.8692910000 3.6576600000 -2.0918000000
H 5.6134190000 1.5015690000 -2.0138730000
O 10.2394090000 1.9318630000 0.4696510000
O 8.8662590000 -0.4625350000 0.5187710000
Mg 10.4884220000 0.2010890000 1.2169130000
C 12.7770780000 2.6023530000 1.7138830000
H 11.8576260000 2.7311970000 1.1358330000
Cl 12.7799990000 3.6528470000 3.1070540000
Cl 12.7173200000 0.8482560000 2.2878660000
Cl 14.1782270000 2.8165310000 0.6963460000
H 10.9845230000 -1.8436610000 2.2009800000
H 10.3264410000 -1.9418060000 1.8586240000
```



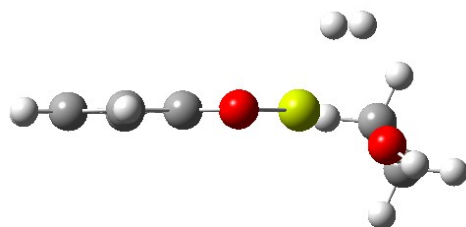
H₂_DMF_Mg

C	-0.0193520000	0.3107050000	0.2370840000
C	-0.0610270000	0.2504850000	1.6368860000
C	1.1391400000	-0.0656640000	2.3610470000
C	2.3001430000	-0.3828190000	1.6403570000
C	2.3218900000	-0.3207630000	0.2394070000
C	1.1540630000	-0.0033940000	-0.4645320000
H	-0.9377290000	0.5630030000	-0.2895310000
H	3.1960410000	-0.6295270000	2.2061060000
H	3.2359950000	-0.5645250000	-0.2969540000
H	1.1638620000	0.0464700000	-1.5508290000
O	1.1119760000	-0.0887330000	3.7172190000
O	-1.1973340000	0.5224950000	2.3342640000
Mg	-0.6929930000	0.3114950000	4.1686520000
N	-4.4529650000	0.1679420000	4.6788790000
C	-5.8491060000	-0.0445610000	5.0506970000
H	-5.9079850000	-0.4218320000	6.0725630000
H	-6.3923100000	0.9017110000	4.9840950000
H	-6.3031730000	-0.7690770000	4.3706980000
C	-4.2035140000	0.7478130000	3.3534670000
H	-4.3133310000	1.8351920000	3.4027800000
H	-3.2087660000	0.4951710000	2.9789630000
H	-4.9514210000	0.3430850000	2.6696210000
C	-3.4859190000	-0.0592010000	5.5573110000
H	-3.8301570000	-0.4667120000	6.5146310000
O	-2.2651680000	0.1507500000	5.3830540000
H	-0.0773350000	1.8661910000	5.9069670000
H	0.5550270000	1.7334360000	5.5346440000



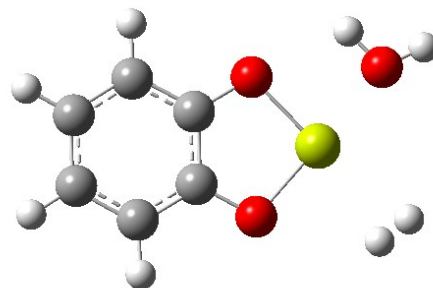
H₂_Ethanol_Mg

C	8.0181840000	0.5235660000	-0.7763180000
C	9.1317470000	1.2975360000	-0.4227200000
C	9.0000830000	2.7273630000	-0.3736560000
C	7.7811890000	3.3109260000	-0.7471800000
C	6.6802670000	2.5196560000	-1.1032180000
C	6.8074000000	1.1259130000	-1.1457890000
H	8.1389520000	-0.5574120000	-0.8005070000
H	7.7062970000	4.3955000000	-0.7089470000
H	5.7438000000	2.9941910000	-1.3863610000
H	5.9582930000	0.5055450000	-1.4223330000
O	10.0704450000	3.4874220000	-0.0107200000
O	10.3184740000	0.7220390000	-0.0783550000
Mg	11.4069170000	2.2051180000	0.3945320000
C	13.1405980000	-0.5922290000	0.9710470000
H	13.3142560000	-1.6037560000	1.3485490000
H	13.8971720000	-0.3759240000	0.2128300000
H	12.1423110000	-0.5642090000	0.5225340000
C	13.2487900000	0.3783300000	2.1240310000
H	12.5084630000	0.1681900000	2.8987900000
H	14.2493450000	0.3739880000	2.5618780000
O	13.0025550000	1.7374490000	1.6219420000
H	13.4395630000	2.3658800000	2.2039890000
H	13.0955020000	3.7865590000	-0.4200230000
H	12.4295650000	4.0875750000	-0.5735220000



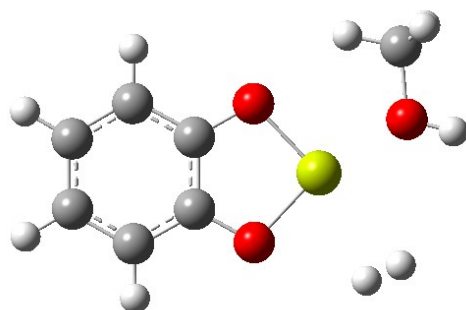
H₂_H₂O_Mg

```
C 6.8787860000 0.5805300000 -0.5680520000
C 8.2355980000 0.7855680000 -0.2826090000
C 8.8891540000 1.9536100000 -0.8046770000
C 8.1723740000 2.8206010000 -1.6402140000
C 6.8165510000 2.5958810000 -1.9172290000
C 6.1776120000 1.4605380000 -1.4040950000
H 6.4016630000 -0.3063250000 -0.1570740000
H 8.6884740000 3.6954610000 -2.0297090000
H 6.2774840000 3.2828020000 -2.5650510000
H 5.1267870000 1.2798180000 -1.6167200000
O 10.2003930000 2.1621960000 -0.5040030000
O 8.9334990000 -0.0751670000 0.5114960000
Mg 10.6641870000 0.6787730000 0.5986030000
H 13.5093780000 1.5144850000 0.7548670000
H 12.3528120000 2.2417310000 -0.0139580000
O 12.5709090000 1.4920970000 0.5642700000
H 11.4459080000 -0.9479860000 2.0495620000
H 10.7282090000 -1.1229960000 1.9345100000
```



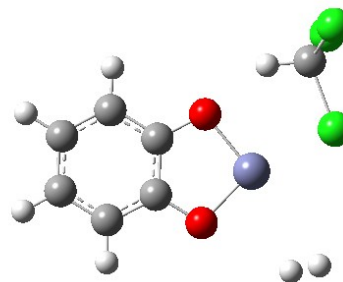
H₂_Methanol_Mg

```
C 6.8220720000 0.6279890000 -0.3777910000
C 8.1513060000 0.8622230000 0.0006210000
C 8.9040390000 1.8767840000 -0.6831340000
C 8.3119760000 2.5546730000 -1.7580140000
C 6.9821220000 2.3039440000 -2.1241550000
C 6.2464660000 1.3196660000 -1.4526670000
H 6.2687960000 -0.1393230000 0.1592050000
H 8.9018040000 3.3136310000 -2.2675980000
H 6.5411610000 2.8448220000 -2.9580070000
H 5.2151150000 1.1193070000 -1.7326920000
O 10.1863900000 2.1249740000 -0.2995470000
O 8.7305590000 0.1807500000 1.0277280000
Mg 10.4748720000 0.9122120000 1.1373370000
C 13.0909770000 2.3838920000 0.9116140000
H 12.3691980000 2.7313300000 0.1732400000
H 13.9678350000 1.9598920000 0.4221990000
H 13.3733780000 3.1941000000 1.5839280000
O 12.4144080000 1.3397170000 1.6747140000
H 13.0113260000 0.9976420000 2.3441080000
H 10.7767710000 -0.6822580000 2.9884080000
H 10.0818670000 -0.7710060000 2.7295750000
```



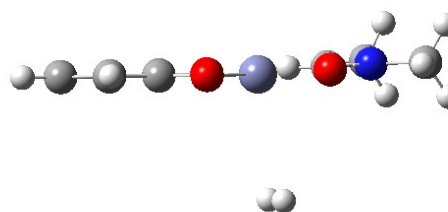
H₂_CHCl₃_Zn

```
C 8.2368530000 0.0010310000 -1.9884470000
C 8.9676710000 -0.0881790000 -0.7980210000
C 8.9853470000 1.0234450000 0.0995940000
C 8.3182340000 2.2029650000 -0.2503330000
C 7.5926730000 2.2781250000 -1.4456130000
C 7.5722950000 1.1868080000 -2.3243530000
H 8.2323600000 -0.8585430000 -2.6538790000
H 8.3495370000 3.0383330000 0.4449170000
H 7.0762240000 3.1987110000 -1.7041280000
H 7.0113830000 1.2431500000 -3.2534530000
O 9.6869040000 0.9198610000 1.2712360000
O 9.6363350000 -1.2400390000 -0.4706450000
Zn 10.3664420000 -0.8201970000 1.1606440000
C 11.2108020000 0.6751360000 3.8359140000
H 10.5817040000 1.1245990000 3.0660410000
Cl 10.3337120000 0.5478670000 5.3376760000
Cl 11.5792920000 -1.0231340000 3.2105570000
Cl 12.7053600000 1.5603180000 3.9886060000
H 10.9364750000 -3.3507010000 0.2661340000
H 11.3543850000 -3.5891580000 0.8315750000
```



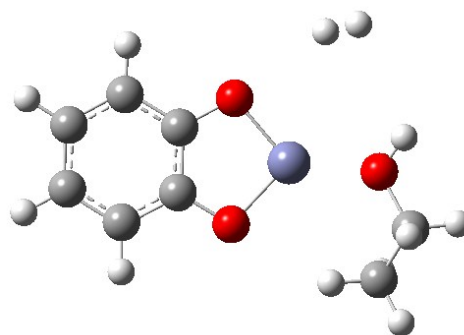
H₂_DMF_Zn

```
C 0.0148850000 0.4435050000 -0.0000280000
C -0.0095470000 0.3795250000 1.3987200000
C 1.1751400000 0.0002350000 2.1084480000
C 2.3165230000 -0.3644550000 1.3811590000
C 2.3256870000 -0.2979690000 -0.0186830000
C 1.1670160000 0.0791730000 -0.7099110000
H -0.8954340000 0.7417820000 -0.5148580000
H 3.2053490000 -0.6570720000 1.9360340000
H 3.2218590000 -0.5807470000 -0.5655520000
H 1.1689590000 0.1305430000 -1.7958340000
O 1.1465650000 -0.0341240000 3.4673400000
O -1.1380860000 0.7125820000 2.0945960000
Zn -0.6331360000 0.4922590000 3.8525230000
N 0.4359330000 0.2438380000 7.7135680000
C 1.7126990000 -0.1130790000 8.3227700000
H 2.4399880000 -0.3345410000 7.5409950000
H 2.0759200000 0.7200330000 8.9301380000
H 1.5834840000 -0.9936230000 8.9572700000
C -0.6675610000 0.5769880000 8.6082570000
H -0.3866180000 1.4348650000 9.2247130000
H -1.5450420000 0.8196440000 8.0119560000
H -0.8805400000 -0.2789210000 9.2537690000
C 0.2958970000 0.2639070000 6.3950380000
H 1.1849240000 -0.0000420000 5.8099860000
O -0.7872040000 0.5668720000 5.8216380000
H -1.1358450000 -2.6155920000 4.2739000000
H -1.8502960000 -2.4232110000 4.2765920000
```



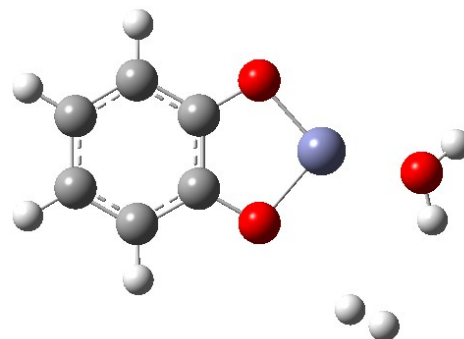
H₂_ Ethanol_Zn

C	7.5556630000	0.8800590000	0.1868550000
C	8.8235100000	1.4687760000	0.2750260000
C	9.0154250000	2.7962260000	-0.2225890000
C	7.9500910000	3.4589310000	-0.8448380000
C	6.6886130000	2.8552660000	-0.9269010000
C	6.4985770000	1.5569730000	-0.4351700000
H	7.4297050000	-0.1272850000	0.5767920000
H	8.1211660000	4.4642890000	-1.2221690000
H	5.8699970000	3.3833070000	-1.4092660000
H	5.5212210000	1.0854070000	-0.4989550000
O	10.2463180000	3.3814840000	-0.1154090000
O	9.8714590000	0.8151410000	0.8579480000
Zn	11.2429710000	2.0634130000	0.7246360000
C	12.9368640000	-0.4446250000	1.9188450000
H	13.2409120000	-1.2300880000	2.6159520000
H	13.2881690000	-0.7132400000	0.9203260000
H	11.8433150000	-0.3984180000	1.9142940000
C	13.5439370000	0.8653910000	2.3636410000
H	13.2207770000	1.1415760000	3.3702060000
H	14.6349600000	0.8379180000	2.3221010000
O	13.1024230000	1.9094700000	1.4390780000
H	13.6441080000	2.6994770000	1.5360200000
H	12.2776890000	4.8053410000	0.0976340000
H	12.9867940000	4.9597050000	0.2554910000



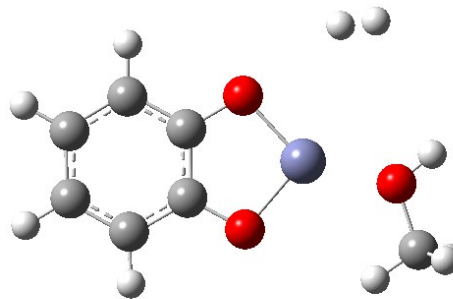
H₂_ H₂O_Zn

C	7.4884770000	0.6374920000	-1.7520130000
C	8.6432570000	1.0183720000	-1.0569350000
C	8.6591490000	2.2654190000	-0.3563730000
C	7.5440170000	3.1094130000	-0.4259370000
C	6.3983480000	2.7149420000	-1.1284880000
C	6.3800430000	1.4916490000	-1.8116320000
H	7.4946030000	-0.3174040000	-2.2720460000
H	7.5819940000	4.0544990000	0.1101730000
H	5.5388570000	3.3789200000	-1.1714260000
H	5.4925090000	1.1834810000	-2.3582740000
O	9.7758940000	2.6363010000	0.3457480000
O	9.7412510000	0.2053160000	-1.0062380000
Zn	10.8929230000	1.1959230000	0.0672620000
H	13.0128470000	-0.3088800000	-0.0631490000
H	13.5519480000	0.9534590000	0.6718860000
O	12.7539550000	0.4734400000	0.4354440000
H	11.4480150000	-1.5572940000	-1.3693040000
H	12.0714640000	-1.9604480000	-1.3270870000



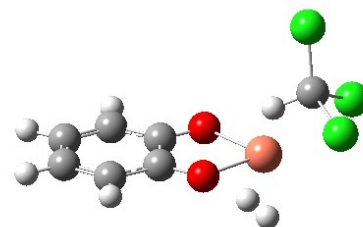
H₂_Methanol_Zn

C	8.0858340000	0.2689170000	-1.7926070000
C	9.3832580000	0.7218770000	-1.5205910000
C	9.5608680000	2.0053180000	-0.9136120000
C	8.4432410000	2.8087860000	-0.6577130000
C	7.1530880000	2.3409340000	-0.9384910000
C	6.9766000000	1.0827730000	-1.5293590000
H	7.9710930000	-0.7117200000	-2.2484040000
H	8.6048040000	3.7825710000	-0.2016610000
H	6.2942010000	2.9742040000	-0.7316570000
H	5.9768680000	0.7172170000	-1.7498140000
O	10.8250900000	2.4455140000	-0.6242170000
O	10.4761820000	-0.0504860000	-1.7897780000
Zn	11.8695190000	1.0325120000	-1.1927460000
C	13.9826850000	-0.9862370000	-1.9671090000
H	13.0095880000	-1.4009250000	-2.2234120000
H	14.4815680000	-1.6217950000	-1.2352560000
H	14.5907400000	-0.8713120000	-2.8646130000
O	13.7252820000	0.3163780000	-1.3841250000
H	14.5445810000	0.7495400000	-1.1308020000
H	13.7757400000	3.4118590000	0.0260270000
H	13.0351540000	3.4439230000	-0.0130600000



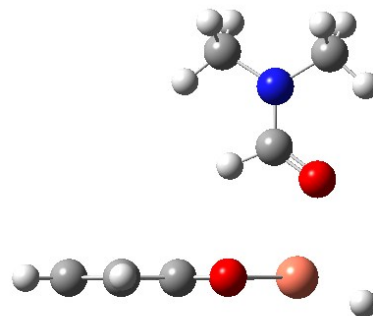
H₂_CHCl₃_Cu

C	6.8077860000	0.3698410000	-1.9458300000
C	7.8685250000	0.1059190000	-1.0409730000
C	8.4177980000	1.2264610000	-0.2460660000
C	7.8563780000	2.5193960000	-0.4310360000
C	6.8346440000	2.7139460000	-1.3159220000
C	6.3074180000	1.6344320000	-2.0765800000
H	6.4173890000	-0.4654360000	-2.5187650000
H	8.2680970000	3.3342990000	0.1565320000
H	6.4128480000	3.7061440000	-1.4466610000
H	5.4944580000	1.8255420000	-2.7706440000
O	9.3639610000	0.9904490000	0.5634920000
O	8.3584330000	-1.0608660000	-0.8948600000
Cu	9.7665530000	-1.1131980000	0.4198580000
C	11.3297130000	0.1349050000	2.6902900000
H	10.9465600000	0.8145900000	1.9277150000
Cl	10.2007700000	0.0789600000	4.0279110000
Cl	11.4004760000	-1.5222660000	1.8648620000
Cl	12.9480770000	0.5928500000	3.1829530000
H	11.6462540000	0.9668540000	-0.3892640000
H	12.3810110000	0.8551310000	-0.4989190000



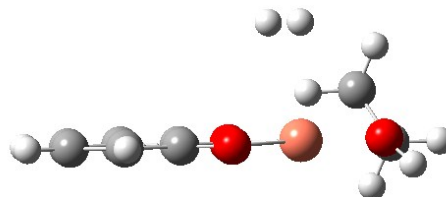
H₂_DMF_Cu

```
C -0.2318150000 1.0303660000 0.3867270000
C -0.0185250000 1.1097710000 1.7900300000
C 0.7358740000 0.0237370000 2.4504620000
C 1.2221460000 -1.0469830000 1.6489090000
C 0.9921970000 -1.0651230000 0.3015580000
C 0.2620650000 -0.0238150000 -0.3316740000
H -0.7853160000 1.8372980000 -0.0845590000
H 1.7789110000 -1.8350270000 2.1471970000
H 1.3714350000 -1.8850900000 -0.3015530000
H 0.1004420000 -0.0707540000 -1.4048490000
O 0.9088590000 0.0855490000 3.7030360000
O -0.4604480000 2.0575090000 2.5077860000
Cu 0.0541370000 1.7675440000 4.4613490000
N -3.6892260000 -0.3000760000 4.5111990000
C -4.3840260000 -0.9910240000 3.4506880000
H -3.8433990000 -0.8663520000 2.5099690000
H -4.4593670000 -2.0620330000 3.6720150000
H -5.3974870000 -0.5913470000 3.3287810000
C -4.2712740000 -0.3599050000 5.8339180000
H -4.3347550000 -1.3994510000 6.1750360000
H -3.6453840000 0.2086770000 6.5213110000
H -5.2810390000 0.0656470000 5.8231230000
C -2.5419600000 0.3622400000 4.2874290000
H -2.2181470000 0.3238180000 3.2314860000
O -1.9022160000 0.9609890000 5.1401090000
H 0.6038070000 2.4029230000 5.8614050000
H 0.1985460000 3.0197470000 5.5019200000
```



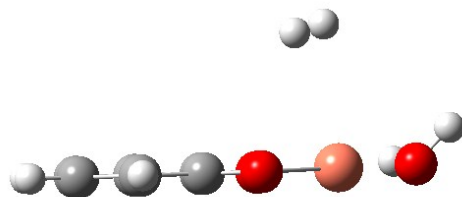
H₂_Ethanol_Cu

```
C 8.3895090000 0.9362940000 0.0630160000
C 9.6677890000 0.4439830000 -0.3056590000
C 10.2215010000 0.8209740000 -1.6252640000
C 9.4348060000 1.6665620000 -2.4618110000
C 8.2100940000 2.1113130000 -2.0533460000
C 7.6840560000 1.7447250000 -0.7854070000
H 8.0006700000 0.6466590000 1.0346390000
H 9.8495120000 1.9367160000 -3.4285070000
H 7.6227490000 2.7548220000 -2.7021030000
H 6.7063100000 2.1155500000 -0.4916750000
O 11.3576120000 0.3831380000 -1.9557090000
O 10.3510970000 -0.3099370000 0.4600050000
Cu 12.0782810000 -0.7849110000 -0.2631440000
C 14.6455290000 0.0269230000 -2.0826930000
H 15.1396090000 0.1693940000 -3.0479100000
H 15.2619200000 0.4932680000 -1.3081530000
H 13.6720660000 0.5267100000 -2.1236340000
C 14.4758250000 -1.4400650000 -1.8137970000
H 13.8384380000 -1.9112800000 -2.5719280000
H 15.4403970000 -1.9603000000 -1.7878840000
O 13.8541870000 -1.5963350000 -0.5157970000
H 13.9273000000 -2.5069330000 -0.2183790000
H 13.3480400000 1.3429080000 0.5124960000
H 12.6761100000 1.6668000000 0.5971690000
```



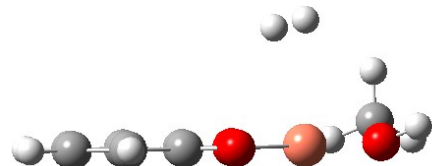
H₂_H₂O_Cu

```
C 7.4551150000 0.3203250000 -1.0618890000
C 8.8719220000 0.3176460000 -1.0932830000
C 9.5852130000 1.6168380000 -1.1402370000
C 8.7950750000 2.8060760000 -1.1414110000
C 7.4324140000 2.7468510000 -1.1083890000
C 6.7574530000 1.4970020000 -1.0694060000
H 6.9543410000 -0.6427580000 -1.0325940000
H 9.3262690000 3.7527630000 -1.1743460000
H 6.8484960000 3.6627110000 -1.1128490000
H 5.6717940000 1.4819780000 -1.0455400000
O 10.8451400000 1.6315670000 -1.1770940000
O 9.5378180000 -0.7729340000 -1.0824630000
Cu 11.4223160000 -0.5023480000 -1.1013800000
H 13.9387900000 -0.5135410000 -0.4457050000
H 13.4297270000 0.8083430000 -1.0872040000
O 13.3673830000 -0.1539890000 -1.1294040000
H 11.5552380000 0.0759160000 1.6626560000
H 10.8276850000 -0.0470020000 1.5292570000
```



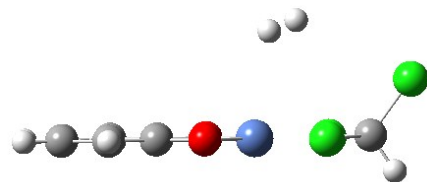
H₂_Methanol_Cu

```
C 0.0472410000 -0.0228320000 0.0785550000
C 1.4635240000 -0.0204660000 0.0224010000
C 2.1718800000 1.2795900000 -0.0135480000
C 1.3822550000 2.4680590000 0.0190600000
C 0.0200700000 2.4047530000 0.0744080000
C -0.6519070000 1.1529850000 0.1032770000
H -0.4518430000 -0.9870270000 0.0997010000
H 1.9111100000 3.4163350000 -0.0059690000
H -0.5657720000 3.3191880000 0.0962020000
H -1.7370280000 1.1359170000 0.1453770000
O 3.4309510000 1.2909020000 -0.0695850000
O 2.1392050000 -1.1027560000 0.0011480000
Cu 4.0306300000 -0.8282260000 -0.0504560000
C 6.5796970000 0.4628180000 0.3088420000
H 5.9194110000 1.2514140000 -0.0519560000
H 7.5719130000 0.5665970000 -0.1382000000
H 6.6457680000 0.5273710000 1.3991770000
O 5.9873310000 -0.7795750000 -0.0954540000
H 6.5024320000 -1.5260950000 0.2190330000
H 4.5212440000 -0.2798590000 2.6547020000
H 3.7926260000 -0.1621470000 2.5193460000
```



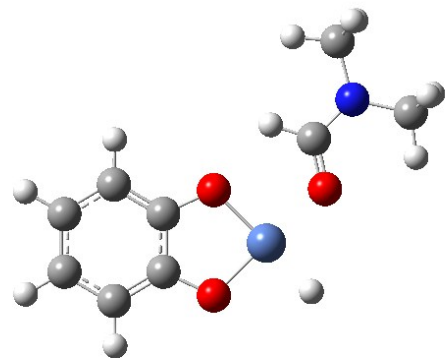
H₂_CHCl₃_Ni

C	7.6542490000	0.1136500000	-0.9311850000
C	8.9892730000	0.4699100000	-1.0042240000
C	9.3620750000	1.7914540000	-1.2530740000
C	8.4048240000	2.7731900000	-1.4372220000
C	7.0587280000	2.4158390000	-1.3666550000
C	6.6878620000	1.1017650000	-1.1153360000
H	7.3841820000	-0.9197180000	-0.7343320000
H	8.7142620000	3.7956350000	-1.6328910000
H	6.2963180000	3.1757010000	-1.5097970000
H	5.6362310000	0.8364440000	-1.0625990000
O	10.6991140000	2.0100530000	-1.2934380000
O	10.0207360000	-0.3950220000	-0.8483110000
Ni	11.5570840000	0.4792610000	-1.0206820000
C	14.3701590000	-0.2851070000	-0.8441420000
H	14.9432480000	-0.6134520000	-1.7084040000
Cl	13.7211600000	1.3573740000	-1.2079550000
Cl	12.9415360000	-1.3741390000	-0.6852840000
Cl	15.3694170000	-0.3008510000	0.5808850000
H	12.6236860000	0.7745940000	1.9282140000
H	12.0079720000	1.0552910000	1.6019360000



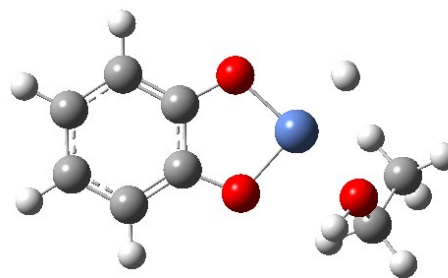
H₂_DMF_Ni

C	-0.0335970000	0.3745410000	0.1440610000
C	-0.0369670000	0.3260100000	1.5287250000
C	1.1427060000	0.0634000000	2.2305630000
C	2.3328590000	-0.1517010000	1.5570060000
C	2.3362850000	-0.1023340000	0.1633110000
C	1.1645670000	0.1582200000	-0.5348610000
H	-0.9600340000	0.5795370000	-0.3845820000
H	3.2402880000	-0.3540890000	2.1194960000
H	3.2639010000	-0.2693120000	-0.3762460000
H	1.1778660000	0.1941930000	-1.6201680000
O	1.0081100000	0.0426430000	3.5753190000
O	-1.1300710000	0.5205220000	2.2918850000
Ni	-0.7052460000	0.3698570000	4.0259560000
N	1.1741230000	-0.1093390000	7.5723340000
C	2.5389660000	-0.3822860000	7.9722740000
H	3.1723700000	-0.4826730000	7.0895900000
H	2.9223820000	0.4347420000	8.5926330000
H	2.5864850000	-1.3110010000	8.5506510000
C	0.1998110000	0.0617670000	8.6326210000
H	0.4786500000	0.9129450000	9.2625500000
H	-0.7813930000	0.2395150000	8.1953680000
H	0.1655360000	-0.8382150000	9.2551020000
C	0.8402900000	-0.0118280000	6.2910060000
H	1.6452960000	-0.1535600000	5.5570730000
O	-0.3165390000	0.2272890000	5.9081240000
H	-2.1590220000	1.0508640000	4.4059150000
H	-2.3164160000	0.2581080000	4.3430070000



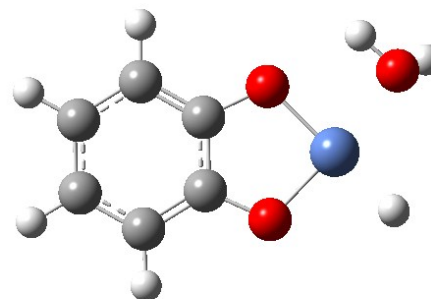
H₂_Ethanol_Ni

```
C 7.9264850000 0.0460780000 -1.1871640000
C 9.2642900000 -0.0460670000 -1.5355130000
C 10.1258080000 1.0326080000 -1.3269760000
C 9.6645410000 2.2121130000 -0.7688750000
C 8.3187500000 2.3049090000 -0.4184650000
C 7.4601260000 1.2329100000 -0.6259820000
H 7.2702110000 -0.8023790000 -1.3561490000
H 10.3518120000 3.0390810000 -0.6152780000
H 7.9420250000 3.2243730000 0.0192770000
H 6.4137130000 1.3166100000 -0.3481860000
O 11.4077280000 0.8141150000 -1.7076290000
O 9.8297150000 -1.1433130000 -2.0840420000
Ni 11.5627440000 -0.8375570000 -2.3854850000
C 14.4407260000 -1.9273530000 -1.2212140000
H 15.1841020000 -2.0542040000 -0.4301350000
H 14.7559150000 -2.5196770000 -2.0854370000
H 13.4891090000 -2.3210360000 -0.8485850000
C 14.3206360000 -0.4755310000 -1.5821940000
H 13.9105400000 0.1188360000 -0.7577300000
H 15.2879130000 -0.0569380000 -1.8804070000
O 13.4299030000 -0.3488880000 -2.7183040000
H 13.2822380000 0.5978150000 -2.8663550000
H 11.7444530000 -2.4521570000 -2.6601860000
H 11.6025600000 -2.1347660000 -3.3944080000
```



H₂_H₂O_Ni

```
C 7.6048410000 0.3617610000 -1.1300750000
C 8.9178400000 0.6168570000 -0.7701010000
C 9.3024860000 1.8924120000 -0.3553220000
C 8.3867920000 2.9272100000 -0.2941670000
C 7.0654120000 2.6708550000 -0.6559470000
C 6.6801140000 1.4022270000 -1.0693110000
H 7.3217680000 -0.6362910000 -1.4505270000
H 8.7075680000 3.9122250000 0.0320490000
H 6.3340570000 3.4720850000 -0.6123830000
H 5.6478840000 1.2151880000 -1.3495170000
O 10.6150840000 2.0053970000 -0.0350370000
O 9.9013710000 -0.3109780000 -0.7877460000
Ni 11.4324440000 0.4263260000 -0.2489450000
H 13.7008440000 1.5981040000 -0.1912150000
H 12.5275650000 2.2322020000 0.6111370000
O 12.9981660000 1.3973970000 0.4352020000
H 12.2171110000 -0.8972380000 -0.8195700000
H 12.0710780000 -1.0691580000 -0.0366040000
```



H₂_Methanol_Ni

C	7.5223720000	0.2832710000	-1.8601810000
C	8.7059930000	0.4180610000	-1.1543900000
C	8.8885530000	1.4995350000	-0.2886030000
C	7.8848180000	2.4268950000	-0.0802460000
C	6.6896760000	2.2837220000	-0.7844670000
C	6.5141550000	1.2258700000	-1.6665690000
H	7.3962510000	-0.5554410000	-2.5381460000
H	8.0458340000	3.2493920000	0.6108760000
H	5.8941500000	3.0082900000	-0.6400360000
H	5.5784810000	1.1247100000	-2.2082860000
O	10.1108630000	1.5559540000	0.3101450000
O	9.7430640000	-0.4440080000	-1.2206830000
Ni	11.0151390000	0.0801880000	-0.1145240000
C	13.1003940000	1.7611670000	0.8480160000
H	13.6175370000	1.6265390000	-0.1014220000
H	13.8298660000	1.9678910000	1.6338410000
H	12.3658930000	2.5651590000	0.7610820000
O	12.4290990000	0.5168760000	1.1343550000
H	11.9923510000	0.5948570000	1.9923400000
H	9.5878740000	0.8173040000	2.5138980000
H	9.4915610000	0.6830830000	3.2480320000

