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

Supporting Information

for

The preference for dual-gold(I) catalysis in the hydro(alkoxylation vs phenoxylation) of alkynes

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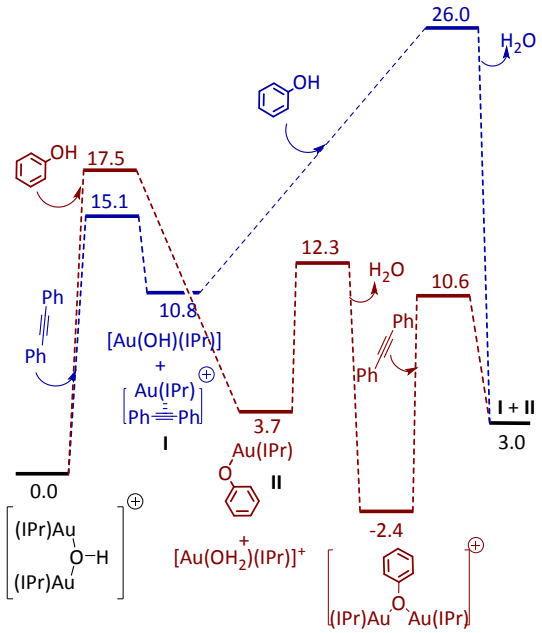


Figure S1. Computed stationary points for the pre-catalytic activation of $[\{Au(IPr)\}_2(\mu\text{-}OH)]^+$ to complexes **I** and **II**. Gibbs free energies in chloroform solution are given in kcal/mol (recalculated from ref. 56 at P = 1 atm).

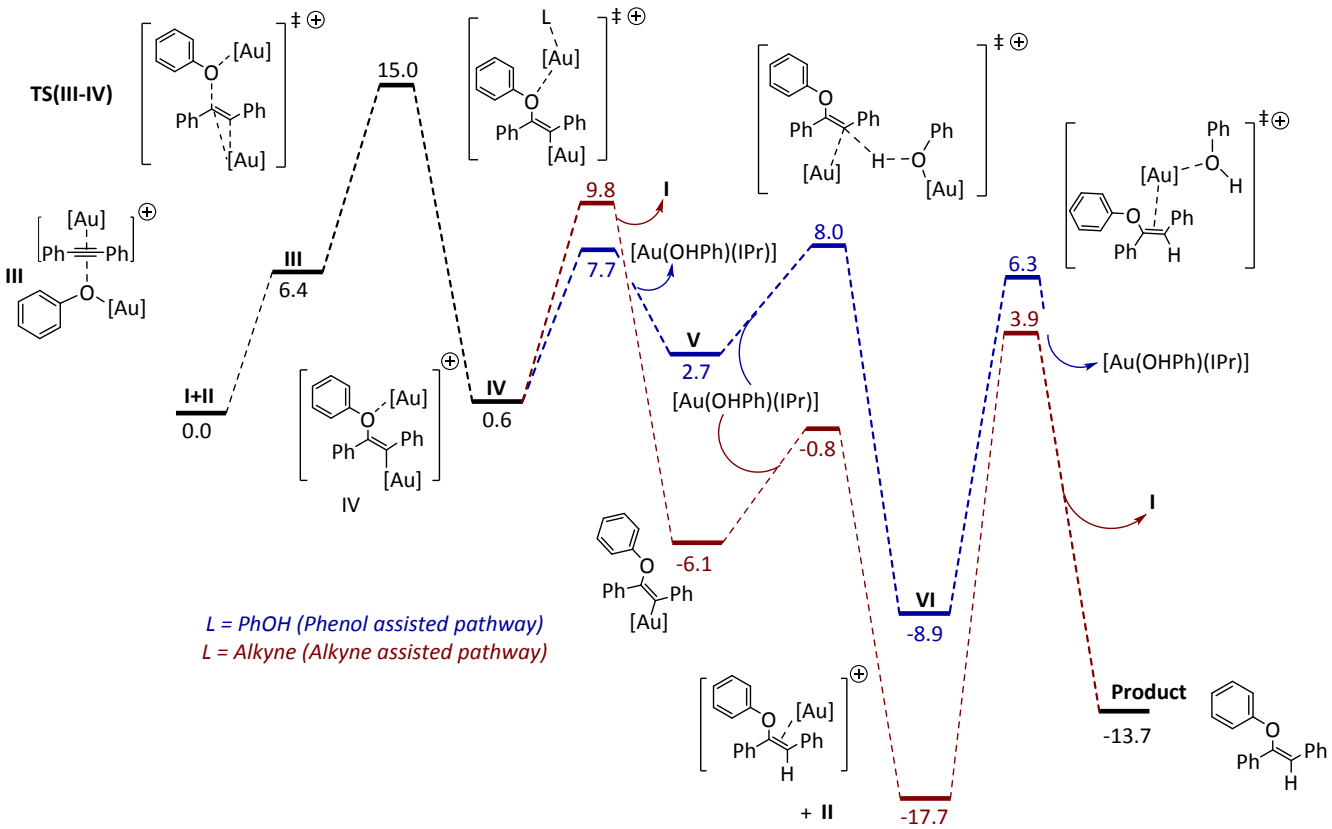


Figure S2. Computed stationary points for the dual-gold catalysed hydrophenoxylation using diphenylacetylene as a substrate and phenol as a nucleophile (Gibbs energies in chloroform solution are given in kcal/mol relative to complex **I** and the neutral [Au(OPh)(IPr)] complex **II**. [Au] = [Au(IPr)].

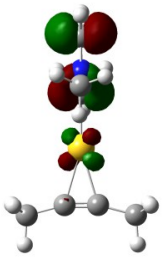
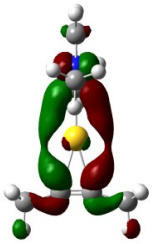
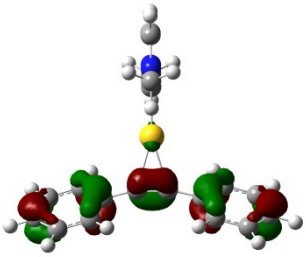
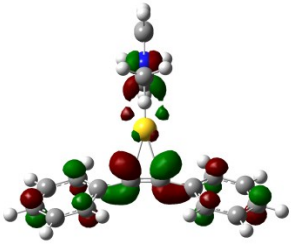
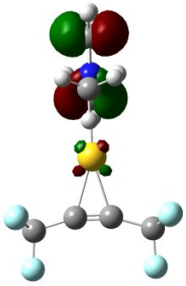
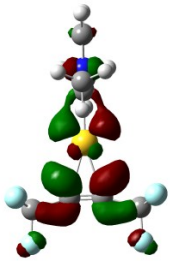
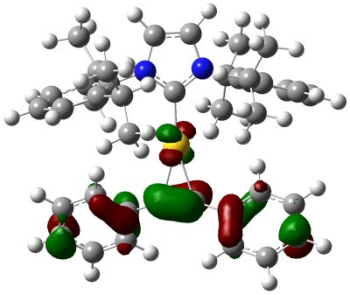
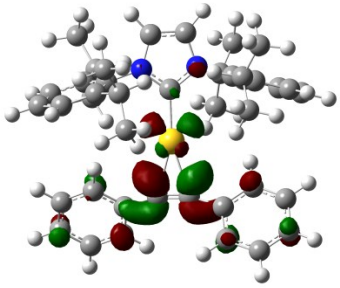
	HOMO	LUMO
CH_3CCCH_3		
PhCCPh		
CF_3CCCF_3		
PhCCPh (real catalyst)		

Figure S3. Frontier molecular orbitals for the cationic π-gold-alkyne complexes **I**.

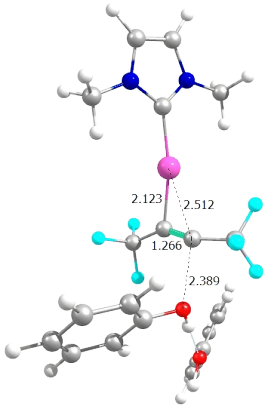
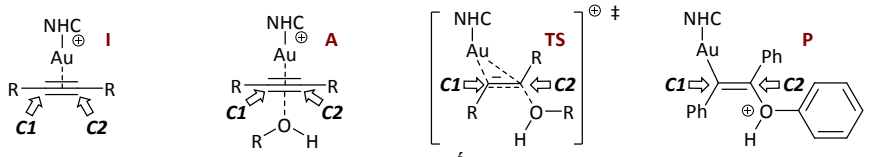


Figure S4. Molecular structures of the computed transition states corresponding to the monoaurated mechanism for the *in silico* NHC = IMe system, involving two molecules of phenol and 1,1,1,3,3,3-hexafluorobut-2-yne. Key distances are indicated in Å.



Distance 1 (d1): ***C1*** ... ***C2***
Distance 2 (d2): ***Au*** ... ***C1***
Distance 3 (d3): ***Au*** ... ***C2***
Distance 4 (d4): ***C1*** ... ***O***

Figure S5. Illustration of key distances (in Å) in the structures considered here.

Table S1. Benchmark for the alcohol nucleophilic attack to π-gold-dimethyl-alkyne species **I** (Enthaylpy (H) and Gibbs (G) energies in chloroform are given in kcal/mol, **A** = adduct; **TS** = transition state; **P** = product).

P 1 atm	E	Alcohol	**I**	**A**	**TS**	**P**
B2PLYP/def2-TZVP// BP86/def2-TZVP	H	2 MeOH	0.0	-5.0	5.1	1.1
B2PLYP/def2-TZVP// BP86/def2-TZVP	G	2 MeOH	0.0	10.4	29.4	27.6
B2PLYP-d3/def2-TZVP// BP86/def2-TZVP	H	2 MeOH	0.0	-7.4	4.1	-0.5
B2PLYP-d3/def2-TZVP// BP86/def2-TZVP	G	2 MeOH	0.0	8.0	24.9	22.4
M06/TZVP// BP86/def2-TZVP	H	2 MeOH	0.0	-4.8	4.2	0.6
M06/TZVP// BP86/def2-TZVP	G	2 MeOH	0.0	10.6	25.0	23.5
B2PLYP/def2-TZVP// BP86/SVP	H	1 MeOH	0.0	-0.7	17.8	18.2
B2PLYP/def2-TZVP// BP86/SVP	G	1 MeOH	0.0	7.7	30.3	30.7
B2PLYP/def2-TZVP// BP86/SVP	H	2 MeOH	0.0	-4.8	7.1	3.9
B2PLYP/def2-TZVP// BP86/SVP	G	2 MeOH	0.0	11.9	27.6	27.0
B2PLYP-d3/def2-TZVP// BP86/SVP	H	1 MeOH	0.0	-2.1	14.9	15.5
B2PLYP-d3/def2-TZVP// BP86/SVP	G	1 MeOH	0.0	6.3	27.4	27.9
B2PLYP-d3/def2-TZVP// BP86/SVP	H	2 MeOH	0.0	-7.5	2.8	-1.3
B2PLYP-d3/def2-TZVP// BP86/SVP	G	2 MeOH	0.0	9.2	23.3	21.8
M06/TZVP//BP86/SVP	H	1 MeOH	0.0	-0.3	14.4	15.3
M06/TZVP//BP86/SVP	G	1 MeOH	0.0	8.0	26.9	27.7
M06/TZVP//BP86/SVP	H	2 MeOH	0.0	-4.7	2.4	0.0
M06/TZVP//BP86/SVP	G	2 MeOH	0.0	12.0	22.9	23.1
P = 1354 atm	E	Alcohol	**I**	**A**	**TS**	**P**
B2PLYP/def2-TZVP// BP86/def2-TZVP	H	2 MeOH	0.0	-5.0	5.1	1.1
B2PLYP/def2-TZVP// BP86/def2-TZVP	G	2 MeOH	0.0	1.8	20.9	19.0
B2PLYP-d3/def2-TZVP// BP86/def2-TZVP	H	2 MeOH	0.0	-7.4	4.1	-0.5
B2PLYP-d3/def2-TZVP// BP86/def2-TZVP	G	2 MeOH	0.0	-0.6	16.4	13.9
M06/TZVP// BP86/def2-TZVP	H	2 MeOH	0.0	-4.8	4.2	0.6
M06/TZVP// BP86/def2-TZVP	G	2 MeOH	0.0	2.0	16.5	15.0
B2PLYP/def2-TZVP// BP86/SVP	H	1 MeOH	0.0	-0.7	17.8	18.2
B2PLYP/def2-TZVP// BP86/SVP	G	1 MeOH	0.0	3.4	26.0	26.4
B2PLYP/def2-TZVP// BP86/SVP	H	2 MeOH	0.0	-4.8	7.1	3.9
B2PLYP/def2-TZVP// BP86/SVP	G	2 MeOH	0.0	3.3	19.1	18.5
B2PLYP-d3/def2-TZVP// BP86/SVP	H	1 MeOH	0.0	-2.1	14.9	15.5
B2PLYP-d3/def2-TZVP// BP86/SVP	G	1 MeOH	0.0	2.0	23.2	23.6
B2PLYP-d3/def2-TZVP// BP86/SVP	H	2 MeOH	0.0	-7.5	2.8	-1.3
B2PLYP-d3/def2-TZVP// BP86/SVP	G	2 MeOH	0.0	0.7	14.7	13.3
M06/TZVP//BP86/SVP	H	1 MeOH	0.0	-0.3	14.4	15.3
M06/TZVP//BP86/SVP	G	1 MeOH	0.0	3.8	22.6	23.4
M06/TZVP//BP86/SVP	H	2 MeOH	0.0	-4.7	2.4	0.0
M06/TZVP//BP86/SVP	G	2 MeOH	0.0	3.4	14.4	14.5

Table S2. Key distances, in Å, in the structures depicted in Figure 6 (d1 = C1 … C2; d2 = Au … C1; d3 = Au … C2; d4 = C1 … O) involved in the nucleophilic attack of η^2-complex **I** by the alcohol. Complex **A** is the adduct formed initially, **TS** is the transition state for nucleophilic attack, and **P** is the complex produced. Mayer Bond Orders are provided for C1 ... C2 (MBO1), Au ... C1 (MBO2), Au ... C2 (MBO3), and C1 ... O (MBO4).

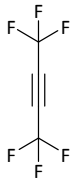
	Alkyne	Alcohol	d1	d2	d3	d4	MBO1	MBO2	MBO3	MBO4
I		-	1.256	2.238	2.238	-	2.008	0.443	0.443	-
A			1.256	2.229	2.229	3.247	1.969	0.465	0.465	-
TS		1 MeOH	1.319	2.897	2.090	1.761	2.006	0.143	0.605	0.507
P			1.336	2.956	2.077	1.609	1.928	0.114	0.645	0.642
A			1.257	2.227	2.226	3.176	1.958	0.471	0.471	-
TS		2 MeOH	1.287	2.729	2.119	2.134	2.133	0.237	0.531	0.272
P			1.346	2.973	2.071	1.538	1.861	0.117	0.697	0.708
A			1.257	2.238	2.235	3.829	1.987	0.450	0.449	-
TS		1 PhOH	-	-	-	-	-	-	-	-
P			-	-	-	-	-	-	-	-
A			1.256	2.235	2.229	3.296	1.970	0.461	0.460	-
TS		2 PhOH	1.309	2.852	2.100	1.858	2.048	0.174	0.592	0.420
P			1.345	2.969	2.069	1.538	1.873	0.111	0.692	0.681
I		-	1.263	2.246	2.246	-	1.796	0.418	0.418	-
A			1.267	2.233	2.233	4.111	1.764	0.438	0.438	-
TS		1 MeOH	1.310	2.875	2.092	1.942	2.035	0.129	0.583	0.428
P			1.350	3.016	2.063	1.556	1.823	0.084	0.674	0.741
A			1.266	2.234	2.232	4.009	1.760	0.439	0.441	-
TS		2 MeOH	1.300	2.771	2.113	2.082	2.051	0.171	0.549	0.318
P			1.359	3.025	2.067	1.474	1.893	0.066	0.599	0.870
A			1.266	2.237	2.236	4.222	1.775	0.432	0.433	-
TS		1 PhOH	-	-	-	-	-	-	-	-
P			-	-	-	-	-	-	-	-
A			1.266	2.190	2.303	3.688	1.793	0.405	0.422	-
TS		2 PhOH	1.324	2.886	2.088	1.760	1.981	0.123	0.625	0.502
P			1.359	3.021	2.067	1.490	1.790	0.088	0.688	0.786
I		-	1.254	2.189	2.189	-	2.328	0.432	0.433	-
A			1.253	2.189	2.190	2.949	2.301	0.445	0.448	-
TS		1 MeOH	1.248	2.425	2.135	2.398	2.300	0.321	0.423	0.189
P			1.343	3.010	2.066	1.489	1.941	0.071	0.558	0.831
A			1.253	2.215	2.175	2.756	2.290	0.448	0.441	-
TS		2 MeOH	1.272	2.312	2.145	2.284	2.071	0.420	0.427	0.217
P			1.349	3.060	2.067	1.446	1.890	0.079	0.607	0.862
A			1.257	2.242	2.229	3.636	1.987	0.450	0.451	-
TS		1 PhOH	1.266	2.545	2.118	2.477	2.357	0.296	0.410	0.174
P			1.342	3.027	2.070	1.490	1.934	0.072	0.563	0.832
A			1.254	2.179	2.192	3.129	2.287	0.430	0.447	-
TS		2 PhOH	1.266	2.512	2.123	2.389	2.304	0.330	0.407	0.169
P			1.348	3.018	2.067	1.443	1.893	0.066	0.599	0.870

Table S3. Grimme dispersion correction on geometry optimizations (Internal Energy (E), Enthaylpy (H) and Gibbs (G) energies in kcal/mol).

	Alkyne	Alcohol	E	H	G
Without dispersion:					
I	CH_3CCCH_3	-	0.0	0.0	0.0
A	CH_3CCCH_3	1 MeOH	-7.3	-5.9	2.4
TS	CH_3CCCH_3	1 MeOH	5.8	6.7	19.2
P	CH_3CCCH_3	1 MeOH	5.6	7.2	19.7
With D3 dispersion:					
I	CH_3CCCH_3	-	0.0	0.0	0.0
A	CH_3CCCH_3	1 MeOH	-10.4	-9.7	0.9
TS	CH_3CCCH_3	1 MeOH	0.3	1.4	14.8
P	CH_3CCCH_3	1 MeOH	0.3	2.1	13.4
With D3bj dispersion:					
I	CH_3CCCH_3	-	0.0	0.0	0.0
A	CH_3CCCH_3	1 MeOH	-9.7	-8.9	1.7
TS	CH_3CCCH_3	1 MeOH	1.1	1.5	16.7
P	CH_3CCCH_3	1 MeOH	0.8	1.9	17.1

Table S4. Alcohol nucleophilic attack to π-gold-alkyne species **I** (Gibbs energies in chloroform are given in kcal/mol, **A** = adduct; **TS** = transition state; **P** = product).

	Alkyne	Alcohol	E	H	G
I	CH_3CCCH_3	-	0.0	0.0	0.0
A	CH_3CCCH_3	1 MeOH	-1.7	-0.3	8.0
TS	CH_3CCCH_3	1 MeOH	13.4	14.4	26.9
P	CH_3CCCH_3	1 MeOH	13.6	15.3	27.7
A	CH_3CCCH_3	2 MeOH	-7.6	-4.7	12.0
TS	CH_3CCCH_3	2 MeOH	0.0	2.4	22.9
P	CH_3CCCH_3	2 MeOH	-2.9	0.0	23.1
A	CH_3CCCH_3	1 PhOH	-1.8	-0.7	6.5
TS	CH_3CCCH_3	1 PhOH	-	-	-
P	CH_3CCCH_3	1 PhOH	-	-	-
A	CH_3CCCH_3	2 PhOH	-8.3	-5.6	11.1
TS	CH_3CCCH_3	2 PhOH	10.5	12.2	34.8
P	CH_3CCCH_3	2 PhOH	8.9	11.0	34.6
I	PhCCPh	-	0.0	0.0	0.0
A	PhCCPh	1 MeOH	-3.2	-1.7	7.4
TS	PhCCPh	1 MeOH	13.0	15.0	29.4
P	PhCCPh	1 MeOH	-4.1	-3.0	11.9
A	PhCCPh	2 MeOH	-9.5	-6.4	10.7
TS	PhCCPh	2 MeOH	-0.4	4.1	25.8
P	PhCCPh	2 MeOH	-8.5	-6.8	18.9
A	PhCCPh	1 PhOH	-2.2	-0.9	7.5
TS	PhCCPh	1 PhOH	-	-	-
P	PhCCPh	1 PhOH	-	-	-
A	PhCCPh	2 PhOH	-9.8	-7.0	12.0
TS	PhCCPh	2 PhOH	8.0	9.6	34.4
P	PhCCPh	2 PhOH	3.6	4.5	31.2
I	CF_3CCCF_3	-	0.0	0.0	0.0
A	CF_3CCCF_3	1 MeOH	-3.9	-2.6	4.9
TS	CF_3CCCF_3	1 MeOH	-4.2	-3.5	7.2
P	CF_3CCCF_3	1 MeOH	-9.6	-7.8	6.3
A	CF_3CCCF_3	2 MeOH	-10.5	-7.6	9.6
TS	CF_3CCCF_3	2 MeOH	-7.0	-4.9	16.6
P	CF_3CCCF_3	2 MeOH	-32.0	-29.8	-5.4
A	CF_3CCCF_3	1 PhOH	-4.9	-3.6	6.4
TS	CF_3CCCF_3	1 PhOH	3.9	4.4	16.0
P	CF_3CCCF_3	1 PhOH	-1.4	-0.1	14.0
A	CF_3CCCF_3	2 PhOH	-11.6	-8.9	11.0
TS	CF_3CCCF_3	2 PhOH	-5.4	-3.7	19.1
P	CF_3CCCF_3	2 PhOH	-18.0	-16.9	8.2
I	HCCH	-	0.0	0.0	0.0
A	HCCH	1 MeOH	-0.7	0.7	9.2
TS	HCCH	1 MeOH	4.1	5.0	14.7
P	HCCH	1 MeOH	2.2	4.8	15.8
A	HCCH	2 MeOH	-11.8	-9.0	7.5
TS	HCCH	2 MeOH	-5.1	-2.9	14.5
P	HCCH	2 MeOH	-13.7	-10.0	10.6
A	HCCH	1 PhOH	-3.5	-2.2	6.4
TS	HCCH	1 PhOH	11.4	12.4	23.3
P	HCCH	1 PhOH	11.5	13.5	24.4
A	HCCH	2 PhOH	-9.8	-7.1	10.6
TS	HCCH	2 PhOH	-1.5	0.4	19.3
P	HCCH	2 PhOH	-0.5	2.6	23.7
I	FCCF	-	0.0	0.0	0.0
A	FCCF	1 MeOH	-2.9	-1.6	4.9
TS	FCCF	1 MeOH	-1.9	-1.3	7.0
P	FCCF	1 MeOH	-25.1	-23.2	-10.6
A	FCCF	2 MeOH	-9.1	-6.3	7.7
TS	FCCF	2 MeOH	-12.0	-9.9	10.5
P	FCCF	2 MeOH	-48.3	-46.0	-23.3
A	FCCF	1 PhOH	-2.4	-1.2	5.4
TS	FCCF	1 PhOH	-0.9	-0.4	8.2
P	FCCF	1 PhOH	-16.0	-14.5	-2.1
A	FCCF	2 PhOH	-8.0	-5.4	11.3
TS	FCCF	2 PhOH	-6.7	-5.2	16.2
P	FCCF	2 PhOH	-32.5	-31.1	-8.6

Table S5. Main distances (d1 = C1···C2; d2 = Au···C1; d3 = Au···C2; d4 = C1···O; in Å, see Figure S5) involved in the nucleophilic attack of the alcohol to the *π*-gold-alkyne complex **I** (**A** = adduct; **TS** = transition state; **P** = product); and the corresponding Mayer Bond Orders (MBO1 = C1···C2; MBO2 = Au···C1; MBO3 = Au···C2; MBO4 = C1···O; in Å).

	Alkyne	Alcohol	d1	d2	d3	d4	MBO1	MBO2	MBO3	MBO4
I	CH_3CCCH_3	-	1.256	2.238	2.238	-	2.008	0.443	0.443	-
A	CH_3CCCH_3	1 MeOH	1.256	2.229	2.229	3.247	1.969	0.465	0.465	-
TS	CH_3CCCH_3	1 MeOH	1.319	2.897	2.090	1.761	2.006	0.143	0.605	0.507
P	CH_3CCCH_3	1 MeOH	1.336	2.956	2.077	1.609	1.928	0.114	0.645	0.642
A	CH_3CCCH_3	2 MeOH	1.257	2.227	2.226	3.176	1.958	0.471	0.471	-
TS	CH_3CCCH_3	2 MeOH	1.287	2.729	2.119	2.134	2.133	0.237	0.531	0.272
P	CH_3CCCH_3	2 MeOH	1.346	2.973	2.071	1.538	1.861	0.117	0.697	0.708
A	CH_3CCCH_3	1 PhOH	1.257	2.238	2.235	3.829	1.987	0.450	0.449	-
TS	CH_3CCCH_3	1 PhOH	-	-	-	-	-	-	-	-
P	CH_3CCCH_3	1 PhOH	-	-	-	-	-	-	-	-
A	CH_3CCCH_3	2 PhOH	1.256	2.235	2.229	3.296	1.970	0.461	0.460	-
TS	CH_3CCCH_3	2 PhOH	1.309	2.852	2.100	1.858	2.048	0.174	0.592	0.420
P	CH_3CCCH_3	2 PhOH	1.345	2.969	2.069	1.538	1.873	0.111	0.692	0.681
I	PhCCPh	-	1.263	2.246	2.246	-	1.796	0.418	0.418	-
A	PhCCPh	1 MeOH	1.267	2.233	2.233	4.111	1.764	0.438	0.438	-
TS	PhCCPh	1 MeOH	1.310	2.875	2.092	1.942	2.035	0.129	0.583	0.428
P	PhCCPh	1 MeOH	1.350	3.016	2.063	1.556	1.823	0.084	0.674	0.741
A	PhCCPh	2 MeOH	1.266	2.234	2.232	4.009	1.760	0.439	0.441	-
TS	PhCCPh	2 MeOH	1.300	2.771	2.113	2.082	2.051	0.171	0.549	0.318
P	PhCCPh	2 MeOH	1.359	3.025	2.067	1.474	1.893	0.066	0.599	0.870
A	PhCCPh	1 PhOH	1.266	2.237	2.236	4.222	1.775	0.432	0.433	-
TS	PhCCPh	1 PhOH	-	-	-	-	-	-	-	-
P	PhCCPh	1 PhOH	-	-	-	-	-	-	-	-
A	PhCCPh	2 PhOH	1.266	2.190	2.303	3.688	1.793	0.405	0.422	-
TS	PhCCPh	2 PhOH	1.324	2.886	2.088	1.760	1.981	0.123	0.625	0.502
P	PhCCPh	2 PhOH	1.359	3.021	2.067	1.490	1.790	0.088	0.688	0.786
I	CF_3CCCF_3	-	1.254	2.189	2.189	-	2.328	0.432	0.433	-
A	CF_3CCCF_3	1 MeOH	1.253	2.189	2.190	2.949	2.301	0.445	0.448	-
TS	CF_3CCCF_3	1 MeOH	1.248	2.425	2.135	2.398	2.300	0.321	0.423	0.189
P	CF_3CCCF_3	1 MeOH	1.343	3.010	2.066	1.489	1.941	0.071	0.558	0.831
A	CF_3CCCF_3	2 MeOH	1.253	2.215	2.175	2.756	2.290	0.448	0.441	-
TS	CF_3CCCF_3	2 MeOH	1.272	2.312	2.145	2.284	2.071	0.420	0.427	0.217
P	CF_3CCCF_3	2 MeOH	1.349	3.060	2.067	1.446	1.890	0.079	0.607	0.862
A	CF_3CCCF_3	1 PhOH	1.257	2.242	2.229	3.636	1.987	0.450	0.451	-
TS	CF_3CCCF_3	1 PhOH	1.266	2.545	2.118	2.477	2.357	0.296	0.410	0.174
P	CF_3CCCF_3	1 PhOH	1.342	3.027	2.070	1.490	1.934	0.072	0.563	0.832
A	CF_3CCCF_3	2 PhOH	1.254	2.179	2.192	3.129	2.287	0.430	0.447	-
TS	CF_3CCCF_3	2 PhOH	1.266	2.512	2.123	2.389	2.304	0.330	0.407	0.169
P	CF_3CCCF_3	2 PhOH	1.348	3.018	2.067	1.443	1.893	0.066	0.599	0.870
I	HCCH	-	1.249	2.215	2.215	-	1.964	0.509	0.509	-
A	HCCH	1 MeOH	1.250	2.228	2.218	2.883	1.901	0.503	0.510	-
TS	HCCH	1 MeOH	1.270	2.614	2.116	2.179	2.111	0.326	0.544	0.267
P	HCCH	1 MeOH	1.325	2.995	2.052	1.559	1.969	0.131	0.717	0.676
A	HCCH	2 MeOH	1.252	2.228	2.221	2.786	1.888	0.505	0.512	-
TS	HCCH	2 MeOH	1.259	2.434	2.141	2.387	2.016	0.419	0.520	0.174
P	HCCH	2 MeOH	1.339	3.012	2.045	1.490	1.926	0.126	0.759	0.785
A	HCCH	1 PhOH	1.250	2.227	2.216	2.970	1.899	0.503	0.511	-
TS	HCCH	1 PhOH	1.295	2.874	2.076	1.863	2.087	0.198	0.639	0.416
P	HCCH	1 PhOH	1.324	2.995	2.052	1.567	1.956	0.131	0.718	0.658
A	HCCH	2 PhOH	1.250	2.228	2.216	2.907	1.885	0.504	0.510	-
TS	HCCH	2 PhOH	1.267	2.564	2.119	2.239	2.098	0.351	0.547	0.219
P	HCCH	2 PhOH	1.335	3.013	2.045	1.497	1.909	0.125	0.769	0.751
I	FCCF	-	1.256	2.159	2.159	-	1.868	0.536	0.536	-
A	FCCF	1 MeOH	1.254	2.166	2.166	2.863	1.872	0.537	0.537	-
TS	FCCF	1 MeOH	1.265	2.316	2.110	2.578	1.852	0.454	0.539	0.065
P	FCCF	1 MeOH	1.348	3.088	2.025	1.472	1.644	0.054	0.710	0.820
A	FCCF	2 MeOH	1.254	2.179	2.164	2.759	1.864	0.532	0.538	-
TS	FCCF	2 MeOH	1.316	2.890	2.064	2.200	1.770	0.142	0.611	0.442
P	FCCF	2 MeOH	1.352	3.060	2.030	1.420	1.609	0.057	0.739	0.909
A	FCCF	1 PhOH	1.254	2.162	2.164	2.980	1.873	0.541	0.542	-
TS	FCCF	1 PhOH	1.265	2.392	2.099	2.604	1.883	0.404	0.536	0.075
P	FCCF	1 PhOH	1.347	3.083	2.026	1.478	1.639	0.054	0.711	0.810
A	FCCF	2 PhOH	1.255	2.181	2.149	2.898	1.864	0.538	0.546	-
TS	FCCF	2 PhOH	1.322	2.926	2.059	2.100	1.764	0.121	0.621	0.431
P	FCCF	2 PhOH	1.352	3.048	2.033	1.419	1.609	0.058	0.736	0.889

Table S6. Chemical hardness (η) and electrophilicity (ω) of the intermediate species involved in the alkoxylation (in a.u.; **A** = Adduct, **P** = Product).

	Alkyne	Alcohol	E_{HOMO}	E_{LUMO}	η	Ω
MeOH			-0.216	0.035	0.251	0.016
PhOH			-0.199	-0.042	0.157	0.046
I	CH_3CCCH_3	-	-0.361	-0.212	0.149	0.275
A	CH_3CCCH_3	1 MeOH	-0.323	-0.204	0.071	0.585
P	CH_3CCCH_3	1 MeOH	-0.326	-0.162	0.164	0.181
A	CH_3CCCH_3	2 MeOH	-0.296	-0.198	0.057	0.647
P	CH_3CCCH_3	2 MeOH	-0.321	-0.144	0.168	0.154
A	CH_3CCCH_3	1 PhOH	-0.286	-0.203	0.083	0.360
P	CH_3CCCH_3	1 PhOH	-0.333	-0.210	0.123	0.299
A	CH_3CCCH_3	2 PhOH	-0.263	-0.201	0.063	0.428
P	CH_3CCCH_3	2 PhOH	-0.310	-0.151	0.158	0.168
I	PhCCPh	-	-0.317	-0.212	0.105	0.333
A	PhCCPh	1 MeOH	-0.303	-0.203	0.100	0.321
P	PhCCPh	1 MeOH	-0.305	-0.185	0.120	0.249
A	PhCCPh	2 MeOH	-0.294	-0.198	0.096	0.315
P	PhCCPh	2 MeOH	-0.293	-0.172	0.121	0.222
A	PhCCPh	1 PhOH	-0.276	-0.205	0.071	0.409
P	PhCCPh	1 PhOH	-0.274	-0.205	0.068	0.419
A	PhCCPh	2 PhOH	-0.276	-0.210	0.066	0.448
P	PhCCPh	2 PhOH	-0.291	-0.174	0.118	0.229
I	CF_3CCCF_3	-	-0.382	-0.265	0.117	0.447
A	CF_3CCCF_3	1 MeOH	-0.323	-0.252	0.071	0.585
P	CF_3CCCF_3	1 MeOH	-0.336	-0.216	0.120	0.317
A	CF_3CCCF_3	2 MeOH	-0.300	-0.243	0.057	0.647
P	CF_3CCCF_3	2 MeOH	-0.324	-0.194	0.130	0.258
A	CF_3CCCF_3	1 PhOH	-0.274	-0.205	0.069	0.413
P	CF_3CCCF_3	1 PhOH	-0.333	-0.210	0.123	0.299
A	CF_3CCCF_3	2 PhOH	-0.287	-0.248	0.039	0.917
P	CF_3CCCF_3	2 PhOH	-0.319	-0.189	0.130	0.248
I	HCCH	-	-0.372	-0.237	0.135	0.344
A	HCCH	1 MeOH	-0.349	-0.216	0.133	0.300
P	HCCH	1 MeOH	-0.327	-0.170	0.156	0.198
A	HCCH	2 MeOH	-0.324	-0.205	0.119	0.293
P	HCCH	2 MeOH	-0.319	-0.205	0.114	0.301
A	HCCH	1 PhOH	-0.293	-0.220	0.074	0.447
P	HCCH	1 PhOH	-0.322	-0.181	0.141	0.224
A	HCCH	2 PhOH	-0.279	-0.212	0.067	0.452
P	HCCH	2 PhOH	-0.307	-0.162	0.145	0.189
I	FCCF	-	-0.383	-0.269	0.114	0.465
A	FCCF	1 MeOH	-0.318	-0.252	0.066	0.620
P	FCCF	1 MeOH	-0.329	-0.180	0.149	0.217
A	FCCF	2 MeOH	-0.291	-0.242	0.049	0.733
P	FCCF	2 MeOH	-0.307	-0.157	0.150	0.179
A	FCCF	1 PhOH	-0.279	-0.257	0.022	1.628
P	FCCF	1 PhOH	-0.324	-0.186	0.138	0.234
A	FCCF	2 PhOH	-0.267	-0.250	0.016	2.044
P	FCCF	2 PhOH	-0.300	-0.160	0.140	0.190

Table S7. Natural Bond Order (NBO) charges (in electrons).

	Alkyne	Alcohol	Au	C1	C2	O
I	CH_3CCCH_3	-	0.406	-0.051	-0.051	-
A	CH_3CCCH_3	1 MeOH	0.401	-0.046	-0.046	-0.748
P	CH_3CCCH_3	1 MeOH	0.271	-0.362	0.197	-0.547
A	CH_3CCCH_3	2 MeOH	0.398	-0.043	-0.045	-0.786
P	CH_3CCCH_3	2 MeOH	0.249	-0.355	0.186	-0.586
A	CH_3CCCH_3	1 PhOH	0.401	-0.052	-0.047	0.401
P	CH_3CCCH_3	1 PhOH	-	-	-	-
A	CH_3CCCH_3	2 PhOH	0.400	-0.040	-0.054	-0.723
P	CH_3CCCH_3	2 PhOH	0.251	-0.349	0.191	-0.572
I	PhCCPh	-	0.404	-0.038	-0.038	-
A	PhCCPh	1 MeOH	0.406	-0.031	-0.031	-0.748
P	PhCCPh	1 MeOH	0.288	-0.344	0.227	-0.562
A	PhCCPh	2 MeOH	0.404	-0.030	-0.028	-0.785
P	PhCCPh	2 MeOH	0.267	-0.356	0.243	-0.587
A	PhCCPh	1 PhOH	0.405	-0.033	-0.034	-0.693
P	PhCCPh	1 PhOH	-	-	-	-
A	PhCCPh	2 PhOH	0.414	-0.120	0.038	-0.710
P	PhCCPh	2 PhOH	0.269	-0.342	0.229	-0.559
I	CF_3CCCF_3	-	0.458	-0.134	-0.134	-
A	CF_3CCCF_3	1 MeOH	0.448	-0.121	-0.123	-0.753
P	CF_3CCCF_3	1 MeOH	0.295	-0.444	1.079	-0.534
A	CF_3CCCF_3	2 MeOH	0.440	-0.143	-0.094	-0.784
P	CF_3CCCF_3	2 MeOH	-0.432	0.111	-0.590	-0.710
A	CF_3CCCF_3	1 PhOH	0.401	-0.064	-0.036	-0.688
P	CF_3CCCF_3	1 PhOH	0.291	-0.448	0.124	-0.534
A	CF_3CCCF_3	2 PhOH	0.454	-0.119	-0.134	-0.703
P	CF_3CCCF_3	2 PhOH	0.273	-0.434	0.118	-0.562
I	HCCH	-	0.420	-0.247	-0.247	-
A	HCCH	1 MeOH	0.415	-0.233	-0.229	-0.736
P	HCCH	1 MeOH	0.290	-0.004	-0.573	-0.529
A	HCCH	2 MeOH	0.398	-0.241	-0.303	-0.777
P	HCCH	2 MeOH	0.271	-0.045	0.546	-0.537
A	HCCH	1 PhOH	0.408	-0.236	-0.277	-0.698
P	HCCH	1 PhOH	0.288	0.008	-0.583	-0.534
A	HCCH	2 PhOH	0.406	-0.233	-0.289	-0.730
P	HCCH	2 PhOH	0.264	0.008	-0.590	-0.562
I	FCCF	-	0.421	0.257	0.257	-
A	FCCF	1 MeOH	0.402	0.267	0.267	-0.752
P	FCCF	1 MeOH	0.271	0.546	-0.045	-0.537
A	FCCF	2 MeOH	0.391	0.281	0.264	-0.789
P	FCCF	2 MeOH	0.237	0.534	-0.035	-0.586
A	FCCF	1 PhOH	0.411	0.266	0.263	-0.690
P	FCCF	1 PhOH	0.268	0.558	-0.052	-0.537
A	FCCF	2 PhOH	0.405	0.288	0.246	-0.725
P	FCCF	2 PhOH	0.235	0.535	-0.018	-0.586

Table S8. Nucleophilic attack of the π-gold-alkyne species **I** by the alcohol. Gibbs energies in chloroform solution are given in kcal/mol, **A** = adduct; **TS** = transition state; **P** = product).

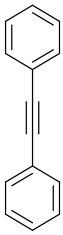
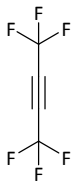
	Alkyne	Alcohol	E	H	G
I		-	0.0	0.0	0.0
A			-1.7	-0.3	8.0
TS		1 MeOH	13.4	14.4	26.9
P			13.6	15.3	27.7
A			-7.6	-4.7	12.0
TS		2 MeOH	0.0	2.4	22.9
P			-2.9	0.0	23.1
A			-1.8	-0.7	6.5
TS		1 PhOH	-	-	-
P			-	-	-
A			-8.3	-5.6	11.1
TS		2 PhOH	10.5	12.2	34.8
P			8.9	11.0	34.6
	Alkyne	**Alcohol**	**E**	**H**	**G**
I		-	0.0	0.0	0.0
A			-3.2	-1.7	7.4
TS		1 MeOH	13.0	15.0	29.4
P			-4.1	-3.0	11.9
A			-9.5	-6.4	10.7
TS		2 MeOH	-0.4	4.1	25.8
P			-8.5	-6.8	18.9
A			-2.2	-0.9	7.5
TS		1 PhOH	-	-	-
P			-	-	-
A			-9.8	-7.0	12.0
TS		2 PhOH	8.0	9.6	34.4
P			3.6	4.5	31.2
	Alkyne	**Alcohol**	**E**	**H**	**G**
I		-	0.0	0.0	0.0
A			-3.9	-2.6	4.9
TS		1 MeOH	-4.2	-3.5	7.2
P			-9.6	-7.8	6.3
A			-10.5	-7.6	9.6
TS		2 MeOH	-7.0	-4.9	16.6
P			-32.0	-29.8	-5.4
A			-4.9	-3.6	6.4
TS		1 PhOH	3.9	4.4	16.0
P			-1.4	-0.1	14.0
A			-11.6	-8.9	11.0
TS		2 PhOH	-5.4	-3.7	19.1
P			-18.0	-16.9	8.2

Table S9. Chemical hardness (η) and electrophilicity (ω) of the intermediate species involved in the hydroalkoxylation/hydrophenoxylation reaction (in a.u.). **A** is the adduct between complex **I** and the alcohol, and **P** is the product complex.

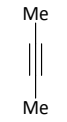
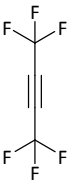
		Alcohol	E_{HOMO}	E_{LUMO}	η	ω
		MeOH	-0.216	0.035	0.251	0.016
		PhOH	-0.199	-0.042	0.157	0.046
	Alkyne	**Alcohol**				
I		-	-0.361	-0.212	0.149	0.275
A		1 MeOH	-0.323	-0.204	0.071	0.585
P			-0.326	-0.162	0.164	0.181
A		2 MeOH	-0.296	-0.198	0.057	0.647
P			-0.321	-0.144	0.168	0.154
A		1 PhOH	-0.286	-0.203	0.083	0.360
P			-0.333	-0.210	0.123	0.299
A		2 PhOH	-0.263	-0.201	0.063	0.428
P			-0.310	-0.151	0.158	0.168
	Alkyne	**Alcohol**				
I		-	-0.317	-0.212	0.105	0.333
A		1 MeOH	-0.303	-0.203	0.100	0.321
P			-0.305	-0.185	0.120	0.249
A		2 MeOH	-0.294	-0.198	0.096	0.315
P			-0.293	-0.172	0.121	0.222
A		1 PhOH	-0.276	-0.205	0.071	0.409
P			-0.274	-0.205	0.068	0.419
A		2 PhOH	-0.276	-0.210	0.066	0.448
P			-0.291	-0.174	0.118	0.229
	Alkyne	**Alcohol**				
I		-	-0.382	-0.265	0.117	0.447
A		1 MeOH	-0.323	-0.252	0.071	0.585
P			-0.336	-0.216	0.120	0.317
A		2 MeOH	-0.300	-0.243	0.057	0.647
P			-0.324	-0.194	0.130	0.258
A		1 PhOH	-0.274	-0.205	0.069	0.413
P			-0.333	-0.210	0.123	0.299
A		2 PhOH	-0.287	-0.248	0.039	0.917
P			-0.319	-0.189	0.130	0.248

Table S10. Benchmark for the nucleophilic attack of **II** to π-gold-dimethyl-alkyne species **I** (Gibbs (G) energies in chloroform are given in kcal/mol).

	Geometry optimization	Thermal correction	E_{gas}	G_{gas}	E_{solv} (M06/TZVP)	G_{solv} (M06/TZVP)	E_{solv} (M06/DEF2TZVP)	G_{solv} (M06/DEF2TZVP)
I+II	BP86/SVP	BP86/SVP	0.0	0.0	0.0	0.0	0.0	0.0
III	BP86/SVP	BP86/SVP	-12.2	0.0	-10.6	1.7	-9.9	2.4
III-IV	BP86/SVP	BP86/SVP	-5.8	7.4	-5.1	8.2	-2.8	10.5
IV	BP86/SVP	BP86/SVP	-17.6	-1.2	-18.2	-1.8	-15.6	0.8
I+II	BP86/Def2TZVP	BP86/Def2TZVP	0.0	0.0	0.0	0.0	0.0	0.0
III	BP86/Def2TZVP	BP86/Def2TZVP	-10.5	2.7	-9.9	3.3	-28.6	-15.4
III-IV	BP86/Def2TZVP	BP86/Def2TZVP	-2.5	13.2	-4.1	11.5	-20.9	-5.3
IV	BP86/Def2TZVP	BP86/Def2TZVP	-11.4	6.3	-17.7	0.1	-34.4	-16.6
I+II	BP86-d3/Def2TZVP	BP86-d3/Def2TZVP	0.0	0.0	0.0	0.0	0.0	0.0
III	BP86-d3/Def2TZVP	BP86-d3/Def2TZVP	-40.5	-19.5	-19.5	1.5	-19.0	1.9
III-IV	BP86-d3/Def2TZVP	BP86-d3/Def2TZVP	-24.0	-7.8	-5.2	11.0	-2.8	13.4
IV	BP86-d3/Def2TZVP	BP86-d3/Def2TZVP	-32.7	-14.7	-18.5	-0.5	-16.0	2.0
I+II	BP86-d3/SVP	BP86-d3/SVP	0.0	0.0	0.0	0.0	0.0	0.0
III	BP86-d3/SVP	BP86-d3/SVP	-43.9	-22.6	-19.4	1.9	-18.9	2.4
III-IV	BP86-d3/SVP	BP86-d3/SVP	39.4	52.4	-4.8	8.2	-2.5	10.5
IV	BP86-d3/SVP	BP86-d3/SVP	-39.1	-21.8	-18.9	-1.6	-16.3	0.9
I+II	BP86/SVP	M06/SVP	0.0	0.0	0.0	0.0	0.0	0.0
III	BP86/SVP	M06/SVP	-21.5	-8.1	-10.6	2.8	-9.9	3.5
III-IV	BP86/SVP	M06/SVP	-18.6	-3.9	-5.1	9.6	-2.8	11.8
IV	BP86/SVP	M06/SVP	-33.3	-16.9	-18.2	-1.8	-15.6	0.7
I+II	BP86/TZVP	BP86/TZVP	0.0	0.0	0.0	0.0	0.0	0.0
III	BP86/TZVP	BP86/TZVP	-11.2	1.8	-10.0	3.0	-9.4	3.6
III-IV	BP86/TZVP	BP86/TZVP	-4.2	10.7	-4.2	10.8	-1.9	13.0
IV	BP86/TZVP	BP86/TZVP	-13.2	3.9	-17.5	-0.4	-15.1	2.0
NHC = IPr								
I+II	BP86/SVP	BP86/Def2TZVP	0.0	0.0	0.0	0.0	0.0	0.0
III	BP86/SVP	BP86/Def2TZVP	-8.6	6.0	-8.2	6.5	-8.0	6.7
III-IV	BP86/SVP	BP86/Def2TZVP	1.0	17.8	-4.3	12.5	-2.0	14.8
IV	BP86/SVP	BP86/Def2TZVP	-7.7	11.6	-20.6	-1.3	-18.2	1.1
NHC = IPr								
I+II	BP86/SVP	BP86-d3/Def2TZVP	0.0	0.0	0.0	0.0	0.0	0.0
III	BP86/SVP	BP86-d3/Def2TZVP	-19.2	-4.4	-8.2	6.7	-8.0	6.9
III-IV	BP86/SVP	BP86-d3/Def2TZVP	-19.1	-2.7	-4.3	12.2	-2.0	14.4
IV	BP86/SVP	BP86-d3/Def2TZVP	-32.0	-13.0	-20.6	-1.6	-18.2	0.8

%V_{bur} calculations

By using SambVca (version 2), developed by Cavallo and coworkers, it is possible to analyse and visualise the first coordination sphere around the metal where the catalysis takes place. The buried volume (%V_{bur}) provides a convenient single number that describes the steric impact of the ligand, and steric maps and per quadrant measures of %V_{bur} provide more information about the way in which the steric bulk is distributed.

Splitting %Vbur into quadrant contributions quantifies any asymmetry in the way the ligand wraps around the metal. This analysis shows how the shape of the reactive pocket is modified when moving from IPr to IMe for species gold-alkyne species **I**.

Structure/Activity Relationships of the monogold systems

With the mono- and digold-catalysed mechanisms described by DFT calculations, and even though the digold mechanism is found to be strongly favored with respect to the monogold one when the catalyst concentration is relatively not low, the role of each species involved was probed. Structure/activity relationships are important because they determine the scope and limitations of the synthetic methodology. The results are collected in Tables S4 and S8 to allow direct comparisons to be made, including the optimised energy in solvent (E) as well as the enthalpy (H) for the sake of consistency with the work of Belanzoni, Zuccaccia and co-workers.[28]

The adduct **A** is formed from the interaction of η^2-alkyne complex **I** with the alcohol, due to the favourable interaction between the carbon atoms of the alkyne and the oxygen of the alcohol, together with hydrogen bonds of the latter atom to hydrogen atoms attached to the alkyne. This interaction is rather weak. In terms of Gibbs free energies, **A** is more stable than the separated species. Mayer Bond Orders (MBO) for these adducts are collected in Table S5 (*vide infra*), and demonstrate that the nature of the bond is neither covalent nor ionic because the corresponding MBOs are null. The nucleophilic attack enjoys a reduced barrier if two molecules of alcohol are involved. However, this favourable effect is not that significant in energy terms once the entropic effects are also considered. Kinetically, the upper energy point on the free energy surface is this transition state. The general trends are that electron-withdrawing substituents on

the alkyne (such as trifluoromethyl groups) increase the barrier by at least 3-5 kcal/mol, and give barriers up to twice as high as the simple but-2-yne substrate. Alkyl alcohols facilitate the alkoxylation, reducing the barrier by around 10 kcal/mol. The combination of diphenylacetylene and phenol leads to prohibitively large barriers and an intermediate that is very high in energy (both > 30 kcal/mol).

The steric properties of the substituents on the alkyne do not play a significant role; the small H and F substituents on acetylene and difluoroacetylene, respectively, lead to completely different behaviour (see Tables S4-S5).

Intermediate **P**, the product of the alkoxylation, is thermodynamically less stable than the initial reactants in all cases except where trifluoromethyl or methyl groups are the substituents on the alkyne. **P** becomes much more thermodynamically stable when it bears electron withdrawing substituents on the alkyne, while larger substituents lead to less stable **P**. In general, for monogold-catalysed hydroalkoxylation, alkyl substituents on the alkyne lead to lower barriers (**TS**) but aryl substituents lead to more thermodynamically stable product complexes **P**. Notably, this key step of the reaction (from **I** to **P**) is not thermodynamically favourable overall unless the alkyne bears highly electron-withdrawing substituents; subsequent protodeauration renders the reaction irreversible. The counterion might compensate for this instability of species

P, and even decrease the barrier. However, in the previous study by Zuccaccia and coworkers,[28] such an effect was not included in the calculations.

The results from the monogold catalysed pathway can be compared to those from the dual gold-catalysed mechanism. In the latter, the highest energy barrier is 15.0 kcal/mol for the hydrophenoxylation of diphenylacetylene and 8.9 kcal/mol for the hydromethoxylation of but-2-yne. The latter value can be compared to 26.9 and 22.9 kcal/mol for the monogold-catalysed pathway, depending on whether one or two methanol molecules participate. Thus, the monoaurated process is at least 14.0 kcal/mol more expensive.

The analysis of the geometry of the transition state (**TS**) turns out to be fundamental, describing early or late transition states. When the C···O distance is close to 1.5 Å which is similar to the C-O bond distance in **P**, the corresponding **TS** can be considered a late transition state. This occurs in all the systems studied here except for those based on fluorinated alkynes. Furthermore, when the alkyne has aryl substituents, the **TS** structures have slightly less late character. On the other hand, when two alcohol molecules are involved, the second alcohol molecule somewhat stabilises the developing

positive charge on the alcohol proton, thus dramatically reducing the later transition state character.

The character of the carbon-carbon bond in η^2-alkyne complex **I** is essentially unaffected once the alcohol bonds to either of the carbon atoms, with a small elongation (< 0.09 Å) in all structures studied. In the corresponding step of the dual gold-catalysed mechanism (see **TS(III-IV)** in Figures 2 and Figure S2), the C···O distance in the transition state is 2.474 Å (versus 2.134 Å for the monogold pathway), confirming that the transition state has less late character in the dual gold-catalysed mechanism.

For a more detailed analysis of the structural changes during the hydroalkoxylation, Mayer Bond Orders (MBO) of the main distances involved in the C-O bond formation are collected in Table S2. The MBO for the former C-C of the alkyne does not change whereas the Au-C MBOs change dramatically. However, the MBOs for the Au-C bonds span a range from 0.6 to 0.7, and

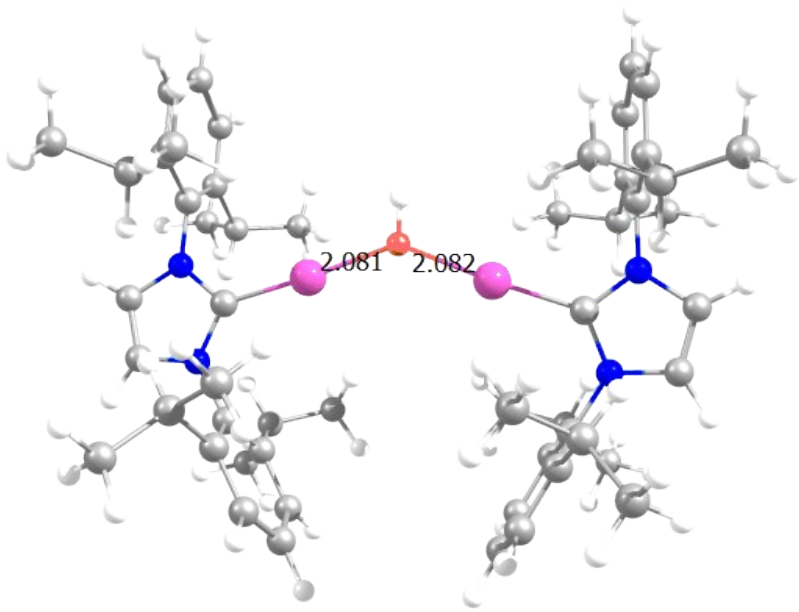
are thus rather far from 1.0 in the initial η^2-alkyne complex **I**. As would be expected, one Au-C bond sees an increase in MBO of around 0.2 – forming a formal Au-C σ-bond in P – while the MBO of the other Au-C bond decreases to 0.1 or lower in P. For the dual gold-catalysed mechanism, in the nucleophilic attack (**III** to **IV**) the MBO of the C-C bond decreases from 2.008 to 1.837. Thus, a significant difference of 0.171 is observed, to be compared with 0.080 and 0.147 for one or two methanol units, in the monogold-catalysed pathway. Furthermore, the new C-O bond in **IV** displays a MBO of 0.772, significantly higher than 0.642 and 0.708 in the monogold-catalysed pathway (with one or two methanol molecules, respectively).

To distinguish between the effects of steric and electronic factors, a natural population analysis has been carried out to evaluate the Natural Bond Orbital (NBO) charges (see Table S7). The charge on the carbon atom in η^2-complex **I** or in adduct **A** would be expected to be slightly positive in order to favour the nucleophilic attack of the alcohol; however, this is not observed – and no trend is evident – even when fluorinated substrates are considered. There is no trend in the charge on gold.

A deeper analysis of the electronic properties was carried out by means of conceptual DFT to discuss the electrophilicity and chemical hardness from the frontier molecular orbitals (Tables S6 and S9). The electrophilicity of the phenol is slightly higher than that of methanol, but more significant differences appear when the different alkynes are evaluated. If there are fluorinated substituents the system is much more electrophilic.

Table S10. 3D view and xyz coordinate data sets and absolute energies in a.u. for DFT optimized complexes.

1A



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H	-5.499039	-3.606052	4.073893
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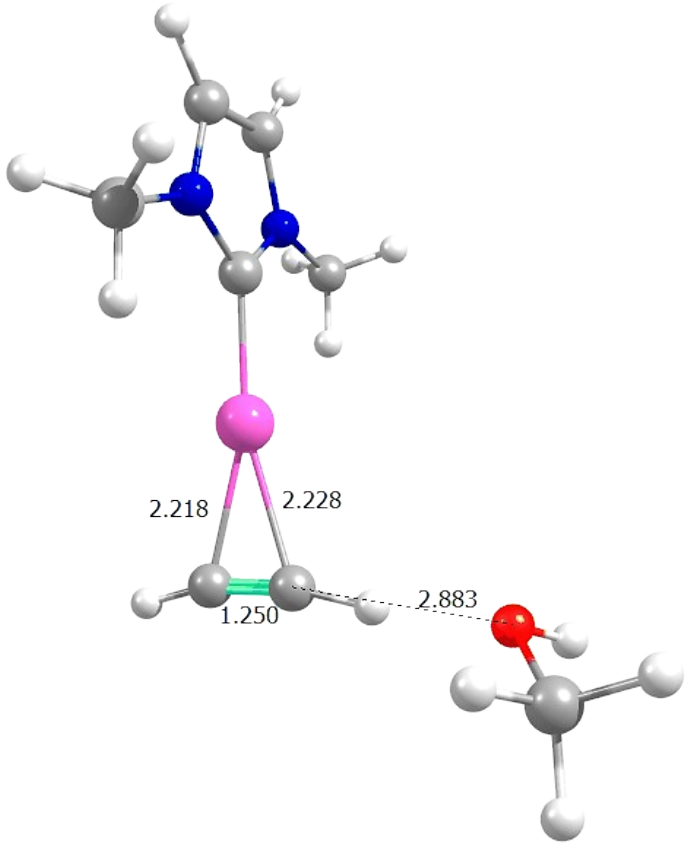

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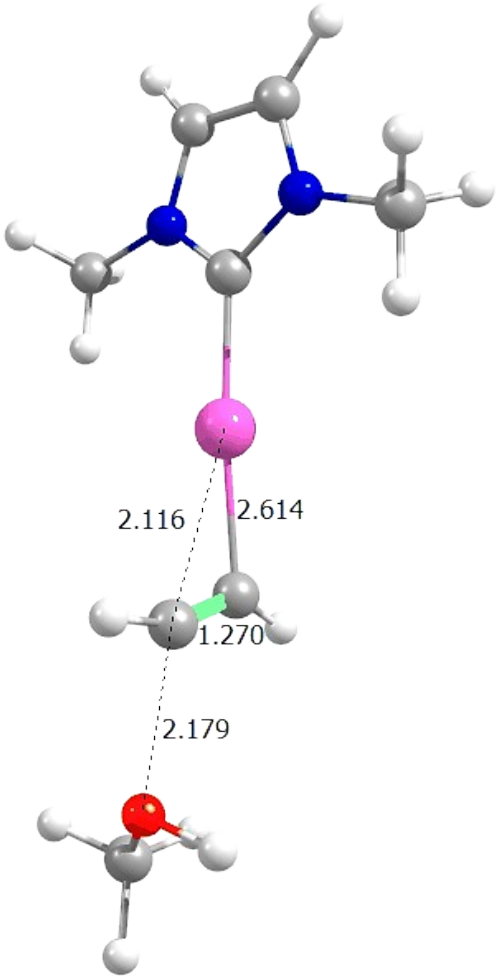

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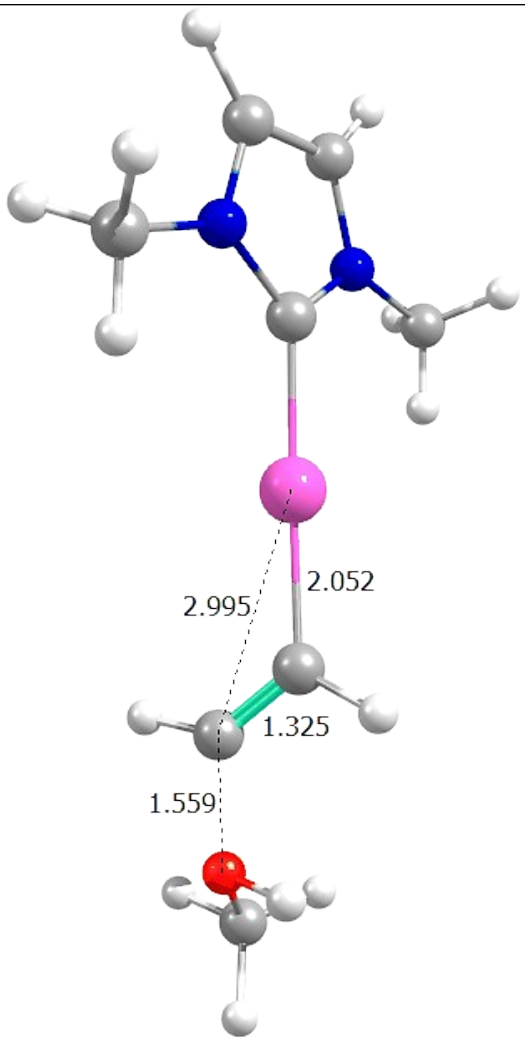

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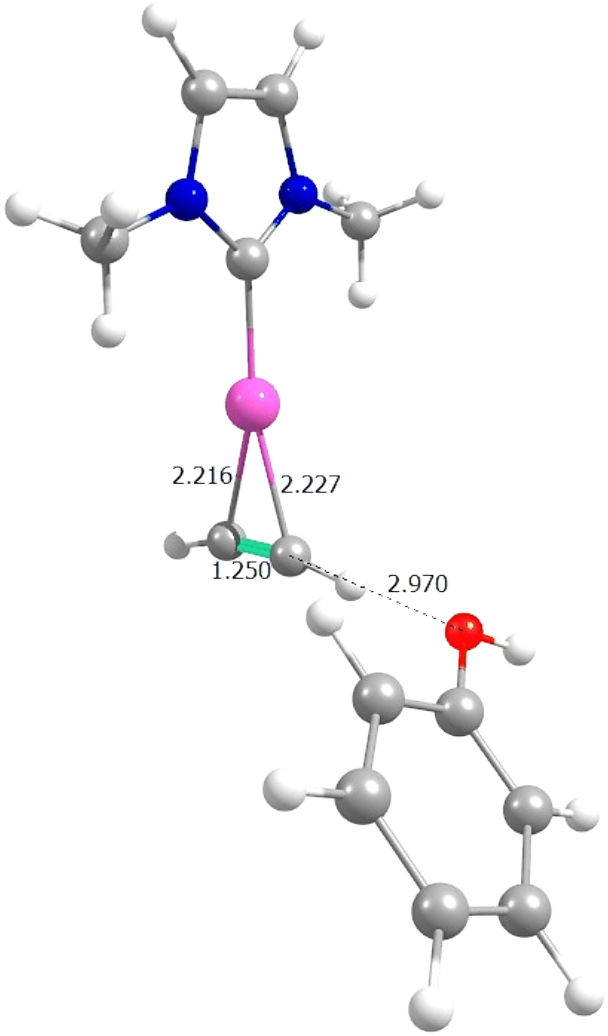
Au	-0.194686000	-0.012327000	-0.192203000
C	-2.220041000	-0.051284000	-0.520691000
C	2.265627000	-2.452112000	0.165255000
C	-3.108514000	-0.326983000	0.423314000
H	4.825849000	-1.329133000	0.462483000
H	4.786871000	1.471714000	0.411530000
H	2.551662000	-2.955134000	1.110082000
H	2.741794000	-2.974495000	-0.688070000
H	1.166779000	-2.490862000	0.048630000
H	1.094973000	2.515286000	-0.022183000
H	2.642629000	3.009837000	-0.809208000
H	2.485334000	3.061189000	0.991493000
O	-4.619338000	-0.433655000	0.054628000
C	-5.543597000	0.547413000	0.667478000
H	-5.259232000	1.571621000	0.359873000
H	-5.442795000	0.414672000	1.758580000
H	-4.683323000	-0.422528000	-0.930490000
H	-6.562991000	0.274784000	0.339797000
H	-2.580254000	0.153274000	-1.551802000
H	-3.056511000	-0.575987000	1.490567000

Zero-point correction= 0.208134 (Hartree/Particle)
Thermal correction to Energy= 0.223866
Thermal correction to Enthalpy= 0.224811
Thermal correction to Gibbs Free Energy= 0.161329
Sum of electronic and zero-point Energies= -633.048722
Sum of electronic and thermal Energies= -633.032990
Sum of electronic and thermal Enthalpies= -633.032046
Sum of electronic and thermal Free Energies= -633.095527

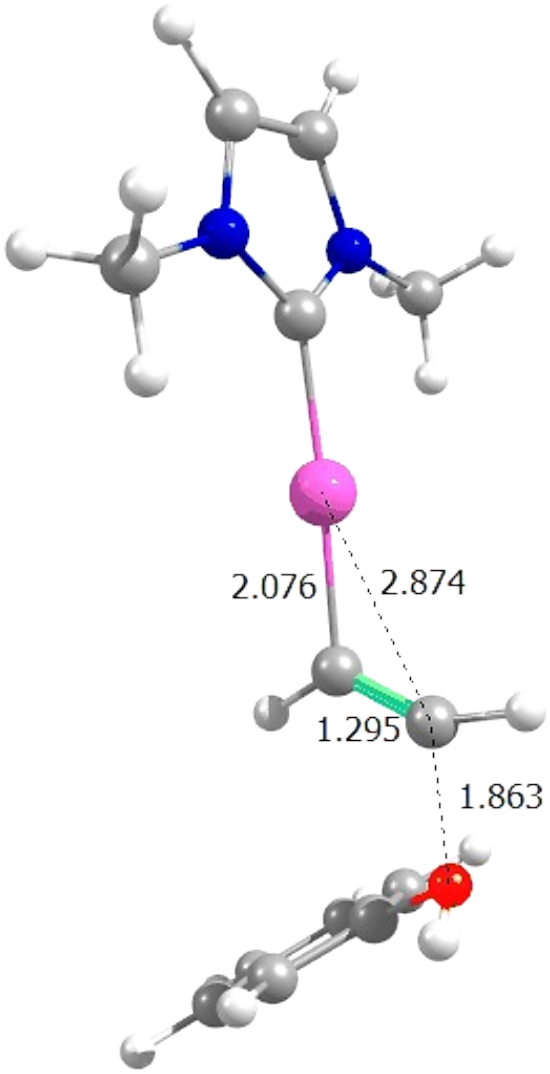
PhOH-CH



C	2.563365000	0.517752000	0.238602000
N	2.900916000	1.773746000	-0.187813000
C	3.996422000	2.244502000	0.517462000
C	4.352681000	1.258130000	1.406217000
N	3.465532000	0.210347000	1.220800000
C	2.217136000	2.532467000	-1.238153000
C	3.506631000	-1.040685000	1.982072000
Au	1.049581000	-0.642327000	-0.443268000
C	-0.931005000	-1.621195000	-0.723726000
C	-0.167362000	-2.093622000	-1.593130000
O	-3.071063000	-0.806698000	1.167303000
H	4.433363000	3.232090000	0.334821000
H	5.159085000	1.222214000	2.146521000
H	2.923422000	2.764595000	-2.059051000
H	1.810665000	3.474946000	-0.821932000
H	1.386632000	1.920074000	-1.633952000
H	2.697505000	-1.701581000	1.621329000
H	3.357234000	-0.834295000	3.059943000
H	4.482423000	-1.542961000	1.833252000
H	-3.378011000	-1.505001000	1.779816000
H	-1.757928000	-1.337503000	-0.035804000
H	0.280493000	-2.643434000	-2.420632000
C	-4.173998000	-0.075636000	0.743105000
C	-5.483804000	-0.451458000	1.091678000
C	-3.941914000	1.058885000	-0.055501000
C	-6.568217000	0.318273000	0.636462000
H	-5.657875000	-1.343811000	1.717090000
C	-5.035289000	1.814778000	-0.509279000
H	-2.909583000	1.347857000	-0.306158000
C	-6.349949000	1.450888000	-0.166411000
H	-7.592341000	0.023473000	0.913361000
H	-4.855048000	2.703869000	-1.133742000
H	-7.201730000	2.049715000	-0.522413000

Zero-point correction= 0.256407 (Hartree/Particle)
Thermal correction to Energy= 0.276286
Thermal correction to Enthalpy= 0.277231
Thermal correction to Gibbs Free Energy= 0.201363
Sum of electronic and zero-point Energies= -824.619446
Sum of electronic and thermal Energies= -824.599567
Sum of electronic and thermal Enthalpies= -824.598622
Sum of electronic and thermal Free Energies= -824.674490

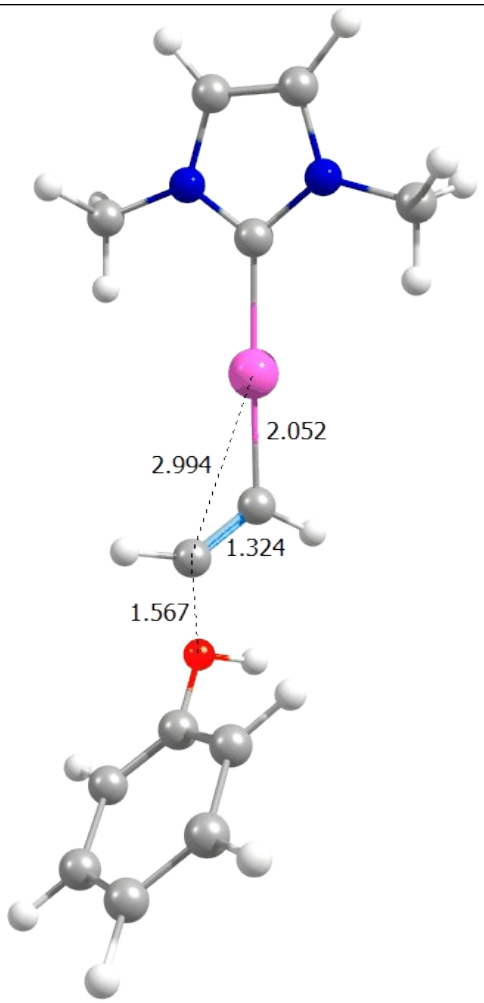
PhOH-CHTs



C	2.847115000	0.061405000	0.170320000
N	3.603994000	1.201269000	0.205963000
C	4.936313000	0.896969000	0.453374000
C	5.014450000	-0.467570000	0.577619000
N	3.727847000	-0.960222000	0.402195000
C	3.096195000	2.559229000	0.009944000
C	3.378155000	-2.379378000	0.466419000
Au	0.834542000	-0.080998000	-0.133439000
C	-1.228153000	-0.225273000	-0.313749000
C	-1.676448000	-0.178742000	-1.527887000
H	5.712797000	1.666280000	0.519550000
H	5.872123000	-1.119388000	0.774236000
H	3.571428000	3.021964000	-0.877548000
H	3.305320000	3.177987000	0.904752000
H	2.003223000	2.504396000	-0.147596000
H	2.297091000	-2.483014000	0.259087000
H	3.597148000	-2.782724000	1.474880000
H	3.952182000	-2.948757000	-0.290882000
H	-1.435440000	-0.049322000	-2.585824000
H	-1.844672000	-0.332042000	0.596824000
C	-5.590209000	-0.951263000	1.257541000
C	-5.903646000	0.366429000	1.633402000
C	-5.413154000	1.452166000	0.883661000
C	-4.613183000	1.230744000	-0.249410000
C	-4.319923000	-0.092728000	-0.605992000
C	-4.779390000	-1.192040000	0.133385000
H	-5.973531000	-1.802309000	1.840863000
H	-6.536364000	0.549160000	2.515163000
H	-5.663804000	2.483663000	1.175000000
H	-4.233473000	2.063061000	-0.860279000
H	-4.522878000	-2.222426000	-0.163973000
O	-3.521490000	-0.287254000	-1.759825000
H	-3.669660000	-1.196703000	-2.102840000

Zero-point correction= 0.257086 (Hartree/Particle)
Thermal correction to Energy= 0.275836
Thermal correction to Enthalpy= 0.276781
Thermal correction to Gibbs Free Energy= 0.204560
Sum of electronic and zero-point Energies= -824.603763
Sum of electronic and thermal Energies= -824.585012
Sum of electronic and thermal Enthalpies= -824.584068
Sum of electronic and thermal Free Energies= -824.656288

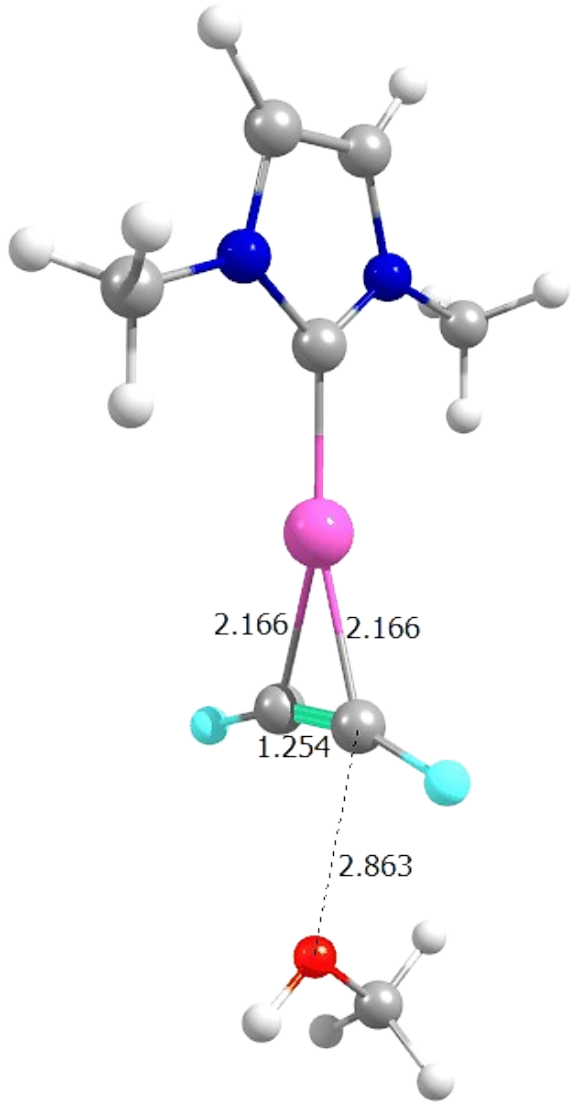
PhOH-CHProd



C	-5.078351000	0.590762000	0.799970000
C	-4.976254000	-0.764354000	0.990083000
N	-3.675798000	-1.118336000	0.654110000
C	-2.959245000	-0.020175000	0.258514000
N	-3.837470000	1.026439000	0.352827000
C	-3.158403000	-2.484810000	0.712309000
Au	-1.008587000	0.040864000	-0.357961000
C	0.927331000	0.125635000	-1.032727000
C	-3.526801000	2.418004000	0.027843000
C	1.929263000	-0.528701000	-0.465853000
H	-5.924238000	1.270955000	0.944503000
H	-5.715973000	-1.495794000	1.331968000
H	-3.661168000	3.059891000	0.920975000
H	-4.186530000	2.777684000	-0.786454000
H	-2.473993000	2.471573000	-0.305593000
H	-2.105449000	-2.473629000	0.375152000
H	-3.747094000	-3.145734000	0.045751000
H	-3.207534000	-2.870691000	1.749883000
H	1.131201000	0.739737000	-1.935324000
H	2.049396000	-1.193715000	0.397524000
C	5.666070000	1.366944000	1.165494000
C	4.538653000	1.090320000	0.371425000
C	4.504492000	-0.142891000	-0.284644000
C	5.502872000	-1.113392000	-0.188322000
C	6.619418000	-0.814785000	0.614432000
C	6.699355000	0.418881000	1.284995000
H	5.731502000	2.329552000	1.695072000
H	3.712496000	1.811509000	0.275952000
H	5.411990000	-2.067934000	-0.727312000
H	7.428850000	-1.554119000	0.712165000
H	7.576423000	0.644268000	1.910636000
O	3.352201000	-0.478843000	-1.121344000
H	3.303384000	0.093544000	-1.924936000

Zero-point correction= 0.258654 (Hartree/Particle)
Thermal correction to Energy= 0.277502
Thermal correction to Enthalpy= 0.278446
Thermal correction to Gibbs Free Energy= 0.206252
Sum of electronic and zero-point Energies= -824.602850
Sum of electronic and thermal Energies= -824.584002
Sum of electronic and thermal Enthalpies= -824.583058
Sum of electronic and thermal Free Energies= -824.655252

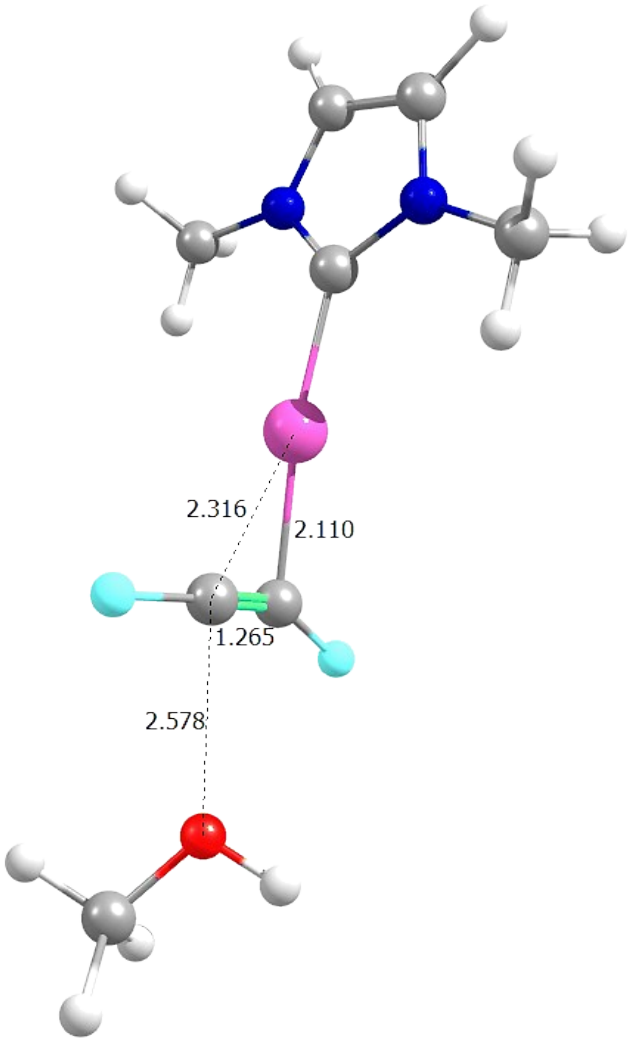
MeOH-FC



C	-2.095212000	-0.057439000	0.000274000
N	-2.865119000	-1.189932000	0.010105000
C	-4.207683000	-0.858818000	0.005691000
C	-4.280726000	0.515840000	-0.006986000
N	-2.980621000	0.987229000	-0.010183000
C	-2.361843000	-2.566808000	0.023093000
C	-2.625319000	2.409430000	-0.022646000
Au	-0.062474000	0.049254000	0.000128000
C	2.008311000	0.160190000	0.626896000
C	2.008421000	0.156346000	-0.626638000
O	4.796431000	0.332544000	-0.001106000
C	5.779358000	-0.701149000	0.000519000
H	-5.001026000	-1.614187000	0.011796000
H	-5.149632000	1.182895000	-0.013746000
H	-2.712091000	-3.106053000	-0.878548000
H	-2.718930000	-3.091218000	0.930758000
H	-1.256991000	-2.542067000	0.027076000
H	-1.524011000	2.500821000	-0.021221000
H	-3.034679000	2.909450000	0.876685000
H	-3.031055000	2.892789000	-0.932679000
H	6.427391000	-0.679968000	-0.906142000
H	5.242555000	-1.670817000	0.007963000
H	5.268837000	1.186057000	-0.006702000
H	6.434611000	-0.670174000	0.901676000
F	2.397352000	0.219293000	1.854718000
F	2.401242000	0.138975000	-1.854590000

Zero-point correction= 0.189803 (Hartree/Particle)
Thermal correction to Energy= 0.209766
Thermal correction to Enthalpy= 0.210711
Thermal correction to Gibbs Free Energy= 0.134226
Sum of electronic and zero-point Energies= -831.337353
Sum of electronic and thermal Energies= -831.317389
Sum of electronic and thermal Enthalpies= -831.316445
Sum of electronic and thermal Free Energies= -831.392930

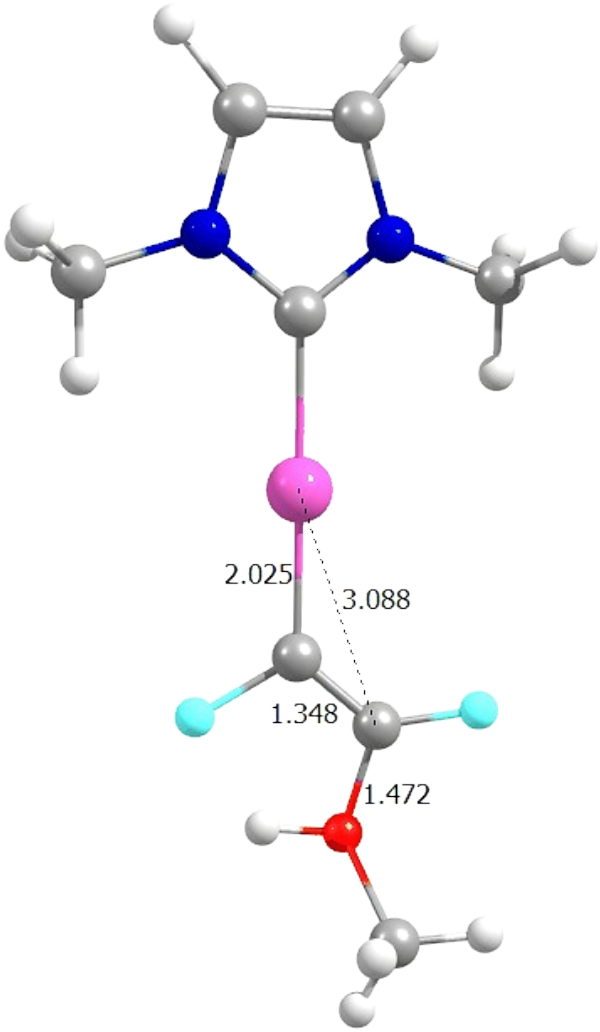
MeOH-FCTs



C	2.089602000	0.020231000	-0.073668000
N	2.883899000	1.128668000	-0.192997000
C	4.215347000	0.760004000	-0.276754000
C	4.254776000	-0.613426000	-0.206949000
N	2.946449000	-1.047227000	-0.081297000
C	2.414582000	2.516565000	-0.229462000
C	2.557780000	-2.456747000	0.020646000
Au	0.065581000	-0.028537000	0.118430000
C	-1.940324000	-0.086804000	0.770003000
C	-2.173168000	-0.057999000	-0.473194000
O	-4.665396000	0.576262000	-0.286893000
C	-5.809469000	-0.268053000	-0.427459000
H	5.023910000	1.491926000	-0.378655000
H	5.103992000	-1.304602000	-0.238050000
H	2.723485000	2.995363000	-1.179047000
H	2.835534000	3.081967000	0.624779000
H	1.311496000	2.520353000	-0.160971000
H	1.458564000	-2.516465000	0.118622000
H	3.028979000	-2.915768000	0.911549000
H	2.873928000	-3.003680000	-0.889013000
H	-5.492892000	-1.161175000	-1.001416000
H	-6.629244000	0.226407000	-0.996062000
H	-4.938978000	1.377134000	0.198180000
H	-6.212831000	-0.612790000	0.552252000
F	-2.457676000	-0.363096000	-1.680690000
F	-2.365754000	0.142316000	1.978252000

Zero-point correction= 0.189703 (Hartree/Particle)
Thermal correction to Energy= 0.208709
Thermal correction to Enthalpy= 0.209654
Thermal correction to Gibbs Free Energy= 0.135996
Sum of electronic and zero-point Energies= -831.336662
Sum of electronic and thermal Energies= -831.317655
Sum of electronic and thermal Enthalpies= -831.316711
Sum of electronic and thermal Free Energies= -831.390368

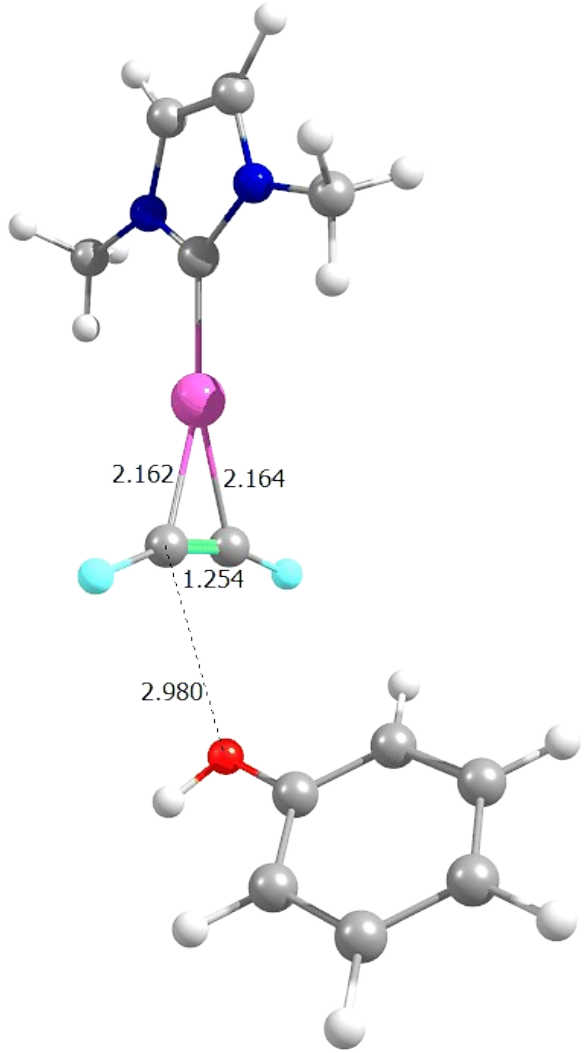
MeOH-FCProd



C	4.180521000	0.999660000	-0.102357000
C	4.326789000	-0.363557000	-0.168400000
N	3.049125000	-0.905615000	-0.128138000
C	2.106707000	0.082835000	-0.038535000
N	2.817510000	1.252321000	-0.022590000
C	2.765472000	-2.340455000	-0.170918000
Au	0.075864000	-0.146382000	0.050763000
C	-1.930799000	-0.397626000	0.145403000
C	2.234965000	2.591582000	0.060789000
C	-2.945190000	0.490248000	0.127207000
H	4.928322000	1.799578000	-0.104594000
H	5.226984000	-0.983096000	-0.238730000
H	2.456786000	3.166024000	-0.860501000
H	2.643110000	3.130790000	0.938122000
H	1.139719000	2.490663000	0.173021000
H	1.670122000	-2.483281000	-0.123933000
H	3.236703000	-2.849746000	0.692812000
H	3.150765000	-2.779120000	-1.112490000
O	-4.301402000	-0.045935000	0.327933000
C	-5.305205000	0.168057000	-0.763646000
H	-4.927775000	-0.296242000	-1.693768000
H	-5.409327000	1.261953000	-0.857465000
H	-4.082373000	-1.025753000	0.460093000
H	-6.240369000	-0.291969000	-0.399737000
F	-2.970653000	1.799992000	0.053113000
F	-2.478317000	-1.691056000	0.281467000

Zero-point correction= 0.193745 (Hartree/Particle)
Thermal correction to Energy= 0.210777
Thermal correction to Enthalpy= 0.211721
Thermal correction to Gibbs Free Energy= 0.144956
Sum of electronic and zero-point Energies= -831.376902
Sum of electronic and thermal Energies= -831.359870
Sum of electronic and thermal Enthalpies= -831.358926
Sum of electronic and thermal Free Energies= -831.425691

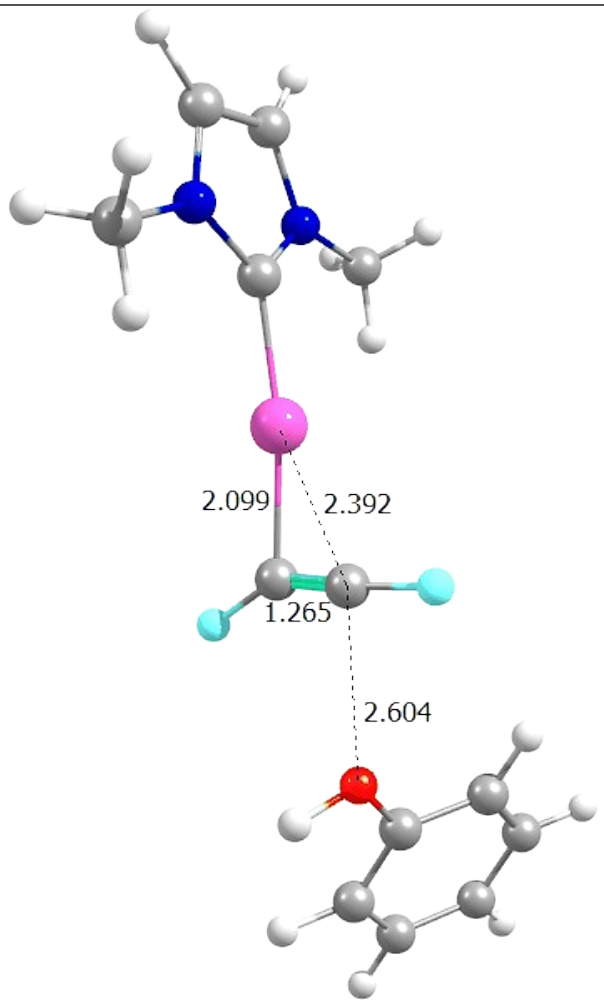
PhOH-FC



C	2.970781000	0.441745000	-0.075020000
N	3.323457000	1.763091000	-0.149951000
C	4.699023000	1.890544000	-0.203867000
C	5.221141000	0.617081000	-0.161511000
N	4.150328000	-0.253968000	-0.083474000
C	2.394662000	2.897513000	-0.170445000
C	4.284914000	-1.712235000	-0.013185000
Au	1.087686000	-0.320979000	0.027252000
C	-0.805261000	-1.076057000	0.755751000
C	-0.864061000	-1.088002000	-0.496944000
O	-3.747270000	-1.521182000	0.120202000
H	5.198991000	2.863161000	-0.268260000
H	6.260926000	0.272763000	-0.181295000
H	2.534330000	3.482749000	-1.100048000
H	2.572874000	3.547856000	0.708026000
H	1.359624000	2.511810000	-0.134872000
H	3.276168000	-2.163072000	0.008062000
H	4.832163000	-1.998137000	0.906280000
H	4.832134000	-2.083558000	-0.901291000
H	-4.137797000	-2.223191000	-0.436176000
F	-1.140483000	-1.165785000	1.998179000
F	-1.279863000	-1.289103000	-1.702029000
C	-4.556768000	-0.407731000	0.040512000
C	-4.279156000	0.670114000	0.905146000
C	-5.626695000	-0.323093000	-0.872316000
C	-5.067655000	1.830295000	0.843699000
H	-3.463002000	0.574726000	1.637868000
C	-6.411168000	0.841991000	-0.920726000
H	-5.846138000	-1.169489000	-1.545738000
C	-6.134728000	1.924857000	-0.068320000
H	-4.852049000	2.666242000	1.527983000
H	-7.247761000	0.898664000	-1.634753000
H	-6.753091000	2.834272000	-0.108329000

Zero-point correction= 0.241614 (Hartree/Particle)
Thermal correction to Energy= 0.264093
Thermal correction to Enthalpy= 0.265037
Thermal correction to Gibbs Free Energy= 0.180064
Sum of electronic and zero-point Energies= -1022.898801
Sum of electronic and thermal Energies= -1022.876321
Sum of electronic and thermal Enthalpies= -1022.875377
Sum of electronic and thermal Free Energies= -1022.960351

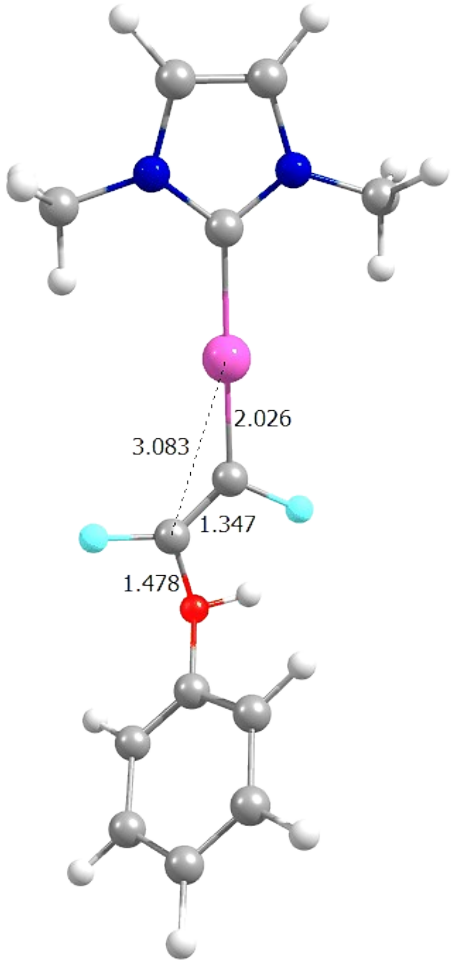
PhOH-FCTs



C	3.135030000	0.237636000	0.023616000
N	3.741310000	1.456477000	0.164460000
C	5.117599000	1.318985000	0.103201000
C	5.377868000	-0.019665000	-0.076421000
N	4.153649000	-0.664837000	-0.121235000
C	3.053988000	2.738169000	0.346211000
C	3.996425000	-2.111345000	-0.296019000
Au	1.141576000	-0.153402000	0.071298000
C	-0.862966000	-0.562587000	0.540321000
C	-1.090411000	-0.527135000	-0.704047000
H	5.798897000	2.172276000	0.190078000
H	6.328908000	-0.554143000	-0.174778000
H	3.273331000	3.410925000	-0.505886000
H	3.386271000	3.213963000	1.289273000
H	1.965296000	2.554248000	0.395765000
H	2.917846000	-2.350341000	-0.329466000
H	4.463219000	-2.649224000	0.552271000
H	4.471144000	-2.431155000	-1.243982000
C	-6.657823000	0.058653000	0.945623000
C	-6.716631000	1.328236000	0.345607000
C	-5.724571000	1.704119000	-0.578605000
C	-4.679873000	0.824741000	-0.904956000
C	-4.626828000	-0.442245000	-0.293195000
C	-5.614037000	-0.829092000	0.632906000
H	-7.430243000	-0.250311000	1.667075000
H	-7.535324000	2.020677000	0.592909000
H	-5.767836000	2.692692000	-1.062188000
H	-3.914286000	1.102922000	-1.645205000
H	-5.568944000	-1.824130000	1.108238000
O	-3.580963000	-1.282710000	-0.635199000
H	-3.735200000	-2.150988000	-0.213018000
F	-1.305101000	-0.246889000	-1.928135000
F	-1.328365000	-0.911921000	1.708133000

Zero-point correction= 0.241319 (Hartree/Particle)
Thermal correction to Energy= 0.262987
Thermal correction to Enthalpy= 0.263931
Thermal correction to Gibbs Free Energy= 0.182226
Sum of electronic and zero-point Energies= -1022.897662
Sum of electronic and thermal Energies= -1022.875995
Sum of electronic and thermal Enthalpies= -1022.875051
Sum of electronic and thermal Free Energies= -1022.956756

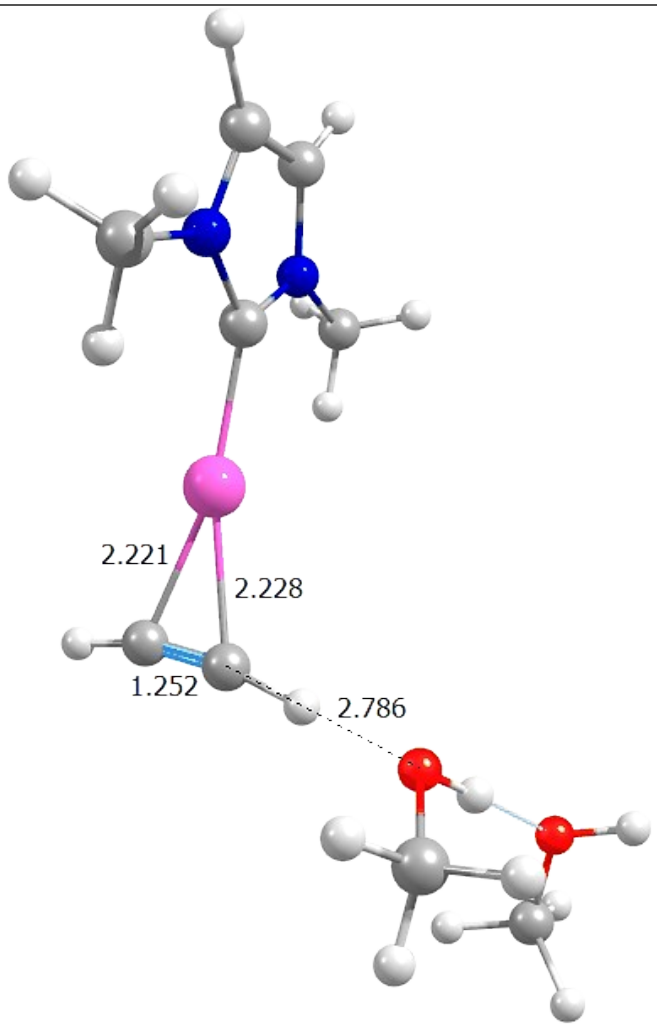
PhOH-FCProd



C	-5.091499000	1.102891000	-0.688750000
C	-5.283971000	-0.255870000	-0.669572000
N	-4.051120000	-0.830752000	-0.390484000
C	-3.091405000	0.132703000	-0.233918000
N	-3.746362000	1.320112000	-0.420443000
C	-3.826401000	-2.271853000	-0.274065000
Au	-1.111539000	-0.148642000	0.195478000
C	0.844292000	-0.446093000	0.633329000
C	-3.128063000	2.643926000	-0.350400000
C	1.873989000	0.418840000	0.716001000
H	-5.795209000	1.922071000	-0.869895000
H	-6.188445000	-0.851960000	-0.829847000
H	-3.612251000	3.250838000	0.439957000
H	-3.223342000	3.163922000	-1.324165000
H	-2.056908000	2.517907000	-0.107491000
H	-2.751046000	-2.445649000	-0.084622000
H	-4.118393000	-2.780929000	-1.213648000
H	-4.416281000	-2.685467000	0.567803000
C	5.421369000	-0.771077000	-1.750556000
C	4.300271000	-0.849275000	-0.904172000
C	4.327170000	-0.059461000	0.244797000
C	5.360485000	0.798662000	0.609699000
C	6.466057000	0.861908000	-0.259775000
C	6.494501000	0.080855000	-1.429063000
H	5.449495000	-1.380858000	-2.666291000
H	3.443686000	-1.500017000	-1.138096000
H	5.307998000	1.390913000	1.534644000
H	7.308354000	1.526121000	-0.013708000
H	7.364906000	0.136446000	-2.100330000
O	3.170755000	-0.121163000	1.175724000
H	2.914297000	-1.076819000	1.377074000
F	1.955154000	1.712110000	0.529788000
F	1.311543000	-1.736220000	0.958569000

Zero-point correction= 0.244436 (Hartree/Particle)
Thermal correction to Energy= 0.264585
Thermal correction to Enthalpy= 0.265529
Thermal correction to Gibbs Free Energy= 0.189975
Sum of electronic and zero-point Energies= -1022.931228
Sum of electronic and thermal Energies= -1022.911079
Sum of electronic and thermal Enthalpies= -1022.910135
Sum of electronic and thermal Free Energies= -1022.985690

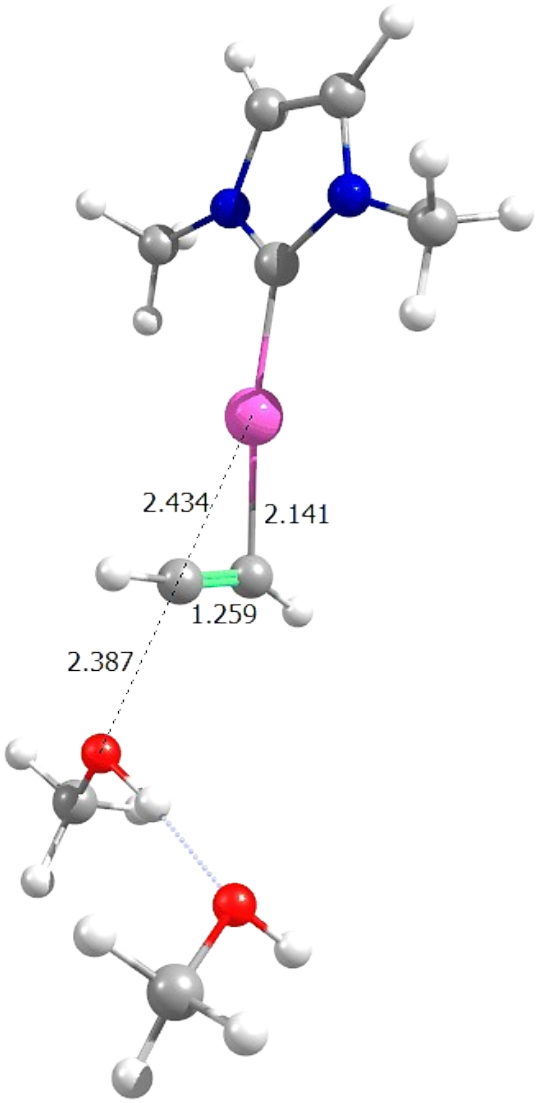
MeOH-CH-MeOH



C	2.180856000	0.306899000	-0.282598000
N	2.701074000	1.572387000	-0.241905000
C	3.888588000	1.630793000	-0.954229000
C	4.115882000	0.370890000	-1.453666000
N	3.061767000	-0.424393000	-1.032539000
C	2.107067000	2.715371000	0.454809000
C	2.927593000	-1.845888000	-1.359117000
Au	0.474820000	-0.346582000	0.590726000
C	-1.009530000	-1.167316000	2.024145000
C	-1.647540000	-0.899988000	0.980827000
H	4.472950000	2.552154000	-1.049611000
H	4.935883000	-0.015807000	-2.068136000
H	1.903580000	3.533334000	-0.263626000
H	2.793720000	3.078830000	1.244391000
H	1.157253000	2.391277000	0.917980000
H	2.013787000	-2.235138000	-0.874120000
H	3.806992000	-2.405438000	-0.984723000
H	2.844296000	-1.978209000	-2.455707000
H	-0.692618000	-1.479792000	3.018312000
H	-2.394604000	-0.721809000	0.133328000
C	-4.150445000	-1.553203000	-1.704401000
H	-4.471173000	-1.298659000	-2.739878000
H	-3.452526000	-2.412408000	-1.771247000
O	-3.466393000	-0.468941000	-1.084455000
H	-4.098777000	0.303052000	-0.988707000
H	-5.047215000	-1.882805000	-1.130604000
C	-6.296863000	1.519469000	0.096021000
H	-6.002217000	0.874212000	0.946058000
H	-6.553660000	2.524644000	0.496339000
H	-7.199864000	1.078495000	-0.382195000
O	-5.176985000	1.575989000	-0.794863000
H	-5.413087000	2.119549000	-1.570314000

Zero-point correction= 0.256156 (Hartree/Particle)
Thermal correction to Energy= 0.277935
Thermal correction to Enthalpy= 0.278879
Thermal correction to Gibbs Free Energy= 0.197173
Sum of electronic and zero-point Energies= -748.660520
Sum of electronic and thermal Energies= -748.638741
Sum of electronic and thermal Enthalpies= -748.637797
Sum of electronic and thermal Free Energies= -748.719504

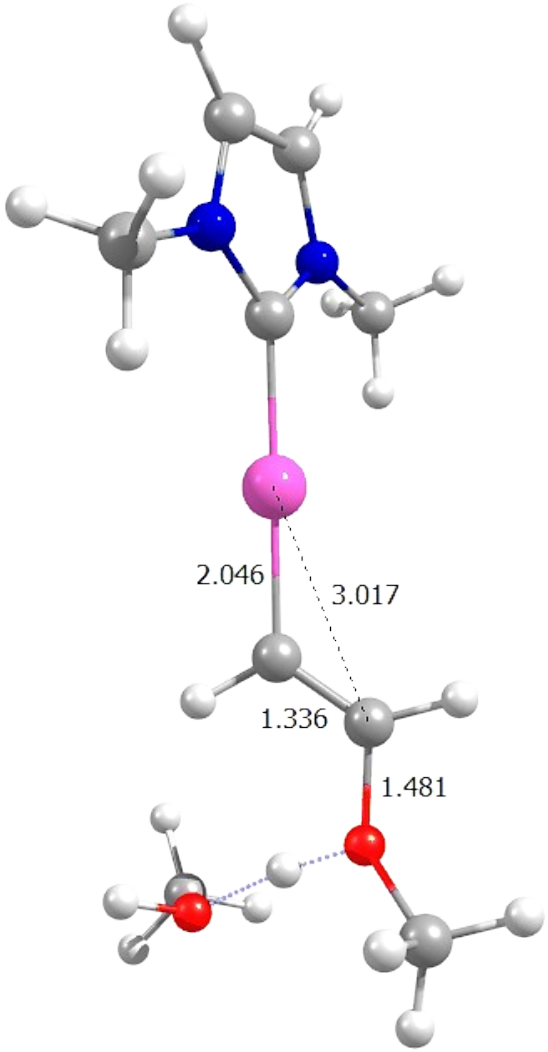
MeOH-CHTs-MeOH



C	-2.470613000	0.189207000	0.129654000
N	-3.114243000	1.396915000	0.123317000
C	-4.463896000	1.228570000	0.394183000
C	-4.668863000	-0.118001000	0.572883000
N	-3.439360000	-0.737286000	0.405601000
C	-2.486359000	2.694028000	-0.135504000
C	-3.227035000	-2.181307000	0.524380000
Au	-0.508412000	-0.160377000	-0.242376000
C	1.447663000	-0.563302000	-1.013769000
C	1.868070000	-0.488538000	0.170125000
O	4.194075000	-0.830096000	0.585694000
C	4.784395000	-2.007186000	0.052773000
H	-5.164488000	2.069192000	0.438088000
H	-5.582200000	-0.676540000	0.803699000
H	-2.640832000	3.369603000	0.728437000
H	-2.919928000	3.152863000	-1.045818000
H	-1.402764000	2.536680000	-0.287091000
H	-2.168493000	-2.402379000	0.295289000
H	-3.875882000	-2.720111000	-0.193370000
H	-3.456465000	-2.517301000	1.554805000
H	4.693004000	-2.079835000	-1.057700000
H	4.274304000	-2.887224000	0.494542000
H	4.702123000	-0.041048000	0.235195000
H	5.865484000	-2.078912000	0.312582000
H	2.085235000	-0.405918000	1.230279000
H	1.639747000	-0.723192000	-2.077546000
C	6.626159000	1.731237000	0.772743000
H	6.816760000	2.823177000	0.683594000
H	6.194120000	1.532968000	1.772425000
H	7.593456000	1.186492000	0.696484000
O	5.666831000	1.281717000	-0.192799000
H	6.042253000	1.392612000	-1.086604000

Zero-point correction= 0.255538 (Hartree/Particle)
Thermal correction to Energy= 0.277032
Thermal correction to Enthalpy= 0.277976
Thermal correction to Gibbs Free Energy= 0.197792
Sum of electronic and zero-point Energies= -748.647365
Sum of electronic and thermal Energies= -748.625872
Sum of electronic and thermal Enthalpies= -748.624927
Sum of electronic and thermal Free Energies= -748.705112

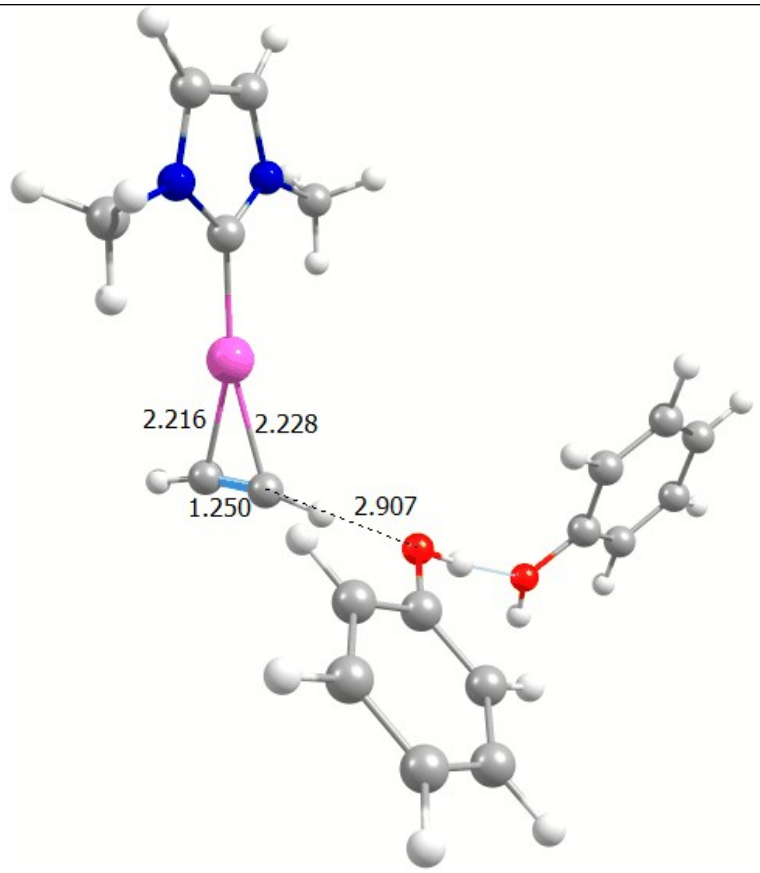
MeOH-CHProd-MeOH



C	-2.381697000	0.043106000	-0.053908000
N	-3.169099000	1.133152000	0.208861000
C	-4.515315000	0.816769000	0.074263000
C	-4.575492000	-0.506966000	-0.281560000
N	-3.264304000	-0.960505000	-0.355156000
C	-2.671120000	2.458360000	0.573800000
C	-2.889264000	-2.330165000	-0.702490000
Au	-0.333274000	-0.061699000	-0.006965000
C	1.709565000	-0.170238000	0.010531000
C	2.475471000	0.003142000	1.091753000
O	3.953758000	-0.008227000	1.010160000
C	4.659246000	-0.894693000	1.934140000
H	-5.312180000	1.549239000	0.240212000
H	-5.435067000	-1.154139000	-0.484838000
H	-3.079763000	2.764427000	1.557205000
H	-2.962445000	3.203733000	-0.192898000
H	-1.568021000	2.409872000	0.634829000
H	-1.785432000	-2.396198000	-0.709627000
H	-3.278930000	-2.591630000	-1.706248000
H	-3.293306000	-3.041660000	0.045023000
H	4.363342000	-1.947317000	1.754810000
H	4.394786000	-0.586448000	2.962420000
H	4.338843000	-0.061366000	-0.006600000
H	5.740008000	-0.743784000	1.760845000
H	2.193733000	0.220027000	2.132359000
H	2.238246000	-0.373141000	-0.943846000
C	5.275812000	1.163493000	-1.910919000
H	4.368859000	1.583325000	-2.392023000
H	5.640344000	1.862988000	-1.136811000
H	6.074545000	1.007993000	-2.662429000
O	4.986904000	-0.089126000	-1.236706000
H	4.676376000	-0.758266000	-1.879420000

Zero-point correction= 0.259457 (Hartree/Particle)
Thermal correction to Energy= 0.279430
Thermal correction to Enthalpy= 0.280374
Thermal correction to Gibbs Free Energy= 0.205257
Sum of electronic and zero-point Energies= -748.669146
Sum of electronic and thermal Energies= -748.649174
Sum of electronic and thermal Enthalpies= -748.648230
Sum of electronic and thermal Free Energies= -748.723347

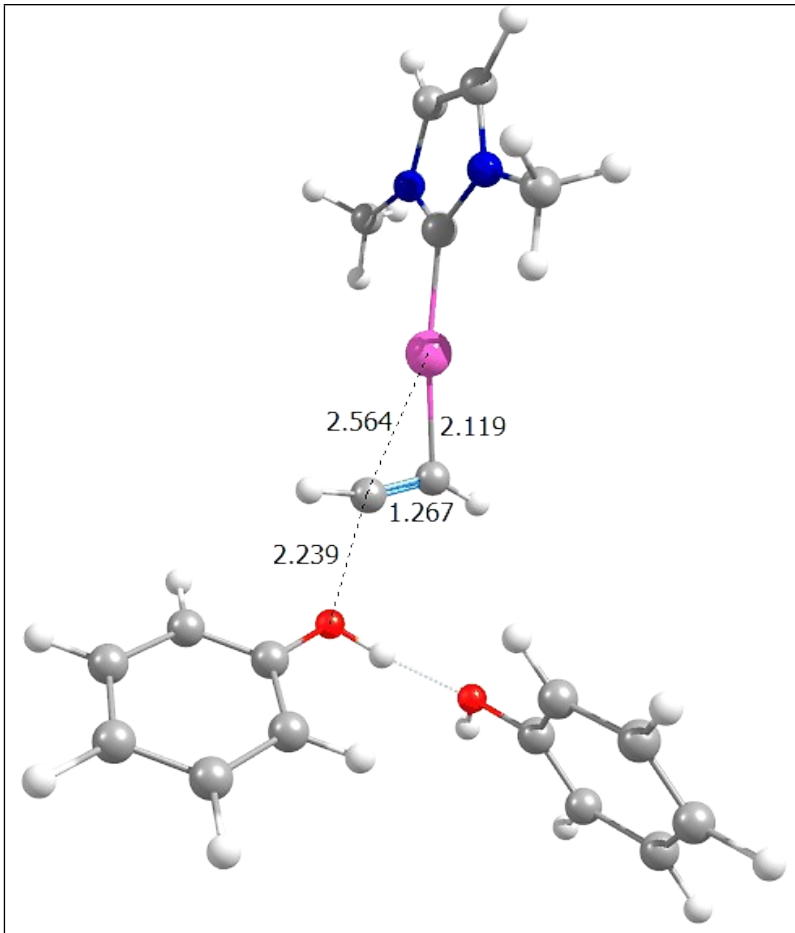
PhOH-CH-PhOH



C	3.340495000	-0.649136000	0.546793000
N	4.150781000	0.058850000	1.392734000
C	4.877694000	-0.802409000	2.198755000
C	4.513091000	-2.080350000	1.847596000
N	3.572522000	-1.966406000	0.836510000
C	4.249517000	1.518938000	1.456243000
C	2.931016000	-3.108949000	0.181927000
Au	2.068987000	0.097428000	-0.842054000
C	0.261039000	0.899327000	-1.868473000
C	1.180923000	0.881216000	-2.715256000
O	-2.131650000	1.095198000	-0.229036000
H	5.589248000	-0.444775000	2.950639000
H	4.846630000	-3.049103000	2.234624000
H	5.289668000	1.837972000	1.249190000
H	3.944749000	1.877282000	2.459002000
H	3.576491000	1.951624000	0.693796000
H	2.221587000	-2.729332000	-0.575904000
H	2.379462000	-3.713241000	0.928390000
H	3.694014000	-3.739863000	-0.314630000
H	-2.898427000	0.529891000	-0.524922000
H	-0.678368000	0.991661000	-1.264119000
H	1.791911000	0.967583000	-3.613179000
C	-2.581276000	2.310946000	0.247565000
C	-3.953621000	2.629588000	0.291476000
C	-1.624831000	3.241667000	0.699901000
C	-4.360211000	3.880900000	0.785044000
H	-4.695829000	1.893468000	-0.055048000
C	-2.045115000	4.490408000	1.185712000
H	-0.556024000	2.977347000	0.673928000
C	-3.412145000	4.817662000	1.231652000
H	-5.434290000	4.122459000	0.818950000
H	-1.293218000	5.215166000	1.536217000
H	-3.736653000	5.796565000	1.615736000
C	-5.110813000	-4.044795000	1.135770000
C	-4.190452000	-3.109068000	1.642349000
C	-3.865881000	-1.954897000	0.911267000
C	-4.475374000	-1.743081000	-0.338557000
C	-5.396783000	-2.668575000	-0.858785000
C	-5.711156000	-3.819186000	-0.114698000
H	-5.363197000	-4.945021000	1.716234000
H	-3.721132000	-3.273564000	2.625118000
H	-3.154569000	-1.210600000	1.300661000
H	-5.870994000	-2.491258000	-1.839168000
H	-6.435535000	-4.542167000	-0.521021000
O	-4.133606000	-0.590951000	-1.034451000
H	-4.643264000	-0.541216000	-1.866708000

Zero-point correction= 0.359423 (Hartree/Particle)
Thermal correction to Energy= 0.386770
Thermal correction to Enthalpy= 0.387715
Thermal correction to Gibbs Free Energy= 0.290780
Sum of electronic and zero-point Energies= -1131.780890
Sum of electronic and thermal Energies= -1131.753543
Sum of electronic and thermal Enthalpies= -1131.752599
Sum of electronic and thermal Free Energies= -1131.849533

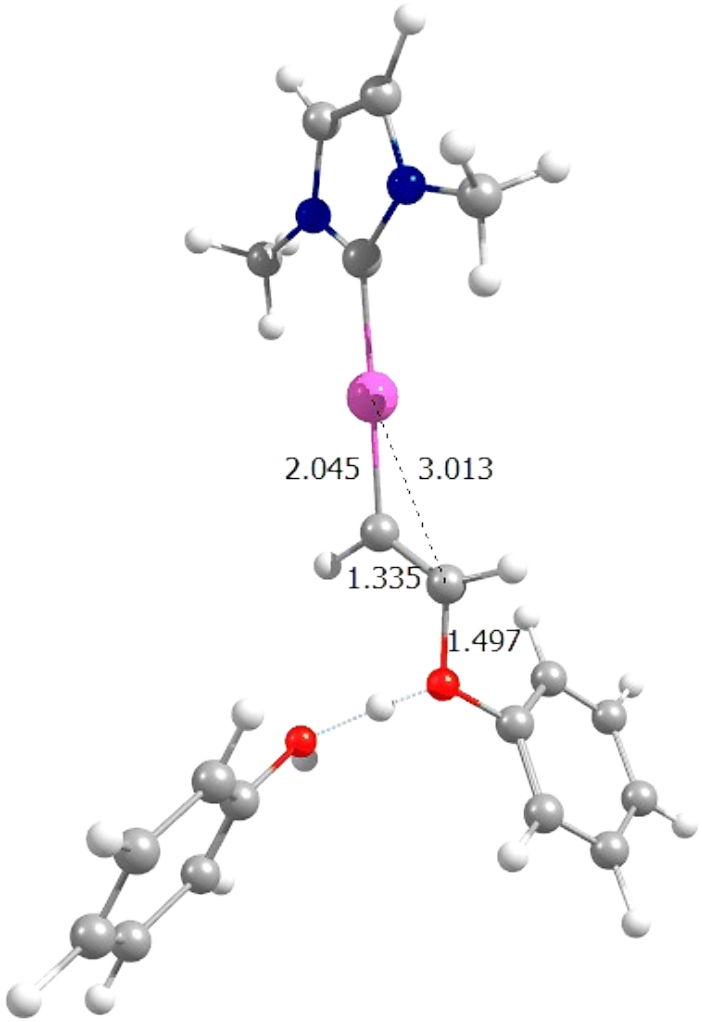
PhOH-CHTs-PhOH



C	3.882256000	-0.264650000	0.271201000
N	4.363472000	-0.910434000	1.377584000
C	5.747023000	-0.820181000	1.429519000
C	6.140134000	-0.102319000	0.326745000
N	4.986541000	0.227571000	-0.369908000
C	3.549159000	-1.598910000	2.380359000
C	4.973529000	0.994476000	-1.616928000
Au	1.947716000	-0.116432000	-0.327419000
C	-0.012088000	-0.219175000	-1.126590000
C	-0.407753000	0.860906000	-0.596042000
H	6.335547000	-1.267235000	2.237648000
H	7.137572000	0.196629000	-0.012454000
H	3.692463000	-1.131217000	3.374288000
H	3.831422000	-2.668837000	2.431404000
H	2.486503000	-1.515610000	2.087323000
H	3.923201000	1.139637000	-1.929625000
H	5.518110000	0.444411000	-2.409486000
H	5.448463000	1.982776000	-1.460347000
H	-0.435318000	1.781153000	-0.013149000
H	-0.339353000	-1.033441000	-1.781814000
C	-4.642820000	2.849739000	1.534739000
C	-4.177490000	4.176503000	1.571516000
C	-3.157707000	4.579669000	0.690865000
C	-2.605206000	3.667962000	-0.224064000
C	-3.074679000	2.338653000	-0.249070000
C	-4.091441000	1.922335000	0.634718000
H	-5.444280000	2.526241000	2.217307000
H	-4.612883000	4.895903000	2.281546000
H	-2.795552000	5.619650000	0.704087000
H	-1.833659000	3.980646000	-0.945194000
H	-4.451547000	0.881339000	0.614664000
O	-2.487039000	1.476298000	-1.152426000
H	-2.985090000	0.609794000	-1.215516000
C	-4.105518000	-2.949744000	1.394042000
C	-3.596507000	-2.003082000	0.489260000
C	-4.209644000	-1.857300000	-0.768185000
C	-5.318853000	-2.643889000	-1.124669000
C	-5.814594000	-3.589183000	-0.210045000
C	-5.212888000	-3.745648000	1.050480000
H	-3.628513000	-3.063986000	2.380089000
H	-2.727942000	-1.378019000	0.747632000
H	-5.795177000	-2.520633000	-2.112164000
H	-6.682809000	-4.205544000	-0.490479000
H	-5.606897000	-4.485226000	1.763648000
O	-3.679824000	-0.912320000	-1.640168000
H	-4.208533000	-0.899000000	-2.463363000

Zero-point correction= 0.358816 (Hartree/Particle)
Thermal correction to Energy= 0.385597
Thermal correction to Enthalpy= 0.386541
Thermal correction to Gibbs Free Energy= 0.291412
Sum of electronic and zero-point Energies= -1131.768197
Sum of electronic and thermal Energies= -1131.741416
Sum of electronic and thermal Enthalpies= -1131.740472
Sum of electronic and thermal Free Energies= -1131.835601

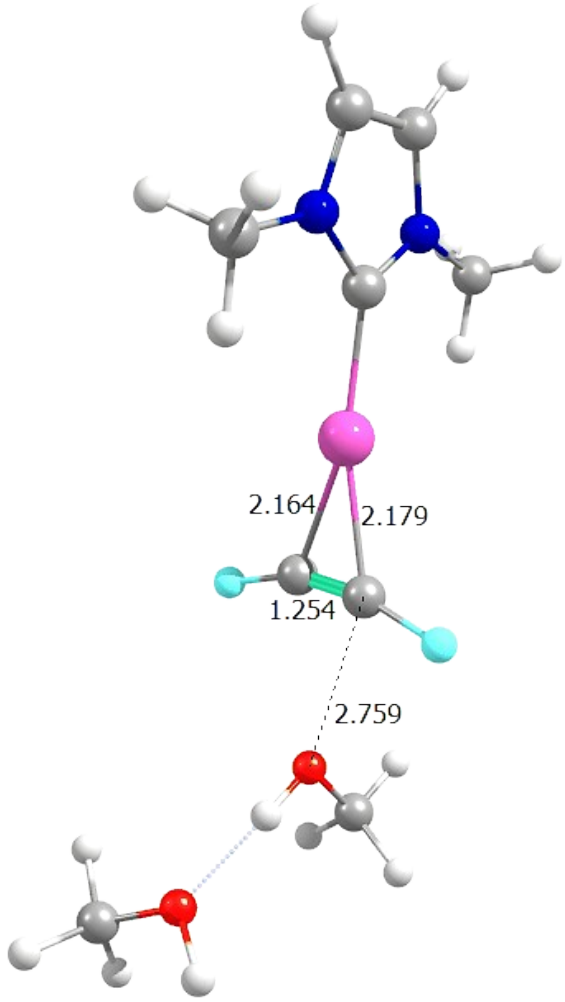
PhOH-CHProd-PhOH



C	-6.129120000	0.684397000	0.441289000
C	-6.097682000	0.139609000	-0.817654000
N	-4.766390000	-0.143381000	-1.096863000
C	-3.959976000	0.208806000	-0.046351000
N	-4.816339000	0.718027000	0.894603000
C	-4.300029000	-0.738816000	-2.347555000
Au	-1.922365000	0.024608000	0.089886000
C	0.109358000	-0.127888000	0.264259000
C	-4.413515000	1.236235000	2.200757000
C	0.880410000	-0.919670000	-0.484062000
H	-6.969528000	1.046400000	1.042689000
H	-6.905410000	-0.066703000	-1.527592000
H	-4.922975000	0.675878000	3.009630000
H	-4.666499000	2.312094000	2.282952000
H	-3.319684000	1.109726000	2.301988000
H	-3.198127000	-0.819504000	-2.302754000
H	-4.585099000	-0.099510000	-3.206547000
H	-4.736637000	-1.748802000	-2.480288000
H	0.623382000	0.495110000	1.023695000
H	0.640287000	-1.625216000	-1.290917000
C	3.248051000	-4.325431000	0.864849000
C	2.524768000	-3.131430000	0.691699000
C	3.072523000	-2.151819000	-0.143615000
C	4.291164000	-2.306157000	-0.813706000
C	5.003712000	-3.502487000	-0.616761000
C	4.483191000	-4.508686000	0.217207000
H	2.839933000	-5.115375000	1.513884000
H	1.556207000	-2.966361000	1.187837000
H	4.666457000	-1.512405000	-1.476850000
H	5.965749000	-3.650583000	-1.130880000
H	5.042377000	-5.446085000	0.359038000
O	2.371370000	-0.907438000	-0.344859000
H	2.756724000	-0.113361000	0.261394000
C	5.857395000	3.571706000	0.338783000
C	5.212523000	2.498299000	0.978824000
C	4.021913000	2.003096000	0.429097000
C	3.460125000	2.543917000	-0.736175000
C	4.122823000	3.611017000	-1.366595000
C	5.317380000	4.127423000	-0.833599000
H	6.790866000	3.970555000	0.764639000
H	5.637194000	2.057328000	1.896456000
H	2.514956000	2.146606000	-1.136734000
H	3.691710000	4.046080000	-2.281411000
H	5.826833000	4.966234000	-1.331233000
O	3.339160000	0.934089000	1.048202000
H	3.782942000	0.685398000	1.884934000

Zero-point correction= 0.361436 (Hartree/Particle)
Thermal correction to Energy= 0.387344
Thermal correction to Enthalpy= 0.388288
Thermal correction to Gibbs Free Energy= 0.296792
Sum of electronic and zero-point Energies= -1131.778686
Sum of electronic and thermal Energies= -1131.752779
Sum of electronic and thermal Enthalpies= -1131.751834
Sum of electronic and thermal Free Energies= -1131.843331

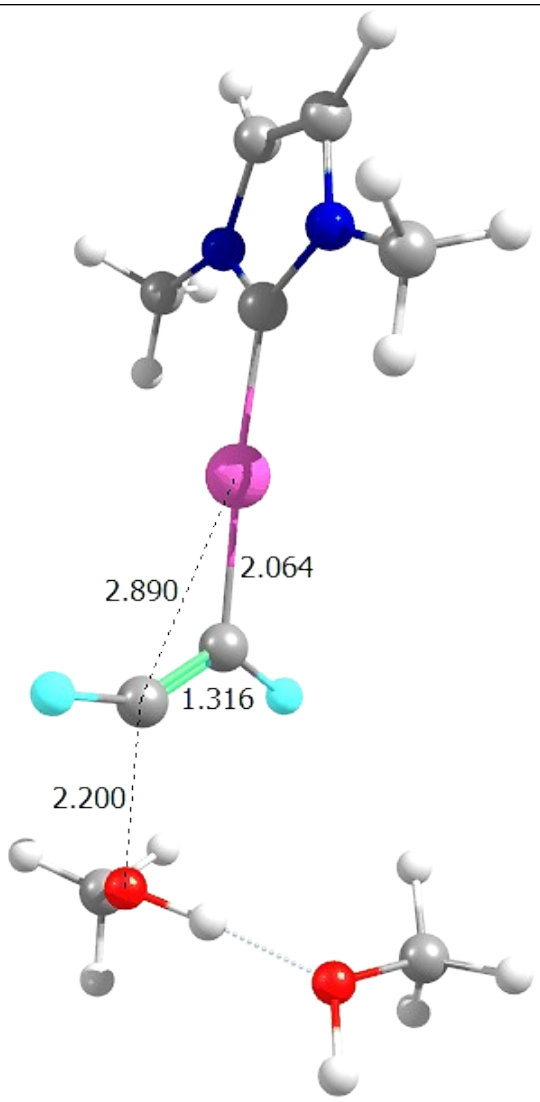
MeOH-FC-MeOH



C	-2.687821000	0.189732000	0.017309000
N	-3.658807000	-0.757261000	0.204701000
C	-4.913638000	-0.176650000	0.157537000
C	-4.723569000	1.168384000	-0.063541000
N	-3.357805000	1.372550000	-0.147164000
C	-3.426503000	-2.188957000	0.416654000
C	-2.737394000	2.680969000	-0.373553000
Au	-0.671567000	-0.098425000	-0.004832000
C	1.402158000	-0.304743000	0.579241000
C	1.370083000	-0.483533000	-0.661903000
O	4.064716000	-0.742470000	-0.126487000
C	4.844577000	-1.922949000	-0.076212000
H	-5.835567000	-0.754833000	0.282673000
H	-5.448675000	1.983103000	-0.165217000
H	-3.861404000	-2.771828000	-0.418794000
H	-3.887820000	-2.508222000	1.371273000
H	-2.337133000	-2.370278000	0.459825000
H	-1.641279000	2.549942000	-0.426614000
H	-2.983754000	3.367112000	0.460244000
H	-3.100471000	3.110862000	-1.327280000
H	5.385314000	-2.132908000	-1.031249000
H	4.169790000	-2.784035000	0.113334000
H	4.682155000	0.018947000	-0.293744000
H	5.601920000	-1.912771000	0.744733000
F	1.851853000	-0.044458000	1.759618000
F	1.670393000	-0.854911000	-1.857997000
C	6.561919000	1.732636000	0.680788000
H	5.911687000	1.582602000	1.564516000
H	6.842686000	2.808480000	0.634136000
H	7.484899000	1.126306000	0.822522000
O	5.807009000	1.328468000	-0.464564000
H	6.374826000	1.393056000	-1.255489000

Zero-point correction= 0.241435 (Hartree/Particle)
Thermal correction to Energy= 0.266071
Thermal correction to Enthalpy= 0.267015
Thermal correction to Gibbs Free Energy= 0.175361
Sum of electronic and zero-point Energies= -946.934035
Sum of electronic and thermal Energies= -946.909400
Sum of electronic and thermal Enthalpies= -946.908456
Sum of electronic and thermal Free Energies= -947.000110

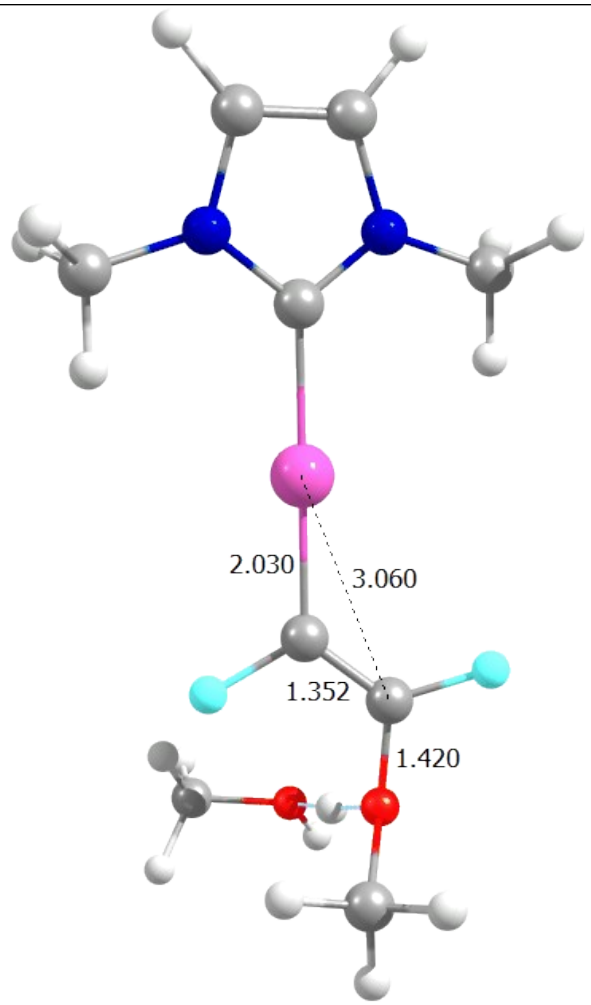
MeOH-FCTs-MeOH



C	2.608190000	0.115414000	0.054116000
N	3.353718000	1.200929000	-0.316588000
C	4.704592000	0.956378000	-0.113155000
C	4.805023000	-0.312862000	0.401248000
N	3.513001000	-0.810190000	0.497560000
C	2.819237000	2.450081000	-0.860900000
C	3.182678000	-2.142639000	1.005725000
Au	0.578501000	-0.076988000	-0.004496000
C	-1.474517000	-0.248049000	0.128418000
C	-2.095587000	-0.562163000	-0.988734000
O	-4.274897000	-0.800010000	-0.804232000
C	-4.660092000	-1.857140000	0.086339000
H	5.478037000	1.694800000	-0.349272000
H	5.682877000	-0.894499000	0.701825000
H	3.207114000	2.617521000	-1.885022000
H	3.106890000	3.301521000	-0.213335000
H	1.716808000	2.374744000	-0.895726000
H	2.087068000	-2.278801000	0.947786000
H	3.507677000	-2.240764000	2.060244000
H	3.680570000	-2.918694000	0.391867000
H	-4.285509000	-2.812869000	-0.326386000
H	-5.770234000	-1.903051000	0.123786000
H	-4.570162000	0.100340000	-0.416111000
H	-4.263791000	-1.716366000	1.113203000
F	-1.967332000	-0.795446000	-2.235535000
F	-2.099076000	-0.074438000	1.304334000
C	-5.038698000	1.964247000	1.441869000
H	-4.094829000	1.581093000	1.871891000
H	-5.020152000	3.073858000	1.482483000
H	-5.891157000	1.588650000	2.049143000
O	-5.093361000	1.498727000	0.083150000
H	-5.901035000	1.838986000	-0.348071000

Zero-point correction= 0.242325 (Hartree/Particle)
Thermal correction to Energy= 0.264738
Thermal correction to Enthalpy= 0.265682
Thermal correction to Gibbs Free Energy= 0.184349
Sum of electronic and zero-point Energies= -946.954047
Sum of electronic and thermal Energies= -946.931634
Sum of electronic and thermal Enthalpies= -946.930690
Sum of electronic and thermal Free Energies= -947.012023

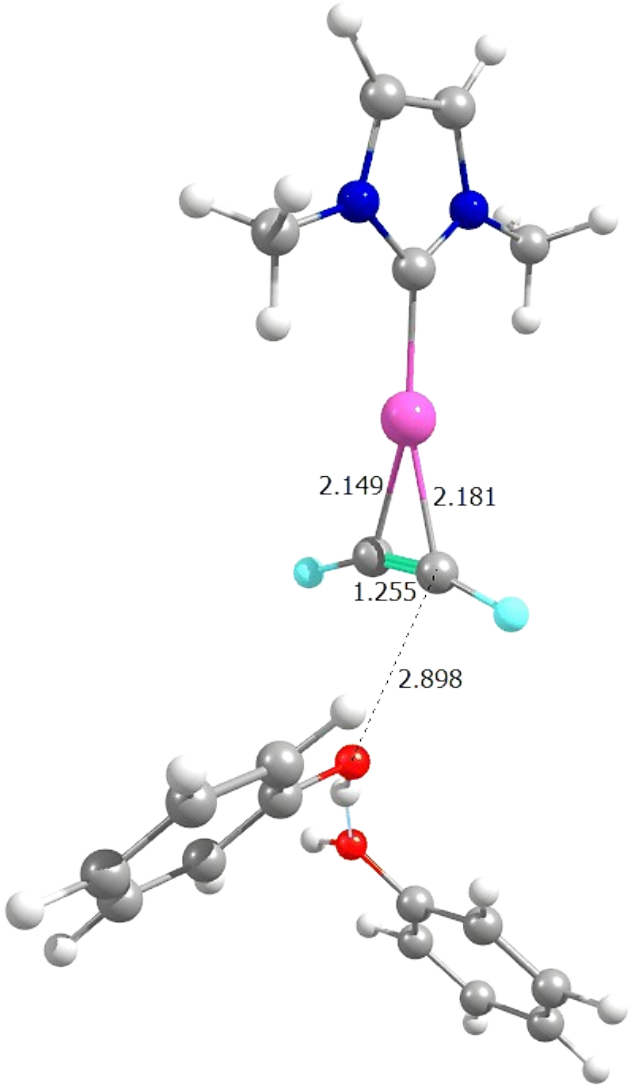
MeOH-FCProd-MeOH



C	-2.536005000	-0.050595000	-0.085057000
N	-3.338361000	0.978189000	-0.501147000
C	-4.675067000	0.600842000	-0.483489000
C	-4.712393000	-0.699165000	-0.045387000
N	-3.397396000	-1.078475000	0.192458000
C	-2.863481000	2.299820000	-0.908974000
C	-2.997933000	-2.400121000	0.674053000
Au	-0.494906000	-0.051961000	0.093542000
C	1.526064000	-0.063495000	0.288663000
C	2.378515000	0.985904000	0.270631000
O	3.786373000	0.855655000	0.400059000
C	4.323838000	0.669126000	1.758914000
H	-5.482428000	1.278615000	-0.779855000
H	-5.558749000	-1.375336000	0.114348000
H	-3.279823000	3.080740000	-0.242094000
H	-3.165536000	2.509972000	-1.954133000
H	-1.760027000	2.310960000	-0.838788000
H	-1.897495000	-2.412912000	0.782344000
H	-3.303674000	-3.181503000	-0.049773000
H	-3.464385000	-2.607350000	1.657526000
H	3.968132000	1.514614000	2.373944000
H	5.425007000	0.698801000	1.667468000
H	4.273220000	0.228830000	-0.450150000
H	3.972801000	-0.299874000	2.159545000
F	2.035352000	2.265942000	0.127059000
F	2.188637000	-1.270284000	0.479608000
C	4.690132000	-1.844889000	-1.521186000
H	3.760657000	-2.143198000	-1.005652000
H	4.644395000	-2.145816000	-2.584977000
H	5.571384000	-2.296957000	-1.023530000
O	4.737854000	-0.390988000	-1.441693000
H	5.532695000	-0.015501000	-1.871146000

Zero-point correction= 0.243874 (Hartree/Particle)
Thermal correction to Energy= 0.265236
Thermal correction to Enthalpy= 0.266180
Thermal correction to Gibbs Free Energy= 0.188453
Sum of electronic and zero-point Energies= -947.003719
Sum of electronic and thermal Energies= -946.982357
Sum of electronic and thermal Enthalpies= -946.981413
Sum of electronic and thermal Free Energies= -947.059140

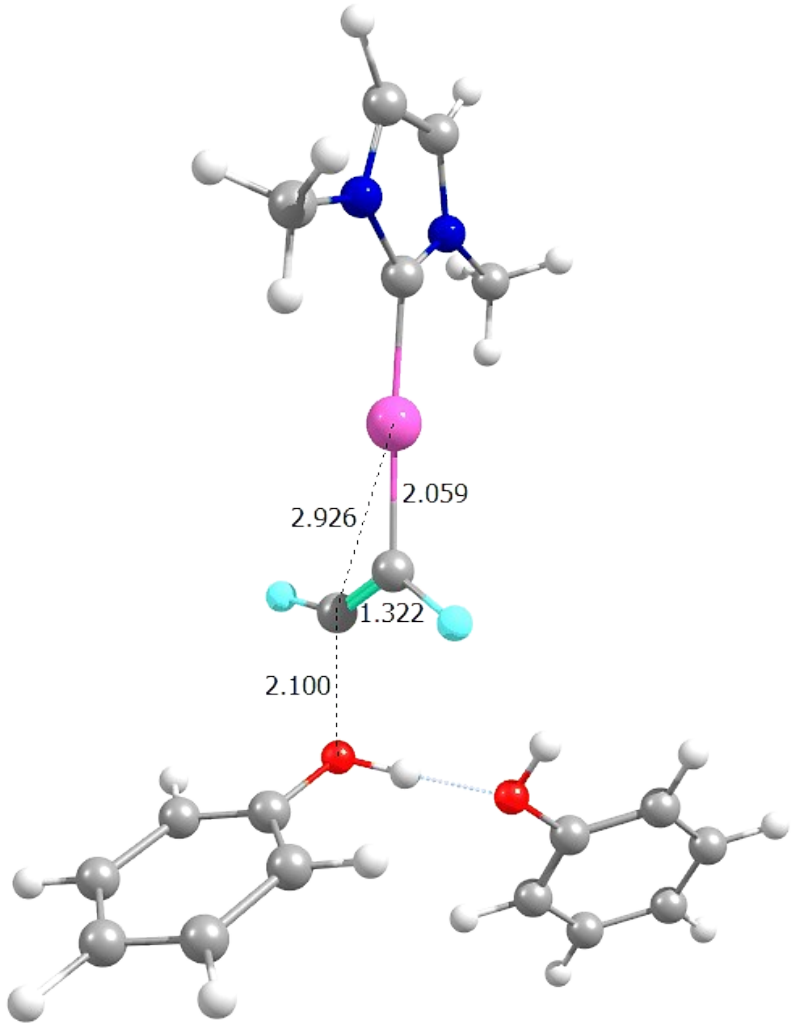
PhOH-FC-PhOH



C	4.251422000	-0.362415000	0.014239000
N	5.061546000	0.741436000	0.041937000
C	6.390655000	0.361486000	0.079567000
C	6.413693000	-1.014940000	0.076320000
N	5.097919000	-1.438725000	0.035086000
C	4.608697000	2.135896000	0.030092000
C	4.691078000	-2.846985000	0.023801000
Au	2.217789000	-0.391783000	-0.051550000
C	0.120780000	-0.407805000	0.548671000
C	0.170958000	-0.397192000	-0.705484000
O	-2.517626000	0.674876000	0.032009000
H	7.210577000	1.087483000	0.105116000
H	7.257327000	-1.713272000	0.100675000
H	4.992183000	2.650794000	-0.872299000
H	4.971073000	2.657897000	0.936965000
H	3.503765000	2.152202000	0.016895000
H	3.588681000	-2.898461000	-0.034066000
H	5.032174000	-3.347343000	0.951091000
H	5.127427000	-3.359001000	-0.855787000
H	-3.223360000	0.262355000	-0.532790000
F	-0.279160000	-0.547239000	1.764148000
F	-0.232087000	-0.253768000	-1.925383000
C	-2.673702000	2.036466000	0.059511000
C	-1.831229000	2.785741000	0.909474000
C	-3.636778000	2.702703000	-0.729390000
C	-1.945524000	4.184222000	0.956381000
H	-1.111001000	2.255346000	1.552274000
C	-3.741987000	4.102442000	-0.672094000
H	-4.307271000	2.115502000	-1.376544000
C	-2.897176000	4.852643000	0.164777000
H	-1.289464000	4.757848000	1.630723000
H	-4.499524000	4.610351000	-1.289966000
H	-2.986636000	5.948706000	0.207537000
C	-7.338905000	-2.653141000	1.081853000
C	-6.251890000	-1.971498000	1.659229000
C	-5.317408000	-1.300774000	0.854377000
C	-5.480706000	-1.316807000	-0.542778000
C	-6.561526000	-1.993364000	-1.135156000
C	-7.488903000	-2.660180000	-0.315327000
H	-8.068445000	-3.175086000	1.719353000
H	-6.128092000	-1.956796000	2.753518000
H	-4.464313000	-0.759918000	1.291326000
H	-6.681864000	-1.998715000	-2.232017000
H	-8.336460000	-3.188158000	-0.779606000
O	-4.535611000	-0.645981000	-1.307405000
H	-4.770566000	-0.710970000	-2.253246000

Zero-point correction= 0.344902 (Hartree/Particle)
Thermal correction to Energy= 0.374784
Thermal correction to Enthalpy= 0.375728
Thermal correction to Gibbs Free Energy= 0.271276
Sum of electronic and zero-point Energies= -1330.058576
Sum of electronic and thermal Energies= -1330.028694
Sum of electronic and thermal Enthalpies= -1330.027750
Sum of electronic and thermal Free Energies= -1330.132202

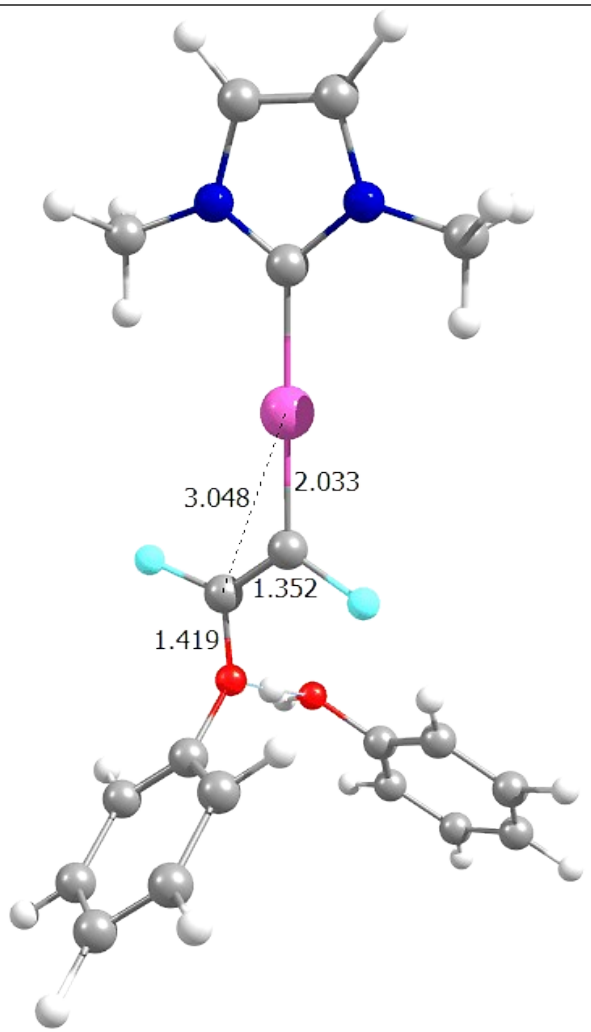
PhOH-FCTs-PhOH



C	-4.069159000	-0.348591000	-0.044751000
N	-5.013187000	0.420256000	-0.668843000
C	-6.279416000	-0.118023000	-0.486154000
C	-6.122514000	-1.253504000	0.269765000
N	-4.764439000	-1.378850000	0.527736000
C	-4.743197000	1.642315000	-1.427923000
C	-4.174802000	-2.465548000	1.310701000
Au	-2.052235000	-0.039577000	-0.001289000
C	-0.011541000	0.219241000	-0.095336000
C	0.604421000	0.716567000	0.962975000
H	-7.180747000	0.344219000	-0.902264000
H	-6.860665000	-1.972218000	0.641021000
H	-5.286175000	2.497466000	-0.979608000
H	-5.060290000	1.515338000	-2.481779000
H	-3.656388000	1.842817000	-1.396061000
H	-3.079728000	-2.317584000	1.345867000
H	-4.396819000	-3.441660000	0.836244000
H	-4.578623000	-2.456577000	2.342292000
C	3.943381000	3.638684000	-1.404215000
C	4.043955000	4.698117000	-0.483249000
C	3.680464000	4.499595000	0.862339000
C	3.219382000	3.246888000	1.294208000
C	3.123213000	2.199230000	0.359530000
C	3.470113000	2.382600000	-0.992771000
H	4.231352000	3.790531000	-2.455940000
H	4.408566000	5.682216000	-0.815148000
H	3.765769000	5.325361000	1.585454000
H	2.947945000	3.064649000	2.344774000
H	3.379307000	1.547979000	-1.703827000
O	2.685691000	0.962756000	0.829898000
H	2.944416000	0.197750000	0.193126000
F	0.391996000	1.172469000	2.140238000
F	0.665522000	-0.126725000	-1.218031000
C	5.948747000	-4.118716000	0.158169000
C	4.811349000	-4.377876000	-0.625208000
C	3.913500000	-3.342515000	-0.939781000
C	4.171109000	-2.047231000	-0.463022000
C	5.303913000	-1.768453000	0.318176000
C	6.189559000	-2.814365000	0.626123000
H	6.648784000	-4.931896000	0.402203000
H	4.614710000	-5.394458000	-0.999555000
H	3.021656000	-3.543639000	-1.557216000
H	5.489826000	-0.743946000	0.674611000
H	7.080219000	-2.602575000	1.237865000
O	3.307646000	-0.988505000	-0.760280000
H	2.537606000	-1.303199000	-1.276748000

Zero-point correction= 0.344995 (Hartree/Particle)
Thermal correction to Energy= 0.372887
Thermal correction to Enthalpy= 0.373831
Thermal correction to Gibbs Free Energy= 0.276778
Sum of electronic and zero-point Energies= -1330.077325
Sum of electronic and thermal Energies= -1330.049433
Sum of electronic and thermal Enthalpies= -1330.048489
Sum of electronic and thermal Free Energies= -1330.145542

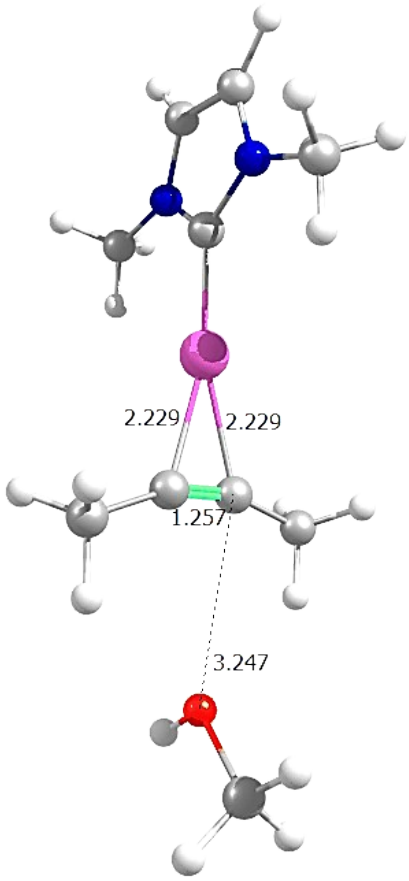
PhOH-FCProd-PhOH



C	-6.244512000	-0.006182000	0.491983000
C	-6.166252000	-0.984215000	-0.467612000
N	-4.818775000	-1.146168000	-0.763952000
C	-4.049366000	-0.295624000	-0.015785000
N	-4.942563000	0.401314000	0.754026000
C	-4.301637000	-2.097890000	-1.746295000
Au	-2.010081000	-0.101668000	-0.044416000
C	0.013651000	0.089324000	-0.088948000
C	-4.584080000	1.436030000	1.722781000
C	0.778652000	0.873972000	0.702932000
H	-7.111207000	0.426444000	1.002554000
H	-6.951499000	-1.570074000	-0.956657000
H	-4.910862000	1.140323000	2.739510000
H	-5.059045000	2.398997000	1.449050000
H	-3.484839000	1.555793000	1.712766000
H	-3.199335000	-2.012076000	-1.767337000
H	-4.705036000	-1.868498000	-2.752566000
H	-4.582717000	-3.131854000	-1.463902000
C	3.416287000	3.014987000	-2.181306000
C	2.734428000	2.002937000	-1.483174000
C	2.879869000	1.966416000	-0.093822000
C	3.658381000	2.871774000	0.631081000
C	4.341369000	3.869153000	-0.089363000
C	4.218479000	3.940507000	-1.488319000
H	3.322587000	3.073506000	-3.276504000
H	2.106456000	1.258996000	-1.994247000
H	3.720390000	2.811086000	1.727846000
H	4.962533000	4.599231000	0.451706000
H	4.750518000	4.727470000	-2.044316000
O	2.195675000	0.920770000	0.641313000
H	2.794888000	0.075667000	1.116761000
F	0.321179000	1.692498000	1.654970000
F	0.739970000	-0.635266000	-1.013176000
C	4.556754000	-3.059912000	-1.088327000
C	5.804026000	-3.494637000	-0.605597000
C	6.261317000	-3.059620000	0.650096000
C	5.479432000	-2.185170000	1.426355000
C	4.242127000	-1.773775000	0.918122000
C	3.755064000	-2.193188000	-0.325011000
H	4.192703000	-3.402352000	-2.069152000
H	6.421259000	-4.177270000	-1.208800000
H	7.235694000	-3.396710000	1.035456000
H	5.836480000	-1.837608000	2.410296000
H	2.770318000	-1.856106000	-0.681290000
O	3.416288000	-0.902104000	1.682349000
H	3.806522000	-0.722969000	2.562950000

Zero-point correction= 0.345274 (Hartree/Particle)
Thermal correction to Energy= 0.372836
Thermal correction to Enthalpy= 0.373780
Thermal correction to Gibbs Free Energy= 0.278593
Sum of electronic and zero-point Energies= -1330.111926
Sum of electronic and thermal Energies= -1330.084364
Sum of electronic and thermal Enthalpies= -1330.083420
Sum of electronic and thermal Free Energies= -1330.178606

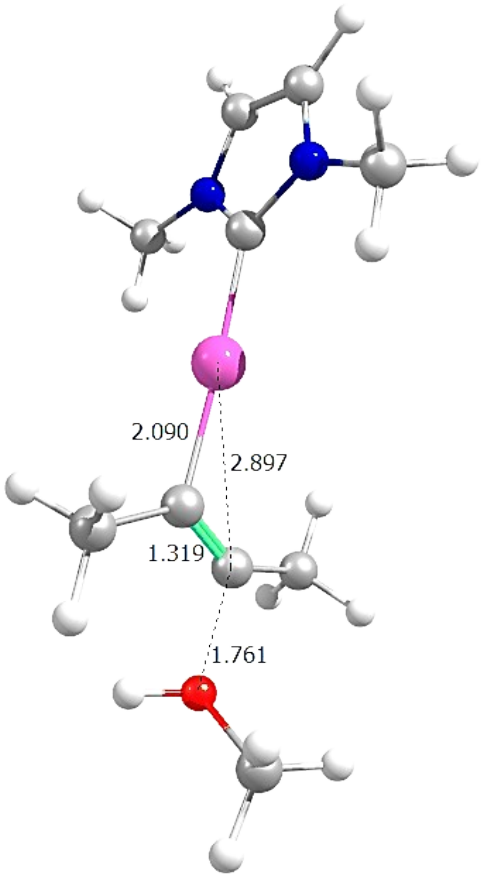
MeOH-MeC



C	2.164839000	0.056573000	-0.000318000
N	3.049026000	-0.988465000	0.002947000
C	4.353785000	-0.520305000	0.001136000
C	4.284064000	0.851996000	-0.003396000
N	2.938764000	1.185731000	-0.004231000
C	2.688859000	-2.407875000	0.007768000
C	2.437769000	2.561876000	-0.009084000
Au	0.136641000	-0.045245000	0.000420000
C	-1.998983000	-0.155818000	-0.627238000
C	-2.455475000	-0.187850000	-2.022847000
C	-1.999069000	-0.147877000	0.629276000
C	-2.455853000	-0.161758000	2.025089000
O	-5.182026000	-0.292979000	0.001744000
C	-6.261114000	0.644438000	-0.004760000
H	5.219737000	-1.190834000	0.003228000
H	5.077575000	1.606874000	-0.006044000
H	-2.172359000	0.731177000	-2.574528000
H	-3.564675000	-0.256923000	-1.976763000
H	-2.056826000	-1.063797000	-2.573118000
H	-2.056923000	-1.030129000	2.587039000
H	-3.565026000	-0.231891000	1.979688000
H	-2.173331000	0.764650000	2.564604000
H	3.092743000	-2.899813000	0.914276000
H	3.094435000	-2.906301000	-0.894421000
H	1.586647000	-2.491068000	0.007017000
H	1.332770000	2.534776000	-0.006070000
H	2.788605000	3.091102000	-0.916670000
H	2.793328000	3.099062000	0.891944000
H	-6.907042000	0.547655000	-0.907450000
H	-5.816286000	1.659111000	-0.012345000
H	-5.572850000	-1.187591000	0.008015000
H	-6.906426000	0.560872000	0.899685000

Zero-point correction= 0.259253 (Hartree/Particle)
Thermal correction to Energy= 0.280223
Thermal correction to Enthalpy= 0.281167
Thermal correction to Gibbs Free Energy= 0.204312
Sum of electronic and zero-point Energies= -711.597565
Sum of electronic and thermal Energies= -711.576595
Sum of electronic and thermal Enthalpies= -711.575651
Sum of electronic and thermal Free Energies= -711.652506

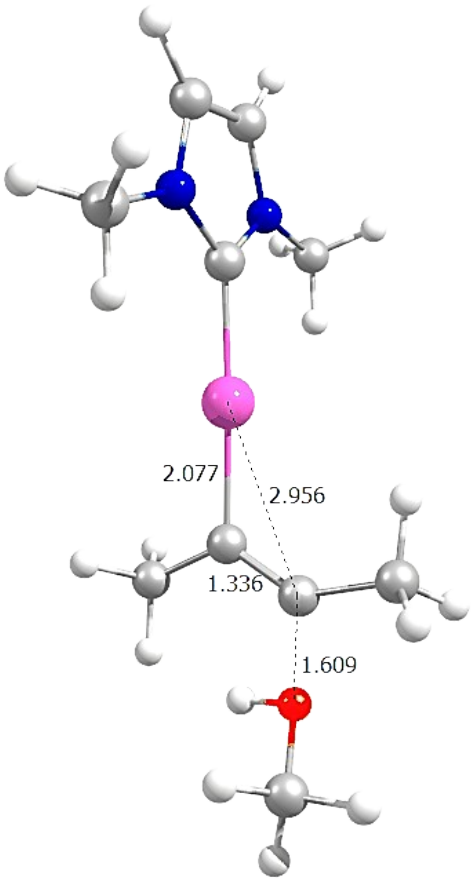
MeOH-MeCTS



C	2.085586000	0.050488000	0.065978000
N	2.961987000	-1.000555000	0.112127000
C	4.266258000	-0.547699000	0.264976000
C	4.205643000	0.822237000	0.315811000
N	2.866026000	1.168420000	0.192230000
C	2.591614000	-2.412110000	0.012323000
C	2.371977000	2.545029000	0.197952000
Au	0.057338000	-0.033000000	-0.169014000
C	-1.999738000	-0.114868000	-0.530226000
C	-2.447484000	-0.007400000	-1.967464000
C	-2.738759000	-0.267053000	0.551843000
C	-2.677777000	-0.441485000	2.020315000
O	-4.465703000	-0.405209000	0.237059000
C	-5.243433000	0.828864000	0.319757000
H	5.122271000	-1.227961000	0.325117000
H	4.998596000	1.568978000	0.428701000
H	-2.100699000	0.948157000	-2.412972000
H	-3.550557000	-0.052038000	-2.127727000
H	-1.992005000	-0.814677000	-2.577501000
H	-1.614817000	-0.392374000	2.326787000
H	-3.090121000	-1.422634000	2.335321000
H	-3.221635000	0.356980000	2.568737000
H	2.913278000	-2.957582000	0.921435000
H	3.064814000	-2.871174000	-0.878257000
H	1.492076000	-2.478060000	-0.084145000
H	1.272122000	2.520884000	0.086614000
H	2.812675000	3.114134000	-0.644404000
H	2.632760000	3.041987000	1.153306000
H	-4.842929000	1.596863000	-0.370721000
H	-5.172401000	1.178160000	1.364619000
H	-4.509833000	-0.757109000	-0.680412000
H	-6.297090000	0.585072000	0.083044000

Zero-point correction= 0.260737 (Hartree/Particle)
Thermal correction to Energy= 0.279612
Thermal correction to Enthalpy= 0.280556
Thermal correction to Gibbs Free Energy= 0.210304
Sum of electronic and zero-point Energies= -711.575273
Sum of electronic and thermal Energies= -711.556398
Sum of electronic and thermal Enthalpies= -711.555454
Sum of electronic and thermal Free Energies= -711.625706

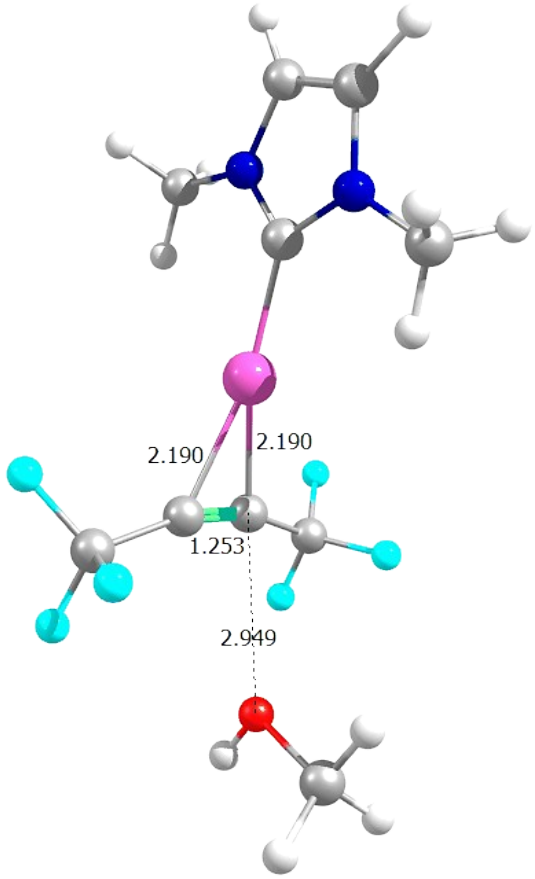
MeOH-MeCprod



C	-5.525691000	0.103205000	0.000470000
C	-5.211633000	1.440931000	0.000458000
N	-3.828235000	1.528799000	0.000197000
C	-3.269181000	0.279334000	0.000050000
N	-4.325838000	-0.590836000	0.000209000
C	-3.088537000	2.792782000	0.000191000
Au	-1.293465000	-0.185390000	-0.000177000
C	0.792385000	-0.674852000	0.627870000
C	1.204371000	-0.770857000	2.034790000
C	-4.225759000	-2.051960000	0.000032000
C	0.792357000	-0.674579000	-0.628501000
C	1.204451000	-0.769961000	-2.035433000
H	-6.497643000	-0.401554000	0.000625000
H	-5.857383000	2.325557000	0.000601000
H	1.050702000	0.183766000	2.577121000
H	2.289076000	-1.011746000	2.036903000
H	0.656289000	-1.570507000	2.572780000
H	1.050949000	0.184939000	-2.577325000
H	0.656339000	-1.569292000	-2.573868000
H	2.289127000	-1.010970000	-2.037595000
H	-4.712701000	-2.466492000	-0.904340000
H	-4.712689000	-2.466704000	0.904312000
H	-3.156397000	-2.331758000	-0.000008000
H	-2.006360000	2.567643000	-0.000976000
H	-3.339128000	3.380200000	0.905198000
H	-3.340872000	3.381149000	-0.903706000
O	4.003941000	-1.292869000	0.000631000
H	4.365922000	-2.200844000	0.000397000
C	5.065564000	-0.408674000	0.000382000
C	4.772620000	0.969218000	0.000479000
C	6.403829000	-0.847589000	0.000068000
C	5.822967000	1.900809000	0.000262000
H	3.721696000	1.297605000	0.000712000
C	7.446221000	0.095433000	-0.000152000
H	6.631604000	-1.927595000	0.000008000
C	7.162829000	1.471910000	-0.000051000
H	5.589650000	2.977369000	0.000341000
H	8.490067000	-0.255607000	-0.000399000
H	7.981751000	2.206952000	-0.000215000

Zero-point correction= 0.261723 (Hartree/Particle)
Thermal correction to Energy= 0.280716
Thermal correction to Enthalpy= 0.281660
Thermal correction to Gibbs Free Energy= 0.211283
Sum of electronic and zero-point Energies= -711.574624
Sum of electronic and thermal Energies= -711.555631
Sum of electronic and thermal Enthalpies= -711.554687
Sum of electronic and thermal Free Energies= -711.625065

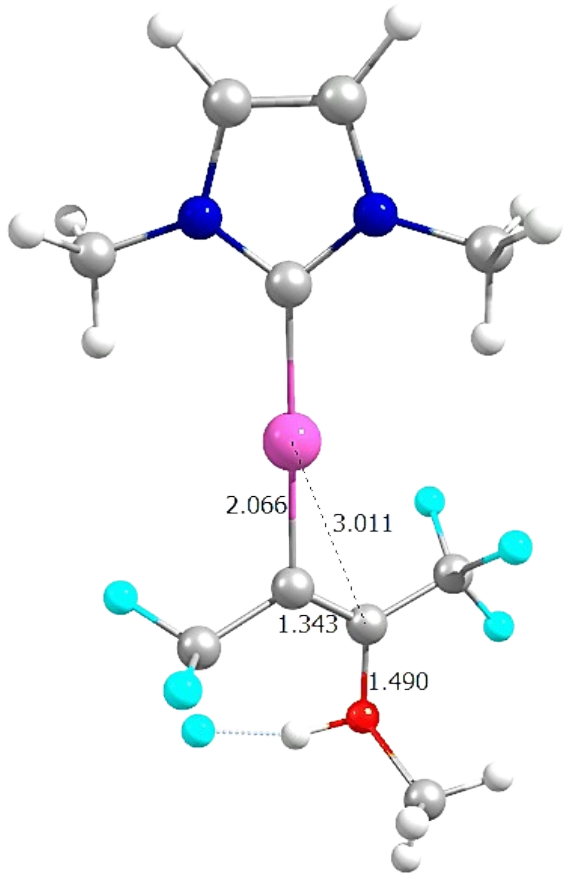
MeOH-CF_3



C	-2.571295000	0.009443000	0.228281000
N	-3.568841000	-0.052332000	-0.706422000
C	-4.806029000	-0.032766000	-0.087826000
C	-4.575301000	0.043618000	1.266976000
N	-3.203045000	0.068963000	1.440699000
C	-3.378155000	-0.123413000	-2.158443000
C	-2.541519000	0.139992000	2.747116000
Au	-0.575476000	0.004459000	-0.115236000
C	1.492030000	-0.634906000	-0.451767000
C	1.910302000	-2.078636000	-0.453606000
C	1.494075000	0.617308000	-0.485680000
C	1.924808000	2.055707000	-0.554527000
O	4.038157000	0.001044000	0.871545000
C	4.440979000	0.017305000	2.239899000
H	-5.745745000	-0.072757000	-0.649322000
H	-5.276222000	0.081930000	2.107914000
H	-3.832547000	0.762323000	-2.643661000
H	-3.845117000	-1.045413000	-2.555956000
H	-2.294514000	-0.141605000	-2.374682000
H	-1.450849000	0.224089000	2.589331000
H	-2.757352000	-0.774880000	3.333053000
H	-2.898950000	1.029137000	3.301579000
H	5.023567000	-0.888308000	2.526293000
H	3.519664000	0.035330000	2.855517000
H	4.847338000	-0.014390000	0.326120000
H	5.040967000	0.919642000	2.499402000
F	3.100845000	-2.211154000	-1.046915000
F	3.122341000	2.148665000	-1.141273000
F	1.028697000	2.762244000	-1.278737000
F	1.982507000	2.579958000	0.679950000
F	1.000533000	-2.810775000	-1.135098000
F	1.975182000	-2.543830000	0.803546000

Zero-point correction= 0.214672 (Hartree/Particle)
Thermal correction to Energy= 0.239828
Thermal correction to Enthalpy= 0.240773
Thermal correction to Gibbs Free Energy= 0.149786
Sum of electronic and zero-point Energies= -1306.605355
Sum of electronic and thermal Energies= -1306.580199
Sum of electronic and thermal Enthalpies= -1306.579255
Sum of electronic and thermal Free Energies= -1306.670242

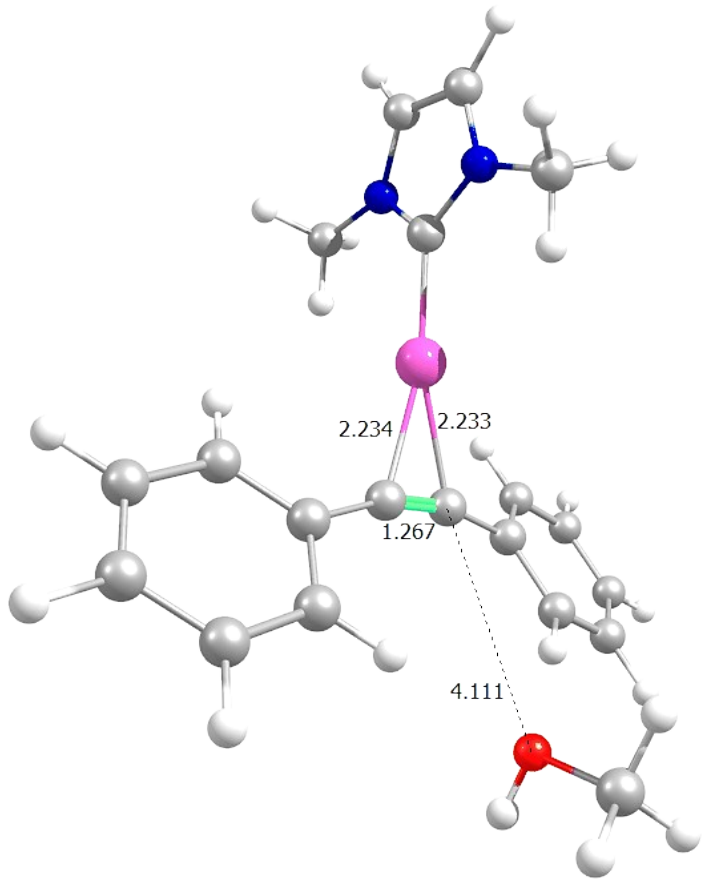
MeOH-CF_3prod



C	-4.844777000	-0.177623000	-0.109535000
C	-4.630646000	1.104371000	0.332625000
N	-3.255830000	1.272034000	0.424836000
C	-2.604612000	0.127402000	0.052553000
N	-3.594954000	-0.758482000	-0.274467000
C	-2.608298000	2.506296000	0.870318000
Au	-0.591536000	-0.194294000	0.003347000
C	1.442730000	-0.555305000	-0.029873000
C	1.837879000	-1.995606000	0.174944000
C	-3.382211000	-2.130345000	-0.737284000
C	2.348724000	0.423449000	-0.187627000
C	2.066729000	1.903570000	-0.447572000
H	-5.775636000	-0.715018000	-0.318911000
H	-5.338685000	1.900774000	0.584766000
H	-3.825990000	-2.267528000	-1.742991000
H	-3.841903000	-2.848564000	-0.030039000
H	-2.294002000	-2.316921000	-0.791174000
H	-1.513476000	2.377542000	0.792013000
H	-2.876567000	2.721436000	1.923656000
H	-2.922774000	3.353295000	0.229524000
O	3.809369000	0.136207000	-0.251550000
C	4.660424000	0.544038000	0.907985000
H	4.265009000	0.073337000	1.827476000
H	4.623595000	1.644166000	0.949998000
H	3.840421000	-0.881263000	-0.351722000
H	5.678136000	0.194118000	0.659898000
F	1.279765000	2.067510000	-1.525661000
F	1.442255000	2.468451000	0.612677000
F	3.218646000	2.581250000	-0.659837000
F	3.225487000	-2.247109000	-0.165595000
F	1.728545000	-2.373635000	1.451910000
F	1.158424000	-2.837819000	-0.601973000

Zero-point correction= 0.218185 (Hartree/Particle)
Thermal correction to Energy= 0.240641
Thermal correction to Enthalpy= 0.241585
Thermal correction to Gibbs Free Energy= 0.161103
Sum of electronic and zero-point Energies= -1306.621470
Sum of electronic and thermal Energies= -1306.599015
Sum of electronic and thermal Enthalpies= -1306.598071
Sum of electronic and thermal Free Energies= -1306.678553

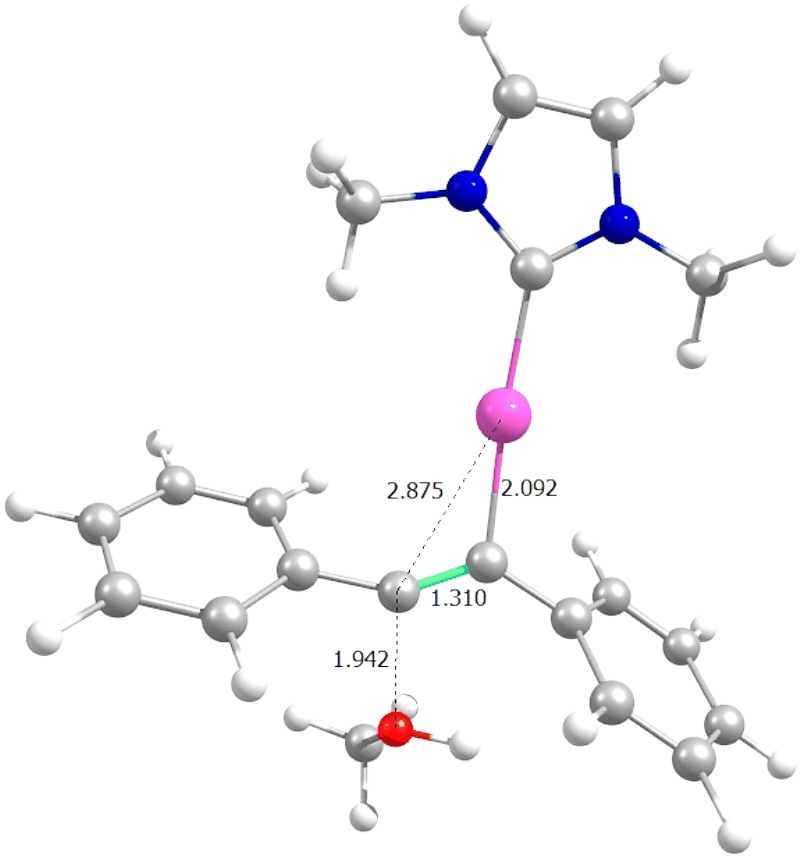
MeOH-PhC



C	2.896044000	-0.000046000	0.394918000
N	3.954512000	-0.001068000	-0.473184000
C	5.153142000	-0.000627000	0.223757000
C	4.835988000	0.000710000	1.560640000
N	3.452253000	0.001058000	1.645395000
C	3.857077000	-0.002389000	-1.934183000
C	2.707496000	0.001967000	2.906477000
Au	0.920435000	-0.000181000	-0.060946000
C	-1.174885000	0.633284000	-0.504861000
C	-1.175018000	-0.633226000	-0.504045000
O	-4.932386000	0.000762000	1.039500000
C	-5.533990000	0.000126000	2.335538000
H	6.126093000	-0.001215000	-0.278997000
H	5.479571000	0.001454000	2.446777000
H	4.344600000	-0.907025000	-2.347561000
H	4.345075000	0.901225000	-2.349232000
H	2.788229000	-0.002368000	-2.215802000
H	1.626284000	0.005068000	2.676199000
H	2.958922000	0.905597000	3.495584000
H	2.954038000	-0.903942000	3.494182000
H	-6.159241000	0.904281000	2.515205000
H	-4.712351000	-0.000759000	3.078347000
H	-5.647522000	0.001156000	0.374525000
H	-6.160045000	-0.903717000	2.513953000
C	-1.550694000	-2.022474000	-0.566331000
C	-0.680707000	-3.012678000	-1.093816000
C	-2.841160000	-2.394386000	-0.097788000
C	-1.094959000	-4.349386000	-1.156014000
H	0.315719000	-2.720434000	-1.460319000
C	-3.239069000	-3.736827000	-0.172692000
H	-3.518774000	-1.627869000	0.315618000
C	-2.373634000	-4.715232000	-0.696025000
H	-0.417576000	-5.112128000	-1.570166000
H	-4.239957000	-4.023622000	0.186229000
H	-2.696393000	-5.766768000	-0.746873000
C	-1.550193000	2.022601000	-0.567211000
C	-0.680288000	3.012439000	-1.095531000
C	-2.840253000	2.394981000	-0.097896000
C	-1.094177000	4.349261000	-1.157679000
H	0.315789000	2.719815000	-1.462679000
C	-3.237811000	3.737523000	-0.172788000
H	-3.517841000	1.628740000	0.316057000
C	-2.372427000	4.715572000	-0.696875000
H	-0.416858000	5.111726000	-1.572444000
H	-4.238375000	4.024684000	0.186744000
H	-2.694900000	5.767198000	-0.747688000

Zero-point correction= 0.363502 (Hartree/Particle)
Thermal correction to Energy= 0.390767
Thermal correction to Enthalpy= 0.391711
Thermal correction to Gibbs Free Energy= 0.297859
Sum of electronic and zero-point Energies= -1094.702086
Sum of electronic and thermal Energies= -1094.674820
Sum of electronic and thermal Enthalpies= -1094.673876
Sum of electronic and thermal Free Energies= -1094.767729

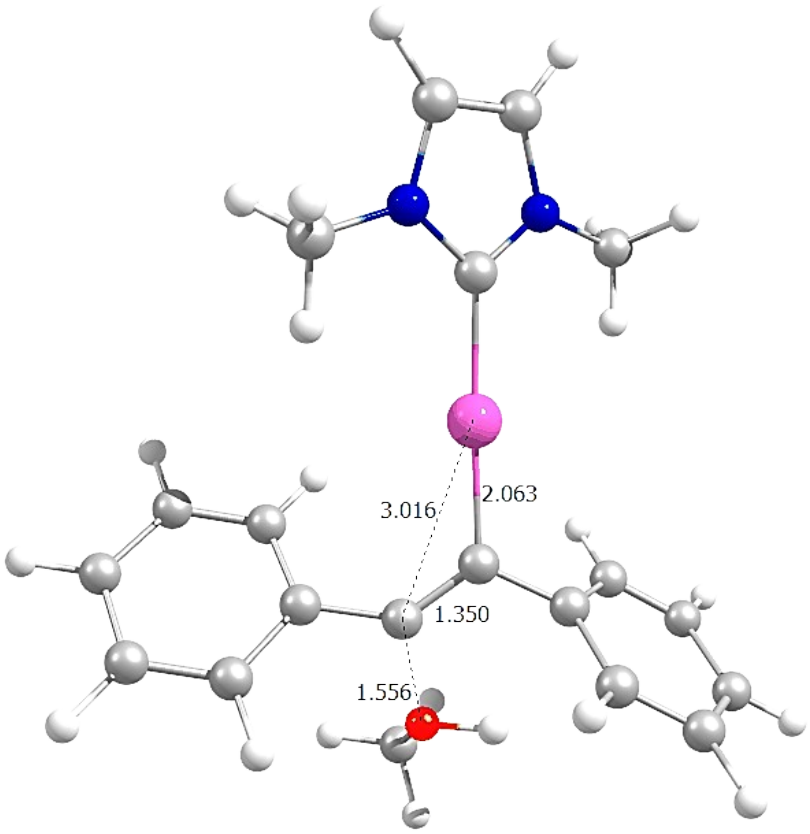
MeOH-PhCTS



Zero-point correction= 0.364032 (Hartree/Particle)
Thermal correction to Energy= 0.388615
Thermal correction to Enthalpy= 0.389559
Thermal correction to Gibbs Free Energy= 0.305221
Sum of electronic and zero-point Energies= -1094.684107
Sum of electronic and thermal Energies= -1094.659524
Sum of electronic and thermal Enthalpies= -1094.658580
Sum of electronic and thermal Free Energies= -1094.742918

C	2.888446000	-0.040672000	-0.043966000
N	3.611199000	-1.200036000	-0.132687000
C	4.974057000	-0.930684000	-0.126739000
C	5.107687000	0.431707000	-0.032588000
N	3.823069000	0.957994000	0.015833000
C	3.042148000	-2.543031000	-0.235828000
C	3.526016000	2.386916000	0.112915000
Au	0.860737000	0.172784000	-0.019769000
C	-1.197908000	0.542617000	-0.038412000
C	-1.920984000	-0.548656000	-0.097594000
O	-3.791742000	-0.065566000	-0.294530000
C	-4.594565000	-0.279739000	0.888495000
H	5.729977000	-1.720339000	-0.190490000
H	6.002910000	1.061286000	0.002837000
H	3.391813000	-3.172609000	0.606154000
H	3.339702000	-3.012502000	-1.194382000
H	1.940418000	-2.459505000	-0.198273000
H	2.428100000	2.517022000	0.100059000
H	3.967110000	2.927559000	-0.747584000
H	3.933680000	2.801155000	1.056335000
H	-4.213324000	0.301481000	1.753056000
H	-4.553994000	-1.361159000	1.115609000
H	-3.698814000	0.907683000	-0.460566000
H	-5.643239000	0.004610000	0.666246000
C	-1.657239000	1.954021000	-0.047730000
C	-1.412734000	2.804328000	1.058591000
C	-2.364495000	2.473802000	-1.165008000
C	-1.889064000	4.124954000	1.058374000
H	-0.854205000	2.415604000	1.924514000
C	-2.830984000	3.802221000	-1.159123000
H	-2.502292000	1.847593000	-2.062522000
C	-2.600477000	4.628669000	-0.046773000
H	-1.700523000	4.769676000	1.931263000
H	-3.368860000	4.192614000	-2.037380000
H	-2.965293000	5.667323000	-0.043743000
C	-2.006617000	-1.989544000	-0.035261000
C	-2.613476000	-2.732992000	-1.082676000
C	-1.483215000	-2.676451000	1.094300000
C	-2.679405000	-4.130104000	-1.004281000
H	-3.031602000	-2.201257000	-1.950022000
C	-1.544017000	-4.075948000	1.155587000
H	-1.027397000	-2.097229000	1.912091000
C	-2.142847000	-4.803746000	0.110224000
H	-3.149239000	-4.701203000	-1.819914000
H	-1.133754000	-4.602694000	2.031244000
H	-2.197290000	-5.902254000	0.166397000

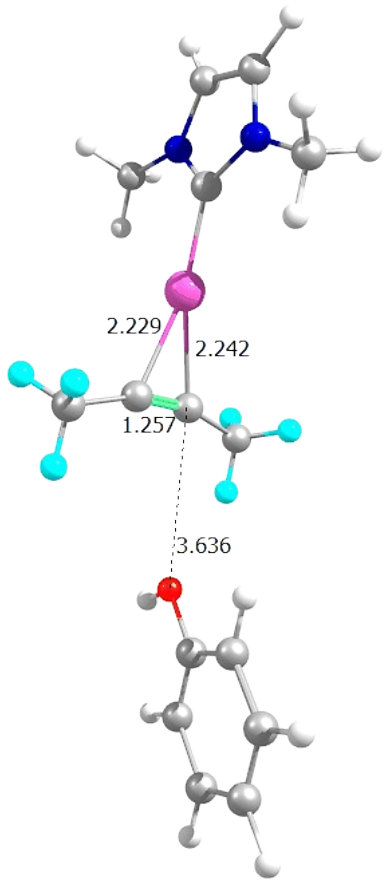
MeOH-PhCprod



Zero-point correction= 0.365549 (Hartree/Particle)
Thermal correction to Energy= 0.390601
Thermal correction to Enthalpy= 0.391545
Thermal correction to Gibbs Free Energy= 0.305864
Sum of electronic and zero-point Energies= -1094.686231
Sum of electronic and thermal Energies= -1094.661179
Sum of electronic and thermal Enthalpies= -1094.660235
Sum of electronic and thermal Free Energies= -1094.745916

C	5.000263000	-0.495083000	-0.419198000
C	5.056464000	0.758142000	0.136770000
N	3.743673000	1.162512000	0.344333000
C	2.864874000	0.194731000	-0.065369000
N	3.654809000	-0.821708000	-0.533709000
C	3.364753000	2.450102000	0.923841000
Au	0.818759000	0.263860000	-0.018385000
C	-1.239380000	0.404678000	-0.044662000
C	3.161630000	-2.073621000	-1.106314000
C	-2.045910000	-0.678444000	-0.048658000
H	5.799865000	-1.171149000	-0.739546000
H	5.914545000	1.385935000	0.398792000
H	3.613567000	-2.936913000	-0.579497000
H	3.411741000	-2.129384000	-2.184629000
H	2.062884000	-2.105594000	-0.986256000
H	2.261163000	2.517697000	0.926972000
H	3.779565000	3.279029000	0.316998000
H	3.740798000	2.531205000	1.963197000
O	-3.558781000	-0.362096000	-0.225061000
C	-4.416721000	-0.556425000	0.960238000
H	-4.055677000	0.081568000	1.789069000
H	-4.350661000	-1.626875000	1.219935000
H	-3.549462000	0.620785000	-0.504948000
H	-5.444088000	-0.291426000	0.651014000
C	-1.865797000	-2.129520000	0.084177000
C	-0.882880000	-2.640965000	0.969884000
C	-2.654122000	-3.042603000	-0.663322000
C	-0.682456000	-4.024505000	1.085453000
H	-0.287521000	-1.937850000	1.573177000
C	-2.453641000	-4.425421000	-0.534463000
H	-3.414988000	-2.664611000	-1.363450000
C	-1.466417000	-4.921043000	0.336260000
H	0.079600000	-4.407412000	1.782281000
H	-3.068105000	-5.121666000	-1.126216000
H	-1.313517000	-6.006883000	0.436427000
C	-1.855527000	1.759761000	-0.138428000
C	-1.733908000	2.694713000	0.921705000
C	-2.631638000	2.130875000	-1.274977000
C	-2.375554000	3.940131000	0.854445000
H	-1.129826000	2.427055000	1.802964000
C	-3.268336000	3.389789000	-1.336761000
H	-2.657171000	1.466059000	-2.156659000
C	-3.148538000	4.292623000	-0.270556000
H	-2.270981000	4.649594000	1.690666000
H	-3.843501000	3.664225000	-2.235074000
H	-3.642276000	5.275350000	-0.317075000

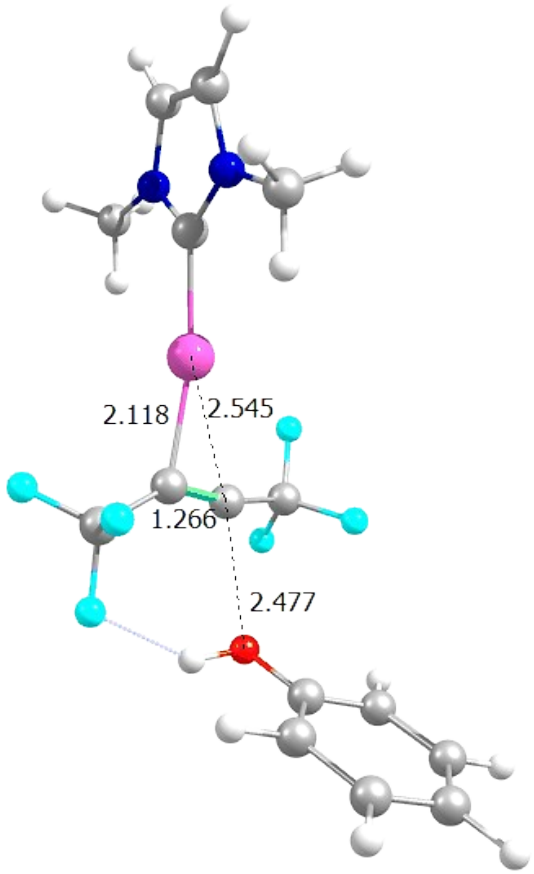
PhOH-CF_3



C	-3.398404000	0.218328000	-0.124900000
N	-4.396917000	-0.711398000	-0.235308000
C	-5.625560000	-0.087444000	-0.386078000
C	-5.389343000	1.266044000	-0.370177000
N	-4.022710000	1.433440000	-0.209096000
C	-4.216551000	-2.164244000	-0.196136000
C	-3.360219000	2.738183000	-0.147087000
Au	-1.415581000	-0.131446000	0.115791000
C	0.605594000	-0.512394000	0.975371000
C	0.834785000	-0.605089000	2.425915000
C	0.762102000	-0.495023000	-0.271402000
C	1.315459000	-0.539671000	-1.630604000
O	4.318868000	-1.231621000	-0.427804000
H	-6.560955000	-0.647366000	-0.491144000
H	-6.079262000	2.111886000	-0.460055000
H	0.561764000	0.335387000	2.945756000
H	1.914798000	-0.797995000	2.597151000
H	0.255038000	-1.433418000	2.880998000
H	0.847265000	-1.339265000	-2.239611000
H	2.405026000	-0.748818000	-1.530731000
H	1.183201000	0.425750000	-2.159718000
H	-4.592866000	-2.618913000	-1.133321000
H	-4.762386000	-2.592747000	0.667270000
H	-3.138072000	-2.382865000	-0.091617000
H	-2.279896000	2.577650000	0.023074000
H	-3.777125000	3.335537000	0.687099000
H	-3.503689000	3.284240000	-1.100164000
H	4.624165000	-2.145044000	-0.594173000
C	5.431087000	-0.429486000	-0.274955000
C	5.227523000	0.940782000	-0.018543000
C	6.738951000	-0.944706000	-0.368038000
C	6.336013000	1.787064000	0.143794000
H	4.200339000	1.330622000	0.052306000
C	7.839914000	-0.087128000	-0.202193000
H	6.896404000	-2.018249000	-0.570772000
C	7.645693000	1.280958000	0.053933000
H	6.172277000	2.857928000	0.343570000
H	8.858963000	-0.498210000	-0.276056000
H	8.510079000	1.949734000	0.182505000

Zero-point correction= 0.266661 (Hartree/Particle)
Thermal correction to Energy= 0.294262
Thermal correction to Enthalpy= 0.295206
Thermal correction to Gibbs Free Energy= 0.199511
Sum of electronic and zero-point Energies= -1498.169291
Sum of electronic and thermal Energies= -1498.141690
Sum of electronic and thermal Enthalpies= -1498.140746
Sum of electronic and thermal Free Energies= -1498.236440

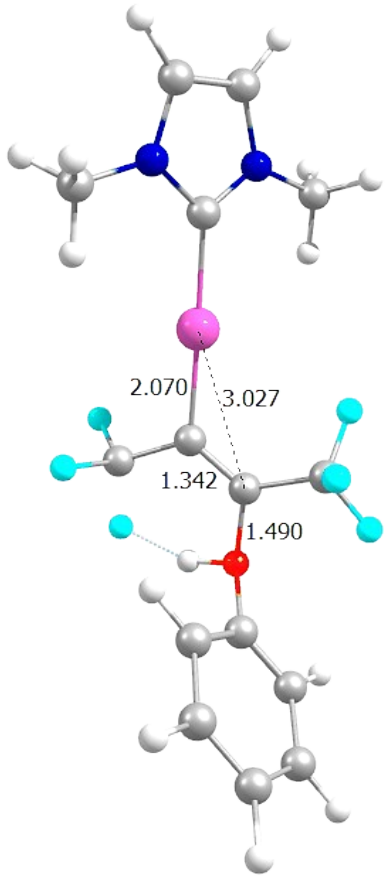
PhOH-CF_3TS



C	-3.309716000	0.124830000	0.552354000
N	-4.401016000	0.467637000	-0.196991000
C	-5.545493000	0.443463000	0.584267000
C	-5.157790000	0.071467000	1.849584000
N	-3.785861000	-0.121563000	1.810165000
C	-4.384934000	0.816362000	-1.620029000
C	-2.978868000	-0.521316000	2.965863000
Au	-1.397854000	-0.050007000	-0.088881000
C	0.492275000	-0.691008000	-0.798265000
O	3.439802000	0.152487000	-1.075858000
H	-6.534800000	0.691609000	0.185112000
H	-5.744685000	-0.066741000	2.763926000
H	-4.780476000	1.840753000	-1.763598000
H	-5.000477000	0.096721000	-2.194419000
H	-3.341774000	0.775079000	-1.983099000
H	-1.927922000	-0.633320000	2.642242000
H	-3.342227000	-1.488384000	3.364704000
H	-3.037779000	0.251978000	3.756653000
H	3.291698000	-0.751316000	-1.424458000
C	1.004558000	0.465666000	-0.752369000
C	0.782394000	-2.148973000	-1.033108000
C	1.261155000	1.947910000	-0.754558000
F	0.796585000	-2.816517000	0.133098000
F	-0.136037000	-2.696248000	-1.841596000
F	2.002626000	-2.307738000	-1.622685000
F	1.880950000	2.322014000	-1.875798000
F	1.990706000	2.301460000	0.312007000
F	0.073875000	2.609545000	-0.690740000
C	4.349355000	0.078472000	-0.030987000
C	4.993011000	1.268395000	0.360330000
C	4.628981000	-1.142146000	0.615424000
C	5.923826000	1.227671000	1.409229000
H	4.770833000	2.204453000	-0.172072000
C	5.571183000	-1.168339000	1.656517000
H	4.120900000	-2.067531000	0.298523000
C	6.216680000	0.014438000	2.060415000
H	6.435202000	2.154160000	1.713459000
H	5.800934000	-2.123142000	2.154460000
H	6.952709000	-0.010222000	2.878260000

Zero-point correction= 0.266482 (Hartree/Particle)
Thermal correction to Energy= 0.293018
Thermal correction to Enthalpy= 0.293962
Thermal correction to Gibbs Free Energy= 0.200775
Sum of electronic and zero-point Energies= -1498.161310
Sum of electronic and thermal Energies= -1498.134775
Sum of electronic and thermal Enthalpies= -1498.133830
Sum of electronic and thermal Free Energies= -1498.227017

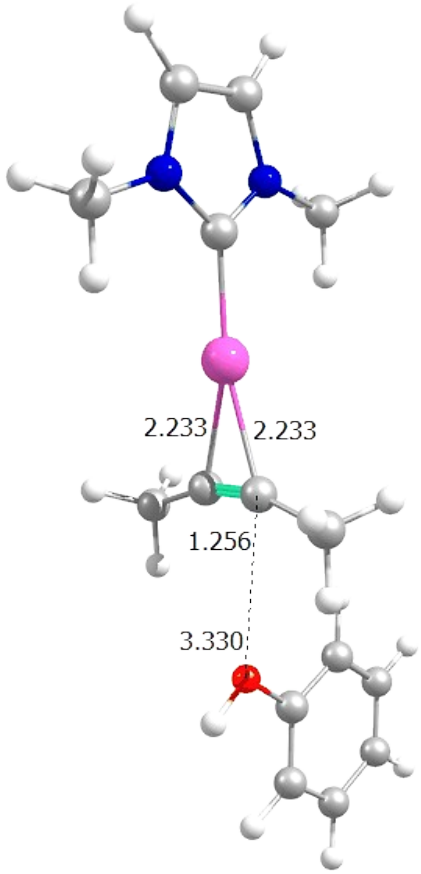
PhOH-CF_3prod



C	5.392152000	-1.108687000	0.438580000
C	5.359234000	-0.075463000	1.341472000
N	4.082922000	0.468418000	1.281252000
C	3.316512000	-0.198973000	0.365117000
N	4.135145000	-1.167991000	-0.148290000
C	3.635103000	1.601482000	2.091184000
Au	1.373443000	0.169165000	-0.136119000
C	-0.588657000	0.588432000	-0.647233000
C	-0.842629000	2.033690000	-0.992302000
C	3.751698000	-2.142179000	-1.170361000
C	-1.573925000	-0.323071000	-0.621078000
C	-1.480646000	-1.805855000	-0.259802000
H	6.200179000	-1.796798000	0.168995000
H	6.133098000	0.312742000	2.011911000
H	3.780243000	-3.168419000	-0.753495000
H	4.439521000	-2.075954000	-2.035997000
H	2.723212000	-1.912808000	-1.504071000
H	2.585762000	1.827441000	1.826498000
H	4.263077000	2.490561000	1.885043000
H	3.694534000	1.349643000	3.168477000
O	-2.970061000	0.021993000	-1.012416000
H	-2.896585000	0.970206000	-1.391151000
C	-4.044052000	-0.051664000	0.003704000
C	-5.173233000	-0.786357000	-0.352160000
C	-3.873369000	0.614914000	1.217174000
C	-6.218330000	-0.843864000	0.587903000
H	-5.232287000	-1.297229000	-1.323639000
C	-4.932902000	0.539029000	2.140024000
H	-2.954272000	1.176268000	1.442745000
C	-6.096731000	-0.185700000	1.825344000
H	-7.129467000	-1.412468000	0.347600000
H	-4.841901000	1.052926000	3.108909000
H	-6.918771000	-0.239719000	2.555166000
F	0.018015000	2.522811000	-1.881730000
F	-2.138126000	2.253893000	-1.597607000
F	-2.538567000	-2.483867000	-0.751840000
F	-1.455639000	-1.978477000	1.079225000
F	-0.359593000	-2.354202000	-0.770809000
F	-0.847834000	2.811648000	0.101606000

Zero-point correction= 0.268549 (Hartree/Particle)
Thermal correction to Energy= 0.294202
Thermal correction to Enthalpy= 0.295146
Thermal correction to Gibbs Free Energy= 0.206038
Sum of electronic and zero-point Energies= -1498.175447
Sum of electronic and thermal Energies= -1498.149794
Sum of electronic and thermal Enthalpies= -1498.148850
Sum of electronic and thermal Free Energies= -1498.237958

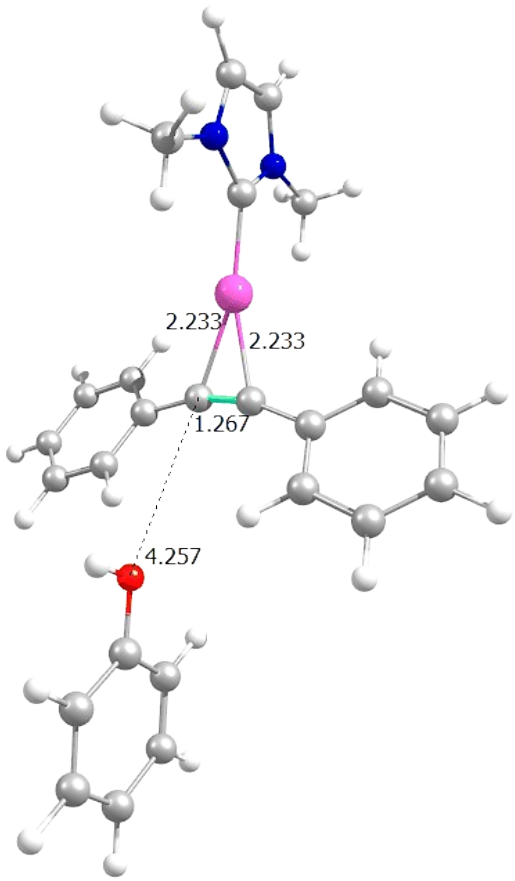
PhOH-MeC



C	-5.525691000	0.103205000	0.000470000
C	-5.211633000	1.440931000	0.000458000
N	-3.828235000	1.528799000	0.000197000
C	-3.269181000	0.279334000	0.000050000
N	-4.325838000	-0.590836000	0.000209000
C	-3.088537000	2.792782000	0.000191000
Au	-1.293465000	-0.185390000	-0.000177000
C	0.792385000	-0.674852000	0.627870000
C	1.204371000	-0.770857000	2.034790000
C	-4.225759000	-2.051960000	0.000032000
C	0.792357000	-0.674579000	-0.628501000
C	1.204451000	-0.769961000	-2.035433000
H	-6.497643000	-0.401554000	0.000625000
H	-5.857383000	2.325557000	0.000601000
H	1.050702000	0.183766000	2.577121000
H	2.289076000	-1.011746000	2.036903000
H	0.656289000	-1.570507000	2.572780000
H	1.050949000	0.184939000	-2.577325000
H	0.656339000	-1.569292000	-2.573868000
H	2.289127000	-1.010970000	-2.037595000
H	-4.712701000	-2.466492000	-0.904340000
H	-4.712689000	-2.466704000	0.904312000
H	-3.156397000	-2.331758000	-0.000008000
H	-2.006360000	2.567643000	-0.000976000
H	-3.339128000	3.380200000	0.905198000
H	-3.340872000	3.381149000	-0.903706000
O	4.003941000	-1.292869000	0.000631000
H	4.365922000	-2.200844000	0.000397000
C	5.065564000	-0.408674000	0.000382000
C	4.772620000	0.969218000	0.000479000
C	6.403829000	-0.847589000	0.000068000
C	5.822967000	1.900809000	0.000262000
H	3.721696000	1.297605000	0.000712000
C	7.446221000	0.095433000	-0.000152000
H	6.631604000	-1.927595000	0.000008000
C	7.162829000	1.471910000	-0.000051000
H	5.589650000	2.977369000	0.000341000
H	8.490067000	-0.255607000	-0.000399000
H	7.981751000	2.206952000	-0.000215000

Zero-point correction= 0.310514 (Hartree/Particle)
Thermal correction to Energy= 0.334450
Thermal correction to Enthalpy= 0.335395
Thermal correction to Gibbs Free Energy= 0.248076
Sum of electronic and zero-point Energies= -903.159169
Sum of electronic and thermal Energies= -903.135233
Sum of electronic and thermal Enthalpies= -903.134289
Sum of electronic and thermal Free Energies= -903.221608

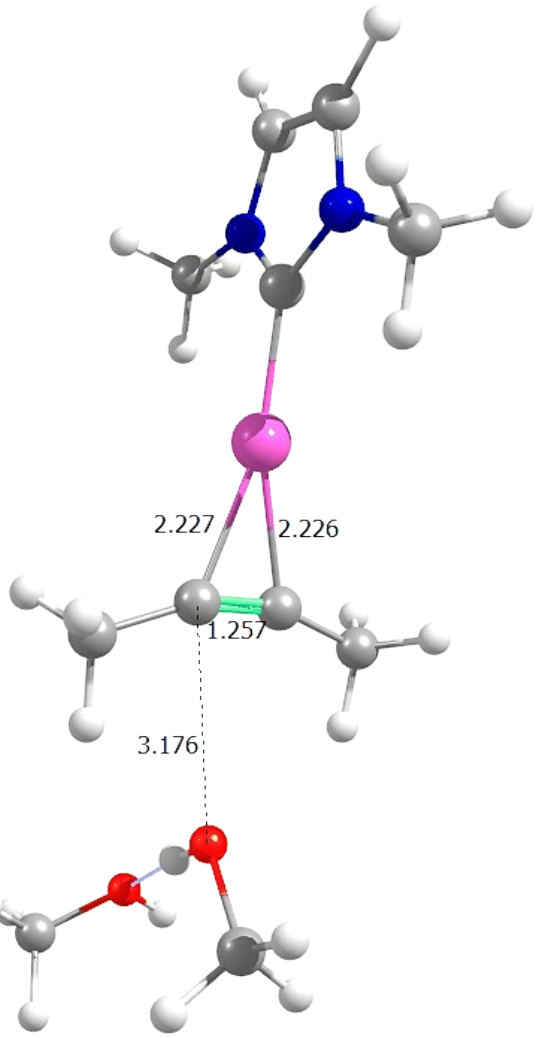
PhOH-PhC



Zero-point correction= 0.414955 (Hartree/Particle)
Thermal correction to Energy= 0.444998
Thermal correction to Enthalpy= 0.445942
Thermal correction to Gibbs Free Energy= 0.343757
Sum of electronic and zero-point Energies= -1286.262936
Sum of electronic and thermal Energies= -1286.232893
Sum of electronic and thermal Enthalpies= -1286.231948
Sum of electronic and thermal Free Energies= -1286.334134

C	-6.131972000	0.000669000	-0.298131000
C	-5.800498000	0.001073000	-1.631574000
N	-4.415995000	0.001129000	-1.701448000
C	-3.873244000	0.000727000	-0.445003000
N	-4.940955000	0.000457000	0.411641000
C	-3.658062000	0.000986000	-2.954565000
Au	-1.902284000	0.000324000	0.032525000
C	0.186807000	0.633121000	0.502232000
C	-4.859402000	0.000010000	1.873705000
C	0.186272000	-0.633697000	0.502280000
H	-7.110284000	0.000613000	0.194128000
H	-6.434529000	0.001376000	-2.524584000
H	-5.351467000	-0.904382000	2.282170000
H	-5.351899000	0.903902000	2.282746000
H	-3.793735000	0.000151000	2.167025000
H	-2.579420000	0.005228000	-2.712664000
H	-3.903945000	0.903663000	-3.547456000
H	-3.897659000	-0.905866000	-3.543700000
O	4.057430000	-0.001480000	-1.153000000
H	3.991614000	-0.001006000	-2.128236000
C	5.396551000	-0.000754000	-0.808113000
C	5.721896000	-0.001102000	0.561972000
C	6.414061000	0.000287000	-1.781545000
C	7.071320000	-0.000405000	0.949302000
H	4.914443000	-0.001936000	1.309938000
C	7.761066000	0.000972000	-1.379468000
H	6.153399000	0.000545000	-2.854205000
C	8.096336000	0.000628000	-0.014832000
H	7.323762000	-0.000686000	2.021481000
H	8.552523000	0.001766000	-2.145297000
H	9.151779000	0.001155000	0.296838000
C	0.566176000	-2.021124000	0.575225000
C	1.866246000	-2.388982000	0.131064000
C	-0.305693000	-3.013934000	1.094495000
C	2.274744000	-3.726893000	0.222765000
H	2.545220000	-1.623573000	-0.277572000
C	0.117456000	-4.347020000	1.173168000
H	-1.309876000	-2.726311000	1.442887000
C	1.406937000	-4.706952000	0.739073000
H	3.285259000	-4.006050000	-0.113955000
H	-0.561402000	-5.111714000	1.581243000
H	1.736810000	-5.755393000	0.805144000
C	0.567419000	2.020323000	0.575515000
C	-0.303921000	3.013578000	1.094793000
C	1.867787000	2.387462000	0.131591000
C	0.120043000	4.346394000	1.173714000
H	-1.308341000	2.726529000	1.442980000
C	2.277099000	3.725103000	0.223541000
H	2.546309000	1.621675000	-0.277090000
C	1.409806000	4.705610000	0.739867000
H	-0.558410000	5.111446000	1.581794000
H	3.287837000	4.003689000	-0.112982000
H	1.740284000	5.753848000	0.806132000

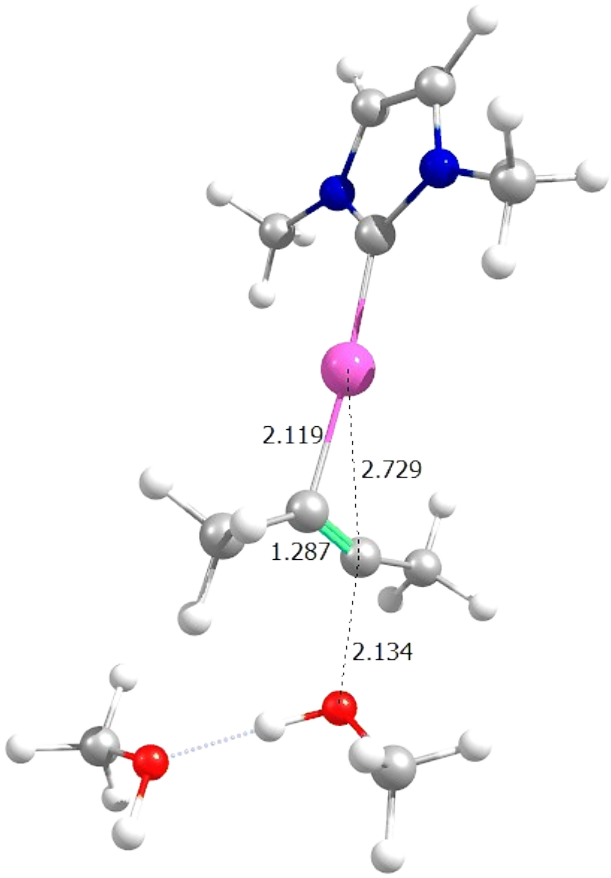
MeOH-MeC-MeOH



C	-4.714624000	0.974729000	0.215494000
C	-4.835009000	-0.325565000	-0.206739000
N	-3.545888000	-0.823059000	-0.345470000
C	-2.621824000	0.132683000	-0.018840000
N	-3.355073000	1.236900000	0.323420000
C	-3.235250000	-2.185083000	-0.780120000
Au	-0.595151000	-0.043228000	-0.067829000
C	1.501109000	-0.180598000	-0.346822000
C	2.075308000	0.074922000	-1.708160000
C	-2.799620000	2.522188000	0.747266000
C	1.942891000	-0.521158000	0.812918000
C	1.888090000	-0.822256000	2.247966000
H	-5.478325000	1.725256000	0.444858000
H	-5.724110000	-0.929165000	-0.417212000
H	1.832729000	-0.764180000	-2.393648000
H	3.175736000	0.197260000	-1.654814000
H	1.642314000	0.989567000	-2.159814000
H	0.845814000	-0.706449000	2.608807000
H	2.536996000	-0.132248000	2.824002000
H	2.213495000	-1.861029000	2.461735000
H	-3.131318000	2.762445000	1.776783000
H	-3.127053000	3.325707000	0.058401000
H	-1.696536000	2.449859000	0.725486000
H	-2.135886000	-2.296691000	-0.818319000
H	-3.657186000	-2.370077000	-1.787611000
H	-3.653879000	-2.920705000	-0.065105000
O	4.049689000	-0.852958000	0.735248000
C	4.411777000	-2.128425000	0.203862000
H	4.139706000	-2.242973000	-0.869303000
H	3.880745000	-2.909476000	0.783219000
C	5.607970000	2.306522000	-0.289299000
H	5.821049000	2.988093000	-1.140221000
H	6.451144000	2.346351000	0.434416000
H	4.523029000	-0.139836000	0.206136000
O	5.351247000	0.968222000	-0.746015000
H	5.504356000	-2.303330000	0.320657000
H	6.138955000	0.641990000	-1.222667000
H	4.689439000	2.657905000	0.218016000

Zero-point correction= 0.310830 (Hartree/Particle)
Thermal correction to Energy= 0.336512
Thermal correction to Enthalpy= 0.337456
Thermal correction to Gibbs Free Energy= 0.246792
Sum of electronic and zero-point Energies= -827.193961
Sum of electronic and thermal Energies= -827.168279
Sum of electronic and thermal Enthalpies= -827.167335
Sum of electronic and thermal Free Energies= -827.257999

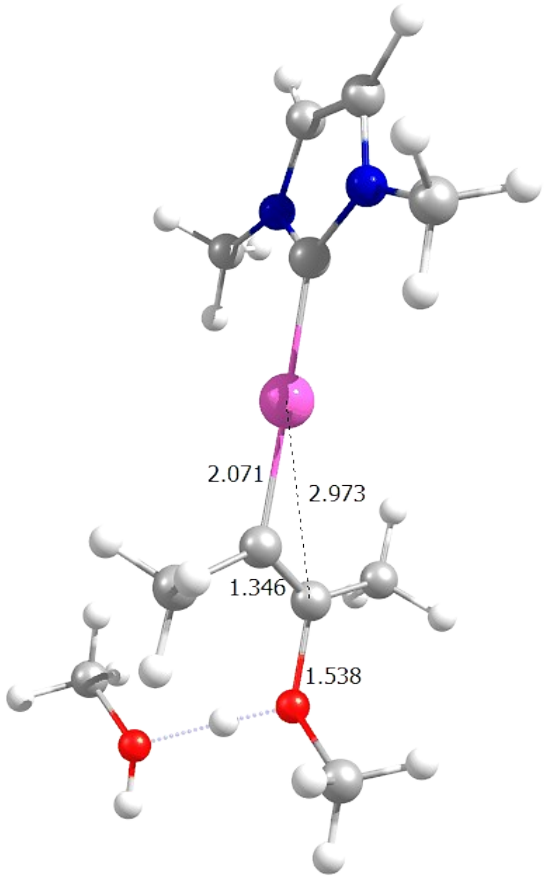
MeOH-MeCTS-MeOH



C	-4.714624000	0.974729000	0.215494000
C	-4.835009000	-0.325565000	-0.206739000
N	-3.545888000	-0.823059000	-0.345470000
C	-2.621824000	0.132683000	-0.018840000
N	-3.355073000	1.236900000	0.323420000
C	-3.235250000	-2.185083000	-0.780120000
Au	-0.595151000	-0.043228000	-0.067829000
C	1.501109000	-0.180598000	-0.346822000
C	2.075308000	0.074922000	-1.708160000
C	-2.799620000	2.522188000	0.747266000
C	1.942891000	-0.521158000	0.812918000
C	1.888090000	-0.822256000	2.247966000
H	-5.478325000	1.725256000	0.444858000
H	-5.724110000	-0.929165000	-0.417212000
H	1.832729000	-0.764180000	-2.393648000
H	3.175736000	0.197260000	-1.654814000
H	1.642314000	0.989567000	-2.159814000
H	0.845814000	-0.706449000	2.608807000
H	2.536996000	-0.132248000	2.824002000
H	2.213495000	-1.861029000	2.461735000
H	-3.131318000	2.762445000	1.776783000
H	-3.127053000	3.325707000	0.058401000
H	-1.696536000	2.449859000	0.725486000
H	-2.135886000	-2.296691000	-0.818319000
H	-3.657186000	-2.370077000	-1.787611000
H	-3.653879000	-2.920705000	-0.065105000
O	4.049689000	-0.852958000	0.735248000
C	4.411777000	-2.128425000	0.203862000
H	4.139706000	-2.242973000	-0.869303000
H	3.880745000	-2.909476000	0.783219000
C	5.607970000	2.306522000	-0.289299000
H	5.821049000	2.988093000	-1.140221000
H	6.451144000	2.346351000	0.434416000
H	4.523029000	-0.139836000	0.206136000
O	5.351247000	0.968222000	-0.746015000
H	5.504356000	-2.303330000	0.320657000
H	6.138955000	0.641990000	-1.222667000
H	4.689439000	2.657905000	0.218016000

Zero-point correction= 0.311557 (Hartree/Particle)
Thermal correction to Energy= 0.335667
Thermal correction to Enthalpy= 0.336611
Thermal correction to Gibbs Free Energy= 0.252063
Sum of electronic and zero-point Energies= -827.182498
Sum of electronic and thermal Energies= -827.158388
Sum of electronic and thermal Enthalpies= -827.157444
Sum of electronic and thermal Free Energies= -827.241991

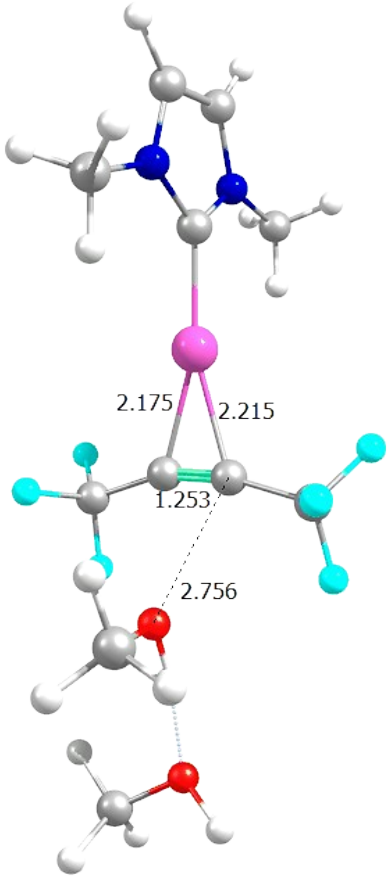
MeOH-MeCprod-MeOH



C	4.604746000	1.018091000	-0.282959000
C	4.763853000	-0.300166000	0.062029000
N	3.488419000	-0.825559000	0.230023000
C	2.531529000	0.127520000	-0.000580000
N	3.236527000	1.259493000	-0.315736000
C	3.216176000	-2.211902000	0.606194000
Au	0.492205000	-0.095520000	0.112825000
C	-1.556720000	-0.331097000	0.301223000
C	-2.119988000	-0.299708000	1.707059000
C	2.640100000	2.553892000	-0.639552000
C	-2.304080000	-0.521345000	-0.801738000
C	-1.990339000	-0.602477000	-2.261253000
H	5.345495000	1.793488000	-0.504542000
H	5.670445000	-0.898592000	0.199881000
H	-1.737126000	-1.164897000	2.290847000
H	-3.229439000	-0.305481000	1.775768000
H	-1.758380000	0.598589000	2.250175000
H	-0.898542000	-0.493807000	-2.403177000
H	-2.502689000	0.196296000	-2.840267000
H	-2.297651000	-1.576100000	-2.702889000
H	2.927301000	2.865452000	-1.663581000
H	2.974200000	3.323131000	0.084889000
H	1.540424000	2.451467000	-0.582360000
H	2.120084000	-2.344973000	0.668645000
H	3.669455000	-2.438689000	1.591628000
H	3.626853000	-2.904891000	-0.154830000
O	-3.823243000	-0.708208000	-0.655317000
C	-4.294949000	-2.037683000	-0.292071000
H	-3.992853000	-2.292438000	0.742248000
H	-3.852319000	-2.752381000	-1.009015000
C	-4.494473000	2.488202000	0.516463000
H	-4.948145000	3.084823000	1.332950000
H	-4.671111000	2.984163000	-0.460831000
H	-4.317319000	0.083772000	-0.139342000
O	-5.027160000	1.141641000	0.533298000
H	-5.396618000	-2.038656000	-0.396496000
H	-5.995782000	1.169384000	0.400966000
H	-3.406986000	2.401416000	0.693399000

Zero-point correction= 0.313433 (Hartree/Particle)
Thermal correction to Energy= 0.336518
Thermal correction to Enthalpy= 0.337462
Thermal correction to Gibbs Free Energy= 0.257101
Sum of electronic and zero-point Energies= -827.188121
Sum of electronic and thermal Energies= -827.165036
Sum of electronic and thermal Enthalpies= -827.164092
Sum of electronic and thermal Free Energies= -827.244453

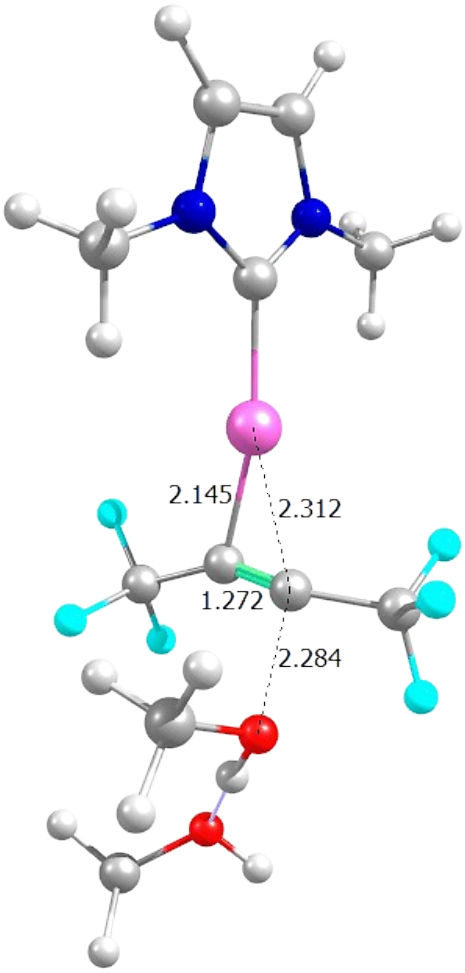
MeOH-CF_3-MeOH



C	3.049254000	-0.065617000	-0.176373000
N	4.029695000	0.125702000	0.758538000
C	5.278622000	0.017331000	0.172141000
C	5.072575000	-0.250281000	-1.161798000
N	3.703105000	-0.296489000	-1.355996000
C	3.811799000	0.410053000	2.180064000
C	3.064844000	-0.558202000	-2.649319000
Au	1.046644000	-0.024868000	0.123989000
C	-1.026872000	-0.577945000	0.475509000
C	-1.510216000	-1.997655000	0.552354000
C	-1.044765000	0.668826000	0.353136000
C	-1.373093000	2.134528000	0.329038000
O	-3.393083000	0.233459000	-1.021977000
C	-3.631206000	0.378213000	-2.410781000
H	6.207700000	0.138076000	0.739644000
H	5.788238000	-0.409113000	-1.975686000
H	4.270188000	1.382637000	2.445039000
H	4.257890000	-0.392438000	2.799287000
H	2.724214000	0.456832000	2.370889000
H	1.968014000	-0.530202000	-2.515840000
H	3.361719000	-1.557559000	-3.022920000
H	3.363785000	0.216431000	-3.382059000
H	-4.362079000	-0.368255000	-2.803535000
H	-2.674720000	0.217262000	-2.951019000
H	-4.267999000	0.348690000	-0.558726000
H	-4.002163000	1.394451000	-2.687866000
O	-5.836118000	0.370391000	0.147223000
H	-6.466098000	1.106662000	0.034691000
C	-6.562320000	-0.857810000	0.240504000
H	-5.812075000	-1.667469000	0.324337000
H	-7.210501000	-0.888935000	1.144378000
H	-7.188663000	-1.054555000	-0.658755000
F	-1.522155000	-2.548902000	-0.673005000
F	-0.681317000	-2.723195000	1.336440000
F	-2.740491000	-2.039092000	1.076515000
F	-1.394303000	2.596635000	-0.929650000
F	-0.413547000	2.811028000	1.011038000
F	-2.549303000	2.362208000	0.918257000

Zero-point correction= 0.266416 (Hartree/Particle)
Thermal correction to Energy= 0.296132
Thermal correction to Enthalpy= 0.297076
Thermal correction to Gibbs Free Energy= 0.194561
Sum of electronic and zero-point Energies= -1422.202544
Sum of electronic and thermal Energies= -1422.172829
Sum of electronic and thermal Enthalpies= -1422.171885
Sum of electronic and thermal Free Energies= -1422.274400

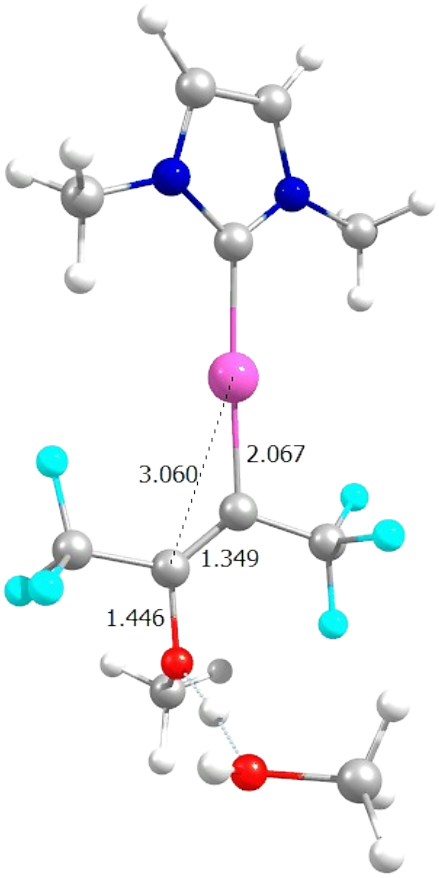
MeOH-CF_3TS-MeOH



C	5.099270000	-0.004632000	0.122035000
C	4.886012000	-0.712480000	-1.037430000
N	3.514137000	-0.814175000	-1.199878000
C	2.866460000	-0.187459000	-0.170732000
N	3.852525000	0.304963000	0.639774000
C	2.868892000	-1.499113000	-2.322366000
Au	0.869414000	-0.040064000	0.124923000
C	-1.175548000	-0.384941000	0.673488000
C	-1.741567000	-1.726069000	1.021165000
C	3.642449000	1.063966000	1.875829000
C	-1.303687000	0.747713000	0.109093000
C	-1.333979000	2.257579000	0.128987000
H	6.031098000	0.298467000	0.611365000
H	5.596496000	-1.146839000	-1.748883000
H	4.139083000	0.551038000	2.722215000
H	2.556824000	1.127177000	2.073508000
H	4.053370000	2.086832000	1.768096000
H	1.773363000	-1.439962000	-2.189219000
H	3.176411000	-2.562796000	-2.345077000
H	3.149165000	-1.011428000	-3.276504000
O	-2.863471000	0.864650000	-1.554984000
C	-2.551527000	0.030420000	-2.664387000
H	-2.259271000	-1.001141000	-2.361249000
H	-1.710549000	0.492675000	-3.218991000
C	-5.712782000	-1.172887000	-0.234813000
H	-6.476708000	-1.022079000	-1.029452000
H	-6.222093000	-1.457064000	0.710911000
H	-3.658485000	0.487630000	-1.064990000
O	-4.880527000	-0.018581000	-0.051052000
H	-3.416972000	-0.042759000	-3.360303000
H	-5.434665000	0.724873000	0.256029000
H	-5.049364000	-2.006797000	-0.532008000
F	-2.761675000	-1.580573000	1.882049000
F	-0.807028000	-2.518404000	1.584624000
F	-2.203229000	-2.362931000	-0.086634000
F	-0.493439000	2.695733000	1.105553000
F	-0.925159000	2.786515000	-1.030715000
F	-2.566136000	2.691951000	0.420613000

Zero-point correction= 0.266700 (Hartree/Particle)
Thermal correction to Energy= 0.294901
Thermal correction to Enthalpy= 0.295845
Thermal correction to Gibbs Free Energy= 0.200004
Sum of electronic and zero-point Energies= -1422.200610
Sum of electronic and thermal Energies= -1422.172409
Sum of electronic and thermal Enthalpies= -1422.171465
Sum of electronic and thermal Free Energies= -1422.267306

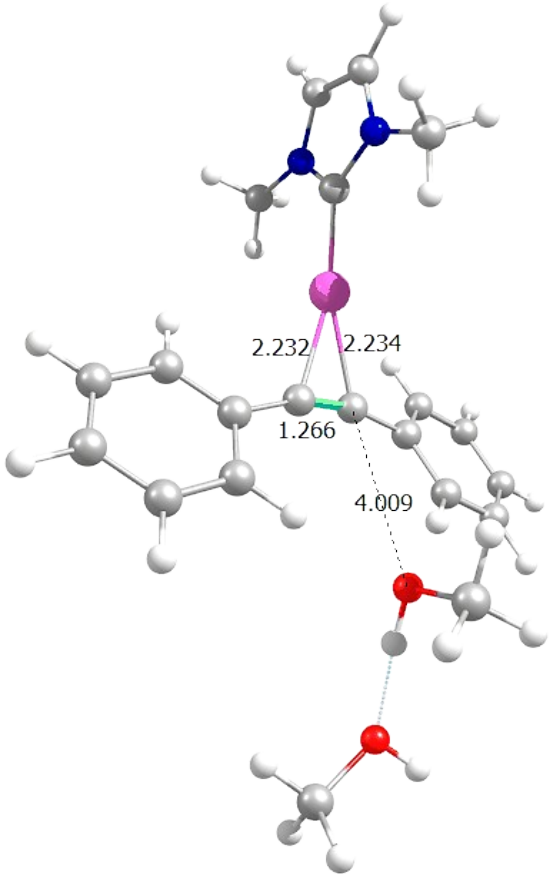
MeOH-CF_3prod-MeOH



C	5.058879000	0.789492000	0.579983000
C	5.180602000	-0.504370000	0.138108000
N	3.895854000	-0.959216000	-0.127079000
C	2.971724000	0.016557000	0.135551000
N	3.702998000	1.089131000	0.571131000
C	3.585438000	-2.299942000	-0.623484000
Au	0.946606000	-0.118556000	-0.079908000
C	-1.096676000	-0.342199000	-0.302025000
C	-1.523465000	-1.795259000	-0.255849000
C	3.144122000	2.376450000	0.982476000
C	-1.994565000	0.658946000	-0.413785000
C	-1.745065000	2.155314000	-0.305297000
H	5.819263000	1.511466000	0.895615000
H	6.068021000	-1.129117000	-0.007503000
H	3.564232000	3.191845000	0.361148000
H	3.373606000	2.571303000	2.048950000
H	2.048271000	2.341195000	0.844899000
H	2.487882000	-2.390357000	-0.721140000
H	3.954039000	-3.065245000	0.087759000
H	4.055286000	-2.460945000	-1.613955000
O	-3.428242000	0.482293000	-0.467885000
C	-4.105296000	0.351226000	-1.761916000
H	-3.864018000	-0.632167000	-2.205066000
H	-3.773464000	1.184771000	-2.405010000
C	-4.538229000	-1.493093000	2.118397000
H	-5.189665000	-1.517928000	3.011674000
H	-3.512185000	-1.832201000	2.357529000
H	-3.957179000	0.118369000	0.517367000
O	-4.528895000	-0.129587000	1.592406000
H	-5.186645000	0.439053000	-1.550748000
H	-4.258627000	0.515563000	2.279284000
H	-4.969881000	-2.129861000	1.327022000
F	-1.343771000	-2.279783000	1.007265000
F	-0.793762000	-2.553510000	-1.099850000
F	-2.840053000	-2.053192000	-0.563331000
F	-0.454425000	2.504368000	-0.424382000
F	-2.446665000	2.833917000	-1.248121000
F	-2.188043000	2.597129000	0.909239000

Zero-point correction= 0.268220 (Hartree/Particle)
Thermal correction to Energy= 0.295065
Thermal correction to Enthalpy= 0.296009
Thermal correction to Gibbs Free Energy= 0.204899
Sum of electronic and zero-point Energies= -1422.242599
Sum of electronic and thermal Energies= -1422.215755
Sum of electronic and thermal Enthalpies= -1422.214810
Sum of electronic and thermal Free Energies= -1422.305921

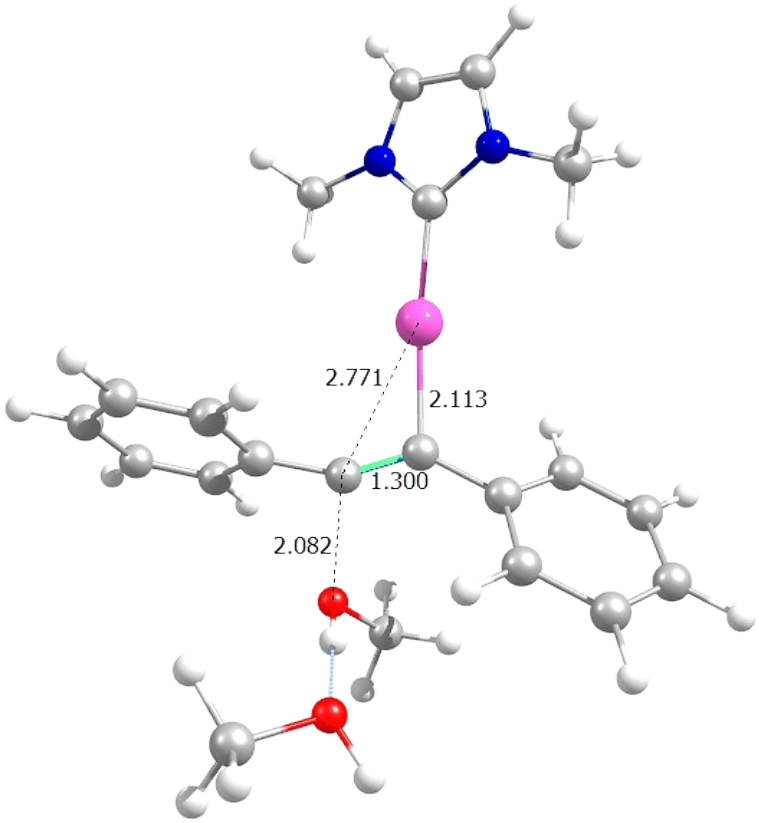
MeOH-PhC-MeOH



C	3.416112000	-0.073847000	-0.320378000
N	4.446578000	-0.138580000	0.578449000
C	5.665761000	-0.158929000	-0.081808000
C	5.390528000	-0.105759000	-1.426829000
N	4.010800000	-0.053769000	-1.552861000
C	4.303108000	-0.175778000	2.035021000
C	3.305546000	0.005950000	-2.835051000
Au	1.428567000	-0.021253000	0.075778000
C	-0.697136000	-0.593164000	0.447183000
C	-0.660367000	0.672547000	0.460221000
O	-4.262679000	0.166906000	-1.224929000
C	-4.638351000	0.159788000	-2.593401000
H	6.622011000	-0.208164000	0.449721000
H	6.061021000	-0.100737000	-2.292738000
H	4.786941000	0.711343000	2.488983000
H	4.767857000	-1.096158000	2.439626000
H	3.225788000	-0.171072000	2.282601000
H	2.221215000	0.089497000	-2.636597000
H	3.500861000	-0.913692000	-3.420956000
H	3.641293000	0.890326000	-3.410919000
H	-5.323668000	-0.682926000	-2.849622000
H	-3.720997000	0.041360000	-3.206162000
H	-5.094213000	0.259678000	-0.685526000
H	-5.133393000	1.108420000	-2.911821000
O	-6.604982000	0.435925000	0.167491000
H	-7.128564000	1.253128000	0.070592000
C	-7.486815000	-0.644304000	0.479046000
H	-6.863860000	-1.554552000	0.575802000
H	-8.014524000	-0.484379000	1.445691000
H	-8.243479000	-0.823861000	-0.318239000
C	-1.120134000	-1.969870000	0.480072000
C	-0.294893000	-2.997840000	1.007012000
C	-2.412636000	-2.286369000	-0.022401000
C	-0.754701000	-4.320728000	1.035435000
H	0.703226000	-2.746276000	1.398522000
C	-2.854393000	-3.616868000	0.017911000
H	-3.054974000	-1.486885000	-0.435061000
C	-2.034383000	-4.634008000	0.540612000
H	-0.112376000	-5.113595000	1.448957000
H	-3.855441000	-3.863512000	-0.369546000
H	-2.392761000	-5.675041000	0.563294000
C	-0.992230000	2.072950000	0.515321000
C	-0.112172000	3.031344000	1.083492000
C	-2.249443000	2.486276000	-0.006190000
C	-0.483060000	4.381195000	1.132286000
H	0.857144000	2.704363000	1.491249000
C	-2.602509000	3.842095000	0.056297000
H	-2.934444000	1.739832000	-0.448528000
C	-1.727818000	4.790239000	0.618460000
H	0.201120000	5.120076000	1.577460000
H	-3.576599000	4.163821000	-0.344571000
H	-2.016380000	5.852268000	0.657846000

Zero-point correction= 0.415007 (Hartree/Particle)
Thermal correction to Energy= 0.447052
Thermal correction to Enthalpy= 0.447996
Thermal correction to Gibbs Free Energy= 0.339929
Sum of electronic and zero-point Energies= -1210.298014
Sum of electronic and thermal Energies= -1210.265968
Sum of electronic and thermal Enthalpies= -1210.265024
Sum of electronic and thermal Free Energies= -1210.373091

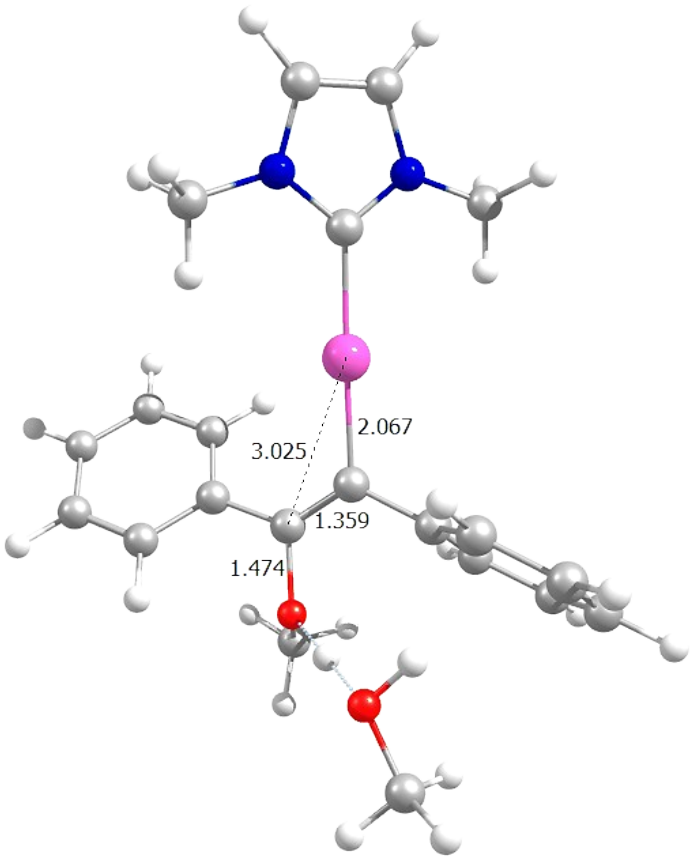
MeOH-PhCTS-MeOH



Zero-point correction= 0.415380 (Hartree/Particle)
Thermal correction to Energy= 0.445765
Thermal correction to Enthalpy= 0.446709
Thermal correction to Gibbs Free Energy= 0.345992
Sum of electronic and zero-point Energies= -1210.283481
Sum of electronic and thermal Energies= -1210.253096
Sum of electronic and thermal Enthalpies= -1210.252152
Sum of electronic and thermal Free Energies= -1210.352869

	5.350183000	-0.411946000	0.687919000
C	5.310383000	0.795821000	0.037727000
N	3.979480000	1.035797000	-0.280961000
C	3.185893000	0.008604000	0.154139000
N	4.042836000	-0.877932000	0.749041000
C	3.506660000	2.222300000	-0.993164000
Au	1.171228000	-0.185427000	-0.052199000
C	-0.892464000	-0.580473000	-0.273005000
C	3.650063000	-2.141331000	1.373283000
C	-1.474277000	0.578558000	-0.357731000
H	6.193500000	-0.970421000	1.107394000
H	6.112314000	1.495272000	-0.220542000
H	3.893370000	-2.127271000	2.454188000
H	4.176600000	-2.986664000	0.888059000
H	2.559180000	-2.270129000	1.246315000
H	2.405040000	2.167393000	-1.069631000
H	3.942784000	2.258444000	-2.011213000
H	3.789964000	3.138502000	-0.438554000
O	-3.475205000	0.407614000	-0.908304000
C	-3.824681000	-0.467828000	-1.984420000
H	-3.755690000	-1.540680000	-1.705151000
H	-3.125520000	-0.277017000	-2.821638000
C	-5.434184000	1.000254000	2.046380000
H	-5.680556000	0.687798000	3.083607000
H	-6.332965000	1.455398000	1.575739000
H	-4.028245000	0.193251000	-0.092203000
O	-4.920512000	-0.101475000	1.279919000
H	-4.856026000	-0.240790000	-2.334843000
H	-5.605217000	-0.795797000	1.224295000
H	-4.634384000	1.763424000	2.090367000
C	-1.483454000	2.013527000	-0.199634000
C	-1.833695000	2.874214000	-1.273632000
C	-1.133898000	2.580590000	1.056943000
C	-1.817350000	4.263239000	-1.097031000
H	-2.119712000	2.438441000	-2.241558000
C	-1.116454000	3.973117000	1.222341000
H	-0.868060000	1.913157000	1.891209000
C	-1.458699000	4.815596000	0.148343000
H	-2.086811000	4.924101000	-1.935496000
H	-0.839027000	4.404418000	2.196867000
H	-1.449322000	5.908778000	0.282301000
C	-1.335110000	-1.987286000	-0.251991000
C	-0.683595000	-2.964354000	-1.044121000
C	-2.400214000	-2.390444000	0.592709000
C	-1.105406000	-4.302883000	-1.016666000
H	0.151590000	-2.659145000	-1.694394000
C	-2.803433000	-3.735481000	0.628331000
H	-2.908814000	-1.644085000	1.222501000
C	-2.163583000	-4.694910000	-0.177399000
H	-0.598334000	-5.047225000	-1.650508000
H	-3.624303000	-4.040303000	1.297187000
H	-2.484959000	-5.747628000	-0.145930000

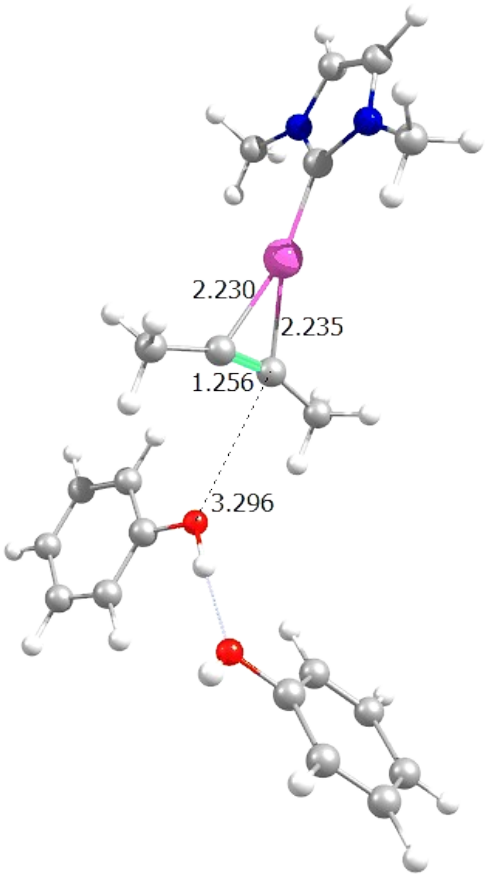
MeOH-PhCprod-MeOH



Zero-point correction= 0.415889 (Hartree/Particle)
Thermal correction to Energy= 0.444785
Thermal correction to Enthalpy= 0.445729
Thermal correction to Gibbs Free Energy= 0.351307
Sum of electronic and zero-point Energies= -1210.300773
Sum of electronic and thermal Energies= -1210.271878
Sum of electronic and thermal Enthalpies= -1210.270934
Sum of electronic and thermal Free Energies= -1210.365356

C	5.230306000	-0.474246000	0.747835000
C	5.131634000	-1.541174000	-0.109312000
N	3.792601000	-1.644340000	-0.465962000
C	3.047569000	-0.669434000	0.144198000
N	3.948957000	0.044393000	0.889193000
C	3.260688000	-2.657940000	-1.375128000
Au	1.028611000	-0.352453000	-0.020134000
C	-1.018258000	-0.099812000	-0.155811000
C	3.615662000	1.191942000	1.731643000
C	-1.606447000	1.124998000	-0.182094000
H	6.098373000	-0.048324000	1.261725000
H	5.897152000	-2.225498000	-0.489777000
H	4.201791000	2.078941000	1.419950000
H	3.830967000	0.964883000	2.794865000
H	2.537375000	1.407525000	1.614800000
H	2.169002000	-2.504665000	-1.463165000
H	3.457680000	-3.672970000	-0.976541000
H	3.726332000	-2.560043000	-2.376020000
O	-3.071069000	1.216998000	-0.043161000
C	-3.836150000	1.730577000	-1.165857000
H	-3.853203000	0.990157000	-1.990553000
H	-3.372105000	2.675768000	-1.504512000
C	-5.494405000	-0.747909000	1.283526000
H	-5.774076000	-1.487887000	2.057112000
H	-5.659831000	-1.174661000	0.273427000
H	-3.608975000	0.428426000	0.677075000
O	-4.106820000	-0.370898000	1.476679000
H	-4.860081000	1.932534000	-0.798625000
H	-3.507763000	-1.172015000	1.421999000
H	-6.103963000	0.163867000	1.423453000
C	-1.823067000	-1.351683000	-0.188105000
C	-1.839163000	-2.238607000	0.927348000
C	-2.580710000	-1.718706000	-1.330908000
C	-2.604303000	-3.422445000	0.903164000
H	-1.215992000	-2.001556000	1.805420000
C	-3.326411000	-2.910919000	-1.357971000
H	-2.547842000	-1.073530000	-2.223480000
C	-3.352177000	-3.764422000	-0.239709000
H	-2.596700000	-4.091308000	1.778793000
H	-3.887971000	-3.179736000	-2.267138000
H	-3.933718000	-4.698849000	-0.264677000
C	-1.001700000	2.474609000	-0.249398000
C	0.112195000	2.724355000	-1.089531000
C	-1.523594000	3.546338000	0.518898000
C	0.698743000	3.998559000	-1.139166000
H	0.504638000	1.907594000	-1.715491000
C	-0.934884000	4.819290000	0.464661000
H	-2.388346000	3.371987000	1.177880000
C	0.179609000	5.049937000	-0.361928000
H	1.558534000	4.176398000	-1.804250000
H	-1.346683000	5.636879000	1.076959000
H	0.636530000	6.050867000	-0.407548000

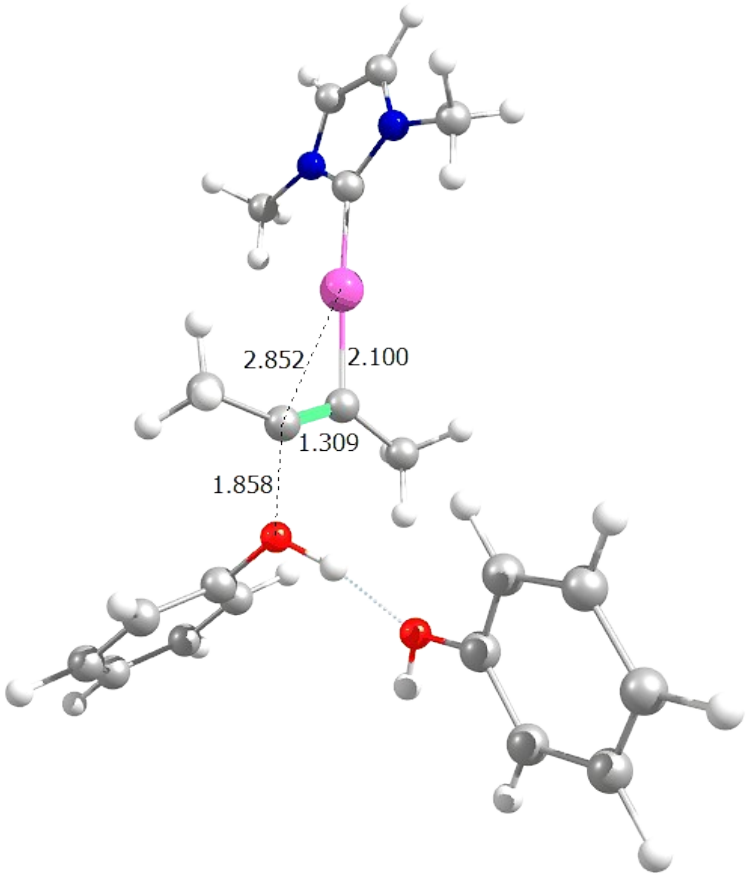
PhOH-MeC-PhOH



C	4.458582000	-0.455624000	-0.132724000
N	5.173251000	-1.561390000	0.241801000
C	6.509146000	-1.413778000	-0.098003000
C	6.633238000	-0.184774000	-0.699767000
N	5.369856000	0.385917000	-0.711776000
C	4.624178000	-2.744253000	0.907902000
C	5.072819000	1.704793000	-1.274714000
Au	2.470322000	-0.131886000	0.114237000
C	0.256101000	-0.081625000	-0.183251000
C	0.484833000	0.506601000	0.903154000
O	-2.872069000	0.829173000	0.316070000
H	7.258590000	-2.184159000	0.112527000
H	7.511618000	0.321453000	-1.114101000
H	5.118120000	-2.891930000	1.888237000
H	4.778416000	-3.641863000	0.277490000
H	3.540910000	-2.589510000	1.064207000
H	4.001845000	1.924393000	-1.111672000
H	5.286933000	1.712569000	-2.361563000
H	5.685481000	2.478240000	-0.771763000
H	-3.607204000	0.280808000	0.695405000
O	-4.899053000	-0.825770000	1.268381000
H	-5.111381000	-1.013290000	2.203462000
C	-3.305570000	2.116698000	0.117030000
C	-2.395248000	3.046485000	-0.429840000
C	-4.615568000	2.531312000	0.442511000
C	-2.794633000	4.375013000	-0.645937000
H	-1.378373000	2.711525000	-0.688725000
C	-5.001995000	3.864049000	0.220940000
H	-5.325932000	1.803410000	0.865323000
C	-4.098133000	4.793654000	-0.322181000
H	-2.077368000	5.092081000	-1.076669000
H	-6.027218000	4.175781000	0.476757000
H	-4.407646000	5.835635000	-0.494572000
C	-5.555895000	-1.731056000	0.448800000
C	-5.409492000	-1.575702000	-0.941816000
C	-6.342473000	-2.769749000	0.977914000
C	-6.059781000	-2.473143000	-1.803714000
H	-4.796737000	-0.748799000	-1.331417000
C	-6.988158000	-3.660104000	0.102054000
H	-6.453901000	-2.882491000	2.069894000
C	-6.849820000	-3.517483000	-1.289086000
H	-5.951161000	-2.348553000	-2.892636000
H	-7.606316000	-4.471187000	0.517636000
H	-7.359701000	-4.215151000	-1.970503000
C	0.318976000	1.238148000	2.167147000
H	0.682184000	0.651467000	3.034965000
H	0.851273000	2.210477000	2.154977000
H	-0.767032000	1.433058000	2.293938000
C	-0.410905000	-0.668171000	-1.352145000
H	-1.491036000	-0.426529000	-1.242528000
H	-0.039846000	-0.236154000	-2.303216000
H	-0.283959000	-1.768910000	-1.391635000

Zero-point correction= 0.413768 (Hartree/Particle)
Thermal correction to Energy= 0.445166
Thermal correction to Enthalpy= 0.446110
Thermal correction to Gibbs Free Energy= 0.338324
Sum of electronic and zero-point Energies= -1210.318113
Sum of electronic and thermal Energies= -1210.286716
Sum of electronic and thermal Enthalpies= -1210.285772
Sum of electronic and thermal Free Energies= -1210.393558

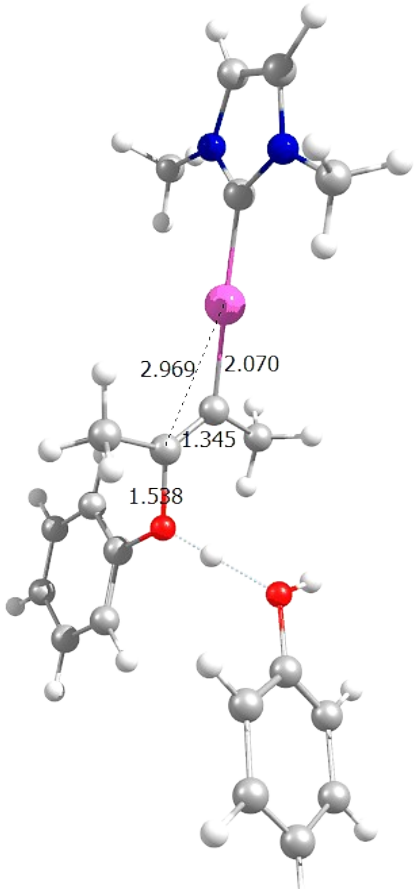
PhOH-MeCTS-PhOH



Zero-point correction= 0.414323 (Hartree/Particle)
Thermal correction to Energy= 0.443653
Thermal correction to Enthalpy= 0.444598
Thermal correction to Gibbs Free Energy= 0.346165
Sum of electronic and zero-point Energies= -1210.296331
Sum of electronic and thermal Energies= -1210.267001
Sum of electronic and thermal Enthalpies= -1210.266057
Sum of electronic and thermal Free Energies= -1210.364490

C	6.060768000	-1.332281000	0.284335000
C	6.273694000	-0.021937000	-0.062669000
N	5.021547000	0.556559000	-0.229046000
C	4.029266000	-0.357432000	0.006123000
N	4.684508000	-1.518145000	0.320700000
C	4.807363000	1.953675000	-0.604668000
Au	2.012895000	-0.064762000	-0.114925000
C	-0.055027000	0.184559000	-0.382962000
C	4.037223000	-2.788238000	0.646978000
C	-0.616544000	0.698336000	0.682462000
H	6.769389000	-2.137382000	0.505130000
H	7.204116000	0.538155000	-0.202926000
H	4.318136000	-3.110881000	1.669100000
H	4.336596000	-3.568726000	-0.080309000
H	2.942160000	-2.643099000	0.596633000
H	3.718605000	2.129492000	-0.684843000
H	5.284566000	2.164603000	-1.582101000
H	5.232471000	2.628077000	0.164979000
O	-2.457436000	0.927374000	0.572842000
H	-2.937560000	0.253471000	-0.019599000
O	-3.960626000	-0.665291000	-0.878857000
H	-4.647021000	-0.199058000	-1.397171000
C	-2.964635000	2.222626000	0.336451000
C	-3.568657000	2.894469000	1.411545000
C	-2.858652000	2.813862000	-0.934340000
C	-4.084185000	4.185904000	1.204215000
H	-3.642999000	2.395616000	2.389471000
C	-3.386255000	4.102470000	-1.129152000
H	-2.359658000	2.277493000	-1.755854000
C	-3.995904000	4.788826000	-0.063225000
H	-4.563304000	4.720167000	2.039242000
H	-3.312331000	4.575465000	-2.120767000
H	-4.402377000	5.799517000	-0.221396000
C	-4.452989000	-1.901273000	-0.450462000
C	-3.618311000	-2.699617000	0.348454000
C	-5.738673000	-2.330565000	-0.817213000
C	-4.088781000	-3.949295000	0.785220000
H	-2.612193000	-2.345634000	0.621206000
C	-6.193770000	-3.584588000	-0.373967000
H	-6.383591000	-1.692897000	-1.445424000
C	-5.373122000	-4.396606000	0.427260000
H	-3.439698000	-4.579805000	1.412661000
H	-7.201188000	-3.924101000	-0.660263000
H	-5.734259000	-5.377012000	0.772531000
C	-0.411166000	1.208611000	2.052743000
H	0.673411000	1.194358000	2.276520000
H	-0.766837000	2.255773000	2.155475000
H	-0.936842000	0.586876000	2.806756000
C	-0.619475000	-0.221806000	-1.717746000
H	-1.724762000	-0.153821000	-1.764509000
H	-0.189824000	0.411325000	-2.522391000
H	-0.334592000	-1.265562000	-1.962861000

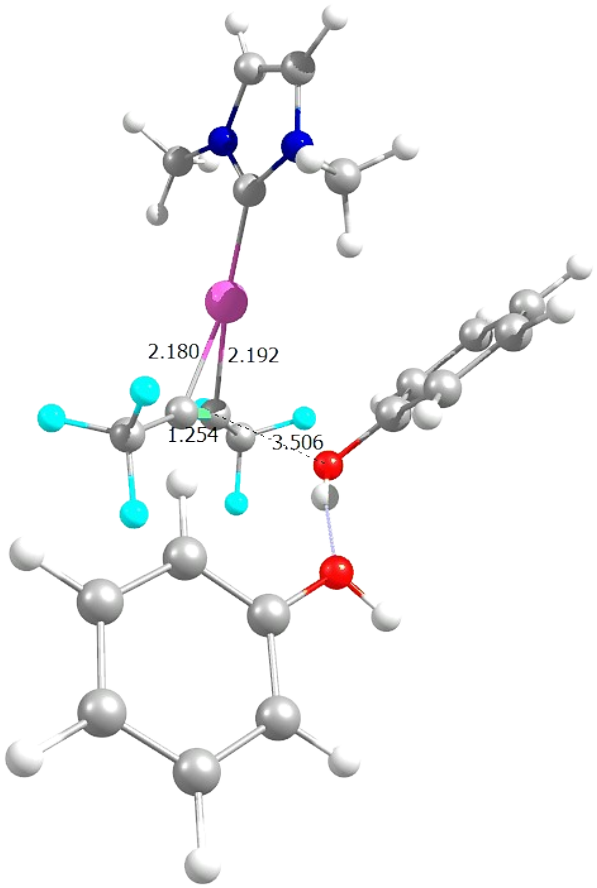
PhOH-MeCprod-PhOH



Zero-point correction= 0.415148 (Hartree/Particle)
Thermal correction to Energy= 0.444262
Thermal correction to Enthalpy= 0.445206
Thermal correction to Gibbs Free Energy= 0.348347
Sum of electronic and zero-point Energies= -1210.299581
Sum of electronic and thermal Energies= -1210.270467
Sum of electronic and thermal Enthalpies= -1210.269523
Sum of electronic and thermal Free Energies= -1210.366381

C	-6.185879000	1.418828000	0.447235000
C	-6.437539000	0.113798000	0.106647000
N	-5.204300000	-0.482372000	-0.127551000
C	-4.184245000	0.413555000	0.056677000
N	-4.806348000	1.581896000	0.410762000
C	-5.030177000	-1.879328000	-0.521417000
Au	-2.168778000	0.082761000	-0.158935000
C	-0.143466000	-0.238264000	-0.438993000
C	-4.120305000	2.837289000	0.710903000
C	0.637890000	-0.481618000	0.627825000
H	-6.869000000	2.233597000	0.709046000
H	-7.382765000	-0.431105000	0.013484000
H	-4.333509000	3.153491000	1.751408000
H	-4.448797000	3.631484000	0.011365000
H	-3.032880000	2.673603000	0.593108000
H	-3.946937000	-2.077658000	-0.622747000
H	-5.529806000	-2.071120000	-1.491874000
H	-5.455711000	-2.551980000	0.249573000
O	2.153186000	-0.613377000	0.399491000
H	2.602143000	0.190070000	-0.122919000
O	3.200303000	1.339733000	-0.784708000
H	3.066111000	1.405576000	-1.752169000
C	2.812567000	-1.879544000	0.276644000
C	2.071522000	-3.023381000	-0.036444000
C	4.195836000	-1.905724000	0.497835000
C	2.756777000	-4.248364000	-0.133959000
H	0.985693000	-2.955366000	-0.199523000
C	4.862411000	-3.137857000	0.378754000
H	4.741153000	-0.987379000	0.764953000
C	4.146587000	-4.307679000	0.067453000
H	2.192883000	-5.162324000	-0.376147000
H	5.949887000	-3.179861000	0.544476000
H	4.674272000	-5.269950000	-0.014660000
C	4.464903000	1.840392000	-0.425207000
C	4.739687000	1.986861000	0.943140000
C	5.407207000	2.177561000	-1.407798000
C	5.998506000	2.479871000	1.328778000
H	3.973216000	1.736531000	1.692161000
C	6.657532000	2.678641000	-1.004349000
H	5.173574000	2.052569000	-2.478399000
C	6.957494000	2.827321000	0.360730000
H	6.223895000	2.602203000	2.399480000
H	7.401148000	2.950456000	-1.769215000
H	7.938229000	3.218488000	0.670423000
C	0.377242000	-0.168017000	-1.858108000
H	1.439487000	-0.478023000	-1.981530000
H	-0.226729000	-0.817981000	-2.524974000
H	0.256100000	0.860379000	-2.263926000
C	0.389127000	-0.630638000	2.092872000
H	0.740590000	-1.614702000	2.473247000
H	0.904183000	0.157948000	2.682899000
H	-0.698397000	-0.556783000	2.282271000

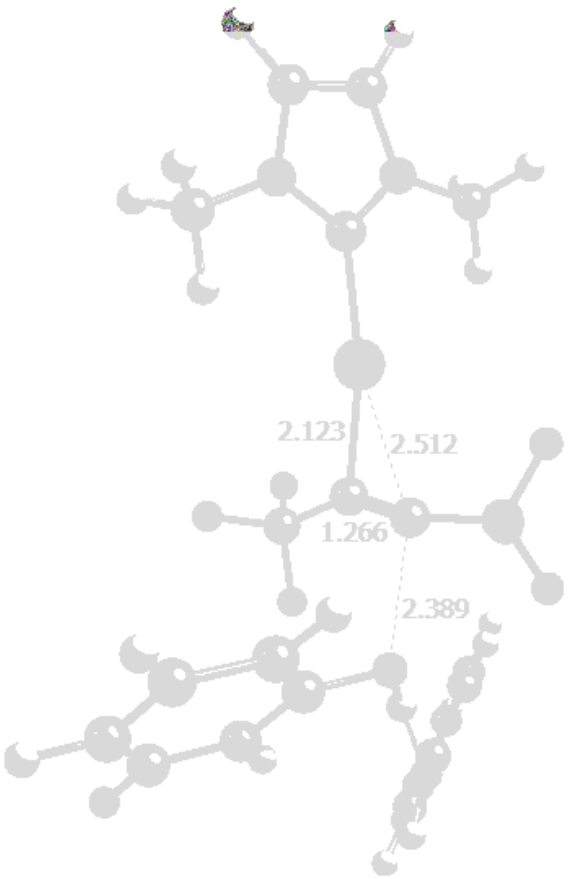
PhOH-CF_3-PhOH



C	2.993866000	0.845718000	-1.157396000
N	4.241838000	0.575673000	-1.650694000
C	4.816082000	1.729794000	-2.153753000
C	3.898524000	2.740824000	-1.979032000
N	2.792598000	2.181662000	-1.364265000
C	4.909320000	-0.728654000	-1.617865000
C	1.558678000	2.913957000	-1.057093000
Au	1.705851000	-0.471224000	-0.316143000
C	-0.014771000	-1.772442000	-0.002918000
C	-1.140190000	-1.914635000	-0.988610000
C	0.753201000	-1.970894000	0.967948000
C	1.375885000	-2.543490000	2.207913000
O	-1.704400000	0.504354000	1.319962000
H	5.822022000	1.746115000	-2.586724000
H	3.947789000	3.801837000	-2.246329000
H	5.719422000	-0.727760000	-0.861895000
H	5.333205000	-0.955106000	-2.614837000
H	4.165930000	-1.503341000	-1.354836000
H	0.997910000	2.376384000	-0.269299000
H	0.933280000	3.003642000	-1.967277000
H	1.815577000	3.920860000	-0.681087000
H	-2.644198000	0.671769000	1.036661000
O	-4.373306000	1.040245000	0.848090000
H	-4.797045000	1.247583000	1.704978000
F	-1.356888000	-0.749306000	-1.634081000
F	-0.817191000	-2.849793000	-1.901241000
F	-2.258812000	-2.283544000	-0.356205000
F	1.841590000	-1.558203000	3.001677000
F	2.407545000	-3.340995000	1.869590000
F	0.467843000	-3.259059000	2.880955000
C	-1.083407000	1.685702000	1.594687000
C	0.145862000	1.645777000	2.296441000
C	-1.615682000	2.937216000	1.201757000
C	0.821503000	2.839769000	2.604562000
H	0.530490000	0.676062000	2.645832000
C	-0.931451000	4.122578000	1.522058000
H	-2.578012000	2.969993000	0.666798000
C	0.290405000	4.085020000	2.220449000
H	1.763295000	2.793492000	3.174884000
H	-1.368131000	5.090293000	1.226909000
H	0.810869000	5.018746000	2.483106000
C	-5.335432000	0.556389000	-0.029419000
C	-4.929541000	0.227121000	-1.334702000
C	-6.675884000	0.403550000	0.366900000
C	-5.881346000	-0.257951000	-2.246299000
H	-3.876163000	0.352898000	-1.624641000
C	-7.617691000	-0.081727000	-0.556826000
H	-6.985293000	0.663474000	1.393662000
C	-7.226218000	-0.414207000	-1.864932000
H	-5.565691000	-0.514377000	-3.269896000
H	-8.667113000	-0.199093000	-0.244740000
H	-7.966825000	-0.793271000	-2.585163000

Zero-point correction= 0.369786 (Hartree/Particle)
Thermal correction to Energy= 0.404789
Thermal correction to Enthalpy= 0.405734
Thermal correction to Gibbs Free Energy= 0.290316
Sum of electronic and zero-point Energies= -1805.329732
Sum of electronic and thermal Energies= -1805.294729
Sum of electronic and thermal Enthalpies= -1805.293785
Sum of electronic and thermal Free Energies= -1805.409202

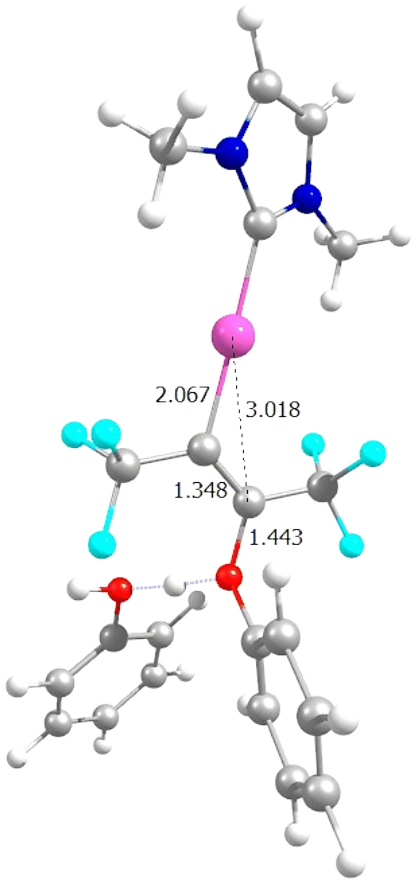
PhOH-CF_3TS-PhOH



C	6.116849000	-1.187650000	-0.236797000
C	6.144877000	0.106449000	-0.698531000
N	4.836103000	0.563699000	-0.694696000
C	3.994197000	-0.413386000	-0.240865000
N	4.791103000	-1.489866000	0.034040000
C	4.432113000	1.902855000	-1.130213000
Au	1.979138000	-0.304104000	-0.076970000
C	-0.119116000	-0.169347000	-0.370341000
C	4.331551000	-2.779674000	0.554660000
C	-0.334619000	-0.072053000	0.873129000
H	6.927528000	-1.906984000	-0.079161000
H	6.984059000	0.729822000	-1.025073000
H	4.617092000	-3.592284000	-0.141420000
H	3.230749000	-2.750407000	0.649703000
H	4.778577000	-2.969532000	1.550129000
H	3.341714000	2.009322000	-0.983006000
H	4.669289000	2.041665000	-2.203257000
H	4.959244000	2.670857000	-0.531360000
O	-2.290162000	1.239402000	1.279772000
H	-3.114629000	0.715430000	1.052522000
O	-4.638094000	-0.063257000	0.874269000
H	-5.425261000	0.514236000	0.930343000
C	-0.301158000	-0.333298000	2.352277000
C	-0.709762000	-0.027835000	-1.749092000
F	0.689846000	-1.227773000	2.622640000
F	-1.457996000	-0.872631000	2.759727000
F	-2.052942000	-0.058193000	-1.698549000
F	-0.291698000	-1.036762000	-2.539862000
F	-0.317749000	1.136682000	-2.301863000
F	-0.050144000	0.781349000	3.050116000
C	-2.296873000	2.461272000	0.646848000
C	-1.385826000	3.439687000	1.098163000
C	-3.181806000	2.748757000	-0.414223000
C	-1.366936000	4.701992000	0.486494000
H	-0.719688000	3.201635000	1.940712000
C	-3.157743000	4.020905000	-1.010305000
H	-3.881402000	1.976121000	-0.767046000
C	-2.251036000	5.000028000	-0.568192000
H	-0.662473000	5.467797000	0.847790000
H	-3.854746000	4.244417000	-1.833214000
H	-2.235958000	5.994154000	-1.040218000
C	-4.967192000	-1.240891000	0.212232000
C	-4.035356000	-2.292884000	0.244690000
C	-6.188444000	-1.380180000	-0.469928000
C	-4.331181000	-3.490729000	-0.426430000
H	-3.101141000	-2.171038000	0.812800000
C	-6.474204000	-2.587705000	-1.130290000
H	-6.914372000	-0.549665000	-0.487651000
C	-5.547591000	-3.644304000	-1.115745000
H	-3.605275000	-4.318546000	-0.398257000
H	-7.432257000	-2.697447000	-1.661795000
H	-5.775647000	-4.587443000	-1.634778000

Zero-point correction= 0.369281 (Hartree/Particle)
Thermal correction to Energy= 0.403293
Thermal correction to Enthalpy= 0.404237
Thermal correction to Gibbs Free Energy= 0.293418
Sum of electronic and zero-point Energies= -1805.323190
Sum of electronic and thermal Energies= -1805.289178
Sum of electronic and thermal Enthalpies= -1805.288233
Sum of electronic and thermal Free Energies= -1805.399053

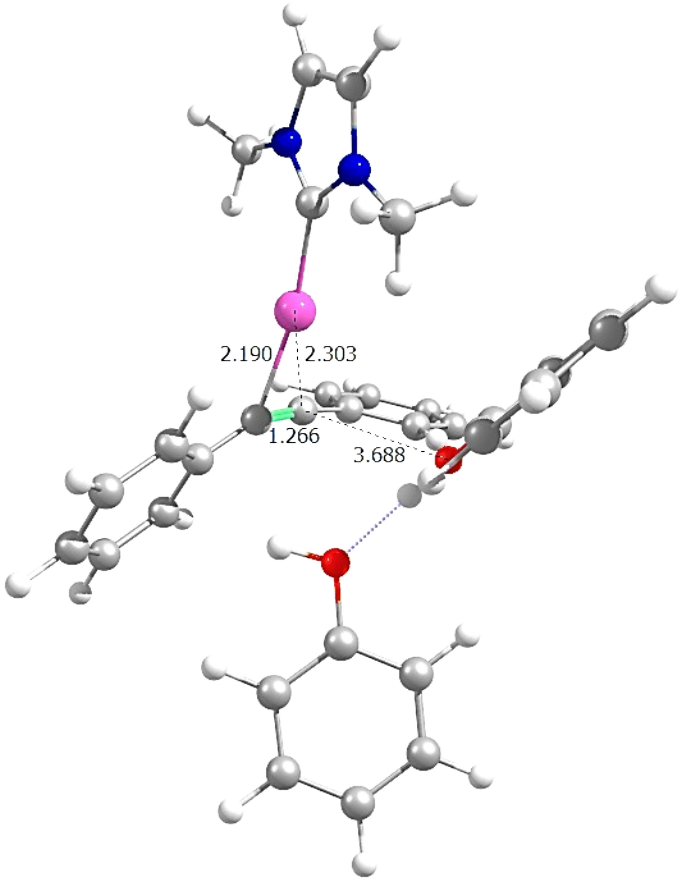
PhOH-CF_3prod-PhOH



C	-6.224655000	0.593239000	1.227127000
C	-6.453791000	0.600317000	-0.126225000
N	-5.216456000	0.465845000	-0.742064000
C	-4.218099000	0.373939000	0.190298000
N	-4.853898000	0.453759000	1.400096000
C	-5.019362000	0.427059000	-2.190874000
Au	-2.216764000	0.166060000	-0.149453000
C	-0.192367000	-0.021694000	-0.519822000
C	-4.190744000	0.404167000	2.703012000
C	0.670962000	-0.532343000	0.380751000
H	-6.919044000	0.674347000	2.069889000
H	-7.386788000	0.688257000	-0.692605000
H	-4.582114000	-0.444199000	3.298430000
H	-4.359122000	1.350163000	3.254885000
H	-3.106530000	0.265100000	2.539464000
H	-3.939496000	0.302644000	-2.392546000
H	-5.371016000	1.371602000	-2.651124000
H	-5.573905000	-0.425641000	-2.630110000
O	2.104104000	-0.570488000	0.217724000
H	2.627907000	0.430781000	-0.099466000
O	3.121775000	1.523414000	-0.448682000
H	3.013602000	1.616628000	-1.421721000
C	2.779734000	-1.797514000	-0.127004000
C	2.114156000	-2.785212000	-0.857048000
C	4.106922000	-1.917868000	0.297195000
C	2.827045000	-3.955469000	-1.176739000
H	1.067965000	-2.653333000	-1.169023000
C	4.803985000	-3.089462000	-0.046254000
H	4.581541000	-1.124533000	0.894222000
C	4.166480000	-4.106915000	-0.778578000
H	2.324815000	-4.750926000	-1.748225000
H	5.849820000	-3.208605000	0.275728000
H	4.715586000	-5.025227000	-1.036041000
C	4.403581000	1.932111000	0.011229000
C	4.602383000	1.975900000	1.396686000
C	5.400686000	2.279531000	-0.907430000
C	5.862180000	2.379725000	1.873277000
H	3.786195000	1.716955000	2.088014000
C	6.650062000	2.692026000	-0.410043000
H	5.214341000	2.233956000	-1.992949000
C	6.883206000	2.738869000	0.975303000
H	6.038320000	2.423509000	2.959007000
H	7.444400000	2.974965000	-1.117507000
H	7.863591000	3.061285000	1.357046000
C	0.225622000	0.503212000	-1.871334000
C	0.266619000	-1.060534000	1.761284000
F	-0.492169000	-0.070035000	-2.858383000
F	0.054665000	1.845152000	-1.941055000
F	1.557938000	0.286010000	-2.217858000
F	1.330704000	-1.561643000	2.422151000
F	-0.260806000	-0.070010000	2.530329000
F	-0.664547000	-2.035649000	1.668592000

Zero-point correction= 0.369537 (Hartree/Particle)
Thermal correction to Energy= 0.402391
Thermal correction to Enthalpy= 0.403335
Thermal correction to Gibbs Free Energy= 0.296062
Sum of electronic and zero-point Energies= -1805.352862
Sum of electronic and thermal Energies= -1805.320008
Sum of electronic and thermal Enthalpies= -1805.319064
Sum of electronic and thermal Free Energies= -1805.426337

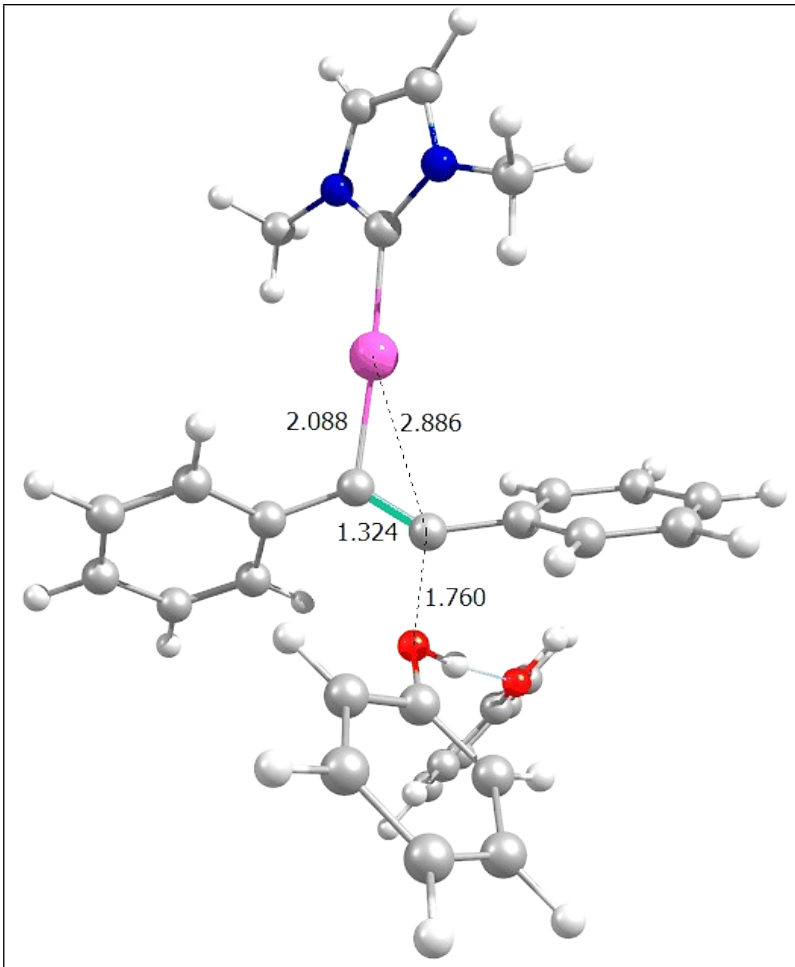
PhOH-PhC-PhOH



Zero-point correction= 0.518283 (Hartree/Particle)
Thermal correction to Energy= 0.555715
Thermal correction to Enthalpy= 0.556659
Thermal correction to Gibbs Free Energy= 0.434424
Sum of electronic and zero-point Energies= -1593.421404
Sum of electronic and thermal Energies= -1593.383972
Sum of electronic and thermal Enthalpies= -1593.383028
Sum of electronic and thermal Free Energies= -1593.505264

C	-3.338978000	-0.169948000	-0.886537000
N	-4.563748000	0.429650000	-1.017072000
C	-5.514289000	-0.494836000	-1.421260000
C	-4.865729000	-1.699070000	-1.552566000
N	-3.537637000	-1.480900000	-1.221142000
C	-4.854958000	1.837628000	-0.742975000
C	-2.501775000	-2.516068000	-1.275242000
Au	-1.609405000	0.728196000	-0.332217000
C	0.329448000	1.743388000	-0.248798000
C	-0.013349000	1.757950000	0.970335000
O	1.109031000	-1.748375000	1.183073000
H	-6.564757000	-0.228103000	-1.578198000
H	-5.240510000	-2.682984000	-1.853636000
H	-5.483262000	1.931875000	0.164997000
H	-5.383716000	2.286844000	-1.605866000
H	-3.899478000	2.370228000	-0.583432000
H	-1.587614000	-2.145256000	-0.777272000
H	-2.271933000	-2.770532000	-2.328663000
H	-2.844871000	-3.423011000	-0.742845000
H	1.780111000	-1.436430000	0.517183000
O	2.987986000	-0.788531000	-0.582406000
H	2.764248000	-0.162541000	-1.303703000
C	1.187227000	2.025570000	-1.382786000
C	2.134960000	3.078851000	-1.282571000
C	1.114080000	1.271389000	-2.583171000
C	2.983697000	3.363989000	-2.361626000
H	2.196694000	3.667832000	-0.355261000
C	1.974581000	1.561601000	-3.654342000
H	0.368481000	0.465045000	-2.668614000
C	2.907773000	2.609784000	-3.548113000
H	3.712426000	4.184852000	-2.275094000
H	1.908632000	0.972356000	-4.582133000
H	3.574217000	2.842238000	-4.393134000
C	-0.233427000	1.829998000	2.385464000
C	-0.734622000	3.028731000	2.965161000
C	0.086111000	0.717625000	3.213448000
C	-0.900978000	3.111632000	4.353047000
H	-0.977556000	3.885846000	2.318724000
C	-0.091203000	0.819692000	4.599457000
H	0.474519000	-0.202947000	2.748623000
C	-0.582306000	2.009536000	5.170022000
H	-1.280305000	4.041900000	4.803312000
H	0.161507000	-0.036563000	5.243851000
H	-0.715762000	2.080611000	6.260930000
C	0.594772000	-2.960926000	0.825419000
C	-0.351074000	-3.561320000	1.687421000
C	0.969319000	-3.623372000	-0.366990000
C	-0.910453000	-4.805922000	1.357332000
H	-0.624220000	-3.046680000	2.621495000
C	0.400082000	-4.869185000	-0.684918000
H	1.722068000	-3.164165000	-1.027476000
C	-0.543579000	-5.468240000	0.169602000
H	-1.634494000	-5.270780000	2.045875000
H	0.712010000	-5.382294000	-1.608913000
H	-0.974155000	-6.450753000	-0.077348000
C	4.336306000	-0.692641000	-0.265960000
C	4.813385000	-1.466880000	0.807272000
C	5.203261000	0.142796000	-0.992578000
C	6.174005000	-1.400429000	1.147269000
H	4.117387000	-2.109889000	1.367034000
C	6.563269000	0.197959000	-0.640201000
H	4.815772000	0.746173000	-1.830697000
C	7.054423000	-0.571481000	0.428156000
H	6.548815000	-2.007135000	1.986485000
H	7.242500000	0.850288000	-1.211205000
H	8.119944000	-0.526337000	0.699625000

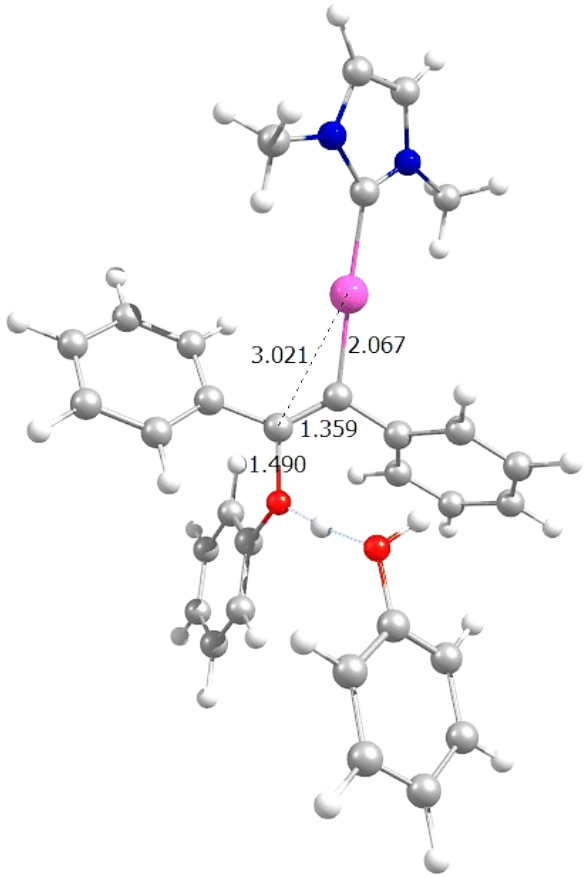
PhOH-PhCTS-PhOH



Zero-point correction= 0.518316 (Hartree/Particle)
Thermal correction to Energy= 0.553829
Thermal correction to Enthalpy= 0.554773
Thermal correction to Gibbs Free Energy= 0.441666
Sum of electronic and zero-point Energies= -1593.399880
Sum of electronic and thermal Energies= -1593.364367
Sum of electronic and thermal Enthalpies= -1593.363423
Sum of electronic and thermal Free Energies= -1593.476530

C	4.260847000	-0.942723000	0.216108000
N	5.428250000	-0.485692000	-0.335467000
C	6.507237000	-1.248681000	0.092976000
C	6.003847000	-2.208150000	0.935054000
N	4.630725000	-2.005013000	0.997484000
C	5.537165000	0.650542000	-1.250265000
C	3.716122000	-2.812742000	1.802764000
Au	2.390719000	-0.171750000	-0.054793000
C	0.546815000	0.767630000	-0.337251000
C	-0.499396000	-0.033200000	-0.215689000
O	-2.067123000	0.843760000	-0.330463000
H	7.533832000	-1.051138000	-0.232778000
H	6.506271000	-3.009030000	1.487494000
H	5.967491000	0.324053000	-2.217642000
H	6.179752000	1.437722000	-0.808561000
H	4.523914000	1.059827000	-1.420055000
H	2.684339000	-2.463644000	1.612345000
H	3.947908000	-2.698520000	2.880509000
H	3.800183000	-3.880748000	1.520521000
H	-2.821901000	0.313206000	-0.780792000
O	-3.970590000	-0.427222000	-1.570651000
H	-3.689642000	-0.891902000	-2.384473000
C	0.580955000	2.215346000	-0.656666000
C	1.350594000	3.106680000	0.131606000
C	-0.110961000	2.732025000	-1.780590000
C	1.399358000	4.475594000	-0.174869000
H	1.904741000	2.713590000	0.999004000
C	-0.040393000	4.097942000	-2.096253000
H	-0.693404000	2.049595000	-2.417800000
C	0.707484000	4.976419000	-1.291998000
H	1.989836000	5.155224000	0.459620000
H	-0.574466000	4.479981000	-2.980747000
H	0.756407000	6.048218000	-1.539810000
C	-0.881481000	-1.435626000	-0.098605000
C	-0.212868000	-2.404713000	-0.895581000
C	-1.886634000	-1.871785000	0.803943000
C	-0.523891000	-3.766800000	-0.767567000
H	0.554513000	-2.070690000	-1.610921000
C	-2.199032000	-3.233793000	0.916713000
H	-2.419558000	-1.137800000	1.427366000
C	-1.516983000	-4.186117000	0.136473000
H	0.005331000	-4.505665000	-1.389752000
H	-2.980259000	-3.554444000	1.622922000
H	-1.765355000	-5.255019000	0.228482000
C	-2.524564000	1.777757000	0.619756000
C	-1.949369000	1.828363000	1.897203000
C	-3.557987000	2.650797000	0.239018000
C	-2.432619000	2.775060000	2.818027000
H	-1.128741000	1.145025000	2.161085000
C	-4.037992000	3.580365000	1.177985000
H	-3.974104000	2.604888000	-0.778582000
C	-3.477741000	3.646435000	2.465905000
H	-1.985522000	2.825543000	3.822956000
H	-4.849848000	4.266302000	0.890232000
H	-3.851623000	4.382890000	3.193308000
C	-5.069486000	-1.087478000	-1.011631000
C	-5.636117000	-0.550936000	0.155985000
C	-5.594762000	-2.243741000	-1.611226000
C	-6.748619000	-1.191589000	0.727285000
H	-5.219005000	0.364824000	0.602250000
C	-6.710841000	-2.870305000	-1.029538000
H	-5.140110000	-2.653338000	-2.529155000
C	-7.289867000	-2.349238000	0.140285000
H	-7.199585000	-0.772230000	1.640113000
H	-7.127883000	-3.773683000	-1.501004000
H	-8.164345000	-2.842143000	0.591136000

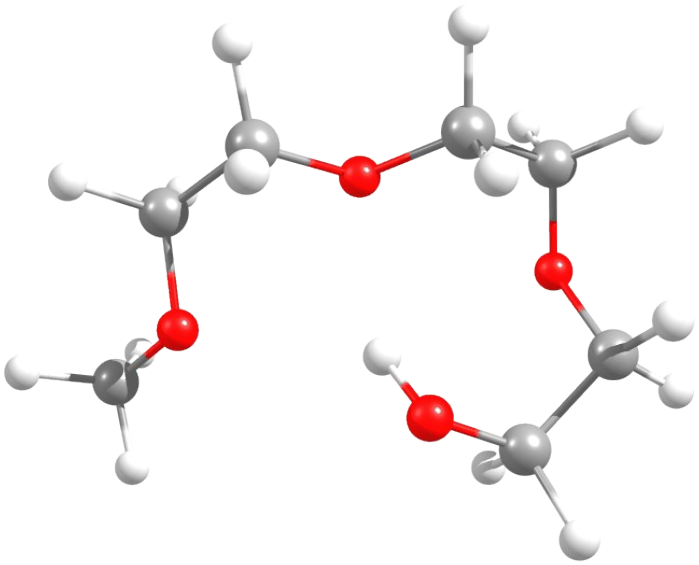
PhOH-PhCprod-PhOH



C	-6.362159000	0.443052000	1.047472000
C	-6.386527000	1.368130000	0.034194000
N	-5.088582000	1.461300000	-0.452940000
C	-4.249603000	0.618466000	0.227792000
N	-5.050172000	-0.003028000	1.149754000
C	-4.683825000	2.340978000	-1.548208000
Au	-2.237303000	0.356776000	-0.058094000
C	-0.194320000	0.180611000	-0.321001000
C	-4.592712000	-0.994182000	2.122399000
C	0.475913000	-0.970793000	-0.053958000
H	-7.163086000	0.071181000	1.694989000
H	-7.213169000	1.958276000	-0.374987000
H	-5.163062000	-1.936648000	2.004703000
H	-4.725092000	-0.611473000	3.154069000
H	-3.519834000	-1.191451000	1.940530000
H	-3.600201000	2.203548000	-1.720840000
H	-4.881888000	3.398891000	-1.284398000
H	-5.237294000	2.083218000	-2.472992000
O	1.963656000	-0.903747000	-0.006814000
H	2.382346000	-0.001941000	0.547472000
O	2.711264000	1.063181000	1.230256000
H	2.194489000	1.819414000	0.831122000
C	0.511993000	1.413994000	-0.769546000
C	0.431225000	2.612242000	-0.002339000
C	1.263145000	1.452177000	-1.972861000
C	1.088215000	3.787197000	-0.417366000
H	-0.181543000	2.617682000	0.914148000
C	1.900413000	2.632554000	-2.393124000
H	1.328448000	0.548279000	-2.597769000
C	1.822829000	3.804433000	-1.618271000
H	1.006960000	4.699517000	0.194874000
H	2.461767000	2.635704000	-3.341018000
H	2.317421000	4.728875000	-1.954458000
C	0.001182000	-2.319212000	0.319082000
C	-1.187286000	-2.843848000	-0.249434000
C	0.714747000	-3.118645000	1.246901000
C	-1.658538000	-4.112382000	0.121483000
H	-1.730435000	-2.249309000	-1.001022000
C	0.240531000	-4.387213000	1.613567000
H	1.643602000	-2.737278000	1.696850000
C	-0.949158000	-4.888476000	1.056116000
H	-2.578290000	-4.506657000	-0.338860000
H	0.805100000	-4.989067000	2.342752000
H	-1.315867000	-5.887278000	1.339939000
C	2.802911000	-1.597989000	-0.926965000
C	2.261358000	-2.177616000	-2.080520000
C	4.167649000	-1.671606000	-0.616952000
C	3.131201000	-2.853185000	-2.955735000
H	1.184058000	-2.113039000	-2.289384000
C	5.020525000	-2.340039000	-1.512322000
H	4.562982000	-1.217821000	0.304834000
C	4.506535000	-2.933503000	-2.678581000
H	2.721049000	-3.319669000	-3.864659000
H	6.095952000	-2.401127000	-1.285293000
H	5.178848000	-3.462703000	-3.370642000
C	4.062157000	1.392751000	1.487786000
C	4.716641000	0.678385000	2.501696000
C	4.707017000	2.391577000	0.744762000
C	6.065385000	0.972876000	2.769195000
H	4.169293000	-0.079723000	3.082161000
C	6.050910000	2.684450000	1.037394000
H	4.167235000	2.927682000	-0.052253000
C	6.732293000	1.975357000	2.042422000
H	6.591721000	0.422041000	3.564026000
H	6.568316000	3.471047000	0.466692000
H	7.785121000	2.207874000	2.263160000

Zero-point correction= 0.517574 (Hartree/Particle)
Thermal correction to Energy= 0.552667
Thermal correction to Enthalpy= 0.553611
Thermal correction to Gibbs Free Energy= 0.443635
Sum of electronic and zero-point Energies= -1593.408661
Sum of electronic and thermal Energies= -1593.373568
Sum of electronic and thermal Enthalpies= -1593.372624
Sum of electronic and thermal Free Energies= -1593.482600

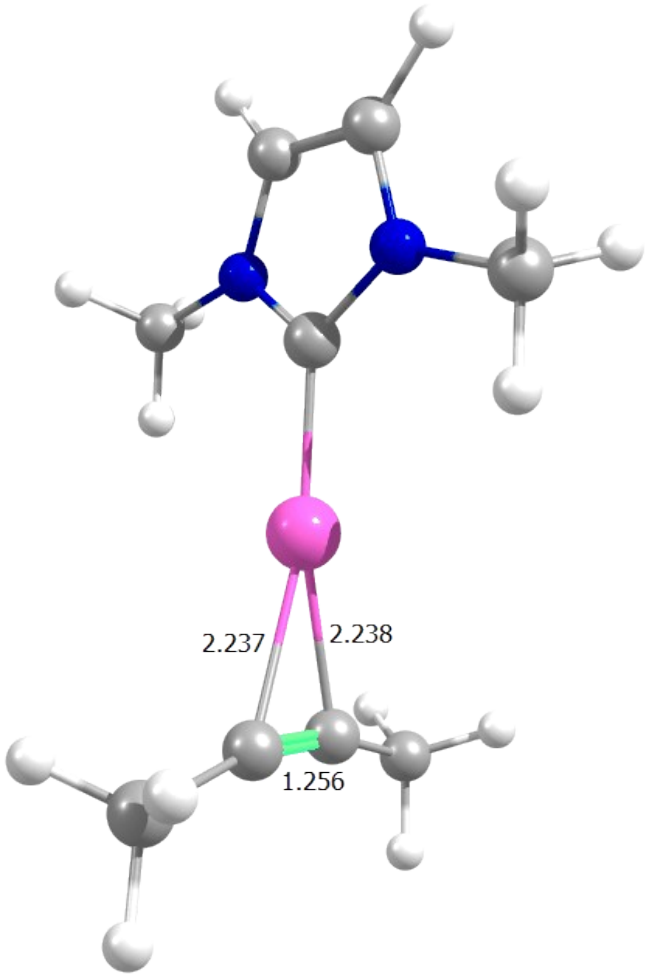
ALCOHOL



O	0.520371	1.460905	-0.931678
C	1.649462	1.979924	-0.260746
C	2.731460	0.936335	0.028389
O	2.267127	-0.023459	0.976643
C	2.148421	-1.359211	0.528628
C	0.997819	-1.609146	-0.446642
O	-0.216757	-1.202813	0.166213
C	-1.372099	-1.475357	-0.609021
C	-2.561302	-0.802304	0.053107
O	-2.395234	0.597162	-0.043292
C	-3.397202	1.334265	0.621413
H	1.376547	2.474153	0.705454
H	2.090277	2.769125	-0.911866
H	3.630786	1.445472	0.453031
H	3.044155	0.447120	-0.924657
H	3.093877	-1.725303	0.052028
H	1.978729	-1.965637	1.443991
H	0.976976	-2.700924	-0.698205
H	1.150893	-1.044910	-1.399020
H	-1.557916	-2.577086	-0.680835
H	-1.257002	-1.081775	-1.649039
H	-2.622328	-1.128248	1.122767
H	-3.504400	-1.137012	-0.451634
H	-3.164332	2.408922	0.487217
H	-3.430393	1.109336	1.716537
H	-4.414683	1.135039	0.201094
H	0.025408	0.890336	-0.300725

Zero-point correction= 0.228999 (Hartree/Particle)
Thermal correction to Energy= 0.242540
Thermal correction to Enthalpy= 0.243484
Thermal correction to Gibbs Free Energy= 0.186795
Sum of electronic and zero-point Energies= -576.558693
Sum of electronic and thermal Energies= -576.545152
Sum of electronic and thermal Enthalpies= -576.544208
Sum of electronic and thermal Free Energies= -576.600896

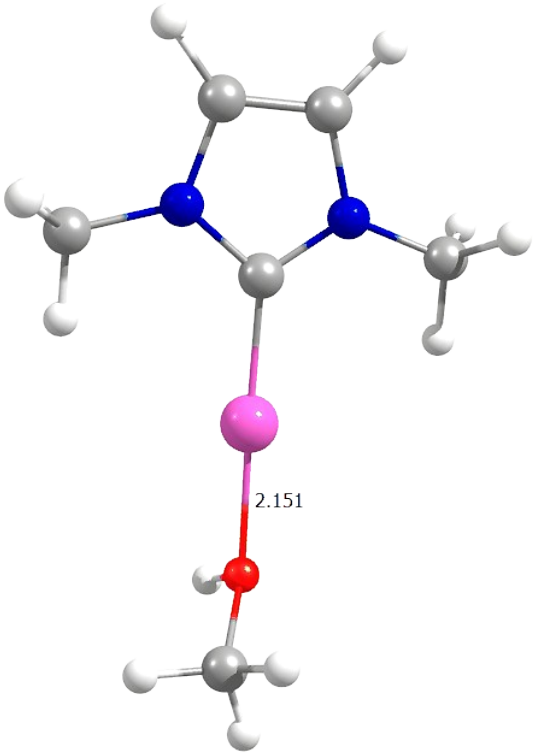
CAT



N	-2.337568	1.086640	-0.073541
C	-3.664017	0.685659	-0.046268
C	-3.664107	-0.685343	0.046723
N	-2.337710	-1.086516	0.073688
C	-1.508634	-0.000003	-0.000028
C	-1.908287	-2.483391	0.173814
Au	0.518007	-0.000071	-0.000156
C	2.665678	-0.072631	-0.623571
C	2.665541	0.072496	0.624190
C	-1.907984	2.483448	-0.173893
C	3.044458	-0.238736	-2.034835
C	3.044214	0.239007	2.035413
H	-4.494923	1.397591	-0.094757
H	-4.495104	-1.397153	0.095443
H	2.659593	-1.191192	-2.452146
H	4.152566	-0.251125	-2.107000
H	2.665479	0.593902	-2.661302
H	2.660307	1.192135	2.452078
H	4.152324	0.250268	2.107711
H	2.664273	-0.592823	2.662362
H	-2.323280	3.068714	0.669562
H	-2.252860	2.920114	-1.131720
H	-0.803987	2.517872	-0.133151
H	-0.804268	-2.517871	0.133739
H	-2.323102	-3.068353	-0.670093
H	-2.253784	-2.920352	1.131279

Zero-point correction= 0.208263 (Hartree/Particle)
Thermal correction to Energy= 0.224268
Thermal correction to Enthalpy= 0.225212
Thermal correction to Gibbs Free Energy= 0.162051
Sum of electronic and zero-point Energies= -596.006756
Sum of electronic and thermal Energies= -595.990751
Sum of electronic and thermal Enthalpies= -595.989807
Sum of electronic and thermal Free Energies= -596.052968

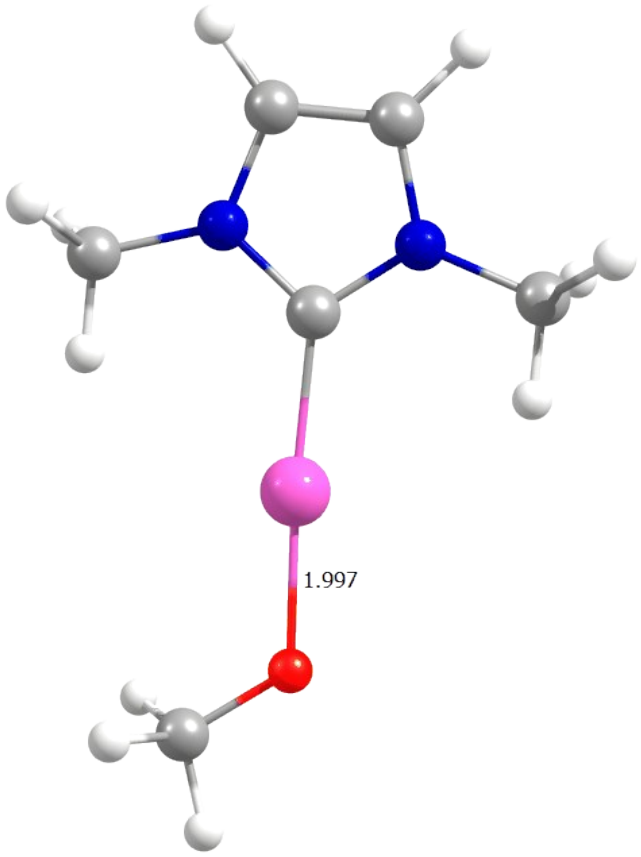
CAT+MeOH



C	1.271710000	0.017204000	0.019724000
N	2.067373000	1.127921000	0.065493000
N	2.118205000	-1.053261000	0.101229000
C	3.400205000	0.755858000	0.175294000
C	3.432131000	-0.616191000	0.197796000
C	1.607451000	2.517320000	0.010805000
C	1.722910000	-2.463934000	0.093230000
H	4.210710000	1.490451000	0.228084000
H	4.275933000	-1.310055000	0.274524000
Au	-0.701251000	-0.037773000	-0.123601000
O	-2.843652000	-0.158468000	-0.273800000
H	-3.205164000	0.148747000	-1.129690000
C	-3.743727000	0.198361000	0.816187000
H	1.906923000	3.052709000	0.933005000
H	2.042605000	3.026987000	-0.871042000
H	0.505333000	2.521588000	-0.072053000
H	2.035156000	-2.950734000	1.037824000
H	0.623281000	-2.523478000	-0.001689000
H	2.192054000	-2.984097000	-0.764614000
H	-3.771147000	1.296150000	0.967712000
H	-4.754625000	-0.190335000	0.585645000
H	-3.356094000	-0.300434000	1.721927000

Zero-point correction= 0.177999 (Hartree/Particle)
Thermal correction to Energy= 0.191219
Thermal correction to Enthalpy= 0.192163
Thermal correction to Gibbs Free Energy= 0.135407
Sum of electronic and zero-point Energies= -555.801500
Sum of electronic and thermal Energies= -555.788280
Sum of electronic and thermal Enthalpies= -555.787336
Sum of electronic and thermal Free Energies= -555.844091

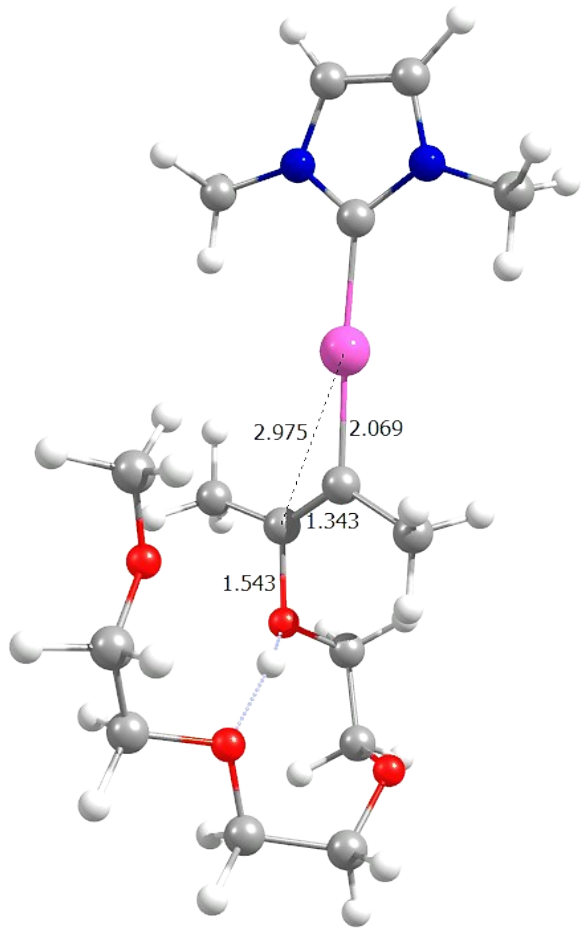
CAT+MeO



C	1.231040000	0.051776000	-0.000554000
N	1.979578000	1.206909000	-0.001009000
N	2.165018000	-0.960181000	0.002499000
C	3.340514000	0.919872000	0.002210000
C	3.457504000	-0.446298000	0.004089000
C	1.418062000	2.553021000	-0.000932000
C	1.839744000	-2.382380000	0.001992000
H	4.105690000	1.702886000	0.002688000
H	4.344840000	-1.087671000	0.005879000
Au	-0.743373000	-0.123363000	-0.001747000
C	-3.651649000	0.602586000	0.010172000
O	-2.714866000	-0.442594000	-0.003400000
H	1.762164000	3.116905000	-0.891580000
H	0.315722000	2.460070000	-0.029505000
H	1.715612000	3.099304000	0.917259000
H	2.254854000	-2.875982000	0.904047000
H	0.737588000	-2.480336000	0.007385000
H	2.245486000	-2.873714000	-0.905611000
H	-3.592083000	1.278354000	-0.883050000
H	-4.681432000	0.167912000	0.008923000
H	-3.586498000	1.260115000	0.916484000

Zero-point correction= 0.164284 (Hartree/Particle)
Thermal correction to Energy= 0.177151
Thermal correction to Enthalpy= 0.178095
Thermal correction to Gibbs Free Energy= 0.121365
Sum of electronic and zero-point Energies= -555.409647
Sum of electronic and thermal Energies= -555.396780
Sum of electronic and thermal Enthalpies= -555.395836
Sum of electronic and thermal Free Energies= -555.452566

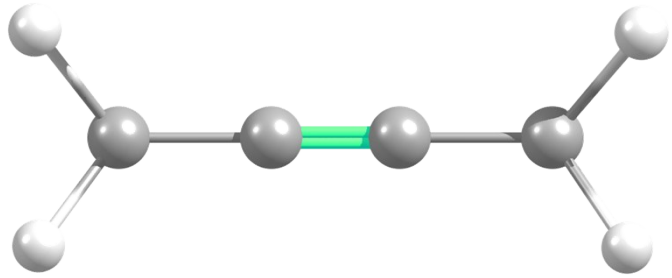
I



Zero-point correction= 0.440607 (Hartree/Particle)
Thermal correction to Energy= 0.469952
Thermal correction to Enthalpy= 0.470896
Thermal correction to Gibbs Free Energy= 0.374878
Sum of electronic and zero-point Energies= -1172.572180
Sum of electronic and thermal Energies= -1172.542835
Sum of electronic and thermal Enthalpies= -1172.541891
Sum of electronic and thermal Free Energies= -1172.637909

C	-5.770958000	0.592073000	0.388350000
C	-5.819912000	-0.305047000	-0.648300000
N	-4.509715000	-0.689730000	-0.905479000
C	-3.636455000	-0.058723000	-0.057463000
N	-4.431718000	0.728939000	0.734006000
C	-4.125865000	-1.643526000	-1.944462000
Au	-1.593458000	-0.279249000	-0.001304000
C	0.453035000	-0.584919000	-0.019284000
C	1.024988000	-1.288929000	-1.232396000
C	-3.948520000	1.597293000	1.804679000
C	1.200444000	-0.166722000	1.015525000
C	0.915251000	0.599159000	2.264560000
H	-6.570801000	1.136767000	0.900796000
H	-6.670963000	-0.695249000	-1.216173000
H	0.567959000	-2.295098000	-1.352401000
H	2.128507000	-1.414013000	-1.230944000
H	0.755638000	-0.729445000	-2.153565000
H	-0.176333000	0.757442000	2.349502000
H	1.415273000	1.591505000	2.238856000
H	1.257134000	0.067590000	3.179405000
H	-4.371643000	1.281356000	2.779092000
H	-4.233147000	2.649673000	1.605385000
H	-2.846575000	1.517601000	1.841948000
H	-3.025788000	-1.753871000	-1.922867000
H	-4.437595000	-1.272788000	-2.941185000
H	-4.596370000	-2.628848000	-1.755179000
O	2.711532000	-0.478868000	1.016253000
C	3.041476000	-1.863803000	1.393618000
H	2.365853000	-2.536141000	0.829653000
H	2.834911000	-1.952146000	2.478503000
C	4.488654000	-2.161334000	1.060399000
H	4.713921000	-3.203521000	1.388352000
H	5.170750000	-1.487156000	1.626363000
O	4.630529000	-2.027767000	-0.347050000
C	5.741106000	-1.279986000	-0.821346000
H	6.716808000	-1.747143000	-0.543878000
H	5.653616000	-1.311587000	-1.925914000
C	5.742800000	0.169632000	-0.341229000
H	6.499622000	0.739521000	-0.926395000
H	6.031205000	0.261460000	0.733409000
C	4.436603000	2.177908000	-0.340479000
H	5.363832000	2.599475000	-0.786707000
H	4.441128000	2.404148000	0.751011000
C	3.238865000	2.812569000	-1.014038000
H	3.226913000	2.533446000	-2.097985000
H	3.368328000	3.924470000	-0.963628000
C	0.882215000	2.929692000	-0.946170000
H	0.019206000	2.459708000	-0.435240000
H	0.817358000	2.694349000	-2.035086000
H	0.830202000	4.038090000	-0.823554000
O	2.061052000	2.394390000	-0.364234000
H	3.305385000	-0.050295000	0.261332000
O	4.438955000	0.744105000	-0.545144000

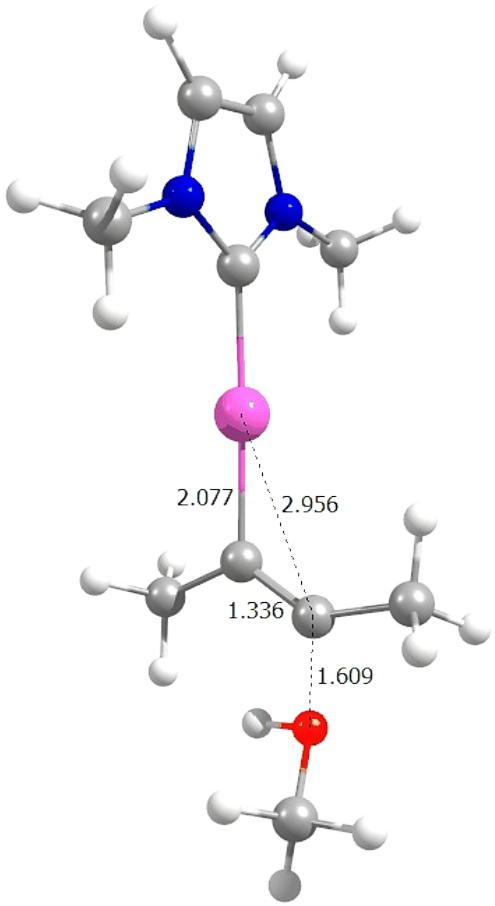
Me-CC-Me



C	0.612503	-0.000481	-0.000129
C	-0.612523	-0.000415	-0.000099
C	-2.073963	0.000234	0.000052
C	2.073958	0.000235	0.000057
H	-2.481687	1.029927	-0.095122
H	-2.482768	-0.596864	-0.843705
H	-2.482299	-0.431852	0.939219
H	2.481640	1.034105	-0.024340
H	2.482552	-0.495205	0.907366
H	2.482710	-0.537548	-0.882704

Zero-point correction= 0.081160 (Hartree/Particle)
Thermal correction to Energy= 0.086980
Thermal correction to Enthalpy= 0.087924
Thermal correction to Gibbs Free Energy= 0.052543
Sum of electronic and zero-point Energies= -155.776771
Sum of electronic and thermal Energies= -155.770951
Sum of electronic and thermal Enthalpies= -155.770007
Sum of electronic and thermal Free Energies= -155.805388

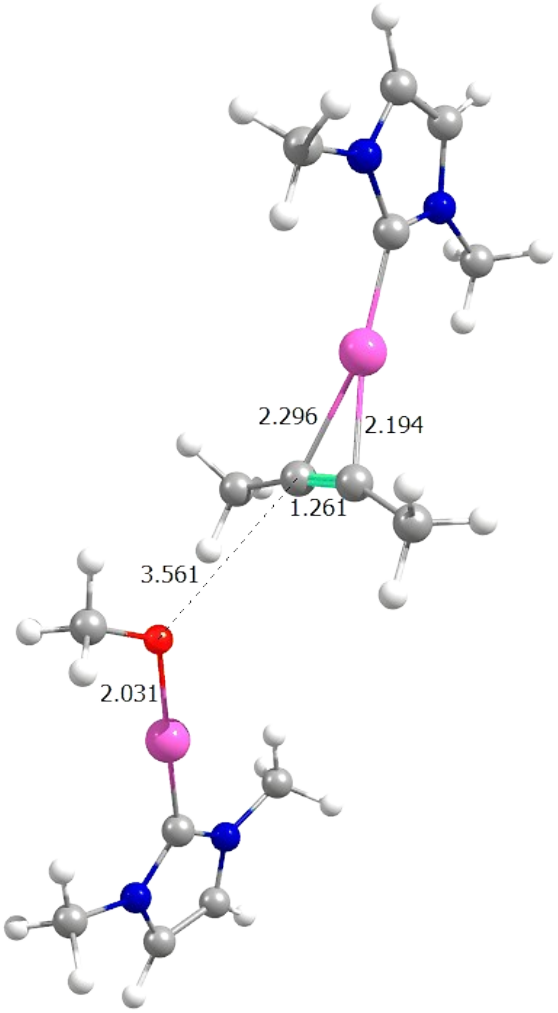
MeOH-I



C	-4.254254000	0.606811000	0.299607000
C	-4.216936000	-0.762417000	0.380748000
N	-2.885395000	-1.134779000	0.244656000
C	-2.086425000	-0.034653000	0.080470000
N	-2.944522000	1.032211000	0.116439000
C	-2.415101000	-2.519153000	0.272073000
Au	-0.056269000	0.008592000	-0.187382000
C	1.988553000	0.052542000	-0.547192000
C	2.429893000	-0.135439000	-1.982145000
C	-2.550736000	2.433882000	-0.022213000
C	2.810940000	0.261280000	0.484359000
C	2.700882000	0.512445000	1.945399000
H	-5.097148000	1.303489000	0.356986000
H	-5.021053000	-1.492055000	0.522662000
H	2.050271000	-1.098019000	-2.383961000
H	3.535020000	-0.149889000	-2.185345000
H	2.006548000	0.661476000	-2.628381000
H	1.624338000	0.560706000	2.197896000
H	3.171816000	1.475900000	2.234694000
H	3.148648000	-0.296262000	2.562829000
H	-2.845607000	3.006079000	0.879614000
H	-3.031582000	2.881575000	-0.914544000
H	-1.452075000	2.477078000	-0.139969000
H	-1.316032000	-2.515540000	0.150473000
H	-2.872956000	-3.096805000	-0.555299000
H	-2.675317000	-2.993615000	1.238964000
O	4.368726000	0.382867000	0.098990000
C	5.291251000	-0.659780000	0.579249000
H	4.895200000	-1.663259000	0.330219000
H	5.380138000	-0.525839000	1.670625000
H	4.347757000	0.380169000	-0.893240000
H	6.268488000	-0.471992000	0.097211000

Zero-point correction= 0.261723 (Hartree/Particle)
Thermal correction to Energy= 0.280716
Thermal correction to Enthalpy= 0.281660
Thermal correction to Gibbs Free Energy= 0.211283
Sum of electronic and zero-point Energies= -711.574624
Sum of electronic and thermal Energies= -711.555631
Sum of electronic and thermal Enthalpies= -711.554687
Sum of electronic and thermal Free Energies= -711.625065

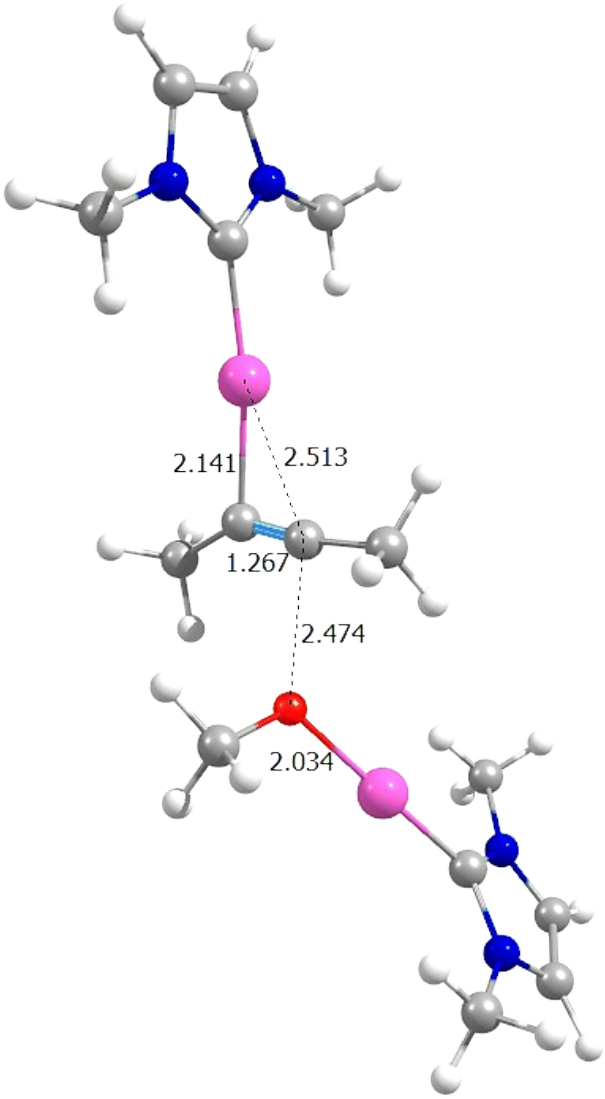
MeOH-I+II



C	5.571241000	0.279766000	0.281513000
N	6.220643000	1.466303000	0.493313000
N	6.500897000	-0.691000000	0.542121000
C	7.533298000	1.240833000	0.880943000
C	7.710283000	-0.120812000	0.911243000
C	5.627719000	2.795840000	0.342023000
C	6.270128000	-2.133738000	0.449886000
H	8.229593000	2.056426000	1.102785000
H	8.590834000	-0.721022000	1.163543000
Au	3.651790000	0.012028000	-0.315008000
C	1.793420000	-0.337603000	-1.427625000
C	1.370838000	-0.239025000	-0.244156000
C	-5.547891000	0.545736000	0.005085000
N	-6.774346000	-0.050472000	-0.153498000
N	-5.810015000	1.893541000	-0.009538000
C	-7.777844000	0.905249000	-0.264267000
C	-7.170233000	2.131000000	-0.174037000
C	-7.004879000	-1.492438000	-0.199550000
C	-4.804253000	2.942318000	0.132211000
H	-8.831233000	0.637542000	-0.396184000
H	-7.589802000	3.141546000	-0.211951000
Au	-3.792028000	-0.356211000	0.227157000
C	-1.894415000	-2.624760000	0.690410000
O	-1.974906000	-1.233417000	0.461126000
C	0.638098000	-0.166208000	1.007259000
C	1.750271000	-0.545267000	-2.889826000
H	4.573740000	2.676013000	0.030730000
H	5.665373000	3.341498000	1.305320000
H	6.174713000	3.371849000	-0.430105000
H	5.221131000	-2.302906000	0.144704000
H	6.947496000	-2.580905000	-0.304051000
H	6.446316000	-2.611471000	1.433647000
H	-7.457582000	-1.779131000	-1.169758000
H	-6.029515000	-2.001396000	-0.086503000
H	-7.676738000	-1.801510000	0.625939000
H	-5.025729000	3.570855000	1.017976000
H	-3.818663000	2.458472000	0.265195000
H	-4.780377000	3.580110000	-0.774199000
H	-0.440133000	-0.509489000	0.790256000
H	1.060844000	-0.840738000	1.779341000
H	0.609493000	0.867146000	1.410192000
H	0.702446000	-0.742169000	-3.197767000
H	2.116437000	0.345984000	-3.438703000
H	2.372755000	-1.410253000	-3.196093000
H	-2.249286000	-3.232485000	-0.178111000
H	-0.825720000	-2.907018000	0.860754000
H	-2.463265000	-2.963154000	1.590804000

Zero-point correction= 0.373326 (Hartree/Particle)
Thermal correction to Energy= 0.403866
Thermal correction to Enthalpy= 0.404810
Thermal correction to Gibbs Free Energy= 0.300702
Sum of electronic and zero-point Energies= -1151.440172
Sum of electronic and thermal Energies= -1151.409632
Sum of electronic and thermal Enthalpies= -1151.408688
Sum of electronic and thermal Free Energies= -1151.512796

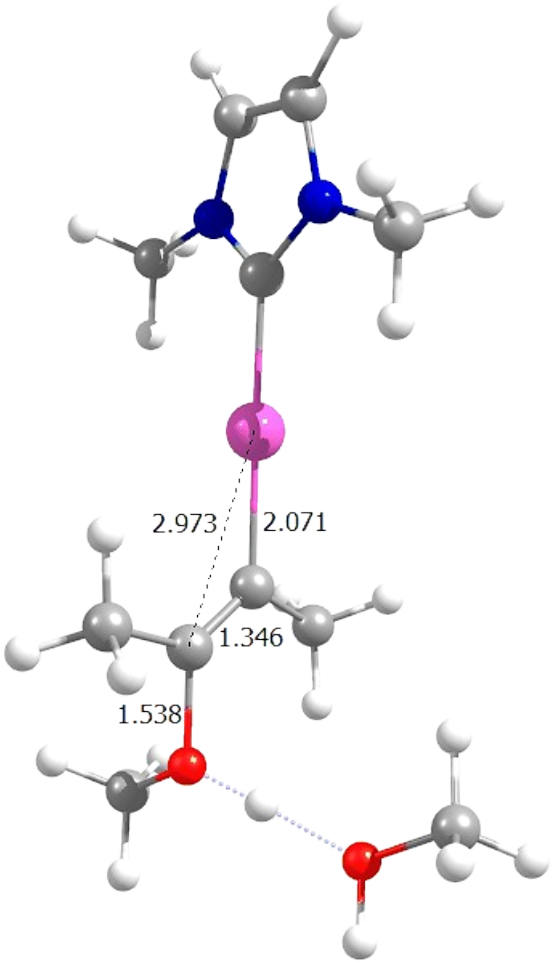
MeOH-I+II--IV



C	5.161882000	0.303414000	-0.261776000
N	5.830682000	1.494671000	-0.350741000
N	6.115684000	-0.658782000	-0.458896000
C	7.179009000	1.280737000	-0.601940000
C	7.358730000	-0.078674000	-0.670565000
C	5.224211000	2.817650000	-0.200350000
C	5.874320000	-2.102252000	-0.455444000
H	7.894949000	2.102289000	-0.709915000
H	8.261538000	-0.671670000	-0.850840000
Au	3.191812000	0.019222000	0.144537000
C	0.737091000	-0.371138000	-0.225884000
C	1.227233000	-0.285416000	0.939267000
C	-5.046205000	0.539551000	-0.188446000
N	-6.191966000	-0.007608000	-0.709323000
N	-5.382242000	1.835709000	0.113712000
C	-7.219802000	0.927805000	-0.730853000
C	-6.709180000	2.090577000	-0.213518000
C	-6.327446000	-1.387015000	-1.172327000
C	-4.476975000	2.820480000	0.700077000
H	-8.220555000	0.691748000	-1.107018000
H	-7.176942000	3.067281000	-0.052293000
Au	-3.297282000	-0.365818000	0.092627000
C	-1.426453000	-2.646680000	0.570242000
O	-1.489651000	-1.244215000	0.408216000
C	0.942609000	-0.382343000	2.395176000
C	0.333677000	-0.365964000	-1.628712000
H	4.141298000	2.686469000	-0.019881000
H	5.676468000	3.349971000	0.659603000
H	5.373581000	3.413051000	-1.122524000
H	4.806339000	-2.277695000	-0.229651000
H	6.115354000	-2.533104000	-1.447317000
H	6.496841000	-2.590660000	0.319755000
H	-6.637224000	-1.405800000	-2.236129000
H	-5.345193000	-1.884251000	-1.067654000
H	-7.077436000	-1.927429000	-0.560908000
H	-4.901056000	3.215559000	1.644594000
H	-3.514221000	2.319812000	0.913692000
H	-4.306694000	3.658853000	-0.005014000
H	-0.141732000	-0.586196000	2.507983000
H	1.522758000	-1.202410000	2.864928000
H	1.205711000	0.556574000	2.922886000
H	-0.672903000	0.094560000	-1.706791000
H	1.041251000	0.220255000	-2.251511000
H	0.267457000	-1.396437000	-2.033131000
H	-1.721222000	-3.217065000	-0.346481000
H	-0.376085000	-2.941915000	0.810249000
H	-2.064226000	-3.019298000	1.408785000

Zero-point correction= 0.373540 (Hartree/Particle)
Thermal correction to Energy= 0.403557
Thermal correction to Enthalpy= 0.404501
Thermal correction to Gibbs Free Energy= 0.303432
Sum of electronic and zero-point Energies= -1151.433346
Sum of electronic and thermal Energies= -1151.403329
Sum of electronic and thermal Enthalpies= -1151.402385
Sum of electronic and thermal Free Energies= -1151.503453

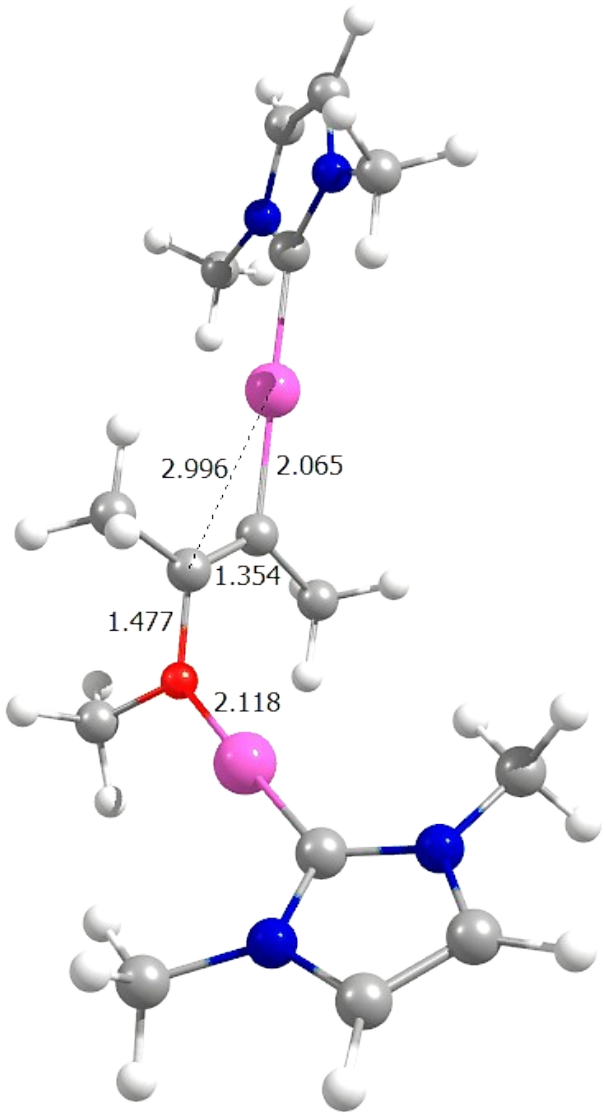
MeOH-I+MeOH



C	4.604746000	1.018091000	-0.282959000
C	4.763853000	-0.300166000	0.062029000
N	3.488419000	-0.825559000	0.230023000
C	2.531529000	0.127520000	-0.000580000
N	3.236527000	1.259493000	-0.315736000
C	3.216176000	-2.211902000	0.606194000
Au	0.492205000	-0.095520000	0.112825000
C	-1.556720000	-0.331097000	0.301223000
C	-2.119988000	-0.299708000	1.707059000
C	2.640100000	2.553892000	-0.639552000
C	-2.304080000	-0.521345000	-0.801738000
C	-1.990339000	-0.602477000	-2.261253000
H	5.345495000	1.793488000	-0.504542000
H	5.670445000	-0.898592000	0.199881000
H	-1.737126000	-1.164897000	2.290847000
H	-3.229439000	-0.305481000	1.775768000
H	-1.758380000	0.598589000	2.250175000
H	-0.898542000	-0.493807000	-2.403177000
H	-2.502689000	0.196296000	-2.840267000
H	-2.297651000	-1.576100000	-2.702889000
H	2.927301000	2.865452000	-1.663581000
H	2.974200000	3.323131000	0.084889000
H	1.540424000	2.451467000	-0.582360000
H	2.120084000	-2.344973000	0.668645000
H	3.669455000	-2.438689000	1.591628000
H	3.626853000	-2.904891000	-0.154830000
O	-3.823243000	-0.708208000	-0.655317000
C	-4.294949000	-2.037683000	-0.292071000
H	-3.992853000	-2.292438000	0.742248000
H	-3.852319000	-2.752381000	-1.009015000
C	-4.494473000	2.488202000	0.516463000
H	-4.948145000	3.084823000	1.332950000
H	-4.671111000	2.984163000	-0.460831000
H	-4.317319000	0.083772000	-0.139342000
O	-5.027160000	1.141641000	0.533298000
H	-5.396618000	-2.038656000	-0.396496000
H	-5.995782000	1.169384000	0.400966000
H	-3.406986000	2.401416000	0.693399000

Zero-point correction= 0.313433 (Hartree/Particle)
Thermal correction to Energy= 0.336518
Thermal correction to Enthalpy= 0.337462
Thermal correction to Gibbs Free Energy= 0.257101
Sum of electronic and zero-point Energies= -827.188121
Sum of electronic and thermal Energies= -827.165036
Sum of electronic and thermal Enthalpies= -827.164092
Sum of electronic and thermal Free Energies= -827.244453

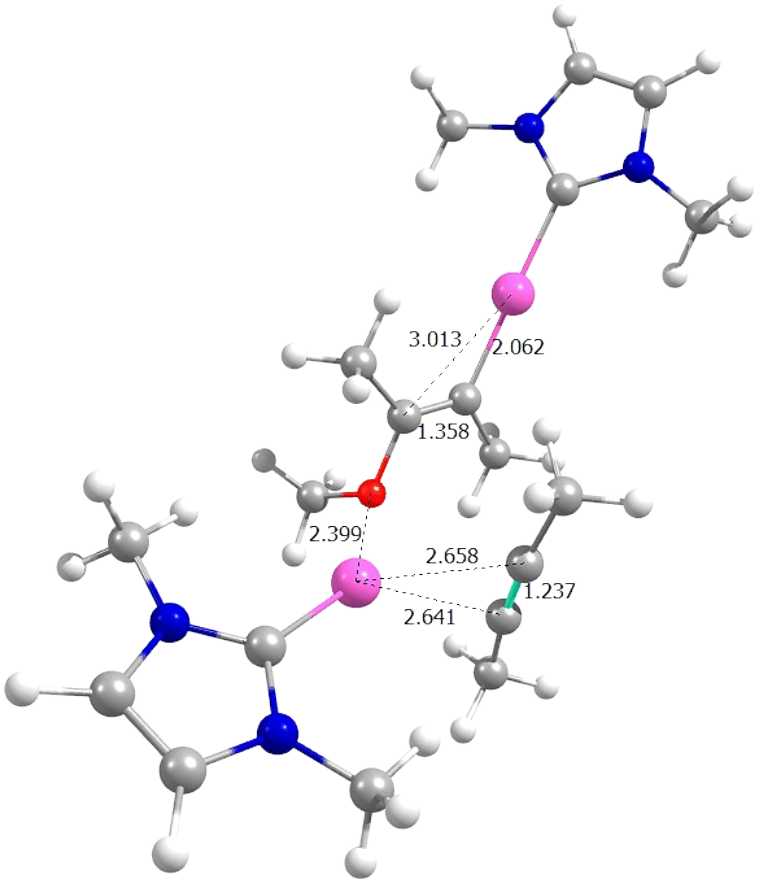
MeOH-IV



C	-4.706228000	0.587737000	0.185860000
N	-5.062889000	1.835351000	0.628449000
N	-5.894590000	-0.082309000	0.050912000
C	-6.442069000	1.941397000	0.767087000
C	-6.967945000	0.728291000	0.401157000
C	-4.121776000	2.913870000	0.919156000
C	-6.023662000	-1.464219000	-0.406879000
H	-6.931993000	2.858652000	1.110019000
H	-8.005935000	0.381762000	0.362191000
Au	-2.813684000	-0.129822000	-0.195280000
C	-0.059541000	-1.176792000	0.347115000
C	-0.940782000	-0.878788000	-0.636968000
C	4.481670000	0.789044000	-0.008851000
N	5.678291000	0.624763000	0.634442000
N	4.585303000	1.978209000	-0.678240000
C	6.519830000	1.697636000	0.369777000
C	5.831549000	2.549929000	-0.456300000
C	6.039465000	-0.511611000	1.482720000
C	3.546639000	2.574098000	-1.519860000
H	7.529853000	1.766600000	0.786921000
H	6.124425000	3.507164000	-0.900005000
Au	2.926784000	-0.436864000	0.010597000
C	1.411339000	-3.159091000	0.156787000
O	1.253092000	-1.733219000	-0.039113000
C	-0.616277000	-1.112627000	-2.098455000
C	-0.172632000	-1.020528000	1.835744000
H	-6.598775000	-1.505362000	-1.353479000
H	-5.007409000	-1.865791000	-0.578244000
H	-6.535974000	-2.077380000	0.360987000
H	-4.184849000	3.204964000	1.986893000
H	-3.101856000	2.546794000	0.698227000
H	-4.339455000	3.796558000	0.285165000
H	2.652821000	1.924247000	-1.489072000
H	3.280626000	3.579881000	-1.139733000
H	3.903252000	2.655997000	-2.565568000
H	5.182819000	-1.209485000	1.515067000
H	6.922055000	-1.034266000	1.064382000
H	6.267417000	-0.164000000	2.509543000
H	-1.165602000	-0.600723000	2.086627000
H	-0.067856000	-1.987375000	2.376394000
H	0.606751000	-0.333890000	2.238640000
H	-0.719467000	-0.168148000	-2.675299000
H	0.402035000	-1.517778000	-2.277819000
H	-1.349427000	-1.814879000	-2.551343000
H	0.508375000	-3.666782000	-0.236872000
H	2.301261000	-3.478348000	-0.418831000
H	1.546995000	-3.406643000	1.230606000

Zero-point correction= 0.377172 (Hartree/Particle)
Thermal correction to Energy= 0.406225
Thermal correction to Enthalpy= 0.407169
Thermal correction to Gibbs Free Energy= 0.308866
Sum of electronic and zero-point Energies= -1151.461311
Sum of electronic and thermal Energies= -1151.432258
Sum of electronic and thermal Enthalpies= -1151.431314
Sum of electronic and thermal Free Energies= -1151.529617

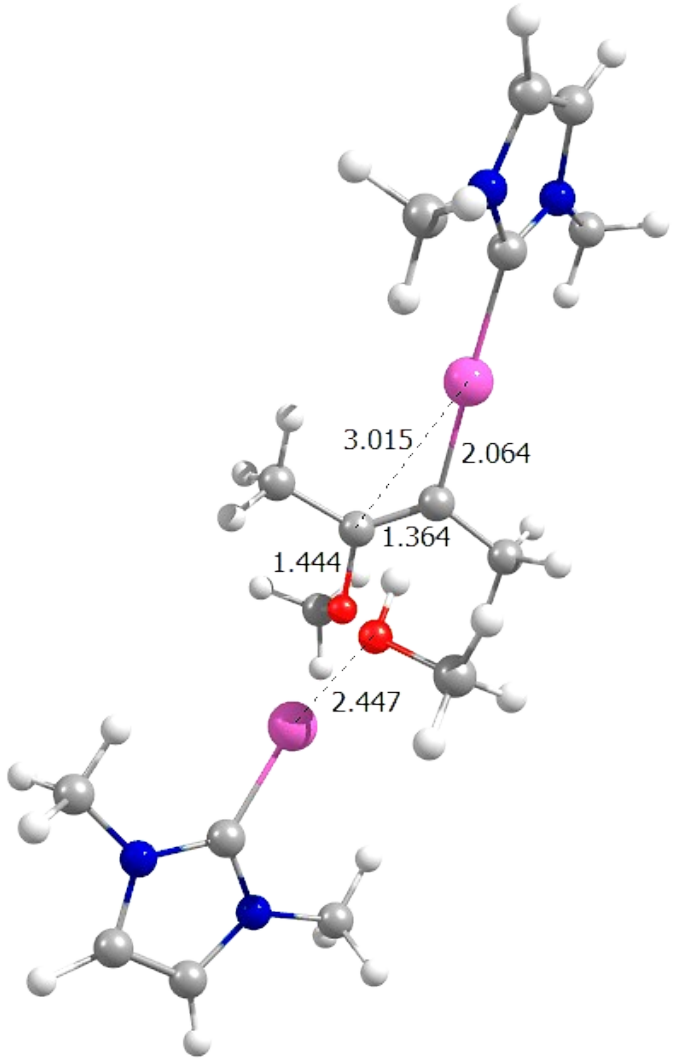
MeOH-IV-VI-ALKYNE



Zero-point correction= 0.458677 (Hartree/Particle)
Thermal correction to Energy= 0.494500
Thermal correction to Enthalpy= 0.495444
Thermal correction to Gibbs Free Energy= 0.383135
Sum of electronic and zero-point Energies= -1307.229841
Sum of electronic and thermal Energies= -1307.194019
Sum of electronic and thermal Enthalpies= -1307.193075
Sum of electronic and thermal Free Energies= -1307.305384

C	-5.047480000	-0.266822000	0.542390000
N	-5.877099000	-1.345007000	0.368956000
N	-5.755814000	0.583173000	1.352696000
C	-7.073591000	-1.172257000	1.055259000
C	-6.997024000	0.047838000	1.677665000
C	-5.554869000	-2.520040000	-0.437257000
C	-5.278399000	1.885976000	1.808982000
H	-7.873292000	-1.920171000	1.044235000
H	-7.717121000	0.571635000	2.314932000
Au	-3.170450000	0.018530000	-0.264846000
C	-0.263814000	-0.463835000	-0.892547000
C	-1.329041000	0.343239000	-1.135163000
C	4.614772000	-0.655083000	0.591142000
N	5.016010000	-1.966109000	0.562941000
N	5.633801000	0.016227000	1.217022000
C	6.261948000	-2.109125000	1.159332000
C	6.652185000	-0.859295000	1.569561000
C	4.249368000	-3.074704000	-0.002380000
C	5.665842000	1.454894000	1.477428000
H	6.764966000	-3.078063000	1.243826000
H	7.562839000	-0.526471000	2.078426000
Au	2.915833000	0.130211000	-0.115347000
C	1.226371000	-0.938991000	-2.739205000
O	1.006608000	-0.190559000	-1.531610000
C	0.638775000	1.896272000	1.819158000
C	-0.179475000	-1.654831000	0.022371000
C	-1.221926000	1.510721000	-2.095442000
C	1.407960000	2.195486000	0.609567000
C	1.977512000	2.580680000	-0.418717000
C	2.546854000	3.189034000	-1.623187000
H	-5.229820000	1.913702000	2.916066000
H	-4.266205000	2.044650000	1.392140000
H	-5.951717000	2.690547000	1.451422000
H	-6.304078000	-2.650281000	-1.243456000
H	-4.557033000	-2.363365000	-0.888354000
H	-5.534944000	-3.430126000	0.195315000
H	3.327754000	-2.660631000	-0.450670000
H	4.842978000	-3.589034000	-0.783622000
H	3.978386000	-3.798878000	0.791350000
H	5.834656000	1.640459000	2.556263000
H	6.475232000	1.934113000	0.891374000
H	4.690780000	1.883301000	1.179048000
H	-0.244349000	1.269838000	1.570606000
H	1.245664000	1.360699000	2.578112000
H	0.276925000	2.840261000	2.279534000
H	2.205655000	4.242447000	-1.711371000
H	3.656577000	3.194018000	-1.606098000
H	2.221531000	2.652230000	-2.538259000
H	0.443334000	-0.691683000	-3.486901000
H	2.220045000	-0.649290000	-3.134171000
H	1.212486000	-2.036164000	-2.553267000
H	-1.515859000	2.459538000	-1.596399000
H	-0.202502000	1.647916000	-2.513715000
H	-1.932012000	1.387354000	-2.942307000
H	-1.154157000	-1.825448000	0.519222000
H	0.095330000	-2.587014000	-0.521391000
H	0.595710000	-1.505028000	0.811201000

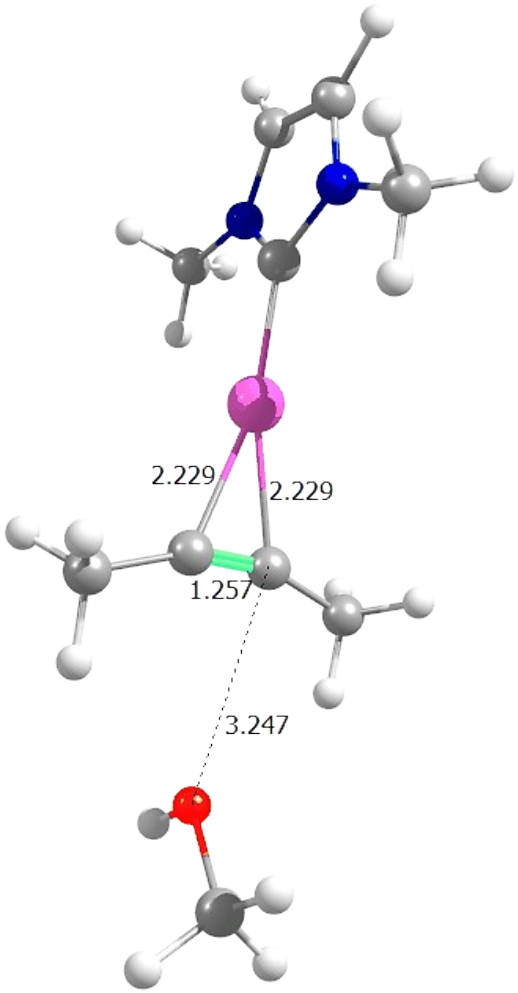
MeOH-IV-VI-MeOH



C	4.993592000	0.456382000	0.047836000
N	6.169923000	-0.247008000	0.025138000
N	5.379319000	1.770520000	0.113684000
C	7.264490000	0.608051000	0.075550000
C	6.764643000	1.884373000	0.131524000
C	6.269194000	-1.703435000	-0.046634000
C	4.462358000	2.906677000	0.158207000
H	8.297432000	0.244725000	0.067818000
H	7.276714000	2.850929000	0.182335000
Au	3.079049000	-0.303406000	-0.005744000
C	0.236483000	-0.713985000	-0.922132000
C	1.180449000	-1.112668000	-0.021824000
C	-4.860088000	0.337740000	0.019960000
N	-5.843969000	-0.408144000	0.614768000
N	-5.508271000	1.396811000	-0.559249000
C	-7.088822000	0.176820000	0.407938000
C	-6.877880000	1.310896000	-0.332803000
C	-5.629857000	-1.636221000	1.377820000
C	-4.866502000	2.462614000	-1.326725000
H	-8.012990000	-0.257481000	0.803052000
H	-7.582597000	2.057092000	-0.714058000
Au	-2.914788000	-0.026644000	0.003939000
C	-1.421841000	-2.243340000	-1.839343000
O	-1.093778000	-1.266846000	-0.830210000
O	-0.941777000	0.887603000	1.125426000
H	-0.142522000	0.411568000	0.766468000
C	-0.864981000	0.969054000	2.552547000
C	0.364290000	0.298839000	-2.027555000
C	0.875157000	-2.200838000	0.991156000
H	-0.633448000	-3.024143000	-1.872647000
H	-2.386342000	-2.700706000	-1.547743000
H	-1.526731000	-1.777705000	-2.842929000
H	1.369893000	0.760650000	-2.001356000
H	0.232241000	-0.163286000	-3.030693000
H	-0.401409000	1.101331000	-1.934782000
H	1.132687000	-1.876865000	2.022304000
H	-0.182584000	-2.538574000	0.979363000
H	1.518221000	-3.087004000	0.795665000
H	-5.157877000	2.400981000	-2.394425000
H	-5.159559000	3.450850000	-0.921387000
H	-3.770566000	2.343535000	-1.239516000
H	-5.887211000	-1.479340000	2.444431000
H	-6.252921000	-2.454273000	0.965770000
H	-4.562204000	-1.913178000	1.298001000
H	4.623926000	3.496296000	1.082675000
H	4.613649000	3.560336000	-0.724104000
H	3.428379000	2.514282000	0.150333000
H	6.799386000	-2.097699000	0.843080000
H	5.244268000	-2.117990000	-0.075985000
H	6.813143000	-2.007481000	-0.963106000
H	-1.748558000	1.535808000	2.905388000
H	-0.867189000	-0.032964000	3.035813000
H	0.049465000	1.517179000	2.867604000

Zero-point correction= 0.428319 (Hartree/Particle)
Thermal correction to Energy= 0.461062
Thermal correction to Enthalpy= 0.462006
Thermal correction to Gibbs Free Energy= 0.356387
Sum of electronic and zero-point Energies= -1267.050109
Sum of electronic and thermal Energies= -1267.017367
Sum of electronic and thermal Enthalpies= -1267.016422
Sum of electronic and thermal Free Energies= -1267.122041

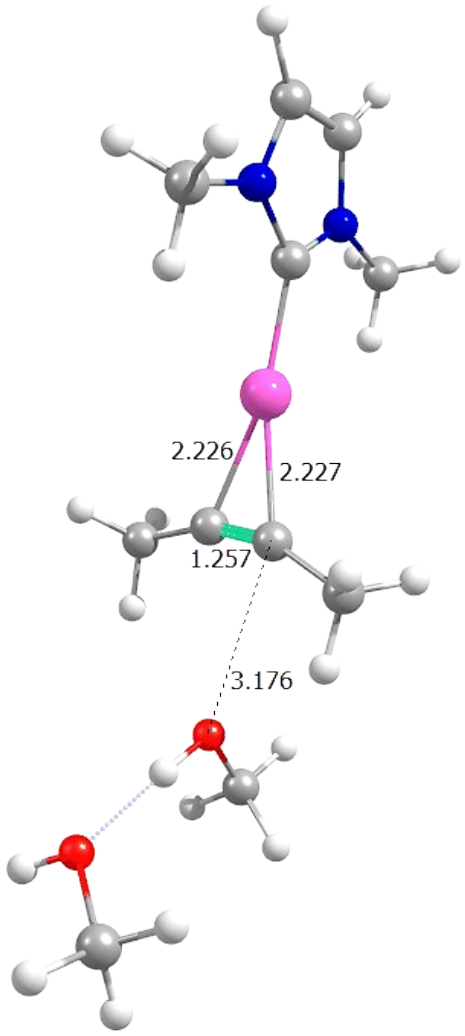
MeOH-RC



C	2.164839	0.056573	-0.000318
N	3.049026	-0.988465	0.002947
C	4.353785	-0.520305	0.001136
C	4.284064	0.851996	-0.003396
N	2.938764	1.185731	-0.004231
C	2.688859	-2.407875	0.007768
C	2.437769	2.561876	-0.009084
Au	0.136641	-0.045245	0.000420
C	-1.998983	-0.155818	-0.627238
C	-2.455475	-0.187850	-2.022847
C	-1.999069	-0.147877	0.629276
C	-2.455853	-0.161758	2.025089
O	-5.182026	-0.292979	0.001744
C	-6.261114	0.644438	-0.004760
H	5.219737	-1.190834	0.003228
H	5.077575	1.606874	-0.006044
H	-2.172359	0.731177	-2.574528
H	-3.564675	-0.256923	-1.976763
H	-2.056826	-1.063797	-2.573118
H	-2.056923	-1.030129	2.587039
H	-3.565026	-0.231891	1.979688
H	-2.173331	0.764650	2.564604
H	3.092743	-2.899813	0.914276
H	3.094435	-2.906301	-0.894421
H	1.586647	-2.491068	0.007017
H	1.332770	2.534776	-0.006070
H	2.788605	3.091102	-0.916670
H	2.793328	3.099062	0.891944
H	-6.907042	0.547655	-0.907450
H	-5.816286	1.659111	-0.012345
H	-5.572850	-1.187591	0.008015
H	-6.906426	0.560872	0.899685

Zero-point correction= 0.259253 (Hartree/Particle)
Thermal correction to Energy= 0.280223
Thermal correction to Enthalpy= 0.281167
Thermal correction to Gibbs Free Energy= 0.204312
Sum of electronic and zero-point Energies= -711.597565
Sum of electronic and thermal Energies= -711.576595
Sum of electronic and thermal Enthalpies= -711.575651
Sum of electronic and thermal Free Energies= -711.652506

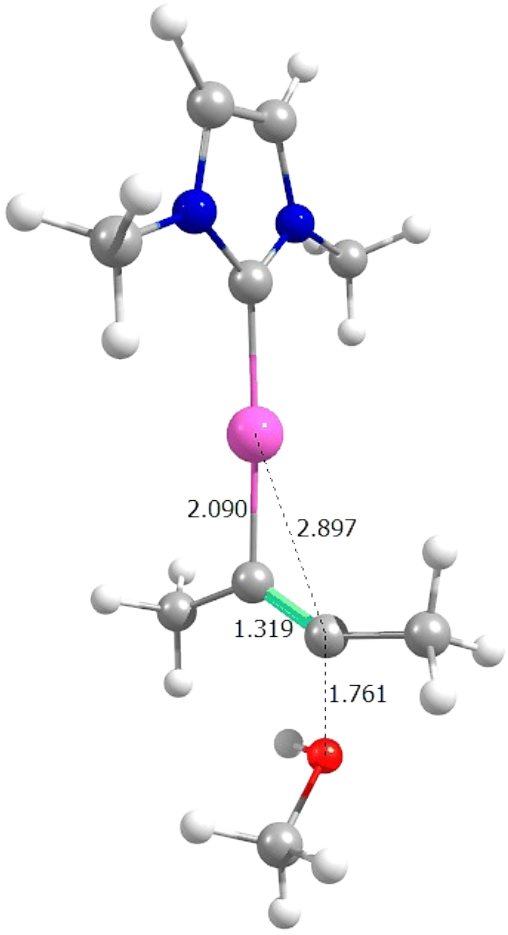
MeOH-RC-MeOH



C	2.802426	0.172277	0.022175
N	3.495376	1.348691	-0.078503
C	4.860102	1.116907	-0.002794
C	5.025454	-0.238818	0.147898
N	3.757334	-0.798784	0.160887
C	2.897752	2.675430	-0.241565
C	3.497243	-2.233034	0.300450
Au	0.786185	-0.077509	-0.017334
C	-1.354427	-0.260875	0.568842
C	-1.873896	-0.144622	1.936661
C	-1.312691	-0.417301	-0.677350
C	-1.741221	-0.649549	-2.062004
O	-4.418362	-0.807733	-0.064803
C	-5.231824	-1.965225	0.049188
H	5.598420	1.923665	-0.061494
H	5.935494	-0.840333	0.245157
H	-1.459756	-0.922352	2.609448
H	-2.973795	-0.289696	1.836661
H	-1.668749	0.850781	2.379471
H	-1.500881	0.206670	-2.723947
H	-2.845831	-0.777294	-2.004119
H	-1.288250	-1.565566	-2.491884
H	3.267398	3.146061	-1.173540
H	3.153642	3.318231	0.623574
H	1.799797	2.561426	-0.300482
H	2.403974	-2.395550	0.284277
H	3.908273	-2.602642	1.260307
H	3.962152	-2.787375	-0.538341
H	-5.931728	-1.922806	0.918062
H	-4.571225	-2.844186	0.199714
H	-5.027940	-0.035438	-0.211700
H	-5.841676	-2.160831	-0.865555
O	-6.176861	1.257502	-0.466267
H	-6.675576	1.277756	-1.304677
C	-7.016102	1.755707	0.578672
H	-6.439207	1.683591	1.521127
H	-7.286275	2.823545	0.420005
H	-7.950941	1.162708	0.698188

Zero-point correction= 0.310830 (Hartree/Particle)
Thermal correction to Energy= 0.336512
Thermal correction to Enthalpy= 0.337456
Thermal correction to Gibbs Free Energy= 0.246792
Sum of electronic and zero-point Energies= -827.193961
Sum of electronic and thermal Energies= -827.168279
Sum of electronic and thermal Enthalpies= -827.167335
Sum of electronic and thermal Free Energies= -827.257999

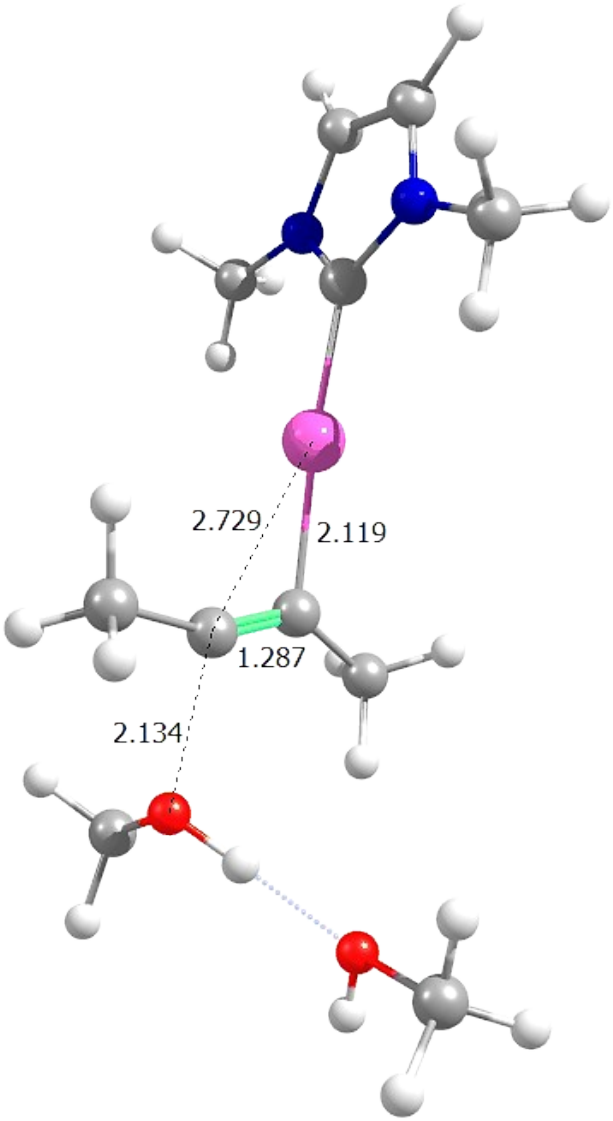
MeOH-TS



C	2.085586	0.050488	0.065978
N	2.961987	-1.000555	0.112127
C	4.266258	-0.547699	0.264976
C	4.205643	0.822237	0.315811
N	2.866026	1.168420	0.192230
C	2.591614	-2.412110	0.012323
C	2.371977	2.545029	0.197952
Au	0.057338	-0.033000	-0.169014
C	-1.999738	-0.114868	-0.530226
C	-2.447484	-0.007400	-1.967464
C	-2.738759	-0.267053	0.551843
C	-2.677777	-0.441485	2.020315
O	-4.465703	-0.405209	0.237059
C	-5.243433	0.828864	0.319757
H	5.122271	-1.227961	0.325117
H	4.998596	1.568978	0.428701
H	-2.100699	0.948157	-2.412972
H	-3.550557	-0.052038	-2.127727
H	-1.992005	-0.814677	-2.577501
H	-1.614817	-0.392374	2.326787
H	-3.090121	-1.422634	2.335321
H	-3.221635	0.356980	2.568737
H	2.913278	-2.957582	0.921435
H	3.064814	-2.871174	-0.878257
H	1.492076	-2.478060	-0.084145
H	1.272122	2.520884	0.086614
H	2.812675	3.114134	-0.644404
H	2.632760	3.041987	1.153306
H	-4.842929	1.596863	-0.370721
H	-5.172401	1.178160	1.364619
H	-4.509833	-0.757109	-0.680412
H	-6.297090	0.585072	0.083044

Zero-point correction= 0.260737 (Hartree/Particle)
Thermal correction to Energy= 0.279612
Thermal correction to Enthalpy= 0.280556
Thermal correction to Gibbs Free Energy= 0.210304
Sum of electronic and zero-point Energies= -711.575273
Sum of electronic and thermal Energies= -711.556398
Sum of electronic and thermal Enthalpies= -711.555454
Sum of electronic and thermal Free Energies= -711.625706

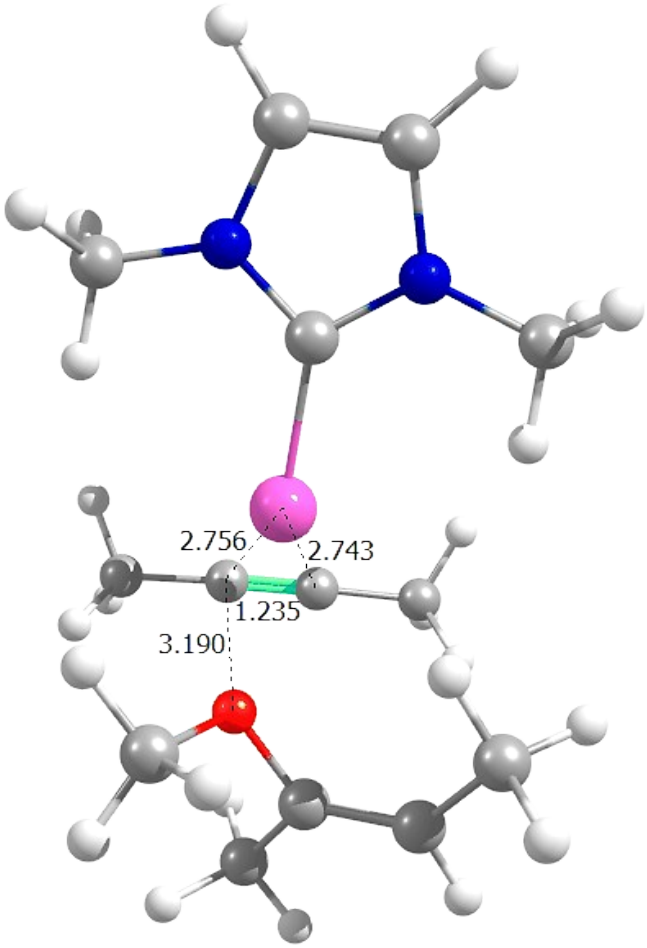
MeOH-TS+MeOH



C	-4.714624	0.974729	0.215494
C	-4.835009	-0.325565	-0.206739
N	-3.545888	-0.823059	-0.345470
C	-2.621824	0.132683	-0.018840
N	-3.355073	1.236900	0.323420
C	-3.235250	-2.185083	-0.780120
Au	-0.595151	-0.043228	-0.067829
C	1.501109	-0.180598	-0.346822
C	2.075308	0.074922	-1.708160
C	-2.799620	2.522188	0.747266
C	1.942891	-0.521158	0.812918
C	1.888090	-0.822256	2.247966
H	-5.478325	1.725256	0.444858
H	-5.724110	-0.929165	-0.417212
H	1.832729	-0.764180	-2.393648
H	3.175736	0.197260	-1.654814
H	1.642314	0.989567	-2.159814
H	0.845814	-0.706449	2.608807
H	2.536996	-0.132248	2.824002
H	2.213495	-1.861029	2.461735
H	-3.131318	2.762445	1.776783
H	-3.127053	3.325707	0.058401
H	-1.696536	2.449859	0.725486
H	-2.135886	-2.296691	-0.818319
H	-3.657186	-2.370077	-1.787611
H	-3.653879	-2.920705	-0.065105
O	4.049689	-0.852958	0.735248
C	4.411777	-2.128425	0.203862
H	4.139706	-2.242973	-0.869303
H	3.880745	-2.909476	0.783219
C	5.607970	2.306522	-0.289299
H	5.821049	2.988093	-1.140221
H	6.451144	2.346351	0.434416
H	4.523029	-0.139836	0.206136
O	5.351247	0.968222	-0.746015
H	5.504356	-2.303330	0.320657
H	6.138955	0.641990	-1.222667
H	4.689439	2.657905	0.218016

Zero-point correction= 0.311557 (Hartree/Particle)
Thermal correction to Energy= 0.335667
Thermal correction to Enthalpy= 0.336611
Thermal correction to Gibbs Free Energy= 0.252063
Sum of electronic and zero-point Energies= -827.182498
Sum of electronic and thermal Energies= -827.158388
Sum of electronic and thermal Enthalpies= -827.157444
Sum of electronic and thermal Free Energies= -827.241991

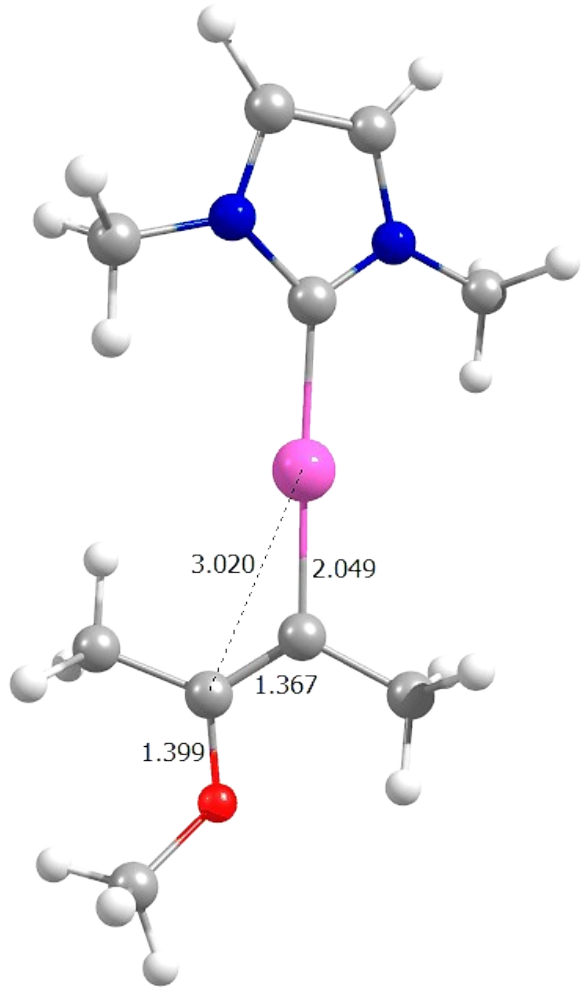
MeOH-VII-6-ALKYNE



C	3.104173	-0.616254	-0.567608
C	3.082323	-1.939475	-0.294936
C	-2.135463	-0.151523	-0.083938
N	-3.094105	0.715600	-0.535827
N	-2.820615	-1.242962	0.377749
C	-4.362095	0.173111	-0.356270
C	-4.190130	-1.059002	0.219095
C	-2.844714	2.033348	-1.117847
C	-2.219240	-2.436416	0.970608
H	-5.273226	0.702098	-0.654604
H	-4.921859	-1.815153	0.522045
Au	-0.163006	0.145554	-0.057090
C	1.929357	0.049616	-2.558824
O	1.951944	0.019452	-1.112383
H	4.010715	-2.354476	0.134493
C	1.373981	3.197657	0.706032
C	1.955744	-2.902913	-0.526609
C	4.254822	0.321353	-0.346441
C	1.361673	1.904975	1.392472
C	1.427268	0.875661	2.071940
C	1.580984	-0.249036	2.996043
H	-2.617847	-3.344344	0.477497
H	-1.125138	-2.391283	0.818695
H	-2.437647	-2.482288	2.056335
H	-3.226512	2.829887	-0.448483
H	-1.753821	2.157619	-1.247841
H	-3.341245	2.112606	-2.104731
H	0.598589	-0.656670	3.312995
H	2.169189	-1.072135	2.540103
H	2.115317	0.084845	3.910864
H	1.061111	0.666154	-2.857731
H	2.861010	0.512061	-2.946190
H	1.823683	-0.974155	-2.975314
H	3.981603	1.109564	0.386913
H	5.140452	-0.222169	0.034541
H	4.551047	0.834865	-1.286806
H	1.032829	-2.399478	-0.880789
H	2.239012	-3.669442	-1.281192
H	1.715523	-3.465171	0.401902
H	0.354350	3.628094	0.622309
H	1.995363	3.922409	1.273949
H	1.800328	3.117090	-0.315520

Zero-point correction= 0.344203 (Hartree/Particle)
Thermal correction to Energy= 0.370026
Thermal correction to Enthalpy= 0.370970
Thermal correction to Gibbs Free Energy= 0.283689
Sum of electronic and zero-point Energies= -867.393856
Sum of electronic and thermal Energies= -867.368034
Sum of electronic and thermal Enthalpies= -867.367090
Sum of electronic and thermal Free Energies= -867.454371

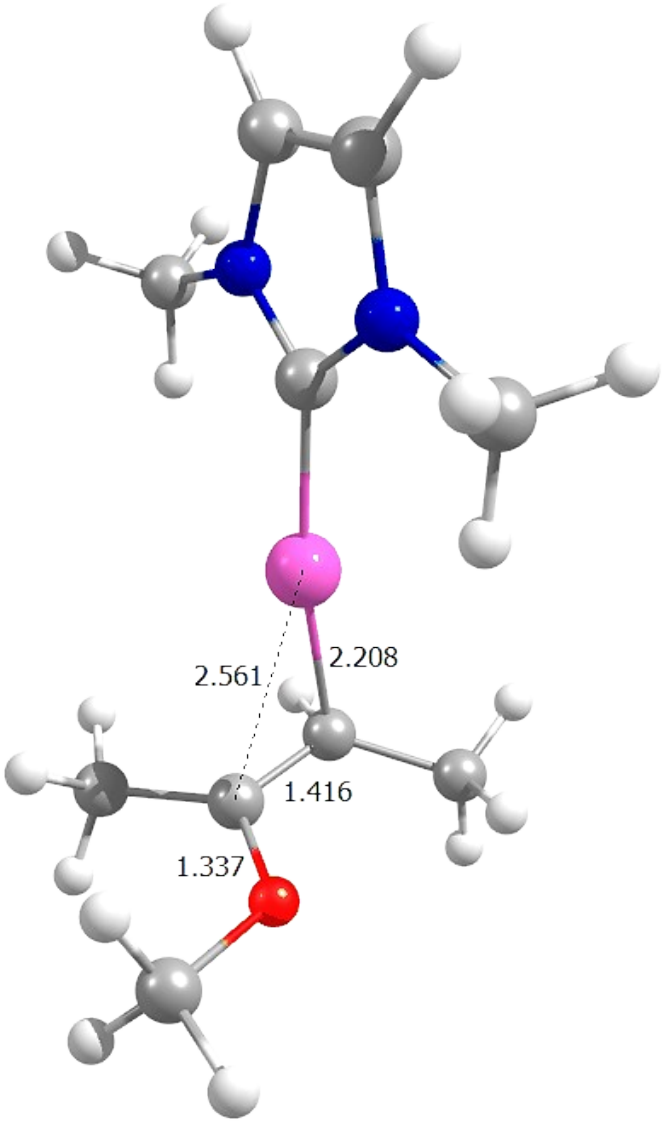
MeOH-VI



C	5.276988	0.767614	-0.171389
O	4.280980	-0.138522	0.262157
C	1.983454	-0.631411	-0.108549
C	2.946244	0.278253	0.230904
C	2.396970	-2.032815	-0.527889
H	3.484892	-2.106373	-0.737258
H	2.164588	-2.775789	0.269625
H	1.841270	-2.367569	-1.430818
C	2.698286	1.696327	0.688135
H	3.161396	1.888625	1.682955
H	3.107575	2.457785	-0.013256
H	1.607427	1.865201	0.774074
C	-2.052663	0.138851	-0.003291
N	-3.057675	-0.778651	0.190757
N	-2.715752	1.332769	-0.158828
C	-4.309407	-0.173385	0.156744
C	-4.093103	1.163425	-0.062921
C	-2.833939	-2.205698	0.398613
C	-2.054587	2.612140	-0.391894
H	-5.240330	-0.734465	0.289619
H	-4.798484	1.995664	-0.157166
Au	-0.021553	-0.212345	-0.042677
H	5.375231	1.662356	0.487848
H	6.240843	0.219409	-0.148340
H	5.101473	1.122535	-1.215830
H	-2.235929	3.306113	0.454074
H	-0.968522	2.419803	-0.481185
H	-2.424321	3.073015	-1.330130
H	-3.302197	-2.535492	1.347909
H	-3.254688	-2.793834	-0.442340
H	-1.740846	-2.372188	0.450145

Zero-point correction= 0.250240 (Hartree/Particle)
Thermal correction to Energy= 0.268435
Thermal correction to Enthalpy= 0.269379
Thermal correction to Gibbs Free Energy= 0.200912
Sum of electronic and zero-point Energies= -711.220351
Sum of electronic and thermal Energies= -711.202156
Sum of electronic and thermal Enthalpies= -711.201212
Sum of electronic and thermal Free Energies= -711.269678

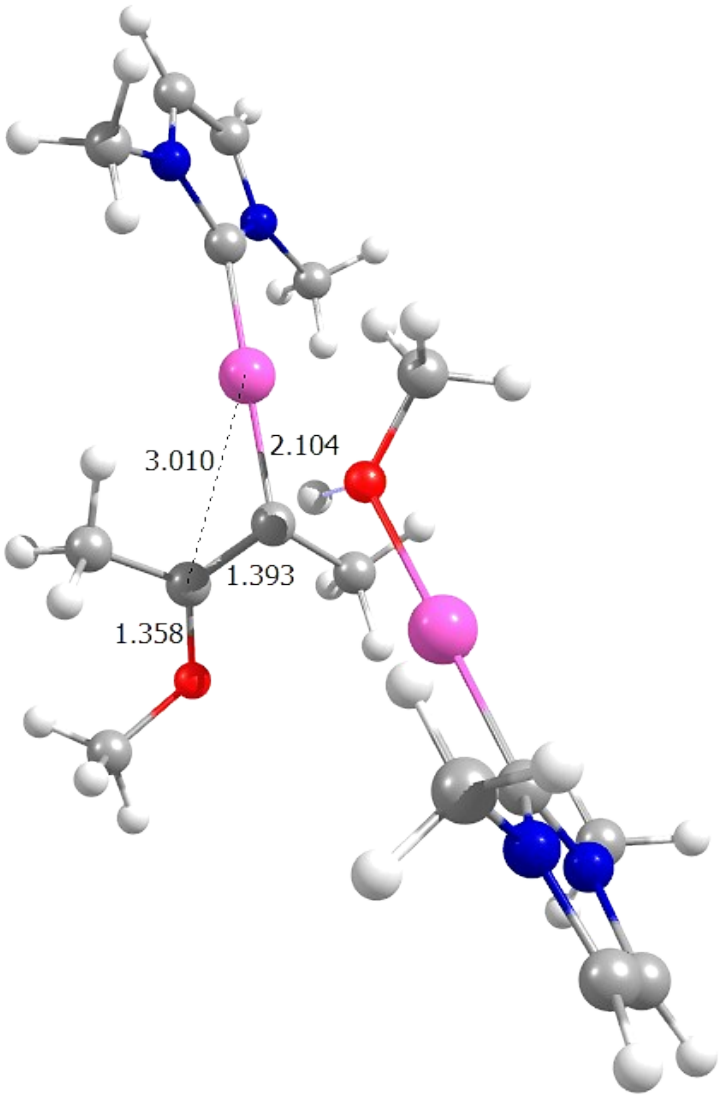
MeOH-VII



C	-1.848677	0.104015	0.102185
N	-2.813004	-0.837382	0.338622
N	-2.504956	1.304645	0.111973
C	-4.052987	-0.234288	0.498486
C	-3.858734	1.117250	0.354940
C	-2.588624	-2.281472	0.420548
C	-1.886802	2.612036	-0.113502
H	-4.964455	-0.807619	0.698282
H	-4.568391	1.949919	0.404272
Au	0.127970	-0.214917	-0.258548
C	3.470774	1.359369	1.829563
O	3.112965	0.924439	0.503333
C	2.164135	-0.575126	-1.031509
C	2.630597	-0.301505	0.277416
H	2.104444	-1.656402	-1.259065
C	2.469594	0.337177	-2.206608
C	2.760167	-1.358157	1.342265
H	2.299143	-2.306353	1.011257
H	3.839626	-1.547923	1.533947
H	2.301610	-1.057069	2.305139
H	2.581571	1.374821	2.493503
H	4.263364	0.719239	2.266137
H	3.857573	2.386965	1.709331
H	1.781013	0.142232	-3.051487
H	2.403267	1.408558	-1.937029
H	3.503518	0.149565	-2.572018
H	-2.820419	-2.648456	1.439952
H	-3.228226	-2.807228	-0.315012
H	-1.527013	-2.485583	0.189909
H	-2.058031	3.270437	0.760652
H	-0.800185	2.466303	-0.255692
H	-2.312701	3.084884	-1.020305

Zero-point correction= 0.263793 (Hartree/Particle)
Thermal correction to Energy= 0.282080
Thermal correction to Enthalpy= 0.283025
Thermal correction to Gibbs Free Energy= 0.214664
Sum of electronic and zero-point Energies= -711.640821
Sum of electronic and thermal Energies= -711.622534
Sum of electronic and thermal Enthalpies= -711.621589
Sum of electronic and thermal Free Energies= -711.689950

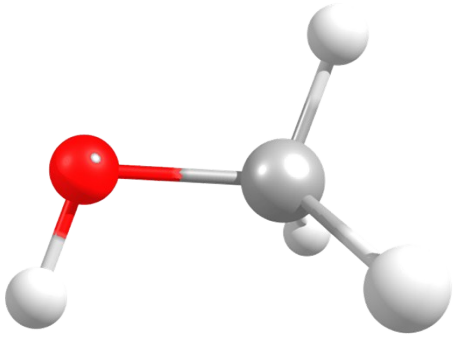
MeOH-VI-VII-MeOH



C	-4.627396	-0.350540	-0.202945
N	-5.611132	-0.826446	0.623804
N	-5.287458	0.332734	-1.190141
C	-6.864243	-0.446619	0.159996
C	-6.660142	0.284350	-0.982935
C	-5.389818	-1.628734	1.826540
C	-4.651018	1.015073	-2.316497
H	-7.789728	-0.724935	0.674692
H	-7.373009	0.768052	-1.658759
Au	-2.669150	-0.621100	-0.023926
C	-0.677056	4.060609	1.691979
O	-0.228256	3.196566	0.643509
C	0.828343	1.264909	-0.176314
C	0.474898	2.065468	0.908130
C	0.410731	1.755435	-1.563490
H	-0.659150	2.060048	-1.593221
H	0.996213	2.646959	-1.879443
H	0.562313	0.970267	-2.331319
C	0.773426	1.735619	2.345624
H	1.432845	2.499977	2.810396
H	-0.151924	1.684576	2.958513
H	1.290520	0.760395	2.401857
C	4.554950	-0.553949	-0.117525
N	5.489972	-0.425320	-1.112228
N	5.168964	-1.322177	0.837885
C	6.660894	-1.098997	-0.784879
C	6.458869	-1.664971	0.448091
C	5.291507	0.318432	-2.354646
C	4.561120	-1.722485	2.104211
H	7.532433	-1.121286	-1.447385
H	7.120317	-2.275689	1.071386
Au	2.681587	0.273624	-0.080851
H	0.101379	0.062776	0.086889
O	-0.625769	-0.906351	0.188116
C	-0.002438	-2.091561	-0.314177
H	1.100777	-1.921784	-0.323390
H	-0.220455	-2.955402	0.349322
H	-0.326643	-2.335413	-1.349302
H	0.168577	4.440765	2.302684
H	-1.168944	4.915533	1.191613
H	-1.413436	3.559534	2.356009
H	-4.300758	-1.771366	1.953912
H	-5.798411	-1.107416	2.714714
H	-5.878644	-2.617554	1.722202
H	-4.993324	0.573548	-3.273316
H	-4.898228	2.094917	-2.299119
H	-3.556331	0.888789	-2.226555
H	5.115443	-1.281825	2.957039
H	3.518729	-1.353769	2.116864
H	4.561305	-2.826613	2.198943
H	6.054667	1.116147	-2.450378
H	5.359230	-0.361688	-3.227150
H	4.285766	0.777595	-2.325522

Zero-point correction= 0.424106 (Hartree/Particle)
Thermal correction to Energy= 0.456748
Thermal correction to Enthalpy= 0.457692
Thermal correction to Gibbs Free Energy= 0.351175
Sum of electronic and zero-point Energies= -1267.068818
Sum of electronic and thermal Energies= -1267.036176
Sum of electronic and thermal Enthalpies= -1267.035232
Sum of electronic and thermal Free Energies= -1267.141749

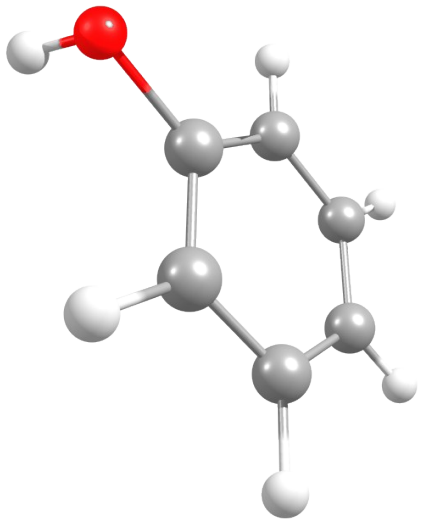
MeOH



O	0.750933	-0.123207	-0.000002
C	-0.656710	0.019394	0.000001
H	-1.053387	0.548113	0.902641
H	-1.094429	-1.000314	-0.000121
H	1.134022	0.773166	0.000000
H	-1.053405	0.548326	-0.902514

Zero-point correction= 0.049540 (Hartree/Particle)
Thermal correction to Energy= 0.052866
Thermal correction to Enthalpy= 0.053811
Thermal correction to Gibbs Free Energy= 0.026786
Sum of electronic and zero-point Energies= -115.580652
Sum of electronic and thermal Energies= -115.577325
Sum of electronic and thermal Enthalpies= -115.576381
Sum of electronic and thermal Free Energies= -115.603406

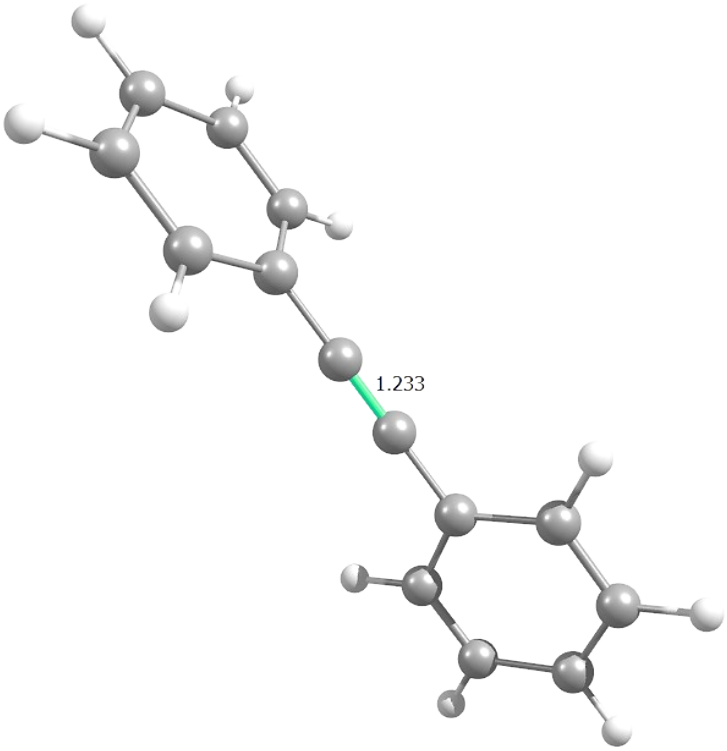
PhOH



C	0.948698	0.000078	-0.015469
C	0.241777	1.219477	-0.011515
C	0.241922	-1.219395	-0.011613
C	-1.163646	1.215977	0.004985
H	0.812550	2.161045	-0.032317
C	-1.163510	-1.216066	0.004946
H	0.812741	-2.160937	-0.032519
C	-1.870426	-0.000088	0.016061
H	-1.710853	2.172516	0.006440
H	-1.710574	-2.172686	0.006354
H	-2.971676	-0.000141	0.027325
O	2.333449	0.000253	-0.089734
H	2.691328	-0.001720	0.818217

Zero-point correction= 0.100680 (Hartree/Particle)
Thermal correction to Energy= 0.105977
Thermal correction to Enthalpy= 0.106922
Thermal correction to Gibbs Free Energy= 0.071786
Sum of electronic and zero-point Energies= -307.139067
Sum of electronic and thermal Energies= -307.133769
Sum of electronic and thermal Enthalpies= -307.132825
Sum of electronic and thermal Free Energies= -307.167961

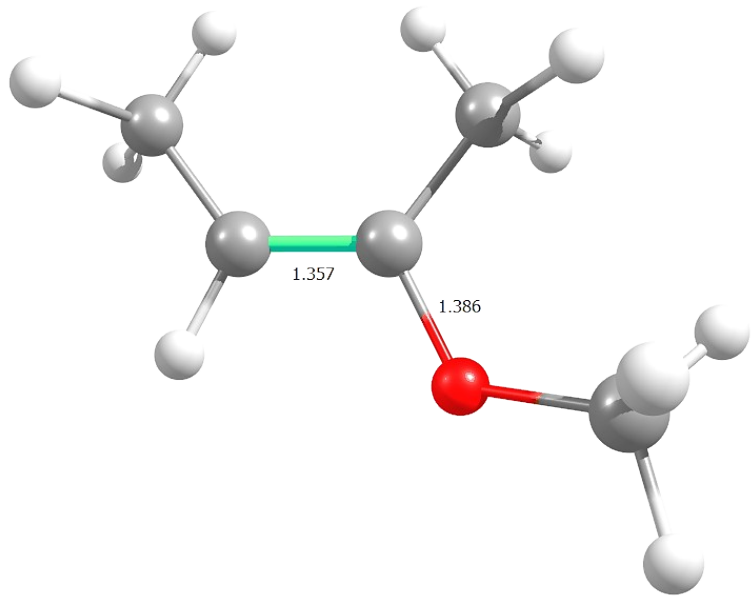
Ph-CC-Ph



C	-0.000044	0.616462	0.000306
C	0.000044	-0.616462	0.000306
C	-0.000028	2.048503	0.000126
C	-0.864550	2.773753	0.863585
C	0.864550	2.773496	-0.863487
C	-0.860606	4.175900	0.859527
H	-1.537254	2.219309	1.535576
C	0.860684	4.175649	-0.859770
H	1.537241	2.218859	-1.535332
C	0.000056	4.882609	-0.000211
H	-1.537075	4.723346	1.535176
H	1.537196	4.722887	-1.535545
H	0.000084	5.984113	-0.000334
C	0.000028	-2.048503	0.000126
C	0.864550	-2.773753	0.863585
C	-0.864550	-2.773496	-0.863487
C	0.860606	-4.175900	0.859527
H	1.537254	-2.219309	1.535576
C	-0.860684	-4.175649	-0.859770
H	-1.537241	-2.218859	-1.535332
C	-0.000056	-4.882609	-0.000211
H	1.537075	-4.723346	1.535176
H	-1.537196	-4.722887	-1.535545
H	-0.000084	-5.984113	-0.000334

Zero-point correction= 0.186042 (Hartree/Particle)
Thermal correction to Energy= 0.196512
Thermal correction to Enthalpy= 0.197456
Thermal correction to Gibbs Free Energy= 0.149346
Sum of electronic and zero-point Energies= -538.880178
Sum of electronic and thermal Energies= -538.869708
Sum of electronic and thermal Enthalpies= -538.868764
Sum of electronic and thermal Free Energies= -538.916875

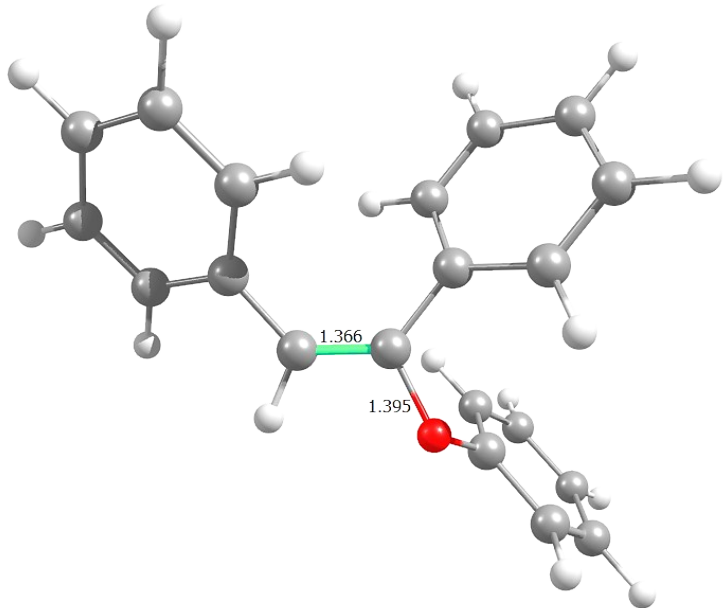
PRODcis



C	-2.344493	-0.275652	-0.266971
O	-1.143405	-0.701642	0.355371
C	1.162714	-0.697350	0.002703
C	0.014962	0.017979	0.108496
H	1.036586	-1.793473	0.052927
C	2.565206	-0.177369	-0.130880
C	-0.109287	1.519842	0.071212
H	0.884092	2.002366	0.016178
H	-0.696250	1.872712	-0.804476
H	-0.624519	1.895421	0.982413
H	-2.690905	0.723486	0.085882
H	-2.255688	-0.246463	-1.379027
H	-3.118861	-1.021058	0.001592
H	3.049251	-0.551851	-1.060885
H	2.620077	0.929618	-0.154819
H	3.208849	-0.522318	0.709880

Zero-point correction= 0.135849 (Hartree/Particle)
Thermal correction to Energy= 0.143902
Thermal correction to Enthalpy= 0.144846
Thermal correction to Gibbs Free Energy= 0.104009
Sum of electronic and zero-point Energies= -271.401980
Sum of electronic and thermal Energies= -271.393927
Sum of electronic and thermal Enthalpies= -271.392983
Sum of electronic and thermal Free Energies= -271.433820

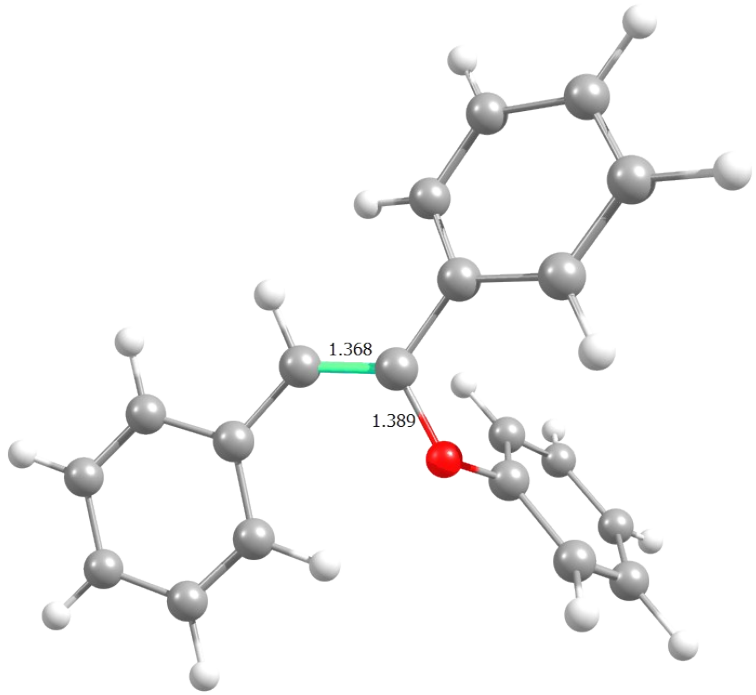
PRODPhcis



Zero-point correction= 0.291236 (Hartree/Particle)
Thermal correction to Energy= 0.308438
Thermal correction to Enthalpy= 0.309383
Thermal correction to Gibbs Free Energy= 0.244026
Sum of electronic and zero-point Energies= -846.061015
Sum of electronic and thermal Energies= -846.043812
Sum of electronic and thermal Enthalpies= -846.042868
Sum of electronic and thermal Free Energies= -846.108225

C	-2.372050	-1.011464	-0.378310
C	-2.430686	-0.863581	1.021098
C	-3.552932	-1.185983	-1.127709
C	-3.681885	-0.878446	1.662092
H	-1.503417	-0.746603	1.600997
C	-4.793304	-1.205429	-0.472615
H	-3.474557	-1.308212	-2.218757
C	-4.866142	-1.047615	0.924311
H	-3.725768	-0.761045	2.756804
H	-5.713962	-1.342709	-1.062092
H	-5.841550	-1.059487	1.434820
O	-1.184588	-1.054597	-1.085441
C	1.048439	-1.335354	-0.466013
C	-0.022739	-0.492593	-0.555907
C	-0.097199	0.959408	-0.245489
C	-0.849931	1.822824	-1.077623
C	-0.936778	3.194573	-0.792409
H	-1.362493	1.407572	-1.958682
C	0.453052	2.874210	1.177301
C	-0.284195	3.726206	0.333763
H	-1.520545	3.853369	-1.454899
H	0.954307	3.280178	2.070421
H	-0.356306	4.801993	0.559634
C	2.471079	-1.049517	-0.218441
C	3.107911	0.161126	-0.598633
C	3.273080	-2.060962	0.372657
C	4.476672	0.357983	-0.366043
H	2.523647	0.946715	-1.100227
C	4.641164	-1.859560	0.610665
H	2.804413	-3.018437	0.653798
C	5.250335	-0.645809	0.246673
H	4.948814	1.303727	-0.677444
H	5.237495	-2.659263	1.078615
H	6.325415	-0.486868	0.426582
H	0.800921	-2.396120	-0.645998
C	0.544176	1.503798	0.893515
H	1.111880	0.839063	1.562654

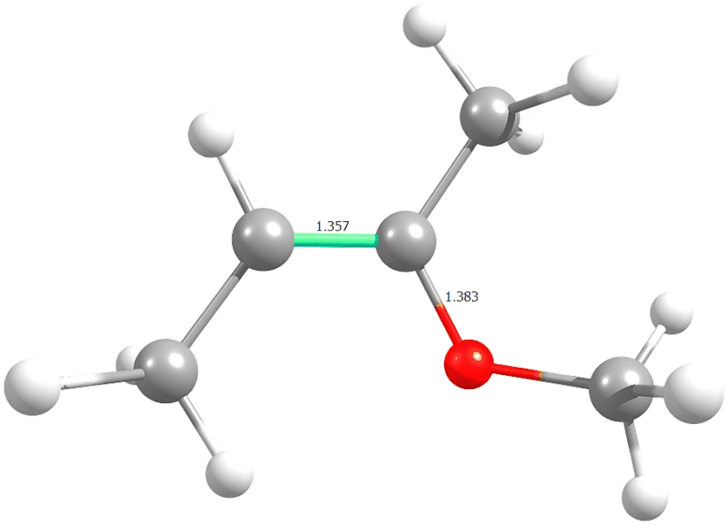
PRODPhtrans



C	0.759209	1.569554	-0.236727
C	1.116155	1.544829	1.124908
C	1.038454	2.699915	-1.030635
C	1.764993	2.659848	1.683594
H	0.879850	0.664002	1.739785
C	1.681870	3.806400	-0.455952
H	0.742903	2.691557	-2.090918
C	2.051646	3.792327	0.902058
H	2.044416	2.639535	2.749179
H	1.898414	4.689016	-1.078825
H	2.559029	4.661297	1.348746
O	0.079399	0.536378	-0.860837
C	-1.140554	-1.315857	0.014693
C	0.057475	-0.732458	-0.295662
C	1.366113	-1.426203	-0.198389
C	2.430855	-1.058745	-1.058649
C	3.662099	-1.729306	-1.003980
H	2.278196	-0.248696	-1.786914
C	2.816063	-3.145880	0.778832
C	3.861289	-2.777227	-0.088094
H	4.473414	-1.431603	-1.687264
H	2.965531	-3.955550	1.510929
H	4.829492	-3.300587	-0.044114
C	-2.507638	-0.790461	-0.022158
C	-2.868467	0.513410	-0.462033
C	-3.553682	-1.650036	0.414682
C	-4.207701	0.928114	-0.451197
H	-2.088034	1.195099	-0.822532
C	-4.890975	-1.231100	0.424327
H	-3.300006	-2.667899	0.754669
C	-5.226570	0.064269	-0.008371
H	-4.460312	1.943364	-0.797299
H	-5.677562	-1.920663	0.770468
H	-6.276355	0.398102	-0.003422
H	-1.068241	-2.371275	0.323188
C	1.585364	-2.475451	0.729444
H	0.788088	-2.752377	1.436881

Zero-point correction= 0.291524 (Hartree/Particle)
Thermal correction to Energy= 0.308710
Thermal correction to Enthalpy= 0.309654
Thermal correction to Gibbs Free Energy= 0.244093
Sum of electronic and zero-point Energies= -846.066597
Sum of electronic and thermal Energies= -846.049412
Sum of electronic and thermal Enthalpies= -846.048468
Sum of electronic and thermal Free Energies= -846.114029

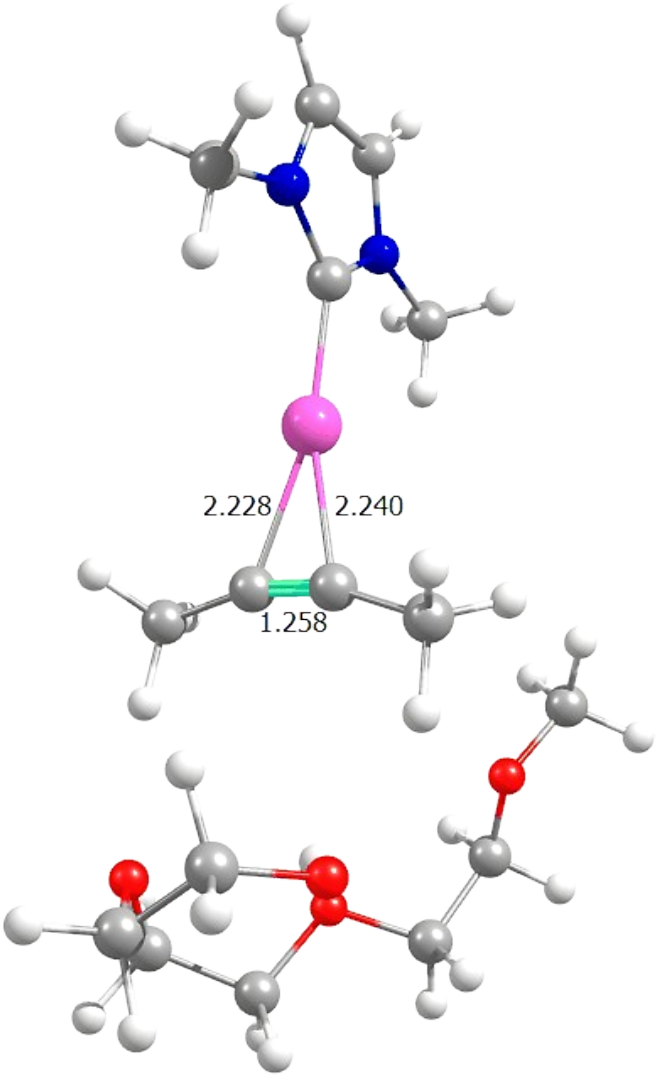
PRODtrans



C	1.855509	-1.087025	0.168487
O	0.552591	-0.800606	-0.313874
C	-1.343805	0.534123	0.082113
C	0.003626	0.440757	-0.051054
H	-1.760386	1.548388	0.201530
C	-2.302055	-0.621490	0.041468
C	0.932286	1.628618	-0.013587
H	0.349525	2.562900	0.096308
H	1.652220	1.582615	0.832511
H	1.532195	1.703368	-0.947724
H	2.639958	-0.442269	-0.289821
H	1.925174	-0.995798	1.277925
H	2.068402	-2.138141	-0.109002
H	-2.958664	-0.581061	-0.857455
H	-1.760921	-1.587207	0.019653
H	-2.981595	-0.617850	0.922505

Zero-point correction= 0.136010 (Hartree/Particle)
Thermal correction to Energy= 0.144050
Thermal correction to Enthalpy= 0.144994
Thermal correction to Gibbs Free Energy= 0.104139
Sum of electronic and zero-point Energies= -271.404511
Sum of electronic and thermal Energies= -271.396471
Sum of electronic and thermal Enthalpies= -271.395527
Sum of electronic and thermal Free Energies= -271.436382

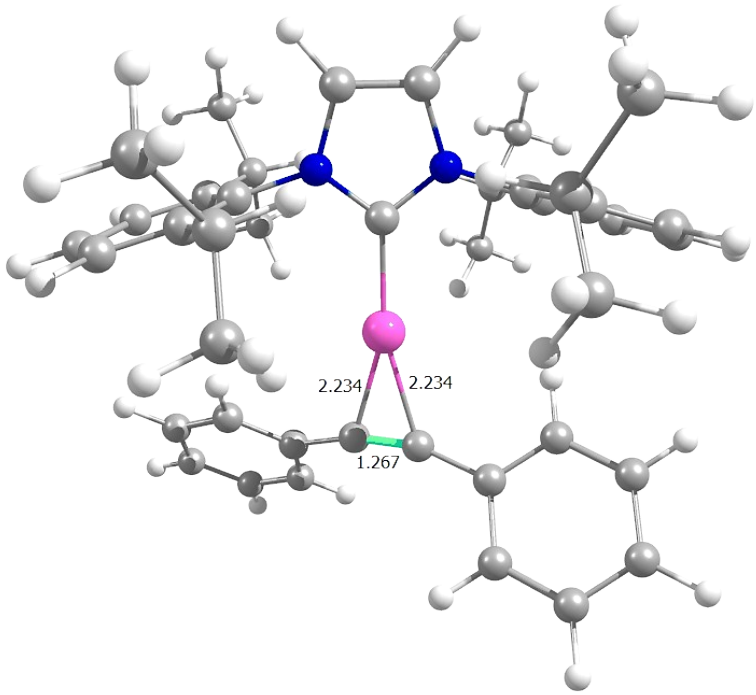
RC



C	-3.739339	0.051449	-0.144804
N	-4.384016	1.173585	-0.590875
C	-5.758088	0.989790	-0.559819
C	-5.978632	-0.279404	-0.082504
N	-4.733547	-0.837196	0.164906
C	-3.731814	2.402347	-1.046492
C	-4.531920	-2.190393	0.686736
Au	-1.738546	-0.241259	0.020994
C	0.385917	-0.784699	-0.374606
C	0.829923	-1.338505	-1.662326
C	0.357705	-0.347373	0.804119
C	0.711377	0.074525	2.164185
O	3.716380	-0.809438	1.573912
C	3.568760	-2.203498	1.359925
C	4.427868	-2.707646	0.202653
O	4.039372	-2.011556	-0.989344
C	5.068157	-1.321518	-1.692835
C	5.610199	-0.100199	-0.954487
O	4.529674	0.782888	-0.667083
C	4.941464	1.947871	0.052661
C	3.887307	3.034121	-0.044180
O	2.717036	2.674214	0.667748
C	1.768457	3.720465	0.687880
H	-6.463049	1.766046	-0.875810
H	-6.912796	-0.821833	0.097753
H	0.248069	-2.238229	-1.947193
H	1.902909	-1.623450	-1.557974
H	0.735753	-0.591601	-2.476776
H	0.206133	-0.547234	2.930901
H	0.457555	1.137334	2.345954
H	1.818210	-0.051792	2.254453
H	-4.062567	3.260115	-0.428665
H	-3.980481	2.594817	-2.108723
H	-2.638335	2.277013	-0.944077
H	-3.445514	-2.376952	0.769682
H	-4.979395	-2.933733	-0.001777
H	-4.997505	-2.286614	1.687270
H	2.502147	-2.480917	1.156635
H	3.864669	-2.726180	2.295488
H	4.279290	-3.803105	0.056999
H	5.504967	-2.539253	0.426738
H	5.918840	-2.000008	-1.943352
H	4.604874	-0.996463	-2.647586
H	6.371752	0.401367	-1.601862
H	6.129909	-0.398271	-0.011387
H	5.886629	2.351484	-0.382926
H	5.137788	1.691668	1.121304
H	3.654985	3.229037	-1.122087
H	4.327933	3.975886	0.372319
H	0.895320	3.378959	1.279421
H	1.417989	3.994971	-0.338297
H	2.174191	4.645778	1.166410
H	3.684067	-0.356998	0.691903

Zero-point correction= 0.439303 (Hartree/Particle)
Thermal correction to Energy= 0.470208
Thermal correction to Enthalpy= 0.471153
Thermal correction to Gibbs Free Energy= 0.370122
Sum of electronic and zero-point Energies= -1172.579705
Sum of electronic and thermal Energies= -1172.548799
Sum of electronic and thermal Enthalpies= -1172.547855
Sum of electronic and thermal Free Energies= -1172.648885

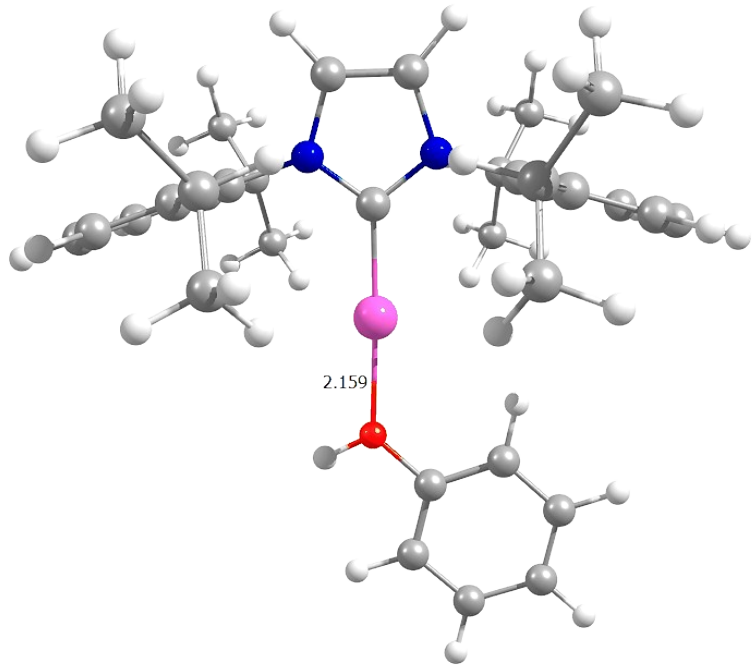
REAL-CAT



Zero-point correction= 0.740374 (Hartree/Particle)
Thermal correction to Energy= 0.786917
Thermal correction to Enthalpy= 0.787861
Thermal correction to Gibbs Free Energy= 0.652876
Sum of electronic and zero-point Energies= -1833.283810
Sum of electronic and thermal Energies= -1833.237267
Sum of electronic and thermal Enthalpies= -1833.236323
Sum of electronic and thermal Free Energies= -1833.371308

C	-0.000096	-1.411726	0.000093
N	-1.052757	-2.239329	-0.279354
N	1.052495	-2.239392	0.279634
C	-0.663675	-3.572078	-0.175250
C	0.663292	-3.572116	0.175693
C	-2.393900	-1.803050	-0.626344
C	2.393710	-1.803198	0.626460
H	-1.362209	-4.393921	-0.360633
H	1.361750	-4.394003	0.361172
C	-2.682025	-1.519715	-1.988464
C	-3.999974	-1.119515	-2.294341
C	-4.981297	-1.024639	-1.297038
C	-4.664577	-1.319482	0.036785
C	-3.362345	-1.713833	0.409198
C	-1.645048	-1.644605	-3.105680
H	-4.265190	-0.892557	-3.338860
H	-6.007119	-0.725691	-1.564576
H	-5.446514	-1.246516	0.808728
C	-3.051382	-2.039922	1.870756
C	2.681999	-1.519767	1.988525
C	4.000018	-1.119671	2.294233
C	4.981252	-1.024988	1.296825
C	4.664370	-1.319923	-0.036940
C	3.362060	-1.714172	-0.409188
C	1.645123	-1.644461	3.105857
H	4.265360	-0.892634	3.338702
H	6.007131	-0.726120	1.564235
H	5.446236	-1.247112	-0.808971
C	3.050916	-2.040341	-1.870690
H	-0.696249	-2.000121	-2.651476
C	-1.352289	-0.277063	-3.759580
C	-2.070056	-2.694691	-4.155465
H	-1.963940	-2.251009	1.948604
C	-3.346393	-0.844065	2.800852
C	-3.800168	-3.310109	2.332042
H	0.696206	-1.999803	2.651763
C	2.070066	-2.694629	4.155589
C	1.352687	-0.276871	3.759796
H	1.963448	-2.251345	-1.948408
C	3.345919	-0.844563	-2.800891
C	3.799555	-3.310615	-2.331969
H	-0.568493	-0.377570	-4.538568
H	-2.255689	0.143902	-4.248552
H	-0.996580	0.461517	-3.010301
H	-1.277204	-2.820397	-4.921668
H	-2.257997	-3.685196	-3.692555
H	-2.997130	-2.391764	-4.685429
H	-3.040460	-1.080124	3.841049
H	-2.800906	0.066782	2.479019
H	-4.428544	-0.598456	2.825071
H	-3.529350	-3.563569	3.377911
H	-4.900460	-3.166645	2.297391
H	-3.558768	-4.185913	1.695047
H	1.277285	-2.820191	4.921889
H	2.257768	-3.685167	3.692653
H	2.997264	-2.391872	4.685434
H	0.568959	-0.377247	4.538871
H	2.256213	0.143930	4.248673
H	0.997027	0.461778	3.010563
H	3.039847	-1.080656	-3.841039
H	2.800542	0.066345	-2.479046
H	4.428087	-0.599041	-2.825249
H	3.528611	-3.564125	-3.377793
H	4.899861	-3.167232	-2.297442
H	3.558154	-4.186357	-1.694890
Au	0.000044	0.614779	0.000000
C	-0.628300	2.757255	0.079402
C	0.628644	2.757117	-0.079475
C	-1.972526	3.164000	0.405271
C	-2.154652	4.319999	1.212803
C	-3.107100	2.464900	-0.081491
C	-3.448625	4.764880	1.513368
H	-1.275442	4.859216	1.596374
C	-4.395573	2.919789	0.231300
H	-2.969018	1.571065	-0.709303
C	-4.570047	4.067747	1.025534
H	-3.583595	5.662916	2.135971
H	-5.271399	2.375331	-0.153346
H	-5.584474	4.422594	1.265528
C	1.972863	3.163877	-0.405398
C	3.107478	2.464202	0.080438
C	2.154928	4.320493	-1.212060
C	4.395927	2.919121	-0.232419
H	2.969475	1.569888	0.707585
C	3.448876	4.765389	-1.512704
H	1.275686	4.860165	-1.594916
C	4.570340	4.067675	-1.025799
H	5.271783	2.374205	0.151509
H	3.583792	5.663893	-2.134643
H	5.584749	4.422537	-1.265850

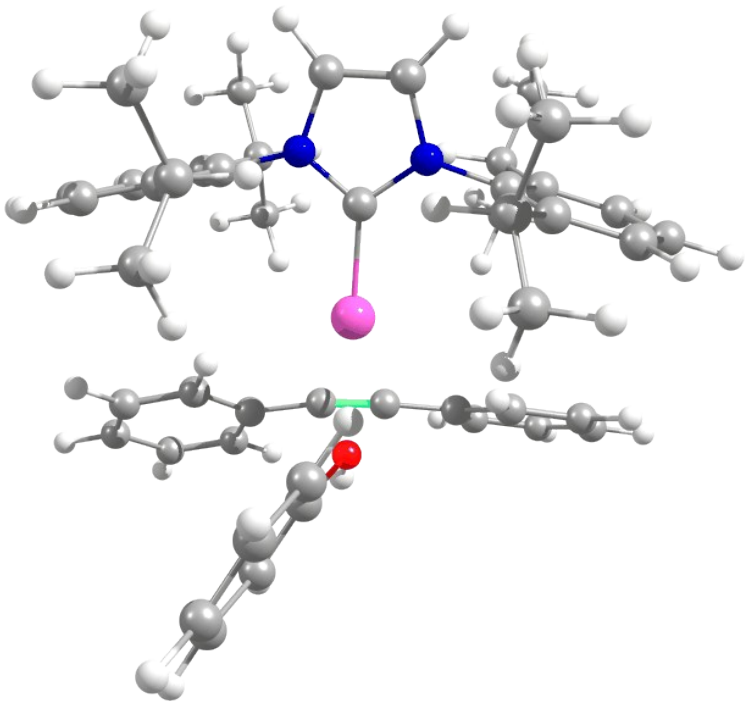
REAL-CAT+PhOH



Zero-point correction= 0.656651 (Hartree/Particle)
Thermal correction to Energy= 0.697419
Thermal correction to Enthalpy= 0.698363
Thermal correction to Gibbs Free Energy= 0.577288
Sum of electronic and zero-point Energies= -1601.534559
Sum of electronic and thermal Energies= -1601.493791
Sum of electronic and thermal Enthalpies= -1601.492847
Sum of electronic and thermal Free Energies= -1601.613923

C	0.780501	0.792238	-0.000267
N	2.143783	0.897974	-0.000857
N	0.302040	2.072764	0.000050
C	2.518089	2.238980	-0.000915
C	1.360619	2.977134	-0.000345
C	3.071591	-0.220832	-0.001137
C	-1.102275	2.450494	0.001275
H	3.569196	2.544210	-0.001392
H	1.193231	4.058650	-0.000149
C	3.510265	-0.733032	-1.251150
C	4.412943	-1.816346	-1.217487
C	4.859630	-2.353026	-0.001632
C	4.413856	-1.816137	1.214464
C	3.511251	-0.732775	1.248626
C	3.038525	-0.171803	-2.593341
H	4.776039	-2.245317	-2.164461
H	5.567703	-3.196536	-0.001828
H	4.777672	-2.244945	2.161242
C	3.040645	-0.171268	2.591111
C	-1.749424	2.639080	1.251810
C	-3.105534	3.025753	1.218996
C	-3.777807	3.219255	0.003880
C	-3.106860	3.029391	-1.212541
C	-1.750822	2.642658	-1.247962
C	-1.044779	2.446843	2.595481
H	-3.643037	3.184275	2.166958
H	-4.835032	3.527828	0.004919
H	-3.645372	3.190642	-2.159484
C	-1.047756	2.454153	-2.592948
H	2.405111	0.717405	-2.388460
C	2.156052	-1.193223	-3.343941
C	4.219119	0.304420	-3.466430
H	2.406597	0.717574	2.386580
C	2.159434	-1.192723	3.343116
C	4.222012	0.305835	3.462707
H	0.006811	2.153170	2.392074
C	-1.003013	3.760476	3.406807
C	-1.686965	1.302469	3.409187
H	0.003417	2.157518	-2.391700
C	-1.692891	1.314333	-3.410712
C	-1.004108	3.770958	-3.399099
H	1.785371	-0.763281	-4.297479
H	2.721707	-2.116027	-3.590632
H	1.274487	-1.488304	-2.735716
H	3.844584	0.776624	-4.398064
H	4.848386	1.047869	-2.935596
H	4.876593	-0.538166	-3.766142
H	1.789667	-0.762517	4.296892
H	1.277286	-1.488393	2.736030
H	2.725708	-2.115199	3.589586
H	3.848343	0.778260	4.394582
H	4.880187	-0.536362	3.761978
H	4.850374	1.049337	2.930884
H	-0.434606	3.616129	4.348825
H	-0.518728	4.580296	2.837557
H	-2.022177	4.102341	3.683729
H	-1.136091	1.143817	4.359301
H	-2.741498	1.529590	3.671049
H	-1.678195	0.347006	2.843749
H	-1.143023	1.158451	-4.361856
H	-1.685669	0.356613	-2.849168
H	-2.747136	1.544610	-3.670949
H	-0.437041	3.629233	-4.342326
H	-2.022882	4.116068	-3.673427
H	-0.517527	4.587519	-2.827124
Au	-0.267415	-0.876693	0.000058
C	-2.724760	-3.021722	-0.000404
C	-3.611711	-1.939141	-0.001133
C	-3.167245	-4.351229	-0.000687
C	-4.992037	-2.205793	-0.002221
H	-3.226865	-0.906410	-0.000852
C	-4.551491	-4.598521	-0.001747
H	-2.449141	-5.188354	-0.000113
C	-5.464548	-3.530134	-0.002517
H	-5.702049	-1.364646	-0.002825
H	-4.911800	-5.638624	-0.001990
H	-6.546490	-3.730287	-0.003370
O	-1.338445	-2.751456	0.000708
H	-0.814583	-3.577007	0.001528

REAL-CAT+PhOH+PhCCPh-CAT+Ph

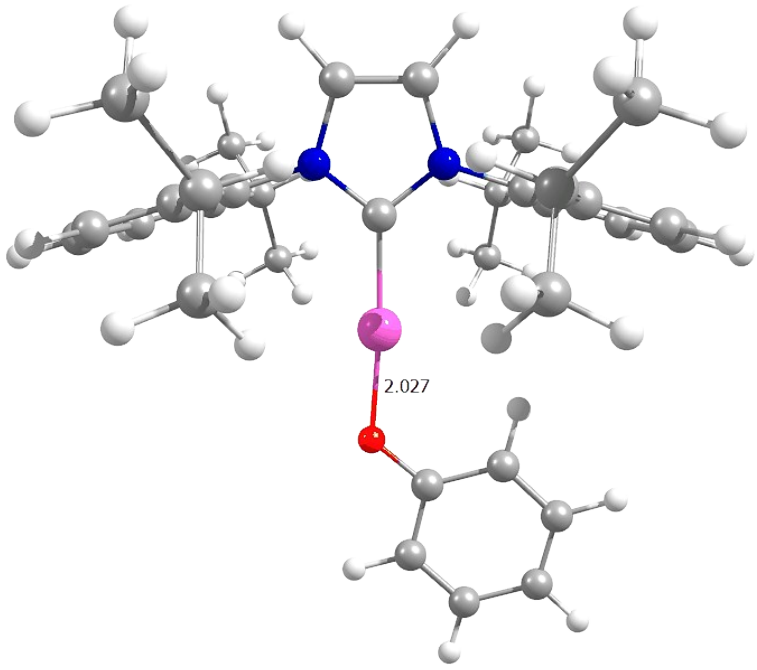


Zero-point correction= 0.842977 (Hartree/Particle)
Thermal correction to Energy= 0.896336
Thermal correction to Enthalpy= 0.897280
Thermal correction to Gibbs Free Energy= 0.746705
Sum of electronic and zero-point Energies= -2140.412635
Sum of electronic and thermal Energies= -2140.359276
Sum of electronic and thermal Enthalpies= -2140.358331
Sum of electronic and thermal Free Energies= -2140.508906

O	0.772862	2.140706	1.584307
Au	0.028636	0.334738	0.137898
C	-0.567926	-1.550153	-0.102786
N	0.198554	-2.614583	-0.501322
C	-0.568164	-3.777554	-0.537333
H	-0.140439	-4.740016	-0.833912
C	-1.837603	-3.430005	-0.155622
H	-2.749319	-4.025988	-0.051432
N	-1.822834	-2.061035	0.105913
C	1.601829	-2.571620	-0.872341
C	2.575871	-2.825924	0.130150
C	3.927082	-2.831264	-0.275128
H	4.712693	-3.031842	0.469836
C	4.286170	-2.601931	-1.611216
H	5.347548	-2.620780	-1.904961
C	3.299148	-2.361017	-2.576921
H	3.595538	-2.189488	-3.623492
C	1.930717	-2.344394	-2.235744
C	2.208817	-3.143012	1.580471
H	1.126594	-2.930082	1.710327
C	2.969473	-2.255248	2.585517
H	2.800667	-1.176523	2.389854
H	4.063636	-2.439727	2.556873
H	2.631564	-2.470306	3.620335
C	2.424692	-4.643191	1.884848
H	1.847664	-5.292271	1.194581
H	2.107531	-4.881078	2.921462
H	3.494626	-4.923373	1.787821
C	0.877939	-2.121762	-3.322618
H	-0.118236	-2.095307	-2.832822
C	0.862540	-3.293480	-4.329628
H	0.689294	-4.267128	-3.826696
H	1.824054	-3.368846	-4.879440
H	0.059240	-3.149933	-5.081874
C	1.066658	-0.767904	-4.038374
H	1.045282	0.077182	-3.320270
H	0.258285	-0.608715	-4.781854
H	2.031525	-0.723111	-4.585222
C	-3.006909	-1.308745	0.481089
C	-3.862228	-0.849763	-0.555749
C	-5.039013	-0.176563	-0.166686
H	-5.729338	0.191936	-0.941222
C	-5.347123	0.024254	1.185744
H	-6.277099	0.543962	1.465546
C	-4.481518	-0.442910	2.185394
H	-4.742253	-0.284654	3.243066
C	-3.290915	-1.126013	1.860920
C	-3.575370	-1.092513	-2.038483
H	-2.551006	-1.513184	-2.122080
C	-3.594350	0.214087	-2.858162
H	-2.889213	0.963861	-2.445520
H	-4.603931	0.674452	-2.877993
H	-3.306903	0.011197	-3.910623
C	-4.553245	-2.135819	-2.624785
H	-4.309661	-2.345944	-3.686963
H	-5.601080	-1.770769	-2.586697
H	-4.515705	-3.095893	-2.069844
C	-2.398600	-1.691233	2.966931
H	-1.414143	-1.935297	2.513868
C	-2.991943	-3.003923	3.529006
H	-3.132088	-3.767936	2.737016
H	-3.982323	-2.823824	3.997516
H	-2.324441	-3.435662	4.303585
C	-2.139345	-0.674651	4.096171
H	-1.744485	0.283567	3.700303
H	-1.402458	-1.082088	4.818877
H	-3.060313	-0.447041	4.672035
C	-1.574027	3.284181	-1.071532
C	-2.423919	2.989720	0.028273
C	-2.049068	4.142110	-2.103211
C	-3.707929	3.547396	0.094503
H	-2.065983	2.322963	0.828145
C	-3.335204	4.691503	-2.023973
H	-1.396470	4.372399	-2.958659
C	-4.166744	4.399522	-0.926489
H	-4.354787	3.315929	0.954350
H	-3.691325	5.357161	-2.825544
H	-5.174536	4.839242	-0.867028
C	-0.236168	2.779464	-1.160949
C	0.961181	2.478593	-1.335710
C	2.363238	2.393723	-1.631757
C	3.212400	1.416888	-1.048167
C	2.923485	3.350157	-2.525427
C	4.583080	1.407041	-1.342055
H	2.784836	0.663581	-0.366536
C	4.293630	3.325459	-2.814522
H	2.271980	4.109785	-2.982922
C	5.128192	2.358633	-2.222680
H	5.229626	0.646118	-0.879123
H	4.715485	4.070995	-3.506414
H	6.205558	2.347383	-2.449892
H	0.955925	2.884185	0.967685
C	1.648225	2.175345	2.672107
C	2.671658	3.136574	2.739323
C	1.466664	1.236580	3.700265
C	3.521304	3.156090	3.859132

	H	2.803226	3.868090	1.924845
	C	2.326169	1.267009	4.811451
	H	0.651664	0.501252	3.630541
	C	3.354255	2.222893	4.896704
	H	4.320561	3.911373	3.915346
	H	2.183863	0.536628	5.623197
	H	4.021273	2.243131	5.771748

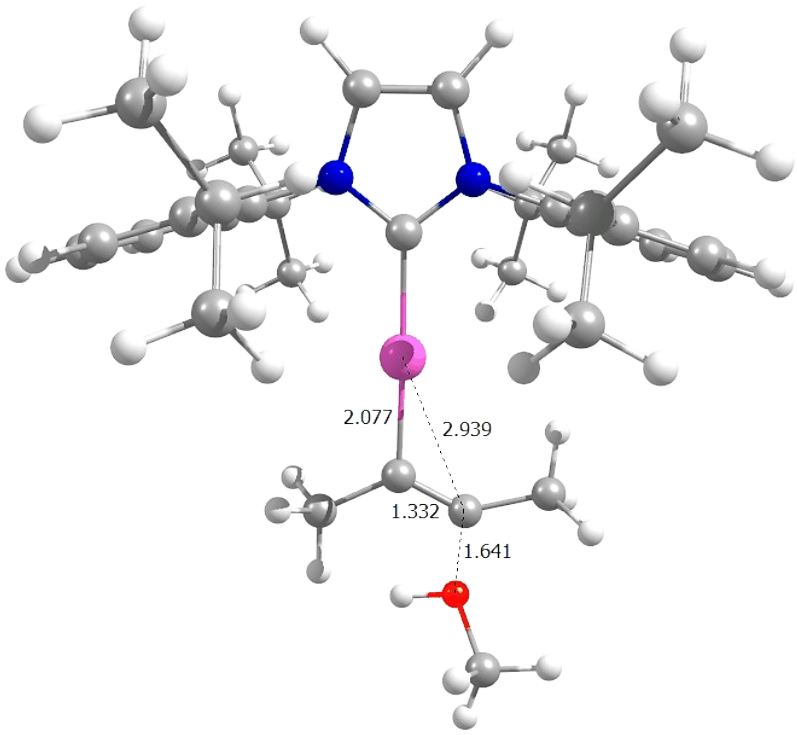
REAL-CAT+PhO



Zero-point correction= 0.644273 (Hartree/Particle)
Thermal correction to Energy= 0.684309
Thermal correction to Enthalpy= 0.685253
Thermal correction to Gibbs Free Energy= 0.566096
Sum of electronic and zero-point Energies= -1601.151247
Sum of electronic and thermal Energies= -1601.111211
Sum of electronic and thermal Enthalpies= -1601.110267
Sum of electronic and thermal Free Energies= -1601.229424

C	-0.726063	-0.795295	0.004052
N	-2.090818	-0.980186	0.000273
N	-0.205422	-2.069081	0.002982
C	-2.409348	-2.338242	-0.003529
C	-1.222247	-3.023482	-0.001159
C	-3.073073	0.084622	-0.000737
C	1.207752	-2.389389	0.007472
H	-3.446014	-2.688537	-0.006740
H	-1.005985	-4.096070	-0.002003
C	-3.541245	0.576437	-1.247381
C	-4.517350	1.593912	-1.216613
C	-5.003295	2.097753	-0.002511
C	-4.518071	1.595453	1.212907
C	-3.542585	0.577697	1.245429
C	-3.016887	0.065746	-2.589916
H	-4.897940	2.003412	-2.165691
H	-5.763600	2.894869	-0.003227
H	-4.899687	2.006961	2.160570
C	-3.001026	0.079166	2.585470
C	1.867641	-2.534892	1.256178
C	3.236243	-2.873859	1.228853
C	3.915039	-3.057653	0.016355
C	3.237080	-2.902437	-1.200803
C	1.868099	-2.566248	-1.237088
C	1.161281	-2.319855	2.594927
H	3.781299	-2.990232	2.178761
H	4.984973	-3.319669	0.019821
H	3.783008	-3.039756	-2.147280
C	1.163782	-2.370043	-2.579864
H	-2.277964	-0.735800	-2.382107
C	-2.271631	1.180832	-3.354748
C	-4.142452	-0.557620	-3.443224
H	-2.345416	-0.793181	2.380342
C	-2.123035	1.160773	3.253015
C	-4.122745	-0.405558	3.526755
H	0.097545	-2.084781	2.381078
C	1.182822	-3.594491	3.465685
C	1.752665	-1.108332	3.347763
H	0.082339	-2.223372	-2.375355
C	1.671835	-1.092532	-3.284143
C	1.289494	-3.609333	-3.490861
H	-1.854929	0.788350	-4.306038
H	-2.949566	2.023224	-3.607802
H	-1.433451	1.587438	-2.751952
H	-3.731222	-0.969588	-4.388665
H	-4.656461	-1.382033	-2.906413
H	-4.912560	0.194184	-3.716820
H	-1.685686	0.779576	4.199709
H	-1.290621	1.467421	2.585459
H	-2.715261	2.068467	3.495283
H	-3.690325	-0.828210	4.457725
H	-4.797066	0.424061	3.826705
H	-4.746974	-1.190832	3.051922
H	0.615202	-3.431567	4.405857
H	0.730268	-4.460244	2.938844
H	2.218111	-3.879061	3.749802
H	1.193009	-0.924315	4.288843
H	2.816157	-1.277609	3.618939
H	1.702833	-0.187578	2.730735
H	1.123968	-0.927397	-4.235693
H	1.529403	-0.197609	-2.643092
H	2.753059	-1.167240	-3.526341
H	0.708623	-3.461903	-4.425340
H	2.342874	-3.799528	-3.786527
H	0.910053	-4.526052	-2.993375
Au	0.258892	0.915452	0.007418
C	2.454208	2.984128	-0.010646
C	3.453930	1.971572	-0.039812
C	2.889071	4.340925	-0.003737
C	4.818180	2.303053	-0.060120
H	3.129082	0.916258	-0.046671
C	4.254124	4.658918	-0.024361
H	2.120434	5.129452	0.018263
C	5.234469	3.647249	-0.052595
H	5.568406	1.494537	-0.082319
H	4.559738	5.718910	-0.018351
H	6.305512	3.903475	-0.068699
O	1.138262	2.741485	0.010371

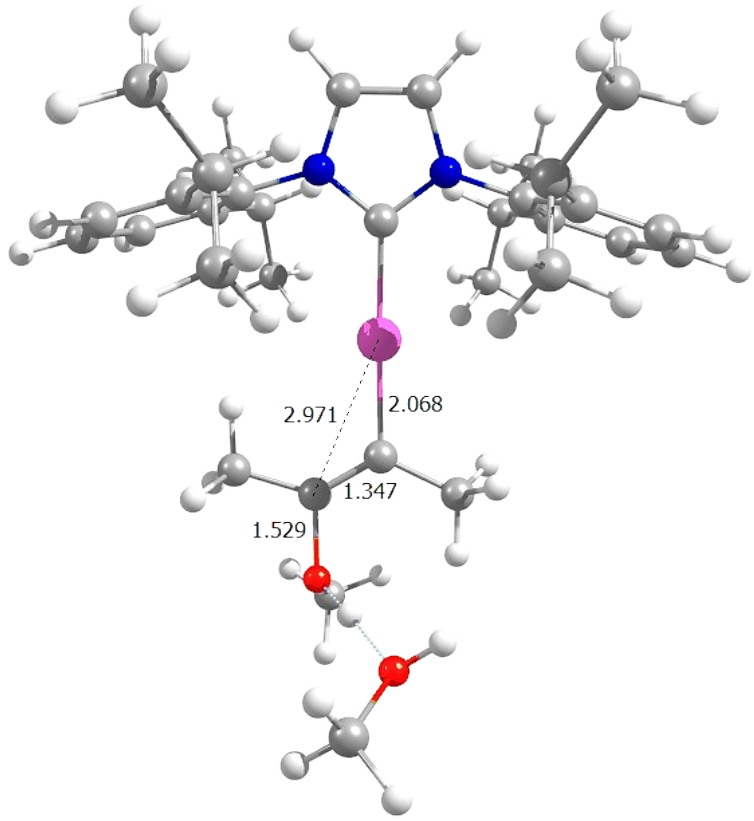
REAL-MeCCMe-MeOH-I



Zero-point correction= 0.689496 (Hartree/Particle)
Thermal correction to Energy= 0.733081
Thermal correction to Enthalpy= 0.734025
Thermal correction to Gibbs Free Energy= 0.606634
Sum of electronic and zero-point Energies= -1565.747677
Sum of electronic and thermal Energies= -1565.704092
Sum of electronic and thermal Enthalpies= -1565.703148
Sum of electronic and thermal Free Energies= -1565.830539

C	-0.452662	-0.919861	-0.087188
N	0.288211	-2.068625	-0.200708
N	-1.757567	-1.334023	-0.166750
C	-0.538653	-3.180068	-0.349084
C	-1.829657	-2.715990	-0.328284
C	1.737271	-2.127292	-0.168269
C	-2.919161	-0.465773	-0.097270
H	-0.136528	-4.192566	-0.454113
H	-2.786832	-3.240005	-0.412256
C	2.379547	-2.311459	1.084886
C	3.789200	-2.368478	1.084122
C	4.520633	-2.254932	-0.106761
C	3.855796	-2.082081	-1.329260
C	2.448006	-2.016512	-1.393017
C	1.610559	-2.440370	2.400607
H	4.323383	-2.512043	2.036435
H	5.620509	-2.310008	-0.082765
H	4.441412	-2.001883	-2.258586
C	1.752040	-1.813382	-2.739366
C	-3.444646	0.060240	-1.307105
C	-4.585237	0.884347	-1.210367
C	-5.175481	1.165049	0.029696
C	-4.635770	0.625016	1.205605
C	-3.496462	-0.205836	1.173805
C	-2.829477	-0.229943	-2.676902
H	-5.022513	1.308936	-2.127774
H	-6.068924	1.807188	0.080118
H	-5.111768	0.850581	2.172649
C	-2.921063	-0.762821	2.476529
H	0.526208	-2.428096	2.162543
C	1.885621	-1.235842	3.327014
C	1.907186	-3.779371	3.109608
H	0.657811	-1.901733	-2.572868
C	2.014067	-0.392103	-3.284690
C	2.145526	-2.896066	-3.766248
H	-1.963567	-0.907989	-2.524612
C	-3.825508	-0.957434	-3.605842
C	-2.284250	1.057857	-3.330961
H	-2.109158	-1.473235	2.213231
C	-2.284380	0.365282	3.318133
C	-3.970388	-1.551342	3.287775
H	1.295137	-1.321180	4.262883
H	2.957214	-1.180044	3.613058
H	1.611844	-0.279159	2.833864
H	1.284580	-3.879177	4.022769
H	1.692382	-4.647614	2.453305
H	2.969180	-3.852098	3.424734
H	1.469297	-0.231905	-4.238427
H	1.677388	0.380644	-2.560831
H	3.094421	-0.228956	-3.484391
H	1.570540	-2.764006	-4.706127
H	3.222546	-2.843534	-4.030040
H	1.943724	-3.917331	-3.383066
H	-3.340891	-1.214304	-4.570694
H	-4.200051	-1.897447	-3.150975
H	-4.707473	-0.323712	-3.836347
H	-1.799898	0.826124	-4.302441
H	-3.094678	1.790419	-3.529969
H	-1.531740	1.549213	-2.679485
H	-1.828680	-0.044653	4.243544
H	-1.490528	0.890331	2.745276
H	-3.042312	1.118220	3.621009
H	-3.502141	-2.008164	4.184224
H	-4.793610	-0.897989	3.645618
H	-4.425200	-2.366078	2.687799
Au	0.246858	0.982164	0.138138
C	2.220901	3.138167	0.441306
C	0.905280	2.937675	0.376781
C	3.330661	5.427210	-0.356167
O	2.664525	4.692189	0.727022
C	-0.153750	4.011635	0.481038
C	3.476248	2.345691	0.417224
H	1.795995	5.122655	0.932254
H	3.449827	6.473186	-0.016819
H	4.322742	4.963542	-0.490391
H	2.734790	5.363917	-1.287399
H	3.198859	1.276325	0.344239
H	4.122195	2.579400	-0.456627
H	4.072141	2.490576	1.343055
H	0.201665	5.073663	0.562927
H	-0.816562	3.992600	-0.408870
H	-0.807240	3.830173	1.359386

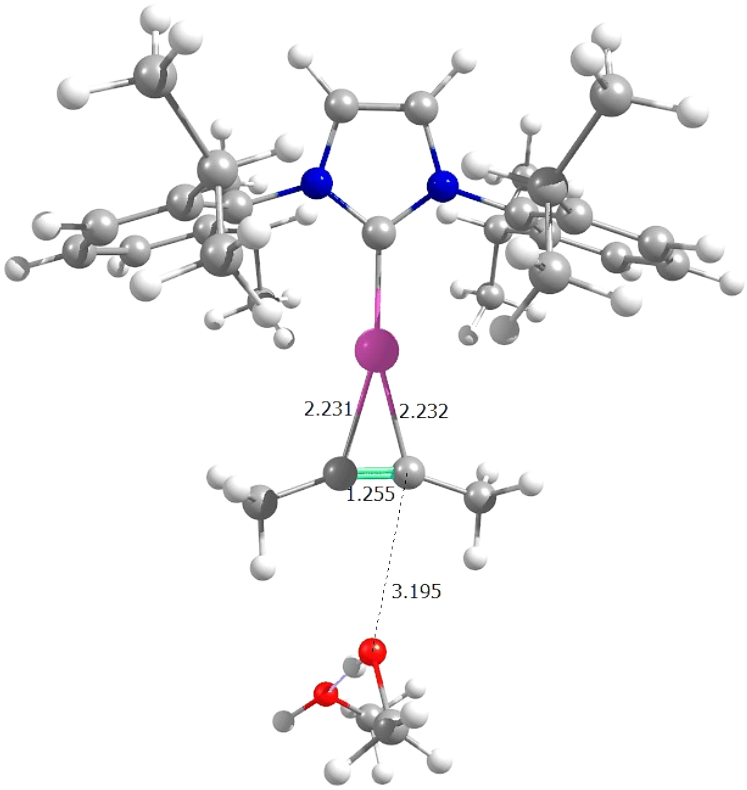
REAL-MeCCMe-MeOH-I+MeOH



Zero-point correction= 0.741463 (Hartree/Particle)
Thermal correction to Energy= 0.788905
Thermal correction to Enthalpy= 0.789849
Thermal correction to Gibbs Free Energy= 0.653847
Sum of electronic and zero-point Energies= -1681.361177
Sum of electronic and thermal Energies= -1681.313736
Sum of electronic and thermal Enthalpies= -1681.312792
Sum of electronic and thermal Free Energies= -1681.448794

C	1.283711	0.382199	0.171970
N	1.676032	1.680403	0.382002
N	2.437967	-0.351383	0.285608
C	3.046934	1.755238	0.622312
C	3.527968	0.471999	0.561002
C	0.794324	2.831879	0.357503
C	2.524886	-1.790918	0.132673
H	3.551221	2.707679	0.812941
H	4.539407	0.072992	0.686135
C	0.180555	3.243260	1.570438
C	-0.656399	4.377537	1.518570
C	-0.867787	5.070330	0.318130
C	-0.243877	4.641662	-0.861922
C	0.604866	3.514849	-0.873157
C	0.377467	2.499415	2.892019
H	-1.147904	4.727900	2.439816
H	-1.521075	5.957064	0.303285
H	-0.414689	5.197494	-1.797287
C	1.261487	3.068526	-2.180279
C	2.778999	-2.321064	-1.159958
C	2.867915	-3.724034	-1.275707
C	2.716438	-4.556667	-0.158020
C	2.473038	-4.001953	1.106290
C	2.372460	-2.606482	1.285124
C	2.940831	-1.441831	-2.400946
H	3.063319	-4.172489	-2.262569
H	2.794463	-5.649363	-0.272769
H	2.361163	-4.667037	1.977161
C	2.103567	-2.032697	2.677011
H	1.147110	1.716100	2.728693
C	-0.920889	1.777824	3.315802
C	0.900604	3.427771	4.008401
H	1.944215	2.224931	-1.946936
C	0.205462	2.535410	-3.172764
C	2.117893	4.188500	-2.808632
H	2.917257	-0.381763	-2.071908
C	4.297884	-1.673185	-3.098633
C	1.759902	-1.638008	-3.376677
H	2.098505	-0.925762	2.592063
C	0.710496	-2.453540	3.192557
C	3.216816	-2.410385	3.677629
H	-0.758936	1.200350	4.249985
H	-1.741255	2.501775	3.506738
H	-1.261103	1.073226	2.527203
H	1.101752	2.846681	4.932280
H	1.841705	3.934892	3.712178
H	0.162916	4.215090	4.269535
H	0.690652	2.176310	-4.104244
H	-0.363653	1.690060	-2.731348
H	-0.518906	3.328001	-3.456071
H	2.636040	3.815669	-3.716452
H	1.499928	5.058151	-3.116247
H	2.889651	4.559539	-2.103290
H	4.416739	-0.975947	-3.953877
H	5.148502	-1.511430	-2.405031
H	4.384281	-2.704491	-3.500249
H	1.864852	-0.967443	-4.254994
H	1.714792	-2.681106	-3.755067
H	0.792342	-1.410076	-2.881508
H	0.505935	-1.994863	4.182559
H	-0.086825	-2.131456	2.490162
H	0.637745	-3.555120	3.313197
H	3.033965	-1.930746	4.661704
H	3.262681	-3.506612	3.847189
H	4.215708	-2.086103	3.320245
Au	-0.598390	-0.311659	-0.230348
C	-3.521919	-0.226697	-0.753554
C	-2.476708	-1.069248	-0.647860
C	-5.301699	-1.051694	-2.390493
O	-4.916095	-0.801154	-1.008082
C	-2.584386	-2.570593	-0.818605
C	-3.654727	1.258149	-0.642614
H	-5.169939	-1.587173	-0.323520
O	-5.567550	-2.585331	0.598355
H	-4.816386	-3.114586	0.934055
C	-6.483222	-2.271237	1.673933
H	-6.356418	-1.384816	-2.381936
H	-5.211992	-0.096913	-2.939514
H	-4.646233	-1.819862	-2.845238
H	-5.991444	-1.675432	2.470780
H	-7.306778	-1.681371	1.231264
H	-6.901041	-3.205233	2.099980
H	-4.313175	1.552600	0.203186
H	-2.653544	1.700784	-0.480147
H	-4.082287	1.711010	-1.564409
H	-3.593760	-2.957081	-1.087717
H	-1.886862	-2.916957	-1.610461
H	-2.246009	-3.093174	0.103231

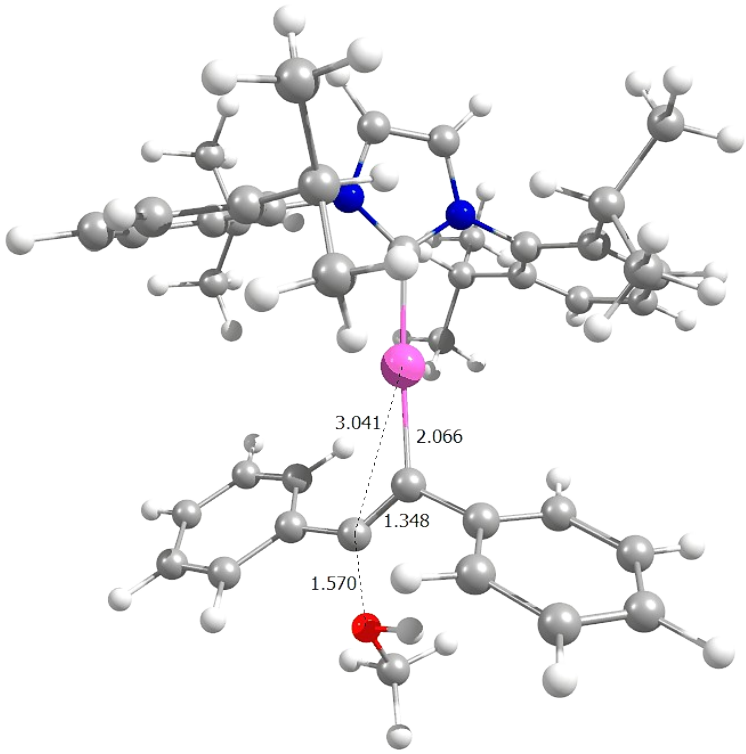
REAL-MeCCMe-MeOH-RC+MeOH



Zero-point correction= 0.738984 (Hartree/Particle)
Thermal correction to Energy= 0.789060
Thermal correction to Enthalpy= 0.790004
Thermal correction to Gibbs Free Energy= 0.644730
Sum of electronic and zero-point Energies= -1681.367601
Sum of electronic and thermal Energies= -1681.317524
Sum of electronic and thermal Enthalpies= -1681.316580
Sum of electronic and thermal Free Energies= -1681.461854

C	1.471582	-0.042111	0.125253
N	2.327376	1.020860	0.225129
N	2.251880	-1.155437	0.276467
C	3.630635	0.577557	0.437071
C	3.583457	-0.793717	0.468098
C	1.939729	2.417378	0.129723
C	1.769994	-2.525434	0.234131
H	4.467548	1.274576	0.544057
H	4.370796	-1.541280	0.605982
C	1.635376	3.117088	1.328077
C	1.281513	4.477003	1.205123
C	1.234548	5.105535	-0.047170
C	1.545235	4.386829	-1.209956
C	1.910032	3.025304	-1.153591
C	1.693647	2.466309	2.711394
H	1.042775	5.056533	2.110743
H	0.958559	6.169456	-0.117101
H	1.510549	4.896018	-2.185813
C	2.259679	2.277153	-2.440920
C	1.763326	-3.200278	-1.015719
C	1.299085	-4.532164	-1.023491
C	0.868387	-5.158661	0.154567
C	0.893142	-4.465235	1.372768
C	1.346730	-3.131627	1.446880
C	2.219301	-2.543075	-2.319493
H	1.279586	-5.090393	-1.972370
H	0.514619	-6.201207	0.123828
H	0.557175	-4.971517	2.291309
C	1.371137	-2.407713	2.793701
H	1.944074	1.393019	2.574709
C	0.327151	2.523726	3.426881
C	2.808636	3.090901	3.579188
H	2.523721	1.233735	-2.167950
C	1.049089	2.204901	-3.396190
C	3.492624	2.894162	-3.136426
H	2.615911	-1.535336	-2.073788
C	3.363812	-3.329996	-2.993593
C	1.030657	-2.339036	-3.284367
H	1.761102	-1.382006	2.622905
C	-0.049571	-2.260569	3.380053
C	2.325647	-3.099792	3.791228
H	0.377613	1.998065	4.402928
H	0.013892	3.568968	3.630828
H	-0.468125	2.042672	2.820376
H	2.872511	2.576464	4.560424
H	3.801416	3.016891	3.089687
H	2.614418	4.165688	3.777875
H	1.302172	1.616623	-4.302503
H	0.176681	1.723333	-2.906574
H	0.734156	3.214671	-3.733250
H	3.771406	2.300461	-4.031655
H	3.293538	3.932019	-3.476234
H	4.371759	2.926755	-2.460630
H	3.723424	-2.791909	-3.894887
H	4.226529	-3.466150	-2.309739
H	3.033750	-4.337762	-3.321541
H	1.363181	-1.827426	-4.211396
H	0.577843	-3.308256	-3.581512
H	0.235185	-1.719723	-2.818234
H	-0.020660	-1.687984	4.330296
H	-0.723681	-1.726913	2.677593
H	-0.504645	-3.248596	3.602134
H	2.379516	-2.525687	4.739411
H	1.981122	-4.124593	4.043030
H	3.354129	-3.184002	3.384069
Au	-0.531697	0.022855	-0.181836
C	-2.654984	0.695252	-0.329563
C	-2.642339	-0.513230	-0.668781
C	-6.524047	0.516175	-2.171395
O	-5.731502	0.204592	-1.037342
C	-3.090582	-1.840316	-1.106396
C	-3.128215	2.051282	-0.028494
H	-6.353872	-0.059988	-0.308749
O	-7.535446	-0.540661	0.897671
H	-8.053319	-1.349316	0.724650
C	-8.371589	0.403017	1.571202
H	-7.206549	1.384113	-2.003067
H	-5.846833	0.786912	-3.008003
H	-7.150211	-0.341998	-2.516615
H	-8.700836	0.029373	2.566470
H	-7.767218	1.317098	1.730741
H	-9.271211	0.681444	0.976744
H	-4.226527	2.022867	-0.207166
H	-2.931122	2.339073	1.023700
H	-2.666058	2.809884	-0.691523
H	-4.189461	-1.741723	-1.254063
H	-2.617416	-2.146526	-2.060825
H	-2.884980	-2.621060	-0.346842

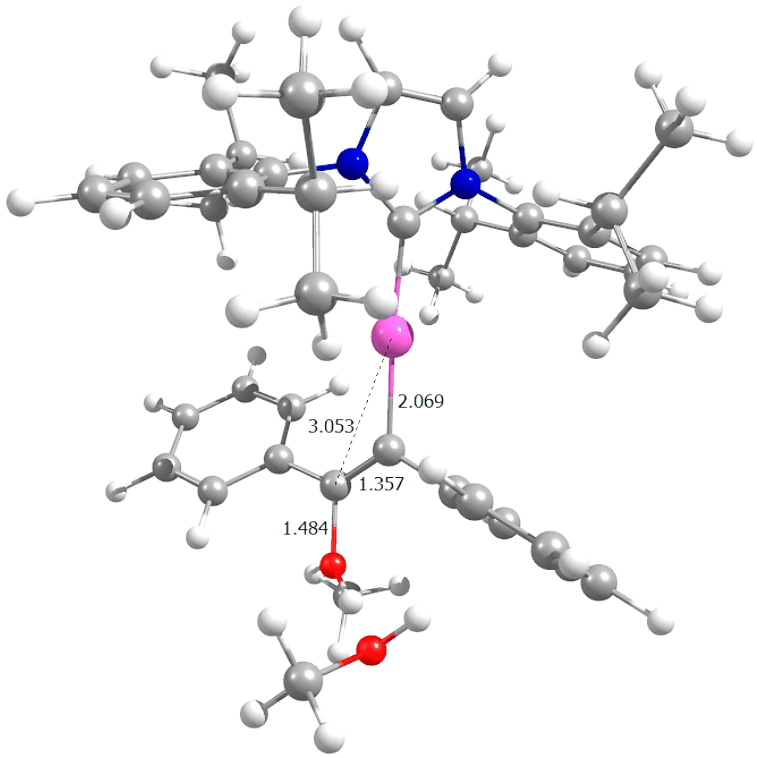
REAL-MeOH-I



Zero-point correction= 0.793823 (Hartree/Particle)
Thermal correction to Energy= 0.843139
Thermal correction to Enthalpy= 0.844083
Thermal correction to Gibbs Free Energy= 0.704026
Sum of electronic and zero-point Energies= -1948.855352
Sum of electronic and thermal Energies= -1948.806036
Sum of electronic and thermal Enthalpies= -1948.805092
Sum of electronic and thermal Free Energies= -1948.945149

C	1.475810	-0.740721	-0.078895
N	1.742865	-1.955949	-0.659084
N	2.686919	-0.313525	0.406321
C	3.093502	-2.276546	-0.541015
C	3.688939	-1.241732	0.133619
C	0.771416	-2.814227	-1.312550
C	2.918989	0.937644	1.102856
H	3.504969	-3.204864	-0.948853
H	4.726497	-1.081671	0.442482
C	0.443484	-2.562357	-2.670995
C	-0.488775	-3.428275	-3.280053
C	-1.055356	-4.499212	-2.575740
C	-0.698713	-4.730876	-1.239975
C	0.222086	-3.896307	-0.573682
C	1.064328	-1.423727	-3.481843
H	-0.769539	-3.262959	-4.332082
H	-1.776998	-5.164836	-3.074956
H	-1.143988	-5.580952	-0.700023
C	0.614171	-4.194794	0.874546
C	2.753932	0.971235	2.512968
C	3.015659	2.194619	3.164402
C	3.428215	3.326238	2.446725
C	3.588464	3.258767	1.055516
C	3.339565	2.064327	0.347682
C	2.313186	-0.247061	3.325077
H	2.901375	2.258981	4.257994
H	3.634718	4.268420	2.978660
H	3.920444	4.152790	0.504360
C	3.542772	2.018302	-1.167271
H	1.774547	-0.884048	-2.820958
C	-0.002503	-0.401670	-3.928389
C	1.872499	-1.960253	-4.683391
H	1.215633	-3.338567	1.246510
C	-0.616043	-4.316232	1.796503
C	1.501224	-5.457199	0.961264
H	2.187367	-1.096974	2.621962
C	3.382031	-0.662328	4.358733
C	0.941634	-0.007396	3.991367
H	3.238443	1.010398	-1.519512
C	2.645391	3.041203	-1.894853
C	5.029576	2.205715	-1.541511
H	0.469392	0.436447	-4.482567
H	-0.756040	-0.864516	-4.600056
H	-0.538092	0.021364	-3.052078
H	2.368025	-1.125649	-5.221755
H	2.658494	-2.674664	-4.363068
H	1.221240	-2.485097	-5.413450
H	-0.295406	-4.438721	2.852147
H	-1.261880	-3.417371	1.730283
H	-1.238908	-5.198916	1.540802
H	1.816361	-5.643357	2.009167
H	0.954691	-6.357370	0.609319
H	2.417125	-5.362576	0.342366
H	3.069043	-1.583273	4.893319
H	4.360536	-0.863982	3.876508
H	3.542819	0.126073	5.123805
H	0.605968	-0.917375	4.531243
H	0.983574	0.821441	4.728987
H	0.173016	0.250629	3.232478
H	2.760623	2.944035	-2.994469
H	1.575114	2.889169	-1.645000
H	2.912327	4.085012	-1.626742
H	5.169041	2.113673	-2.638735
H	5.402078	3.207578	-1.240997
H	5.676048	1.449199	-1.050902
Au	-0.289500	0.289419	-0.029206
C	-3.224073	1.026862	0.269529
C	-2.000596	1.444792	-0.113646
C	-4.965650	2.740785	1.113443
O	-4.383175	2.037929	-0.043306
C	-1.867241	2.805151	-0.713223
C	-1.122368	3.821834	-0.061529
C	-2.535604	3.136831	-1.927958
C	-1.068730	5.119581	-0.591030
H	-0.585187	3.577989	0.867914
C	-2.467272	4.443825	-2.458323
H	-3.040125	2.341752	-2.505037
C	-1.742659	5.439217	-1.787284
H	-0.488674	5.894615	-0.065399
H	-2.973913	4.671368	-3.409516
H	-1.688591	6.458946	-2.198438
C	-3.797640	-0.141725	0.946935
C	-5.055155	-0.671776	0.557400
C	-3.100895	-0.751734	2.020069
C	-5.594013	-1.783992	1.220927
H	-5.604749	-0.216323	-0.280629
C	-3.645734	-1.865296	2.676573
H	-2.132642	-0.334327	2.335642
C	-4.892428	-2.384056	2.282039
H	-6.567207	-2.189268	0.902821
H	-3.099641	-2.322292	3.516243
H	-5.320106	-3.253269	2.805516
H	-3.930751	2.701743	-0.673289
H	-5.760624	3.398439	0.716927
H	-5.394373	1.962278	1.767765
H	-4.177187	3.315054	1.636275

REAL-MeOH-I+MeOH

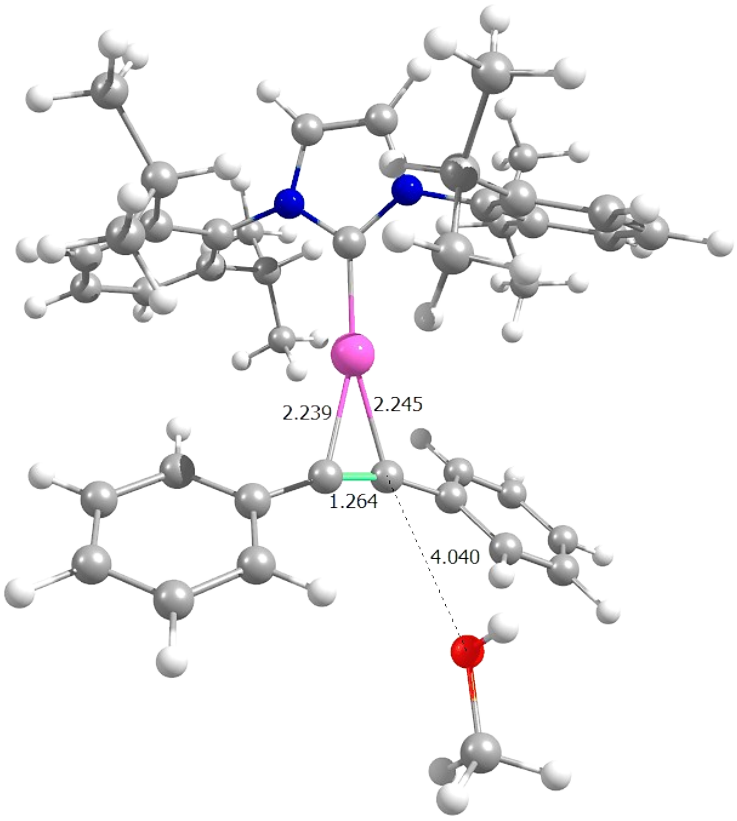


Zero-point correction= 0.844575 (Hartree/Particle)
Thermal correction to Energy= 0.897794
Thermal correction to Enthalpy= 0.898738
Thermal correction to Gibbs Free Energy= 0.751354
Sum of electronic and zero-point Energies= -2064.468426
Sum of electronic and thermal Energies= -2064.415207
Sum of electronic and thermal Enthalpies= -2064.414262
Sum of electronic and thermal Free Energies= -2064.561646

C	-1.803785	0.126849	0.238852
N	-2.587812	-0.770037	0.923774
N	-2.665305	1.137693	-0.113736
C	-3.906131	-0.324938	0.998340
C	-3.955747	0.876931	0.340655
C	-2.138974	-2.024917	1.496391
C	-2.308209	2.329674	-0.860807
H	-4.682685	-0.899434	1.512285
H	-4.786108	1.564683	0.153796
C	-1.540364	-2.014679	2.783892
C	-1.140638	-3.256225	3.320895
C	-1.337448	-4.451151	2.615613
C	-1.945691	-4.430365	1.352826
C	-2.363299	-3.220210	0.761695
C	-1.349924	-0.737295	3.602998
H	-0.673948	-3.286931	4.318214
H	-1.021125	-5.409198	3.057355
H	-2.103260	-5.376669	0.812630
C	-3.066128	-3.235927	-0.597310
C	-2.355380	2.282434	-2.279138
C	-2.045948	3.469439	-2.975505
C	-1.713222	4.647109	-2.292178
C	-1.679503	4.662762	-0.890821
C	-1.974474	3.506694	-0.139260
C	-2.740151	1.022855	-3.055480
H	-2.073280	3.471672	-4.076590
H	-1.482553	5.563840	-2.857484
H	-1.420665	5.595379	-0.365744
C	-1.957005	3.562139	1.389039
H	-1.673299	0.120177	2.976715
C	0.133845	-0.502579	3.954378
C	-2.235107	-0.746730	4.868697
H	-3.123651	-2.188083	-0.960859
C	-2.283074	-4.038043	-1.655737
C	-4.513009	-3.763492	-0.462990
H	-2.887947	0.203463	-2.321352
C	-4.073999	1.211901	-3.810515
C	-1.610104	0.576913	-4.006817
H	-2.061893	2.522734	1.764764
C	-0.620770	4.106432	1.934490
C	-3.154824	4.374231	1.930839
H	0.257071	0.459701	4.494281
H	0.533347	-1.304869	4.609868
H	0.754090	-0.471311	3.033960
H	-2.127907	0.206664	5.426994
H	-3.307678	-0.875867	4.616730
H	-1.952443	-1.571113	5.556601
H	-2.771721	-3.942414	-2.647776
H	-1.238379	-3.678651	-1.746767
H	-2.249612	-5.121058	-1.414037
H	-5.033542	-3.733498	-1.442927
H	-4.522736	-4.815335	-0.107508
H	-5.109120	-3.165400	0.256477
H	-4.365865	0.274378	-4.328166
H	-4.898034	1.492256	-3.122615
H	-3.996978	2.008047	-4.580441
H	-1.877558	-0.376198	-4.508913
H	-1.420757	1.327885	-4.802307
H	-0.661421	0.424377	-3.451508
H	-0.612322	4.063093	3.043674
H	0.240412	3.517654	1.557746
H	-0.458783	5.166769	1.647991
H	-3.160913	4.369632	3.040917
H	-3.107006	5.433002	1.599526
H	-4.124183	3.960649	1.584167
Au	0.214250	0.082021	-0.101857
C	3.045705	-0.806661	-0.818901
C	2.266469	0.193989	-0.335885
C	5.295386	-0.528345	-1.931734
O	4.520096	-0.682080	-0.709752
C	2.865285	1.484543	0.110315
C	3.405979	2.404124	-0.824367
C	2.893722	1.850712	1.486244
C	3.968653	3.623064	-0.405652
H	3.354576	2.165805	-1.898758
C	3.472027	3.067071	1.903478
H	2.424511	1.179708	2.224054
C	4.015863	3.958358	0.958717
H	4.373348	4.319939	-1.156830
H	3.479232	3.326336	2.974518
H	4.458390	4.912210	1.284213
C	2.697138	-2.097326	-1.452425
C	3.430966	-3.275705	-1.162480
C	1.649300	-2.171347	-2.402293
C	3.116853	-4.489985	-1.791503
H	4.251346	-3.238339	-0.429131
C	1.342468	-3.386525	-3.034516
H	1.089094	-1.257566	-2.652783
C	2.073033	-4.549792	-2.732110
H	3.691441	-5.396924	-1.545855
H	0.537533	-3.420953	-3.785043
H	1.834748	-5.500252	-3.234600
H	4.956114	-0.148318	0.227307
O	5.477861	0.407962	1.238704
H	4.822306	1.120042	1.491081
C	5.765178	-0.446255	2.373208

	H	6.361806	-0.561355	-1.640560
	H	5.058548	-1.373743	-2.604200
	H	5.053838	0.437896	-2.416503
	H	4.844452	-0.921085	2.770329
	H	6.467533	-1.225861	2.025617
	H	6.256293	0.153697	3.163482

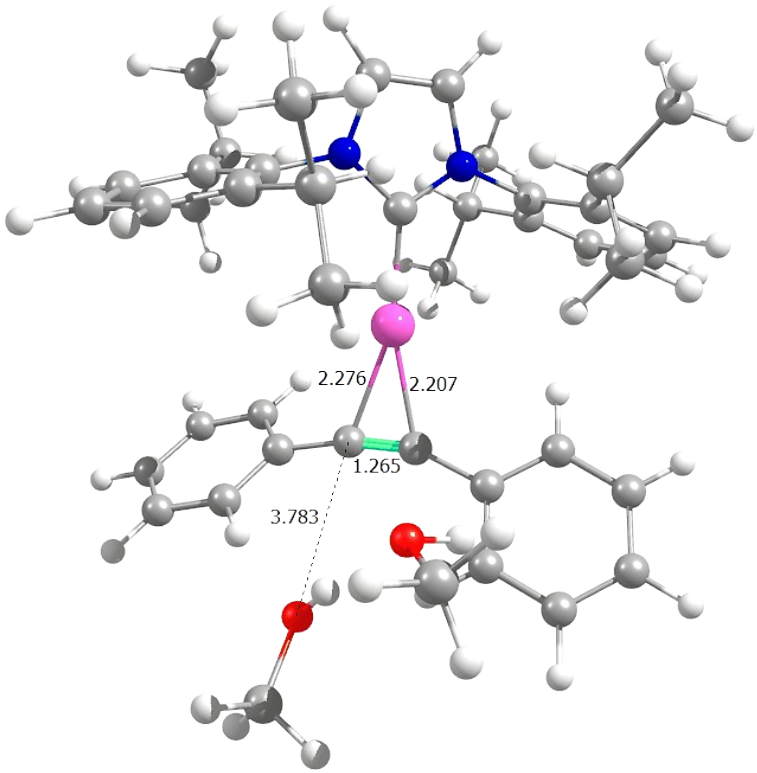
REAL-MeOH-RC



Zero-point correction= 0.791647 (Hartree/Particle)
Thermal correction to Energy= 0.843304
Thermal correction to Enthalpy= 0.844248
Thermal correction to Gibbs Free Energy= 0.695192
Sum of electronic and zero-point Energies= -1948.874004
Sum of electronic and thermal Energies= -1948.822348
Sum of electronic and thermal Enthalpies= -1948.821403
Sum of electronic and thermal Free Energies= -1948.970459

C	1.406089	-0.847208	0.301905
N	1.451467	-2.044738	0.965514
N	2.714223	-0.491250	0.105077
C	2.770473	-2.430734	1.181216
C	3.566207	-1.451929	0.639708
C	0.299843	-2.820599	1.394201
C	3.168873	0.727450	-0.541007
H	3.022813	-3.359204	1.702376
H	4.654771	-1.352594	0.587373
C	-0.147367	-3.880455	0.559734
C	-1.250035	-4.632239	1.014447
C	-1.873158	-4.343208	2.236782
C	-1.401767	-3.295325	3.038844
C	-0.299900	-2.508465	2.642674
C	0.545074	-4.248594	-0.754014
H	-1.627165	-5.463024	0.398683
H	-2.732523	-4.945840	2.570207
H	-1.894990	-3.086155	4.001052
C	0.204355	-1.390569	3.556474
C	3.482981	1.844920	0.278509
C	3.952497	3.004776	-0.372502
C	4.099829	3.047255	-1.766420
C	3.783950	1.924895	-2.544929
C	3.315374	0.732780	-1.953602
C	3.364718	1.816103	1.803581
H	4.213750	3.890574	0.226986
H	4.472831	3.963099	-2.251324
H	3.913067	1.970391	-3.637616
C	3.010836	-0.484225	-2.828227
H	1.201326	-3.398985	-1.041005
C	-0.450836	-4.463290	-1.911624
C	1.445874	-5.491757	-0.568316
H	1.071503	-0.906216	3.059350
C	-0.868902	-0.299937	3.759874
C	0.705552	-1.948607	4.906455
H	2.858358	0.869327	2.087656
C	4.759500	1.809096	2.468950
C	2.493538	2.969438	2.342365
H	2.640903	-1.294780	-2.165452
C	1.891648	-0.186169	-3.848345
C	4.286061	-1.008222	-3.524648
H	0.097258	-4.620695	-2.863517
H	-1.083793	-5.360724	-1.751356
H	-1.125733	-3.592791	-2.039394
H	1.979775	-5.733548	-1.510829
H	2.207323	-5.340858	0.224066
H	0.843333	-6.379657	-0.283463
H	-0.467061	0.531477	4.375342
H	-1.203779	0.120845	2.788562
H	-1.762625	-0.700115	4.283027
H	1.123331	-1.133206	5.532857
H	-0.116512	-2.421916	5.483227
H	1.498143	-2.712075	4.766328
H	4.664217	1.734135	3.572121
H	5.380207	0.957359	2.122180
H	5.319079	2.741221	2.243992
H	2.362437	2.872168	3.439956
H	2.958067	3.960240	2.156199
H	1.488243	2.974216	1.873556
H	1.649636	-1.095841	-4.436352
H	0.964933	0.155348	-3.341336
H	2.191617	0.603149	-4.568633
H	4.061433	-1.924859	-4.108540
H	4.703755	-0.259090	-4.229399
H	5.081028	-1.256535	-2.791769
Au	-0.234483	0.204359	-0.246828
C	-1.714340	1.853197	-0.571318
C	-2.250970	0.805149	-1.030159
C	-6.603866	2.908318	0.889623
O	-5.370324	2.221822	1.110395
C	-3.159715	-0.147361	-1.614757
C	-4.502058	-0.179416	-1.147741
C	-2.756125	-1.012782	-2.665122
C	-5.414944	-1.065619	-1.737460
H	-4.814697	0.505815	-0.341653
C	-3.683349	-1.890410	-3.242504
H	-1.718517	-0.975241	-3.030240
C	-5.012194	-1.921373	-2.779432
H	-6.456701	-1.086096	-1.380850
H	-3.369865	-2.551983	-4.064904
H	-5.737664	-2.612158	-3.236840
C	-1.452944	3.212951	-0.170875
C	-2.458615	3.910234	0.552910
C	-0.245203	3.872532	-0.518738
C	-2.247571	5.250944	0.905614
H	-3.397826	3.394256	0.815666
C	-0.054599	5.213284	-0.158063
H	0.530209	3.330247	-1.081210
C	-1.052025	5.904877	0.554132
H	-3.028756	5.794164	1.460195
H	0.878996	5.724544	-0.439094
H	-0.897768	6.958677	0.834218
H	-5.376226	1.880354	2.024851
H	-6.735126	3.779734	1.571320
H	-6.585980	3.287441	-0.150944
H	-7.488892	2.240183	0.997340

REAL-MeOH-RC+MeOH

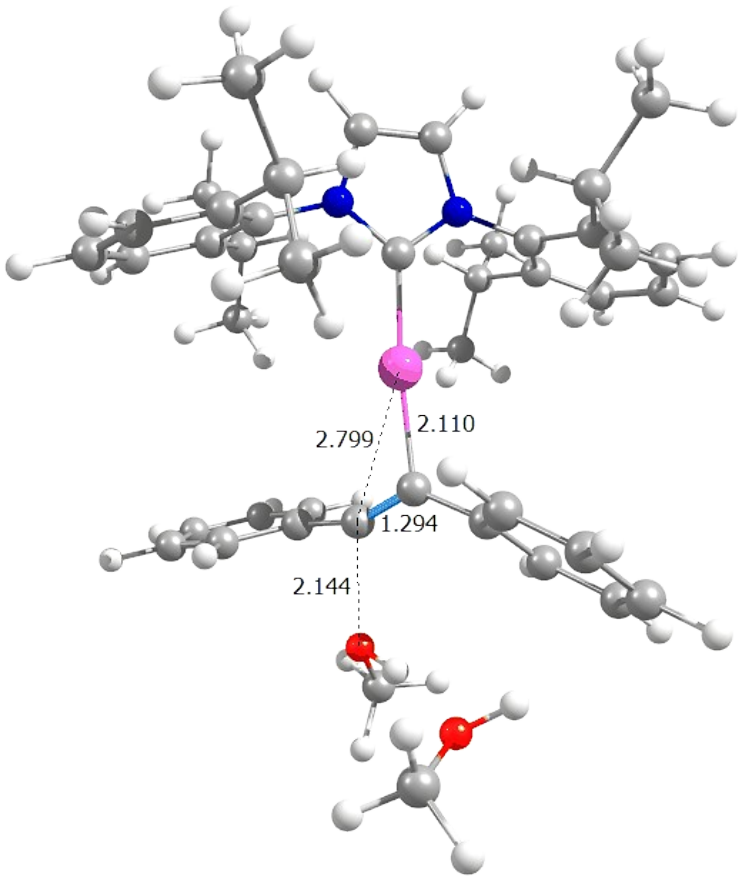


Zero-point correction= 0.843520 (Hartree/Particle)
Thermal correction to Energy= 0.899488
Thermal correction to Enthalpy= 0.900433
Thermal correction to Gibbs Free Energy= 0.742452
Sum of electronic and zero-point Energies= -2064.468775
Sum of electronic and thermal Energies= -2064.412806
Sum of electronic and thermal Enthalpies= -2064.411862
Sum of electronic and thermal Free Energies= -2064.569843

C	-1.751364	-0.241840	0.463969
N	-2.162198	-1.298996	1.230799
N	-2.818536	0.615812	0.424403
C	-3.469940	-1.104270	1.664658
C	-3.884042	0.102021	1.156888
C	-1.357449	-2.462261	1.563869
C	-2.831569	1.902905	-0.247454
H	-3.983575	-1.835574	2.296169
H	-4.833309	0.638398	1.252085
C	-0.472734	-2.377759	2.671256
C	0.285850	-3.527948	2.974270
C	0.157048	-4.703302	2.222496
C	-0.738294	-4.757833	1.144809
C	-1.519453	-3.640502	0.785788
C	-0.332696	-1.126212	3.539286
H	0.987198	-3.501942	3.822951
H	0.757394	-5.589366	2.481885
H	-0.833425	-5.689871	0.567042
C	-2.521891	-3.740274	-0.366029
C	-3.164748	1.947621	-1.627406
C	-3.169301	3.215680	-2.245564
C	-2.869981	4.378747	-1.522200
C	-2.560243	4.300848	-0.156675
C	-2.533684	3.062314	0.518043
C	-3.525260	0.702464	-2.438815
H	-3.423499	3.293093	-3.314288
H	-2.889020	5.357899	-2.026106
H	-2.340661	5.223845	0.402422
C	-2.208856	3.015213	2.012692
H	-1.005803	-0.344524	3.127801
C	1.101188	-0.559009	3.493499
C	-0.787171	-1.398434	4.990629
H	-2.830823	-2.707675	-0.636602
C	-1.914079	-4.376774	-1.632246
C	-3.790634	-4.505441	0.077570
H	-3.474467	-0.173902	-1.758879
C	-4.971038	0.779493	-2.976934
C	-2.511504	0.455164	-3.576430
H	-2.244507	1.954130	2.337443
C	-0.782079	3.527092	2.303162
C	-3.261690	3.781831	2.843061
H	1.169253	0.368523	4.098894
H	1.839356	-1.278621	3.904889
H	1.414779	-0.314880	2.457689
H	-0.731806	-0.469224	5.595018
H	-1.831268	-1.771272	5.031513
H	-0.142714	-2.155047	5.485091
H	-2.640122	-4.329055	-2.470077
H	-0.985633	-3.858709	-1.947223
H	-1.667654	-5.448023	-1.478817
H	-4.536309	-4.538315	-0.743855
H	-3.546159	-5.552344	0.354871
H	-4.275334	-4.035313	0.957736
H	-5.236340	-0.156456	-3.510841
H	-5.705839	0.926040	-2.158884
H	-5.096872	1.617564	-3.693830
H	-2.761178	-0.477538	-4.123772
H	-2.513768	1.284316	-4.314441
H	-1.478415	0.358027	-3.180504
H	-0.551799	3.436367	3.385043
H	-0.020865	2.949087	1.739599
H	-0.666759	4.596516	2.028680
H	-3.046830	3.684058	3.927396
H	-3.263058	4.865307	2.601165
H	-4.287101	3.399120	2.662206
Au	0.047067	0.038623	-0.426083
C	1.977679	-0.325145	-1.576011
C	1.929561	0.884198	-1.209415
C	6.751033	-0.377578	0.314384
O	5.351236	-0.228192	0.132232
C	2.349866	2.258533	-1.050141
C	3.739288	2.516740	-0.880001
C	1.434126	3.339382	-1.094624
C	4.187362	3.842602	-0.766706
H	4.444284	1.668007	-0.831448
C	1.901853	4.657261	-0.983906
H	0.360083	3.139302	-1.229712
C	3.275188	4.913836	-0.819584
H	5.264297	4.041416	-0.647292
H	1.186317	5.492658	-1.030580
H	3.636598	5.950763	-0.737441
C	2.300053	-1.628020	-2.086146
C	3.511349	-2.239707	-1.659945
C	1.467975	-2.278647	-3.036717
C	3.873036	-3.484785	-2.194223
H	4.157730	-1.710987	-0.936663
C	1.847334	-3.523111	-3.555191
H	0.539575	-1.791016	-3.370667
C	3.047356	-4.128508	-3.134607
H	4.814507	-3.957631	-1.873750
H	1.208283	-4.022730	-4.299648
H	3.342326	-5.105621	-3.548442
H	4.966507	0.186619	0.949101
O	4.127931	1.260615	2.123471
H	3.845593	1.995681	1.539807
C	4.776621	1.811114	3.272778

	H	7.007251	-1.054532	1.163996
	H	7.173387	-0.825933	-0.608151
	H	7.273918	0.594491	0.481832
	H	4.085782	2.439309	3.878151
	H	5.107146	0.962288	3.902585
	H	5.672430	2.418748	3.010520

REAL-MeOH-TS+MeOH

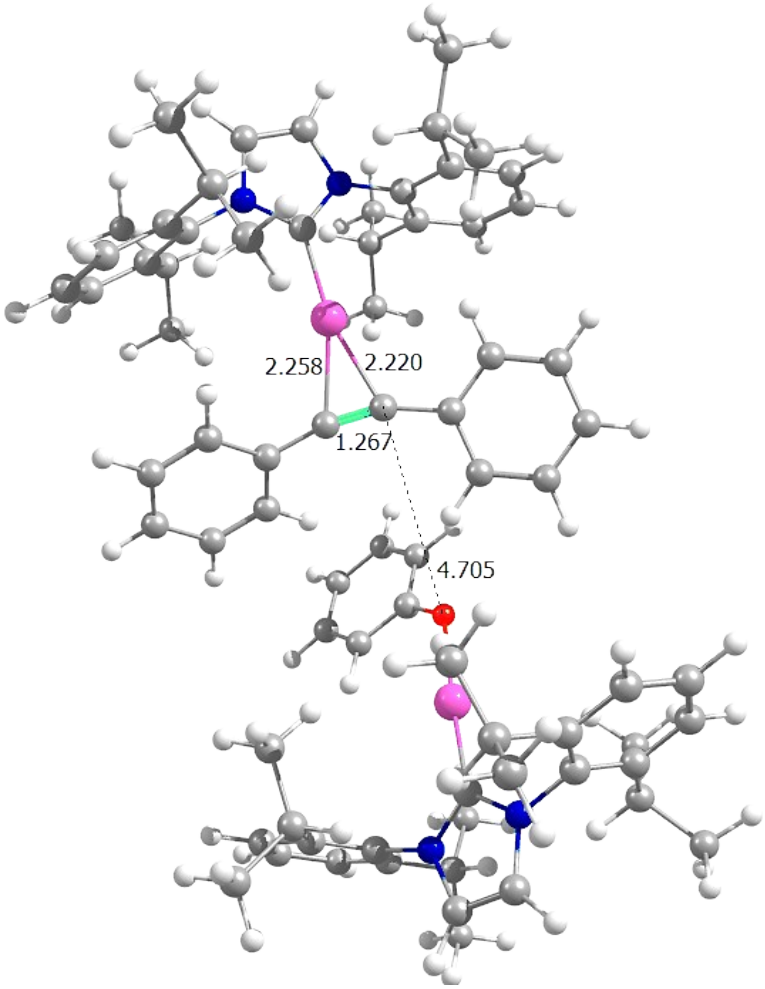


Zero-point correction= 0.843681 (Hartree/Particle)
Thermal correction to Energy= 0.898177
Thermal correction to Enthalpy= 0.899121
Thermal correction to Gibbs Free Energy= 0.745522
Sum of electronic and zero-point Energies= -2064.457326
Sum of electronic and thermal Energies= -2064.402829
Sum of electronic and thermal Enthalpies= -2064.401885
Sum of electronic and thermal Free Energies= -2064.555484

C	-1.930602	0.224373	0.143544
N	-2.805206	-0.639098	0.751889
N	-2.709741	1.257857	-0.310373
C	-4.108566	-0.153291	0.677345
C	-4.048271	1.042309	0.007290
C	-2.449182	-1.896990	1.382558
C	-2.225600	2.429506	-1.018169
H	-4.954400	-0.699471	1.106322
H	-4.830695	1.755000	-0.271303
C	-2.058565	-1.886446	2.747467
C	-1.739333	-3.128393	3.334831
C	-1.814104	-4.320458	2.600850
C	-2.212348	-4.297453	1.257079
C	-2.542232	-3.086880	0.613065
C	-1.970538	-0.605317	3.577585
H	-1.431759	-3.161918	4.391778
H	-1.564936	-5.278611	3.083534
H	-2.272710	-5.241744	0.693435
C	-2.984597	-3.096486	-0.850685
C	-2.117214	2.370745	-2.432845
C	-1.663320	3.531910	-3.092239
C	-1.339949	4.693870	-2.377769
C	-1.465170	4.721419	-0.981907
C	-1.912637	3.592065	-0.265146
C	-2.457471	1.118276	-3.241295
H	-1.566472	3.526078	-4.189289
H	-0.991566	5.589775	-2.915355
H	-1.212019	5.642515	-0.433896
C	-2.046435	3.658987	1.257020
H	-2.322787	0.235732	2.943952
C	-0.508371	-0.297904	3.966617
C	-2.888677	-0.658487	4.817305
H	-3.170034	-2.045615	-1.157065
C	-1.875372	-3.646227	-1.771621
C	-4.309147	-3.868413	-1.037259
H	-2.857186	0.357413	-2.538410
C	-3.553844	1.390093	-4.293178
C	-1.189228	0.517418	-3.885351
H	-2.387730	2.664368	1.613510
C	-0.687195	3.939533	1.932219
C	-3.113405	4.690110	1.685552
H	-0.444994	0.661355	4.521704
H	-0.084450	-1.091265	4.617630
H	0.132756	-0.221030	3.062555
H	-2.857731	0.306818	5.363954
H	-3.943211	-0.858989	4.537321
H	-2.574255	-1.450811	5.528272
H	-2.190433	-3.589801	-2.834486
H	-0.934183	-3.070049	-1.658140
H	-1.649104	-4.709934	-1.548894
H	-4.643448	-3.817994	-2.094412
H	-4.197166	-4.941255	-0.774387
H	-5.119750	-3.453521	-0.403445
H	-3.827935	0.451794	-4.818763
H	-4.473305	1.802829	-3.829642
H	-3.213818	2.112621	-5.064118
H	-1.431988	-0.421926	-4.424738
H	-0.735115	1.217956	-4.617443
H	-0.424321	0.287970	-3.113264
H	-0.794124	3.928628	3.037063
H	0.069905	3.179143	1.649350
H	-0.287831	4.935371	1.647603
H	-3.239609	4.684756	2.788239
H	-2.827070	5.720763	1.388397
H	-4.100736	4.473991	1.228052
Au	0.088329	0.065697	-0.022916
C	2.604445	-1.037086	-0.560210
C	2.194883	0.112325	-0.128307
C	5.476390	-1.161539	-1.626926
O	4.742358	-1.096474	-0.407676
C	2.891106	1.359936	0.243916
C	3.582415	2.107710	-0.740061
C	2.898775	1.815205	1.583977
C	4.294776	3.265177	-0.382243
H	3.557837	1.774079	-1.788578
C	3.621354	2.966529	1.938687
H	2.349337	1.247441	2.350368
C	4.327588	3.693388	0.959659
H	4.830511	3.836376	-1.156738
H	3.630351	3.302673	2.987547
H	4.886291	4.600633	1.238010
C	2.477635	-2.358698	-1.105280
C	2.759886	-3.499698	-0.306291
C	2.111398	-2.534151	-2.467937
C	2.661354	-4.782427	-0.857857
H	3.062556	-3.358919	0.741505
C	2.014434	-3.823792	-3.009083
H	1.899173	-1.648899	-3.086570
C	2.289818	-4.946933	-2.207045
H	2.878768	-5.664041	-0.235191
H	1.727437	-3.954925	-4.063886
H	2.218630	-5.958510	-2.636900
H	5.142825	-0.362059	0.165584
O	6.060824	0.714124	0.978997
H	5.704078	1.628250	0.983734
C	6.580999	0.399792	2.273903

	H	6.524101	-1.481360	-1.433724
	H	5.000918	-1.923170	-2.277799
	H	5.495764	-0.189992	-2.170106
	H	5.811145	0.486268	3.073050
	H	6.935062	-0.648778	2.240185
	H	7.445304	1.049772	2.532485

REAL-PhOH-I+II

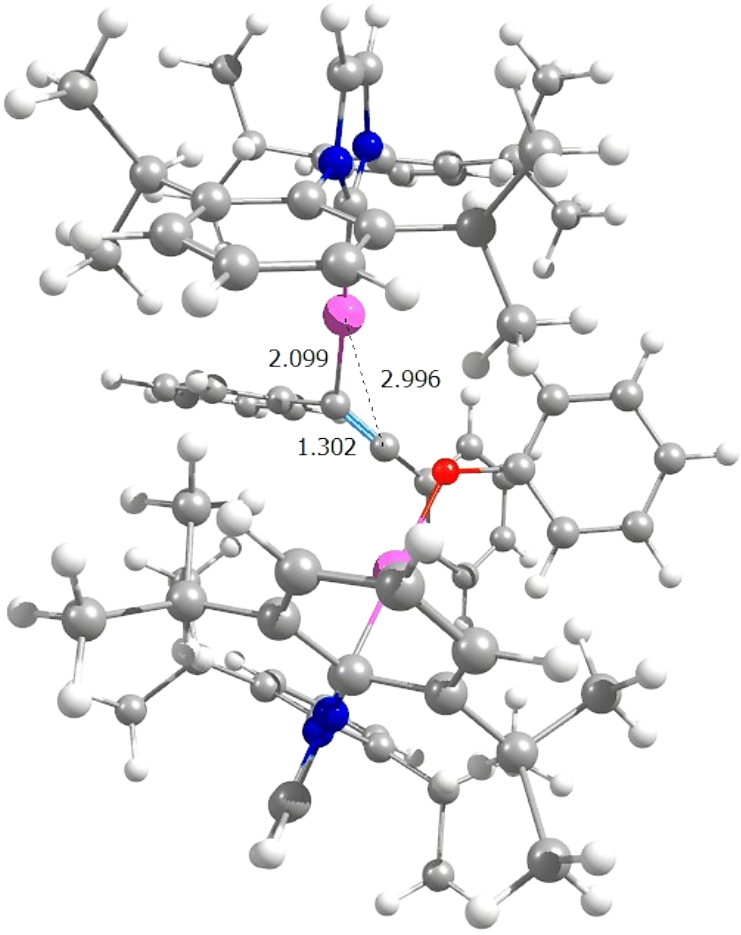


Zero-point correction= 1.385889 (Hartree/Particle)
Thermal correction to Energy= 1.474496
Thermal correction to Enthalpy= 1.475440
Thermal correction to Gibbs Free Energy= 1.249030
Sum of electronic and zero-point Energies= -3434.450039
Sum of electronic and thermal Energies= -3434.361432
Sum of electronic and thermal Enthalpies= -3434.360488
Sum of electronic and thermal Free Energies= -3434.586899

C	-6.074024	0.055985	0.106026
N	-6.895835	-0.883363	0.667899
N	-6.912191	0.991281	-0.439587
C	-8.231892	-0.542946	0.472038
C	-8.241853	0.638381	-0.225521
C	-6.457714	-2.069209	1.381007
C	-6.491299	2.197105	-1.130128
H	-9.047383	-1.169399	0.846201
H	-9.068201	1.256745	-0.589038
C	-6.207037	-1.962326	2.775228
C	-5.810204	-3.137300	3.447465
C	-5.685560	-4.356915	2.766590
C	-5.946868	-4.428523	1.391050
C	-6.338465	-3.287161	0.660644
C	-6.351382	-0.650657	3.549194
H	-5.607073	-3.096907	4.529131
H	-5.387842	-5.263674	3.316558
H	-5.847449	-5.393349	0.869775
C	-6.631379	-3.400319	-0.836398
C	-6.193433	2.117113	-2.516267
C	-5.804846	3.311526	-3.158657
C	-5.730916	4.523063	-2.458392
C	-6.040701	4.569271	-1.091329
C	-6.426278	3.408515	-0.389021
C	-6.284417	0.817239	-3.316555
H	-5.561075	3.290708	-4.232306
H	-5.432376	5.443125	-2.984864
H	-5.986532	5.529629	-0.555407
C	-6.791946	3.495403	1.094731
H	-6.742437	0.116946	2.848095
C	-4.983465	-0.146405	4.058639
C	-7.371022	-0.776392	4.701823
H	-6.842076	-2.379603	-1.220047
C	-5.415594	-3.935994	-1.621915
C	-7.890102	-4.258047	-1.095083
H	-6.630350	0.016123	-2.629465
C	-7.325139	0.924607	-4.452705
C	-4.902029	0.390410	-3.855980
H	-6.880823	2.459101	1.484917
C	-5.703096	4.197930	1.931957
C	-8.164241	4.182158	1.282556
H	-5.097927	0.822624	4.587368
H	-4.525742	-0.863734	4.771813
H	-4.269731	0.002775	3.221123
H	-7.511541	0.203970	5.202507
H	-8.361375	-1.120008	4.338731
H	-7.029351	-1.495259	5.475575
H	-5.635517	-3.948322	-2.709525
H	-4.514665	-3.309404	-1.460195
H	-5.160077	-4.974786	-1.326195
H	-8.120905	-4.292985	-2.180050
H	-7.745364	-5.303453	-0.750499
H	-8.780175	-3.854621	-0.569635
H	-7.420038	-0.045384	-4.983506
H	-8.327592	1.203207	-4.067478
H	-7.031322	1.686077	-5.205104
H	-4.974646	-0.582286	-4.385077
H	-4.497952	1.132625	-4.575730
H	-4.162495	0.280837	-3.034945
H	-5.971098	4.172480	3.008423
H	-4.714512	3.708700	1.815216
H	-5.588965	5.265782	1.651159
H	-8.448391	4.202419	2.355219
H	-8.138545	5.231406	0.920566
H	-8.969641	3.659092	0.726992
Au	-4.047628	0.042419	0.037306
C	-1.902982	-0.665056	0.022790
C	-1.905866	0.585866	-0.176127
C	6.125248	0.174443	0.584767
N	7.030366	-0.857204	0.648879
N	6.688634	1.181861	1.331007
C	8.136592	-0.498990	1.418149
C	7.921316	0.784890	1.848087
C	6.865550	-2.148763	0.012279
C	6.100343	2.488290	1.552105
H	8.969849	-1.187689	1.587779
H	8.528060	1.450356	2.469708
C	7.358759	-2.323865	-1.307398
C	7.206361	-3.600100	-1.888460
C	6.594027	-4.648968	-1.188722
C	6.115860	-4.443759	0.113227
C	6.241043	-3.190614	0.747905
C	8.026828	-1.199533	-2.099744
H	7.574220	-3.773754	-2.912025
H	6.488733	-5.637322	-1.663528
H	5.635378	-5.275661	0.652049
C	5.689787	-2.989099	2.160069
C	5.272134	2.676993	2.689632
C	4.734723	3.965065	2.891406
C	5.012577	5.015228	2.005333
C	5.834335	4.797245	0.890865
C	6.400303	3.530824	0.635998
C	4.940556	1.550159	3.668664
H	4.086587	4.147334	3.763146
H	4.585442	6.014396	2.186086
H	6.044627	5.629439	0.200773

	C	7.276402	3.321946	-0.599926
	H	8.022189	-0.289062	-1.464446
	C	7.232942	-0.863439	-3.380295
	C	9.501667	-1.530182	-2.416261
	H	5.995779	-1.978215	2.502444
	C	4.145677	-3.017182	2.156141
	C	6.274435	-4.004688	3.163851
	H	5.505153	0.648626	3.351102
	C	5.386987	1.887458	5.107199
	C	3.440344	1.189609	3.609223
	H	7.677335	2.287279	-0.560732
	C	6.439323	3.435236	-1.892992
	C	8.486598	4.279409	-0.620762
	H	7.698640	-0.006265	-3.909858
	H	7.215496	-1.719967	-4.086577
	H	6.182004	-0.594661	-3.146676
	H	9.984814	-0.683342	-2.946911
	H	10.084415	-1.732128	-1.493729
	H	9.589167	-2.424291	-3.068963
	H	3.749305	-2.820029	3.174385
	H	3.733261	-2.248277	1.469486
	H	3.761010	-4.006815	1.830461
	H	5.913148	-3.785989	4.190405
	H	5.970157	-5.045142	2.923410
	H	7.383496	-3.974988	3.178772
	H	5.191079	1.030538	5.785126
	H	6.470536	2.121113	5.156680
	H	4.837209	2.762528	5.513470
	H	3.217011	0.338375	4.286085
	H	2.805219	2.044541	3.924018
	H	3.139684	0.902344	2.580434
	H	7.070236	3.235737	-2.784259
	H	5.601624	2.706811	-1.892677
	H	6.008048	4.452119	-2.008522
	H	9.134912	4.062263	-1.494987
	H	8.171266	5.340966	-0.700813
	H	9.104358	4.181455	0.295735
	Au	4.406492	0.201045	-0.393987
	C	2.197803	-0.568238	-2.283181
	C	1.153706	-0.212006	-3.187697
	C	2.708707	-1.895749	-2.360891
	C	0.653276	-1.140418	-4.114489
	H	0.767444	0.818775	-3.159118
	C	2.204029	-2.812887	-3.296978
	H	3.520661	-2.184105	-1.671396
	C	1.167922	-2.450440	-4.179529
	H	-0.143810	-0.829249	-4.810294
	H	2.635051	-3.827222	-3.341280
	H	0.780986	-3.169861	-4.917688
	O	2.629625	0.345937	-1.405658
	C	-1.410415	1.929601	-0.356217
	C	-2.267195	3.059385	-0.374104
	C	-0.010396	2.105817	-0.531774
	C	-1.733136	4.343635	-0.545906
	H	-3.353875	2.920806	-0.262283
	C	0.505513	3.397590	-0.709473
	H	0.680138	1.246390	-0.550131
	C	-0.346652	4.516964	-0.712359
	H	-2.405996	5.214947	-0.556988
	H	1.590392	3.518213	-0.852359
	H	0.069054	5.527305	-0.852378
	C	-1.611969	-2.068475	0.138267
	C	-2.210484	-2.872921	1.145212
	C	-0.676538	-2.646577	-0.763665
	C	-1.870707	-4.227487	1.250110
	H	-2.937022	-2.424763	1.840154
	C	-0.344849	-4.003085	-0.638864
	H	-0.210575	-2.031611	-1.549058
	C	-0.937824	-4.795018	0.361183
	H	-2.335218	-4.844407	2.034596
	H	0.386299	-4.435626	-1.338612
	H	-0.672375	-5.860409	0.449477

REAL-PhOH-I+II--IVcis

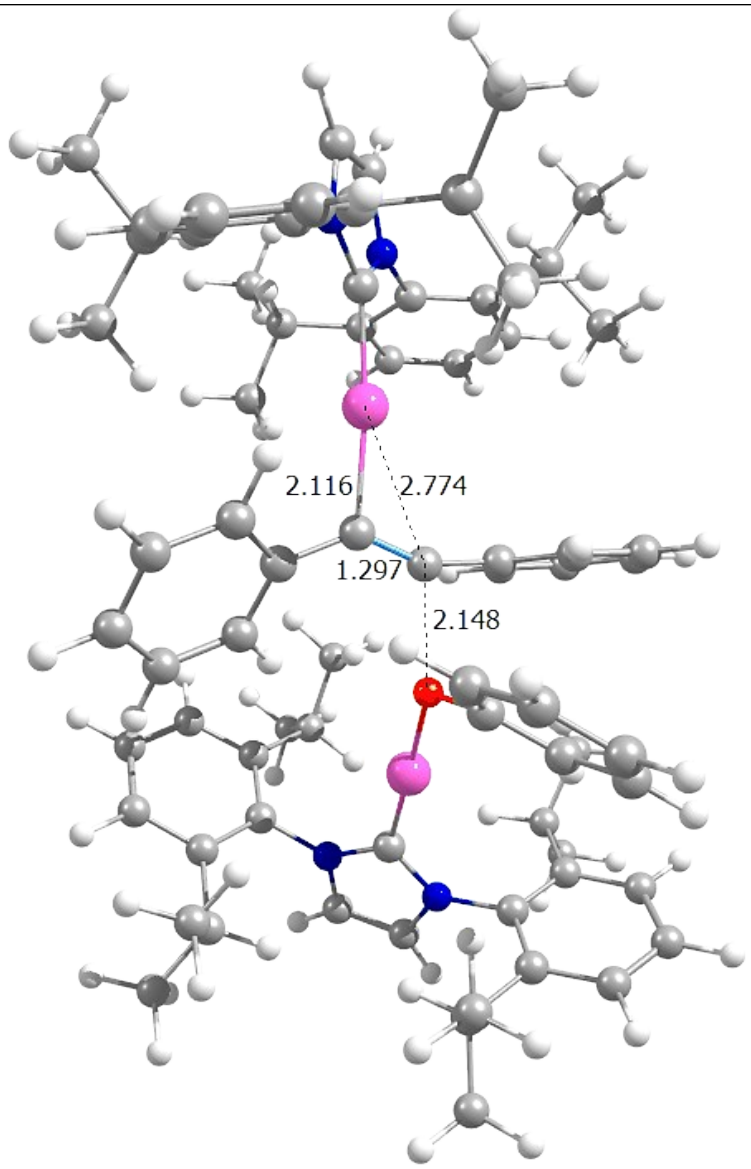


Zero-point correction= 1.385821 (Hartree/Particle)
Thermal correction to Energy= 1.473158
Thermal correction to Enthalpy= 1.474102
Thermal correction to Gibbs Free Energy= 1.247556
Sum of electronic and zero-point Energies= -3434.416671
Sum of electronic and thermal Energies= -3434.329335
Sum of electronic and thermal Enthalpies= -3434.328390
Sum of electronic and thermal Free Energies= -3434.554937

C	3.991943	0.905740	0.171041
N	4.143226	2.270936	0.135323
N	5.240692	0.431822	0.509228
C	5.452263	2.637261	0.445727
C	6.142810	1.478348	0.678775
C	3.151522	3.268880	-0.219675
C	5.629376	-0.962913	0.624490
H	5.766877	3.684987	0.467548
H	7.190031	1.302010	0.941346
C	2.360728	3.841063	0.810698
C	1.514378	4.911687	0.454412
C	1.463284	5.390775	-0.861555
C	2.240609	4.790763	-1.862062
C	3.104632	3.715996	-1.567556
C	2.409175	3.359590	2.259961
H	0.892160	5.384852	1.229859
H	0.815701	6.246396	-1.110622
H	2.186444	5.171610	-2.894058
C	3.938615	3.085306	-2.683817
C	6.079470	-1.635609	-0.542609
C	6.481778	-2.979835	-0.397535
C	6.451801	-3.616330	0.850143
C	6.025796	-2.917398	1.988462
C	5.607211	-1.573304	1.907361
C	6.200426	-0.946107	-1.902021
H	6.832680	-3.535094	-1.281070
H	6.773719	-4.665920	0.939231
H	6.023263	-3.425716	2.964665
C	5.215271	-0.808844	3.172957
H	3.109196	2.499277	2.306811
C	1.028638	2.850379	2.724993
C	2.959162	4.452287	3.202614
H	4.573560	2.296243	-2.230616
C	3.031892	2.391282	-3.722682
C	4.883449	4.108519	-3.349529
H	5.669147	0.026829	-1.837787
C	7.681483	-0.644344	-2.226896
C	5.532440	-1.749829	-3.034077
H	4.631838	0.083350	2.859445
C	4.321247	-1.632641	4.119035
C	6.473741	-0.305750	3.918754
H	1.090921	2.448766	3.757381
H	0.272901	3.663737	2.729381
H	0.651987	2.040729	2.067315
H	3.031886	4.067594	4.241185
H	3.968762	4.794165	2.894054
H	2.296688	5.343256	3.224379
H	3.644377	1.880919	-4.494929
H	2.381544	1.633852	-3.238451
H	2.376469	3.120817	-4.243178
H	5.510680	3.613453	-4.119732
H	4.319665	4.920894	-3.854262
H	5.561852	4.582373	-2.610545
H	7.767040	-0.099539	-3.190345
H	8.159644	-0.023876	-1.441052
H	8.271339	-1.580961	-2.316282
H	5.575921	-1.179921	-3.985496
H	6.043364	-2.718913	-3.213132
H	4.467913	-1.960857	-2.809018
H	3.987509	-1.004002	4.970331
H	3.420293	-2.018644	3.601227
H	4.862825	-2.498707	4.553477
H	6.188991	0.284290	4.814928
H	7.100677	-1.157136	4.258184
H	7.108343	0.338922	3.277470
Au	2.375787	-0.273000	-0.240965
C	0.170333	-2.268745	0.118164
C	1.037059	-1.811189	-0.738509
C	-4.047984	0.619420	-0.569770
N	-4.521621	1.906401	-0.635873
N	-4.994085	-0.135990	-1.219842
C	-5.735432	1.953486	-1.317409
C	-6.031691	0.667813	-1.687250
C	-3.875334	3.084440	-0.089176
C	-4.963749	-1.573688	-1.404957
H	-6.270240	2.894418	-1.478646
H	-6.879202	0.252126	-2.240362
C	-3.001129	3.820328	-0.931814
C	-2.434268	4.995172	-0.397647
C	-2.728533	5.416574	0.907053
C	-3.594979	4.666027	1.713283
C	-4.194016	3.481596	1.235576
C	-2.649675	3.364416	-2.348399
H	-1.752731	5.593769	-1.020538
H	-2.283094	6.345098	1.298117
H	-3.819793	5.009761	2.735076
C	-5.157405	2.699022	2.128290
C	-5.643221	-2.390109	-0.460856
C	-5.648872	-3.780451	-0.699155
C	-5.005276	-4.329229	-1.818051
C	-4.345180	-3.495630	-2.731345
C	-4.313686	-2.096366	-2.554211
C	-6.390339	-1.813098	0.743456
H	-6.176727	-4.444766	0.002885
H	-5.024372	-5.417913	-1.983751
H	-3.850339	-3.938641	-3.609415

C	-3.642946	-1.206907	-3.601347
H	-3.370272	2.569444	-2.635424
C	-1.238519	2.736583	-2.384781
C	-2.792450	4.494466	-3.388204
H	-5.456008	1.780762	1.580128
C	-4.479218	2.243714	3.437468
C	-6.443789	3.506915	2.408308
H	-6.088614	-0.749591	0.849776
C	-7.917964	-1.843781	0.508708
C	-6.020569	-2.520273	2.063003
H	-3.612993	-0.173026	-3.198577
C	-2.185441	-1.625667	-3.878297
C	-4.475586	-1.172900	-4.903285
H	-1.006846	2.359766	-3.403139
H	-0.460771	3.479359	-2.110433
H	-1.152921	1.886718	-1.674914
H	-2.620294	4.099065	-4.410712
H	-3.803176	4.951409	-3.364401
H	-2.052240	5.305655	-3.225075
H	-5.179061	1.629038	4.041130
H	-3.573503	1.635482	3.235959
H	-4.174834	3.107429	4.065044
H	-7.158198	2.906256	3.009043
H	-6.224981	4.433386	2.979850
H	-6.954500	3.806517	1.469861
H	-8.455043	-1.387214	1.366055
H	-8.207632	-1.289708	-0.407610
H	-8.284605	-2.885887	0.396854
H	-6.511134	-2.014579	2.920240
H	-6.357583	-3.578160	2.075159
H	-4.925687	-2.509374	2.239360
H	-1.712062	-0.917692	-4.589568
H	-1.578022	-1.633642	-2.950665
H	-2.122407	-2.635639	-4.334250
H	-4.011390	-0.489944	-5.645040
H	-4.539263	-2.179586	-5.367408
H	-5.513002	-0.823699	-4.721034
Au	-2.393401	0.005836	0.342853
C	-0.693774	-0.818565	2.681501
C	0.518536	-0.811612	3.422298
C	-1.901833	-1.101289	3.370851
C	0.508860	-1.054699	4.803277
H	1.455494	-0.595174	2.885529
C	-1.901079	-1.337123	4.755275
H	-2.841580	-1.119664	2.794071
C	-0.697688	-1.315298	5.481609
H	1.457894	-1.036465	5.362228
H	-2.852870	-1.544540	5.270329
H	-0.697691	-1.500872	6.566730
O	-0.645886	-0.575363	1.351003
C	1.402181	-2.572795	-1.982408
C	1.615044	-1.878572	-3.197199
C	1.514272	-3.984572	-1.983379
C	1.906704	-2.576356	-4.381457
H	1.538932	-0.780458	-3.202897
C	1.824035	-4.677172	-3.164680
H	1.362747	-4.542078	-1.046265
C	2.015526	-3.977879	-4.370387
H	2.060347	-2.017743	-5.318498
H	1.912645	-5.775124	-3.143144
H	2.253794	-4.523778	-5.296758
C	-0.490004	-3.276683	0.871552
C	-1.879040	-3.556540	0.721641
C	0.277440	-4.060339	1.784776
C	-2.460623	-4.615131	1.427547
H	-2.477978	-2.946988	0.027801
C	-0.324048	-5.100102	2.505219
H	1.347727	-3.837459	1.907684
C	-1.689555	-5.384186	2.322219
H	-3.527591	-4.841871	1.281815
H	0.275541	-5.696646	3.210054
H	-2.158415	-6.208886	2.882007

REAL-PhOH-I+II-IV

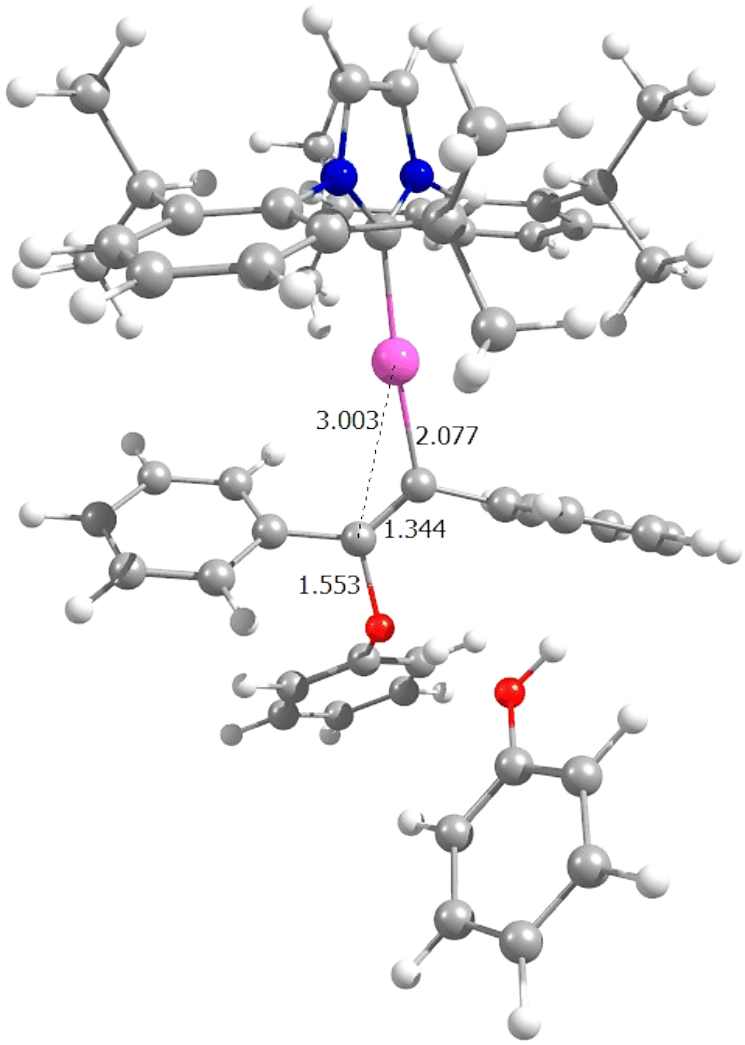


Zero-point correction= 1.386225 (Hartree/Particle)
Thermal correction to Energy= 1.472802
Thermal correction to Enthalpy= 1.473746
Thermal correction to Gibbs Free Energy= 1.249769
Sum of electronic and zero-point Energies= -3434.437646
Sum of electronic and thermal Energies= -3434.351069
Sum of electronic and thermal Enthalpies= -3434.350125
Sum of electronic and thermal Free Energies= -3434.574101

C	-5.087539	-0.280508	0.351335
N	-5.619538	-1.097932	1.315929
N	-6.173809	0.303450	-0.250916
C	-7.011436	-1.028705	1.311941
C	-7.360783	-0.145865	0.322439
C	-4.863536	-1.925694	2.236034
C	-6.113993	1.269635	-1.331789
H	-7.620661	-1.610004	2.010845
H	-8.338660	0.201561	-0.024795
C	-4.416038	-1.349890	3.454550
C	-3.716399	-2.190642	4.344865
C	-3.482068	-3.538677	4.039479
C	-3.940032	-4.077373	2.829085
C	-4.642098	-3.286250	1.896196
C	-4.661614	0.113979	3.821968
H	-3.355222	-1.780541	5.301139
H	-2.940419	-4.177527	4.754948
H	-3.751556	-5.138247	2.601305
C	-5.133880	-3.905038	0.586864
C	-6.075972	0.791968	-2.668567
C	-6.037243	1.756856	-3.696625
C	-6.044766	3.128609	-3.406309
C	-6.090902	3.567674	-2.075615
C	-6.127547	2.651312	-1.003890
C	-6.075422	-0.696831	-3.017315
H	-6.005594	1.424568	-4.746169
H	-6.019909	3.863289	-4.226586
H	-6.101970	4.647942	-1.861597
C	-6.192961	3.162996	0.435993
H	-5.269688	0.569856	3.012857
C	-3.335855	0.902401	3.887481
C	-5.469143	0.247919	5.130944
H	-5.623516	-3.103618	-0.005379
C	-3.961184	-4.439528	-0.261824
C	-6.192815	-4.999880	0.842010
H	-6.142951	-1.266621	-2.066745
C	-7.302015	-1.082340	-3.872029
C	-4.754633	-1.111024	-3.700827
H	-6.170366	2.281287	1.110384
C	-4.968745	4.033765	0.788905
C	-7.515971	3.913634	0.704770
H	-3.530189	1.972908	4.107393
H	-2.669793	0.511507	4.685561
H	-2.787921	0.842270	2.923675
H	-5.689978	1.314761	5.343149
H	-6.434886	-0.295422	5.074874
H	-4.909938	-0.153324	6.002202
H	-4.332184	-4.824987	-1.234415
H	-3.213115	-3.646667	-0.467578
H	-3.435145	-5.274831	0.246272
H	-6.574709	-5.403418	-0.118888
H	-5.769074	-5.850915	1.415691
H	-7.058266	-4.609335	1.416176
H	-7.314941	-2.175968	-4.061034
H	-8.253757	-0.811186	-3.370361
H	-7.288180	-0.576125	-4.860097
H	-4.743972	-2.203546	-3.896718
H	-4.619940	-0.595963	-4.675343
H	-3.880392	-0.865608	-3.062128
H	-5.005071	4.336610	1.856159
H	-4.018685	3.488391	0.614960
H	-4.939044	4.963588	0.183192
H	-7.572802	4.235104	1.765637
H	-7.600668	4.824387	0.075483
H	-8.400672	3.278468	0.492462
Au	-3.138656	0.057639	-0.113191
C	-0.475065	-0.437781	-0.710049
C	-1.179604	0.649621	-0.651396
C	4.870121	0.281035	0.745191
N	6.008465	-0.471477	0.587234
N	5.176884	1.181788	1.735152
C	7.004050	-0.049205	1.464955
C	6.480437	0.990299	2.189284
C	6.189865	-1.538559	-0.379610
C	4.306736	2.234194	2.223184
H	7.989765	-0.523583	1.490513
H	6.912225	1.610697	2.980492
C	6.629254	-1.200121	-1.687125
C	6.833887	-2.262323	-2.592253
C	6.618479	-3.594114	-2.211907
C	6.189408	-3.895064	-0.911564
C	5.964151	-2.876772	0.037659
C	6.909098	0.237912	-2.125600
H	7.174586	-2.038247	-3.615167
H	6.790938	-4.406687	-2.935206
H	6.027891	-4.945517	-0.623237
C	5.518516	-3.237565	1.455018
C	3.434206	1.949711	3.305897
C	2.626901	3.004862	3.779223
C	2.692985	4.282705	3.206609
C	3.572149	4.534018	2.143699
C	4.402838	3.518793	1.624815
C	3.346219	0.569152	3.956319
H	1.937451	2.821704	4.618247
H	2.056476	5.092731	3.596077
H	3.622072	5.544569	1.708361

C	5.361967	3.831108	0.475026
H	6.599222	0.911215	-1.299020
C	6.080354	0.633953	-3.365356
C	8.419902	0.461060	-2.359453
H	5.291900	-2.291206	1.989897
C	4.224441	-4.077205	1.454183
C	6.649049	-3.949978	2.230632
H	4.075041	-0.093609	3.444844
C	3.735895	0.615080	5.449377
C	1.948990	-0.054167	3.752624
H	5.896800	2.893929	0.214068
C	4.605711	4.286064	-0.791081
C	6.429643	4.864225	0.897581
H	6.247891	1.702088	-3.615427
H	6.365029	0.038947	-4.258375
H	4.994468	0.485206	-3.193552
H	8.620849	1.519417	-2.627109
H	9.016880	0.217517	-1.456261
H	8.798628	-0.170942	-3.190133
H	3.886867	-4.264667	2.495082
H	3.406280	-3.560749	0.911919
H	4.377185	-5.067406	0.975551
H	6.334611	-4.162581	3.273830
H	6.915214	-4.918114	1.756345
H	7.571902	-3.335406	2.271649
H	3.721993	-0.404973	5.887109
H	4.752904	1.034058	5.594541
H	3.030587	1.238499	6.038220
H	1.917097	-1.082607	4.169328
H	1.159060	0.537956	4.260813
H	1.692972	-0.107147	2.673833
H	5.315330	4.443573	-1.629727
H	3.858514	3.531183	-1.110947
H	4.072777	5.246303	-0.626793
H	7.149786	5.039067	0.071344
H	5.971964	5.843384	1.152070
H	7.003438	4.524110	1.784302
Au	3.194538	0.118771	-0.297862
C	1.581580	-0.353438	-2.768237
C	0.799975	0.296772	-3.756912
C	2.430601	-1.419696	-3.157851
C	0.878718	-0.108381	-5.097963
H	0.148029	1.128945	-3.450658
C	2.508305	-1.809480	-4.506379
H	3.030426	-1.930933	-2.386858
C	1.732463	-1.161133	-5.483182
H	0.273371	0.413844	-5.856560
H	3.179994	-2.634889	-4.792295
H	1.793311	-1.470182	-6.538199
O	1.473806	0.048650	-1.472011
C	-0.937206	2.088235	-0.865470
C	-1.842680	2.860551	-1.634989
C	0.188724	2.729974	-0.294118
C	-1.610128	4.228013	-1.853280
H	-2.729413	2.374304	-2.071502
C	0.402926	4.101762	-0.498012
H	0.894349	2.144727	0.313457
C	-0.489227	4.855521	-1.282184
H	-2.316168	4.807548	-2.468528
H	1.281268	4.582633	-0.040208
H	-0.313199	5.930625	-1.444530
C	-0.255215	-1.852989	-0.603775
C	0.108232	-2.436234	0.641043
C	-0.389914	-2.688947	-1.746968
C	0.315593	-3.817859	0.738925
H	0.209597	-1.790420	1.525461
C	-0.173338	-4.070453	-1.637549
H	-0.672926	-2.241159	-2.710365
C	0.177737	-4.637333	-0.399203
H	0.580818	-4.263131	1.710354
H	-0.281812	-4.710034	-2.527200
H	0.341599	-5.723614	-0.317979

REAL-PhOH-I+PhOH

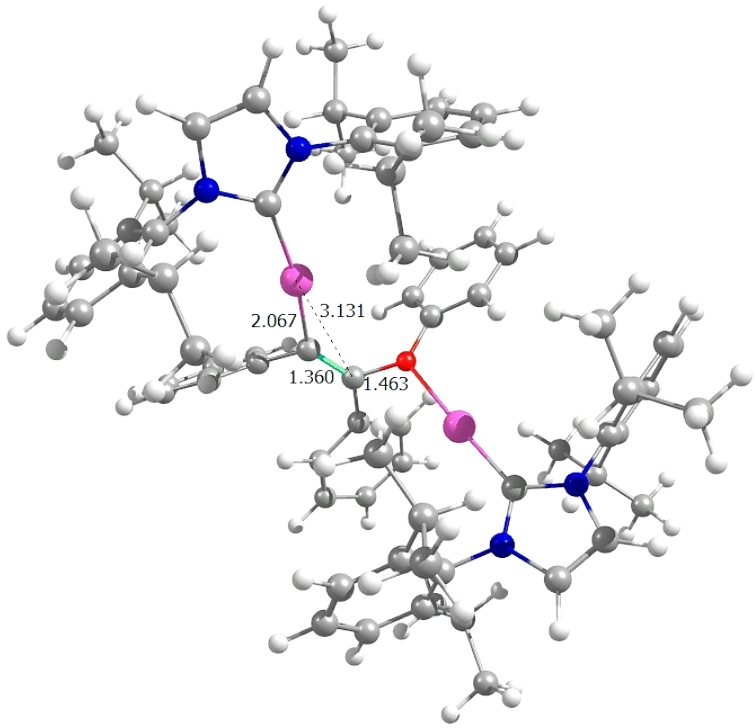


Zero-point correction= 0.946530 (Hartree/Particle)
Thermal correction to Energy= 1.006267
Thermal correction to Enthalpy= 1.007211
Thermal correction to Gibbs Free Energy= 0.840828
Sum of electronic and zero-point Energies= -2447.571802
Sum of electronic and thermal Energies= -2447.512065
Sum of electronic and thermal Enthalpies= -2447.511121
Sum of electronic and thermal Free Energies= -2447.677504

C	2.744037	0.042477	0.311293
N	3.436515	1.055501	0.928773
N	3.698614	-0.900897	0.020282
C	4.791932	0.745573	1.024365
C	4.957515	-0.487967	0.449313
C	2.868346	2.297246	1.418865
C	3.453595	-2.172589	-0.633663
H	5.509226	1.426018	1.493197
H	5.849421	-1.105662	0.306352
C	2.287014	2.318561	2.714077
C	1.772392	3.549779	3.170986
C	1.845403	4.705974	2.382412
C	2.438880	4.655951	1.113364
C	2.964982	3.453275	0.598519
C	2.212898	1.084367	3.613396
H	1.312920	3.603431	4.170614
H	1.442249	5.657556	2.763321
H	2.497314	5.572663	0.506210
C	3.643640	3.440750	-0.772559
C	3.530811	-2.235491	-2.049963
C	3.321115	-3.493357	-2.652495
C	3.054353	-4.633251	-1.881325
C	2.990617	-4.539306	-0.484127
C	3.189595	-3.308940	0.175717
C	3.833351	-1.014795	-2.919778
H	3.373750	-3.581760	-3.749149
H	2.899821	-5.606011	-2.374365
H	2.786254	-5.443192	0.111094
C	3.134336	-3.243507	1.702415
H	2.687728	0.240280	3.071205
C	0.748922	0.680417	3.887456
C	3.000128	1.287825	4.926092
H	3.818064	2.380711	-1.053962
C	2.757328	4.060089	-1.871746
C	5.021172	4.139165	-0.712234
H	3.957134	-0.140892	-2.246481
C	5.155756	-1.185378	-3.698236
C	2.656768	-0.692568	-3.864928
H	3.235988	-2.178691	2.000041
C	1.776696	-3.735106	2.246048
C	4.310882	-4.015806	2.338958
H	0.707454	-0.250645	4.490785
H	0.206575	1.469779	4.449469
H	0.206663	0.503415	2.934259
H	2.984090	0.361098	5.536897
H	4.060531	1.549166	4.731162
H	2.563870	2.100218	5.544564
H	3.248818	3.958979	-2.861858
H	1.766306	3.565715	-1.925110
H	2.587344	5.144186	-1.702705
H	5.529867	4.088042	-1.697529
H	4.915355	5.211169	-0.442774
H	5.690104	3.673022	0.040000
H	5.387102	-0.267780	-4.278339
H	6.009115	-1.383042	-3.017408
H	5.101111	-2.028500	-4.418535
H	2.867129	0.228578	-4.447554
H	2.477694	-1.512599	-4.591805
H	1.719628	-0.534929	-3.291790
H	1.740123	-3.624696	3.350002
H	0.935663	-3.156055	1.812226
H	1.605682	-4.807757	2.016194
H	4.288116	-3.920376	3.444665
H	4.264603	-5.098180	2.095596
H	5.291399	-3.636386	1.984414
Au	0.733373	-0.131759	-0.022496
C	-2.087352	0.461073	-0.865456
C	-1.305649	-0.448312	-0.258932
O	-3.625993	0.253966	-0.863157
C	-1.798572	-1.728437	0.321076
C	-2.027927	-2.862949	-0.496315
C	-2.000793	-1.865761	1.722281
C	-2.472712	-4.077060	0.058164
H	-1.836817	-2.789973	-1.578379
C	-2.455989	-3.081341	2.271281
H	-1.773702	-1.012858	2.382035
C	-2.699850	-4.192165	1.440447
H	-2.639926	-4.944401	-0.600239
H	-2.598193	-3.166677	3.360867
H	-3.047289	-5.143433	1.871694
C	-1.794626	1.738531	-1.549123
C	-2.363010	2.952757	-1.090669
C	-0.958731	1.760493	-2.689422
C	-2.097524	4.158146	-1.757721
H	-3.010807	2.947658	-0.199903
C	-0.699806	2.968803	-3.357731
H	-0.525901	0.816364	-3.053578
C	-1.269538	4.168403	-2.896231
H	-2.536281	5.097437	-1.385820
H	-0.057388	2.970772	-4.252061
H	-1.069192	5.114148	-3.423788
H	-4.055336	-0.270416	-0.021472
O	-4.746617	-0.941377	1.006210
H	-4.096157	-1.501555	1.507259
C	-5.649846	-0.285384	1.854208
C	-5.596374	-0.474256	3.244197

	C	-6.612868	0.548100	1.263907
	C	-6.531110	0.190216	4.057461
	H	-4.837919	-1.138572	3.688311
	C	-7.535626	1.209249	2.091834
	H	-6.646173	0.664859	0.169938
	C	-7.499487	1.033843	3.486768
	H	-6.497404	0.042845	5.148078
	H	-8.295801	1.862830	1.636462
	H	-8.228877	1.550953	4.128301
	C	-4.337473	-0.021560	-2.080600
	C	-4.717290	1.054273	-2.893593
	C	-4.667004	-1.349144	-2.384350
	C	-5.440952	0.777383	-4.067217
	H	-4.452526	2.082969	-2.613539
	C	-5.404113	-1.603933	-3.554092
	H	-4.360886	-2.165333	-1.713897
	C	-5.784412	-0.545295	-4.397791
	H	-5.745043	1.608754	-4.721703
	H	-5.680272	-2.639795	-3.804638
	H	-6.356797	-0.751826	-5.315101

REAL-PhOH-IVcis

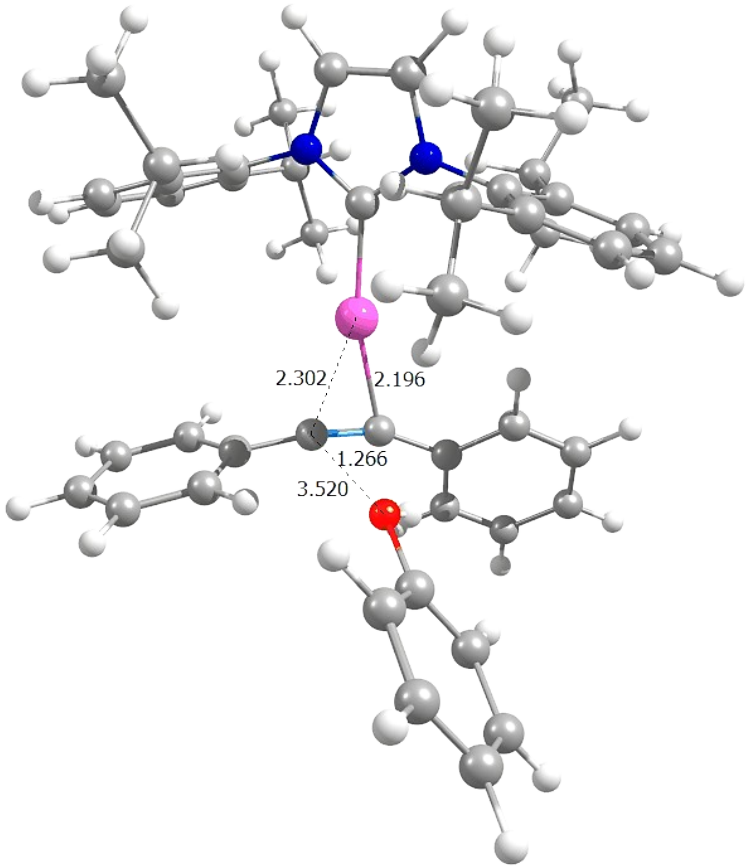


Zero-point correction= 1.388785 (Hartree/Particle)
Thermal correction to Energy= 1.475741
Thermal correction to Enthalpy= 1.476685
Thermal correction to Gibbs Free Energy= 1.251535
Sum of electronic and zero-point Energies= -3434.445083
Sum of electronic and thermal Energies= -3434.358127
Sum of electronic and thermal Enthalpies= -3434.357183
Sum of electronic and thermal Free Energies= -3434.582333

C	-4.121630	0.873669	0.645898
N	-4.382074	2.216137	0.783481
N	-5.222950	0.260270	1.200111
C	-5.612968	2.432334	1.402413
C	-6.142438	1.196712	1.665854
C	-3.528464	3.303633	0.352484
C	-5.445110	-1.169988	1.296775
H	-5.994269	3.439876	1.594930
H	-7.083096	0.899070	2.139110
C	-3.687847	3.812109	-0.962228
C	-2.872815	4.901903	-1.333670
C	-1.958164	5.463785	-0.433065
C	-1.837492	4.949714	0.866426
C	-2.623544	3.860675	1.294235
C	-4.700449	3.237092	-1.952761
H	-2.965188	5.322961	-2.346983
H	-1.340724	6.321940	-0.742684
H	-1.126128	5.412043	1.568143
C	-2.481667	3.304652	2.712106
C	-5.024581	-1.842156	2.474650
C	-5.310617	-3.219900	2.569758
C	-5.989131	-3.892340	1.543768
C	-6.390454	-3.200722	0.392515
C	-6.131026	-1.823175	0.238902
C	-4.303638	-1.132224	3.621007
H	-5.003187	-3.773915	3.470925
H	-6.210560	-4.966737	1.644045
H	-6.920371	-3.740887	-0.407223
C	-6.611433	-1.088475	-1.012933
H	-5.264102	2.435056	-1.432291
C	-3.996719	2.581693	-3.159180
C	-5.726427	4.299970	-2.400806
H	-3.376349	2.679751	2.917366
C	-1.250714	2.378513	2.818043
C	-2.450183	4.409271	3.787402
H	-4.175589	-0.067856	3.333295
C	-5.138021	-1.161065	4.920153
C	-2.891171	-1.712138	3.845695
H	-6.195214	-0.059741	-0.979635
C	-6.088257	-1.744531	-2.307085
C	-8.151522	-0.964450	-1.024222
H	-4.742264	2.117975	-3.838458
H	-3.421772	3.326850	-3.748082
H	-3.289342	1.793072	-2.828797
H	-6.493404	3.843662	-3.060850
H	-6.249649	4.756920	-1.535554
H	-5.245030	5.120892	-2.973220
H	-1.179552	1.941341	3.836279
H	-1.306128	1.546378	2.085391
H	-0.313796	2.941716	2.623980
H	-2.457295	3.958196	4.801439
H	-1.535338	5.034701	3.717584
H	-3.326411	5.085219	3.709060
H	-4.625773	-0.594305	5.725667
H	-6.141903	-0.712217	4.772909
H	-5.287700	-2.198464	5.286642
H	-2.366855	-1.154814	4.650131
H	-2.931861	-2.778554	4.153099
H	-2.279064	-1.644289	2.922804
H	-6.390866	-1.144099	-3.190325
H	-4.982101	-1.824899	-2.304335
H	-6.499785	-2.765768	-2.448031
H	-8.490765	-0.391471	-1.912457
H	-8.636961	-1.962488	-1.063776
H	-8.530267	-0.445816	-0.119076
Au	-2.582940	-0.129376	-0.280709
C	0.015988	-1.236087	-1.630869
C	-1.285452	-1.398305	-1.270990
C	4.237377	-0.029558	0.820039
N	5.150744	0.993684	0.854864
N	4.742185	-0.996107	1.651243
C	6.210672	0.669801	1.697850
C	5.951220	-0.578701	2.201346
C	5.057688	2.246078	0.126330
C	4.138277	-2.287946	1.927101
H	7.049975	1.353362	1.857548
H	6.512231	-1.207116	2.899369
C	4.525255	3.378862	0.798985
C	4.490514	4.593768	0.084319
C	4.960983	4.675089	-1.234174
C	5.484380	3.539894	-1.867249
C	5.553093	2.297063	-1.203500
C	4.042230	3.327360	2.249296
H	4.091566	5.495697	0.573927
H	4.926208	5.635882	-1.771461
H	5.857109	3.619236	-2.900332
C	6.172036	1.091051	-1.911227
C	4.640982	-3.424699	1.238791
C	4.048339	-4.668518	1.537923
C	3.012547	-4.773986	2.476838
C	2.552467	-3.634683	3.150902
C	3.108488	-2.362758	2.901364
C	5.804272	-3.348219	0.248107
H	4.407443	-5.573242	1.023603
H	2.564365	-5.756951	2.690969
H	1.747594	-3.733716	3.895987

C	2.617547	-1.148890	3.690478
H	3.961610	2.259277	2.542443
C	2.641468	3.947195	2.422649
C	5.065008	3.995079	3.196502
H	6.069241	0.211258	-1.241858
C	5.428989	0.753214	-3.220046
C	7.682046	1.306032	-2.157641
H	5.992308	-2.276089	0.026427
C	7.094284	-3.928528	0.872184
C	5.482603	-4.033424	-1.094112
H	3.182410	-0.260479	3.337657
C	1.123353	-0.870252	3.431375
C	2.912168	-1.304926	5.198910
H	2.287585	3.812005	3.465510
H	2.642353	5.038045	2.216922
H	1.901869	3.473101	1.745360
H	4.732166	3.915200	4.252345
H	6.067162	3.525711	3.119956
H	5.184676	5.073378	2.960355
H	5.857413	-0.160203	-3.682015
H	4.350724	0.571158	-3.033944
H	5.512447	1.572356	-3.964489
H	8.131607	0.405921	-2.626082
H	7.864482	2.163427	-2.838978
H	8.227980	1.508315	-1.213154
H	7.948633	-3.825351	0.171183
H	7.367152	-3.418325	1.818978
H	6.975394	-5.008393	1.101374
H	6.319287	-3.886384	-1.808389
H	5.344921	-5.128730	-0.976342
H	4.561043	-3.623186	-1.552530
H	0.799024	0.043133	3.971536
H	0.920701	-0.719836	2.350212
H	0.485220	-1.708657	3.779981
H	2.602539	-0.393271	5.751330
H	2.359550	-2.162544	5.636566
H	3.992193	-1.470969	5.391039
Au	2.542113	-0.047529	-0.201652
C	0.416321	1.170731	-2.122842
C	-0.202255	1.061648	-3.378802
C	0.865887	2.410931	-1.641143
C	-0.342759	2.216407	-4.168724
H	-0.561643	0.086801	-3.735135
C	0.717123	3.554225	-2.442918
H	1.338709	2.473398	-0.647963
C	0.117830	3.462826	-3.711524
H	-0.814913	2.130418	-5.159892
H	1.076727	4.523827	-2.066178
H	0.010233	4.359015	-4.341452
O	0.668426	0.036507	-1.322337
C	-1.995799	-2.646340	-1.694657
C	-2.560425	-3.527045	-0.737807
C	-2.162455	-2.962244	-3.066970
C	-3.220258	-4.700469	-1.138031
H	-2.469480	-3.284621	0.332951
C	-2.841991	-4.124657	-3.465681
H	-1.746664	-2.285124	-3.829764
C	-3.364986	-5.006723	-2.503562
H	-3.633759	-5.377312	-0.373691
H	-2.958330	-4.345560	-4.538874
H	-3.890051	-5.922990	-2.816361
C	0.957775	-2.169724	-2.299777
C	0.911696	-3.564813	-2.042583
C	1.922975	-1.697756	-3.229519
C	1.757560	-4.450697	-2.724294
H	0.200092	-3.954009	-1.301429
C	2.768737	-2.589207	-3.910192
H	1.990740	-0.621594	-3.450807
C	2.682393	-3.971258	-3.670793
H	1.694268	-5.529695	-2.512349
H	3.492231	-2.198281	-4.643017
H	3.336605	-4.671482	-4.213506

REAL-PhOH-I

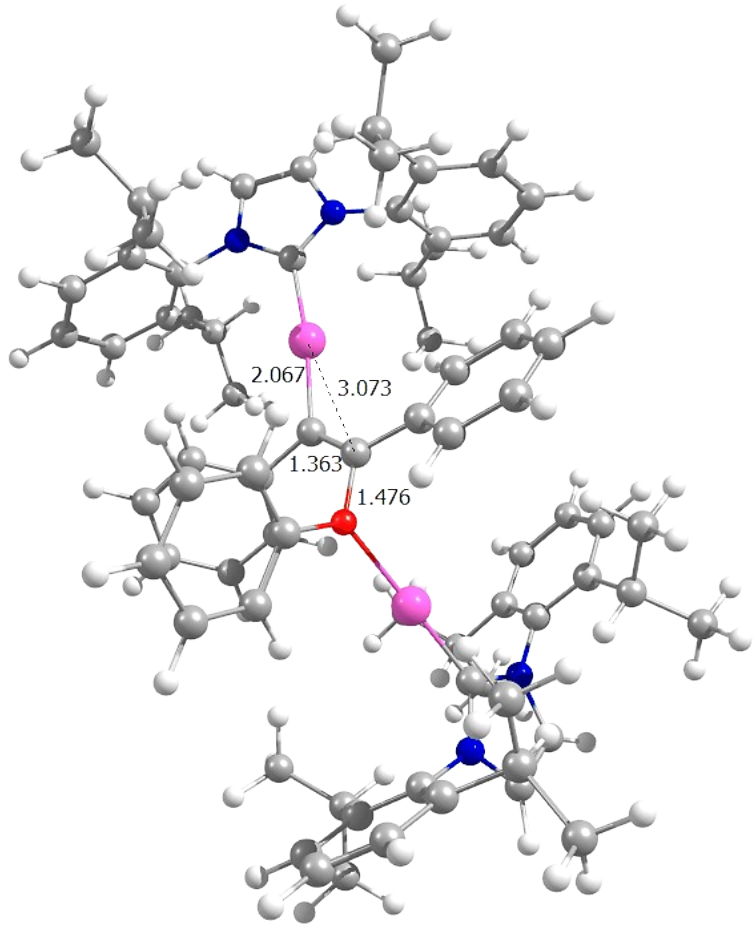


Zero-point correction= 0.843020 (Hartree/Particle)
Thermal correction to Energy= 0.897450
Thermal correction to Enthalpy= 0.898394
Thermal correction to Gibbs Free Energy= 0.741653
Sum of electronic and zero-point Energies= -2140.434202
Sum of electronic and thermal Energies= -2140.379773
Sum of electronic and thermal Enthalpies= -2140.378828
Sum of electronic and thermal Free Energies= -2140.535570

C	-1.692405	-0.751198	-0.702246
N	-2.925857	-0.247420	-1.013721
N	-1.594374	-1.930244	-1.390164
C	-3.590879	-1.099299	-1.890653
C	-2.752458	-2.160436	-2.126458
C	-3.472586	1.004471	-0.519050
C	-0.456284	-2.832160	-1.348470
H	-4.594925	-0.874668	-2.263645
H	-2.875139	-3.053563	-2.746703
C	-3.278482	2.177882	-1.295558
C	-3.835629	3.374230	-0.798560
C	-4.547039	3.398200	0.409318
C	-4.723408	2.220374	1.148983
C	-4.195920	0.990699	0.702860
C	-2.533306	2.176049	-2.631112
H	-3.711208	4.305084	-1.373460
H	-4.975991	4.344595	0.774456
H	-5.291731	2.252552	2.091675
C	-4.411063	-0.278301	1.529449
C	-0.460520	-3.877809	-0.385813
C	0.648924	-4.749584	-0.383570
C	1.704391	-4.585253	-1.292443
C	1.673194	-3.545736	-2.232931
C	0.590501	-2.643513	-2.290374
C	-1.622087	-4.109643	0.582823
H	0.680183	-5.579154	0.339877
H	2.557710	-5.281427	-1.273998
H	2.505188	-3.434155	-2.945023
C	0.552438	-1.557359	-3.366629
H	-2.092589	1.166595	-2.773271
C	-1.364842	3.183538	-2.645836
C	-3.503880	2.425920	-3.807417
H	-3.989614	-1.132532	0.958310
C	-3.646968	-0.207263	2.869598
C	-5.910111	-0.574551	1.748965
H	-2.298477	-3.230760	0.519409
C	-2.439374	-5.354826	0.168796
C	-1.157811	-4.212248	2.050066
H	-0.268296	-0.854172	-3.110588
C	1.853940	-0.732521	-3.425467
C	0.217993	-2.175357	-4.744180
H	-0.804350	3.108050	-3.600578
H	-1.722342	4.230590	-2.557063
H	-0.654329	2.997242	-1.814493
H	-2.964931	2.372463	-4.776106
H	-4.324234	1.679334	-3.831933
H	-3.970762	3.430869	-3.738397
H	-3.775555	-1.148993	3.442524
H	-2.559656	-0.050784	2.705377
H	-4.017606	0.624074	3.505388
H	-6.038415	-1.532889	2.293435
H	-6.401675	0.215930	2.353570
H	-6.458438	-0.650899	0.787740
H	-3.315317	-5.486395	0.837350
H	-2.813242	-5.276992	-0.872812
H	-1.825455	-6.277686	0.233476
H	-2.034197	-4.309944	2.723538
H	-0.516448	-5.101961	2.220816
H	-0.584036	-3.315852	2.362691
H	1.750206	0.085031	-4.168618
H	2.104378	-0.274767	-2.446693
H	2.720905	-1.348201	-3.743647
H	0.145312	-1.384367	-5.519242
H	1.005723	-2.889191	-5.064501
H	-0.744533	-2.727272	-4.728074
Au	-0.308411	0.056585	0.536070
C	0.938724	1.596281	1.707167
C	1.282022	0.414824	2.007098
O	3.560035	1.139133	-0.597578
C	2.010254	-0.618188	2.716372
C	2.585442	-0.302996	3.977099
C	2.184811	-1.916955	2.174910
C	3.321716	-1.271956	4.671784
H	2.447406	0.702966	4.401672
C	2.927708	-2.875756	2.879490
H	1.739919	-2.165072	1.198264
C	3.495259	-2.558264	4.126522
H	3.764089	-1.020913	5.648337
H	3.064189	-3.879860	2.449623
H	4.075843	-3.314936	4.676835
C	0.740857	2.997742	1.463993
C	1.537410	3.667711	0.494444
C	-0.210269	3.728145	2.227177
C	1.385521	5.048523	0.310688
H	2.272680	3.090183	-0.088103
C	-0.346522	5.108225	2.031017
H	-0.824964	3.204790	2.974867
C	0.448593	5.769262	1.075440
H	2.009325	5.569196	-0.432256
H	-1.075904	5.674905	2.630056
H	0.338914	6.855164	0.927937
H	3.471001	0.727094	0.284941
C	4.899441	1.222891	-0.915819
C	5.242902	1.787232	-2.160368
C	5.907334	0.769005	-0.042020
C	6.594966	1.894746	-2.521756

	H	4.443182	2.136427	-2.831120
	C	7.257492	0.882998	-0.416471
	H	5.635008	0.329118	0.932795
	C	7.608858	1.445086	-1.655587
	H	6.858925	2.337316	-3.495366
	H	8.040090	0.527686	0.272439
	H	8.666947	1.533366	-1.945055

REAL-PhOH-IV

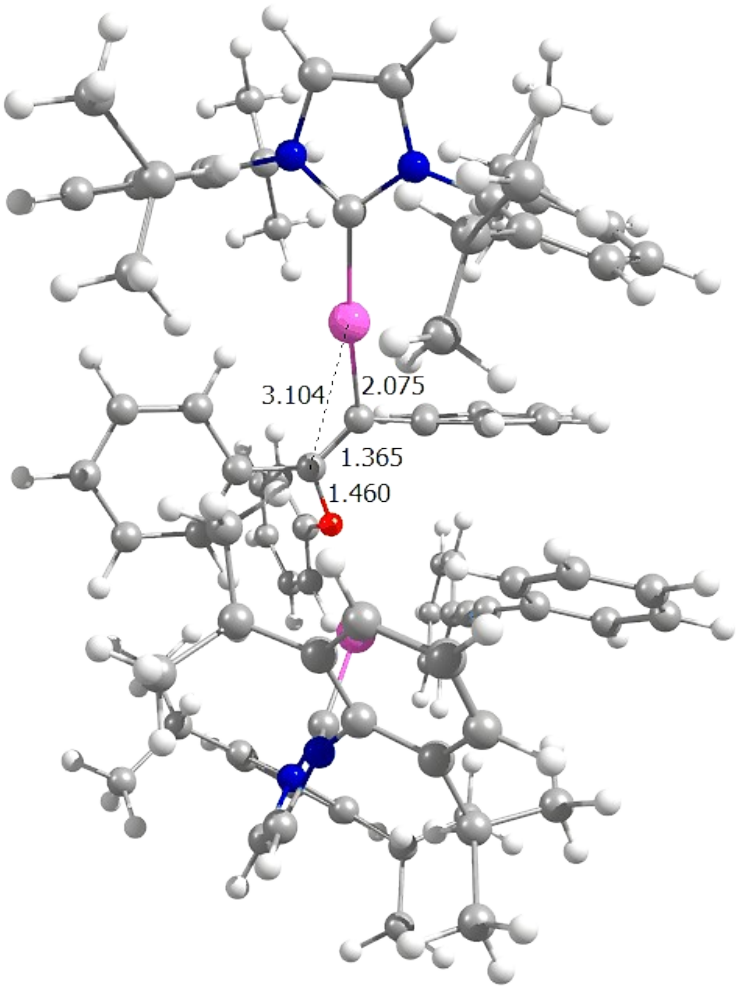


Zero-point correction= 1.388759 (Hartree/Particle)
Thermal correction to Energy= 1.475710
Thermal correction to Enthalpy= 1.476655
Thermal correction to Gibbs Free Energy= 1.252657
Sum of electronic and zero-point Energies= -3434.453854
Sum of electronic and thermal Energies= -3434.366903
Sum of electronic and thermal Enthalpies= -3434.365958
Sum of electronic and thermal Free Energies= -3434.589956

C	4.930464	0.157710	0.176442
N	5.650758	1.318755	0.029953
N	5.868694	-0.779392	0.539254
C	7.002979	1.109258	0.298329
C	7.139939	-0.216197	0.619481
C	5.119984	2.609832	-0.358788
C	5.600456	-2.181561	0.796098
H	7.737586	1.917852	0.234580
H	8.018963	-0.807286	0.894277
C	4.676693	3.495806	0.658448
C	4.225358	4.769513	0.253816
C	4.226850	5.145706	-1.097109
C	4.671272	4.247852	-2.078143
C	5.128557	2.958296	-1.735291
C	4.682077	3.122709	2.141673
H	3.877761	5.485518	1.015392
H	3.883765	6.151602	-1.387250
H	4.670122	4.554540	-3.135955
C	5.613299	2.004465	-2.827889
C	5.710844	-3.098608	-0.282629
C	5.483123	-4.460858	0.002969
C	5.168245	-4.887851	1.300947
C	5.067928	-3.957411	2.344490
C	5.282100	-2.581620	2.120414
C	6.041651	-2.661191	-1.710455
H	5.559674	-5.202141	-0.807971
H	5.003016	-5.958233	1.501837
H	4.819307	-4.305334	3.359268
C	5.164436	-1.591372	3.279196
H	5.107386	2.101522	2.232357
C	3.248961	3.065840	2.712299
C	5.583075	4.068826	2.964180
H	5.932224	1.061761	-2.335965
C	4.474859	1.643244	-3.805649
C	6.841906	2.571141	-3.572137
H	6.277585	-1.576575	-1.686965
C	7.285730	-3.385625	-2.266684
C	4.819539	-2.837756	-2.637839
H	5.388501	-0.578864	2.882770
C	3.725251	-1.550230	3.836517
C	6.195941	-1.886832	4.389330
H	3.267786	2.751948	3.776939
H	2.752034	4.057865	2.664644
H	2.622766	2.340775	2.152199
H	5.622218	3.743163	4.024581
H	6.621775	4.087171	2.574648
H	5.202963	5.112038	2.951926
H	4.827567	0.901906	-4.552772
H	3.605024	1.210452	-3.270548
H	4.118027	2.533900	-4.364305
H	7.212717	1.841853	-4.322298
H	6.595937	3.508269	-4.114616
H	7.675655	2.797733	-2.875917
H	7.542711	-2.995309	-3.273399
H	8.169419	-3.245922	-1.610454
H	7.115193	-4.477685	-2.371430
H	5.051715	-2.479063	-3.662497
H	4.521424	-3.904809	-2.714449
H	3.947170	-2.264030	-2.260060
H	3.641356	-0.783289	4.634932
H	2.992914	-1.305427	3.039547
H	3.429743	-2.525078	4.278020
H	6.133561	-1.121283	5.190697
H	6.017772	-2.875770	4.861705
H	7.233817	-1.886529	3.996777
Au	2.924096	-0.199121	-0.034092
C	0.007433	-0.239480	-0.999778
C	0.947941	-0.788440	-0.180437
C	-4.697585	0.639845	0.531494
N	-5.958782	0.117538	0.404172
N	-4.850061	1.785521	1.268377
C	-6.888117	0.928504	1.049366
C	-6.190914	1.977195	1.592551
C	-6.300114	-1.111615	-0.289466
C	-3.785505	2.688776	1.667901
H	-7.954928	0.685353	1.061094
H	-6.524318	2.840443	2.176192
C	-6.360823	-2.315116	0.462601
C	-6.721754	-3.488655	-0.231863
C	-7.011539	-3.461753	-1.603412
C	-6.948149	-2.255497	-2.314448
C	-6.594382	-1.048061	-1.677076
C	-6.079419	-2.374025	1.965087
H	-6.781545	-4.442074	0.316059
H	-7.295337	-4.390573	-2.122815
H	-7.182377	-2.248008	-3.390428
C	-6.552958	0.252284	-2.480396
C	-3.453222	3.765369	0.803579
C	-2.434641	4.640826	1.233556
C	-1.790092	4.456676	2.464314
C	-2.151588	3.390723	3.300006
C	-3.160188	2.479398	2.926033
C	-4.190054	4.026013	-0.510898
H	-2.144303	5.485961	0.590890
H	-0.999696	5.156002	2.779163
H	-1.642044	3.264153	4.267410

C	-3.582588	1.363292	3.883661
H	-5.756332	-1.363149	2.292407
C	-4.927780	-3.345956	2.296622
C	-7.358207	-2.726672	2.757314
H	-6.226954	1.066122	-1.798901
C	-5.519970	0.176599	-3.624778
C	-7.953888	0.632525	-3.008664
H	-4.765384	3.110083	-0.763866
C	-5.205722	5.180190	-0.344606
C	-3.231705	4.296526	-1.686711
H	-4.175177	0.624503	3.302733
C	-2.383400	0.606428	4.487989
C	-4.497914	1.921687	4.998161
H	-4.712139	-3.331117	3.385277
H	-5.181826	-4.392361	2.026802
H	-3.995540	-3.074178	1.759895
H	-7.156457	-2.715363	3.848617
H	-8.179483	-2.008824	2.554325
H	-7.729563	-3.739925	2.496542
H	-5.456478	1.149161	-4.155609
H	-4.509687	-0.073091	-3.239430
H	-5.795684	-0.594386	-4.374383
H	-7.917845	1.606493	-3.539504
H	-8.337774	-0.123056	-3.725766
H	-8.694060	0.718824	-2.186689
H	-5.771003	5.341415	-1.286165
H	-5.939741	4.975864	0.461980
H	-4.690979	6.131243	-0.092624
H	-3.805233	4.389887	-2.632136
H	-2.671552	5.245613	-1.553841
H	-2.491787	3.480958	-1.813883
H	-2.739103	-0.255871	5.088842
H	-1.702154	0.221400	3.702731
H	-1.786297	1.248806	5.168346
H	-4.837980	1.107305	5.671398
H	-3.958442	2.669521	5.616676
H	-5.398722	2.420289	4.585308
Au	-3.044917	-0.111573	-0.245638
C	-1.310984	-2.158373	-1.876504
C	-0.332888	-2.440331	-2.844134
C	-2.366438	-3.048655	-1.626911
C	-0.426229	-3.639579	-3.571400
H	0.492443	-1.735906	-3.020818
C	-2.446737	-4.240851	-2.366360
H	-3.114804	-2.809748	-0.853969
C	-1.478581	-4.542395	-3.339686
H	0.336825	-3.863677	-4.333216
H	-3.273120	-4.940806	-2.168394
H	-1.542264	-5.479197	-3.914003
O	-1.279079	-0.946787	-1.152632
C	0.613564	-1.979635	0.654057
C	-0.397972	-1.913030	1.645595
C	1.331628	-3.194553	0.523886
C	-0.686433	-3.017528	2.464512
H	-0.947291	-0.966968	1.785225
C	1.025703	-4.306058	1.325173
H	2.139831	-3.259934	-0.221250
C	0.017286	-4.224379	2.302153
H	-1.464561	-2.932756	3.240175
H	1.590986	-5.241925	1.191853
H	-0.211414	-5.092194	2.940730
C	0.037328	0.976430	-1.836999
C	-0.763821	1.082201	-3.005109
C	0.871094	2.074584	-1.502512
C	-0.699315	2.220190	-3.825429
H	-1.429355	0.253146	-3.287282
C	0.930601	3.210009	-2.322909
H	1.476015	2.024359	-0.583355
C	0.151612	3.288176	-3.492749
H	-1.317360	2.268017	-4.736035
H	1.592020	4.043215	-2.038957
H	0.201459	4.180477	-4.136550

REAL-PhOH-IV-VI-ALKYNE



Zero-point correction= 1.575319 (Hartree/Particle)
Thermal correction to Energy= 1.674439
Thermal correction to Enthalpy= 1.675384
Thermal correction to Gibbs Free Energy= 1.426297
Sum of electronic and zero-point Energies= -3973.304742
Sum of electronic and thermal Energies= -3973.205622
Sum of electronic and thermal Enthalpies= -3973.204677
Sum of electronic and thermal Free Energies= -3973.453764

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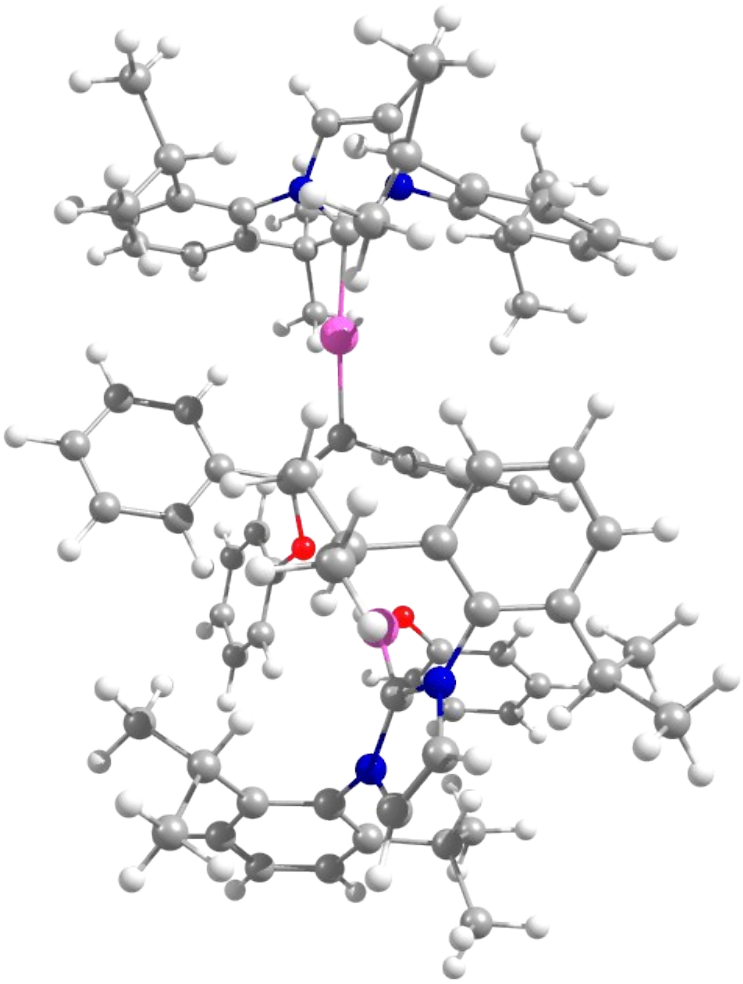
N	6.182347	-0.505016	-0.829717
N	5.912916	1.257923	0.406069
C	7.433457	0.099667	-0.715245
C	7.262739	1.213975	0.064062
C	5.967205	-1.722095	-1.586796
C	5.340510	2.281131	1.258255
H	8.324064	-0.318864	-1.193867
H	7.972291	1.973251	0.406861
C	5.784321	-1.618194	-2.991266
C	5.638120	-2.819811	-3.715829
C	5.668933	-4.064932	-3.071340
C	5.850262	-4.134161	-1.682981
C	6.013008	-2.967830	-0.906135
C	5.746145	-0.275961	-3.723588
H	5.501643	-2.777466	-4.808044
H	5.556211	-4.990830	-3.657267
H	5.877621	-5.117702	-1.188145
C	6.238749	-3.085204	0.601557
C	5.365923	2.081235	2.663544
C	4.834621	3.108534	3.470589
C	4.308189	4.277658	2.904773
C	4.302947	4.447462	1.512823
C	4.822858	3.456930	0.654390
C	5.945275	0.823133	3.311163
H	4.836336	2.987908	4.565155
H	3.902498	5.068238	3.555739
H	3.891881	5.373952	1.082090
C	4.800542	3.664073	-0.860566
H	5.885904	0.525190	-2.968151
C	4.373091	-0.036527	-4.386516
C	6.897192	-0.152147	-4.745088
H	6.387124	-2.061616	1.004020
C	4.998167	-3.670454	1.309463
C	7.513273	-3.894647	0.924410
H	6.281545	0.147864	2.496651
C	7.183796	1.152781	4.173150
C	4.878282	0.058135	4.121634
H	5.371956	2.832574	-1.323854
C	3.358653	3.578529	-1.406599
C	5.489938	4.979286	-1.279633
H	4.340780	0.968117	-4.857920
H	4.168051	-0.782973	-5.182596
H	3.551374	-0.098900	-3.644190
H	6.887232	0.849201	-5.223982
H	7.888517	-0.291278	-4.266528
H	6.808063	-0.907854	-5.553555
H	5.161077	-3.712741	2.406519
H	4.102237	-3.042320	1.119978
H	4.778294	-4.702187	0.962178
H	7.693123	-3.912628	2.019543
H	7.427873	-4.948853	0.586253
H	8.410368	-3.458708	0.438179
H	7.626552	0.223493	4.588515
H	7.969202	1.671386	3.585156
H	6.921887	1.807750	5.030886
H	5.305056	-0.882014	4.529530
H	4.510284	0.655811	4.981517
H	4.001378	-0.201646	3.493997
H	3.353859	3.681838	-2.512204
H	2.891160	2.605769	-1.146046
H	2.722506	4.387430	-0.988476
H	5.527640	5.061880	-2.385938
H	4.945596	5.870436	-0.902187
H	6.530123	5.036548	-0.898013
Au	3.250565	-0.258931	0.190082
C	0.358922	-1.380254	0.062183
C	1.313009	-0.713792	0.775594
C	-4.003389	0.583178	-1.521986
N	-5.187237	-0.032418	-1.860837
N	-3.835363	1.572589	-2.463841
C	-5.737762	0.554138	-2.998007
C	-4.888071	1.556025	-3.378327
C	-5.905074	-1.021073	-1.074957
C	-2.855050	2.648152	-2.481363
H	-6.689407	0.215566	-3.417787
H	-4.939143	2.271385	-4.204309
C	-6.823768	-0.542884	-0.100503
C	-7.546099	-1.508453	0.631469
C	-7.374059	-2.878398	0.391765
C	-6.482323	-3.316158	-0.598110
C	-5.730194	-2.401032	-1.363627
C	-7.108050	0.945491	0.119541
H	-8.270112	-1.177156	1.392715
H	-7.952922	-3.614462	0.971625
H	-6.373258	-4.394112	-0.788193
C	-4.833410	-2.891189	-2.502234
C	-1.586178	2.428605	-3.081409
C	-0.712642	3.533208	-3.157033
C	-1.091387	4.797218	-2.682210
C	-2.354134	4.983838	-2.106850
C	-3.269397	3.917112	-1.990770
C	-1.195407	1.084192	-3.695288
H	0.279303	3.401425	-3.612864
H	-0.395524	5.646815	-2.768652
H	-2.642689	5.980940	-1.739837

C	-4.655541	4.181061	-1.396255
H	-6.387033	1.526383	-0.492809
C	-6.902123	1.385698	1.582263
C	-8.526926	1.304954	-0.377905
H	-4.060103	-2.110471	-2.672971
C	-4.103458	-4.207956	-2.177017
C	-5.649277	-3.038458	-3.809342
H	-1.722857	0.290799	-3.123348
C	-1.669979	0.998184	-5.165740
C	0.310828	0.786044	-3.598346
H	-5.179907	3.207083	-1.301457
C	-4.580285	4.786944	0.019747
C	-5.500513	5.070684	-2.336029
H	-7.108326	2.470783	1.689079
H	-7.588080	0.854672	2.275261
H	-5.860174	1.206458	1.916612
H	-8.710104	2.395094	-0.277629
H	-8.673221	1.030412	-1.442847
H	-9.307329	0.779036	0.211178
H	-3.385315	-4.455648	-2.984589
H	-3.538388	-4.145872	-1.225653
H	-4.807607	-5.063134	-2.104722
H	-4.992829	-3.364106	-4.643101
H	-6.448563	-3.799986	-3.690500
H	-6.134856	-2.089696	-4.115030
H	-1.407559	0.010073	-5.597461
H	-2.767159	1.128602	-5.263771
H	-1.181754	1.780713	-5.784361
H	0.509846	-0.251137	-3.934064
H	0.909013	1.460550	-4.246455
H	0.684673	0.878959	-2.558569
H	-5.600575	4.901655	0.441314
H	-3.991374	4.146557	0.705796
H	-4.114515	5.794125	0.013608
H	-6.520561	5.215872	-1.923230
H	-5.043584	6.075248	-2.457631
H	-5.602940	4.628743	-3.348515
Au	-2.755827	-0.038422	-0.079512
C	-1.357358	-2.821522	1.027721
C	-0.423110	-3.863079	1.188568
C	-2.721895	-3.054245	1.270262
C	-0.867416	-5.128832	1.609227
H	0.641373	-3.687470	0.979641
C	-3.151606	-4.320859	1.698569
H	-3.450143	-2.237457	1.127150
C	-2.227338	-5.365656	1.871914
H	-0.131524	-5.939352	1.730714
H	-4.222141	-4.483374	1.896316
H	-2.565456	-6.359109	2.204065
O	-0.969238	-1.528171	0.649907
C	-2.187573	2.505732	2.268102
C	-2.537847	3.473358	3.250219
C	-1.348200	2.898513	1.196406
C	-2.050129	4.784496	3.162802
H	-3.187787	3.175942	4.086873
C	-0.864079	4.213166	1.116962
H	-1.068855	2.159511	0.428541
C	-1.208311	5.158798	2.098624
H	-2.326806	5.519695	3.934940
H	-0.212698	4.497242	0.276909
H	-0.823456	6.188867	2.034984
C	0.450338	-2.006012	-1.283744
C	1.696364	-2.391058	-1.841249
C	-0.713957	-2.285963	-2.044788
C	1.777536	-2.991563	-3.106046
H	2.617529	-2.220753	-1.260120
C	-0.633048	-2.886152	-3.311855
H	-1.702169	-2.020340	-1.638449
C	0.613170	-3.240743	-3.855008
H	2.764969	-3.280516	-3.497855
H	-1.556530	-3.080958	-3.879969
H	0.675667	-3.721093	-4.844203
C	1.095723	-0.304161	2.197762
C	1.177030	1.057374	2.586197
C	0.944063	-1.270283	3.225288
C	1.064152	1.439989	3.932179
H	1.342462	1.824373	1.814521
C	0.869778	-0.889235	4.576574
H	0.914356	-2.338507	2.963252
C	0.913789	0.468934	4.938356
H	1.112598	2.508011	4.196814
H	0.786168	-1.665309	5.354994
H	0.848881	0.766790	5.996825
C	-2.663718	1.155250	2.442548
C	-3.144133	0.153064	3.002212
C	-3.634807	-0.978418	3.726503
C	-2.749726	-1.718860	4.556711
C	-5.004278	-1.353633	3.674014
C	-3.227797	-2.797953	5.311384
H	-1.689488	-1.429394	4.593325
C	-5.469851	-2.436546	4.432596
H	-5.693866	-0.786178	3.033690
C	-4.585912	-3.160940	5.253487
H	-2.533208	-3.363236	5.952266
H	-6.534330	-2.715508	4.387434
H	-4.957099	-4.008553	5.850925

REAL-PhOH-IV-VI-PhOH

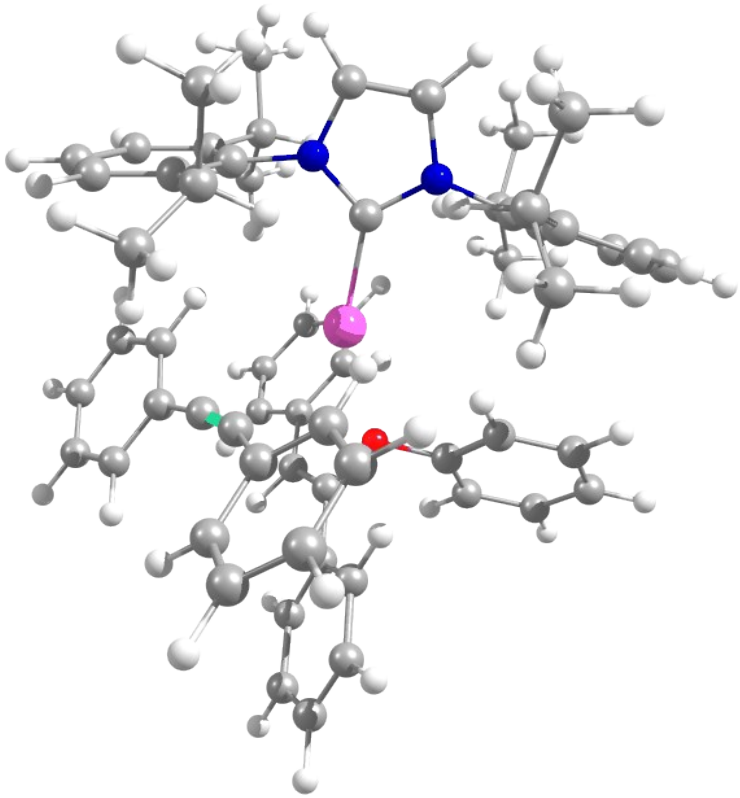


Zero-point correction= 1.491020 (Hartree/Particle)
Thermal correction to Energy= 1.584736
Thermal correction to Enthalpy= 1.585681
Thermal correction to Gibbs Free Energy= 1.346853
Sum of electronic and zero-point Energies= -3741.589726
Sum of electronic and thermal Energies= -3741.496009
Sum of electronic and thermal Enthalpies= -3741.495065
Sum of electronic and thermal Free Energies= -3741.733893

C	5.000155	0.370941	0.099896
N	6.089983	-0.468949	0.093366
N	5.548562	1.630725	0.175855
C	7.282245	0.248648	0.166868
C	6.940653	1.574205	0.218253
C	6.052667	-1.915219	0.004660
C	4.817609	2.882224	0.197506
H	8.257102	-0.248011	0.176747
H	7.555508	2.477441	0.277516
C	6.212994	-2.513946	-1.273685
C	6.227494	-3.923281	-1.329600
C	6.084729	-4.698198	-0.169469
C	5.929525	-4.077096	1.077707
C	5.917512	-2.671594	1.198901
C	6.398120	-1.694573	-2.552217
H	6.358252	-4.422911	-2.302546
H	6.100635	-5.797486	-0.237340
H	5.824877	-4.696775	1.982287
C	5.786233	-2.026624	2.578828
C	4.428715	3.422677	1.451708
C	3.776942	4.673489	1.440365
C	3.536438	5.357173	0.240250
C	3.937623	4.799676	-0.982133
C	4.588383	3.549293	-1.034672
C	4.737357	2.730709	2.779853
H	3.459708	5.124393	2.393439
H	3.040563	6.340876	0.259668
H	3.751323	5.350372	-1.918004
C	5.022485	2.969644	-2.381348
H	6.245925	-0.626381	-2.291600
C	5.349270	-2.048057	-3.626566
C	7.835226	-1.837143	-3.101393
H	5.775996	-0.925763	2.438536
C	4.453749	-2.405462	3.258561
C	6.997077	-2.366249	3.475369
H	5.088168	1.703160	2.549550
C	5.881940	3.456631	3.522986
C	3.488295	2.593521	3.672178
H	5.544147	2.010064	-2.184886
C	3.802514	2.642154	-3.268321
C	6.021511	3.893807	-3.109833
H	5.465708	-1.385940	-4.509816
H	5.461618	-3.093104	-3.984820
H	4.317042	-1.931166	-3.239085
H	7.974878	-1.200337	-3.999868
H	8.595956	-1.538054	-2.350941
H	8.053307	-2.885241	-3.396616
H	4.354290	-1.884128	4.233324
H	3.590294	-2.116034	2.623749
H	4.389576	-3.496429	3.456132
H	6.915566	-1.845861	4.452492
H	7.059340	-3.455404	3.682514
H	7.954465	-2.060416	3.005236
H	6.134504	2.925670	4.464644
H	6.803738	3.515032	2.908034
H	5.593090	4.495269	3.789749
H	3.731826	2.011370	4.585067
H	3.110245	3.581897	4.008042
H	2.663322	2.074555	3.143968
H	4.125883	2.165258	-4.217158
H	3.111214	1.946346	-2.749809
H	3.236772	3.560688	-3.534282
H	6.372004	3.422025	-4.051467
H	5.559627	4.866866	-3.379789
H	6.912164	4.109163	-2.484264
Au	3.014953	-0.147578	0.205066
C	0.307139	-1.613733	0.009108
C	1.032239	-0.613927	0.574956
C	-4.006634	0.841671	-1.291953
N	-5.202772	0.394830	-1.801982
N	-3.762727	2.029413	-1.934822
C	-5.691464	1.292782	-2.749524
C	-4.786525	2.317496	-2.834353
C	-5.906940	-0.814915	-1.413502
C	-2.619896	2.895421	-1.716580
H	-6.636881	1.121158	-3.272330
H	-4.775535	3.221953	-3.449559
C	-6.840308	-0.737552	-0.344205
C	-7.539361	-1.917537	-0.014709
C	-7.327029	-3.109652	-0.720624
C	-6.409999	-3.149594	-1.780328
C	-5.679207	-2.003718	-2.158300
C	-7.148062	0.570365	0.386972
H	-8.269865	-1.898474	0.808068
H	-7.889270	-4.016607	-0.447459
H	-6.262803	-4.089497	-2.333353
C	-4.738424	-2.051402	-3.363700
C	-1.428662	2.639946	-2.446012
C	-0.341391	3.508884	-2.220051
C	-0.444628	4.584191	-1.326055
C	-1.643244	4.822013	-0.639199
C	-2.763937	3.983936	-0.815939
C	-1.327525	1.523168	-3.485190
H	0.604903	3.338925	-2.754765
H	0.421665	5.243784	-1.163880
H	-1.713285	5.678541	0.049001

C	-4.077883	4.292565	-0.095038
H	-6.284632	1.252511	0.232053
C	-7.317681	0.387843	1.906949
C	-8.398625	1.247546	-0.222415
H	-4.027171	-1.203140	-3.267396
C	-3.904306	-3.345394	-3.424939
C	-5.526493	-1.855149	-4.680428
H	-2.149285	0.803401	-3.286424
C	-1.541979	2.092757	-4.907232
C	-0.007294	0.734496	-3.398251
H	-4.742959	3.410669	-0.211240
C	-3.889251	4.519849	1.418142
C	-4.788594	5.500436	-0.748196
H	-7.417779	1.376687	2.398973
H	-8.233162	-0.188430	2.155983
H	-6.450649	-0.130333	2.363021
H	-8.606696	2.211976	0.286199
H	-8.278633	1.454726	-1.305342
H	-9.294082	0.601863	-0.103154
H	-3.151887	-3.274116	-4.236985
H	-3.368249	-3.538644	-2.473875
H	-4.531492	-4.234264	-3.645782
H	-4.838380	-1.856842	-5.551380
H	-6.261762	-2.674172	-4.827065
H	-6.086365	-0.898308	-4.694644
H	-1.515759	1.279358	-5.662152
H	-2.515737	2.615910	-5.003937
H	-0.745046	2.821291	-5.166690
H	-0.033922	-0.132979	-4.088983
H	0.864650	1.354566	-3.692698
H	0.179652	0.349404	-2.375036
H	-4.874154	4.654199	1.911184
H	-3.378695	3.660710	1.897854
H	-3.293103	5.432114	1.629345
H	-5.761671	5.697499	-0.251918
H	-4.173009	6.420523	-0.661735
H	-4.984870	5.333299	-1.827133
Au	-2.864897	-0.075001	0.041911
C	-1.451547	-3.000610	0.955128
C	-0.540509	-3.783386	1.693814
C	-2.790591	-3.420833	0.804423
C	-0.980385	-4.981120	2.281253
H	0.502092	-3.450958	1.799223
C	-3.216505	-4.619344	1.407007
H	-3.487882	-2.812691	0.202759
C	-2.315201	-5.404828	2.146169
H	-0.265318	-5.589510	2.857081
H	-4.261865	-4.941408	1.280309
H	-2.648804	-6.345352	2.610354
O	-1.086730	-1.777763	0.396709
O	-2.834284	-0.784820	2.463415
H	-2.675294	-1.755193	2.413613
C	-3.740796	-0.508877	3.473052
C	-4.424945	-1.540656	4.144240
C	-3.944876	0.836219	3.829486
C	-5.316868	-1.216580	5.181790
H	-4.254422	-2.592074	3.859342
C	-4.843594	1.144630	4.863347
H	-3.374182	1.618008	3.307780
C	-5.533098	0.124252	5.544409
H	-5.845376	-2.025531	5.710437
H	-4.997819	2.197597	5.147858
H	-6.230962	0.372806	6.358431
C	0.704574	-2.584602	-1.043105
C	2.001744	-3.150186	-1.076297
C	-0.223501	-2.985059	-2.036178
C	2.359171	-4.071091	-2.073894
H	2.731087	-2.868447	-0.300132
C	0.137349	-3.901759	-3.035880
H	-1.238289	-2.559963	-2.024221
C	1.431125	-4.451352	-3.059643
H	3.371168	-4.504587	-2.067260
H	-0.599897	-4.192911	-3.800843
H	1.711540	-5.179523	-3.836974
C	0.442776	0.237728	1.652104
C	-0.047506	1.537311	1.367387
C	0.440145	-0.192181	3.002707
C	-0.507098	2.375859	2.399354
H	-0.025469	1.906507	0.329943
C	-0.021799	0.646269	4.030116
H	0.829540	-1.192976	3.248004
C	-0.493899	1.938051	3.735465
H	-0.858704	3.389760	2.151069
H	-0.006164	0.289712	5.072585
H	-0.839306	2.600728	4.544457

REAL-PhOH-VII-6-ALKYNE

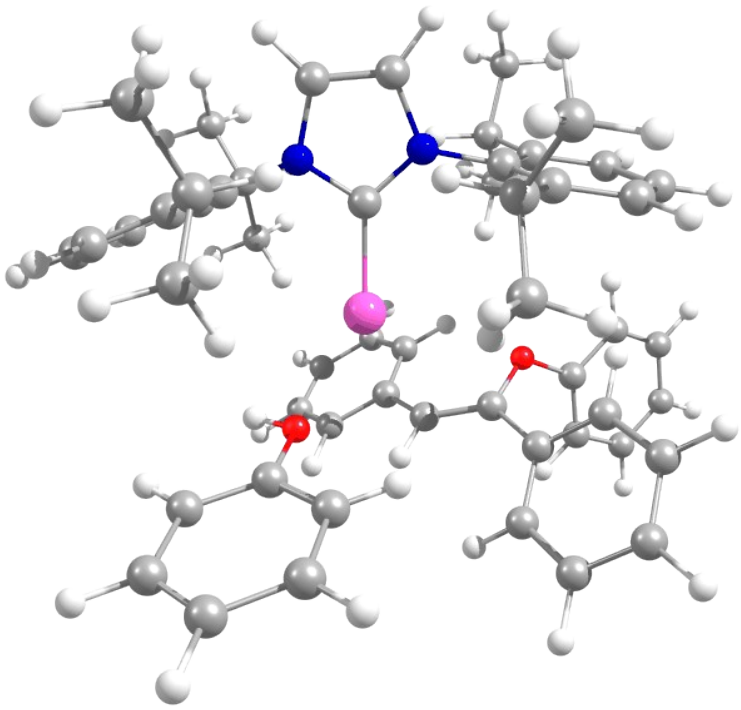


Zero-point correction= 1.575319 (Hartree/Particle)
Thermal correction to Energy= 1.674439
Thermal correction to Enthalpy= 1.675384
Thermal correction to Gibbs Free Energy= 1.426297
Sum of electronic and zero-point Energies= -3973.304742
Sum of electronic and thermal Energies= -3973.205622
Sum of electronic and thermal Enthalpies= -3973.204677
Sum of electronic and thermal Free Energies= -3973.453764

C	-3.006158	-0.657398	-1.234571
C	-3.308268	0.505669	-1.883095
C	2.143089	0.380261	0.283770
N	3.244687	-0.361533	-0.080988
N	2.656797	1.518806	0.861090
C	4.417049	0.309571	0.259493
C	4.048327	1.486182	0.851126
C	3.294699	-1.658015	-0.739858
C	1.935259	2.671911	1.377427
H	5.403282	-0.111771	0.044704
H	4.644544	2.307305	1.259598
C	3.297243	-1.696466	-2.160934
C	3.476097	-2.955320	-2.770275
C	3.656888	-4.115722	-2.006286
C	3.654685	-4.045406	-0.607037
C	3.479741	-2.816414	0.063489
C	3.189868	-0.437141	-3.022398
H	3.483322	-3.026536	-3.868017
H	3.807121	-5.084765	-2.507650
H	3.805617	-4.963705	-0.019540
C	3.565078	-2.765089	1.590221
C	1.466815	2.645136	2.720439
C	0.845801	3.815105	3.203623
C	0.726019	4.961388	2.405087
C	1.223773	4.964584	1.096175
C	1.839484	3.820669	0.545468
C	1.691851	1.446649	3.645241
H	0.460089	3.833553	4.233269
H	0.244985	5.864315	2.812360
H	1.137642	5.876496	0.485279
C	2.418283	3.879758	-0.870301
H	2.719279	0.356697	-2.402860
C	2.297233	-0.638572	-4.261923
C	4.594875	0.058155	-3.440296
H	3.117629	-1.803831	1.923644
C	2.773236	-3.901669	2.266863
C	5.038326	-2.787959	2.061369
H	1.712125	0.534449	3.010287
C	3.063125	1.558348	4.355220
C	0.571311	1.257523	4.684424
H	2.695089	2.846931	-1.170492
C	1.396398	4.392441	-1.904854
C	3.704890	4.737087	-0.901345
H	2.170842	0.323017	-4.800380
H	2.745902	-1.347838	-4.987986
H	1.293150	-1.022496	-3.990792
H	4.518551	0.991037	-4.036826
H	5.242709	0.268241	-2.565123
H	5.111648	-0.701019	-4.064282
H	2.760084	-3.752440	3.366151
H	1.725296	-3.948668	1.907117
H	3.235580	-4.894015	2.085103
H	5.096812	-2.721014	3.167664
H	5.536251	-3.730601	1.751506
H	5.626282	-1.947553	1.641328
H	3.235436	0.676922	5.007495
H	3.907858	1.617417	3.639497
H	3.100555	2.465064	4.994864
H	0.708900	0.295821	5.218884
H	0.583083	2.057693	5.453620
H	-0.430938	1.245181	4.212113
H	1.834944	4.360204	-2.923549
H	0.473929	3.777767	-1.916928
H	1.106990	5.446570	-1.711488
H	4.148791	4.738781	-1.918518
H	3.489377	5.791023	-0.626666
H	4.474647	4.362809	-0.195775
Au	0.205802	-0.096245	0.067161
C	-1.372083	-2.292569	-1.918983
C	-2.085220	-2.616711	-3.085199
C	-0.340633	-3.116651	-1.444405
C	-1.759685	-3.797461	-3.774891
H	-2.887981	-1.957030	-3.445365
C	-0.027284	-4.293586	-2.145465
H	0.205353	-2.836665	-0.528216
C	-0.736689	-4.640672	-3.308496
H	-2.318500	-4.057100	-4.687532
H	0.775203	-4.944762	-1.767938
H	-0.494114	-5.568121	-3.849337
O	-1.662998	-1.112746	-1.198123
H	-4.348082	0.835863	-1.735528
C	-1.700644	-1.250006	3.007021
C	-2.796982	-1.520556	3.874146
C	-0.550568	-2.075970	3.085913
C	-2.733438	-2.577476	4.790980
H	-3.694762	-0.887619	3.817362
C	-0.499682	-3.134655	4.005178
H	0.301354	-1.869621	2.418379
C	-1.586456	-3.389570	4.860649
H	-3.588693	-2.769705	5.457560
H	0.398079	-3.768587	4.056289
H	-1.539246	-4.220920	5.581068
C	-2.539367	1.382247	-2.765753
C	-1.207384	1.145933	-3.204437
C	-3.206383	2.531954	-3.273671
C	-0.591912	2.014044	-4.118288

	H	-0.661007	0.263937	-2.843580
	C	-2.585835	3.398697	-4.182244
	H	-4.239030	2.735021	-2.947548
	C	-1.272453	3.141258	-4.614082
	H	0.433066	1.800140	-4.457680
	H	-3.133030	4.274960	-4.563938
	H	-0.783998	3.810843	-5.339184
	C	-3.986689	-1.517003	-0.534260
	C	-3.561699	-2.543351	0.346057
	C	-5.382969	-1.359316	-0.743978
	C	-4.491985	-3.366740	0.999302
	H	-2.489516	-2.697953	0.526561
	C	-6.309257	-2.174870	-0.081365
	H	-5.752790	-0.606574	-1.456338
	C	-5.869733	-3.185324	0.794518
	H	-4.132375	-4.157232	1.676054
	H	-7.385784	-2.033012	-0.265625
	H	-6.599101	-3.834368	1.303792
	C	-1.813176	-0.132606	2.114861
	C	-2.144146	0.921764	1.545440
	C	-2.691474	2.145743	1.047068
	C	-1.902030	3.129378	0.398533
	C	-4.077447	2.399591	1.252606
	C	-2.483410	4.330933	-0.029386
	H	-0.829011	2.943538	0.244068
	C	-4.645257	3.606330	0.823748
	H	-4.695918	1.640387	1.754336
	C	-3.852116	4.576141	0.181424
	H	-1.858764	5.084878	-0.532267
	H	-5.716938	3.793806	0.995254
	H	-4.302155	5.524158	-0.152510

REAL-PhOH-VII-6-PhOH

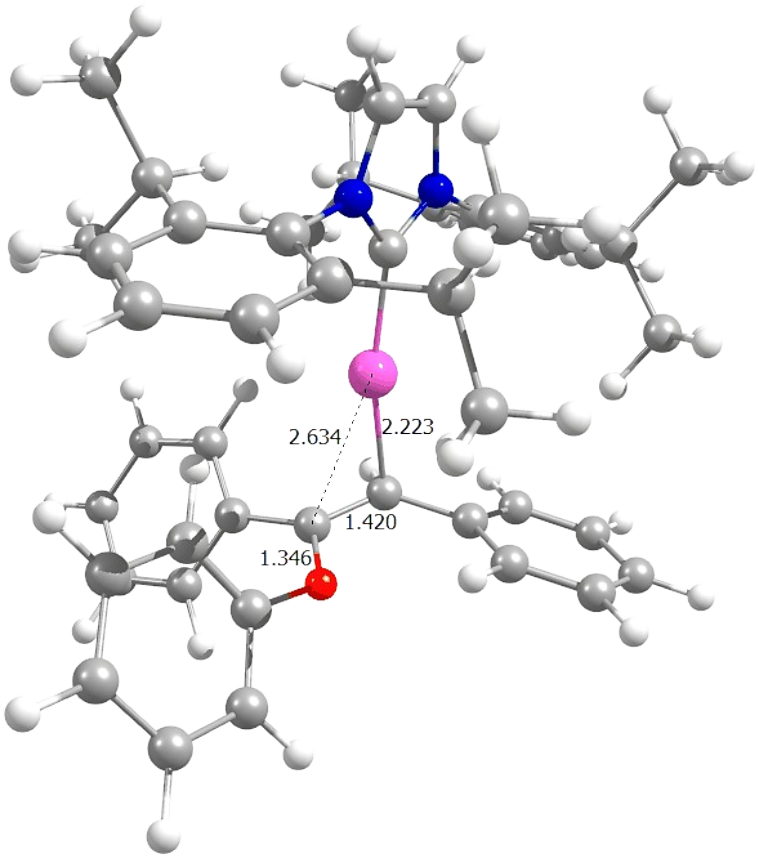


Zero-point correction= 0.948826 (Hartree/Particle)
Thermal correction to Energy= 1.007101
Thermal correction to Enthalpy= 1.008045
Thermal correction to Gibbs Free Energy= 0.848535
Sum of electronic and zero-point Energies= -2447.589459
Sum of electronic and thermal Energies= -2447.531184
Sum of electronic and thermal Enthalpies= -2447.530240
Sum of electronic and thermal Free Energies= -2447.689750

C	1.275904	-1.362094	0.832753
N	2.544467	-1.868874	0.693002
N	0.677050	-2.141518	1.786957
C	2.735816	-2.948581	1.547629
C	1.563105	-3.118113	2.238194
C	3.564438	-1.334888	-0.191631
C	-0.672604	-2.013098	2.307670
H	3.683252	-3.494867	1.584870
H	1.276868	-3.837937	3.010959
C	4.456354	-0.357271	0.327018
C	5.437947	0.144976	-0.552594
C	5.528533	-0.310307	-1.876545
C	4.643931	-1.289695	-2.349875
C	3.641906	-1.834176	-1.518319
C	4.418085	0.106613	1.784198
H	6.150748	0.900785	-0.188064
H	6.308014	0.092057	-2.542799
H	4.737603	-1.650555	-3.386145
C	2.721606	-2.933656	-2.048118
C	-1.667470	-2.900113	1.815350
C	-2.952110	-2.801091	2.388126
C	-3.230910	-1.864504	3.394450
C	-2.222866	-1.010081	3.861391
C	-0.913093	-1.069280	3.340223
C	-1.383714	-3.953073	0.742212
H	-3.747980	-3.480529	2.044764
H	-4.242059	-1.809577	3.827510
H	-2.450160	-0.291346	4.664309
C	0.175877	-0.165921	3.921492
H	3.468983	-0.257181	2.231259
C	4.419181	1.642226	1.920532
C	5.579064	-0.527029	2.585147
H	1.976183	-3.165656	-1.258249
C	1.934605	-2.475927	-3.292449
C	3.513956	-4.231128	-2.325432
H	-0.365200	-3.761475	0.342266
C	-1.387423	-5.376870	1.343377
C	-2.359030	-3.853436	-0.448653
H	1.131137	-0.405858	3.409671
C	-0.117111	1.323956	3.650645
C	0.387101	-0.438575	5.427069
H	4.308954	1.931751	2.985932
H	5.367758	2.090884	1.559585
H	3.585979	2.104763	1.352612
H	5.522387	-0.233327	3.653905
H	5.561368	-1.635291	2.535308
H	6.563255	-0.192790	2.194995
H	1.244618	-3.276578	-3.629090
H	1.324745	-1.572694	-3.083458
H	2.607879	-2.243082	-4.143629
H	2.828893	-5.043509	-2.645181
H	4.260299	-4.086010	-3.134453
H	4.061086	-4.579967	-1.425474
H	-1.124108	-6.126710	0.568730
H	-0.662999	-5.480317	2.177209
H	-2.389691	-5.643307	1.739527
H	-2.063946	-4.567984	-1.244462
H	-3.399555	-4.105570	-0.155510
H	-2.362875	-2.833388	-0.881358
H	0.708425	1.958482	4.034823
H	-0.227918	1.519465	2.563700
H	-1.053474	1.654946	4.145734
H	1.216246	0.185214	5.820920
H	-0.519915	-0.196287	6.019596
H	0.638101	-1.501975	5.619889
Au	0.658725	0.239602	-0.174272
C	-4.665160	-0.011163	-0.942576
C	-5.386406	-1.050052	-0.329137
C	-5.319553	0.977556	-1.698254
C	-6.782597	-1.094097	-0.473520
H	-4.842214	-1.807367	0.253830
C	-6.718244	0.923359	-1.827653
H	-4.739712	1.773713	-2.188809
C	-7.454219	-0.107749	-1.218643
H	-7.351523	-1.906725	0.005096
H	-7.234370	1.695450	-2.419609
H	-8.548888	-0.144874	-1.327105
O	-3.272114	-0.050400	-0.821936
C	-1.572110	1.284424	-1.830449
C	-2.556384	1.127398	-0.878334
H	-1.025670	2.236854	-1.766308
O	1.308064	2.229477	-1.329486
H	1.853864	1.927581	-2.084555
C	1.887919	3.364522	-0.748329
C	1.238794	3.941449	0.354084
C	3.066828	3.915173	-1.276129
C	1.791372	5.094772	0.936867
H	0.306361	3.499639	0.738965
C	3.604082	5.071586	-0.683463
H	3.563360	3.448266	-2.143125
C	2.971748	5.662576	0.423751
H	1.286637	5.554869	1.800462
H	4.526440	5.509680	-1.095343
H	3.396863	6.566867	0.884738
C	-1.284904	0.497504	-3.041315
C	-0.457833	1.095218	-4.033883

	C	-1.819978	-0.790060	-3.317150
	C	-0.189503	0.448634	-5.248900
	H	-0.056823	2.107364	-3.857005
	C	-1.551083	-1.431794	-4.535037
	H	-2.458361	-1.274482	-2.567467
	C	-0.738355	-0.820399	-5.507666
	H	0.437950	0.944504	-6.006532
	H	-1.988694	-2.423654	-4.730703
	H	-0.538826	-1.327603	-6.464486
	C	-2.880209	2.149615	0.149193
	C	-3.439584	1.752359	1.389478
	C	-2.663780	3.531989	-0.082652
	C	-3.763186	2.706163	2.365820
	H	-3.608284	0.683673	1.587493
	C	-2.984123	4.481814	0.899247
	H	-2.277630	3.871198	-1.056355
	C	-3.536947	4.073573	2.127300
	H	-4.200895	2.379053	3.322018
	H	-2.823759	5.551937	0.693967
	H	-3.802166	4.821645	2.890741

REAL-PhOH-VII

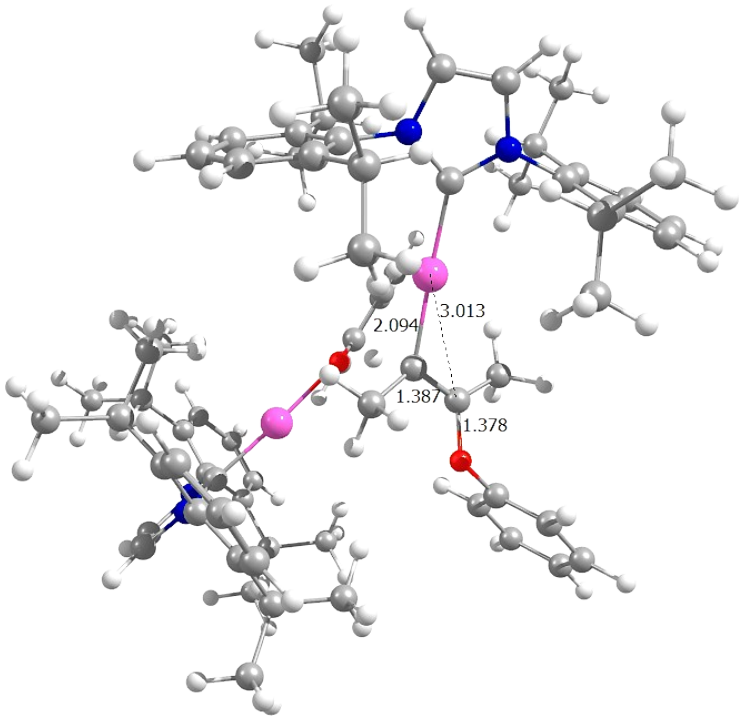


Zero-point correction= 0.846629 (Hartree/Particle)
Thermal correction to Energy= 0.898805
Thermal correction to Enthalpy= 0.899749
Thermal correction to Gibbs Free Energy= 0.754419
Sum of electronic and zero-point Energies= -2140.461810
Sum of electronic and thermal Energies= -2140.409634
Sum of electronic and thermal Enthalpies= -2140.408690
Sum of electronic and thermal Free Energies= -2140.554021

C	-1.247577	1.269841	-0.217057
N	-2.599261	1.406632	-0.036719
N	-0.830993	2.463426	-0.743205
C	-3.022408	2.667445	-0.444764
C	-1.908919	3.333676	-0.890109
C	-3.487256	0.378338	0.477563
C	0.528405	2.815723	-1.111144
H	-4.071325	2.973002	-0.383120
H	-1.784526	4.341536	-1.297874
C	-3.719156	0.319491	1.877874
C	-4.610030	-0.671870	2.339085
C	-5.237375	-1.555708	1.449540
C	-4.989321	-1.467499	0.072723
C	-4.109617	-0.497771	-0.451375
C	-3.084867	1.300734	2.864753
H	-4.821437	-0.748280	3.416903
H	-5.932792	-2.318371	1.833935
H	-5.494076	-2.163889	-0.614652
C	-3.891425	-0.395990	-1.961674
C	0.976542	2.502771	-2.421950
C	2.279834	2.915108	-2.769769
C	3.088398	3.613101	-1.862218
C	2.614711	3.908345	-0.575965
C	1.322372	3.518304	-0.165711
C	0.108164	1.778452	-3.451229
H	2.664812	2.692877	-3.777190
H	4.096542	3.937668	-2.164330
H	3.257412	4.464271	0.124599
C	0.822373	3.884049	1.232833
H	-2.294242	1.863261	2.323692
C	-2.401945	0.583785	4.047603
C	-4.125645	2.329154	3.363177
H	-3.055562	0.314484	-2.136375
C	-3.475676	-1.743127	-2.586782
C	-5.143573	0.181135	-2.660313
H	-0.856759	1.521723	-2.965607
C	-0.214574	2.691628	-4.654963
C	0.753484	0.452898	-3.906814
H	-0.174358	3.414725	1.372758
C	1.742870	3.323244	2.336747
C	0.637103	5.410938	1.378971
H	-1.880106	1.318832	4.694856
H	-3.134239	0.049099	4.687723
H	-1.655932	-0.160426	3.699228
H	-3.651134	3.072033	4.037681
H	-4.593368	2.882098	2.522814
H	-4.941166	1.832374	3.929655
H	-3.250864	-1.610659	-3.665366
H	-2.574364	-2.164877	-2.097153
H	-4.284748	-2.499547	-2.514390
H	-4.964367	0.296270	-3.749526
H	-6.019052	-0.489749	-2.533065
H	-5.424160	1.174754	-2.254177
H	-0.889597	2.172225	-5.366375
H	-0.711978	3.630840	-4.336652
H	0.703843	2.972341	-5.211738
H	0.081099	-0.084548	-4.607082
H	1.714517	0.625111	-4.434953
H	0.955869	-0.215133	-3.044197
H	1.323966	3.547272	3.339786
H	1.857479	2.222949	2.250689
H	2.756691	3.773659	2.297471
H	0.220113	5.659530	2.376958
H	1.603537	5.947760	1.277338
H	-0.051990	5.817885	0.610697
Au	-0.195379	-0.406922	0.220856
C	3.786357	-1.473575	-0.591664
C	3.902701	-0.103474	-0.310857
C	4.812959	-2.189683	-1.227982
C	5.099043	0.550388	-0.654812
H	3.075007	0.446608	0.161302
C	5.997998	-1.517859	-1.569233
H	4.673370	-3.259619	-1.443538
C	6.146724	-0.149590	-1.278143
H	5.204005	1.623427	-0.433881
H	6.810925	-2.071286	-2.064309
H	7.079145	0.372355	-1.542141
O	2.609946	-2.197112	-0.330686
C	0.487529	-2.474513	0.670425
C	1.827395	-2.009929	0.748592
H	0.037519	-2.618855	1.668491
C	-0.113421	-3.348461	-0.377914
C	-1.210533	-4.159003	0.015935
C	0.341616	-3.442708	-1.719466
C	-1.810389	-5.052660	-0.882637
H	-1.585538	-4.093562	1.050205
C	-0.266134	-4.335007	-2.615656
H	1.179589	-2.821204	-2.059472
C	-1.338210	-5.147358	-2.203776
H	-2.649391	-5.682088	-0.547215
H	0.106568	-4.399185	-3.650049
H	-1.804833	-5.850761	-2.910864
C	2.444841	-1.629869	2.051787
C	3.703883	-2.185492	2.392417
C	1.766474	-0.839339	3.009001
C	4.256700	-1.961143	3.661746

	H	4.240846	-2.819717	1.672193
	C	2.326595	-0.615069	4.275430
	H	0.798917	-0.381164	2.742463
	C	3.573695	-1.174798	4.606169
	H	5.229503	-2.409986	3.915287
	H	1.789136	0.008627	5.006323
	H	4.014364	-0.995682	5.599188

REAL-PhOH-VI-VII-PhOH

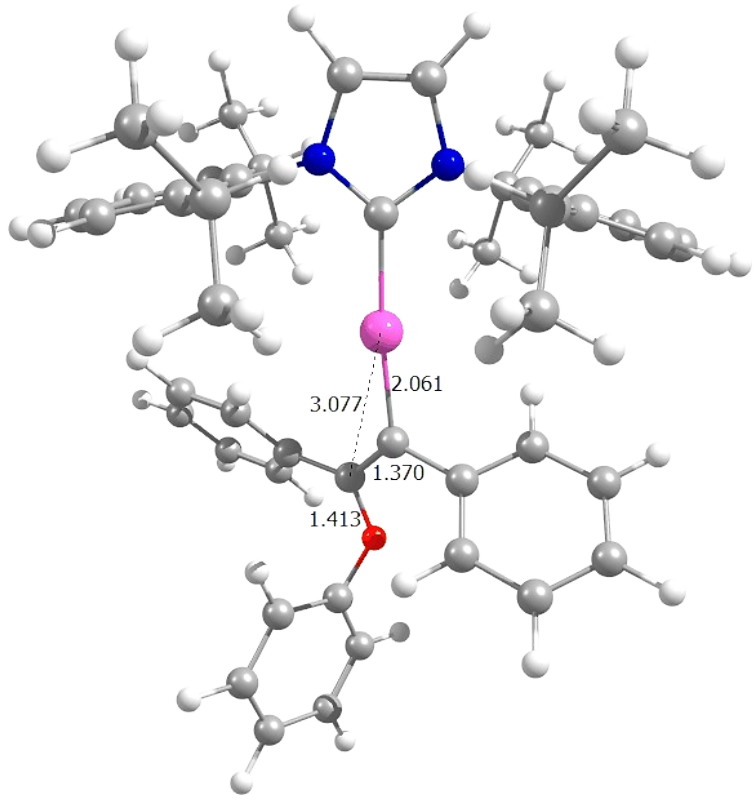


Zero-point correction= 1.486738 (Hartree/Particle)
Thermal correction to Energy= 1.580396
Thermal correction to Enthalpy= 1.581340
Thermal correction to Gibbs Free Energy= 1.341410
Sum of electronic and zero-point Energies= -3741.607478
Sum of electronic and thermal Energies= -3741.513821
Sum of electronic and thermal Enthalpies= -3741.512877
Sum of electronic and thermal Free Energies= -3741.752806

C	-4.453439	-0.587262	-0.456368
N	-5.644392	-0.607865	0.224829
N	-4.762757	-0.971853	-1.734226
C	-6.681384	-1.001413	-0.617378
C	-6.126642	-1.229459	-1.851014
C	-5.815936	-0.265847	1.624425
C	-3.817239	-1.097364	-2.827058
H	-7.712469	-1.085160	-0.260988
H	-6.571897	-1.553190	-2.796794
C	-6.140829	1.078652	1.950351
C	-6.324104	1.385056	3.314422
C	-6.190235	0.400237	4.303714
C	-5.873399	-0.918144	3.948445
C	-5.683459	-1.288313	2.600251
C	-6.304199	2.170526	0.891394
H	-6.578431	2.415901	3.606459
H	-6.339872	0.662358	5.362978
H	-5.775793	-1.681624	4.736128
C	-5.353020	-2.739442	2.248522
C	-3.133157	-2.331331	-2.984978
C	-2.232145	-2.432738	-4.064384
C	-2.033140	-1.361228	-4.946773
C	-2.726597	-0.156730	-4.762741
C	-3.634240	0.009934	-3.696063
C	-3.337908	-3.516387	-2.040082
H	-1.680696	-3.373338	-4.217214
H	-1.329132	-1.465404	-5.787337
H	-2.557541	0.678967	-5.459949
C	-4.369751	1.338545	-3.519397
H	-6.043678	1.728505	-0.093552
C	-5.335953	3.348015	1.128502
C	-7.767845	2.656767	0.806257
H	-5.287781	-2.817303	1.142997
C	-3.978543	-3.155870	2.815062
C	-6.470175	-3.702334	2.705169
H	-4.140853	-3.243539	-1.323602
C	-3.812440	-4.778346	-2.791813
C	-2.063241	-3.791956	-1.214467
H	-4.953208	1.282131	-2.575742
C	-3.386738	2.521216	-3.380143
C	-5.372344	1.581154	-4.669335
H	-5.435977	4.100839	0.319495
H	-5.544157	3.863440	2.089375
H	-4.281587	3.002362	1.148452
H	-7.883983	3.403924	-0.006261
H	-8.468364	1.820847	0.603049
H	-8.090332	3.139748	1.752732
H	-3.725157	-4.189335	2.499471
H	-3.174677	-2.478911	2.458073
H	-3.970834	-3.134233	3.924988
H	-6.229367	-4.743992	2.407385
H	-6.593560	-3.693323	3.808173
H	-7.449575	-3.436199	2.256865
H	-4.018900	-5.599816	-2.074656
H	-4.739922	-4.587694	-3.369667
H	-3.044130	-5.146943	-3.503736
H	-2.233096	-4.623191	-0.498868
H	-1.211718	-4.076848	-1.866600
H	-1.758996	-2.894580	-0.634993
H	-3.941899	3.463884	-3.193153
H	-2.670367	2.373769	-2.546426
H	-2.791103	2.667578	-4.305673
H	-5.931862	2.525657	-4.506066
H	-4.850942	1.667441	-5.645795
H	-6.110549	0.757280	-4.755653
Au	-2.677296	-0.137772	0.286109
C	-0.255677	4.498913	-1.323533
C	-1.173862	4.931515	-0.349520
C	0.326069	5.408939	-2.223006
C	-1.491916	6.298114	-0.265484
H	-1.634926	4.196828	0.328466
C	-0.004862	6.772031	-2.132683
H	1.026588	5.037507	-2.986124
C	-0.908819	7.220459	-1.153149
H	-2.206593	6.643061	0.498330
H	0.448597	7.488536	-2.835562
H	-1.163548	8.289291	-1.084620
O	0.028624	3.141664	-1.478465
C	0.923828	1.076594	-0.774916
C	0.835544	2.449682	-0.600913
C	0.160241	0.479530	-1.957677
H	-0.893857	0.834692	-2.010951
H	0.627634	0.765988	-2.925997
H	0.144704	-0.627035	-1.913752
C	1.545700	3.253814	0.450842
H	2.194356	4.022786	-0.021186
H	0.842499	3.797819	1.114637
H	2.181877	2.586130	1.059631
C	4.471636	-0.825294	0.157196
N	4.732524	-2.174255	0.126018
N	5.699224	-0.246483	0.382310
C	6.088164	-2.430538	0.320665
C	6.698601	-1.214152	0.481197
C	3.754608	-3.213992	-0.128757
C	5.971044	1.175132	0.473458
H	6.489217	-3.448643	0.324172

H	7.746159	-0.948071	0.652019
C	3.526832	-3.609247	-1.473530
C	2.597852	-4.647619	-1.693717
C	1.936121	-5.267836	-0.625135
C	2.190550	-4.862582	0.692860
C	3.105434	-3.827399	0.975701
C	4.240339	-2.961035	-2.660705
H	2.395388	-4.980382	-2.724118
H	1.221441	-6.082988	-0.820146
H	1.669245	-5.362257	1.523982
C	3.403744	-3.439693	2.424671
C	6.056258	1.765710	1.762986
C	6.376352	3.137408	1.827411
C	6.601637	3.886844	0.664341
C	6.513938	3.275895	-0.593765
C	6.201120	1.906073	-0.722761
C	5.848708	0.971509	3.053563
H	6.455217	3.628279	2.810050
H	6.854530	4.956216	0.740256
H	6.699825	3.873783	-1.500298
C	6.139829	1.272550	-2.112702
H	4.967643	-2.224505	-2.258205
C	3.248794	-2.180990	-3.550632
C	5.042165	-3.993439	-3.481737
H	3.949175	-2.472854	2.407883
C	2.123984	-3.221719	3.255687
C	4.327076	-4.485809	3.090278
H	5.440997	-0.023074	2.776546
C	7.189319	0.737444	3.786226
C	4.817843	1.638459	3.986619
H	5.874040	0.202000	-1.985773
C	5.034896	1.919836	-2.973914
C	7.511122	1.326222	-2.820402
H	3.786963	-1.666163	-4.373941
H	2.499355	-2.857743	-4.013340
H	2.700112	-1.414593	-2.965122
H	5.610961	-3.488756	-4.290255
H	5.766130	-4.548524	-2.850392
H	4.375899	-4.739386	-3.963199
H	2.383296	-2.859528	4.272023
H	1.454505	-2.472655	2.786627
H	1.547322	-4.161739	3.384941
H	4.585051	-4.179334	4.125630
H	3.830863	-5.477858	3.145275
H	5.274699	-4.618630	2.528763
H	7.035422	0.122311	4.697388
H	7.926275	0.213170	3.143928
H	7.647511	1.698342	4.102159
H	4.628631	0.996158	4.872098
H	5.174049	2.618768	4.366796
H	3.851885	1.807741	3.468775
H	4.967443	1.418571	-3.961847
H	4.045947	1.843162	-2.477183
H	5.242934	2.995032	-3.158381
H	7.463126	0.807380	-3.800670
H	7.829602	2.372058	-3.014145
H	8.305196	0.841007	-2.216167
Au	2.688374	0.108933	-0.194906
H	0.082746	0.630219	0.411103
O	-0.779361	0.275024	1.115008
C	-0.601103	0.585036	2.453347
C	-1.698105	0.973674	3.248520
C	0.687192	0.499220	3.022168
C	-1.506209	1.271731	4.608024
H	-2.702079	1.034949	2.795750
C	0.865788	0.815499	4.379992
H	1.533537	0.178429	2.392929
C	-0.224170	1.200394	5.180525
H	-2.371654	1.567950	5.221521
H	1.873855	0.748904	4.818062
H	-0.075897	1.438691	6.244893

REAL-PhOH-VI

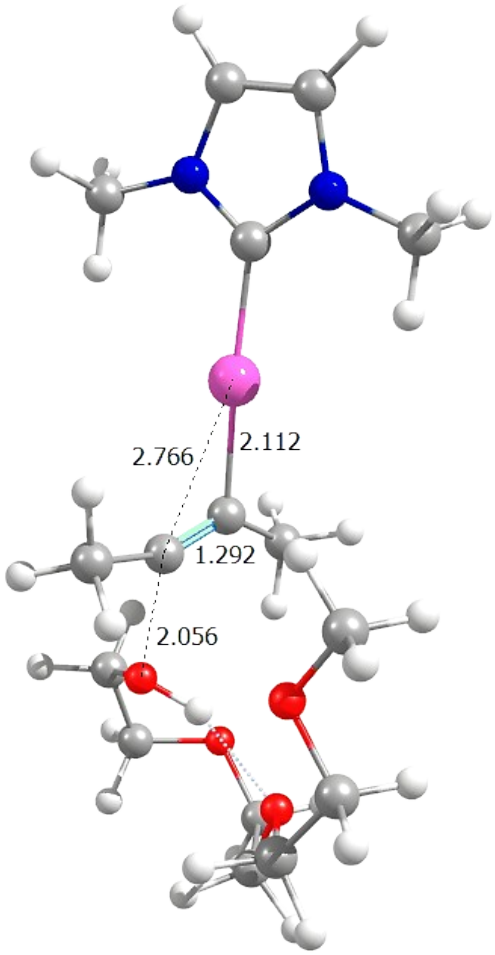


Zero-point correction= 0.833458 (Hartree/Particle)
Thermal correction to Energy= 0.885387
Thermal correction to Enthalpy= 0.886331
Thermal correction to Gibbs Free Energy= 0.740863
Sum of electronic and zero-point Energies= -2140.051192
Sum of electronic and thermal Energies= -2139.999262
Sum of electronic and thermal Enthalpies= -2139.998318
Sum of electronic and thermal Free Energies= -2140.143787

C	2.136393	0.326969	0.117031
N	2.741611	1.512513	0.463404
N	3.188445	-0.535061	-0.093319
C	4.131605	1.390388	0.468766
C	4.413401	0.096111	0.117439
C	2.057128	2.749215	0.776994
C	3.062367	-1.925060	-0.482818
H	4.785075	2.231407	0.720088
H	5.364802	-0.431413	-0.001038
C	1.680094	2.997434	2.122940
C	1.053798	4.230216	2.401529
C	0.825914	5.173782	1.389935
C	1.212342	4.900253	0.070132
C	1.836976	3.682764	-0.270057
C	1.905434	1.981518	3.243366
H	0.741633	4.455511	3.433369
H	0.340692	6.132546	1.633103
H	1.021606	5.646445	-0.716903
C	2.216740	3.390907	-1.722370
C	3.045011	-2.243164	-1.866719
C	2.958343	-3.606659	-2.215716
C	2.896100	-4.605094	-1.233406
C	2.912785	-4.259248	0.124646
C	2.998846	-2.912732	0.534693
C	3.080101	-1.174046	-2.959436
H	2.935938	-3.890863	-3.279710
H	2.828859	-5.663885	-1.530102
H	2.851656	-5.051628	0.886946
C	2.992031	-2.566389	2.024106
H	2.540172	1.166734	2.836288
C	0.569415	1.340192	3.679317
C	2.661744	2.591841	4.441628
H	2.841736	2.473324	-1.727746
C	0.958777	3.089855	-2.566121
C	3.064069	4.518943	-2.346358
H	3.267658	-0.196520	-2.467670
C	4.226585	-1.405462	-3.965888
C	1.712019	-1.070694	-3.668812
H	3.154969	-1.472212	2.117038
C	1.618285	-2.875111	2.658531
C	4.139721	-3.264311	2.784306
H	0.740547	0.579215	4.469390
H	-0.129113	2.101048	4.087759
H	0.070294	0.839616	2.822477
H	2.879315	1.809620	5.198714
H	3.626154	3.045181	4.131422
H	2.067241	3.380862	4.948902
H	1.242776	2.829492	-3.607498
H	0.381122	2.243762	-2.139586
H	0.280457	3.967619	-2.607604
H	3.387476	4.235663	-3.369839
H	2.491087	5.465854	-2.436788
H	3.973784	4.731897	-1.747043
H	4.267701	-0.574933	-4.701352
H	5.212712	-1.463857	-3.459921
H	4.087831	-2.345419	-4.540790
H	1.726556	-0.261637	-4.429026
H	1.454321	-2.017772	-4.188580
H	0.902139	-0.848142	-2.942532
H	1.611960	-2.582287	3.729620
H	0.805067	-2.324569	2.141728
H	1.377739	-3.957365	2.602381
H	4.151313	-2.942810	3.846926
H	4.026199	-4.369001	2.777051
H	5.130474	-3.026217	2.344057
Au	0.148392	-0.163383	-0.023950
C	-2.878318	-0.149713	-0.576875
C	-1.785755	-0.862113	-0.156865
C	-5.240045	-0.595602	-0.262363
C	-6.395812	-1.183248	-0.823002
C	-5.345316	0.182383	0.910444
C	-7.644098	-0.988914	-0.215209
H	-6.285562	-1.793982	-1.732047
C	-6.605495	0.370549	1.505561
H	-4.444269	0.634796	1.349922
C	-7.759778	-0.208537	0.951443
H	-8.539239	-1.453532	-0.659719
H	-6.679831	0.981383	2.420026
H	-8.742231	-0.055596	1.424657
O	-4.054208	-0.865309	-0.897200
C	-1.946232	-2.310964	0.168424
C	-1.127602	-3.291540	-0.448901
C	-2.885862	-2.758652	1.132968
C	-1.260596	-4.654947	-0.139487
H	-0.379527	-2.966870	-1.190086
C	-3.007566	-4.119783	1.455724
H	-3.525286	-2.020676	1.642317
C	-2.200099	-5.078716	0.817704
H	-0.618483	-5.392351	-0.648373
H	-3.745345	-4.434157	2.212152
H	-2.300170	-6.147369	1.067488
C	-2.952047	1.294664	-0.920758
C	-3.793227	1.728769	-1.977385
C	-2.228253	2.277724	-0.202184
C	-3.890689	3.087325	-2.313725
H	-4.368957	0.980511	-2.542396

	C	-2.332648	3.637609	-0.535528
	H	-1.591202	1.962852	0.639605
	C	-3.162647	4.051360	-1.593315
	H	-4.545650	3.396298	-3.144551
	H	-1.766820	4.380579	0.048197
	H	-3.250672	5.119998	-1.847602

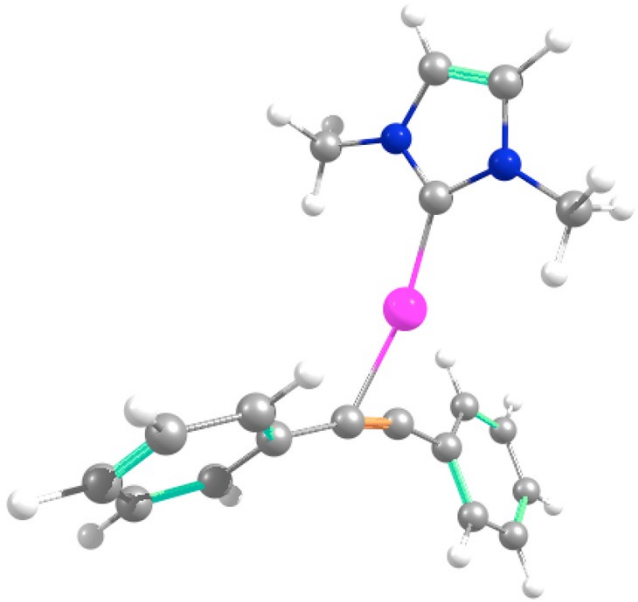
TS



C	-3.703326	0.016539	-0.119467
N	-4.406806	1.046081	-0.685244
C	-5.772757	0.861231	-0.512792
C	-5.928771	-0.314285	0.177761
N	-4.654100	-0.816016	0.407827
C	-3.816031	2.188302	-1.381489
C	-4.381219	-2.064267	1.119851
Au	-1.682696	-0.245007	-0.099803
C	0.395555	-0.577456	-0.276306
C	0.951899	-0.885180	-1.637749
C	0.880758	-0.459187	0.915782
C	0.833769	-0.095871	2.337333
O	2.878968	-0.941661	0.958164
C	3.119021	-2.337551	0.698146
C	4.478548	-2.539206	0.042957
O	4.469117	-1.791860	-1.170551
C	5.621808	-1.010304	-1.459166
C	5.836503	0.134229	-0.469786
O	4.618524	0.867350	-0.340918
C	4.745335	1.995171	0.533777
C	3.600233	2.965776	0.324215
O	2.381853	2.404683	0.775854
C	1.281895	3.274521	0.578513
H	-6.515074	1.571599	-0.891521
H	-6.833678	-0.827756	0.519207
H	0.482961	-1.798798	-2.058526
H	2.051276	-1.025005	-1.618273
H	0.717805	-0.060083	-2.341494
H	-0.196622	0.219347	2.599718
H	1.522482	0.754284	2.522360
H	1.121335	-0.941325	2.994457
H	-4.096036	3.132830	-0.874341
H	-4.163922	2.218343	-2.433007
H	-2.716384	2.074785	-1.363708
H	-3.287755	-2.228477	1.129395
H	-4.873286	-2.912927	0.605040
H	-4.752152	-2.000705	2.162044
H	2.324209	-2.744119	0.034450
H	3.067742	-2.875047	1.668013
H	4.639007	-3.624171	-0.161020
H	5.289281	-2.204715	0.729602
H	6.548950	-1.630858	-1.503172
H	5.442536	-0.597910	-2.472839
H	6.654612	0.791842	-0.851225
H	6.169095	-0.240199	0.529888
H	5.696990	2.533404	0.314059
H	4.782725	1.659492	1.598084
H	3.537453	3.231996	-0.760746
H	3.838131	3.907580	0.881484
H	0.371824	2.749090	0.928864
H	1.148199	3.537069	-0.498854
H	1.394141	4.225209	1.154299
H	3.346477	-0.372502	0.274261

Zero-point correction= 0.439693 (Hartree/Particle)
Thermal correction to Energy= 0.469302
Thermal correction to Enthalpy= 0.470247
Thermal correction to Gibbs Free Energy= 0.373849
Sum of electronic and zero-point Energies= -1172.567823
Sum of electronic and thermal Energies= -1172.538213
Sum of electronic and thermal Enthalpies= -1172.537269
Sum of electronic and thermal Free Energies= -1172.633667

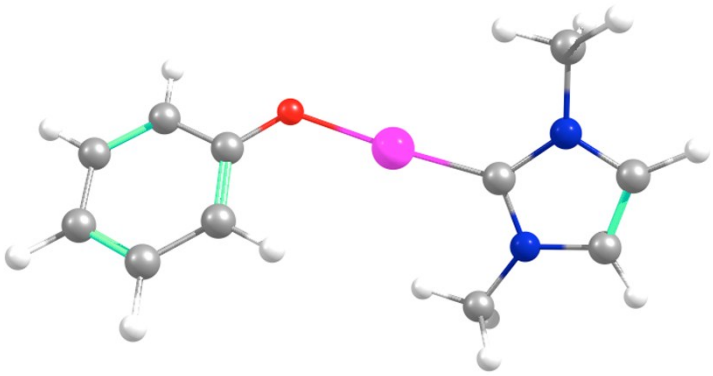
I-s



Zero-point correction= 0.312416
(Hartree/Particle)
Thermal correction to Energy= 0.334556
Thermal correction to Enthalpy= 0.335500
Thermal correction to Gibbs Free Energy= 0.255233
Sum of electronic and zero-point Energies= -979.110519
Sum of electronic and thermal Energies= -979.088380
Sum of electronic and thermal Enthalpies= -979.087436
Sum of electronic and thermal Free Energies= -979.167702

6	-2.537548000	0.001089000	-0.000013000
7	-3.366706000	-0.448164000	-0.991881000
7	-3.366396000	0.450638000	0.991974000
6	-4.693748000	-0.283589000	-0.624919000
6	-4.693552000	0.286592000	0.625193000
6	-2.932928000	-1.043744000	-2.257447000
1	-5.524610000	-0.582936000	-1.272619000
1	-5.524211000	0.586237000	1.273013000
79	-0.511091000	0.000404000	-0.000064000
6	1.627633000	0.627109000	-0.089632000
6	1.626733000	-0.628577000	0.089383000
6	2.022144000	2.013896000	-0.110950000
6	3.113542000	2.427930000	0.700621000
6	1.367517000	2.962381000	-0.939640000
6	3.538753000	3.762489000	0.669115000
1	3.618984000	1.695175000	1.347541000
6	1.799760000	4.295270000	-0.956745000
1	0.528224000	2.638925000	-1.574523000
6	2.884233000	4.697290000	-0.155129000
1	4.387711000	4.077265000	1.295553000
1	1.291658000	5.025925000	-1.604762000
1	3.222770000	5.744916000	-0.173653000
6	2.019998000	-2.015741000	0.110874000
6	1.364367000	-2.963541000	0.939554000
6	3.111120000	-2.430858000	-0.700499000
6	1.795392000	-4.296820000	0.956876000
1	0.525264000	-2.639243000	1.574259000
6	3.535103000	-3.765805000	-0.668791000
1	3.617321000	-1.698643000	-1.347437000
6	2.879615000	-4.699918000	0.155459000
1	1.286532000	-5.026944000	1.604897000
1	4.383854000	-4.081428000	-1.295083000
1	3.217190000	-5.747851000	0.174146000
1	-3.405307000	-0.511497000	-3.105730000
1	-3.211087000	-2.115651000	-2.292264000
1	-1.834093000	-0.949904000	-2.333381000
6	-2.932192000	1.046421000	2.257296000
1	-1.833664000	0.949856000	2.334296000
1	-3.406679000	0.516221000	3.105672000
1	-3.207631000	2.119078000	2.290812000

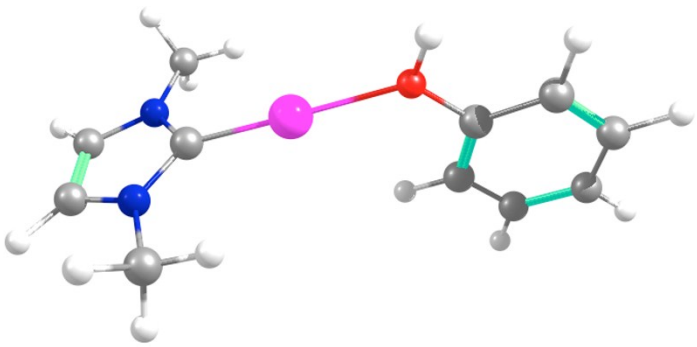
II-s



Zero-point correction= 0.216312 (Hartree/Particle)
Thermal correction to Energy= 0.231935
Thermal correction to Enthalpy= 0.232879
Thermal correction to Gibbs Free Energy= 0.169561
Sum of electronic and zero-point Energies= -746.982050
Sum of electronic and thermal Energies= -746.966428
Sum of electronic and thermal Enthalpies= -746.965484
Sum of electronic and thermal Free Energies= -747.028802

6	2.145208000	0.185738000	-0.018245000
7	3.224197000	-0.595895000	-0.355472000
7	2.672975000	1.438104000	0.183773000
6	4.395532000	0.152934000	-0.362098000
6	4.047656000	1.435785000	-0.023787000
6	3.153032000	-2.022862000	-0.656941000
6	1.895237000	2.615305000	0.560385000
1	5.370175000	-0.283482000	-0.603407000
1	4.659085000	2.337331000	0.085382000
79	0.248634000	-0.368354000	0.129792000
6	-2.760227000	-0.371445000	0.077084000
6	-2.782857000	0.906803000	-0.548427000
6	-4.011651000	-0.953131000	0.430461000
6	-3.994708000	1.570100000	-0.798687000
1	-1.820466000	1.362265000	-0.841761000
6	-5.215416000	-0.281917000	0.174515000
1	-4.003088000	-1.943675000	0.911848000
6	-5.223443000	0.985812000	-0.440369000
1	-3.976953000	2.559677000	-1.286066000
1	-6.168007000	-0.758068000	0.461999000
1	-6.172430000	1.508199000	-0.638789000
8	-1.642854000	-1.060782000	0.340266000
1	3.567826000	-2.223562000	-1.665009000
1	2.089260000	-2.325902000	-0.631826000
1	3.717122000	-2.607769000	0.097418000
1	2.300544000	3.060630000	1.490834000
1	0.850372000	2.294957000	0.732516000
1	1.916935000	3.371414000	-0.250313000

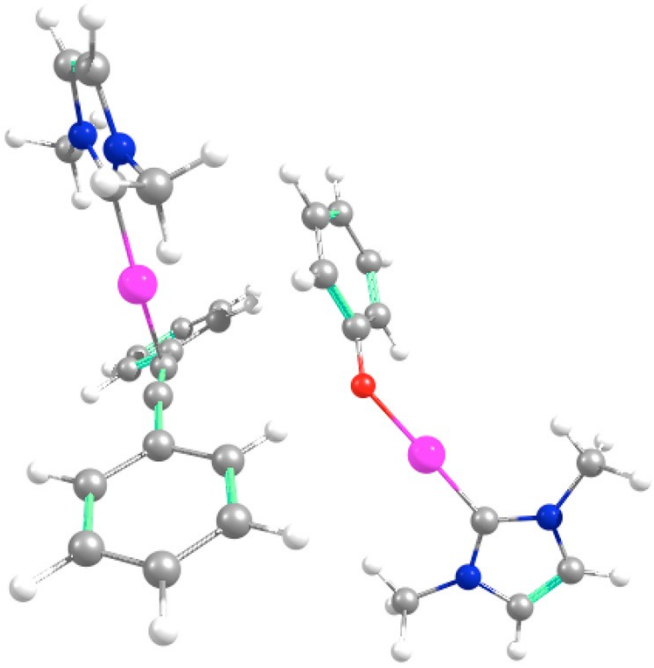
II+-s



Zero-point correction= 0.228260 (Hartree/Particle)
Thermal correction to Energy= 0.244795
Thermal correction to Enthalpy= 0.245739
Thermal correction to Gibbs Free Energy= 0.178555
Sum of electronic and zero-point Energies= -747.358034
Sum of electronic and thermal Energies= -747.341499
Sum of electronic and thermal Enthalpies= -747.340555
Sum of electronic and thermal Free Energies= -747.407740

6	-2.196597000	0.067905000	0.132424000
7	-2.929397000	1.221975000	0.134474000
7	-3.043644000	-0.914752000	0.563451000
6	-4.224128000	0.963825000	0.563040000
6	-4.296153000	-0.380338000	0.832398000
6	-2.704791000	-2.331046000	0.722364000
1	-4.982473000	1.750019000	0.641244000
1	-5.129596000	-0.993550000	1.191063000
79	-0.299606000	-0.139020000	-0.388684000
6	2.938648000	-0.118825000	-0.257363000
6	2.817780000	0.216703000	1.095640000
6	4.180277000	-0.207242000	-0.899305000
6	3.989272000	0.472404000	1.829382000
1	1.823259000	0.275767000	1.567681000
6	5.341658000	0.051920000	-0.149371000
1	4.251408000	-0.474602000	-1.966904000
6	5.249598000	0.390796000	1.211383000
1	3.910452000	0.737044000	2.894930000
1	6.324263000	-0.014114000	-0.640964000
1	6.162429000	0.591878000	1.791793000
8	1.755113000	-0.384623000	-0.989572000
1	1.953528000	-0.591739000	-1.924963000
6	-2.443854000	2.548412000	-0.253902000
1	-3.031170000	2.931022000	-1.111432000
1	-1.381505000	2.464754000	-0.547531000
1	-2.532955000	3.249706000	0.598716000
1	-2.875380000	-2.645585000	1.770422000
1	-1.637874000	-2.469931000	0.468967000
1	-3.325375000	-2.948763000	0.043992000

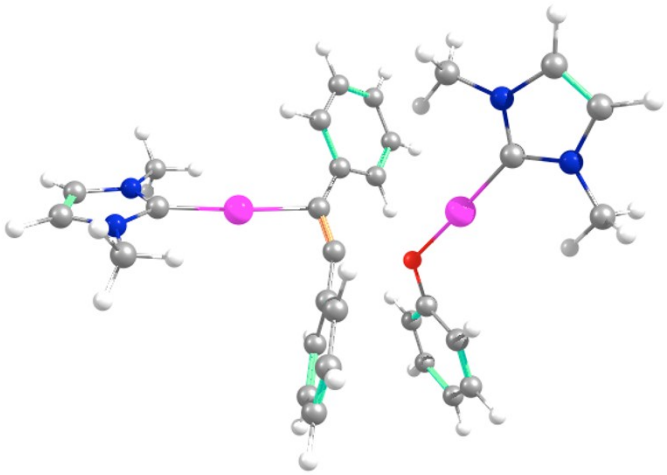
III-s



Zero-point correction= 0.529608 (Hartree/Particle)
Thermal correction to Energy= 0.569654
Thermal correction to Enthalpy= 0.570598
Thermal correction to Gibbs Free Energy= 0.444333
Sum of electronic and zero-point Energies= -1726.111169
Sum of electronic and thermal Energies= -1726.071123
Sum of electronic and thermal Enthalpies= -1726.070179
Sum of electronic and thermal Free Energies= -1726.196445

6	-4.612172000	-0.458576000	1.174551000
7	-5.724161000	0.330606000	1.278430000
7	-4.681132000	-1.326272000	2.229457000
6	-6.478316000	-0.036891000	2.385985000
6	-5.821874000	-1.082716000	2.984230000
6	-6.080244000	1.418948000	0.367485000
6	-3.702215000	-2.370114000	2.535533000
1	-7.410506000	0.470223000	2.655910000
1	-6.071684000	-1.667645000	3.875529000
79	-3.163907000	-0.352910000	-0.230841000
6	-1.746297000	0.330725000	-1.845276000
6	-1.501758000	-0.894015000	-1.680419000
6	5.557841000	-0.039068000	0.093019000
7	6.587755000	0.210458000	0.963679000
7	6.165333000	-0.284141000	-1.112252000
6	7.813028000	0.122717000	0.313914000
6	7.546935000	-0.190556000	-0.994659000
6	6.430456000	0.533001000	2.380906000
6	5.465805000	-0.607270000	-2.353808000
1	8.764282000	0.289812000	0.829623000
1	8.220943000	-0.352471000	-1.842163000
79	3.611954000	-0.025435000	0.491260000
6	0.897621000	0.905622000	1.390420000
6	-0.383536000	0.649818000	1.963178000
6	1.340537000	2.259233000	1.359439000
6	-1.168441000	1.694737000	2.477829000
1	-0.721446000	-0.397078000	2.023888000
6	0.548166000	3.294947000	1.880070000
1	2.330375000	2.475932000	0.921915000
6	-0.715782000	3.027889000	2.441168000
1	-2.146154000	1.461492000	2.932161000
1	0.928519000	4.329435000	1.850108000
1	-1.328232000	3.841851000	2.858392000
8	1.604269000	-0.121878000	0.906654000
6	-0.976519000	-2.234674000	-1.618602000
6	-1.554787000	-3.268770000	-2.402310000
6	0.135555000	-2.512522000	-0.777265000
6	-1.017899000	-4.562008000	-2.353411000
1	-2.417718000	-3.044562000	-3.047898000
6	0.654140000	-3.815896000	-0.740117000
1	0.585603000	-1.704621000	-0.169782000
6	0.084467000	-4.838336000	-1.522024000
1	-1.462181000	-5.360985000	-2.967134000
1	1.516966000	-4.032820000	-0.090824000
1	0.500481000	-5.857556000	-1.484496000
6	-1.815586000	1.702481000	-2.285617000
6	-2.325807000	2.004340000	-3.576323000
6	-1.357422000	2.749823000	-1.442706000
6	-2.363997000	3.334294000	-4.016625000
1	-2.680158000	1.189006000	-4.225225000
6	-1.402565000	4.074305000	-1.900446000
1	-0.958991000	2.515953000	-0.443013000
6	-1.904587000	4.370274000	-3.181331000
1	-2.753321000	3.564646000	-5.020540000
1	-1.038945000	4.882516000	-1.247328000
1	-1.937050000	5.413619000	-3.532539000
1	-5.316331000	1.475313000	-0.429695000
1	-6.105663000	2.382332000	0.913868000
1	-7.071462000	1.225428000	-0.087716000
1	-3.249087000	-2.189068000	3.529994000
1	-2.909619000	-2.347045000	1.765302000
1	-4.190276000	-3.364539000	2.526309000
1	5.353143000	0.494546000	2.627827000
1	6.817566000	1.550333000	2.589251000
1	6.976064000	-0.203675000	3.003262000
1	4.378467000	-0.522015000	-2.170473000
1	5.703744000	-1.641344000	-2.674505000
1	5.759766000	0.102295000	-3.152346000

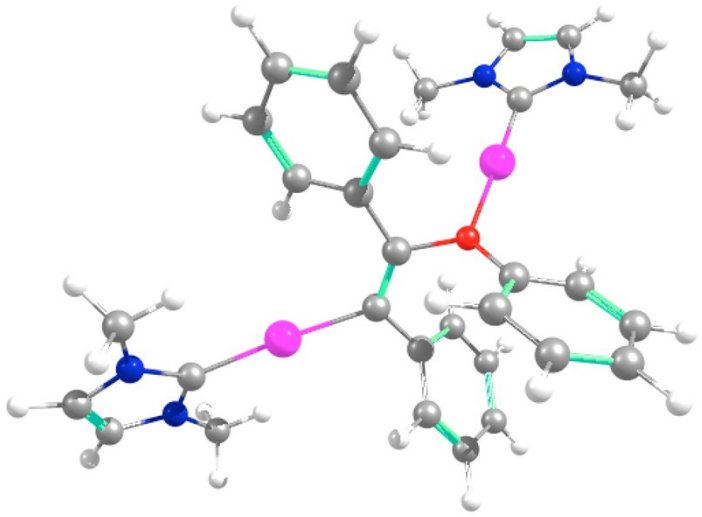
III-IV-s



Zero-point correction= 0.529350
(Hartree/Particle)
Thermal correction to Energy= 0.568418
Thermal correction to Enthalpy= 0.569362
Thermal correction to Gibbs Free Energy= 0.445954
Sum of electronic and zero-point Energies= -1726.101265
Sum of electronic and thermal Energies= -1726.062196
Sum of electronic and thermal Enthalpies= -1726.061252
Sum of electronic and thermal Free Energies= -1726.184661

6	-4.903116000	-0.381763000	-0.519470000
7	-5.925782000	-0.934002000	0.204889000
7	-5.496245000	0.117590000	-1.648182000
6	-7.136710000	-0.781096000	-0.458859000
6	-6.865836000	-0.117080000	-1.628630000
6	-5.778909000	-1.586660000	1.505659000
6	-4.796499000	0.804536000	-2.732579000
1	-8.082413000	-1.151462000	-0.049626000
1	-7.529301000	0.203838000	-2.438443000
79	-2.934634000	-0.332885000	-0.006335000
6	-0.461751000	0.751989000	0.277961000
6	-0.921272000	-0.403011000	0.657056000
6	3.996588000	-1.537833000	-1.069221000
7	3.716975000	-2.835579000	-1.408867000
7	5.277126000	-1.320167000	-1.506826000
6	4.803677000	-3.416927000	-2.051152000
6	5.786910000	-2.462434000	-2.112164000
6	2.455079000	-3.524058000	-1.140198000
6	6.020323000	-0.070428000	-1.352686000
1	4.790591000	-4.453094000	-2.404587000
1	6.799094000	-2.504030000	-2.527494000
79	2.813720000	-0.259626000	-0.122455000
6	1.950232000	2.252388000	1.311205000
6	1.509794000	2.787518000	2.548582000
6	2.754388000	3.057982000	0.467068000
6	1.891223000	4.080943000	2.937465000
1	0.880091000	2.164174000	3.202477000
6	3.132004000	4.350108000	0.866451000
1	3.076549000	2.650489000	-0.505622000
6	2.704927000	4.869222000	2.102319000
1	1.553892000	4.475980000	3.909213000
1	3.764881000	4.960011000	0.201827000
1	3.004743000	5.881759000	2.413351000
8	1.573144000	0.990085000	0.974020000
6	-0.457947000	-1.569622000	1.430627000
6	-0.966896000	-2.861177000	1.137185000
6	0.469502000	-1.435245000	2.495882000
6	-0.552629000	-3.983441000	1.872484000
1	-1.696776000	-2.972810000	0.318790000
6	0.867420000	-2.558511000	3.237727000
1	0.872666000	-0.439919000	2.725266000
6	0.363292000	-3.835787000	2.929717000
1	-0.958965000	-4.977656000	1.627234000
1	1.579314000	-2.433006000	4.069037000
1	0.676616000	-4.712216000	3.518730000
6	-0.533944000	2.003851000	-0.420614000
6	-0.146897000	2.081895000	-1.787683000
6	-0.954103000	3.185611000	0.247764000
6	-0.208545000	3.303707000	-2.469081000
1	0.196742000	1.169113000	-2.298236000
6	-1.007220000	4.405031000	-0.443498000
1	-1.248118000	3.129620000	1.305747000
6	-0.638664000	4.466752000	-1.799050000
1	0.084416000	3.354777000	-3.529565000
1	-1.336276000	5.315094000	0.081369000
1	-0.681144000	5.426740000	-2.337344000
1	5.382535000	0.647736000	-0.804949000
1	6.278060000	0.348692000	-2.345632000
1	6.948750000	-0.247189000	-0.774584000
1	1.821341000	-2.870958000	-0.511532000
1	2.649131000	-4.469646000	-0.597465000
1	1.926866000	-3.745096000	-2.089313000
1	-4.705389000	-1.597124000	1.771469000
1	-6.154166000	-2.627801000	1.455082000
1	-6.341571000	-1.029414000	2.280772000
1	-4.906095000	0.238963000	-3.679263000
1	-3.725100000	0.872551000	-2.468471000
1	-5.204927000	1.825910000	-2.864712000

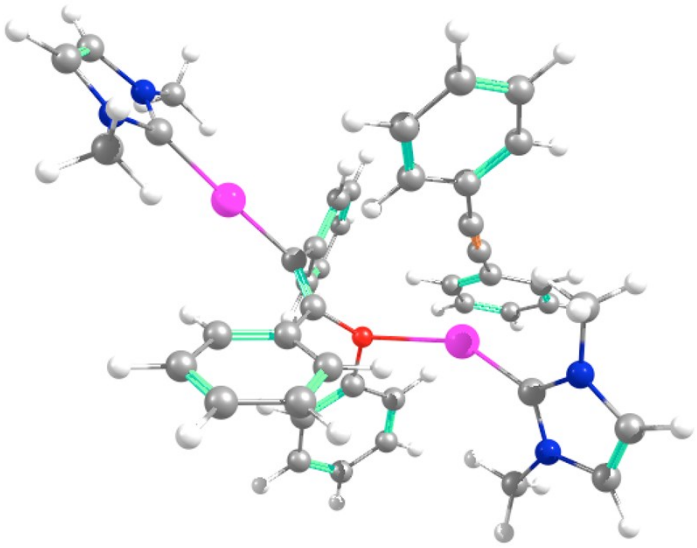
IV-s



Zero-point correction=	0.531810 (Hartree/Particle)
Thermal correction to Energy=	0.570404
Thermal correction to Enthalpy=	0.571349
Thermal correction to Gibbs Free Energy=	0.450942
Sum of electronic and zero-point Energies=	-1726.117504
Sum of electronic and thermal Energies=	-1726.078909
Sum of electronic and thermal Enthalpies=	-1726.077965
Sum of electronic and thermal Free Energies=	-1726.198372

6	4.970210000	-0.697123000	-0.333116000
7	5.669481000	-1.466139000	0.560396000
7	5.881038000	-0.381034000	-1.307500000
6	6.988550000	-1.626387000	0.152944000
6	7.121770000	-0.941280000	-1.028589000
6	5.113357000	-2.024627000	1.791006000
6	5.591027000	0.432856000	-2.486725000
1	7.717349000	-2.206076000	0.728967000
1	7.988629000	-0.809690000	-1.684505000
79	3.006266000	-0.113003000	-0.228314000
6	0.073648000	-0.010040000	0.557862000
6	1.073183000	0.603871000	-0.134456000
6	-4.535898000	-1.089196000	-0.895122000
7	-5.848681000	-0.750404000	-0.711115000
7	-4.548754000	-2.168770000	-1.735518000
6	-6.672815000	-1.606855000	-1.430441000
6	-5.854483000	-2.499148000	-2.075714000
6	-6.334814000	0.348343000	0.124198000
6	-3.366087000	-2.877781000	-2.226511000
1	-7.763804000	-1.514600000	-1.421296000
1	-6.092615000	-3.335825000	-2.740632000
79	-2.947220000	-0.211944000	-0.108457000
6	-1.258535000	1.876200000	1.515595000
6	-0.383808000	2.053585000	2.598249000
6	-2.234485000	2.831813000	1.195436000
6	-0.507238000	3.215282000	3.380359000
1	0.386329000	1.300132000	2.818904000
6	-2.349070000	3.983721000	1.992554000
1	-2.878951000	2.679265000	0.314739000
6	-1.487880000	4.179151000	3.086323000
1	0.172867000	3.361799000	4.233956000
1	-3.108962000	4.740518000	1.742914000
1	-1.576362000	5.085048000	3.705016000
8	-1.205996000	0.700436000	0.735127000
6	0.836784000	1.891811000	-0.846980000
6	-0.142471000	1.989414000	-1.868762000
6	1.624988000	3.038087000	-0.573566000
6	-0.329350000	3.185205000	-2.581639000
1	-0.744668000	1.101330000	-2.122617000
6	1.421439000	4.239764000	-1.270472000
1	2.401916000	2.977054000	0.205391000
6	0.445635000	4.319564000	-2.280431000
1	-1.084237000	3.230173000	-3.383414000
1	2.037516000	5.120483000	-1.028419000
1	0.296563000	5.258200000	-2.836873000
6	0.008657000	-1.345929000	1.186979000
6	-0.800546000	-1.581638000	2.330693000
6	0.733138000	-2.442061000	0.648264000
6	-0.855356000	-2.851574000	2.928168000
1	-1.376351000	-0.753700000	2.772227000
6	0.677435000	-3.708175000	1.250157000
1	1.333228000	-2.286021000	-0.262357000
6	-0.114356000	-3.920588000	2.394688000
1	-1.478812000	-3.003602000	3.823442000
1	1.245914000	-4.543686000	0.810885000
1	-0.159653000	-4.916446000	2.862794000
1	-5.464475000	0.846299000	0.589751000
1	-6.999267000	-0.043198000	0.919330000
1	-6.889578000	1.081185000	-0.494233000
1	-2.477504000	-2.495801000	-1.691023000
1	-3.240177000	-2.708632000	-3.314409000
1	-3.469894000	-3.962451000	-2.029731000
1	4.029271000	-1.805832000	1.811274000
1	5.595538000	-1.565069000	2.677102000
1	5.268012000	-3.121422000	1.817441000
1	4.540144000	0.772034000	-2.422559000
1	5.728423000	-0.163377000	-3.410896000
1	6.259564000	1.316023000	-2.516820000

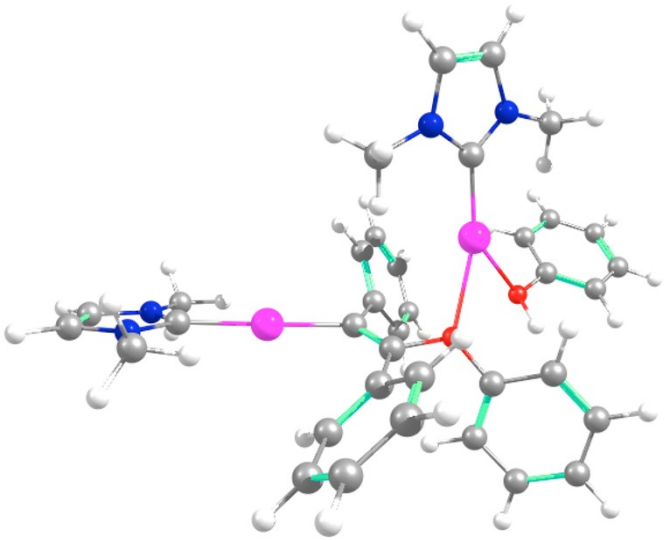
IV-V-alkyne-s TS



Zero-point correction= 0.717777 (Hartree/Particle)
Thermal correction to Energy= 0.769228
Thermal correction to Enthalpy= 0.770172
Thermal correction to Gibbs Free Energy= 0.619449
Sum of electronic and zero-point Energies= -2264.986433
Sum of electronic and thermal Energies= -2264.934982
Sum of electronic and thermal Enthalpies= -2264.934037
Sum of electronic and thermal Free Energies= -2265.084761

6	-5.461934000	0.219770000	-0.230942000
7	-6.140100000	1.392103000	-0.016290000
7	-6.391363000	-0.619978000	-0.789274000
6	-7.462608000	1.286144000	-0.431111000
6	-7.621061000	0.013752000	-0.919339000
6	-5.557507000	2.597513000	0.567906000
6	-6.134537000	-2.003543000	-1.185965000
1	-8.175347000	2.113036000	-0.346085000
1	-8.499446000	-0.485368000	-1.341616000
79	-3.502274000	-0.222927000	0.189758000
6	-0.614410000	-0.035716000	1.179029000
6	-1.546203000	-0.798240000	0.536106000
6	4.104833000	1.923050000	0.049481000
7	5.146558000	1.894625000	0.937708000
7	4.359798000	2.983267000	-0.778273000
6	6.042152000	2.922045000	0.666222000
6	5.545356000	3.609601000	-0.411535000
6	5.315692000	0.922885000	2.017748000
1	6.950530000	3.077895000	1.257293000
1	5.932130000	4.486233000	-0.941330000
79	2.554460000	0.663039000	-0.028811000
6	1.299561000	-1.074657000	2.324395000
6	0.686380000	-0.981813000	3.587343000
6	2.496556000	-1.800304000	2.164011000
6	1.296049000	-1.606705000	4.691349000
1	-0.252140000	-0.426546000	3.714377000
6	3.092435000	-2.416854000	3.276889000
1	2.930553000	-1.913784000	1.157179000
6	2.498002000	-2.319852000	4.548103000
1	0.815618000	-1.528326000	5.679360000
1	4.020277000	-2.994739000	3.140407000
1	2.962586000	-2.807292000	5.418766000
8	0.768968000	-0.480826000	1.170766000
6	0.633227000	0.923301000	-2.988184000
6	1.006217000	1.448316000	-4.257871000
6	-0.498169000	1.468443000	-2.323267000
6	0.265502000	2.486232000	-4.839830000
1	1.874807000	1.021548000	-4.782508000
6	-1.228266000	2.508539000	-2.917207000
1	-0.803259000	1.060380000	-1.346932000
6	-0.851973000	3.022030000	-4.171854000
1	0.559055000	2.877338000	-5.826780000
1	-2.103932000	2.919549000	-2.391075000
1	-1.430812000	3.837864000	-4.632576000
6	-0.834388000	1.266174000	1.864519000
6	-2.031206000	1.497630000	2.593948000
6	0.131451000	2.302075000	1.848224000
6	-2.260354000	2.719919000	3.245396000
1	-2.771891000	0.685706000	2.668778000
6	-0.097621000	3.525212000	2.499196000
1	1.080591000	2.149063000	1.304327000
6	-1.297349000	3.744391000	3.198043000
1	-3.190331000	2.863979000	3.818695000
1	0.670131000	4.314539000	2.460736000
1	-1.473178000	4.699511000	3.717477000
6	-1.251159000	-2.171448000	0.033590000
6	-1.434315000	-2.507563000	-1.333420000
6	-0.903776000	-3.215589000	0.929058000
6	-1.272514000	-3.827054000	-1.785169000
1	-1.714892000	-1.714097000	-2.044424000
6	-0.765585000	-4.540786000	0.479417000
1	-0.778752000	-2.988584000	1.998942000
6	-0.947750000	-4.854698000	-0.879256000
1	-1.412349000	-4.057805000	-2.853492000
1	-0.519332000	-5.335308000	1.202207000
1	-0.843527000	-5.893312000	-1.230549000
6	1.404895000	-0.145529000	-2.422507000
6	2.116396000	-1.117523000	-2.117637000
6	2.949185000	-2.260890000	-1.889241000
6	2.473559000	-3.381458000	-1.156757000
6	4.266109000	-2.291778000	-2.427303000
6	3.300643000	-4.499125000	-0.972737000
1	1.452712000	-3.369130000	-0.748091000
6	5.080343000	-3.415915000	-2.235730000
1	4.633541000	-1.428021000	-3.002159000
6	4.601734000	-4.521857000	-1.507653000
1	2.919294000	-5.365235000	-0.409872000
1	6.095590000	-3.432847000	-2.662279000
1	5.243122000	-5.405370000	-1.362836000
1	-6.121332000	2.894491000	1.474625000
1	-5.578492000	3.430784000	-0.162937000
1	-4.509143000	2.379020000	0.844539000
1	-5.067863000	-2.226351000	-0.995805000
1	-6.351954000	-2.139601000	-2.264007000
1	-6.764120000	-2.697300000	-0.593841000
6	3.503261000	3.429570000	-1.876437000
1	3.076067000	4.426394000	-1.649121000
1	2.680624000	2.702316000	-2.003283000
1	4.089422000	3.485401000	-2.814309000
1	5.496398000	1.451831000	2.973573000
1	6.169234000	0.250203000	1.800557000
1	4.389991000	0.323362000	2.101910000

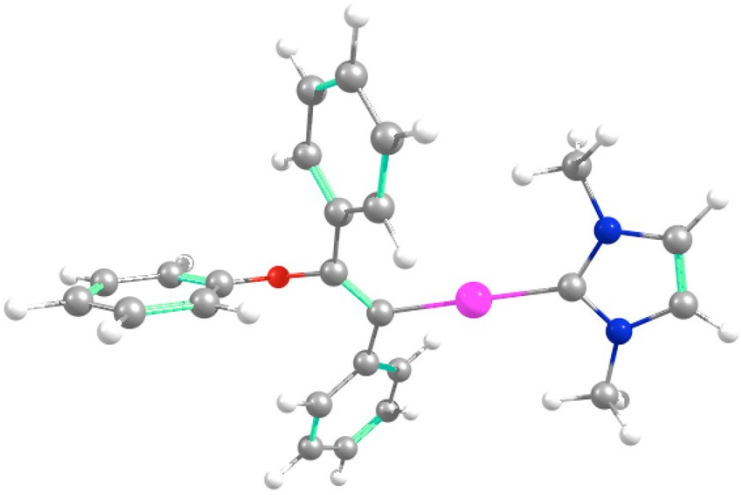
IV-V-phoh-s TS



Zero-point correction= 0.634025 (Hartree/Particle)
Thermal correction to Energy= 0.679437
Thermal correction to Enthalpy= 0.680381
Thermal correction to Gibbs Free Energy= 0.543311
Sum of electronic and zero-point Energies= -2033.262962
Sum of electronic and thermal Energies= -2033.217550
Sum of electronic and thermal Enthalpies= -2033.216606
Sum of electronic and thermal Free Energies= -2033.353676

6	5.061930000	-0.974793000	-0.515112000
7	6.058835000	-0.620872000	0.357510000
7	5.654912000	-1.862567000	-1.375912000
6	7.246567000	-1.273675000	0.048570000
6	6.991270000	-2.057596000	-1.048160000
6	5.897434000	0.304968000	1.476475000
6	4.982355000	-2.505475000	-2.503238000
1	8.166082000	-1.128984000	0.625243000
1	7.645934000	-2.726782000	-1.616152000
79	3.117692000	-0.318319000	-0.553378000
6	0.654494000	1.363497000	0.010127000
6	1.144652000	0.278699000	-0.654969000
6	-2.197283000	-1.748504000	2.269654000
7	-3.322618000	-2.427927000	2.652934000
7	-1.208774000	-2.169694000	3.119590000
6	-3.041983000	-3.259770000	3.729847000
6	-1.711241000	-3.098604000	4.022471000
6	-4.646502000	-2.284621000	2.047093000
6	0.177836000	-1.703883000	3.104682000
1	-3.803610000	-3.895598000	4.192965000
1	-1.086281000	-3.568361000	4.788968000
79	-2.022587000	-0.415957000	0.814398000
6	-1.327656000	2.776009000	-0.299893000
6	-0.744740000	3.594005000	-1.285862000
6	-2.534822000	3.154130000	0.325092000
6	-1.387073000	4.789629000	-1.650289000
1	0.204125000	3.295066000	-1.754865000
6	-3.170357000	4.350158000	-0.059932000
1	-2.941327000	2.528343000	1.137247000
6	-2.600903000	5.170260000	-1.049639000
1	-0.930548000	5.429782000	-2.421457000
1	-4.107376000	4.648641000	0.436174000
1	-3.095340000	6.107990000	-1.344895000
8	-0.776019000	1.552094000	0.063758000
8	-3.305072000	0.544282000	-1.118782000
1	-3.337098000	1.525384000	-1.028028000
6	-4.545286000	0.041850000	-1.480002000
6	-5.684325000	0.865578000	-1.546276000
6	-4.628315000	-1.328585000	-1.789684000
6	-6.917034000	0.306537000	-1.926911000
1	-5.606035000	1.939139000	-1.307710000
6	-5.868868000	-1.872963000	-2.162917000
1	-3.712483000	-1.939817000	-1.763346000
6	-7.016805000	-1.062142000	-2.232240000
1	-7.806893000	0.952885000	-1.984511000
1	-5.934168000	-2.943121000	-2.416057000
1	-7.984117000	-1.493520000	-2.531378000
6	1.395762000	2.344145000	0.843110000
6	2.655535000	2.845340000	0.430243000
6	0.859364000	2.809030000	2.070023000
6	3.365591000	3.754342000	1.231448000
1	3.062977000	2.528880000	-0.543033000
6	1.572637000	3.714991000	2.870717000
1	-0.125151000	2.444521000	2.402177000
6	2.830462000	4.189968000	2.457207000
1	4.335814000	4.144172000	0.883853000
1	1.141233000	4.055878000	3.825314000
1	3.383667000	4.909856000	3.080696000
6	0.266391000	-0.564015000	-1.519063000
6	0.127181000	-1.958028000	-1.277556000
6	-0.368904000	-0.032307000	-2.671627000
6	-0.614298000	-2.778894000	-2.144531000
1	0.640810000	-2.399570000	-0.408464000
6	-1.093658000	-0.855958000	-3.547646000
1	-0.263720000	1.040373000	-2.896236000
6	-1.222206000	-2.233001000	-3.289949000
1	-0.698807000	-3.857549000	-1.934517000
1	-1.559650000	-0.418307000	-4.444860000
1	-1.781217000	-2.878391000	-3.985648000
1	-5.092283000	-3.284868000	1.885533000
1	-4.539747000	-1.772934000	1.072239000
1	-5.310538000	-1.687803000	2.704155000
1	0.398050000	-1.129228000	4.026199000
1	0.323562000	-1.050956000	2.223335000
1	0.866296000	-2.568700000	3.036173000
1	3.916977000	-2.208514000	-2.485136000
1	5.059056000	-3.607580000	-2.417061000
1	5.436001000	-2.180091000	-3.460786000
1	4.894863000	0.767050000	1.406668000
1	6.669685000	1.097828000	1.428415000
1	5.987033000	-0.232841000	2.441998000

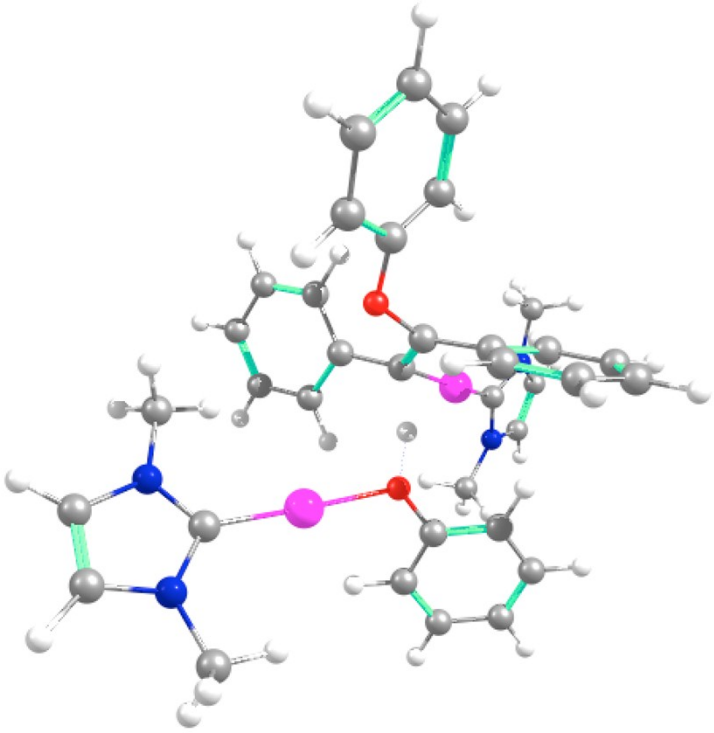
V-s



Zero-point correction= 0.405261 (Hartree/Particle)
Thermal correction to Energy= 0.432936
Thermal correction to Enthalpy= 0.433881
Thermal correction to Gibbs Free Energy= 0.342038
Sum of electronic and zero-point Energies= -1285.886332
Sum of electronic and thermal Energies= -1285.858656
Sum of electronic and thermal Enthalpies= -1285.857712
Sum of electronic and thermal Free Energies= -1285.949555

6	-3.455523000	-0.210580000	0.171485000
7	-4.095286000	-1.386276000	-0.132632000
7	-4.462153000	0.632159000	0.572944000
6	-5.466458000	-1.277815000	0.070763000
6	-5.698526000	-0.001680000	0.518766000
6	-3.425454000	-2.580307000	-0.642600000
6	-4.255209000	2.010212000	1.009591000
1	-6.157277000	-2.106505000	-0.116224000
1	-6.630431000	0.497629000	0.803576000
79	-1.453254000	0.206463000	0.014644000
6	1.515950000	-0.253132000	-0.378444000
6	0.535283000	0.689952000	-0.207984000
6	3.922235000	-0.133316000	-0.134432000
6	5.145948000	0.069073000	-0.809957000
6	3.922604000	-0.569404000	1.207529000
6	6.357718000	-0.170843000	-0.146856000
1	5.118177000	0.420864000	-1.852520000
6	5.146751000	-0.809600000	1.856848000
1	2.969494000	-0.716290000	1.736250000
6	6.367991000	-0.615385000	1.189405000
1	7.307408000	-0.008860000	-0.682104000
1	5.139090000	-1.151971000	2.904456000
1	7.321581000	-0.805808000	1.706018000
8	2.782391000	0.158532000	-0.841881000
6	0.870109000	2.140058000	-0.276147000
6	0.106194000	3.020282000	-1.086631000
6	1.922343000	2.707224000	0.489208000
6	0.391422000	4.393849000	-1.147617000
1	-0.719012000	2.600189000	-1.685268000
6	2.198179000	4.082943000	0.441408000
1	2.521097000	2.056495000	1.145296000
6	1.438753000	4.935306000	-0.380588000
1	-0.212260000	5.048226000	-1.798012000
1	3.017689000	4.493577000	1.053804000
1	1.659034000	6.014290000	-0.419545000
6	1.344834000	-1.729893000	-0.320566000
6	2.016428000	-2.562835000	-1.250539000
6	0.523656000	-2.349792000	0.655197000
6	1.841401000	-3.955210000	-1.231334000
1	2.670484000	-2.099743000	-2.004817000
6	0.353630000	-3.744387000	0.676109000
1	0.038405000	-1.720887000	1.418632000
6	1.006308000	-4.554952000	-0.270776000
1	2.364367000	-4.579445000	-1.973904000
1	-0.277119000	-4.204178000	1.454824000
1	0.879371000	-5.649297000	-0.249439000
1	-3.178848000	2.243831000	0.901584000
1	-4.551597000	2.130422000	2.071253000
1	-4.847076000	2.706358000	0.381991000
1	-2.334315000	-2.455517000	-0.505719000
1	-3.640863000	-2.718377000	-1.721790000
1	-3.766824000	-3.473652000	-0.083371000

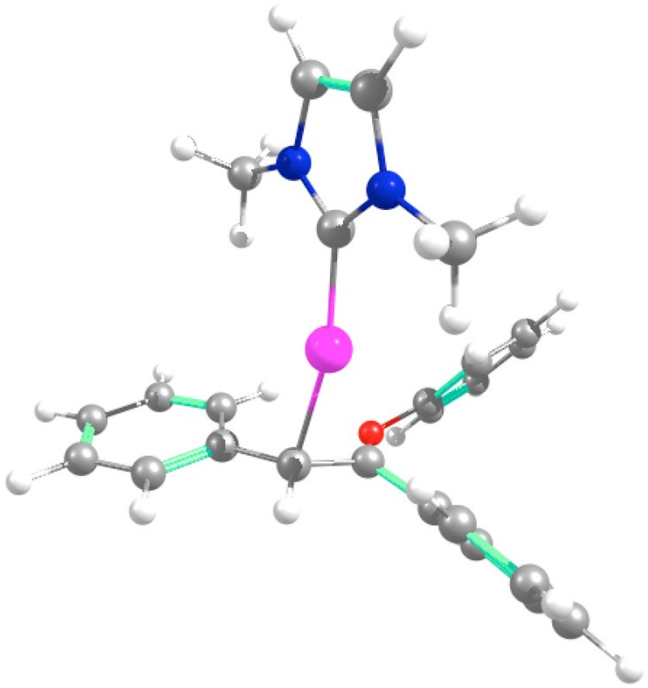
V-VI-s



Zero-point correction= 0.629646 (Hartree/Particle)
Thermal correction to Energy= 0.674166
Thermal correction to Enthalpy= 0.675110
Thermal correction to Gibbs Free Energy= 0.540869
Sum of electronic and zero-point Energies= -2033.278803
Sum of electronic and thermal Energies= -2033.234284
Sum of electronic and thermal Enthalpies= -2033.233339
Sum of electronic and thermal Free Energies= -2033.367581

6	-4.451808000	-1.224398000	-0.236011000
7	-5.494998000	-1.832729000	0.410355000
7	-5.009832000	-0.596042000	-1.316692000
6	-6.688479000	-1.586842000	-0.257212000
6	-6.382677000	-0.806432000	-1.343502000
6	-5.382315000	-2.636736000	1.626855000
6	-4.279575000	0.209263000	-2.297593000
1	-7.647207000	-1.985973000	0.089630000
1	-7.023777000	-0.389032000	-2.126797000
79	-2.540563000	-1.233659000	0.279859000
6	-0.936307000	4.019347000	0.155759000
6	-2.209638000	4.594971000	0.316543000
6	0.221938000	4.818540000	0.148640000
6	-2.319690000	5.984594000	0.484253000
1	-3.098119000	3.945780000	0.308616000
6	0.095310000	6.207710000	0.322575000
1	1.210891000	4.357818000	0.004874000
6	-1.170091000	6.795659000	0.491823000
1	-3.315468000	6.437314000	0.612694000
1	1.000159000	6.835626000	0.318653000
1	-1.261158000	7.884352000	0.625457000
8	-0.892058000	2.648525000	-0.080123000
6	0.557221000	0.823645000	-0.534075000
6	0.172685000	1.866460000	0.310245000
6	4.343434000	-0.869077000	-0.766871000
7	4.669019000	-2.198651000	-0.789855000
7	5.531714000	-0.212214000	-0.949209000
6	6.035057000	-2.369199000	-0.973867000
6	6.581285000	-1.114231000	-1.075879000
6	3.706545000	-3.289159000	-0.618827000
6	5.686179000	1.239389000	-1.014119000
1	6.503407000	-3.357621000	-1.023960000
1	7.616398000	-0.795349000	-1.235326000
79	2.488391000	-0.064931000	-0.522957000
1	0.143896000	-0.278861000	0.253928000
8	-0.519463000	-1.150724000	0.841441000
6	0.018973000	0.735595000	-1.933023000
6	-0.270174000	-0.536488000	-2.497333000
6	-0.141660000	1.870555000	-2.771224000
6	-0.718664000	-0.667975000	-3.822791000
1	-0.119928000	-1.440658000	-1.886190000
6	-0.581944000	1.738819000	-4.097384000
1	0.102657000	2.871284000	-2.385825000
6	-0.881063000	0.470968000	-4.631087000
1	-0.928029000	-1.670418000	-4.229877000
1	-0.684246000	2.638350000	-4.725504000
1	-1.218881000	0.371739000	-5.674751000
6	0.632138000	2.058031000	1.710569000
6	1.990407000	1.930863000	2.086605000
6	-0.321974000	2.352199000	2.719728000
6	2.381697000	2.071524000	3.428134000
1	2.744766000	1.736693000	1.306438000
6	0.069958000	2.486084000	4.058510000
1	-1.383307000	2.452498000	2.448505000
6	1.423556000	2.347745000	4.418810000
1	3.445336000	1.979678000	3.699252000
1	-0.687045000	2.700111000	4.829080000
1	1.731077000	2.463579000	5.469966000
6	0.178407000	-2.208031000	1.381158000
6	1.225512000	-1.945701000	2.292138000
6	-0.137030000	-3.541027000	1.038450000
6	1.937982000	-3.016756000	2.859598000
1	1.448607000	-0.905124000	2.571582000
6	0.575379000	-4.603240000	1.621115000
1	-0.953637000	-3.732319000	0.322245000
6	1.617630000	-4.347739000	2.531758000
1	2.741141000	-2.805197000	3.583635000
1	0.310949000	-5.640544000	1.360501000
1	2.167887000	-5.182140000	2.993458000
1	-3.193707000	0.062184000	-2.146389000
1	-4.522746000	1.283004000	-2.172416000
1	-4.550140000	-0.113025000	-3.321416000
1	-5.696157000	-3.680683000	1.427956000
1	-6.016015000	-2.207628000	2.427858000
1	-4.325901000	-2.628403000	1.953266000
1	3.394368000	-3.379226000	0.441001000
1	4.174166000	-4.235315000	-0.948309000
1	2.811324000	-3.091004000	-1.236788000
1	6.192027000	1.526786000	-1.956892000
1	6.280203000	1.605660000	-0.152838000
1	4.679434000	1.696131000	-0.988111000

VI-s



Zero-point correction= 0.418055 (Hartree/Particle)
Thermal correction to Energy= 0.446016
Thermal correction to Enthalpy= 0.446961
Thermal correction to Gibbs Free Energy= 0.354246
Sum of electronic and zero-point Energies= -1286.291512
Sum of electronic and thermal Energies= -1286.263551
Sum of electronic and thermal Enthalpies= -1286.262607
Sum of electronic and thermal Free Energies= -1286.355322

6	2.368463000	-1.532655000	-0.299761000
7	2.638036000	-2.805604000	0.123044000
7	3.313301000	-1.257794000	-1.250530000
6	3.734773000	-3.320414000	-0.555048000
6	4.160003000	-2.344170000	-1.421445000
6	1.896914000	-3.534760000	1.152156000
6	3.428239000	-0.005406000	-2.000885000
1	4.120546000	-4.328208000	-0.368705000
1	4.987438000	-2.336598000	-2.138738000
79	0.924612000	-0.268538000	0.356397000
6	-2.423418000	0.396725000	-1.611396000
6	-2.153906000	-0.975162000	-1.742981000
6	-3.291709000	1.064799000	-2.489838000
6	-2.788112000	-1.690538000	-2.774299000
1	-1.456008000	-1.475771000	-1.054729000
6	-3.915168000	0.334535000	-3.514813000
1	-3.469942000	2.142918000	-2.360217000
6	-3.668846000	-1.043116000	-3.658258000
1	-2.586297000	-2.767323000	-2.886097000
1	-4.600233000	0.849733000	-4.205765000
1	-4.161070000	-1.611691000	-4.461800000
8	-1.784137000	1.203363000	-0.654517000
6	-0.284117000	1.419934000	1.168757000
6	-1.391546000	0.767011000	0.562609000
1	-0.238559000	1.257417000	2.259579000
6	0.450376000	2.636092000	0.723663000
6	1.271565000	3.273449000	1.692709000
6	0.385893000	3.202624000	-0.577965000
6	1.991395000	4.435165000	1.382147000
1	1.333792000	2.850669000	2.708844000
6	1.110034000	4.365573000	-0.881944000
1	-0.244796000	2.739694000	-1.347212000
6	1.913625000	4.987547000	0.091089000
1	2.612204000	4.915463000	2.154393000
1	1.038703000	4.796845000	-1.892934000
1	2.474302000	5.902711000	-0.155034000
6	-2.295079000	-0.128533000	1.342428000
6	-3.695851000	-0.013080000	1.161800000
6	-1.808165000	-1.006538000	2.340873000
6	-4.577660000	-0.752804000	1.963821000
1	-4.100519000	0.679629000	0.410017000
6	-2.693562000	-1.745584000	3.137922000
1	-0.720232000	-1.119335000	2.482099000
6	-4.082706000	-1.622456000	2.950872000
1	-5.663293000	-0.642748000	1.817877000
1	-2.297833000	-2.426400000	3.907486000
1	-4.778320000	-2.205065000	3.574477000
1	4.436506000	0.429694000	-1.857492000
1	2.669552000	0.705335000	-1.624481000
1	3.254840000	-0.189486000	-3.079499000
1	1.550258000	-4.507428000	0.751820000
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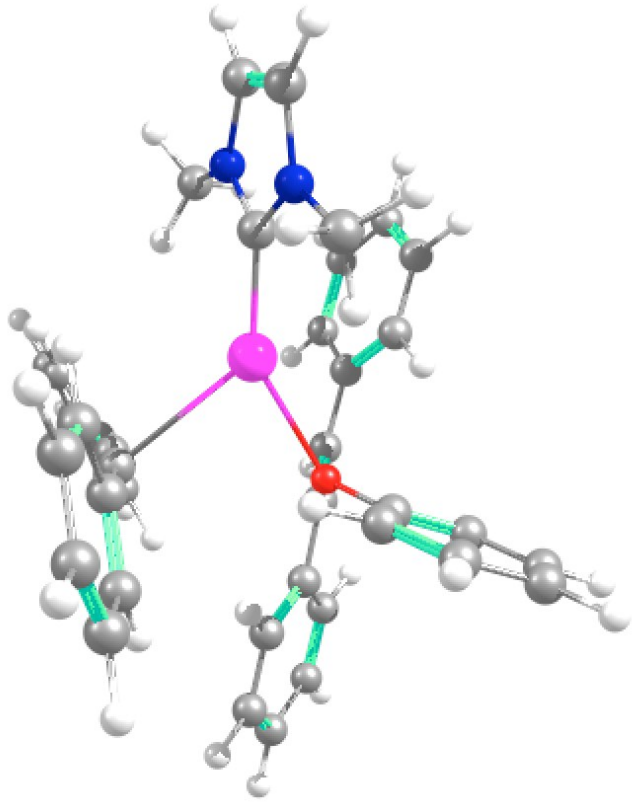

Zero-point correction= 0.604037 (Hartree/Particle)
Thermal correction to Energy= 0.645038
Thermal correction to Enthalpy= 0.645982
Thermal correction to Gibbs Free Energy= 0.521575
Sum of electronic and zero-point Energies= -1825.155549
Sum of electronic and thermal Energies= -1825.114547
Sum of electronic and thermal Enthalpies= -1825.113603
Sum of electronic and thermal Free Energies= -1825.238011

6	2.004823000	-0.857439000	-1.078324000
6	1.537455000	-2.116394000	-1.325566000
6	-3.045728000	0.120970000	-0.102226000
7	-3.878957000	1.086886000	-0.597459000
7	-3.858568000	-0.918315000	0.254937000
6	-5.199965000	0.654568000	-0.550890000
6	-5.185846000	-0.610089000	-0.019318000
6	-3.459650000	2.399724000	-1.086830000
6	-3.390171000	-2.208756000	0.762743000
1	-6.033075000	1.277542000	-0.892415000
1	-6.003941000	-1.309064000	0.183125000
79	-1.057755000	0.185093000	0.055963000
6	1.274983000	1.281502000	-1.973365000
6	1.848720000	1.060428000	-3.235471000
6	0.811106000	2.550948000	-1.591042000
6	1.951863000	2.141003000	-4.130229000
1	2.209650000	0.059269000	-3.514771000
6	0.915834000	3.617728000	-2.500030000
1	0.395405000	2.698480000	-0.580922000
6	1.485651000	3.417235000	-3.770519000
1	2.401031000	1.975662000	-5.121900000
1	0.561552000	4.617357000	-2.203435000
1	1.571511000	4.256575000	-4.477173000
8	1.100194000	0.228026000	-1.053246000
1	2.262792000	-2.917903000	-1.112171000
6	0.112177000	2.401239000	2.335583000
6	1.212938000	3.291194000	2.209608000
6	-1.183155000	2.940441000	2.568004000
6	1.018584000	4.676515000	2.310228000
1	2.222220000	2.882000000	2.053929000
6	-1.364136000	4.326648000	2.671396000
1	-2.035640000	2.254198000	2.684653000
6	-0.267362000	5.199245000	2.538890000
1	1.881655000	5.354337000	2.219613000
1	-2.369068000	4.732177000	2.868468000
1	-0.413697000	6.287239000	2.624284000
6	0.225663000	-2.584212000	-1.788622000
6	-0.682902000	-1.792930000	-2.544661000
6	-0.131511000	-3.935127000	-1.526337000
6	-1.892112000	-2.334858000	-3.008656000
1	-0.416227000	-0.762986000	-2.821703000
6	-1.346274000	-4.469097000	-1.979128000
1	0.566832000	-4.572511000	-0.960320000
6	-2.234941000	-3.669773000	-2.723681000
1	-2.565660000	-1.711765000	-3.618376000
1	-1.593440000	-5.521418000	-1.767414000
1	-3.177702000	-4.094158000	-3.103774000
6	3.400285000	-0.525853000	-0.716615000
6	3.698564000	0.628941000	0.049584000
6	4.473785000	-1.359613000	-1.123071000
6	5.020440000	0.925240000	0.415168000
1	2.880100000	1.290081000	0.368386000
6	5.792153000	-1.063626000	-0.749168000
1	4.276623000	-2.234466000	-1.761803000
6	6.072422000	0.079120000	0.022756000
1	5.232396000	1.825145000	1.013659000
1	6.611419000	-1.721488000	-1.078924000
1	7.109572000	0.314780000	0.307532000
6	0.311324000	0.979558000	2.276216000
6	0.571463000	-0.226634000	2.426366000
6	0.852539000	-1.594116000	2.738752000
6	-0.126829000	-2.387800000	3.399011000
6	2.120546000	-2.165665000	2.446427000
6	0.156928000	-3.715060000	3.747291000
1	-1.099360000	-1.939614000	3.655126000
6	2.392070000	-3.493830000	2.802407000
1	2.885590000	-1.553149000	1.946646000
6	1.414327000	-4.272954000	3.448818000
1	-0.604085000	-4.317725000	4.267429000
1	3.380895000	-3.924053000	2.579313000
1	1.635687000	-5.314345000	3.730142000
1	-3.713075000	3.189687000	-0.352022000
1	-3.962823000	2.617036000	-2.048708000
1	-2.365103000	2.384517000	-1.242862000
1	-2.482407000	-2.049843000	1.373623000
1	-3.141820000	-2.887463000	-0.078134000
1	-4.180412000	-2.661186000	1.390438000

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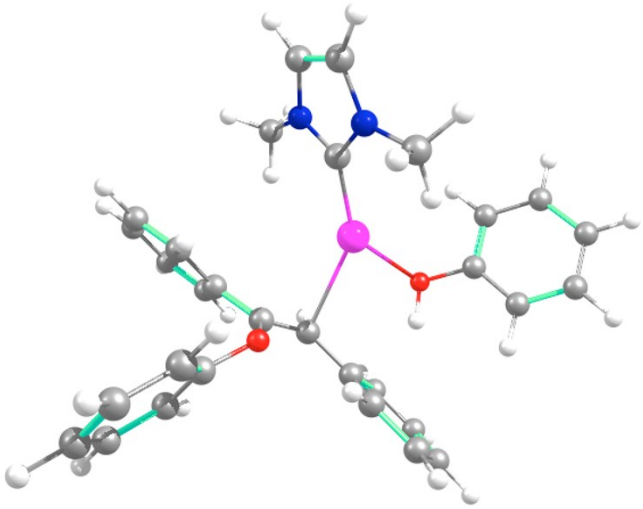

Zero-point correction= 0.519988 (Hartree/Particle)
Thermal correction to Energy= 0.554946
Thermal correction to Enthalpy= 0.555890
Thermal correction to Gibbs Free Energy= 0.444408
Sum of electronic and zero-point Energies= -1593.430083
Sum of electronic and thermal Energies= -1593.395125
Sum of electronic and thermal Enthalpies= -1593.394181
Sum of electronic and thermal Free Energies= -1593.505663

6	-0.603460000	-2.485710000	0.683401000
7	-0.921499000	-2.830958000	1.969169000
7	-0.109409000	-3.625533000	0.109719000
6	-0.631525000	-4.171900000	2.195787000
6	-0.124081000	-4.672893000	1.024103000
6	-1.474273000	-1.925783000	2.976221000
6	0.321308000	-3.751897000	-1.282316000
1	-0.807968000	-4.654601000	3.162664000
1	0.221480000	-5.679736000	0.767603000
79	-0.818646000	-0.691352000	-0.177865000
6	3.395193000	1.403265000	1.088910000
6	3.785948000	1.102625000	2.404293000
6	4.267427000	2.045716000	0.194500000
6	5.083481000	1.439415000	2.823470000
1	3.071854000	0.614031000	3.084340000
6	5.564928000	2.369548000	0.627892000
1	3.934316000	2.300657000	-0.822748000
6	5.977436000	2.067497000	1.937393000
1	5.397235000	1.207505000	3.853212000
1	6.254793000	2.873137000	-0.067071000
1	6.993402000	2.328631000	2.270395000
8	2.067453000	1.107776000	0.745645000
6	0.572403000	1.323803000	-1.081662000
6	1.714649000	0.751822000	-0.525350000
1	0.356387000	0.991175000	-2.111554000
8	-2.538875000	0.753744000	-1.006812000
1	-2.218087000	1.692360000	-1.014828000
6	-3.832705000	0.681047000	-0.487282000
6	-4.542766000	-0.519601000	-0.656289000
6	-4.407810000	1.778743000	0.176081000
6	-5.848985000	-0.617464000	-0.148935000
1	-4.071835000	-1.358263000	-1.191440000
6	-5.719915000	1.667905000	0.670222000
1	-3.834644000	2.711872000	0.303784000
6	-6.442899000	0.472874000	0.513208000
1	-6.412159000	-1.554218000	-0.283983000
1	-6.176411000	2.527958000	1.184617000
1	-7.469259000	0.392141000	0.902129000
6	-0.142781000	2.546934000	-0.657038000
6	-0.914751000	3.233186000	-1.640653000
6	-0.115155000	3.087404000	0.657805000
6	-1.611534000	4.413777000	-1.328311000
1	-0.932016000	2.853475000	-2.676244000
6	-0.814644000	4.265576000	0.960852000
1	0.462212000	2.578022000	1.439581000
6	-1.565556000	4.935559000	-0.023631000
1	-2.184717000	4.930858000	-2.113708000
1	-0.772011000	4.668023000	1.985301000
1	-2.107202000	5.861534000	0.223895000
6	2.544199000	-0.262685000	-1.227270000
6	3.231154000	-1.259634000	-0.488978000
6	2.666926000	-0.258089000	-2.639185000
6	4.007083000	-2.225419000	-1.146002000
1	3.148803000	-1.278187000	0.607558000
6	3.440639000	-1.229526000	-3.292929000
1	2.181380000	0.533942000	-3.230244000
6	4.114538000	-2.215516000	-2.549552000
1	4.539591000	-2.988881000	-0.557232000
1	3.535480000	-1.202964000	-4.389660000
1	4.734317000	-2.967243000	-3.062920000
1	-0.447450000	-4.281167000	-1.880685000
1	1.275847000	-4.309635000	-1.328994000
1	0.476971000	-2.738719000	-1.696724000
1	-2.359825000	-2.389197000	3.452610000
1	-1.780504000	-0.989108000	2.474752000
1	-0.716031000	-1.696748000	3.751556000