

## SUPPORTING INFORMATION

# Assessing the Whole Range of CuAAC Mechanisms by DFT Calculations. On the Intermediacy of Copper Acetylides

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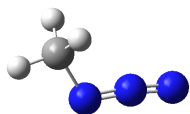
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### Contents:

Cartesian coordinates, energies, and imaginary frequency (transition states) for all optimized geometries

## Methyl azide

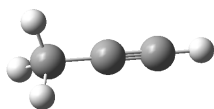


E(Hartree) = -204.148400947

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.547488	0.281699	-0.000009
2	1	0	-2.436372	-0.345008	-0.002407
3	1	0	-1.563398	0.914283	0.893806
4	1	0	-1.560910	0.917819	-0.891319
5	7	0	1.792408	0.271265	0.000021
6	7	0	0.717806	-0.095894	-0.000023
7	7	0	-0.389413	-0.629269	-0.000002

## Propine

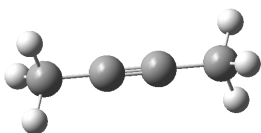


E(Hartree) = -116.690769971

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.420077	-0.000041	-0.000727
2	6	0	0.219173	-0.000496	0.001214
3	1	0	2.482123	0.001215	0.000555
4	6	0	-1.238143	0.000156	-0.000237
5	1	0	-1.628694	0.982934	-0.278559
6	1	0	-1.629148	-0.731593	-0.712646
7	1	0	-1.630924	-0.250273	0.989151

## Butyne



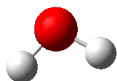
E(Hartree) = -156.024915322

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.601483	0.000226	0.000372

2	6	0	0.601484	0.000116	-0.000338
3	6	0	2.060360	-0.000030	0.000054
4	1	0	2.455975	-0.519704	0.877876
5	1	0	2.456340	-0.500807	-0.888518
6	1	0	2.456611	1.019785	0.010945
7	6	0	-2.060361	-0.000102	-0.000035
8	1	0	-2.456742	0.455848	0.912159
9	1	0	-2.456212	0.561984	-0.851239
10	1	0	-2.455972	-1.018368	-0.061545

## Water

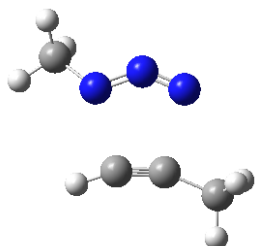


E(Hartree) = -76.4474480045

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	0.000000	0.000000	0.118697
2	1	0	0.000000	0.757048	-0.474786
3	1	0	0.000000	-0.757048	-0.474786

## Structure 3

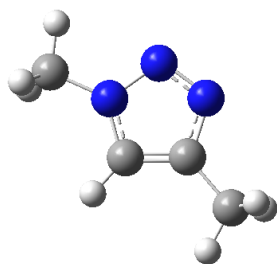


Imaginary Frequency:  $-479.34 \text{ cm}^{-1}$   
E(RB+HF-LYP) = -320.805441731

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.473419	1.319920	-0.101499
2	6	0	1.392604	0.504959	-0.003673
3	1	0	-0.044425	2.244805	-0.194650
4	6	0	2.772862	0.013972	0.122010
5	1	0	3.027744	-0.639463	-0.715718
6	1	0	3.484044	0.843796	0.147126
7	1	0	2.889339	-0.574466	1.035277
8	7	0	0.348552	-1.392400	-0.014261
9	7	0	-0.743759	-0.992458	-0.092111
10	7	0	-1.320102	0.111040	-0.274516
11	6	0	-2.680484	0.309060	0.216990
12	1	0	-3.397894	-0.311435	-0.328483
13	1	0	-2.773094	0.112233	1.290500
14	1	0	-2.928952	1.353795	0.029202

### Structure 4

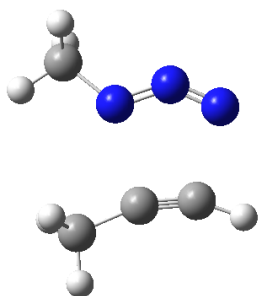


E(RB+HF-LYP) = -320.940108734

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.014848	-0.929604	-0.000118
2	6	0	1.105436	-0.088626	-0.000246
3	1	0	-0.077791	-2.002696	-0.000309
4	6	0	2.565229	-0.406766	0.000127
5	1	0	3.052350	0.003972	0.888439
6	1	0	2.733836	-1.485232	-0.014678
7	1	0	3.057377	0.029405	-0.873010
8	7	0	0.642287	1.195410	-0.000156
9	7	0	-0.658621	1.187314	0.000091
10	7	0	-1.059462	-0.098950	0.000187
11	6	0	-2.475430	-0.420463	0.000025
12	1	0	-3.014980	0.524448	0.000418
13	1	0	-2.740351	-0.991400	-0.892196
14	1	0	-2.740364	-0.992160	0.891752

### Structure 5



Imaginary Frequency: -440.9561 cm<sup>-1</sup>

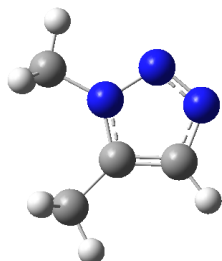
E(RB+HF-LYP) = -320.805356982

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.411641	1.193025	0.063650
2	6	0	-1.373655	-0.037976	0.019790
3	1	0	-1.872096	2.151973	0.115566
4	6	0	1.874478	-1.317966	0.081652
5	1	0	2.328285	-1.247848	1.076172
6	1	0	1.384719	-2.288118	-0.006407
7	1	0	2.661335	-1.266595	-0.677799
8	6	0	-1.801185	-1.439641	-0.024643
9	1	0	-1.401474	-2.005169	0.820778

10	1	0	-2.893079	-1.499752	0.012371
11	1	0	-1.463883	-1.924515	-0.943654
12	7	0	0.844407	-0.308179	-0.133901
13	7	0	1.125437	0.913292	-0.048634
14	7	0	0.534186	1.922798	0.005432

### Structure 6

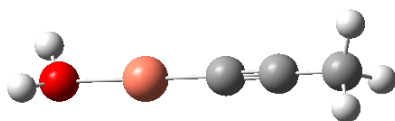


E(RB+HF-LYP) = -320.939784601

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.977712	-1.206309	-0.000015
2	6	0	0.302278	-0.695135	-0.000018
3	1	0	-1.296251	-2.236396	-0.000035
4	6	0	1.078297	1.724564	-0.000008
5	1	0	0.520698	2.658764	0.000003
6	1	0	1.708411	1.677075	0.891080
7	1	0	1.708388	1.677085	-0.891113
8	6	0	1.645794	-1.342641	0.000014
9	1	0	2.230551	-1.067595	0.883708
10	1	0	1.534272	-2.427340	-0.000484
11	1	0	2.230970	-1.066824	-0.883158
12	7	0	0.102329	0.651047	-0.000003
13	7	0	-1.221487	0.943893	0.000016
14	7	0	-1.870698	-0.180317	0.000010

### Structure 7



E(Hartree) = -388.724366481

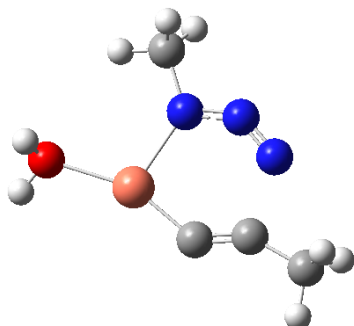
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.003719	0.000470	-0.006246
2	6	0	-2.221914	-0.000936	0.008556
3	6	0	-3.681623	-0.001872	0.024219
4	1	0	-4.085645	0.981731	-0.238657
5	1	0	-4.089840	-0.724892	-0.690197
6	1	0	-4.072271	-0.262604	1.013817
7	29	0	0.845521	0.002230	-0.023209
8	8	0	2.830836	-0.003773	-0.032425
9	1	0	3.259260	-0.782432	0.340212

10                    1                    0                    3.265225                    0.767732                    0.348121

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### Structure 8



Imaginary Frequency:  $-297.4081 \text{ cm}^{-1}$   
E(Hartree) =  $-592.859396785$

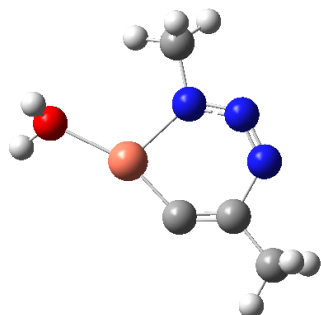
Standard orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.012179	-1.200292	-0.026895
2	6	0	2.118105	-0.589605	0.003567
3	7	0	-0.499334	1.250561	-0.006202
4	7	0	0.708623	1.695508	0.022542
5	7	0	1.807957	1.241032	0.034846
6	29	0	-0.785928	-0.770184	-0.030498
7	6	0	-1.524712	2.299059	-0.032282
8	1	0	-1.376135	2.996533	-0.862771
9	1	0	-2.488083	1.806401	-0.171039
10	1	0	-1.555897	2.869620	0.903205
11	6	0	3.594622	-0.666546	0.023085
12	1	0	3.924204	-1.706515	0.002151
13	1	0	4.016777	-0.144126	-0.839628
14	1	0	3.992151	-0.187376	0.921861
15	8	0	-2.837793	-1.092939	0.017277
16	1	0	-3.242257	-0.939722	0.878573
17	1	0	-3.098390	-1.981378	-0.249271

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### Structure 9

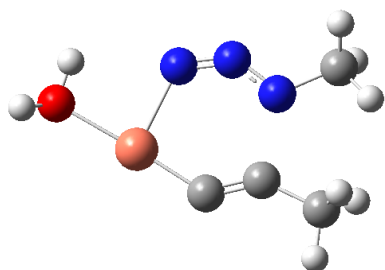


E(Hartree) =  $-592.864586404$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.929358	-1.146226	-0.020929
2	6	0	2.017033	-0.425088	0.007978
3	7	0	-0.335111	1.210369	-0.017960
4	7	0	0.870878	1.693168	0.011703
5	7	0	1.936562	1.059566	0.023332
6	29	0	-0.838857	-0.715836	-0.026659
7	6	0	-1.367365	2.255781	-0.017037
8	1	0	-1.142534	3.033238	-0.751954
9	1	0	-2.320998	1.795272	-0.282106
10	1	0	-1.466399	2.726287	0.968250
11	6	0	3.450342	-0.874782	0.026143
12	1	0	3.528929	-1.961801	0.013011
13	1	0	3.973441	-0.465554	-0.842399
14	1	0	3.944378	-0.488856	0.921965
15	8	0	-2.891467	-0.983107	0.007403
16	1	0	-3.331075	-0.757275	0.834702
17	1	0	-3.209680	-1.857049	-0.244028

### Structure 10

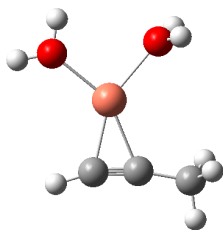


Imaginary Frequency:  $-380.8120 \text{ cm}^{-1}$   
E(Hartree) =  $-592.843897605$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.153602	-1.407054	0.037629
2	6	0	-1.382717	-1.086247	-0.016697
3	7	0	0.570540	1.356023	-0.034536
4	7	0	-0.607671	1.532556	-0.064901
5	7	0	-1.649550	0.808976	-0.117479
6	29	0	1.428507	-0.487445	0.051547
7	6	0	-2.742308	-1.684371	-0.071232
8	1	0	-2.651886	-2.771253	-0.064572
9	1	0	-3.357336	-1.395832	0.786872
10	1	0	-3.277439	-1.398694	-0.982326
11	8	0	3.251465	0.457800	0.024470
12	1	0	2.952874	1.371695	-0.091481
13	1	0	3.883880	0.273956	-0.677837
14	6	0	-2.943324	1.457016	0.112382
15	1	0	-3.722610	0.760219	-0.187193
16	1	0	-3.089309	1.715421	1.166933
17	1	0	-3.038129	2.359035	-0.495102

### Structure 13

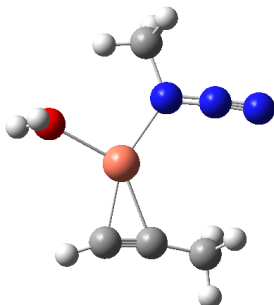


E(Hartree) = -465.596556561

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.140903	-1.522790	-0.000454
2	6	0	-1.769771	-0.469786	-0.000019
3	29	0	0.343129	-0.117787	-0.000063
4	8	0	2.286475	-0.775500	0.000366
5	8	0	1.020208	1.855966	-0.000286
6	1	0	0.970856	2.429328	0.773944
7	1	0	0.969395	2.429192	-0.774521
8	1	0	3.033246	-0.166502	0.000517
9	1	0	2.637038	-1.672436	0.000672
10	6	0	-2.762094	0.606776	0.000426
11	1	0	-2.671196	1.234080	0.889266
12	1	0	-2.671241	1.234786	-0.887919
13	1	0	-3.759331	0.157826	0.000271
14	1	0	-0.876361	-2.559382	-0.000771

### Structure 14



E(Hartree) = -593.294733282

Standard orientation:

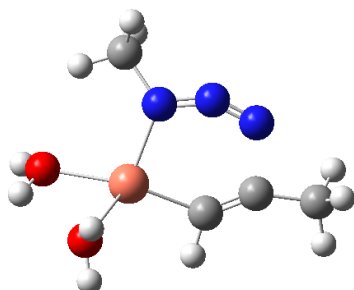
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.397181	-0.683964	-0.051536
2	6	0	-2.222338	0.525121	0.043477
3	7	0	1.555099	1.556261	-0.106949
4	7	0	1.466570	0.316190	0.022766
5	7	0	1.572510	2.674042	-0.234679
6	29	0	-0.349637	-0.589402	-0.021484
7	6	0	2.773448	-0.371188	0.249459
8	1	0	2.554969	-1.434093	0.278865
9	1	0	3.463148	-0.159543	-0.569631
10	1	0	3.208670	-0.056992	1.199983
11	6	0	-2.284533	1.981988	0.159467
12	1	0	-1.804425	2.474510	-0.688448
13	1	0	-3.336707	2.280843	0.173610
14	1	0	-1.820187	2.330925	1.083936



15	1	0	-2.861321	-1.643813	-0.134065
16	8	0	0.348628	-2.609736	-0.076975
17	1	0	0.417371	-3.110938	-0.898537
18	1	0	0.153294	-3.247548	0.619944

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### Structure 15



Imaginary Frequency:  $-366.2242 \text{ cm}^{-1}$   
E(Hartree) =  $-669.726561606$

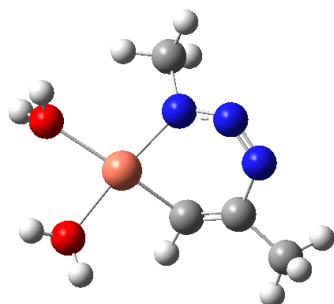
Standard orientation:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.067592	-1.144908	-0.441930
2	6	0	2.235011	-0.712356	-0.208317
3	7	0	1.156874	1.514568	0.526163
4	7	0	-0.072464	1.442608	0.344814
5	7	0	2.179576	0.956874	0.569667
6	29	0	-0.753030	-0.413479	-0.239118
7	6	0	-0.814294	2.670998	-0.022622
8	1	0	-1.852563	2.377909	-0.152599
9	1	0	-0.744405	3.396436	0.789216
10	1	0	-0.429309	3.104428	-0.947551
11	8	0	-2.696411	-0.025481	-0.832027
12	8	0	-2.022769	-1.694880	1.230168
13	1	0	-1.999585	-1.417597	2.154514
14	1	0	-1.944732	-2.656589	1.249925
15	1	0	-3.301583	-0.591460	-0.334808
16	1	0	-3.048058	0.087316	-1.722138
17	6	0	3.691794	-0.944746	-0.274910
18	1	0	4.144755	-0.861288	0.714628
19	1	0	3.871135	-1.945761	-0.672319
20	1	0	4.169455	-0.213045	-0.930135
21	1	0	0.797671	-2.138839	-0.797261

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### Structure 16

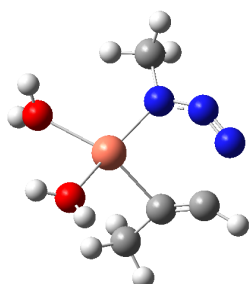


E(Hartree) = -669.732101319

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.979558	-0.883593	0.600737
2	6	0	-2.105962	-0.453060	0.093577
3	7	0	-1.213591	1.580106	-0.569695
4	7	0	-0.010170	1.402227	-0.179410
5	7	0	-2.168737	0.822511	-0.648303
6	29	0	0.825309	-0.341309	0.069064
7	6	0	0.607185	2.566364	0.498386
8	1	0	1.660798	2.350457	0.651886
9	1	0	0.505123	3.438433	-0.149263
10	1	0	0.123870	2.763752	1.456595
11	8	0	2.884545	0.190214	-0.098474
12	8	0	1.542191	-2.256150	-0.254592
13	1	0	0.991816	-2.995864	-0.537434
14	1	0	2.423091	-2.385035	-0.625409
15	1	0	3.221728	0.772618	-0.790160
16	1	0	3.503279	0.242233	0.640433
17	6	0	-3.477327	-1.060018	0.182078
18	1	0	-3.850698	-1.268758	-0.823634
19	1	0	-3.471612	-1.979920	0.764643
20	1	0	-4.162848	-0.344971	0.644018
21	1	0	-0.810933	-1.819565	1.123183

### Structure 17



Imaginary Frequency: -381.8584 cm<sup>-1</sup>

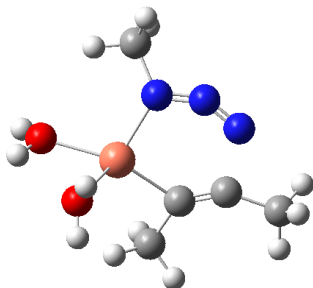
E(Hartree) = -669.714928868

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.359051	-1.676026	0.482310
2	6	0	-1.424535	-1.982354	-0.097586
3	7	0	-2.168085	0.448374	-0.461718
4	7	0	-1.169508	1.070267	0.002105
5	7	0	-2.537071	-0.622789	-0.757505
6	29	0	0.578422	0.161639	-0.111097
7	6	0	-1.411188	2.392018	0.613152
8	1	0	-0.444211	2.777208	0.927705
9	1	0	-1.848478	3.076083	-0.116680
10	1	0	-2.065526	2.310563	1.483113
11	1	0	-2.090443	-2.777454	-0.369431
12	6	0	0.713287	-2.151262	1.408402
13	1	0	0.688380	-1.603376	2.353057
14	1	0	0.539751	-3.209092	1.628036
15	1	0	1.710900	-2.054493	0.976632

16	8	0	2.049582	1.739879	0.307485
17	8	0	2.110702	-0.716717	-1.218600
18	1	0	1.990348	-1.376135	-1.911375
19	1	0	2.945664	-0.263262	-1.379759
20	1	0	2.082854	2.577444	-0.169886
21	1	0	2.445821	1.904442	1.171492

### Structure 18

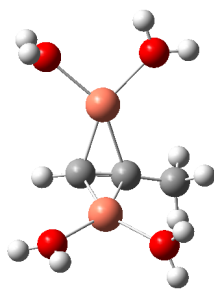


Imaginary Frequency:  $-327.3856 \text{ cm}^{-1}$   
 $E(\text{Hartree}) = -709.051461404$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.159150	-0.928173	-0.334918
2	6	0	2.213894	-0.306503	-0.037837
3	7	0	0.871615	1.914054	0.340341
4	7	0	-0.323771	1.640856	0.083821
5	7	0	1.941653	1.483916	0.511654
6	29	0	-0.765844	-0.314451	-0.110500
7	6	0	-1.200245	2.710907	-0.437276
8	1	0	-2.192293	2.278705	-0.544529
9	1	0	-1.246800	3.536696	0.274432
10	1	0	-0.849890	3.073058	-1.405991
11	6	0	0.841019	-2.310960	-0.864010
12	1	0	0.656361	-2.273614	-1.939818
13	1	0	1.694634	-2.970738	-0.681119
14	1	0	-0.030172	-2.779980	-0.397392
15	8	0	-2.755593	-0.437193	-0.719874
16	8	0	-1.735738	-1.345121	1.698094
17	1	0	-1.758799	-0.794773	2.490740
18	1	0	-1.477542	-2.222619	2.005315
19	1	0	-3.303207	-0.932661	-0.098523
20	1	0	-3.164411	-0.484657	-1.590859
21	6	0	3.685843	-0.361763	0.075574
22	1	0	4.021672	-1.368105	-0.189876
23	1	0	4.156277	0.358751	-0.596594
24	1	0	4.009852	-0.135309	1.093041

### Structure 19

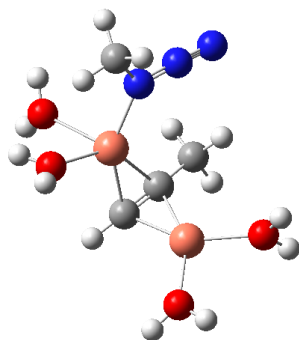


E (Hartree) = -814.390894295

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.035468	1.061311	-0.990291
2	6	0	-0.007900	-0.123346	-1.403432
3	29	0	1.572439	-0.168234	-0.047278
4	8	0	2.741520	0.865961	1.299678
5	1	0	2.636022	0.936048	2.256729
6	1	0	3.536578	1.362771	1.066540
7	29	0	-1.568016	-0.091466	-0.042417
8	8	0	-2.737113	-1.810098	-0.011898
9	8	0	-2.760696	0.824729	1.310681
10	1	0	-3.520314	0.344108	1.664249
11	1	0	-2.858587	1.747319	1.574778
12	1	0	-2.588185	-2.616295	0.498268
13	1	0	-3.401613	-2.022512	-0.680513
14	6	0	0.088823	2.529685	-0.912881
15	1	0	0.170064	2.893780	0.111645
16	1	0	0.956051	2.883099	-1.478855
17	1	0	-0.811941	2.949143	-1.370165
18	1	0	-0.038597	-0.896887	-2.153228
19	8	0	2.636224	-1.905852	0.019055
20	1	0	2.705617	-2.603974	-0.643662
21	1	0	3.348788	-2.049111	0.654873

## Structure 20



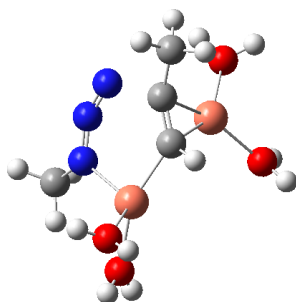
E (Hartree) = -1018.56953219

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.806934	-1.058819	1.157907
2	6	0	-0.666803	0.140598	1.483530

3	7	0	2.099067	2.058544	-0.425816
4	7	0	2.167558	0.856515	-0.760489
5	7	0	1.984656	3.122891	-0.077121
6	29	0	0.978498	-0.573301	0.123857
7	6	0	3.164870	0.571037	-1.840184
8	1	0	3.116912	-0.498519	-2.020656
9	1	0	2.905076	1.109473	-2.753184
10	1	0	4.169621	0.847086	-1.515654
11	6	0	-0.536926	1.398359	2.235898
12	1	0	-0.414018	2.266395	1.587939
13	1	0	-1.430558	1.545554	2.849100
14	1	0	0.327737	1.333258	2.902223
15	1	0	-0.952946	-2.114802	1.300436
16	8	0	1.479309	-2.309311	-0.981992
17	1	0	1.260853	-2.734651	-1.818665
18	1	0	2.139279	-2.848705	-0.528650
19	29	0	-2.162463	-0.070593	-0.071315
20	8	0	-3.017219	1.732391	-0.631292
21	8	0	-3.423483	-1.221579	-1.186942
22	1	0	-4.088770	-0.832340	-1.768159
23	1	0	-3.654429	-2.151726	-1.076516
24	1	0	-2.791883	2.294859	-1.382476
25	1	0	-3.727478	2.176213	-0.150470
26	8	0	2.573857	-1.578974	1.497425
27	1	0	3.462058	-1.208450	1.574534
28	1	0	2.429641	-2.063652	2.319957

## Structure 21



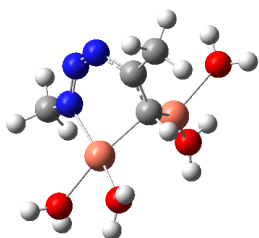
Imaginary Frequency:  $-357.0782 \text{ cm}^{-1}$   
E(Hartree) =  $-1018.53496766$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.172948	-0.246495	-1.157920
2	6	0	0.981214	-1.243692	-0.941823
3	7	0	-0.307422	-1.718863	1.226451
4	7	0	-1.266015	-0.947604	1.322095
5	7	0	0.580849	-2.142419	0.595155
6	29	0	-1.565380	0.289232	-0.308936
7	6	0	-1.886249	-0.655887	2.642641
8	1	0	-2.716551	0.017184	2.451472
9	1	0	-2.263469	-1.585820	3.069634
10	1	0	-1.165612	-0.190520	3.316364
11	8	0	-3.003377	1.588059	0.373749
12	8	0	-3.204954	-0.149630	-1.790925
13	1	0	-3.641031	-1.011574	-1.806797
14	1	0	-3.290729	0.200623	-2.686987
15	1	0	-3.833780	1.544374	-0.118371
16	1	0	-2.988926	2.417324	0.865887
17	6	0	1.926635	-2.188626	-1.595715
18	1	0	1.398390	-3.113762	-1.841059

19	1	0	2.310931	-1.740170	-2.513901
20	1	0	2.757993	-2.445305	-0.939365
21	1	0	0.034774	0.229221	-2.131538
22	29	0	1.790694	0.572055	-0.116323
23	8	0	1.988955	2.616566	0.002915
24	8	0	3.505847	0.201053	0.988293
25	1	0	1.886634	3.264934	-0.704119
26	1	0	2.443545	3.059148	0.730480
27	1	0	3.638061	-0.507137	1.630572
28	1	0	4.384720	0.506181	0.728948

## Structure 22

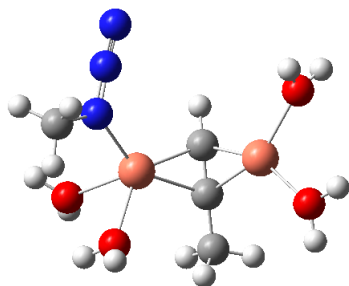


E(Hartree) = -1018.54674207

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.312746	0.899334	-0.730933
2	6	0	-0.347957	2.117121	-0.059493
3	7	0	0.357858	1.251954	1.936156
4	7	0	0.980656	0.231390	1.591696
5	7	0	0.029294	2.259536	1.254082
6	29	0	1.402790	-0.166041	-0.336911
7	6	0	1.087254	-0.854625	2.597151
8	1	0	2.135613	-0.951588	2.881547
9	1	0	0.478720	-0.616991	3.466962
10	1	0	0.751823	-1.786054	2.140993
11	8	0	2.907182	-1.627684	-0.043740
12	8	0	2.184681	0.083813	-2.218177
13	1	0	2.296102	0.895766	-2.728780
14	1	0	2.808735	-0.564963	-2.568334
15	1	0	3.798828	-1.402386	0.253477
16	1	0	2.836929	-2.589772	-0.002503
17	6	0	-0.810098	3.405579	-0.677122
18	1	0	-0.059861	4.183314	-0.509910
19	1	0	-1.014427	3.304373	-1.741546
20	1	0	-1.722433	3.737838	-0.173001
21	1	0	-0.211782	1.024734	-1.812154
22	29	0	-1.469803	-0.633968	-0.356819
23	8	0	-3.622252	-0.329758	0.067207
24	8	0	-2.030862	-2.569667	-0.182707
25	1	0	-4.249116	-0.088326	-0.627527
26	1	0	-3.978520	0.045727	0.882949
27	1	0	-1.741488	-3.385936	-0.606040
28	1	0	-2.969129	-2.663712	0.030205

## Structure 23

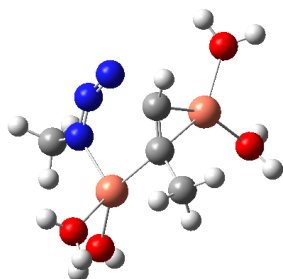


E(Hartree) = -1018.53776356

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.291542	1.351187	0.368759
2	6	0	-0.170099	1.441280	1.773650
3	7	0	0.119332	-0.766247	2.251395
4	7	0	0.765121	-1.197415	1.279826
5	7	0	0.052170	0.449869	2.639135
6	29	0	1.357632	0.074660	-0.205480
7	6	0	0.643566	-2.650420	1.026175
8	1	0	1.569642	-3.124906	1.359082
9	1	0	-0.201184	-3.066658	1.571753
10	1	0	0.536435	-2.803904	-0.046489
11	8	0	2.668212	-1.318405	-1.209468
12	8	0	2.512159	1.477437	-1.135892
13	1	0	2.633417	2.417046	-0.950823
14	1	0	3.318122	1.157338	-1.561281
15	1	0	3.384515	-1.797154	-0.771994
16	1	0	2.602611	-1.679872	-2.102681
17	29	0	-1.463702	0.059991	-0.529341
18	8	0	-3.589944	-0.047331	0.038692
19	8	0	-2.052108	-1.357944	-1.847543
20	1	0	-4.231764	0.614113	-0.252851
21	1	0	-3.907175	-0.356198	0.897667
22	1	0	-1.798403	-1.551287	-2.757523
23	1	0	-2.984219	-1.594531	-1.745895
24	1	0	-0.246497	2.407907	2.269879
25	6	0	-0.164019	2.677975	-0.339095
26	1	0	-1.151551	3.161410	-0.256197
27	1	0	0.544639	3.370751	0.126387
28	1	0	0.037084	2.587426	-1.404976

## Structure 24

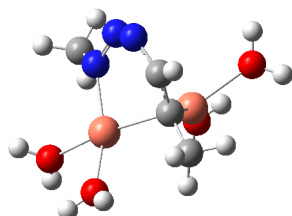


Imaginary Frequency:  $-355.4178 \text{ cm}^{-1}$   
E(Hartree) = -1018.52414973

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.145288	-0.864630	-0.953573
2	6	0	-0.897356	-0.077137	-1.644490
3	7	0	0.207050	2.069216	-0.771890
4	7	0	1.101702	1.721424	0.013103
5	7	0	-0.609683	1.752288	-1.547924
6	29	0	1.530867	-0.256440	0.115871
7	6	0	1.638247	2.687510	1.009291
8	1	0	2.402598	2.161922	1.574379
9	1	0	2.090563	3.530423	0.485542
10	1	0	0.848910	3.033188	1.677917
11	8	0	2.720363	-0.505529	1.807227
12	8	0	3.276318	-1.011717	-1.000818
13	1	0	3.665702	-0.515637	-1.732244
14	1	0	3.676112	-1.890014	-1.031927
15	1	0	3.665756	-0.668336	1.698707
16	1	0	2.522854	-0.565925	2.749539
17	29	0	-1.980892	-0.320407	0.090812
18	8	0	-2.431112	-1.168981	1.894980
19	8	0	-3.700529	0.843460	0.025840
20	1	0	-2.459933	-2.106203	2.122395
21	1	0	-2.927564	-0.696177	2.574852
22	1	0	-3.774588	1.680910	-0.448936
23	1	0	-4.596637	0.491684	0.103565
24	6	0	0.198195	-2.344022	-1.026819
25	1	0	0.999481	-2.478866	-1.756734
26	1	0	0.523823	-2.765256	-0.074752
27	1	0	-0.671344	-2.910196	-1.369655
28	1	0	-1.491584	-0.041640	-2.543757

## Structure 25



E(Hartree) = -1018.53776356

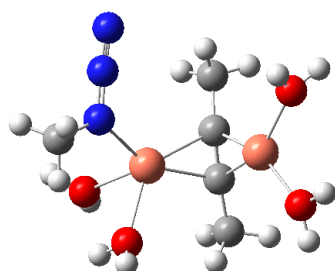
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.291542	1.351187	0.368759
2	6	0	-0.170099	1.441280	1.773650
3	7	0	0.119332	-0.766247	2.251395
4	7	0	0.765121	-1.197415	1.279826
5	7	0	0.052170	0.449869	2.639135
6	29	0	1.357632	0.074660	-0.205480
7	6	0	0.643566	-2.650420	1.026175
8	1	0	1.569642	-3.124906	1.359082
9	1	0	-0.201184	-3.066658	1.571753
10	1	0	0.536435	-2.803904	-0.046489
11	8	0	2.668212	-1.318405	-1.209468
12	8	0	2.512159	1.477437	-1.135892
13	1	0	2.633417	2.417046	-0.950823
14	1	0	3.318122	1.157338	-1.561281
15	1	0	3.384515	-1.797154	-0.771994
16	1	0	2.602611	-1.679872	-2.102681



17	29	0	-1.463702	0.059991	-0.529341
18	8	0	-3.589944	-0.047331	0.038692
19	8	0	-2.052108	-1.357944	-1.847543
20	1	0	-4.231764	0.614113	-0.252851
21	1	0	-3.907175	-0.356198	0.897667
22	1	0	-1.798403	-1.551287	-2.757523
23	1	0	-2.984219	-1.594531	-1.745895
24	1	0	-0.246497	2.407907	2.269879
25	6	0	-0.164019	2.677975	-0.339095
26	1	0	-1.151551	3.161410	-0.256197
27	1	0	0.544639	3.370751	0.126387
28	1	0	0.037084	2.587426	-1.404976

## Structure 26

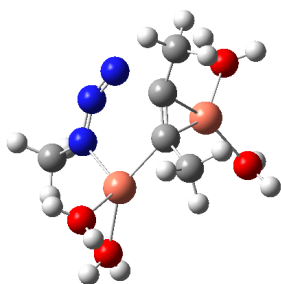


E (Hartree) = -1057.90860973

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.877694	-1.194132	0.959603
2	6	0	-0.651126	-0.062492	1.451724
3	7	0	2.222726	2.113218	0.031500
4	7	0	2.211776	1.020928	-0.576743
5	7	0	2.180103	3.069899	0.623079
6	29	0	0.941280	-0.496387	-0.002022
7	6	0	3.164148	0.948043	-1.728235
8	1	0	3.059521	-0.048551	-2.146566
9	1	0	2.909238	1.690487	-2.486547
10	1	0	4.190711	1.098252	-1.389288
11	8	0	1.262146	-2.026377	-1.460451
12	1	0	1.176185	-2.142846	-2.413530
13	1	0	1.981244	-2.592802	-1.149997
14	29	0	-1.999713	0.237548	-0.148103
15	8	0	-2.730110	2.187526	-0.331960
16	8	0	-3.218213	-0.421542	-1.644724
17	1	0	-3.850375	0.185710	-2.049284
18	1	0	-3.492807	-1.315400	-1.880541
19	1	0	-2.398823	2.896910	-0.896260
20	1	0	-3.373820	2.586101	0.267493
21	8	0	2.604905	-1.887671	0.961247
22	1	0	3.494810	-1.526540	1.060741
23	1	0	2.512622	-2.523450	1.682008
24	6	0	-1.196456	-2.636034	0.863528
25	1	0	-0.982122	-3.037392	-0.126321
26	1	0	-0.593921	-3.181374	1.595264
27	1	0	-2.248765	-2.805882	1.103539
28	6	0	-0.456938	0.985683	2.480894
29	1	0	0.387198	0.716801	3.120936
30	1	0	-0.268147	1.969667	2.053163
31	1	0	-1.351852	1.046429	3.105993

## Structure 27

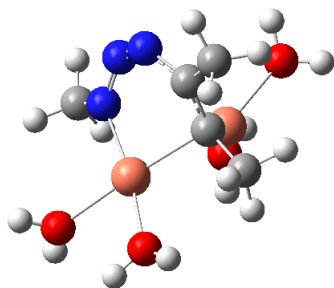


Imaginary Frequency:  $-326.3842 \text{ cm}^{-1}$   
E(Hartree) =  $-1057.86248384$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.178697	-0.932799	0.748287
2	6	0	1.011889	-0.263691	1.485671
3	7	0	-0.184803	1.972420	0.964205
4	7	0	-1.152293	1.714767	0.230737
5	7	0	0.705349	1.545510	1.596756
6	29	0	-1.536644	-0.241797	-0.138736
7	6	0	-1.836037	2.801025	-0.518709
8	1	0	-2.626924	2.332234	-1.097485
9	1	0	-2.274648	3.507697	0.186881
10	1	0	-1.139238	3.311314	-1.184777
11	8	0	-2.858244	-0.283374	-1.734808
12	8	0	-3.305976	-1.133398	0.918213
13	1	0	-3.701120	-0.683858	1.676215
14	1	0	-3.592927	-2.053259	0.980778
15	1	0	-3.766173	-0.545432	-1.536769
16	1	0	-2.779811	-0.179162	-2.690263
17	29	0	1.740502	-0.250177	-0.507299
18	8	0	1.882668	-0.879250	-2.461976
19	8	0	3.440467	0.947795	-0.651806
20	1	0	1.852914	-1.783136	-2.798060
21	1	0	2.319724	-0.341618	-3.134408
22	1	0	3.561114	1.790804	-0.197102
23	1	0	4.324606	0.612850	-0.848966
24	6	0	-0.152345	-2.423019	0.738123
25	1	0	-0.864249	-2.635682	1.538660
26	1	0	-0.576075	-2.774177	-0.203586
27	1	0	0.754983	-3.003158	0.931487
28	6	0	1.980570	-0.452013	2.602571
29	1	0	2.337250	-1.485283	2.603047
30	1	0	2.831053	0.224083	2.521381
31	1	0	1.481904	-0.247046	3.553457

## Structure 28

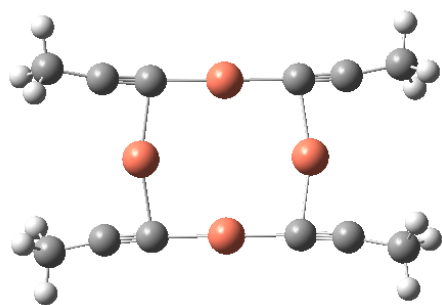


E(Hartree) = -1057.87441588

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.381363	1.140242	-0.437033
2	6	0	-0.412181	1.962619	0.717233
3	7	0	-0.046224	0.269548	2.233167
4	7	0	0.692565	-0.518182	1.609282
5	7	0	-0.232534	1.502181	1.977412
6	29	0	1.438297	-0.063832	-0.186284
7	6	0	0.671175	-1.927859	2.062774
8	1	0	1.682734	-2.207060	2.356516
9	1	0	-0.011671	-2.038749	2.902643
10	1	0	0.354160	-2.557606	1.229450
11	8	0	3.164953	-1.447989	-0.062894
12	8	0	2.500739	0.544697	-1.785958
13	1	0	2.470895	1.327898	-2.348258
14	1	0	3.379126	0.148672	-1.858086
15	1	0	3.851000	-1.356337	0.611899
16	1	0	3.245852	-2.346715	-0.408078
17	29	0	-1.426179	-0.519173	-0.547976
18	8	0	-3.570076	-0.649754	-0.059573
19	8	0	-1.701948	-2.508156	-0.935770
20	1	0	-4.251254	-0.358119	-0.680169
21	1	0	-3.930307	-0.479140	0.820607
22	1	0	-1.382726	-3.062763	-1.657662
23	1	0	-2.600516	-2.796629	-0.724315
24	6	0	-0.211653	1.846684	-1.759120
25	1	0	-1.178250	2.328412	-1.977749
26	1	0	0.523675	2.657862	-1.750593
27	1	0	-0.019648	1.168640	-2.588700
28	6	0	-0.701311	3.437486	0.659426
29	1	0	0.071034	3.960040	0.086802
30	1	0	-1.656486	3.635172	0.165454
31	1	0	-0.733028	3.843292	1.668657

**Structure 29**

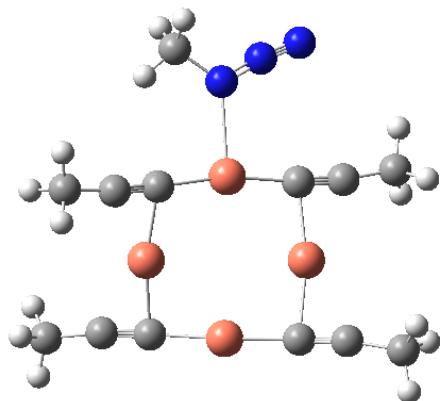


E(Hartree) = -1249.21005913

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.875773	-1.965313	-0.367311
2	6	0	-3.079224	-2.034380	-0.627712
3	6	0	1.875752	1.965279	-0.367132
4	6	0	3.079131	2.034475	-0.627837
5	6	0	3.076209	-2.036255	0.627695
6	6	0	1.872818	-1.966809	0.366951
7	6	0	-3.076248	2.036377	0.627794
8	6	0	-1.872932	1.966727	0.366796
9	29	0	-2.139994	0.000729	0.000274
10	29	0	0.001364	1.965406	-0.000331
11	29	0	2.140155	-0.000756	0.000524
12	29	0	-0.001407	-1.965617	-0.000431
13	6	0	-4.469903	2.312106	0.975725
14	1	0	-4.578611	3.364359	1.254935
15	1	0	-5.141936	2.118305	0.135248
16	1	0	-4.800740	1.705573	1.823189
17	6	0	-4.473157	-2.308974	-0.975348
18	1	0	-4.582807	-3.361193	-1.254309
19	1	0	-5.144909	-2.114423	-0.134820
20	1	0	-4.803586	-1.702336	-1.822899
21	6	0	4.469903	-2.311807	0.975638
22	1	0	4.578835	-3.364151	1.254415
23	1	0	5.141978	-2.117493	0.135314
24	1	0	4.800508	-1.705545	1.823388
25	6	0	4.472964	2.309333	-0.975659
26	1	0	4.582365	3.361578	-1.254625
27	1	0	5.144863	2.114908	-0.135221
28	1	0	4.803404	1.702770	-1.823260

### Structure 30

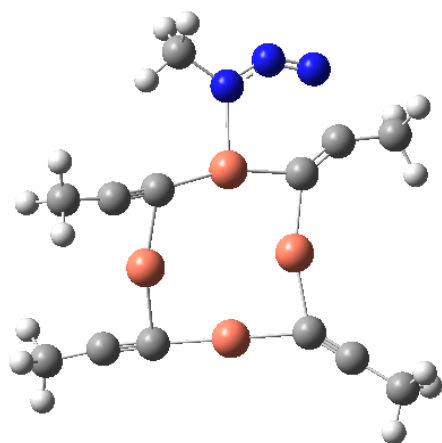


E(Hartree) = -1453.36397562

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.922183	-1.204782	-0.719894
2	6	0	-3.905403	-0.570147	-1.106599
3	6	0	-2.020983	2.499176	1.167701
4	6	0	-0.977939	1.987077	0.750384
5	6	0	2.241079	0.147925	-0.266962
6	6	0	3.282577	-0.425005	-0.595233
7	6	0	0.135084	-3.198612	0.393708
8	6	0	1.116907	-3.836357	0.779766
9	6	0	1.268662	4.663767	-0.003910
10	1	0	1.321052	5.226683	-0.940935
11	1	0	0.226797	4.492747	0.255980
12	1	0	1.751957	5.236230	0.793879
13	7	0	1.871293	3.326848	-0.145726
14	7	0	3.060596	3.283062	-0.465987
15	7	0	4.138039	3.082156	-0.753986
16	29	0	-2.114754	0.497816	0.000913
17	29	0	0.716359	1.238130	0.202030
18	29	0	-1.414441	-2.237961	-0.168541
19	29	0	1.356190	-1.612524	0.093702
20	6	0	-3.142843	3.241462	1.745524
21	1	0	-2.771660	4.103001	2.309068
22	1	0	-3.821810	3.614331	0.973525
23	1	0	-3.722551	2.620011	2.433402
24	6	0	-5.136167	0.019257	-1.631381
25	1	0	-5.735326	-0.753158	-2.122880
26	1	0	-5.745118	0.458332	-0.836240
27	1	0	-4.926160	0.798687	-2.368989
28	6	0	2.157961	-4.740421	1.267168
29	1	0	1.709745	-5.691648	1.569576
30	1	0	2.902709	-4.952322	0.494982
31	1	0	2.677267	-4.324828	2.134988
32	6	0	4.583624	-0.940448	-1.020699
33	1	0	5.237760	-0.108713	-1.297708
34	1	0	5.076272	-1.501583	-0.221726
35	1	0	4.490039	-1.597943	-1.889501

### Structure 31

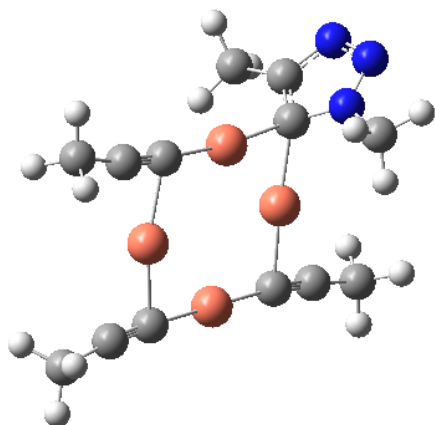


Imaginary Frequency: -341.5132  $\text{cm}^{-1}$   
E(Hartree) = -1453.34429963

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.150935	0.156180	-0.717165
2	6	0	3.942885	-0.711580	-1.085270
3	6	0	1.037951	-2.956361	1.130659
4	6	0	0.199342	-2.150471	0.712391
5	6	0	-2.291257	0.616852	-0.187342
6	6	0	-3.476903	0.920569	-0.491316
7	6	0	0.749135	2.969455	0.345410
8	6	0	0.650435	4.138809	0.696114
9	6	0	-2.863462	-3.596835	-0.053643
10	1	0	-3.192771	-4.082625	-0.976650
11	1	0	-1.826434	-3.862055	0.137835
12	1	0	-3.480425	-3.949212	0.778800
13	7	0	-2.913189	-2.132684	-0.174518
14	7	0	-4.045118	-1.640061	-0.475000
15	7	0	-4.541179	-0.582989	-0.660474
16	29	0	1.835764	-1.178549	0.003856
17	29	0	-1.268721	-0.959182	0.183849
18	29	0	1.958212	1.563966	-0.203262
19	29	0	-0.611138	1.567312	0.109997
20	6	0	1.848493	-4.026417	1.718308
21	1	0	2.374809	-4.601767	0.951830
22	1	0	2.592350	-3.631156	2.415043
23	1	0	1.205167	-4.716355	2.272601
24	6	0	4.975657	-1.619514	-1.578345
25	1	0	5.769246	-1.045718	-2.066317
26	1	0	5.429931	-2.193813	-0.766187
27	1	0	4.573924	-2.323871	-2.311889
28	6	0	0.545576	5.528700	1.114771
29	1	0	1.541119	5.957335	1.266136
30	1	0	0.031672	6.136445	0.364149
31	1	0	0.000068	5.618205	2.058950
32	6	0	-4.452669	1.993711	-0.787681
33	1	0	-4.882069	1.853868	-1.782816
34	1	0	-5.276330	1.968654	-0.069786
35	1	0	-3.969988	2.970767	-0.741871

### Structure 32



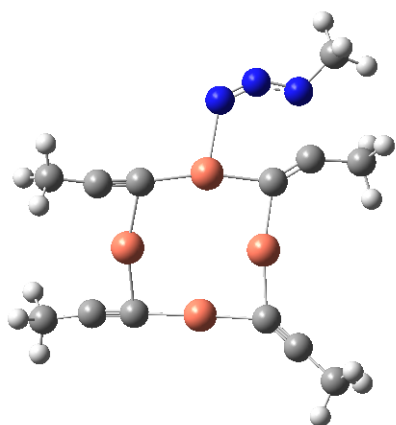
E(Hartree) = -1453.44158597

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
			X	Y	Z

Number	Number	Type	X	Y	Z
1	6	0	0.677427	2.741954	0.007939
2	6	0	-2.941436	1.505982	-0.030730
3	6	0	-4.135516	1.200629	-0.042290
4	6	0	-2.541633	-2.752896	0.064449
5	6	0	-1.442280	-2.193671	0.039609
6	6	0	1.784612	3.279425	0.025773
7	6	0	2.246639	-0.954712	0.002798
8	6	0	3.117303	-1.249970	1.064453
9	6	0	2.710368	-1.208776	-2.503879
10	1	0	3.612014	-1.459986	-3.059074
11	1	0	1.921831	-1.924651	-2.743518
12	1	0	2.378459	-0.205143	-2.773404
13	7	0	3.042677	-1.269139	-1.088495
14	7	0	4.248512	-1.709541	-0.725960
15	7	0	4.304457	-1.699277	0.580682
16	29	0	-1.130406	2.115460	-0.012744
17	29	0	-2.445109	-0.441393	0.007548
18	29	0	0.329013	-1.463496	0.013377
19	29	0	1.384741	0.870694	0.011386
20	6	0	-3.737243	-3.595057	0.101113
21	1	0	-4.343437	-3.394436	0.988542
22	1	0	-4.364131	-3.443820	-0.781689
23	1	0	-3.443640	-4.648589	0.127413
24	6	0	-5.586627	1.023266	-0.059024
25	1	0	-6.075863	2.001318	-0.091243
26	1	0	-5.913989	0.457478	-0.935471
27	1	0	-5.939815	0.502854	0.835347
28	6	0	3.035708	4.031483	0.051845
29	1	0	3.638455	3.776519	0.927582
30	1	0	3.636878	3.843813	-0.841877
31	1	0	2.821368	5.103667	0.092981
32	6	0	2.881674	-1.139970	2.537361
33	1	0	2.951626	-2.121462	3.014297
34	1	0	3.633676	-0.498347	3.004069
35	1	0	1.894142	-0.726313	2.748516

### Structure 33



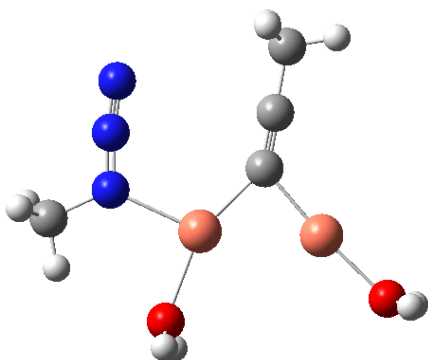
Imaginary Frequency:  $-382.2625 \text{ cm}^{-1}$   
 E(Hartree) =  $-1453.33053656$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	3.227168	0.391623	-0.678612
2	6	0	4.116960	-0.386926	-1.025195
3	6	0	1.504567	-3.089516	0.967351
4	6	0	0.595634	-2.315812	0.649552
5	6	0	-2.179504	0.226445	-0.113940
6	6	0	-3.388731	0.460740	-0.397711
7	6	0	0.552659	2.973658	0.329805
8	6	0	0.420686	4.148110	0.651245
9	7	0	-2.618742	-2.502914	0.002122
10	7	0	-3.718050	-2.182694	-0.236526
11	7	0	-4.422693	-1.180099	-0.530728
12	29	0	2.108283	-1.144980	-0.014752
13	29	0	-0.961617	-1.209042	0.237614
14	29	0	1.873220	1.653457	-0.187692
15	29	0	-0.690569	1.466857	0.117860
16	6	0	2.402472	-4.152945	1.423834
17	1	0	2.952966	-4.601080	0.592079
18	1	0	3.130027	-3.783139	2.151367
19	1	0	1.820040	-4.944714	1.904288
20	6	0	5.261798	-1.164443	-1.496029
21	1	0	5.994159	-0.498493	-1.962216
22	1	0	5.760363	-1.686930	-0.674911
23	1	0	4.963947	-1.907037	-2.241320
24	6	0	0.277006	5.544706	1.036060
25	1	0	-0.237523	6.124333	0.263662
26	1	0	-0.287146	5.643049	1.968535
27	1	0	1.259117	6.000673	1.195439
28	6	0	-4.393817	1.497340	-0.735387
29	1	0	-4.849858	1.314182	-1.712681
30	1	0	-5.194547	1.553142	0.008109
31	1	0	-3.903846	2.470958	-0.770861
32	6	0	-5.878109	-1.288984	-0.392688
33	1	0	-6.317884	-0.407979	-0.854280
34	1	0	-6.250295	-2.171607	-0.916226
35	1	0	-6.186051	-1.331872	0.657348

### Structure 34



E (Hartree) = -865.361758111

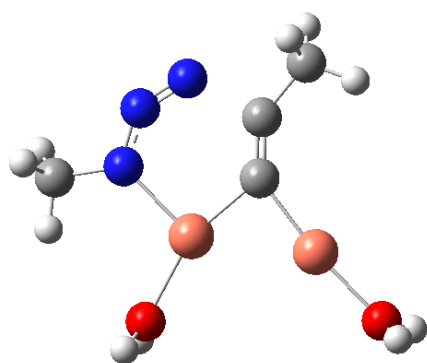
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.536786	1.030287	0.015417
2	6	0	-0.414584	2.251793	0.026512
3	7	0	2.531758	-0.377122	-0.010922
4	7	0	2.880896	0.816474	-0.048741



5	7	0	3.067776	1.927496	-0.087370
6	29	0	0.414742	-0.677049	0.004377
7	6	0	3.638249	-1.363787	0.066044
8	1	0	4.229392	-1.218300	0.973112
9	1	0	3.168165	-2.342622	0.095222
10	1	0	4.283896	-1.296515	-0.812600
11	6	0	-0.251591	3.697517	0.041447
12	1	0	-1.226762	4.189831	0.098595
13	1	0	0.335499	4.017949	0.906164
14	1	0	0.248763	4.047850	-0.865114
15	29	0	-2.140834	-0.008517	-0.002975
16	8	0	0.565611	-2.768065	-0.003881
17	1	0	0.404893	-3.279523	-0.805197
18	1	0	0.256294	-3.304692	0.734759
19	8	0	-3.900123	-0.906492	-0.018974
20	1	0	-4.479259	-0.897486	0.752235
21	1	0	-4.462873	-0.901399	-0.802264

### Structure 35



Imaginary Frequency:  $-325.9294 \text{ cm}^{-1}$

E(Hartree) =  $-865.334429959$

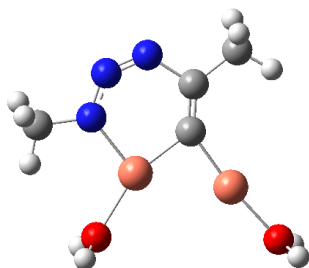
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.309559	0.881138	0.000064
2	6	0	0.181862	2.052800	0.000041
3	7	0	2.360593	-0.166824	-0.000139
4	7	0	2.553847	1.086531	-0.000125
5	7	0	1.922702	2.088570	-0.000055
6	29	0	0.473218	-0.852915	0.000073
7	6	0	3.561335	-1.022969	-0.000236
8	1	0	4.166131	-0.849876	0.892368
9	1	0	3.220258	-2.056448	-0.000401
10	1	0	4.166162	-0.849616	-0.892767
11	6	0	-0.180135	3.493812	0.000197
12	1	0	-1.262329	3.618549	-0.000089
13	1	0	0.240621	3.982890	0.881518
14	1	0	0.241140	3.983228	-0.880683
15	29	0	-2.007671	0.010045	-0.000020
16	8	0	0.589253	-2.894369	0.000254
17	1	0	0.643217	-3.458926	-0.778612
18	1	0	0.644224	-3.458673	0.779234
19	8	0	-3.852166	-0.673590	-0.000226
20	1	0	-4.418983	-0.705179	-0.779614

21                    1                    0                    -4.419017                    -0.705685                    0.779115

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### Structure 36



E(Hartree) = -865.336283712 cm<sup>-1</sup>

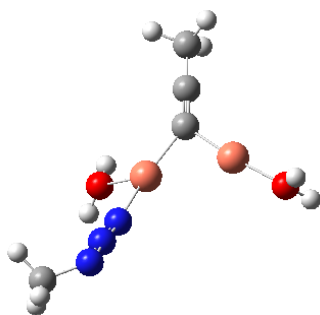
Standard orientation:

---

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.268327	0.839175	-0.001110
2	6	0	0.288910	2.013052	-0.000384
3	7	0	2.309283	-0.080558	0.000927
4	7	0	2.537912	1.175101	0.001302
5	7	0	1.790924	2.136986	0.001177
6	29	0	0.504459	-0.871087	-0.000644
7	6	0	3.504939	-0.946549	0.000353
8	1	0	4.108945	-0.769999	0.892424
9	1	0	3.167951	-1.981685	0.000077
10	1	0	4.108641	-0.769401	-0.891807
11	6	0	-0.307202	3.390235	-0.001082
12	1	0	-1.395596	3.360986	-0.001322
13	1	0	0.041758	3.933484	0.880422
14	1	0	0.042090	3.932708	-0.882941
15	29	0	-1.976267	0.002360	0.000087
16	8	0	0.595673	-2.911230	-0.000464
17	1	0	0.727674	-3.463738	-0.779202
18	1	0	0.728457	-3.463179	0.778541
19	8	0	-3.826062	-0.658299	0.001242
20	1	0	-4.390066	-0.712813	0.781488
21	1	0	-4.391063	-0.713220	-0.778258

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### Structure 37



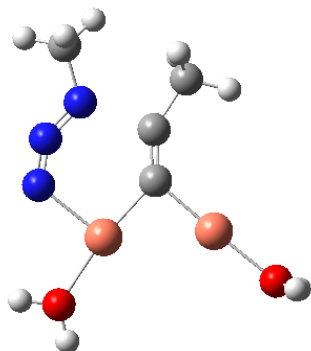
E(Hartree) = -865.362876592

Standard orientation:

---

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.706138	-0.639957	-0.226129
2	6	0	2.660116	-1.320623	-0.589891
3	7	0	-2.073826	-0.069903	0.084670
4	7	0	-3.117255	0.290188	-0.208889
5	7	0	-4.149658	0.814659	-0.540719
6	29	0	-0.201410	-0.643172	0.166411
7	6	0	3.768748	-2.151528	-1.032486
8	1	0	4.345350	-1.647863	-1.813271
9	1	0	4.443697	-2.394679	-0.207581
10	1	0	3.394825	-3.089250	-1.454664
11	29	0	1.632806	1.249864	0.081599
12	8	0	-0.522465	-2.534340	1.247074
13	1	0	-1.088004	-2.706032	2.008087
14	1	0	0.286717	-3.039033	1.385612
15	8	0	1.716008	3.198896	0.355381
16	1	0	2.136643	3.617783	1.114570
17	1	0	1.687669	3.843523	-0.360472
18	6	0	-5.416278	0.049182	-0.546375
19	1	0	-5.667668	-0.280451	0.464259
20	1	0	-6.183012	0.728112	-0.907556
21	1	0	-5.342224	-0.809678	-1.217046

### Structure 38



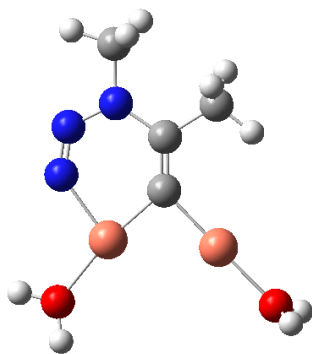
Imaginary Frequency:  $-364.4125 \text{ cm}^{-1}$   
E(Hartree) =  $-865.333251355$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.022352	-0.576843	-0.032855
2	6	0	0.996609	-1.386493	-0.059623
3	7	0	1.834033	1.662941	0.002452
4	7	0	2.589555	0.772106	-0.005674
5	7	0	2.703731	-0.466500	-0.071925
6	29	0	-0.188411	1.306974	-0.011886
7	6	0	1.409454	-2.809569	-0.113185
8	1	0	0.517275	-3.435886	-0.114378
9	1	0	1.975297	-3.029809	-1.021751
10	1	0	2.017299	-3.092335	0.749421
11	29	0	-1.868497	-0.837747	0.010793
12	8	0	-0.720253	3.236608	0.010261
13	1	0	-0.009400	3.887971	-0.001766
14	1	0	-1.540196	3.679985	-0.228515
15	8	0	-3.809254	-1.170928	0.068772
16	1	0	-4.290102	-1.407312	0.870108
17	1	0	-4.327866	-1.469945	-0.686740

18	6	0	4.012587	-1.101507	0.161282
19	1	0	4.182091	-1.260537	1.228999
20	1	0	4.018180	-2.058670	-0.353341
21	1	0	4.806568	-0.479843	-0.250294

### Structure 39



E (Hartree) = -865.351757750

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.156825	-0.443693	0.009561
2	6	0	1.311954	-1.092433	0.011094
3	7	0	1.611243	1.641811	-0.026112
4	7	0	2.574199	0.925158	-0.023918
5	7	0	2.570918	-0.398768	-0.006119
6	29	0	-0.305497	1.365907	0.010358
7	6	0	1.452742	-2.602209	0.030546
8	1	0	0.470311	-3.065751	0.040979
9	1	0	1.988135	-2.962410	-0.851423
10	1	0	1.995229	-2.938450	0.917645
11	29	0	-1.671501	-0.970231	-0.003339
12	8	0	-1.110404	3.204086	-0.010057
13	1	0	-1.981100	3.536064	0.230198
14	1	0	-0.504094	3.952861	-0.049840
15	8	0	-3.557835	-1.541376	-0.022507
16	1	0	-4.036507	-1.817952	-0.812323
17	1	0	-4.041027	-1.863716	0.746862
18	6	0	3.885265	-1.057591	-0.008561
19	1	0	4.012743	-1.663908	0.888554
20	1	0	4.001609	-1.679893	-0.896250
21	1	0	4.638312	-0.274981	-0.020244