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Electronic Supplementary Information

Theoretical Studies on Thermally Activated Delayed Fluorescence of "Carbene-Metal-Amide" Cu and Au Complexes: Geometric Structures, Excitation Characters and Mechanisms

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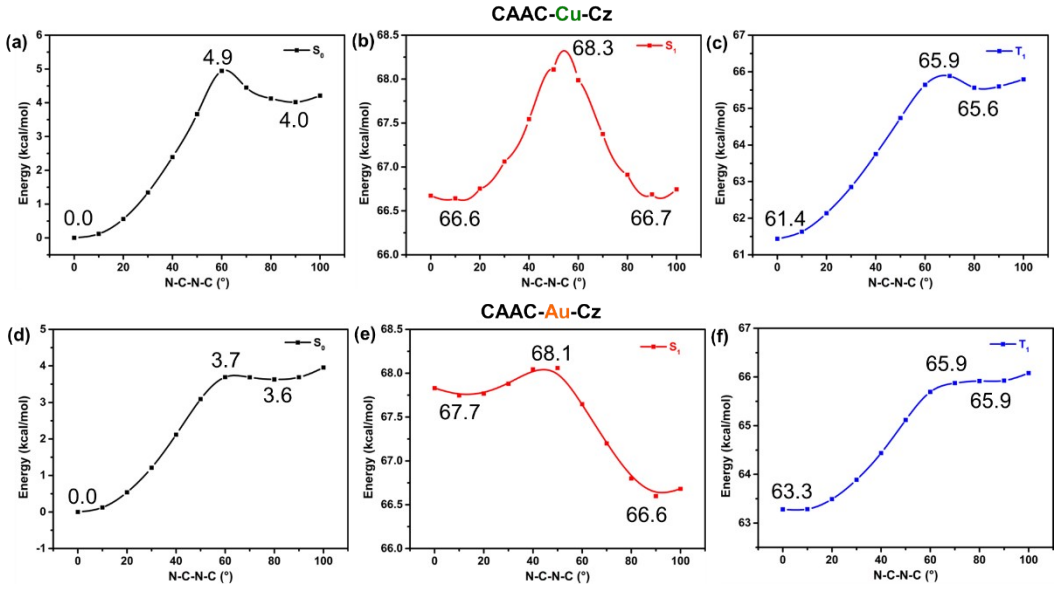

Fig. S1. Relaxed potential energy scan of the S_0, S_1, and T_1 states of (a-c) CAAC-Cu-Cz and (d-f) CAAC-Au-Cz with respect to their N1-C1-N2-C3 dihedral angles by DFT/PCM, TD-DFT/PCM and UDFT/PCM methods, respectively. The energetic zero point is assigned to the energy of the coplanar S_0 geometries.

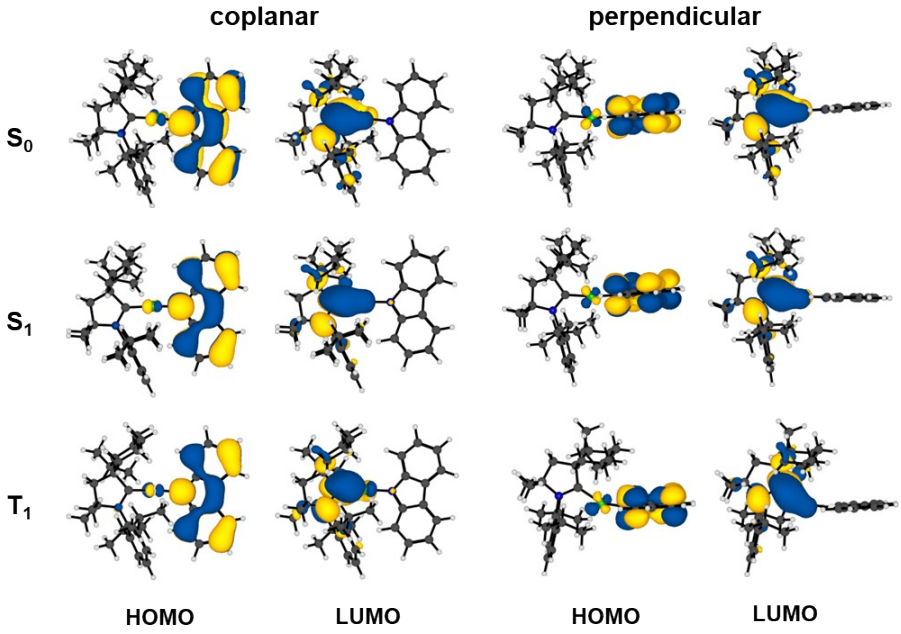

Fig. S2. HOMO and LUMO distributions at the coplanar and perpendicular S_0, S_1 and T_1 minima of the CAAC-Cu-Cz complex.

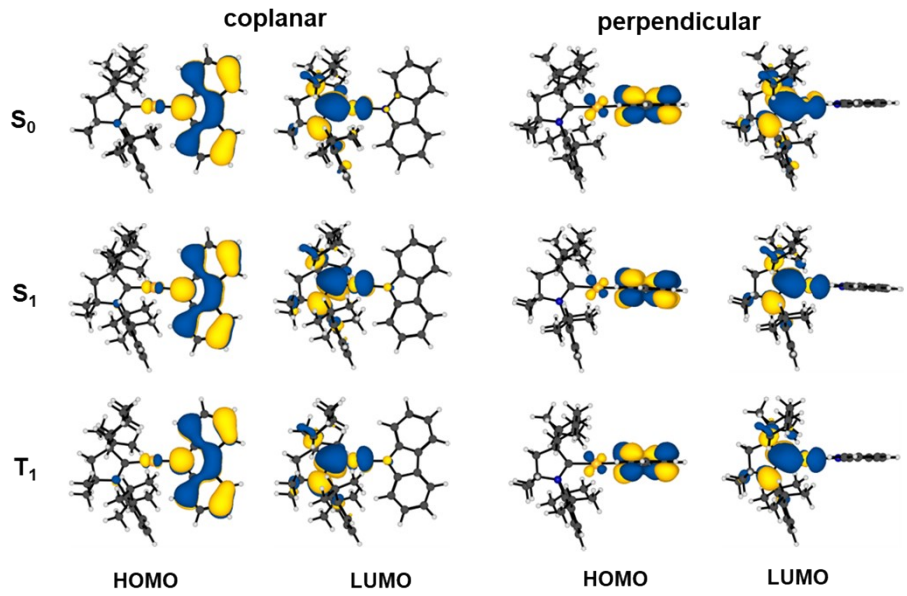

Fig. S3. HOMO and LUMO distributions at the coplanar and perpendicular S_0, S_1 and T_1 minima of the CAAC-Au-Cz complex.

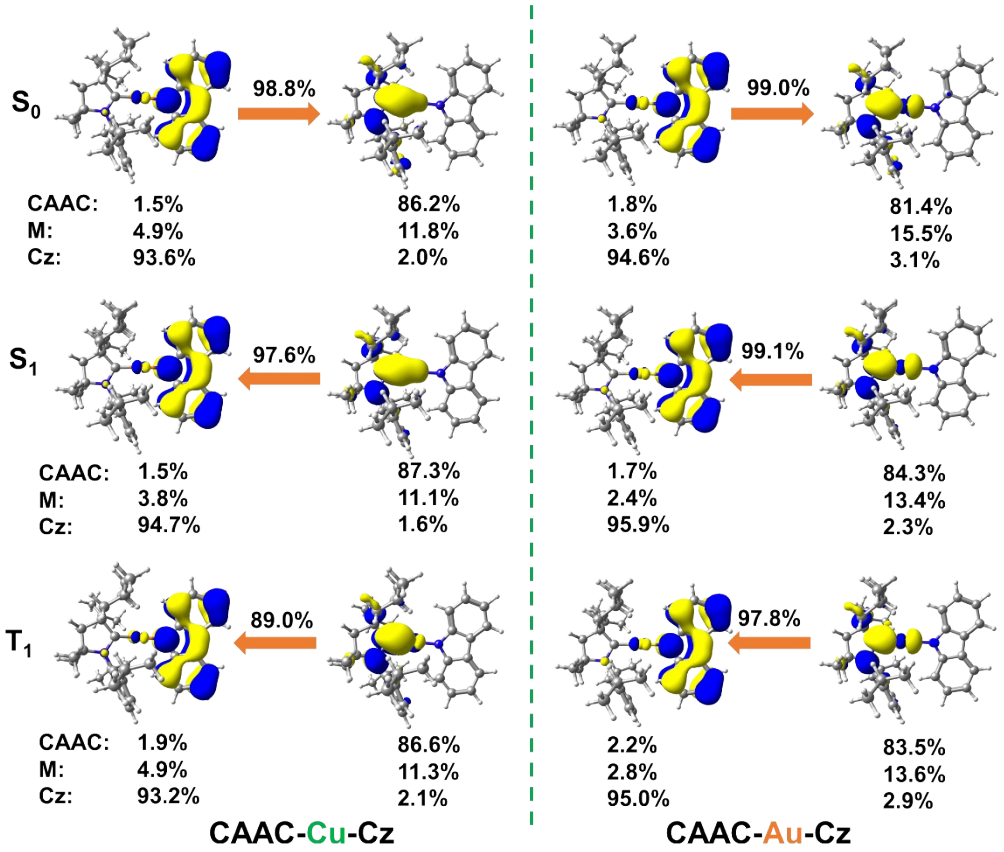

Fig. S4. Composition analysis and distribution of selected frontier molecular orbitals at the S_0, S_1 and T_1 minima of two CMA complexes.

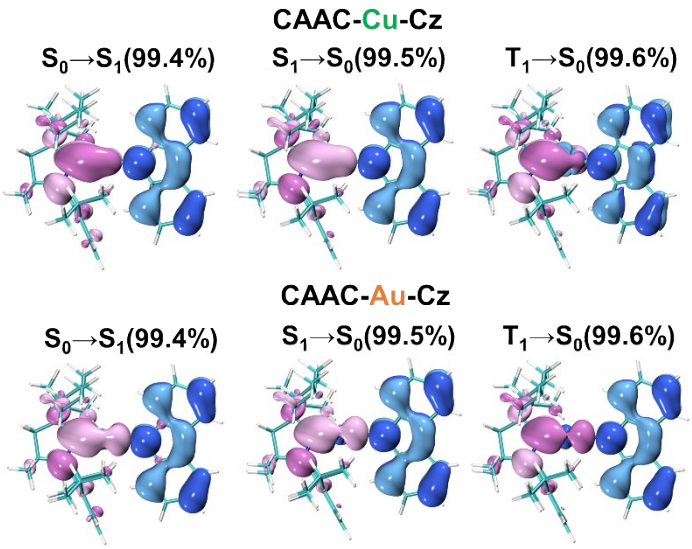

Fig. S5. The corresponding NTO distributions and weights of the CAAC-Cu-Cz and CAAC-Au-Cz complexes. Blue and pink are for hole and electron, respectively.

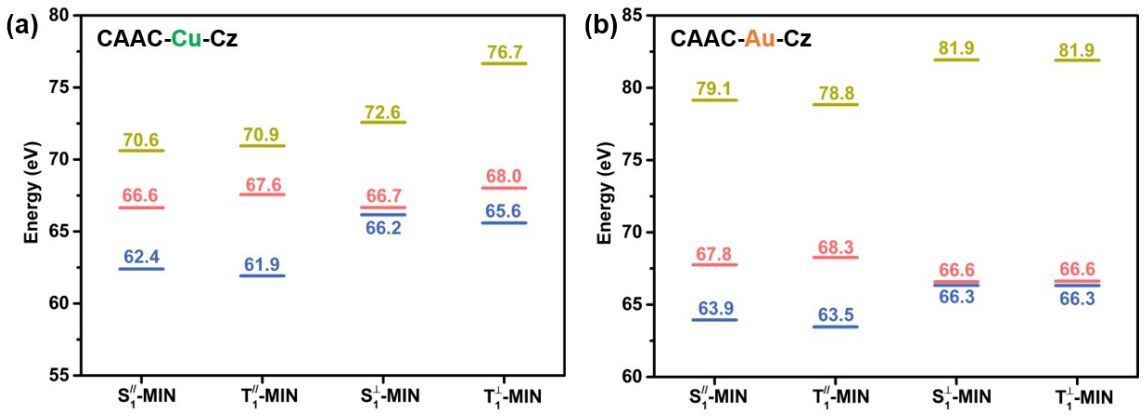

Fig. S6. Related energies of the S_1 (red), T_1 (blue), and T_2 (yellow) states at the coplanar and perpendicular S_1 and T_1 minima with respect to the energy of the coplanar S_0 minima of the two CMA complexes.

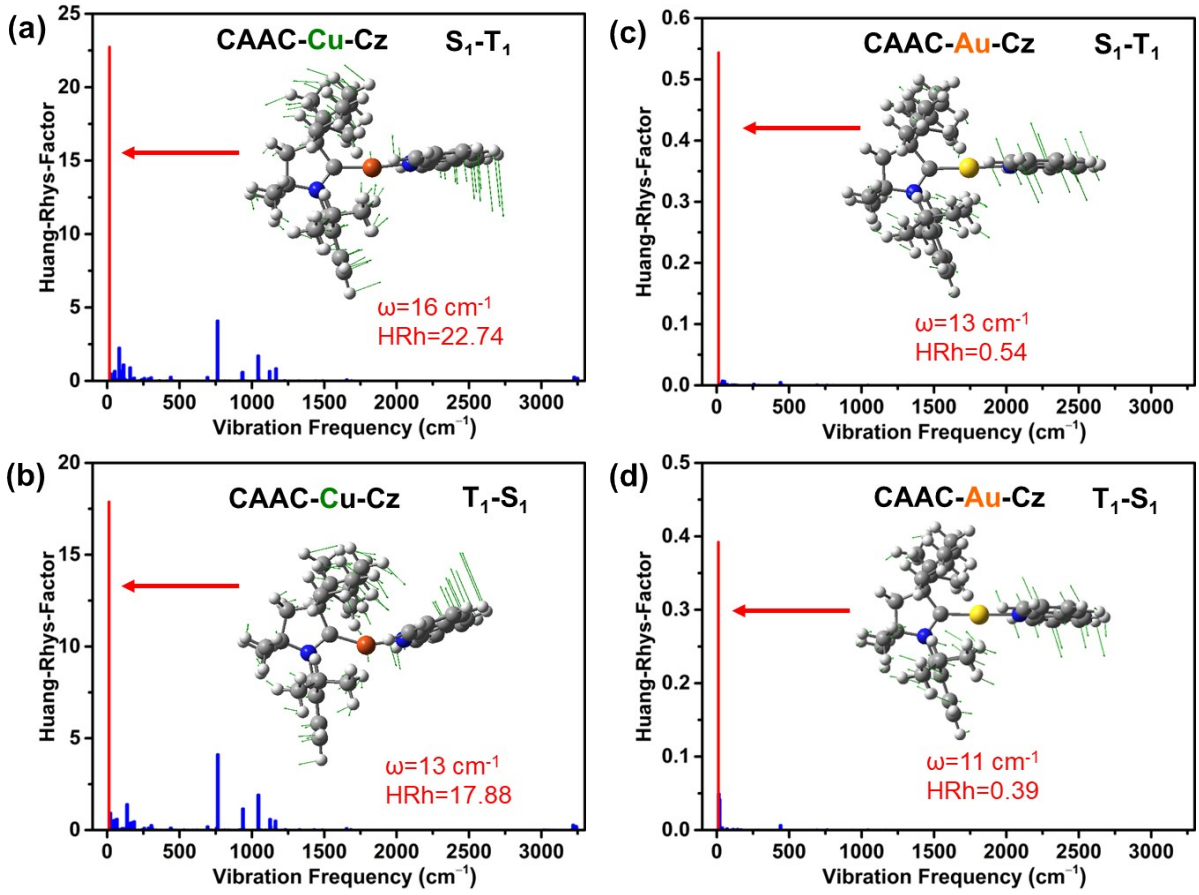

Fig. S7. Huang-Rhys factor distributions corresponding to different vibrational modes at the perpendicular structures: (a) ISC and (b) rISC in CAAC-Cu-Cz; (c) ISC and (d) rISC in CAAC-Au-Cz. The red lines represent the vibrational mode that has largest impact on the Huang-Rhys factor, the inset is the corresponding vibrational mode.

II Tables

Table S1. Calculate Key Bond Angel (C-Cu-N, in degree) and Dihedral Angeles (N-C-N-C, in degree) at the Different S_0, S_1 and T_1 Minimum-Energy Geometry and Crystal Structures of Two CMA Complexes.

Complexes	Geometry State	Crystal	Coplanar			Perpendicular		
			$S_0^{//}$	$S_1^{//}$	$T_1^{//}$	$S_0^{\perp}$	$S_1^{\perp}$	$T_1^{\perp}$
CAAC-Cu-Cz	C-Cu-N	173.5	175.8	171.9	167.9	173.2	173.0	154.8
	N-C-N-C	-1.3	1.7	8.0	4.1	88.1	93.2	105.7
CAAC-Au-Cz	C-Au-N	176.2	176.5	174.6	175.4	176.5	177.6	177.9
	N-C-N-C	0.3	1.1	14.5	6.0	80.3	91.8	89.3

Table S2. The RMSD Values (in Å) between S_0, S_1 and T_1 Minima at Perpendicular Minima of the Two CMA Complexes.

Complexes	S_0-S_1	S_0-T_1	S_1-T_1
CAAC-Cu-Cz	0.0974	0.3549	0.3944
CAAC-Au-Cz	0.1983	0.1397	0.0727

Table S3. TD-PBE0/PCM Calculated Vertical Energies ($E_{\perp}$, kcal/mol), Wavelength (λ, nm) Oscillator Strengths (ƒ) and Electronic Configurations at the S_0, S_1 and T_1 Minima and Available Experiment Data of Two CMA Complexes.

Structure		State	$E_{\perp}$ (kcal/mol)	λ (nm)	ƒ	Configuration	Exp.[a] (nm)
CAAC-Cu-Cz							
Coplanar Geometry	$S_0^{//}$-MIN	S_1	73.6	389	0.1138	HOMO->LUMO (98.8%)	388
		T_1	68.6	417	0	HOMO->LUMO (89.6%)	-
	$S_1^{//}$-MIN	S_1	58.8	486	0.1019	HOMO←LUMO (97.6%)	474
	$T_1^{//}$-MIN	T_1	55.0	520	0	HOMO←LUMO (89.0%)	-
Perpendicular Geometry	$S_0^{\perp}$-MIN	S_1	69.8	409	0.0027	HOMO->LUMO (97.1%)	
		T_1	69.8	409	0	HOMO->LUMO (94.8%)	
	$S_1^{\perp}$-MIN	S_1	55.3	517	0.0012	HOMO←LUMO (97.6%)	
	$T_1^{\perp}$-MIN	T_1	52.9	540	0	HOMO←LUMO (80.8%)	

CAAC-Au-Cz							
Coplanar Geometry	$S_0^{//}$-MIN	S_1	74.7	383	0.1690	HOMO->LUMO (99.0%)	388
		T_1	69.8	409	0	HOMO->LUMO (88.5%)	-
	$S_1^{//}$-MIN	S_1	59.7	479	0.1479	HOMO←LUMO (99.1%)	502
	$T_1^{//}$-MIN	T_1	56.1	509	0	HOMO←LUMO (97.8%)	-
Perpendicular Geometry	$S_0^{\perp}$-MIN	S_1	70.2	407	0.0082	HOMO->LUMO (98.9%)	
		T_1	69.8	409	0	HOMO->LUMO (98.5%)	
	$S_1^{\perp}$-MIN	S_1	55.3	517	0.0005	HOMO←LUMO (99.2%)	
	$T_1^{\perp}$-MIN	T_1	55.1	519	0	HOMO←LUMO (99.0%)	

[a]Experimental values in the 2-MeTHF solution in ref[54]

Table S4. Percentage of Each Excitation Character Estimated by NTOs at the Coplanar S_0, S_1 and T_1 minima of Two CMA complexes.

Complex	CAAC-Cu-Cz			CAAC-Au-Cz		
Excitation State	S_1 (FC)	S_1-MIN	T_1-MIN	S_1 (FC)	S_1-MIN	T_1-MIN
Cz->M	11.8%	10.20%	9.7%	16.0%	14.4%	13.9%
CAAC->M	0.2%	0.50%	0.7%	0.4%	0.3%	0.5%
Cz->CAAC	77.9%	77.10%	63.4%	73.9%	78.1%	74.4%
CAAC->Cz	0.0%	0.1%	0.1%	0.1%	0.1%	0.1%
M->Cz	0.20%	0.1%	0.4%	0.2%	0.1%	0.2%
M->CAAC	5.3%	5.8%	17.2%	3.3%	2.2%	5.1%
Cz->Cz	2.4%	1.9%	1.5%	3.8%	2.7%	2.4%
CAAC->CAAC	1.4%	3.5%	4.4%	1.7%	1.7%	2.5%
M->M	0.8%	0.8%	2.6%	0.7%	0.4%	1.0%

Table S5. Percentage of Excitation Character Estimated by NTOs at the Coplanar S_0, S_1 and T_1 minima of Two CMA complexes.

Structure	Excitation State	LMCT[a]	LLCT[b]	MLCT[c]	LE[d]	CT[e]
			CAAC-Cu-Cz			
S_0-MIN	S_1 (FC)	12.0%	77.9%	5.4%	4.6%	95.4%
S_1-MIN	S_1-MIN	10.7%	77.2%	6.0%	6.1%	93.9%
T_1-MIN	T_1-MIN	10.3%	63.5%	17.6%	8.5%	91.5%
			CAAC-Au-Cz			
S_0-MIN	S_1 (FC)	16.4%	74.0%	3.5%	6.2%	93.8%
S_1-MIN	S_1-MIN	14.8%	78.2%	2.3%	4.8%	95.2%
T_1-MIN	T_1-MIN	14.3%	74.5%	5.3%	5.9%	94.1%

Note: LMCT[a] includes Cz->M and CAAC->M; LLCT[b] includes Cz->CAAC and CAAC->Cz; MLCT[c] includes M->Cz and M->CAAC; LE[d] includes Cz->Cz, CAAC->CAAC, and M->M; CT[e] includes LMCT, MLCT and LLCT

Table S6. Related Energies (kcal/mol) of the S_1, T_1, and T_2 States at the S_1 and T_1 Minima with Respect to the Energy of Coplanar S_0 minima of Two CMA Complexes in Solution.

		At S∥ 1	At T∥ 1	At S⊥ 1	At T⊥ 1
CAAC-Cu-Cz	S_1	66.6	67.6	66.7	68.0
	T_1	62.4	61.9	66.2	65.6
	T_2	70.6	70.9	72.6	76.7
CAAC-Au-Cz	S_1	67.8	68.3	66.6	66.6
	T_1	63.9	63.5	66.3	66.3
	T_2	79.1	78.8	81.9	81.9

Table S7. Boltzmann Distribution (300 K) of T_2:T_1 at T_1 Minima of Two CMA Complexes.

	CAAC-Cu-Cz		CAAC-Au-Cz	
	coplanar	perpendicular	coplanar	perpendicular
T_2:T_1	1:3.6×10^{6}	1:1.2×10^{8}	1:1.4×10^{11}	1:2.3×10^{11}

Table S8. Reorganization Energies (in eV) between S_1 and T_1 Minima of Two CMA Complexes.

Compound	coplanar		perpendicular	
	S_1-T_1	T_1-S_1	S_1-T_1	T_1-S_1
CAAC-Cu-Cz	0.417	0.356	1.598	1.581
CAAC-Au-Cz	0.024	0.027	0.002	0.002

Table S9. Temperature-Dependence of (Reverse) Intersystem Crossing Rates ($k_{(r)ISC}$, s^{-1}) between Coplanar S_1 and T_1 States of Two CMA Complexes.

Temperature (K)	CAAC-Cu-Cz		CAAC-Au-Cz	
	k_{ISC} (s^{-1})	k_{rISC} (s^{-1})	k_{ISC} (s^{-1})	k_{rISC} (s^{-1})
300	1.64×10^{10}	4.78×10^{7}	5.36×10^{10}	1.10×10^{8}
250	2.28×10^{10}	1.47×10^{6}	5.65×10^{10}	2.81×10^{7}
200	3.15×10^{10}	2.13×10^{6}	5.92×10^{10}	3.52×10^{6}
150	4.26×10^{10}	6.98×10^{4}	6.12×10^{10}	1.08×10^{5}
100	5.57×10^{10}	5.61×10^{1}	6.14×10^{10}	1.03×10^{2}
77	6.20×10^{10}	3.04×10^{0}	5.98×10^{10}	3.81

III Modified Parameters of 2-MeTHF solution

PCM model with two modified parameters in Gaussian 16:

Eps=7.0 # Dielectric constant at 298 K (ε=7.0).

Epsinf=1.976836 # Square of the index of refraction at optical frequencies at 293 K (n_{20}^{D}).

CPCM model with two modified parameters in ORCA 5.0.1:

Eps=7.0 # Dielectric constant

Refrac=1.406 # The index of refraction at optical frequencies at 293 K (n_{20}^{D})

IV Cartesian Coordinates of Optimized Structures

In xyz format (unit: Angstrom)

CAAC-Cu-Cz

S0-MIN

Coplanar Geometry				Perpendicular Geometry			
Energy	-1820.764292 Hatree			Energy	-1820.757866 Hatree		
Atom	x	y	z	Atom	x	y	z
C	3.328775	1.090803	-0.138497	C	3.238474	1.180626	0.399320
C	3.224687	2.488596	-0.047074	C	2.968042	2.173241	1.357395
H	2.243754	2.964153	0.027566	H	1.949775	2.332478	1.718103
C	4.389612	3.246641	-0.050625	C	4.018605	2.947756	1.834869
H	4.319283	4.335687	0.020674	H	3.814892	3.722670	2.579279
C	5.658241	2.641015	-0.143152	C	5.337879	2.756528	1.379813
H	6.555556	3.264976	-0.143834	H	6.142291	3.381460	1.775852
C	5.773750	1.257248	-0.231029	C	5.618300	1.781113	0.428545
H	6.758891	0.786819	-0.300209	H	6.641137	1.634539	0.069501
C	4.613333	0.472420	-0.228234	C	4.574197	0.990997	-0.069551
C	4.354529	-0.944024	-0.293646	C	4.491707	-0.063771	-1.045968
C	5.160253	-2.086962	-0.385811	C	5.424081	-0.705961	-1.871251
H	6.249351	-1.994379	-0.428931	H	6.480946	-0.426476	-1.832117
C	4.557536	-3.340646	-0.419915	C	4.988732	-1.698360	-2.743264
H	5.174182	-4.240308	-0.491014	H	5.704648	-2.207521	-3.393435
C	3.154579	-3.461015	-0.360959	C	3.625157	-2.047770	-2.799789
H	2.697389	-4.454450	-0.384905	H	3.298949	-2.823391	-3.498440
C	2.335659	-2.342404	-0.270787	C	2.683328	-1.425045	-1.989608
H	1.248918	-2.442796	-0.221430	H	1.627216	-1.694510	-2.050959
C	2.934788	-1.072796	-0.238876	C	3.112142	-0.429790	-1.095062
C	-1.389161	0.545089	0.156558	C	-1.377383	0.399658	0.200282
C	-3.626768	-0.290298	0.393699	C	-3.626444	-0.005831	0.934163
C	-3.694094	1.245087	0.353787	C	-3.668728	1.102771	-0.126745
H	-4.222336	1.575444	-0.550490	H	-4.187984	0.742382	-1.024599
H	-4.264858	1.632820	1.208607	H	-4.236148	1.970709	0.235719
C	-2.240717	1.773229	0.369837	C	-2.207332	1.486042	-0.450516
C	-4.411376	-0.936680	-0.741257	C	-4.463846	-1.215797	0.540103
H	-4.272310	-2.027557	-0.755926	H	-4.350489	-2.038506	1.260932
H	-4.124203	-0.529070	-1.719961	H	-4.205516	-1.582398	-0.462448
H	-5.481748	-0.733832	-0.592406	H	-5.523059	-0.920900	0.527070
C	-4.107604	-0.862125	1.723680	C	-4.070269	0.483380	2.309471
H	-3.933232	-1.946268	1.778710	H	-3.920629	-0.290253	3.076007
H	-5.189835	-0.689367	1.810463	H	-5.143860	0.716625	2.270508
H	-3.621638	-0.379317	2.581889	H	-3.540647	1.395303	2.615439
C	-1.601543	-1.854958	0.174015	C	-1.661966	-1.399618	1.795693
C	-1.475484	-2.511290	-1.068088	C	-1.621330	-2.720418	1.304957
C	-1.044757	-3.842608	-1.062985	C	-1.263422	-3.739017	2.194140
H	-0.940183	-4.372725	-2.012293	H	-1.226780	-4.770705	1.836962
C	-0.716343	-4.490728	0.121799	C	-0.927126	-3.459278	3.513238
H	-0.385333	-5.531763	0.103346	H	-0.657319	-4.270259	4.193898
C	-0.758392	-3.793993	1.323934	C	-0.890451	-2.140707	3.951015

H	-0.430783	-4.286784	2.241914	H	-0.563569	-1.921860	4.970059
C	-1.185776	-2.463152	1.378873	C	-1.241845	-1.083588	3.105098
C	-1.645155	-1.800964	-2.398502	C	-1.793442	-3.054506	-0.164581
H	-2.065059	-0.804369	-2.203561	H	-2.170473	-2.159266	-0.678540
C	-0.268088	-1.589802	-3.036678	C	-0.414636	-3.362023	-0.755171
H	-0.359627	-1.013073	-3.969585	H	-0.473960	-3.491499	-1.846732
H	0.209620	-2.552938	-3.275006	H	0.004421	-4.284107	-0.322764
H	0.409579	-1.042476	-2.362294	H	0.293713	-2.547191	-0.540791
C	-2.584592	-2.527364	-3.359126	C	-2.771570	-4.196430	-0.429113
H	-2.721991	-1.932794	-4.275375	H	-2.892949	-4.346117	-1.512971
H	-3.574765	-2.700397	-2.913547	H	-3.763643	-3.995569	0.000238
H	-2.176854	-3.504225	-3.662079	H	-2.408773	-5.146556	-0.007576
C	-1.065356	-1.708868	2.691459	C	-1.028391	0.340304	3.585042
H	-1.552087	-0.732444	2.569457	H	-1.462080	1.020915	2.840596
C	0.409881	-1.431565	2.997653	C	0.473451	0.633525	3.631743
H	0.504445	-0.834302	3.918027	H	0.655922	1.691951	3.874836
H	0.894631	-0.875618	2.179389	H	0.951467	0.416203	2.664046
H	0.970144	-2.369031	3.138848	H	0.974988	0.017724	4.394718
C	-1.738156	-2.424063	3.861763	C	-1.684302	0.638536	4.931597
H	-1.691046	-1.797105	4.765375	H	-1.549098	1.699944	5.190452
H	-1.234843	-3.374308	4.098268	H	-1.232518	0.045962	5.742090
H	-2.795282	-2.646214	3.656255	H	-2.762931	0.425725	4.921198
C	-1.905533	2.309355	1.787691	C	-1.857363	2.816092	0.271322
H	-2.688710	3.047146	2.039748	H	-2.636984	3.544855	-0.015121
H	-2.010421	1.491860	2.521274	H	-1.957261	2.677996	1.361462
C	-0.545215	2.980181	1.941360	C	-0.495313	3.414408	-0.058626
H	0.239040	2.229511	1.720761	H	0.284585	2.690843	0.245333
C	-0.416216	4.100196	0.915233	C	-0.373882	3.600496	-1.566202
H	0.580268	4.567359	0.988509	H	0.624048	3.995756	-1.817403
H	-1.149902	4.892370	1.154964	H	-1.108062	4.359890	-1.895203
C	-0.654408	3.587350	-0.496083	C	-0.616213	2.291057	-2.300488
H	0.146761	2.873553	-0.756259	H	0.194234	1.587903	-2.038791
H	-0.567592	4.412619	-1.220928	H	-0.539740	2.445848	-3.388646
C	-2.013119	2.907825	-0.667701	C	-1.975025	1.665777	-1.978796
H	-2.779092	3.658433	-0.394863	H	-2.738861	2.415823	-2.259610
C	-0.332855	3.469429	3.366019	C	-0.256066	4.702586	0.713508
H	0.655950	3.940239	3.478899	H	0.740713	5.114578	0.492494
H	-0.396654	2.640134	4.088097	H	-0.318268	4.535366	1.800759
H	-1.094999	4.216926	3.643613	H	-1.004670	5.467892	0.447945
C	-2.292933	2.508284	-2.138056	C	-2.267272	0.408426	-2.834391
H	-3.063049	1.717390	-2.126202	H	-3.071930	-0.155845	-2.331539
C	-2.883324	3.683937	-2.913364	C	-2.803568	0.801487	-4.209309
H	-3.086142	3.407387	-3.959762	H	-3.025350	-0.089667	-4.816877
H	-2.187032	4.538629	-2.928317	H	-2.067747	1.403816	-4.766726
H	-3.827882	4.029160	-2.464537	H	-3.728185	1.393916	-4.126614
C	-1.085816	1.938430	-2.878380	C	-1.085094	-0.545214	-2.979428
H	-1.394702	1.517082	-3.847270	H	-1.402583	-1.480730	-3.465098
H	-0.590424	1.136090	-2.311019	H	-0.650317	-0.811934	-2.004088
H	-0.329561	2.712323	-3.081420	H	-0.279180	-0.110821	-3.590433
Cu	0.477327	0.412302	-0.026478	Cu	0.500904	0.255462	0.041122

N	2.321729	0.155557	-0.150018	N	2.363536	0.313094	-0.212421
N	-2.146464	-0.519818	0.215079	N	-2.153290	-0.345974	0.941816

S1-MIN

Coplanar Geometry				Perpendicular Geometry			
Energy	-1820.658086 Hartree			Energy	-1820.658066 Hartree		
Atom	x	y	z	Atom	x	y	z
C	3.357889	1.176394	-0.045495	C	3.294721	1.129420	0.414254
C	3.183772	2.563441	0.074089	C	3.004901	2.095860	1.386197
H	2.180924	2.988829	0.144565	H	1.976758	2.259660	1.710740
C	4.324050	3.365379	0.095395	C	4.064309	2.835117	1.911393
H	4.219707	4.448335	0.188005	H	3.866257	3.594246	2.670663
C	5.601524	2.800722	-0.003866	C	5.376240	2.618189	1.476170
H	6.477896	3.452191	0.012022	H	6.188145	3.209751	1.904460
C	5.780992	1.410359	-0.123451	C	5.670573	1.657164	0.492856
H	6.786240	0.989327	-0.196654	H	6.699326	1.505989	0.158818
C	4.660497	0.597264	-0.142629	C	4.628495	0.917115	-0.039132
C	4.431117	-0.837997	-0.235119	C	4.526567	-0.119578	-1.057819
C	5.239777	-1.956570	-0.339039	C	5.433034	-0.764848	-1.881407
H	6.327606	-1.866902	-0.379730	H	6.499720	-0.534945	-1.837498
C	4.630417	-3.225286	-0.388448	C	4.949770	-1.727534	-2.785296
H	5.259129	-4.114461	-0.471458	H	5.653305	-2.244381	-3.441384
C	3.239045	-3.369973	-0.332076	C	3.586444	-2.032010	-2.863589
H	2.794998	-4.366910	-0.369263	H	3.240671	-2.778719	-3.581060
C	2.407092	-2.256159	-0.231033	C	2.661980	-1.392715	-2.038073
H	1.320524	-2.355533	-0.189270	H	1.596068	-1.613870	-2.095544
C	3.011810	-0.990100	-0.184770	C	3.140029	-0.439645	-1.129599
C	-1.387123	0.516985	0.039278	C	-1.321337	0.379455	0.154971
C	-3.618420	-0.432958	0.221389	C	-3.583073	-0.011735	0.974351
C	-3.728722	1.089137	0.005605	C	-3.637281	0.986945	-0.194834
H	-4.086457	1.283545	-1.015150	H	-4.065854	0.486164	-1.073959
H	-4.469198	1.534982	0.686694	H	-4.300417	1.834613	0.034890
C	-2.321199	1.697192	0.210272	C	-2.192414	1.451440	-0.487294
C	-4.366024	-1.204398	-0.866583	C	-4.471624	-1.226176	0.702195
H	-4.198579	-2.288663	-0.773035	H	-4.357171	-1.990041	1.486888
H	-4.050035	-0.888809	-1.870137	H	-4.233797	-1.685346	-0.266896
H	-5.447837	-1.021037	-0.779122	H	-5.528564	-0.919586	0.680688
C	-4.181767	-0.862941	1.578978	C	-4.043091	0.623053	2.290520
H	-4.003563	-1.934783	1.751592	H	-3.911122	-0.079164	3.127055
H	-5.268993	-0.693251	1.605491	H	-5.111773	0.880202	2.231476
H	-3.731975	-0.298764	2.406953	H	-3.486843	1.542200	2.518636
C	-1.549873	-1.916808	0.149393	C	-1.642806	-1.393560	1.831212
C	-1.305030	-2.588227	-1.073210	C	-1.562261	-2.718721	1.341324
C	-0.795418	-3.892515	-1.037772	C	-1.169953	-3.742071	2.212183
H	-0.619518	-4.424748	-1.976310	H	-1.121637	-4.770670	1.844526
C	-0.484305	-4.511576	0.168211	C	-0.822328	-3.470190	3.530972
H	-0.095166	-5.533122	0.177931	H	-0.528875	-4.282248	4.201550
C	-0.631547	-3.807230	1.359029	C	-0.813202	-2.153812	3.979573
H	-0.330174	-4.274228	2.300372	H	-0.484482	-1.935799	4.999323
C	-1.142589	-2.503756	1.372513	C	-1.199960	-1.100076	3.142869

C	-1.472474	-1.898087	-2.414198	C	-1.774620	-3.039281	-0.125948
H	-1.952581	-0.928448	-2.222839	H	-2.154104	-2.125794	-0.605292
C	-0.096306	-1.596430	-3.014599	C	-0.421347	-3.348981	-0.770215
H	-0.199135	-1.041063	-3.960216	H	-0.521689	-3.470997	-1.860569
H	0.464133	-2.522863	-3.221498	H	0.016499	-4.274008	-0.360875
H	0.501853	-0.981475	-2.324580	H	0.284685	-2.526990	-0.577562
C	-2.332054	-2.689281	-3.398527	C	-2.765698	-4.175296	-0.369876
H	-2.487338	-2.110007	-4.322415	H	-2.931093	-4.314228	-1.450117
H	-3.319411	-2.928601	-2.977451	H	-3.739616	-3.975154	0.099969
H	-1.851531	-3.638181	-3.685977	H	-2.392642	-5.132502	0.028224
C	-1.157626	-1.732985	2.679826	C	-1.020062	0.326539	3.626072
H	-1.658971	-0.776556	2.483173	H	-1.460085	0.982767	2.864358
C	0.272470	-1.401661	3.115379	C	0.473642	0.655774	3.686376
H	0.266406	-0.790294	4.031983	H	0.631610	1.720821	3.922431
H	0.798044	-0.830360	2.332779	H	0.950260	0.443477	2.717124
H	0.855651	-2.314702	3.318250	H	0.987574	0.057391	4.456270
C	-1.904487	-2.456804	3.799044	C	-1.691653	0.613201	4.967245
H	-1.957614	-1.821209	4.697047	H	-1.580222	1.676850	5.231401
H	-1.394700	-3.389524	4.088878	H	-1.239248	0.026036	5.782374
H	-2.932295	-2.715044	3.505907	H	-2.766422	0.381689	4.945151
C	-2.236298	2.262248	1.653513	C	-1.973101	2.823664	0.204678
H	-3.067448	2.979379	1.803554	H	-2.767601	3.521777	-0.125663
H	-2.402845	1.438995	2.367785	H	-2.102565	2.695657	1.292202
C	-0.931064	2.972812	1.986256	C	-0.625349	3.473918	-0.076268
H	-0.113856	2.236712	1.840629	H	0.152177	2.764163	0.268326
C	-0.710492	4.109951	0.995398	C	-0.449684	3.649358	-1.580020
H	0.254774	4.608697	1.193774	H	0.543344	4.077742	-1.801274
H	-1.493575	4.876615	1.150577	H	-1.195342	4.381925	-1.944422
C	-0.760668	3.608470	-0.439850	C	-0.628681	2.327685	-2.312450
H	0.086308	2.919269	-0.606288	H	0.190676	1.646571	-2.018384
H	-0.614989	4.447583	-1.140716	H	-0.520379	2.480031	-3.399556
C	-2.057857	2.871293	-0.777433	C	-1.972263	1.657483	-2.016360
H	-2.881395	3.587959	-0.586808	H	-2.749710	2.391752	-2.307886
C	-0.893154	3.444677	3.431559	C	-0.447839	4.776670	0.688205
H	0.061839	3.941628	3.667337	H	0.541492	5.223075	0.496650
H	-1.016922	2.601753	4.130544	H	-0.542562	4.618394	1.774828
H	-1.703164	4.166428	3.633195	H	-1.210616	5.517137	0.392377
C	-2.141214	2.501895	-2.281860	C	-2.212687	0.411295	-2.908187
H	-2.804531	1.624354	-2.367027	H	-2.945881	-0.228350	-2.388279
C	-2.784881	3.635223	-3.078131	C	-2.837103	0.818184	-4.241731
H	-2.850020	3.387518	-4.149997	H	-3.017205	-0.058264	-4.885058
H	-2.194944	4.563629	-2.990994	H	-2.173650	1.502256	-4.797740
H	-3.803147	3.854745	-2.718995	H	-3.799435	1.334776	-4.096780
C	-0.815650	2.092987	-2.920795	C	-0.984217	-0.463361	-3.144458
H	-0.986735	1.708753	-3.939415	H	-1.266450	-1.382869	-3.682574
H	-0.329454	1.300338	-2.333269	H	-0.534883	-0.750731	-2.182732
H	-0.119104	2.942811	-3.004371	H	-0.219144	0.050279	-3.748548
Cu	0.489028	0.426366	0.102598	Cu	0.541532	0.250244	0.034025
N	2.383922	0.218031	-0.076625	N	2.407390	0.299991	-0.231456
N	-2.156197	-0.633398	0.139646	N	-2.148133	-0.363655	0.996565

T1-MIN

Coplanar Geometry				Perpendicular Geometry			
Energy	-1820.665611 Hartree			Energy	-1820.659761 Hartree		
Atom	x	y	z	Atom	x	y	z
C	3.284649	1.189463	-0.250573	C	3.179235	1.212008	0.376346
C	3.103190	2.572862	-0.136143	C	2.937603	2.073620	1.453454
H	2.098476	2.998385	-0.107555	H	2.024679	1.981120	2.043380
C	4.239352	3.376770	-0.053694	C	3.889749	3.048871	1.743932
H	4.127169	4.459233	0.037242	H	3.719297	3.732533	2.578555
C	5.521903	2.814668	-0.082210	C	5.058396	3.167864	0.979603
H	6.394865	3.467548	-0.014620	H	5.786121	3.943829	1.227374
C	5.707108	1.427687	-0.193417	C	5.307385	2.306491	-0.096124
H	6.713948	1.004570	-0.213338	H	6.222746	2.404924	-0.684408
C	4.586815	0.613761	-0.275890	C	4.366968	1.328728	-0.398078
C	4.371538	-0.822542	-0.390078	C	4.275911	0.287138	-1.407137
C	5.200809	-1.932185	-0.458066	C	5.096421	-0.127716	-2.449376
H	6.287796	-1.826729	-0.436451	H	6.049020	0.369933	-2.645517
C	4.612213	-3.204049	-0.552882	C	4.677601	-1.199945	-3.246850
H	5.253390	-4.086833	-0.604097	H	5.310166	-1.536785	-4.071177
C	3.220987	-3.362155	-0.575655	C	3.458212	-1.846861	-3.004406
H	2.789551	-4.363465	-0.638764	H	3.153606	-2.679417	-3.642416
C	2.372584	-2.257929	-0.508035	C	2.624136	-1.441192	-1.964326
H	1.286669	-2.373152	-0.505302	H	1.669311	-1.934480	-1.779785
C	2.958580	-0.989161	-0.423772	C	3.038620	-0.371117	-1.162970
C	-1.353188	0.512318	0.140168	C	-1.260115	0.265102	0.261970
C	-3.534579	-0.426564	0.660077	C	-3.586613	0.041089	0.909760
C	-3.674923	1.093821	0.449534	C	-3.474371	1.070747	-0.231432
H	-4.206387	1.280688	-0.493898	H	-3.907005	0.644551	-1.146729
H	-4.284066	1.548319	1.245222	H	-4.057699	1.975460	-0.004605
C	-2.253358	1.704419	0.400879	C	-1.976903	1.404284	-0.441920
C	-4.455221	-1.207126	-0.277528	C	-4.531103	-1.101030	0.536117
H	-4.279638	-2.290940	-0.194818	H	-4.532297	-1.885506	1.308696
H	-4.307157	-0.909250	-1.324569	H	-4.247897	-1.556608	-0.422670
H	-5.507041	-1.015041	-0.016403	H	-5.559347	-0.720292	0.439885
C	-3.866118	-0.833565	2.098980	C	-4.096562	0.679470	2.203866
H	-3.658611	-1.902067	2.259403	H	-4.078217	-0.046918	3.029923
H	-4.934781	-0.663088	2.299933	H	-5.136826	1.013943	2.072152
H	-3.288363	-0.253832	2.831390	H	-3.495301	1.551843	2.493532
C	-1.498311	-1.919278	0.302815	C	-1.790951	-1.465031	1.909043
C	-1.448958	-2.632489	-0.919593	C	-1.758602	-2.799428	1.437268
C	-0.924928	-3.931619	-0.923709	C	-1.467313	-3.828997	2.339465
H	-0.899020	-4.496355	-1.859445	H	-1.456798	-4.864012	1.987554
C	-0.416276	-4.505931	0.236344	C	-1.171691	-3.556127	3.670546
H	-0.018983	-5.524173	0.217443	H	-0.957093	-4.372894	4.364655
C	-0.375837	-3.760731	1.410373	C	-1.111220	-2.236003	4.104270
H	0.080404	-4.192457	2.305006	H	-0.822900	-2.022518	5.136996
C	-0.891000	-2.459946	1.462869	C	-1.396590	-1.174326	3.238116
C	-1.849730	-1.995463	-2.237568	C	-1.912756	-3.129518	-0.035001
H	-2.288433	-1.015648	-2.002917	H	-2.201689	-2.201394	-0.547829

C	-0.605498	-1.731137	-3.090235	C	-0.553355	-3.548078	-0.601134
H	-0.877395	-1.210968	-4.022246	H	-0.604379	-3.680224	-1.693306
H	-0.094275	-2.669744	-3.359663	H	-0.206623	-4.495027	-0.156956
H	0.114115	-1.096370	-2.549221	H	0.205707	-2.780384	-0.383371
C	-2.871435	-2.819962	-3.019169	C	-2.968630	-4.196490	-0.316506
H	-3.188459	-2.279081	-3.924790	H	-3.080728	-4.346979	-1.401850
H	-3.767968	-3.034083	-2.419826	H	-3.950538	-3.915494	0.090697
H	-2.448920	-3.783678	-3.345713	H	-2.689995	-5.168444	0.120949
C	-0.702073	-1.644186	2.728703	C	-1.170393	0.246899	3.718774
H	-1.239158	-0.697880	2.585164	H	-1.503045	0.917133	2.915190
C	0.775447	-1.287491	2.913674	C	0.328378	0.491875	3.911676
H	0.909219	-0.648324	3.801246	H	0.524996	1.551196	4.142978
H	1.157773	-0.737464	2.040467	H	0.887509	0.232137	2.998591
H	1.395100	-2.188965	3.048110	H	0.735377	-0.116515	4.735277
C	-1.248985	-2.334413	3.977259	C	-1.935108	0.591281	4.995620
H	-1.162540	-1.668884	4.850659	H	-1.782490	1.649877	5.258834
H	-0.688138	-3.253526	4.210776	H	-1.587389	-0.011199	5.849829
H	-2.307849	-2.608541	3.864294	H	-3.015641	0.422797	4.885279
C	-1.932840	2.332272	1.781109	C	-1.673594	2.757673	0.251123
H	-2.724501	3.064928	2.034406	H	-2.371066	3.522742	-0.142649
H	-1.980184	1.543281	2.550091	H	-1.890908	2.661653	1.328236
C	-0.586678	3.041516	1.854339	C	-0.250679	3.260661	0.055658
H	0.189873	2.291174	1.604927	H	0.424135	2.479262	0.453260
C	-0.538705	4.134829	0.792562	C	0.042185	3.398680	-1.433595
H	0.443737	4.639283	0.804425	H	1.088760	3.713915	-1.586730
H	-1.286137	4.910627	1.045572	H	-0.593838	4.203150	-1.850031
C	-0.831356	3.577280	-0.592488	C	-0.226307	2.095505	-2.172258
H	-0.018079	2.885632	-0.880441	H	0.501880	1.340149	-1.831146
H	-0.814277	4.388327	-1.339613	H	-0.041027	2.228587	-3.251247
C	-2.162852	2.829532	-0.670987	C	-1.645555	1.565251	-1.956065
H	-2.941690	3.559104	-0.373574	H	-2.330560	2.365605	-2.299775
C	-0.297991	3.574958	3.249169	C	0.016693	4.544429	0.825346
H	0.685848	4.069381	3.294235	H	1.059254	4.877016	0.696400
H	-0.302947	2.764328	3.995519	H	-0.162755	4.408111	1.904261
H	-1.057645	4.314562	3.554790	H	-0.641369	5.359226	0.478263
C	-2.508156	2.391558	-2.120553	C	-1.950487	0.332961	-2.845876
H	-3.127032	1.481138	-2.049031	H	-2.783756	-0.215513	-2.374625
C	-3.349983	3.460473	-2.814577	C	-2.428853	0.772053	-4.228468
H	-3.605723	3.166800	-3.845494	H	-2.653087	-0.096085	-4.868974
H	-2.802601	4.416944	-2.870753	H	-1.657715	1.369171	-4.743804
H	-4.290708	3.648488	-2.272642	H	-3.339151	1.389347	-4.164381
C	-1.312893	2.018400	-2.994748	C	-0.804161	-0.665417	-2.973987
H	-1.659906	1.602550	-3.954383	H	-1.139626	-1.570350	-3.505940
H	-0.689749	1.255122	-2.504782	H	-0.448376	-0.966603	-1.978279
H	-0.678525	2.889281	-3.224606	H	0.047972	-0.249984	-3.534614
Cu	0.458670	0.427489	-0.291628	Cu	0.577438	-0.070325	0.369723
N	2.309972	0.222532	-0.350584	N	2.376796	0.186471	-0.086059
N	-2.107446	-0.638009	0.342314	N	-2.187871	-0.419881	1.033904

CAAC-Au-Cz

S0-MIN

Coplanar Geometry				Perpendicular Geometry			
Energy	-1759.220187 Hartree			Energy	-1759.214382 Hartree		
Atom	x	y	z	Atom	x	y	z
C	-3.099946	1.085672	-0.169080	C	-3.277772	0.489034	-1.021104
C	-2.535602	2.371119	-0.196718	C	-2.895031	1.502860	-1.913947
H	-1.451475	2.504262	-0.143250	H	-1.838764	1.735605	-2.065172
C	-3.388821	3.463982	-0.291897	C	-3.886259	2.191701	-2.603075
H	-2.962839	4.471127	-0.313958	H	-3.599357	2.983710	-3.300438
C	-4.786688	3.301049	-0.359825	C	-5.250377	1.888837	-2.425537
H	-5.429668	4.181689	-0.434392	H	-6.005141	2.449443	-2.982692
C	-5.351984	2.029931	-0.331947	C	-5.638993	0.878198	-1.552349
H	-6.437276	1.904643	-0.384151	H	-6.697394	0.636363	-1.419413
C	-4.513242	0.911637	-0.235808	C	-4.657940	0.169656	-0.846687
C	-4.731734	-0.513175	-0.180942	C	-4.688338	-0.916543	0.099080
C	-5.868636	-1.331237	-0.202483	C	-5.709984	-1.680701	0.677558
H	-6.866310	-0.889200	-0.276884	H	-6.756281	-1.483241	0.427338
C	-5.712844	-2.711878	-0.128063	C	-5.377279	-2.694521	1.570023
H	-6.591584	-3.361433	-0.144012	H	-6.164234	-3.298986	2.027945
C	-4.428478	-3.282191	-0.030860	C	-4.029071	-2.951691	1.886486
H	-4.328160	-4.369530	0.027909	H	-3.786829	-3.756169	2.586523
C	-3.285176	-2.491733	-0.007659	C	-2.998149	-2.205901	1.327044
H	-2.289188	-2.936351	0.068375	H	-1.954534	-2.413688	1.576160
C	-3.433825	-1.098159	-0.084341	C	-3.324489	-1.176126	0.428862
C	1.544721	-0.460303	0.160267	C	1.547971	-0.356885	0.155150
C	3.760126	0.432585	0.297962	C	3.720547	0.193714	0.992644
C	3.863911	-1.100043	0.258814	C	3.877261	-0.945859	-0.021663
H	4.479016	-1.469587	1.090309	H	4.471523	-1.767107	0.400723
H	4.363982	-1.418767	-0.665371	H	4.422060	-0.586663	-0.904725
C	2.428842	-1.672483	0.334372	C	2.460261	-1.424838	-0.410319
C	1.688703	1.950417	0.133053	C	1.646626	1.539770	1.664126
C	1.486027	2.571635	-1.117878	C	1.574794	2.824400	1.086374
C	0.997134	3.882575	-1.124181	C	1.106273	3.873871	1.883104
H	0.833896	4.385095	-2.080227	H	1.043183	4.878399	1.458685
C	0.686726	4.544724	0.057240	C	0.695731	3.657884	3.192960
H	0.307896	5.569090	0.028649	H	0.338730	4.492960	3.800354
C	0.814089	3.881945	1.271989	C	0.700221	2.369548	3.713306
H	0.507728	4.384536	2.192106	H	0.320414	2.197272	4.722934
C	1.301144	2.572302	1.340800	C	1.159650	1.281281	2.963825
C	1.648063	1.853038	-2.445834	C	1.846554	3.089494	-0.383421
H	2.077282	0.860351	-2.249279	H	2.282689	2.181212	-0.822838
C	0.272299	1.628497	-3.082304	C	0.515015	3.335162	-1.098098
H	0.368854	1.037434	-4.005756	H	0.665286	3.421745	-2.185114
H	-0.206330	2.586214	-3.340091	H	0.039966	4.262942	-0.742682
H	-0.402894	1.089818	-2.399776	H	-0.186144	2.509131	-0.909404
C	2.573234	2.586448	-3.416690	C	2.814400	4.245818	-0.627864
H	3.564610	2.776668	-2.981969	H	3.771265	4.102624	-0.106119
H	2.148822	3.556304	-3.719399	H	2.389430	5.204314	-0.291935
H	2.710588	1.989932	-4.331748	H	3.023579	4.341712	-1.704427

C	1.275559	1.860851	2.683167	C	0.999220	-0.114276	3.542270
H	1.748130	0.877319	2.558209	H	1.464870	-0.828673	2.849580
C	-0.171402	1.604914	3.116993	C	-0.487624	-0.474447	3.620112
H	-0.723584	1.036184	2.352925	H	-0.979310	-0.354831	2.643211
H	-0.709362	2.550491	3.287894	H	-1.014661	0.167940	4.342877
H	-0.192030	1.028089	4.054759	H	-0.614285	-1.520043	3.941601
C	2.033886	2.615672	3.775027	C	1.658426	-0.281052	4.911301
H	2.051786	2.022507	4.702254	H	1.568929	-1.325125	5.248750
H	1.547208	3.574788	4.010698	H	1.169880	0.349667	5.670073
H	3.073086	2.829944	3.488230	H	2.725649	-0.019382	4.896370
C	4.277294	1.017163	1.607854	C	4.097132	-0.230193	2.408105
H	3.827880	0.531329	2.484046	H	3.577872	-1.146753	2.717759
H	4.089041	2.098607	1.662702	H	3.879890	0.566870	3.132651
H	5.364210	0.860368	1.657229	H	5.177785	-0.429145	2.438677
C	4.488687	1.092955	-0.865198	C	4.531239	1.424090	0.608250
H	5.567567	0.912628	-0.753767	H	5.599545	1.172711	0.675216
H	4.326122	2.180435	-0.875276	H	4.338086	2.265243	1.289469
H	4.175913	0.677102	-1.832267	H	4.326630	1.743974	-0.421971
C	2.177053	-2.234466	1.760039	C	2.150198	-2.754555	0.331819
H	3.018555	-2.916992	1.977074	H	3.013277	-3.418956	0.146697
H	2.254347	-1.414276	2.494417	H	2.136728	-2.572491	1.420184
C	0.875548	-3.001777	1.963200	C	0.885928	-3.492116	-0.093651
H	0.033064	-2.306855	1.786320	H	0.015673	-2.845814	0.125752
C	0.777860	-4.119348	0.930500	C	0.915388	-3.723651	-1.600065
H	1.575054	-4.860828	1.127789	H	1.747770	-4.411900	-1.840962
H	-0.180227	-4.653781	1.043763	H	-0.011209	-4.227049	-1.921568
C	0.912707	-3.581618	-0.485720	C	1.089212	-2.415934	-2.356859
H	0.050541	-2.928649	-0.703306	H	0.199225	-1.786973	-2.186570
H	0.860623	-4.408734	-1.212111	H	1.126489	-2.607243	-3.441592
C	2.212394	-2.807916	-0.707317	C	2.350644	-1.655925	-1.946238
H	3.034031	-3.510274	-0.470090	H	3.197873	-2.340393	-2.142561
C	0.767858	-3.519521	3.389881	C	0.720327	-4.784348	0.692007
H	-0.178339	-4.061200	3.543315	H	-0.202895	-5.307972	0.399358
H	0.807343	-2.695604	4.119931	H	0.669892	-4.591751	1.775596
H	1.593193	-4.213848	3.621640	H	1.566601	-5.468616	0.511646
C	2.416716	-2.383205	-2.184838	C	2.604362	-0.394442	-2.811970
H	3.102531	-1.517816	-2.190159	H	3.255524	0.282646	-2.231338
C	3.108018	-3.496551	-2.969192	C	3.373460	-0.762099	-4.079386
H	2.502254	-4.417868	-2.963038	H	2.804244	-1.480084	-4.692576
H	4.093014	-3.740843	-2.541273	H	4.346030	-1.221491	-3.842662
H	3.257199	-3.208168	-4.021405	H	3.560571	0.126369	-4.702383
C	1.146101	-1.942058	-2.907003	C	1.351613	0.401483	-3.169129
H	1.397285	-1.519809	-3.892206	H	1.630127	1.346977	-3.659507
H	0.590748	-1.175259	-2.347015	H	0.748820	0.650745	-2.282974
H	0.461540	-2.787595	-3.076101	H	0.702141	-0.152592	-3.864239
Au	-0.441278	-0.357764	0.037454	Au	-0.442440	-0.277740	-0.052504
N	-2.459409	-0.128984	-0.079970	N	-2.484273	-0.318845	-0.242099
N	2.271890	0.629121	0.176624	N	2.237886	0.465379	0.901912

S1-MIN

Coplanar Geometry				Perpendicular Geometry			
Energy	-1759.112216 Hartree			Energy	-1759.114077 Hartree		
Atom	x	y	z	Atom	x	y	z
C	-3.186743	0.958466	-0.243068	C	-3.269686	0.439409	-1.139904
C	-2.613086	2.237257	-0.352449	C	-2.779392	1.321467	-2.112281
H	-1.528900	2.367490	-0.311217	H	-1.705045	1.467898	-2.230035
C	-3.474342	3.321358	-0.512229	C	-3.704789	1.988029	-2.914711
H	-3.058005	4.327085	-0.599710	H	-3.352129	2.681279	-3.680697
C	-4.861480	3.137540	-0.560020	C	-5.078341	1.778914	-2.751047
H	-5.513319	4.004677	-0.686033	H	-5.782284	2.315297	-3.390735
C	-5.438677	1.856715	-0.445870	C	-5.573848	0.887672	-1.780800
H	-6.523959	1.738318	-0.480480	H	-6.649413	0.733653	-1.671566
C	-4.602938	0.765854	-0.287479	C	-4.668454	0.216532	-0.978804
C	-4.794615	-0.669215	-0.127989	C	-4.779573	-0.767229	0.090974
C	-5.889778	-1.513260	-0.074498	C	-5.833021	-1.409897	0.715925
H	-6.907324	-1.126643	-0.165520	H	-6.868171	-1.204951	0.434738
C	-5.669061	-2.892894	0.102796	C	-5.542797	-2.343931	1.728134
H	-6.526530	-3.567849	0.145394	H	-6.365069	-2.858365	2.229828
C	-4.376108	-3.416946	0.224879	C	-4.224755	-2.630206	2.100013
H	-4.242039	-4.492012	0.360590	H	-4.033359	-3.365593	2.883797
C	-3.259058	-2.584617	0.172889	C	-3.151827	-1.989837	1.480984
H	-2.241833	-2.972628	0.260263	H	-2.116764	-2.204935	1.751149
C	-3.476255	-1.208582	-0.002073	C	-3.437991	-1.050921	0.480488
C	1.564794	-0.416095	0.039462	C	1.509603	-0.340910	0.109061
C	3.721596	0.633949	0.324905	C	3.691645	0.209032	1.006994
C	3.911132	-0.871275	0.055537	C	3.849937	-0.800075	-0.143123
H	4.660561	-1.305937	0.733343	H	4.569763	-1.590985	0.114755
H	4.294469	-1.008001	-0.965184	H	4.257385	-0.279659	-1.021032
C	2.535438	-1.561580	0.207114	C	2.454633	-1.380258	-0.467753
C	1.584219	2.028397	0.192237	C	1.635267	1.507114	1.738616
C	1.331021	2.678178	-1.040705	C	1.488026	2.799661	1.180433
C	0.733757	3.944685	-1.025305	C	0.983025	3.829732	1.982177
H	0.548234	4.459915	-1.971462	H	0.880062	4.834126	1.562726
C	0.353774	4.549171	0.167948	C	0.594852	3.594978	3.296683
H	-0.103971	5.541874	0.160858	H	0.212349	4.413529	3.912192
C	0.525902	3.865999	1.366668	C	0.663877	2.305252	3.811397
H	0.177426	4.319666	2.298209	H	0.309583	2.112649	4.827693
C	1.118412	2.597937	1.402633	C	1.161067	1.243598	3.046054
C	1.598409	2.016328	-2.380519	C	1.767013	3.081643	-0.284346
H	2.104877	1.061922	-2.178921	H	2.218156	2.174342	-0.710151
C	0.276776	1.678722	-3.076634	C	0.446655	3.308669	-1.024304
H	0.464484	1.143390	-4.020856	H	0.617797	3.408435	-2.108191
H	-0.297428	2.589951	-3.311372	H	-0.058922	4.222868	-0.672701
H	-0.346674	1.033895	-2.438563	H	-0.230650	2.457873	-0.858066
C	2.483400	2.861923	-3.296667	C	2.717286	4.257765	-0.505191
H	3.430201	3.140069	-2.811933	H	3.664785	4.127437	0.037259
H	1.977247	3.792643	-3.598988	H	2.269587	5.207554	-0.171552
H	2.722031	2.306459	-4.217443	H	2.950008	4.366019	-1.576498
C	1.153666	1.850376	2.723655	C	1.074466	-0.163642	3.608001

H	1.674892	0.900509	2.544070	H	1.549508	-0.832273	2.877658
C	-0.266296	1.502192	3.180627	C	-0.392281	-0.588856	3.716927
H	-0.791948	0.915945	2.410389	H	-0.901382	-0.459174	2.750250
H	-0.857422	2.409437	3.386294	H	-0.930006	0.009401	4.470498
H	-0.236314	0.901791	4.103983	H	-0.469956	-1.649029	4.008284
C	1.888416	2.615723	3.824497	C	1.774438	-0.326239	4.956622
H	1.960788	2.000909	4.735538	H	1.738932	-1.378063	5.282152
H	1.353521	3.540066	4.095389	H	1.283781	0.274335	5.739233
H	2.907729	2.897240	3.524529	H	2.829646	-0.021105	4.915458
C	4.222944	1.034586	1.714305	C	4.139201	-0.379830	2.347565
H	3.761743	0.431445	2.507662	H	3.616820	-1.317533	2.579253
H	4.008921	2.094693	1.912508	H	3.954353	0.332710	3.164355
H	5.313039	0.894298	1.771964	H	5.219228	-0.590451	2.322377
C	4.465555	1.478744	-0.708453	C	4.517562	1.468907	0.748419
H	5.550801	1.339884	-0.589179	H	5.589859	1.222627	0.776254
H	4.245548	2.549964	-0.581553	H	4.327065	2.236951	1.513842
H	4.198502	1.185954	-1.732486	H	4.295810	1.897424	-0.237959
C	2.447611	-2.173448	1.632610	C	2.310239	-2.744759	0.258319
H	3.336969	-2.815015	1.789045	H	3.186992	-3.372157	0.003599
H	2.517023	-1.359531	2.373125	H	2.355745	-2.573383	1.346529
C	1.207823	-3.014576	1.906219	C	1.055137	-3.535774	-0.085340
H	0.325317	-2.360092	1.764146	H	0.184253	-2.906687	0.185488
C	1.121571	-4.134572	0.875556	C	1.003847	-3.769409	-1.590928
H	1.974541	-4.824621	1.024016	H	1.850088	-4.422242	-1.880291
H	0.206893	-4.731628	1.036622	H	0.082961	-4.314335	-1.862133
C	1.146685	-3.582186	-0.541788	C	1.082553	-2.456274	-2.355552
H	0.236758	-2.978252	-0.702590	H	0.176222	-1.864881	-2.136532
H	1.103909	-4.408862	-1.270870	H	1.070672	-2.650143	-3.441615
C	2.377682	-2.718587	-0.824397	C	2.322692	-1.633625	-2.000187
H	3.255325	-3.367610	-0.633890	H	3.189628	-2.282231	-2.236265
C	1.189012	-3.537426	3.334589	C	0.971614	-4.831587	0.707103
H	0.282188	-4.131599	3.532427	H	0.053167	-5.391245	0.466608
H	1.217004	-2.711558	4.063685	H	0.975268	-4.638122	1.792118
H	2.060907	-4.184863	3.530925	H	1.829800	-5.488544	0.483789
C	2.469939	-2.288264	-2.312825	C	2.474835	-0.371359	-2.892202
H	3.017862	-1.330959	-2.343995	H	3.014877	0.385944	-2.298815
C	3.283507	-3.303320	-3.113348	C	3.330783	-0.684781	-4.117953
H	2.813619	-4.301086	-3.076699	H	2.867480	-1.478586	-4.728701
H	4.306924	-3.404142	-2.717658	H	4.335977	-1.032602	-3.830258
H	3.357508	-3.013827	-4.174092	H	3.450561	0.199857	-4.764229
C	1.130453	-2.029322	-2.998925	C	1.166696	0.289464	-3.321172
H	1.295354	-1.601311	-4.000943	H	1.375480	1.235617	-3.846406
H	0.521135	-1.318715	-2.421947	H	0.539811	0.516259	-2.446605
H	0.549808	-2.956498	-3.130513	H	0.587377	-0.347215	-4.008859
Au	-0.433255	-0.400212	0.044617	Au	-0.474145	-0.312629	-0.027232
N	-2.535941	-0.225494	-0.070713	N	-2.542839	-0.312928	-0.252047
N	2.254537	0.773111	0.203911	N	2.238627	0.474454	0.972620

T1-MIN

Coplanar Geometry				Perpendicular Geometry			
Energy	-1759.119055 Hartree			Energy	-1759.114496 Hartree		
Atom	x	y	z	Atom	x	y	z
C	-3.160334	0.976888	-0.148447	C	-3.290638	0.469972	-1.086114
C	-2.589408	2.257858	-0.175416	C	-2.825267	1.404424	-2.020697
H	-1.505498	2.388260	-0.133048	H	-1.754655	1.575903	-2.139762
C	-3.454529	3.348651	-0.258515	C	-3.769785	2.089936	-2.783867
H	-3.040503	4.358767	-0.280971	H	-3.436862	2.824355	-3.519731
C	-4.840319	3.164359	-0.313454	C	-5.137814	1.847571	-2.619091
H	-5.494845	4.036145	-0.378554	H	-5.857092	2.399469	-3.227783
C	-5.413318	1.877407	-0.286798	C	-5.608096	0.903382	-1.687372
H	-6.497808	1.756056	-0.329829	H	-6.679524	0.723598	-1.577036
C	-4.571277	0.783153	-0.204545	C	-4.683332	0.213493	-0.924159
C	-4.761756	-0.662489	-0.152039	C	-4.766891	-0.820076	0.100247
C	-5.860020	-1.503687	-0.164434	C	-5.803281	-1.509276	0.704081
H	-6.875936	-1.107904	-0.226989	H	-6.844307	-1.311368	0.439861
C	-5.641378	-2.892857	-0.093617	C	-5.487678	-2.480864	1.672149
H	-6.499790	-3.567849	-0.102851	H	-6.296140	-3.032251	2.156770
C	-4.350177	-3.426609	-0.011743	C	-4.161608	-2.756908	2.022635
H	-4.217378	-4.508933	0.041546	H	-3.950261	-3.520756	2.773386
C	-3.231623	-2.593693	0.001913	C	-3.105689	-2.069858	1.424583
H	-2.215755	-2.989268	0.063322	H	-2.064665	-2.273950	1.680833
C	-3.448222	-1.210858	-0.068916	C	-3.417321	-1.095993	0.466088
C	1.543434	-0.423739	0.066600	C	1.508820	-0.333210	0.099418
C	3.717236	0.626066	0.257353	C	3.688655	0.199918	1.012264
C	3.891345	-0.891057	0.052485	C	3.846156	-0.810953	-0.136156
H	4.653069	-1.299649	0.733015	H	4.562215	-1.604574	0.123903
H	4.252424	-1.075653	-0.968892	H	4.257308	-0.292300	-1.013499
C	2.515910	-1.566461	0.263379	C	2.448943	-1.384577	-0.464061
C	1.589546	2.030262	0.110065	C	1.638647	1.525644	1.715592
C	1.315131	2.638384	-1.139514	C	1.515268	2.817426	1.150022
C	0.726431	3.908916	-1.158405	C	1.008563	3.856621	1.938770
H	0.525769	4.391402	-2.118645	H	0.923440	4.860166	1.513361
C	0.374931	4.558898	0.019561	C	0.596549	3.631849	3.247709
H	-0.075660	5.554380	-0.014069	H	0.212913	4.457118	3.853459
C	0.565716	3.917196	1.238469	C	0.643750	2.343829	3.769096
H	0.238227	4.406046	2.159835	H	0.271766	2.159910	4.780673
C	1.150434	2.646683	1.307754	C	1.141280	1.273079	3.016719
C	1.554341	1.927058	-2.459049	C	1.822163	3.089253	-0.311051
H	2.054631	0.975614	-2.229844	H	2.274360	2.176574	-0.723772
C	0.218855	1.578039	-3.122120	C	0.516857	3.319774	-1.075723
H	0.386161	1.002635	-4.046489	H	0.707907	3.414988	-2.156643
H	-0.348477	2.485796	-3.385304	H	0.008265	4.236778	-0.735927
H	-0.401524	0.966610	-2.448949	H	-0.165423	2.471413	-0.918564
C	2.432584	2.730404	-3.418568	C	2.784707	4.257139	-0.521488
H	3.390308	3.014500	-2.959502	H	3.721245	4.122877	0.038844
H	1.931212	3.655741	-3.744659	H	2.338207	5.212172	-0.201513
H	2.649945	2.140861	-4.323339	H	3.037585	4.357358	-1.588990
C	1.205766	1.944838	2.652864	C	1.033270	-0.129523	3.586925

H	1.723365	0.989129	2.496722	H	1.504557	-0.808785	2.863858
C	-0.207085	1.612766	3.142162	C	-0.438846	-0.537393	3.692819
H	-0.741381	0.997351	2.401452	H	-0.944177	-0.410443	2.723695
H	-0.796654	2.526477	3.322481	H	-0.972536	0.072071	4.440203
H	-0.163575	1.046861	4.086566	H	-0.529020	-1.594270	3.992299
C	1.957912	2.745958	3.715683	C	1.723862	-0.290657	4.940785
H	2.044275	2.162020	4.645655	H	1.674067	-1.339585	5.273730
H	1.428398	3.679698	3.964085	H	1.235681	0.321529	5.715919
H	2.972690	3.015473	3.390176	H	2.782734	0.001806	4.903811
C	4.248134	1.081971	1.618854	C	4.112357	-0.394308	2.358277
H	3.799027	0.515440	2.445454	H	3.571967	-1.322578	2.586171
H	4.042963	2.150657	1.776935	H	3.930408	0.322858	3.171596
H	5.338423	0.938076	1.662392	H	5.188981	-0.622676	2.345229
C	4.451754	1.416965	-0.824639	C	4.534724	1.448478	0.764247
H	5.537841	1.273281	-0.719333	H	5.603035	1.187581	0.807498
H	4.243499	2.494882	-0.741085	H	4.344015	2.219615	1.526512
H	4.162880	1.082886	-1.830068	H	4.333213	1.879460	-0.225328
C	2.455878	-2.119517	1.711935	C	2.292081	-2.743938	0.268843
H	3.342098	-2.763033	1.878540	H	3.167125	-3.377415	0.023518
H	2.545575	-1.277199	2.417834	H	2.331153	-2.567121	1.356326
C	1.213662	-2.936487	2.041449	C	1.035275	-3.530644	-0.078446
H	0.335342	-2.279903	1.885118	H	0.165909	-2.895274	0.182180
C	1.102461	-4.099131	1.061312	C	0.992775	-3.773050	-1.582764
H	1.953534	-4.787900	1.225665	H	1.838361	-4.430654	-1.863035
H	0.186932	-4.682479	1.262847	H	0.071519	-4.315920	-1.856809
C	1.107908	-3.609842	-0.379393	C	1.080992	-2.464215	-2.353485
H	0.197556	-3.010281	-0.553380	H	0.175710	-1.868468	-2.142213
H	1.051578	-4.467673	-1.070637	H	1.074154	-2.663270	-3.438636
C	2.335563	-2.762098	-0.718515	C	2.322277	-1.644294	-1.995869
H	3.213523	-3.408265	-0.519938	H	3.188043	-2.296469	-2.226245
C	1.212163	-3.398315	3.490928	C	0.939134	-4.820773	0.721729
H	0.303599	-3.975256	3.727980	H	0.019065	-5.376652	0.478673
H	1.258782	-2.542561	4.183737	H	0.936715	-4.620348	1.805492
H	2.081493	-4.044814	3.701299	H	1.794979	-5.484035	0.508357
C	2.402335	-2.387856	-2.224518	C	2.481030	-0.384469	-2.890489
H	2.920560	-1.416500	-2.297063	H	3.011394	0.376391	-2.292949
C	3.239227	-3.409763	-2.991480	C	3.352124	-0.699112	-4.105150
H	2.798174	-4.418194	-2.911180	H	2.898241	-1.496270	-4.718638
H	4.267549	-3.465945	-2.599516	H	4.354891	-1.043126	-3.804664
H	3.298406	-3.160921	-4.063484	H	3.476863	0.183810	-4.752858
C	1.052347	-2.193925	-2.912023	C	1.175932	0.270884	-3.337173
H	1.201794	-1.812265	-3.935055	H	1.388438	1.216750	-3.861411
H	0.431161	-1.468341	-2.367082	H	0.536093	0.497702	-2.471957
H	0.491873	-3.138971	-2.994080	H	0.608246	-0.369011	-4.031536
Au	-0.442745	-0.396730	0.040957	Au	-0.474256	-0.300361	-0.035698
N	-2.501342	-0.221563	-0.065608	N	-2.541907	-0.309563	-0.240629
N	2.251562	0.772776	0.153658	N	2.239635	0.483600	0.960446