Collision-Induced Dissociation of Singly and Doubly Charged Cu^{II}-Cytidine Complexes in the Gas Phase: an Experimental and Computational Study

Shuqin Zhang,[a,b] Li Xu, [a] Junguo Dong,[a] Zhen Zhou,[a] Ping Cheng[a*]

a: School of Environmental and Chemical Engineering, Shanghai University, Shanghai, 200444, China

b:College of Resources and Environmental Engineering, Wuhan University of Science and Technology, Wuhan 430081, China;

Table 1S. B3LYP/LANDL2DZ6-311+G(d) optimized geometries of cytidine and Cu^{II}-Cytidine Complexes (L=Cytidine, B=Cytosine, R=Ribose)

	L（=*keto*-L）				$[L+H]^+$		
	X	Y	Z		X	Y	Z
O	-1.91982100	2.74729600	-0.23664000	C	-2.71682600	-0.69768800	0.38775500
C	-2.89896100	1.82047500	-0.69572900	C	-1.29402400	-1.12237400	0.79429900
H	-3.78612300	1.96046100	-0.07432500	O	-1.13470000	0.41847000	-1.01241300
H	-3.17653500	2.03520200	-1.73425400	C	-2.48683000	0.55178200	-0.47901400
C	-2.44108500	0.37570800	-0.57758400	O	-3.20998200	-1.80146300	-0.37043600
H	-3.19083300	-0.27817200	-1.04128900	C	-2.64327300	1.87391800	0.25116700
O	-1.17866100	0.23110400	-1.24189200	O	-2.49192400	2.89845600	-0.71341100
C	-0.40624200	-0.80514600	-0.62956400	C	-0.52568700	-0.71012600	-0.48255000
H	-0.23535000	-1.62591400	-1.32149700	C	3.19385300	-0.88915600	-0.93149300
N	0.91909800	-0.28018400	-0.27455200	C	1.84853600	-1.11037100	-1.00304600
C	1.07968000	0.97421800	0.21697100	N	0.92915800	-0.42487500	-0.28440300
H	0.18168100	1.56999100	0.31481600	C	1.31704500	0.59188500	0.59903700
C	2.30551800	1.45166400	0.54855100	N	2.71361700	0.81502600	0.62567400
H	2.42752700	2.45071500	0.94623400	C	3.65213800	0.13334400	-0.07511600
C	3.41299300	0.56679600	0.33011900	N	4.93755900	0.44962500	0.06678100
N	4.67216200	0.97795700	0.64336600	O	0.58468000	1.23327500	1.29757400
H	4.87314200	1.95158700	0.79199200	O	-1.14895700	-2.47665000	1.10715000
H	5.42835300	0.37844900	0.35361300	H	-3.35220700	-0.50617900	1.25708900
N	3.28215000	-0.65244700	-0.14473600	H	-0.95880000	-0.53670400	1.64856100
C	2.05136200	-1.16533900	-0.44336100	H	-3.15867300	0.55037000	-1.34102700
O	1.84977400	-2.29690700	-0.83722800	H	-4.16460200	-1.73985000	-0.48088200
C	-2.18690200	-0.13119000	0.84164000	H	-1.89747600	1.95609800	1.05098500
H	-1.71651400	0.65067500	1.44531200	H	-3.64588500	1.89426900	0.70523800
C	-1.22484700	-1.30679700	0.57688700	H	-2.56920100	3.75417800	-0.27823700
H	-0.57768700	-1.54994600	1.42770800	H	-0.54181400	-1.55239200	-1.18369800
O	-3.41755200	-0.55250200	1.42507100	H	3.88321600	-1.47062000	-1.52607900
H	-1.22438500	2.77441400	-0.90392400	H	1.44808100	-1.87117000	-1.66104000
H	-3.35774700	-0.47695500	2.38320400	H	5.64500100	-0.05069200	-0.44860100
O	-1.97082100	-2.43378400	0.16470300	H	-1.84257900	-2.95430000	0.62615700
H	-2.81185100	-2.40177300	0.64417600	H	5.25709700	1.18872500	0.67417300
				H	2.97298200	1.55584900	1.26705000
	$[R]^+$				$[B+H]^+$		
	X	Y	Z		X	Y	Z

* Corresponging author: Pingcheng@shu.edu.cn

C	-0.15076900	0.66626500	-0.11035200	C	-1.02510900	1.20292100	-0.00001200
C	-1.57743800	0.13435900	0.17498100	C	0.25880700	1.71982600	-0.00007900
O	-0.16906700	-1.70166300	0.23362700	N	1.32408200	0.88386100	-0.00002300
C	0.73047200	-0.48575600	0.41952300	C	1.14909500	-0.51184500	-0.00001300
O	0.03687800	1.86657100	0.56530700	N	-0.09073200	-1.04360500	-0.00005000
C	2.03915100	-0.71242900	-0.31363900	C	-1.19038900	-0.21855400	-0.00003400
O	2.61435600	0.58374700	-0.28895400	N	-2.37617800	-0.82769500	0.00003700
C	-1.36066700	-1.33371000	0.10938100	O	2.20530700	-1.24553200	0.00004100
O	-2.60045000	0.51827900	-0.67787700	H	-1.87586200	1.87183500	0.00012500
H	-0.02524600	0.76641900	-1.19630600	H	0.45634400	2.78408700	0.00026200
H	-1.78935800	0.35339800	1.24150500	H	-2.40479200	-1.84060900	0.00000000
H	0.86564400	-0.40142900	1.49863700	H	-3.25229700	-0.32453600	0.00013900
H	0.89394000	2.23818100	0.31413500	H	2.27952700	1.23146900	0.00023500
H	1.84506700	-1.05881600	-1.33719800				
H	2.65400900	-1.45627500	0.20262000				
H	3.51872100	0.55888700	-0.62172400				
H	-2.11541700	-2.10438000	-0.04436600				
H	-2.98558500	1.35617000	-0.39348400				

	[R-H]$^+$				[CuB(MeOH)]$^+$		
	X	Y	Z		X	Y	Z
C	0.16772800	0.65145500	0.30208800	Cu	-1.20962800	0.12093500	-0.20280300
C	1.62551800	0.22070800	0.11348900	C	3.20507000	0.39315000	0.02883700
O	0.21525400	-1.67740700	-0.00147900	C	3.24708400	-1.01189700	0.15380300
C	-0.57283300	-0.53180000	-0.33602900	N	2.14170400	-1.70688800	0.31873500
O	-0.09540500	1.90664100	-0.25888900	C	0.96941300	-1.07008500	-0.01803000
C	-1.98228400	-0.73103600	0.18136800	N	0.82538500	0.30060700	-0.10409600
O	-2.65377300	0.51476100	-0.02676900	C	1.91065200	1.06678900	0.05353300
C	1.58545500	-1.29574900	-0.09905000	N	1.85991100	2.38559100	0.12353200
O	2.60175800	0.91656900	0.10091300	O	-0.05687900	-1.72391000	-0.24660200
H	-0.02651100	0.63430900	1.39024400	H	4.12143400	0.96790900	-0.07416400
H	2.00067100	-1.53338600	-1.08854500	H	4.19839900	-1.53163000	0.24520400
H	-0.59617000	-0.37534500	-1.42516000	H	0.98289600	2.89089100	0.06314900
H	-1.05313300	2.02974300	-0.20404900	H	2.69629900	2.95024700	0.21991500
H	-1.93853700	-0.99023600	1.24705600	O	-3.11895200	0.22938000	-0.31692600
H	-2.47703400	-1.54801400	-0.35696400	H	-3.54254000	0.15241800	-1.18387500
H	-3.55652900	0.45001800	0.29980300	C	-4.12003600	0.00285000	0.74569200
C	0.16772800	0.65145500	0.30208800	H	-4.93248700	0.71260000	0.59424200
				H	-4.47698300	-1.02425100	0.68259300
				H	-3.62325200	0.19092000	1.69223100

	[Cu(MeOH)(BCOH)]$^+$				[L-CH_2OH]$^+$		
	X	Y	Z		X	Y	Z
Cu	1.62297700	0.37956600	-0.00002400	C	2.97486500	-0.37983800	0.34477200
C	-2.48387600	1.74043900	-0.00009800	C	1.72620100	0.39877200	0.80654200
C	-3.02253200	0.50495600	-0.00015000	O	1.27697100	-0.79174100	-1.25003100
N	-2.25325400	-0.63370800	-0.00009900	C	2.39423900	-1.43038600	-0.58932300
C	-0.83549900	-0.53766200	-0.00020900	O	3.75919400	0.60063900	-0.32524700
N	-0.29435100	0.74608000	0.00001800	C	0.86884300	0.33273100	-0.55577100
C	-1.05317700	1.84433000	0.00006200	C	-2.69639900	1.29397200	-0.44513400
N	-0.46686900	3.04421100	0.00023600	C	-1.33280100	1.34832100	-0.62478700
O	-0.10544100	-1.50237400	-0.00047500	N	-0.56569700	0.29250400	-0.32441700
H	-3.11109800	2.62101700	-0.00016700	C	-1.17748900	-0.90480100	0.35010100
H	-4.09482100	0.34690900	-0.00022800	N	-2.51833400	-0.96514500	0.40726200
H	0.53766800	3.12722800	0.00042200	C	-3.26898700	0.04872100	0.03018100
H	-1.00744300	3.89373400	0.00038500	N	-4.59815300	-0.07372900	0.09839900
C	3.94816900	-1.52115300	0.00011000	O	-0.39818000	-1.70259200	0.81336300
H	3.06269900	-2.15011800	-0.00172100	O	1.97203500	1.68574400	1.22211400
H	4.53533800	-1.70415400	0.89954500	H	3.50749800	-0.81179400	1.19734200
H	4.53844200	-1.70334900	-0.89745500	H	1.17534400	-0.13373500	1.58023100
O	3.47822200	-0.14080500	-0.00014700	H	3.08887500	-1.74990900	-1.36641200
H	4.21678700	0.47529900	0.00114300	H	4.67380700	0.31250700	-0.41688500
C	-2.93759400	-1.91567100	0.00012400	H	1.08306900	1.24590100	-1.11903500
H	-4.02882400	-1.75498700	-0.00003800	H	-3.31038000	2.15135700	-0.69051300
O	-2.41111800	-2.97513400	0.00046000	H	-0.84310100	2.22517600	-1.03277900
				H	-5.22989300	0.66234900	-0.17202000
				H	2.78607700	1.98432300	0.77846600
				H	-4.98828800	-0.94286000	0.43454100
				H	2.02128800	-2.30006200	-0.04272500

	[CuL]$^{2+}$	[CuL(MeOH)]$^{2+}$

	X	Y	Z
Cu	-3.48898635	-1.16319853	-1.94439675
C	3.64570025	0.98637207	-0.20784095
C	0.95291817	0.20482009	1.77090478
O	1.52237995	-0.13166378	-0.56300296
C	2.88187420	-0.35050325	-0.17727681
O	4.74193745	1.20406667	0.68422019
C	3.54024050	-1.34037192	-1.15621188
O	4.89973477	-1.55921136	-0.77048573
C	0.91103985	0.78750002	0.34600817
C	-2.36905967	2.37822659	-0.16819366
C	-1.07896098	2.18145362	0.20211645
N	-0.48648219	1.01246098	-0.05050757
C	-1.24320597	-0.04471068	-0.72722683
N	-2.51283242	0.17755262	-1.08044661
C	-3.08838417	1.35947206	-0.81688578
N	-4.35978347	1.57134765	-1.17478777
O	-0.70146069	-1.15343464	-0.97383135
O	1.02429543	1.08009368	2.89948859
H	3.35614914	1.75234963	-0.89656335
H	0.92860734	-0.85495397	1.91646553
H	2.91097152	-0.75535228	0.81274875
H	5.37380938	1.79996912	0.27527260
H	3.51114317	-0.93552290	-2.14623744
H	3.00953021	-2.26923983	-1.13497573
H	5.31014493	-2.17627240	-1.38073091
H	1.44175022	1.71636789	0.32477206
H	-2.84268681	3.31592914	0.03500885
H	-0.53767682	2.96149672	0.69551711
H	-4.87608483	0.85006103	-1.63650035
H	-4.79391775	2.45102356	-0.98062877
H	0.59030966	0.66942639	3.65089310

	X	Y	Z
Cu	-2.24693779	-0.65031929	-1.47408670
C	4.30149420	0.22116334	0.65043173
C	1.34575339	0.11805688	2.39120728
O	2.01724168	-0.39798843	0.11800817
C	3.25446419	-0.90778982	0.62227298
O	5.33995224	0.20887081	1.63346468
C	3.75060949	-2.04542750	-0.28943990
O	4.98783200	-2.55522889	0.21482490
C	1.55653532	0.65838936	0.96459877
C	-1.30138197	2.96871513	0.13194271
C	-0.08712307	2.48073551	0.62460646
N	0.28470523	1.18245101	0.44622862
C	-0.64912934	0.34823681	-0.28255420
N	-1.78596866	0.89312130	-0.74882509
C	-2.19404828	2.12962319	-0.58951415
N	-3.36185073	2.56890050	-1.07191874
O	-0.67591601	-0.97613010	-0.64124849
O	1.51917315	0.98336941	3.51640051
H	4.25194806	1.01476377	-0.06555957
H	1.06953936	-0.90484055	2.54049448
H	3.10801187	-1.28321556	1.61348801
H	6.12248721	0.63622985	1.27765114
H	3.89706180	-1.67000176	-1.28065492
H	3.02312761	-2.82983002	-0.30900473
H	5.29711736	-3.26440563	-0.35351561
H	2.28401724	1.44279185	0.98416372
H	-1.56315382	3.99244862	0.30030316
H	0.56495453	3.14256352	1.15534038
H	-3.96098749	1.94613801	-1.57511057
H	-3.63570672	3.52004553	-0.92934937
H	0.94202598	0.70057933	4.22951404
O	-3.48948662	-1.42132662	-2.57432310
H	-3.04736786	-1.99761635	-3.20203413
C	-4.41004882	-2.18606908	-1.79161357
H	-3.87956528	-2.94980430	-1.26227840
H	-4.90282706	-1.54374615	-1.09197733
H	-5.13656641	-2.63687669	-2.43492119

	[CuL(B-H)]$^+$		
	X	Y	Z
C	-4.65318376	-1.75281929	-0.48661163
C	-3.23921446	-1.48988816	-0.12425499
O	-4.19407452	0.35954976	-1.30544517
C	-5.10669358	-0.28992332	-0.39139962
O	-4.79929372	-2.27899744	-1.80823504
C	-4.92616723	0.23711436	1.04430283
O	-5.26627897	1.62536831	1.08874355
C	-2.90710610	-0.32424030	-1.07806931
C	-1.17160199	2.30008388	0.97446943
C	-2.17424881	1.52603838	0.39279981
N	-1.86946935	0.50527891	-0.44869832
C	-0.45771946	0.28553375	-0.68898524
N	0.44136430	1.03307069	-0.10383969
C	0.20036838	2.03879886	0.71069035
N	1.18213185	2.76600480	1.25544101
O	0.24575249	-0.56103052	-1.43028756
O	-2.33345125	-2.59225841	-0.22055050
H	-5.15745816	-2.42231969	0.17850229
H	-3.23659667	-1.14221835	0.88768317
H	-6.12984870	-0.15102748	-0.67204451
H	-4.35504932	-1.70163454	-2.43345420
H	-3.90739303	0.10967049	1.34556219
H	-5.56502157	-0.30801669	1.70732414
H	-6.18031937	1.73971048	0.81845478
H	-2.55791952	-0.65096633	-2.03526252
H	-1.43873015	3.10268132	1.62974029
H	-3.19941770	1.74001134	0.61221799
H	2.13674233	2.55279012	1.04745465

	[CuL(R-2H)]$^+$		
	X	Y	Z
Cu	-1.01896836	-0.44814119	0.60493152
C	5.11738789	0.37338409	-0.21056554
C	4.01059898	-0.33311616	-0.93831663
O	3.41671611	-0.16598924	1.35089827
C	4.26500439	0.94965064	0.90978098
O	5.81720568	1.35684691	-0.97734840
C	5.08799469	1.56700098	2.05571532
O	5.89054837	2.63459059	1.54477502
C	3.48946343	-1.13232883	0.24643705
C	0.94017778	-3.70436008	-0.77243629
C	2.15528732	-3.06980197	-0.52025201
N	2.20701182	-1.80204225	-0.01375869
C	1.05089301	-1.20065719	0.23068548
N	-0.11523923	-1.84158861	0.00563941
C	-0.27388971	-3.04047897	-0.49003755
N	-1.47458702	-3.58869402	-0.70735645
O	0.71597186	0.04783251	0.69497141
O	4.42774970	-1.13530606	-2.04618694
H	5.84158432	-0.32402879	0.15556941
H	3.28460165	0.36402010	-1.30139917
H	3.63799248	1.70708983	0.48783080
H	6.45641667	1.80371254	-0.41759807
H	5.72115472	0.81813597	2.48374522
H	4.42614043	1.94597840	2.80619853
H	6.40358128	3.01943235	2.25912371
H	4.22261939	-1.87259604	0.49013109
H	0.92723473	-4.69405717	-1.17892385
H	3.06840958	-3.58692841	-0.72926865

H	-2.32866793	-2.92476664	-1.12111444	H	-2.30511113	-3.07625466	-0.48910064
Cu	1.83429371	0.16099707	-0.84335592	H	-1.54164631	-4.51095216	-1.08807021
C	5.09164527	-1.60992039	0.93822623	H	4.80923258	-0.57197923	-2.72348576
C	6.00098489	-0.95662912	0.08957981	C	-4.45677116	-0.78870499	-0.31603251
N	5.59104643	-0.10288763	-0.89248901	C	-3.69511335	0.27721429	-1.04695354
C	4.16354634	0.08379276	-0.99840958	O	-2.70982637	0.11330006	1.02288236
N	3.30372344	-0.58504812	-0.10969635	C	-3.62778000	-1.01350595	0.95923054
C	3.68143568	-1.41492207	0.83167613	O	-4.73024018	-2.01015057	-1.00754202
N	2.80897235	-2.03328741	1.63533859	C	-4.65075730	-1.13562944	2.10387164
O	3.33471997	0.76385917	-1.76665138	O	-5.48123223	-2.27824476	1.88106769
H	5.46783751	-2.27400464	1.68814056	C	-3.04353094	0.98128015	-0.07927809
H	7.04830514	-1.13487099	0.21705580	O	-3.70049981	0.53384253	-2.45372748
H	1.82823522	-1.86948236	1.52893096	H	-5.38499762	-0.31979439	-0.06420223
H	3.13749798	-2.65935255	2.34252552	H	-3.00008909	-1.88002761	0.95257142
H	6.23624101	0.36157197	-1.49912008	H	-5.22926503	-2.59724545	-0.43492189
				H	-5.25722430	-0.25467331	2.13571578
				H	-4.13365592	-1.24647370	3.03404351
				H	-6.11893241	-2.35437369	2.59461017
				H	-2.78341939	2.01724651	-0.14264739
				H	-4.54277804	0.26178463	-2.82541537

	$[Cu(L-H)(B+H)]^+$				$[CuL(B+COH)]^+$		
	X	Y	Z		X	Y	Z
C	-4.35380063	-2.53837136	0.70490238	C	-5.07102772	-1.71093257	0.57993545
C	-5.45103160	-1.74164344	0.34087046	C	-3.70584370	-1.21468022	0.87951881
N	-5.30587923	-0.43452601	-0.01782384	O	-4.52285279	-0.32352747	-1.18584592
C	-3.95258751	0.06707613	0.00065539	C	-5.53155702	-0.44643179	-0.15745955
N	-2.89477802	-0.77834064	0.34340596	O	-5.06990682	-2.86153602	-0.26918786
C	-3.01887598	-2.03244172	0.70702428	C	-5.51112664	0.76696584	0.79061683
N	-1.96842762	-2.78503974	1.05285049	O	-5.85336396	1.94804030	0.06066032
O	-3.34877664	1.20670047	-0.22255148	C	-3.26939435	-0.70875176	-0.51056786
H	-4.52321734	-3.55607701	0.98858037	C	-1.77589292	2.72388679	0.00662120
H	-6.43028754	-2.17283658	0.34637268	C	-2.70063137	1.68399139	-0.17861910
H	-1.04791844	-2.39450603	1.04075636	N	-2.30755016	0.38670191	-0.32152550
Cu	-1.64294071	0.50471836	0.08139904	C	-0.88272306	0.16147466	-0.27184911
C	4.19730799	-1.41992004	0.68199618	N	-0.00641818	1.23617915	-0.11328139
C	2.94937446	-0.64705787	0.99626835	C	-0.36848874	2.48740881	0.04192117
O	3.60946685	-0.13728692	-1.22529452	N	0.51880437	3.47282058	0.21831848
C	3.99211592	-1.49657537	-0.82212121	O	-0.07153244	-0.86256539	-0.32732931
O	5.36694829	-0.67394402	1.02892749	O	-2.79554846	-2.14757632	1.46770873
C	2.80595280	-2.44118266	-1.09107124	H	-5.64630563	-1.95805964	1.44762406
O	2.53362644	-2.47675759	-2.49445030	H	-3.81531120	-0.38689226	1.54861068
C	3.19600042	0.50419097	0.03134352	H	-6.51719832	-0.53604292	-0.56413025
C	1.05564173	3.55788584	-0.57497410	H	-4.55876054	-2.67505808	-1.06010851
C	2.16906880	2.71680760	-0.42429457	H	-4.53211994	0.87688764	1.20818493
N	2.03618506	1.39211114	-0.13396251	H	-6.21985852	0.61637798	1.57796836
C	0.67877015	0.92109394	0.00300848	H	-6.73172504	1.84941864	-0.31398027
N	-0.39116767	1.79202734	-0.18567993	H	-2.81635529	-1.46943565	-1.11141358
C	-0.28102384	3.07291431	-0.44835588	H	-2.13690373	3.72427246	0.12409343
N	-1.34711839	3.86836389	-0.59028428	H	-3.74468605	1.91643731	-0.20723349
O	0.07959201	-0.20004034	0.29314043	H	1.49729206	3.26729862	0.23627900
O	2.81108663	-0.24630716	2.36198258	H	-2.69107160	-2.90343880	0.88516562
H	4.27132170	-2.37396846	1.16075873	Cu	1.47035827	0.18925992	-0.20559112
H	2.07582973	-1.20728036	0.73555707	C	4.66146584	-2.39964365	-0.20959939
H	4.84835790	-1.86053944	-1.35059054	C	5.60299622	-1.36750069	-0.19649156
H	6.14759592	-1.14416730	0.72713394	N	5.25484079	0.04787725	-0.53940994
H	1.94198002	-2.08640134	-0.56897810	C	3.82836093	0.21701931	-0.34092471
H	3.04954196	-3.42566303	-0.74995143	N	2.94144045	-0.86842162	-0.29526383
H	1.79420007	-3.06560369	-2.66210746	C	3.27048802	-2.13661544	-0.30199328
H	4.01830892	1.07620664	0.40751744	N	2.35916215	-3.11348538	-0.37019602
H	1.21340978	4.59366246	-0.79217457	O	3.02309805	1.23095338	-0.17104935
H	3.15026412	3.12778997	-0.53939990	H	4.99685178	-3.41302562	-0.13561802
H	-2.26844518	3.49135700	-0.49529619	H	6.61507060	-1.59884339	0.06251787
H	-1.22275246	4.84001050	-0.79137127	H	1.38675512	-2.88708157	-0.42646258
H	3.58379935	0.25775730	2.62737674	H	2.65030604	-4.07015011	-0.36491488
H	-6.08430124	0.13844524	-0.27426704	C	6.01084897	0.99182315	0.29624413
				H	5.58809746	1.94253178	0.54591223
				O	7.15522075	0.68178778	0.71798082
				H	0.20361436	4.41498869	0.33222424

	[CuL(B+CH_2COH)]$^+$		
	X	Y	Z
C	3.60960276	-2.62467282	-0.79036572
C	4.74711585	-1.82353479	-0.60428980
N	4.65350240	-0.50822983	-0.25999639
C	3.31055097	-0.00206556	-0.10507279
N	2.21526262	-0.83308820	-0.33761637
C	2.28734798	-2.10548374	-0.64881495
N	1.19830870	-2.86232506	-0.82421738
O	2.74391693	1.12472218	0.23734589
H	3.73752200	-3.65546363	-1.04704961
H	5.71592034	-2.25854115	-0.73512382
H	0.28811536	-2.46184765	-0.71747876
Cu	1.00652566	0.48190204	-0.02708903
C	-4.86877738	-1.24138962	-0.76008977
C	-3.59516900	-0.49318772	-1.02621683
O	-4.27440304	-0.05013641	1.20368653
C	-4.68976392	-1.38118659	0.74294682
O	-6.01123235	-0.44977758	-1.09570565
C	-3.53585655	-2.36969106	0.99377007
O	-3.28742739	-2.46582255	2.39864554
C	-3.82358670	0.62674751	-0.02098393
C	-1.60017696	3.58842496	0.73229570
C	-2.73678679	2.78747844	0.53824504
N	-2.64075152	1.47265176	0.19305064
C	-1.29732954	0.96679940	0.04694661
N	-0.20261065	1.79768750	0.28370394
C	-0.27677760	3.06977225	0.59666469
N	0.81060052	3.82734832	0.77894490
O	-0.73061454	-0.16037653	-0.29145637
O	-3.42423572	-0.04427990	-2.37307646
H	-4.96185608	-2.17407055	-1.27612469
H	-2.74207551	-1.08817823	-0.77488525
H	-5.56443413	-1.73981181	1.24416668
H	-6.80954595	-0.90914894	-0.82488629
H	-2.65381590	-2.02111416	0.49856154
H	-3.80212689	-3.33310135	0.61207493
H	-2.56854626	-3.08246867	2.55507200
H	-4.62335109	1.23686409	-0.38558929
H	-1.72947842	4.61879864	0.99061028
H	-3.70640962	3.22221283	0.66357222
H	1.72123312	3.42767416	0.67607117
H	0.71267364	4.79337756	1.01801426
H	-4.17809687	0.49158289	-2.62990920
C	5.83949970	0.33572208	-0.05721590
O	5.70416083	1.54508857	0.26257957
C	7.24785457	-0.26013549	-0.23619838
H	7.58966049	-0.65433539	0.69791616
H	7.21362744	-1.04430732	-0.96314658
H	7.91905252	0.50444007	-0.56770097

	[CH_2OH]$^\bullet$		
	X	Y	Z
C	-0.62501000	0.03399100	-0.00001200
H	-1.07560200	1.02911300	0.00001500
H	-1.21964900	-0.87920700	0.00004500
O	0.61003900	-0.12935700	-0.00000300
H	1.16499600	0.68100300	0.00003400

	[CuL(L-H)]$^+$		
	X	Y	Z
Cu	0.00001300	0.00021200	-0.06910400
C	5.88496264	0.28256092	-0.29530081
C	4.73969212	-0.42476603	-0.95997695
O	4.34293729	-0.38553897	1.37714550
C	5.11727291	0.77694159	0.92126601
O	6.48684869	1.32360920	-1.06914650
C	6.01895334	1.36613121	2.02192105
O	6.74305512	2.48244100	1.49807928

	[CuL(L-H)-CH_2O]$^+$		
	X	Y	Z
C	6.19202565	1.29204110	0.50544734
C	4.80612835	0.87529057	0.81589474
O	5.54569821	-0.03010279	-1.26739573
C	6.56461054	0.00730255	-0.25110504
O	6.24172260	2.45340981	-0.33117674
C	6.46891403	-1.20868229	0.68842880
O	6.68040851	-2.41028913	-0.05568291
C	4.32927090	0.41882411	-0.57535318
C	2.47540633	-2.83746637	-0.18951622
C	3.52856634	-1.93114128	-0.31883147
N	3.28611776	-0.60047483	-0.39517915
C	1.90705507	-0.21555020	-0.29815806
N	0.95422486	-1.07756207	-0.19838806
C	1.12577063	-2.38860089	-0.14176268
N	0.09215511	-3.23663281	-0.04518994
O	1.29003670	0.93541365	-0.25491285
O	3.96192484	1.84810615	1.42583750
H	6.79365844	1.49274645	1.36890144
H	4.86573954	0.03910401	1.46756296
H	7.54981097	0.02467774	-0.66708855
H	5.70427738	2.30448473	-1.11632322
H	5.49641961	-1.24067722	1.13763295
H	7.21399322	-1.12127963	1.45105736
H	7.54187352	-2.37759556	-0.47294618
H	3.92478361	1.21179428	-1.16624147
H	2.68549831	-3.88545811	-0.13094630
H	4.53064497	-2.28260442	-0.36226844
H	-0.84385082	-2.88814419	-0.01414025
H	3.87793067	2.60598682	0.84801715
Cu	-0.38594776	0.16134735	-0.15077142
C	-6.57318357	-1.57121500	0.06859562
C	-5.31256278	-1.01253394	-0.52215819
O	-5.49558960	-0.26261968	1.72459689
C	-6.11174854	-1.58759423	1.51588730
O	-7.66567559	-0.66271965	-0.13195379
C	-5.26968387	0.22622035	0.35149045
C	-3.10274106	3.24283051	0.06603870
C	-4.18009451	2.38825732	0.26608677
N	-4.06230776	1.03944936	0.22334747
C	-2.71506456	0.53145857	0.04450263
N	-1.66649736	1.44524604	-0.09191456
C	-1.79121808	2.75331557	-0.13932437
N	-0.75997189	3.58051134	-0.35684450
O	-2.09180966	-0.62332343	-0.04392590
O	-5.36907313	-0.72904524	-1.92176911
H	-6.86964145	-2.53007924	-0.31221879
H	-4.47885560	-1.66836885	-0.36790625
H	-6.89291121	-1.79243800	2.21548878
H	-8.43622727	-0.96242507	0.35600682
H	-6.09778139	0.82896471	0.06237565
H	-3.26535115	4.29756069	0.07162891
H	-5.13771607	2.80072217	0.45354663
H	0.16364554	3.22019881	-0.49214475
H	-0.91629098	4.57162492	-0.38228516
H	-6.09774723	-0.12827745	-2.09997226
H	-5.36014510	-2.34543318	1.60557288

	[CuL_2]$^{2+}$		
	X	Y	Z
Cu	0.00001300	0.00021200	-0.06910400
C	5.77367800	0.61267900	-0.37268100
C	4.91458100	-0.40651500	-1.12166900
O	4.65855900	-0.73517600	1.22645700
C	5.12236400	0.62504800	1.01741300
O	5.73352400	1.85059000	-1.03651100
C	6.07478300	1.02379400	2.12968500
O	6.56705700	2.29987600	1.72559800

C	4.34689553	-1.29574206	0.22369818	C	4.56020400	-1.38995300	0.00190500
C	1.87304008	-3.85883307	-0.68205639	C	1.82831700	-3.97290000	-0.28745300
C	3.04881296	-3.21360114	-0.51314282	C	3.04215600	-3.36844500	-0.22337800
N	3.06642338	-1.99429316	0.04127117	N	3.18851600	-2.00646200	-0.12869500
C	1.92510584	-1.40418871	0.43201938	C	2.06122900	-1.25033300	-0.09509400
N	0.74503041	-2.02215378	0.27589185	N	0.83229600	-1.81891900	-0.14270500
C	0.69079189	-3.23888364	-0.27317813	C	0.66114500	-3.15341700	-0.24155100
N	-0.48503801	-3.85727095	-0.42970454	N	-0.56978000	-3.64803900	-0.29294800
O	1.96329839	-0.25825531	0.95063090	O	2.03463500	0.01710900	-0.03290400
O	5.08156631	-1.15957014	-2.13814979	O	5.53603100	-1.14133200	-2.14657600
H	6.65798646	-0.40719439	-0.02776684	H	6.79985100	0.22473200	-0.30100600
H	3.96512907	0.26450594	-1.22432722	H	4.02575100	0.12202300	-1.48579500
H	4.43446735	1.53247118	0.59288928	H	4.25979200	1.29856200	1.00102200
H	7.15931540	1.76431021	-0.54456777	H	6.27656900	2.46617300	-0.52390600
H	6.70817719	0.61906992	2.35626665	H	6.87973800	0.28261000	2.20733800
H	5.41441325	1.68728187	2.84429021	H	5.55457700	1.07590400	3.09275800
H	7.30512797	2.84973456	2.18420055	H	7.22168800	2.61511600	2.35801700
H	5.11945139	-2.02216132	0.36648961	H	5.23811500	-2.24590600	-0.04353000
H	1.84871374	-4.83307180	-1.12384006	H	1.75587300	-5.04929600	-0.36456500
H	3.96326591	-3.67572929	-0.82153610	H	3.96461900	-3.93385400	-0.24760400
H	-1.32892123	-3.40880592	-0.13519677	H	-1.37958400	-3.04580100	-0.26304700
H	-0.52014394	-4.76801590	-0.84120790	H	-0.73218600	-4.64032000	-0.37223600
H	5.38624155	-0.55262400	-2.81668203	H	5.81877500	-0.53919000	-2.84606000
C	-5.88988858	-0.28947571	-0.29072616	C	-5.77348400	-0.61296500	-0.37265300
C	-4.75296802	0.41893800	-0.96842151	C	-4.91465100	0.40656500	-1.12146700
O	-4.33900860	0.39719987	1.36594521	O	-4.65837500	0.73465800	1.22670300
C	-5.11092961	-0.77203185	0.92341679	C	-5.12195900	-0.62557100	1.01736200
O	-6.49229762	-1.33854757	-1.05324058	O	-5.73312900	-1.85070600	-1.03682100
C	-6.00167376	-1.35831744	2.03446938	C	-6.07415900	-1.02479100	2.12965400
O	-6.72401542	-2.48160522	1.52325799	O	-6.56631300	-2.30080700	1.72525100
C	-4.35578337	1.29964918	0.20653864	C	-4.56029800	1.38977500	0.00231800
C	-1.90094915	3.86812819	-0.73496853	C	-1.82892200	3.97318900	-0.28748400
C	-3.07235992	3.21859382	-0.55276983	C	-3.04265400	3.36853400	-0.22328900
N	-3.08004911	2.00303753	0.01001833	N	-3.18874600	2.00654300	-0.12833400
C	-1.93308369	1.42102737	0.39635088	C	-2.06131500	1.25062900	-0.09471400
N	-0.75715604	2.04342848	0.22718146	N	-0.83248900	1.81940900	-0.14224500
C	-0.71275408	3.25650896	-0.33078043	C	-0.66160000	3.15393300	-0.24132400
N	0.45896641	3.87914259	-0.50055081	N	0.56922600	3.64880300	-0.29266900
O	-1.96199339	0.27856313	0.92314624	O	-2.03455900	-0.01683500	-0.03261800
O	-5.10700401	1.14423687	-2.14889254	O	-5.53627700	1.14158200	-2.14612100
H	-6.66430021	0.39828966	-0.02210316	H	-6.79973400	-0.22529300	-0.30074500
H	-3.97700853	-0.26833173	-1.23387022	H	-4.02577900	-0.12175700	-1.48580100
H	-4.42682193	-1.52638193	0.59504924	H	-4.25927300	-1.29894100	1.00066400
H	-7.15873047	-1.77902605	-0.52084573	H	-6.27609900	-2.46651000	-0.52440400
H	-6.69213721	-0.61244080	2.36890061	H	-6.87920900	-0.28374000	2.20763900
H	-5.38960573	-1.67105344	2.85450988	H	-5.55381200	-1.07709600	3.09264100
H	-7.27926214	-2.84713109	2.21584574	H	-7.22040300	-2.61658900	2.35795900
H	-5.13076997	2.02330524	0.35017622	H	-5.23837700	2.24561600	-0.04278600
H	-1.88453722	4.83939939	-1.18359761	H	-1.75666300	5.04958500	-0.36477500
H	-3.99127645	3.67433660	-0.85736107	H	-3.96522500	3.93376300	-0.24758500
H	1.30710629	3.43661453	-0.20930992	H	1.37917100	3.04677900	-0.26228700
C	5.88496264	0.28256092	-0.29530081	H	0.73142600	4.64111400	-0.37200600
				H	-5.81884900	0.53962800	-2.84583700

	$[CuLB]^{2+}$			$[CuL_4]^{2+}$			
	X	Y	Z		X	Y	Z
Cu	-1.70908100	0.55736700	-0.07864900	C	-7.21777100	-1.22966600	1.39328900
C	3.72707400	-1.34816400	0.64513600	C	-5.78146800	-1.38003900	0.84809300
C	3.10365600	-0.07710100	1.22339000	O	-5.61387300	-1.28328600	3.21262500
O	3.03046600	0.02508000	-1.15754200	C	-7.06847800	-1.40314200	2.92280500
C	3.15099300	-1.37177100	-0.77792400	O	-7.59360900	0.11671400	1.00837600
O	3.36508100	-2.45593600	1.42959200	C	-7.81397800	-0.33983000	3.73067200
C	4.02835500	-2.10617300	-1.77520800	O	-9.12990300	-0.21018300	3.10266400
O	4.18183100	-3.40648700	-1.21032200	C	-4.92051500	-0.83325700	2.01944700
C	3.04363200	0.82296900	-0.01767900	C	-2.07862400	-3.20341900	2.52899500
C	1.00406100	3.99213900	-0.18526700	C	-3.32054800	-2.64537900	2.56361800
C	2.03836400	3.11671600	-0.10629800	N	-3.55203200	-1.38208200	2.07151500
N	1.85542300	1.75637100	-0.04409600	C	-2.48759000	-0.59248800	1.59161700
C	0.58267000	1.29115900	-0.06861500	N	-1.26356400	-1.21056100	1.43348200

N	-0.47547200	2.13123300	-0.15331800
C	-0.32444300	3.47202500	-0.21542900
N	-1.39880200	4.24548300	-0.30106800
O	0.25014700	0.06474800	-0.00198100
O	3.83443500	0.60909200	2.20808100
H	4.81806400	-1.21949500	0.60365500
H	2.09905600	-0.34012100	1.57594900
H	2.15356600	-1.82212500	-0.75143900
H	3.77208400	-3.23610000	1.02675400
H	4.98975600	-1.58684000	-1.87064500
H	3.55408100	-2.14549600	-2.76232600
H	4.77581400	-3.93385300	-1.75537900
H	3.90438300	1.49629100	-0.01542600
H	1.19006100	5.05668800	-0.23157800
H	3.06838500	3.44812900	-0.08572800
H	-2.32899500	3.85415800	-0.32841100
H	-1.31782300	5.25008800	-0.34791100
H	3.93891700	0.04376200	2.98361500
C	-4.45344800	-2.88311500	0.23293400
C	-5.48867700	-2.01880800	0.10502400
N	-5.26855300	-0.66948100	-0.03822700
C	-4.00259300	-0.18474600	-0.05581600
N	-2.94999100	-1.02731900	0.06485800
C	-3.11820100	-2.35901700	0.21520200
N	-2.05212100	-3.13508900	0.34206700
O	-3.70190600	1.03398600	-0.17930100
H	-4.63467800	-3.94319500	0.34739200
H	-6.52425900	-2.33344100	0.10947600
H	-1.11833200	-2.74961500	0.33835000
H	-2.13993500	-4.13355300	0.45974900
H	-6.03928900	-0.01784300	-0.13172500

	$[Cu(L-H)]^+$		
	X	Y	Z
C	-3.27371600	-1.07962000	0.45415100
C	-1.75452900	-1.13081200	0.76659400
O	-2.17505800	0.27601100	-1.12360600
C	-3.40265000	0.21075600	-0.34280800
O	-3.62246900	-2.25319900	-0.26757700
C	-3.57973700	1.45214900	0.55206600
O	-3.12568700	2.64603800	-0.06021400
C	-1.16665200	-0.50006800	-0.54939600
C	1.02697700	2.46386200	0.12526200
C	-0.08615300	1.69886600	-0.14439600
N	0.02596200	0.36232100	-0.29916500
C	1.28555000	-0.27759700	-0.25261300
N	2.38175200	0.47997000	0.02270500
C	2.29884400	1.82836100	0.22191800
N	3.34919200	2.59714600	0.49542000
O	1.39470800	-1.48771500	-0.45894200
O	-1.29373700	-2.40049600	1.07135600
H	-3.86628200	-1.08676300	1.37097600
H	-1.50849400	-0.48293600	1.61272500
H	-4.20926100	0.16447900	-1.07928300
H	-3.62075500	-2.08964000	-1.21865000
H	-2.99335800	1.36158000	1.46949200
H	-4.63196900	1.52204600	0.85135000
H	-3.72018000	2.90535100	-0.77426100
H	-0.82235900	-1.27936600	-1.22991700
H	0.95670400	3.53358100	0.26058500
H	-1.08282300	2.11823700	-0.25660600
H	4.20039900	2.02904200	0.55127700
H	-1.83717700	-3.03549400	0.57772000
Cu	3.63198400	-1.10264400	-0.06692900
C	-3.27371600	-1.07962000	0.45415100
C	-1.75452900	-1.13081200	0.76659400
O	-2.17505800	0.27601100	-1.12360600
C	-3.40265000	0.21075600	-0.34280800
C	-1.01573400	-2.45725000	1.91833100
N	0.22114300	-2.95488300	1.80219500
O	-2.66694800	0.61077900	1.27197600
O	-5.61751100	-0.66605300	-0.38866300
H	-7.91256900	-1.95887700	0.96815100
H	-5.53205100	-2.42975200	0.66715400
H	-7.36649000	-2.40829900	3.22987400
H	-8.46063600	0.33142300	1.43132600
H	-7.26894600	0.60803100	3.67588000
H	-7.90085200	-0.64124400	4.77826500
H	-9.80903600	0.12466500	3.71719600
H	-4.83117300	0.25214900	1.97100400
H	-1.89764100	-4.18306800	2.94860900
H	-4.17760600	-3.13401500	3.00538000
H	0.99155300	-2.37991200	1.44886700
H	0.42488600	-3.89821400	2.09475500
H	-6.29914200	0.05202800	-0.38816600
Cu	-0.10610500	-0.21891500	0.03228400
C	2.83672700	-4.97912300	-3.23247100
C	1.69235700	-4.09861000	-3.73768900
O	0.98520200	-5.32529900	-1.78115100
C	2.46455300	-5.23303300	-1.76429600
O	4.09167300	-4.29798800	-3.39645700
C	3.04337400	-6.52579300	-1.21952200
O	4.47679500	-6.39282700	-1.47449900
C	0.48115100	-4.59708900	-2.92672800
C	-2.69206500	-2.66166000	-2.50156300
C	-1.79029800	-3.61946300	-2.85123100
N	-0.45991400	-3.52935000	-2.50686800
C	-0.00793700	-2.46119600	-1.71102200
N	-0.91304300	-1.47712000	-1.37890600
C	-2.21934600	-1.51828600	-1.77439300
N	-3.01945000	-0.50047100	-1.45586800
O	1.17967900	-2.41238500	-1.29532300
O	1.35254500	-4.26541700	-5.12977400
H	2.82098400	-5.92901600	-3.78708100
H	1.93551300	-3.05759100	-3.50672000
H	2.76125200	-4.37436800	-1.15715400
H	4.78265600	-4.85585800	-2.97493400
H	2.61948400	-7.38164400	-1.75950800
H	2.83694500	-6.64195200	-0.14924700
H	4.97536100	-7.16989900	-1.15914200
H	-0.10153000	-5.27562100	-3.55350000
H	-3.72606700	-2.72628600	-2.80900000
H	-2.06913100	-4.48740900	-3.43424100
H	-2.61915000	0.36416000	-1.09449200
H	-4.03773500	-0.58630600	-1.43440200
H	2.10575500	-4.00622900	-5.69752200
C	-1.02179700	6.10742500	-2.28670900
C	-1.35997200	4.64564900	-1.94212400
O	-0.14080600	4.76284200	-4.01683600
C	0.15362900	6.00609900	-3.26288900
O	-0.70310300	6.83272200	-1.08773800
C	0.24908200	7.17230400	-4.22789500
O	0.28414300	8.33259900	-3.34159000
C	-0.77882300	3.83015800	-3.12275100
C	2.41516600	1.81650900	-2.99697000
C	1.49304800	2.77165500	-3.30981800
N	0.26283200	2.81379900	-2.69768900
C	-0.08463700	1.83450500	-1.76299200
N	0.85063400	0.88372900	-1.42726600
C	2.07034500	0.82272600	-2.02190500
N	2.90637700	-0.16599300	-1.68211900
O	-1.22409600	1.81180700	-1.21707900
O	-2.78017800	4.39187500	-1.91360200
H	-1.88533300	6.54353400	-2.80747800
H	-0.88095300	4.38162800	-0.99410100
H	1.08926200	5.89006000	-2.70089200

O	-3.62246900	-2.25319900	-0.26757700
C	-3.57973700	1.45214900	0.55206600
O	-3.12568700	2.64603800	-0.06021400
C	-1.16665200	-0.50006800	-0.54939600
C	1.02697700	2.46386200	0.12526200
C	-0.08615300	1.69886600	-0.14439600
N	0.02596200	0.36232100	-0.29916500
C	1.28555000	-0.27759700	-0.25261300
N	2.38175200	0.47997000	0.02270500
C	2.29884400	1.82836100	0.22191800
N	3.34919200	2.59714600	0.49542000
O	1.39470800	-1.48771500	-0.45894200
O	-1.29373700	-2.40049600	1.07135600
H	-3.86628200	-1.08676300	1.37097600
H	-1.50849400	-0.48293600	1.61272500
H	-4.20926100	0.16447900	-1.07928300
H	-3.62075500	-2.08964000	-1.21865000
H	-2.99335800	1.36158000	1.46949200
H	-4.63196900	1.52204600	0.85135000
H	-3.72018000	2.90535100	-0.77426100
H	-0.82235900	-1.27936600	-1.22991700
H	0.95670400	3.53358100	0.26058500
H	-1.08282300	2.11823700	-0.25660600
H	4.20039900	2.02904200	0.55127700
H	-1.83717700	-3.03549400	0.57772000
Cu	3.63198400	-1.10264400	-0.06692900

	$[Cu(CH_2OH)(MeOH)]^+$		
	X	Y	Z
Cu	0.08525900	0.07709900	-0.00062900
O	-1.78582400	0.47236000	-0.01312300
H	-2.09698600	1.38148000	0.05190500
C	-2.91152700	-0.46146600	0.00526500
H	-2.49778300	-1.45561400	-0.13400600
H	-3.41916000	-0.39559300	0.96652200
H	-3.58565000	-0.22078800	-0.81519600
C	3.05478900	0.04649800	0.00181300
H	3.24004800	1.12857200	0.00365300
O	1.92527800	-0.41572900	0.00088300
H	3.91180500	-0.63717000	0.00081500

	$[L_2 + H]^+$		
	X	Y	Z
C	-6.19090900	-0.38612400	-0.48140300
C	-5.17909900	0.52847800	-1.16826700
O	-4.94936400	0.68902600	1.20450900
C	-5.55524200	-0.58237000	0.89940000
O	-6.37079800	-1.57191500	-1.21982600
C	-6.55523600	-0.93696000	1.98318800
O	-7.21266900	-2.11582000	1.51094900
C	-4.66943700	1.37586600	0.00823100
C	-1.60990700	3.48755900	-0.09205700
C	-2.89985600	3.07705600	-0.06854200
N	-3.23803000	1.75776100	-0.05794000
C	-2.22973000	0.77697000	-0.06286200
N	-0.92989000	1.17359000	-0.07466500
C	-0.60400400	2.47313500	-0.08866700
N	0.69328100	2.80060400	-0.09782000
O	-2.55526000	-0.41718400	-0.06628800
O	-5.70570400	1.41336500	-2.13865100
H	-7.13822300	0.16474500	-0.37466300
H	-4.38488300	-0.09532400	-1.58520000
H	-4.78106100	-1.35212200	0.83030100
H	-6.93985700	-2.14601200	-0.68844800
H	-7.26168200	-0.10754500	2.11420000
H	-6.04773300	-1.11698400	2.93810300
H	-7.89273400	-2.37955500	2.13894000
H	-5.21120800	2.32492400	-0.00127500
H	-1.36044300	4.53971200	-0.10353500
H	-0.42977500	7.73845700	-1.35478800
H	-0.63424300	7.18852700	-4.87776600
H	1.14968300	7.11231500	-4.84904200
H	0.38369500	9.16699000	-3.83741000
H	-1.57071900	3.30497900	-3.65676800
H	3.37347300	1.79112800	-3.49684000
H	1.65621500	3.53451200	-4.05732000
H	2.57009500	-0.93702500	-1.10738200
H	3.80659300	-0.26155400	-2.12685500
H	-3.19832500	4.90066800	-1.19042200
O	5.07931000	3.15543200	4.88390500
C	5.90954700	2.06784300	5.40109900
H	6.94867400	2.39739900	5.52538800
H	5.52858900	1.71325800	6.36487400
C	5.86956800	0.94044200	4.39334000
H	6.55906300	0.14521100	4.69440200
O	4.49593100	0.39055300	4.36491700
C	4.11161100	0.03191900	3.02649600
H	3.85720600	-1.02381400	2.95600500
N	2.87545500	0.80384200	2.68161900
C	2.60702500	2.02654000	3.25298300
H	3.35578500	2.40921600	3.94249700
C	1.44923800	2.69158300	2.96479000
H	1.23382800	3.64491100	3.42719200
C	0.50625900	2.08532500	2.07351500
N	-0.67724200	2.64578800	1.79210300
H	-1.38951300	2.11626900	1.28732500
H	-0.93501100	3.52962600	2.20340700
N	0.81576300	0.89398900	1.49391200
C	1.96655000	0.21481800	1.80228400
O	2.19227900	-0.92044000	1.27999200
C	6.16625400	1.33941600	2.93828700
H	5.87758900	2.37852600	2.76223400
C	5.30631600	0.35142300	2.10742300
H	4.98134300	0.76483100	1.14462100
O	7.57337200	1.11644000	2.66438400
H	5.09776000	3.92501000	5.48474000
H	7.98776100	1.86490100	2.19596000
O	6.03194100	-0.87579700	1.92070900
H	6.99488100	-0.66512100	1.93867600

	$[R\text{-}CH_2O]$		
	X	Y	Z
C	0.52673500	-0.70618700	0.45154600
C	-0.71324100	-0.54420800	-0.45562000
O	0.22703100	1.57489700	-0.06276400
C	0.63339500	0.73206700	0.98615300
O	1.64021500	-1.05256200	-0.36580800
C	-0.28849400	0.67524800	-1.17656500
O	-1.93420900	-0.43998700	0.39709200
H	0.43160000	-1.46458000	1.24186000
H	-0.84850500	-1.40933000	-1.12058200
H	-0.02611000	0.84941700	1.86729100
H	1.42066900	-0.51123500	-1.17360000
H	-1.11521700	1.22882000	-1.63989000
H	-1.94818100	-1.23724200	0.95369400
H	1.67107000	0.94384200	1.28998600

H	-3.72626000	3.77625600	-0.06109900
H	1.40955000	2.08173300	-0.08514100
H	0.97915200	3.76479400	-0.11201000
H	-6.01018000	0.89220400	-2.89077300
C	6.27184900	0.24107400	-0.48497800
C	5.19839500	-0.60971500	-1.16121800
O	4.93147600	-0.70283000	1.20772800
C	5.63373100	0.51970900	0.88160700
O	6.54423700	1.38630300	-1.25300500
C	6.64162000	0.82888000	1.97231300
O	7.39967400	1.92899400	1.46698100
C	4.63676200	-1.39965000	0.02975600
C	1.44433700	-3.34885300	-0.11671400
C	2.75305900	-2.99393500	-0.08036000
N	3.17552500	-1.69932600	-0.04843700
C	2.25342200	-0.64991300	-0.04915600
N	0.91854500	-1.03154500	-0.06888000
C	0.46771900	-2.31428100	-0.10472700
N	-0.83188200	-2.53132000	-0.12444800
O	2.58086700	0.51961200	-0.04327300
O	5.64959900	-1.54402500	-2.11941900
H	7.17305800	-0.37691600	-0.35051400
H	4.45076800	0.06780300	-1.58415700
H	4.91545700	1.33853400	0.78350200
H	7.14987900	1.93522200	-0.73545800
H	7.27418800	-0.05086300	2.14619100
H	6.13510300	1.08607500	2.90963300
H	8.06751300	2.18700200	2.11036200
H	5.11350800	-2.38303400	0.04601900
H	1.15073600	-4.38838900	-0.14384600
H	3.53888900	-3.73848800	-0.07923000
H	-1.51813300	-1.75032600	-0.10616000
H	-1.17744900	-3.47768600	-0.15634200
H	6.00117400	-1.06092500	-2.87673100
H	0.23671600	-0.22895400	-0.06826200

$[C_3H_5O_2]^+$

	X	Y	Z
C	0.90265900	0.09847900	0.33902700
C	-0.43939800	0.02577100	-0.32135600
O	2.00639200	-0.06942800	-0.18091100
C	-1.00220900	1.31867800	-0.00831500
O	-1.21963500	-1.20847400	0.14323300
H	0.83165500	0.37387300	1.41926500
H	-0.27699300	-0.10323900	-1.40167800
H	-1.23315100	1.50186000	1.04240900
H	-1.71245000	1.76279400	-0.70896200
H	-0.66943500	-1.96963100	-0.10574900

B

	X	Y	Z
C	-1.02510900	1.20292100	-0.00001200
C	0.25880700	1.71982600	-0.00007900
N	1.32408200	0.88386100	-0.00002300
C	1.14909500	-0.51184500	-0.00001300
N	-0.09073200	-1.04360500	-0.00005000
C	-1.19038900	-0.21855400	-0.00003400
N	-2.37617800	-0.82769500	0.00003700
O	2.20530700	-1.24553200	0.00004100
H	-1.87586200	1.87183500	0.00012500
H	0.45634400	2.78408700	0.00026200
H	-2.40479200	-1.84060900	0.00000000
H	-3.25229700	-0.32453600	0.00013900

$[CuL_3\text{-}H]^+$

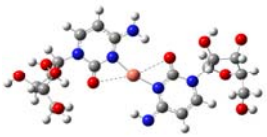
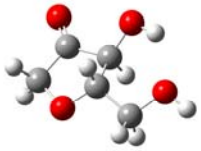
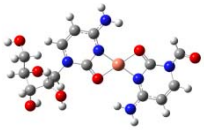
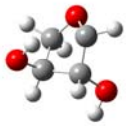
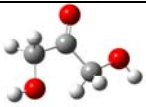
	X	Y	Z
C	5.19070300	-3.16890400	-0.99532200
C	3.70009500	-2.91328500	-0.70984000
O	4.92709300	-1.59439000	0.82650000
C	5.92108600	-2.09870700	-0.15016800
O	5.43369100	-4.52570400	-0.52937700
C	7.12019900	-2.64706400	0.62284900
O	7.87178400	-3.49076300	-0.31308100
C	3.74649500	-2.46662600	0.76578000
C	1.67225900	-0.96787500	3.42621200
C	2.68568000	-1.52756000	2.73888700
N	2.61823900	-1.75105000	1.35169300
C	1.51223800	-1.27929000	0.64244400
N	0.45251500	-0.78880300	1.34713600
C	0.43130700	-0.61076800	2.75023600
N	-0.58813000	-0.18467700	3.43312700
O	1.43824000	-1.33756900	-0.62983800
O	2.89188200	-4.08485400	-0.93017600
H	5.43454300	-3.08487500	-2.05803500
H	3.31087700	-2.11217800	-1.32914900
H	6.21134800	-1.24926800	-0.77289000
H	6.40337600	-4.69660400	-0.58207700
H	6.76338100	-3.24331800	1.46937600
H	7.74059400	-1.82837000	1.00011800
H	8.79236800	-3.62832300	-0.02135300
H	3.92412700	-3.35160800	1.39023100
H	1.73124200	-0.79306300	4.49062500
H	3.61704300	-1.82619600	3.19953100
H	-1.41570600	0.01674900	2.85810100
H	3.47668600	-4.86113000	-0.76299900
Cu	-0.95518900	-0.19188900	0.10203800

$[CuL_3]^{2+}$

	X	Y	Z
C	5.49646600	-2.32580300	-0.86545300
C	3.95570100	-2.21817600	-0.69261300
O	5.00333300	-2.23120400	1.49878600
C	6.07462100	-1.91781800	0.50456900
O	5.74559300	-3.71896200	-1.19432600
C	7.33024700	-2.70273500	0.91760000
O	8.11218700	-2.89047100	-0.31330700
C	3.75113400	-2.48294700	0.83253500
C	1.88144600	-0.73446700	3.60352600
C	2.87260400	-1.33487200	2.86683100
N	2.70575400	-1.62492600	1.52912500
C	1.51297200	-1.27635700	0.87993900
N	0.49017400	-0.70102200	1.62777800
C	0.63636400	-0.43270400	2.95192100
N	-0.39691700	0.10573300	3.64571500
O	1.32344500	-1.47005700	-0.34752800
O	3.26472500	-3.19929700	-1.49567700
H	5.86830500	-1.67240000	-1.66118900
H	3.59950900	-1.22801300	-0.97615200
H	6.25102200	-0.83610600	0.53324000
H	6.72123200	-3.85252300	-1.27288300
H	7.02986600	-3.67324800	1.32890200
H	7.90874600	-2.15034500	1.66653200
H	9.05783600	-3.06416400	-0.13317200
H	3.45200900	-3.52686900	0.98745600
H	2.03241400	-0.51580400	4.65293800
H	3.83313300	-1.60947700	3.28469100
H	-1.28298300	0.31871500	3.20452700
H	-0.30641200	0.29043000	4.63652900
H	3.93199900	-3.89580300	-1.72387900

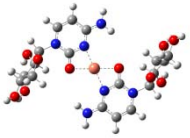
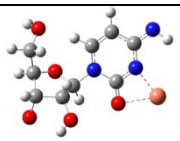
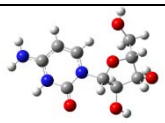
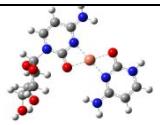
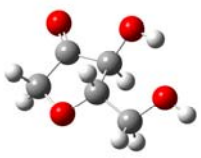
C	3.68108300	4.19134600	-0.64096500	Cu	-1.01264800	-0.30066200	0.28331800
C	2.84832700	3.79045200	0.57966000	C	3.48759200	3.99597300	-0.82873300
O	1.43312700	4.73514600	-1.12959000	C	2.61417500	3.86102400	0.42810000
C	2.64424400	4.16921000	-1.77184600	O	1.22660000	4.35907400	-1.49609900
O	4.77571700	3.28235900	-0.82960200	C	2.48801000	3.73291100	-1.97594700
C	3.01914800	5.03424500	-2.95945600	O	4.57037900	3.04170700	-0.77361500
O	4.34794200	4.55283800	-3.34271400	C	2.90674800	4.37937200	-3.29120000
C	1.49131900	4.46038700	0.29171700	O	4.27867500	3.88583800	-3.48982500
C	-1.78516900	3.64923700	1.89377100	C	1.24094700	4.38983200	-0.05018800
C	-0.62758500	4.27702000	1.54425700	C	-2.06549700	3.70163200	1.62234400
N	0.29592600	3.69324300	0.71535400	C	-0.92831200	4.32430100	1.16973700
C	0.07320300	2.39961900	0.19387400	N	0.05801600	3.64736400	0.48989800
N	-1.07843300	1.73761400	0.60769900	C	-0.07909500	2.27054000	0.22852900
C	-2.02530000	2.33647700	1.37731200	N	-1.21836700	1.62865200	0.72292200
N	-3.16753700	1.67993700	1.63313500	C	-2.22112800	2.29660000	1.36263200
O	0.87389800	1.85510700	-0.59131500	N	-3.32474500	1.61759000	1.75524400
O	3.31614000	4.31988500	1.83922500	O	0.77025200	1.59960400	-0.40891000
H	4.03967800	5.22228900	-0.49397600	O	2.99867600	4.68939700	1.55343200
H	2.77126500	2.70039300	0.60397000	H	3.86931100	5.02645600	-0.89989200
H	2.44270800	3.13766400	-2.07107300	H	2.58250700	2.80174200	0.70516100
H	5.16497400	3.47867200	-1.71083000	H	2.32871200	2.65558500	-2.09167500
H	3.05332700	6.08847300	-2.65690700	H	5.04863500	3.09376400	-1.63358300
H	2.30190100	4.91967700	-3.77995000	H	2.89247000	5.47411900	-3.20142600
H	4.67203100	4.99629200	-4.14858900	H	2.25340200	4.07021700	-4.11655600
H	1.44877200	5.40335400	0.84177100	H	4.65051100	4.17645000	-4.34669400
H	-2.51005200	4.13227400	2.53302900	H	1.12473200	5.42367300	0.29109300
H	-0.38630200	5.27170900	1.89563600	H	-2.83631800	4.26368700	2.13350100
H	-3.41197200	0.83952500	1.11763600	H	-0.76448000	5.38540500	1.32191500
H	-3.88715800	2.08008600	2.21433500	H	-3.55752900	0.71134800	1.34979500
H	4.16153300	3.89389400	2.08392100	H	-4.08569200	2.10311000	2.21452100
C	-6.50407100	-0.27529300	0.33639800	H	3.91664500	4.49038700	1.83428200
C	-5.73545400	-1.57820100	0.60243500	C	-6.51635300	-0.45877800	0.34688300
O	-5.78411200	-1.10555100	-1.77336300	C	-5.76662300	-1.79737400	0.50661600
C	-6.06865900	0.16143300	-1.07018200	O	-5.66772000	-1.06004300	-1.81134600
O	-6.19614400	0.72748500	1.33362400	C	-6.02270600	0.12281300	-0.99570500
C	-7.14878600	0.92500300	-1.81237400	O	-6.22011100	0.42815900	1.46030100
O	-7.46979400	2.02301400	-0.89656200	C	-7.09218800	0.94480000	-1.70648400
C	-5.39637200	-2.10858000	-0.81149800	O	-7.48427200	1.92597500	-0.68115200
C	-2.33166500	-4.09022500	-1.70575700	C	-5.34377900	-2.16648000	-0.94103300
C	-3.62748200	-3.72691900	-1.51192600	C	-2.22395200	-3.96683400	-2.07776500
N	-3.96845000	-2.48962000	-0.98910300	C	-3.53285800	-3.65785000	-1.83584000
C	-2.95131200	-1.60102600	-0.69434100	N	-3.89488900	-2.53395500	-1.09514600
N	-1.65134500	-1.94596500	-0.84398900	C	-2.88756700	-1.72933300	-0.62153400
C	-1.28434900	-3.16063200	-1.35757600	N	-1.57056900	-2.02434900	-0.79617900
N	0.00265100	-3.42320800	-1.50813500	C	-1.17891200	-3.10841400	-1.54907200
O	-3.17564700	-0.42044600	-0.23448000	N	0.11058900	-3.34802300	-1.78270000
O	-6.51993600	-2.61626500	1.23409800	O	-3.09546500	-0.62035100	0.03500900
H	-7.57745600	-0.50820700	0.33966900	O	-6.59053600	-2.90246200	0.95413600
H	-4.83957800	-1.35492200	1.18583600	H	-7.59401100	-0.66425800	0.29129000
H	-5.15210100	0.75155600	-1.00405500	H	-4.91233500	-1.64814200	1.17449400
H	-6.69729800	1.53282600	1.07152000	H	-5.12401900	0.72678100	-0.82762600
H	-8.02078100	0.28107400	-1.98036000	H	-6.78424900	1.22679600	1.33737300
H	-6.78681600	1.30032100	-2.77549600	H	-7.94155000	0.30930300	-1.99097400
H	-8.13695300	2.62516600	-1.27569900	H	-6.69209100	1.44336600	-2.59762600
H	-5.97331900	-3.01536500	-0.99756300	H	-8.16162600	2.54865900	-1.01433700
H	-2.08730600	-5.05954300	-2.11736700	H	-5.90969000	-3.04545400	-1.26107900
H	-4.45569600	-4.38032500	-1.75090200	H	-1.97071700	-4.84214000	-2.66315700
H	0.70123200	-2.70169200	-1.25102600	H	-4.34844000	-4.26493900	-2.21093900
H	0.35039100	-4.31563800	-1.82548100	H	0.84945100	-2.73347800	-1.40792700
H	-6.70059300	-2.39207500	2.16867200	H	0.39391700	-4.14036800	-2.34714800
				H	-6.89717000	-2.77511600	1.87665500

Table 2S B3LYP/LANDL2DZ6-311+G(d) calculations fo potential structures of reactant and products and final reaction energies associated with the fragmentation pathway for the CID of $[CuL(L\text{-}H)]^+$

Compound	**Structure**	E_{zpe} **(kcal mol^{-1})**	$E_{thermal}$ **(kcal mol^{-1})**	S **(kcal mol^{-1} K^{-1})**
$[CuL(L\text{-}H)]^+$		-12.4×10^{11}	314.166	224.572
$[Cu(L\text{-}H)(B+H)]^+$		-9.30×10^{11}	220.986	180.611
[R-H]		-3.11×10^{11}	90.164	91.563
△(Reaction 2a)		-3.76	-3.016	+47.602
$[CuL(B+COH)]^+$		-10.0×10^{11}	237.858	181.903
$[R\text{-}CH_2O]$		-2.40×10^{11}	67.174	78.177
△(Reaction 2b)		-9.86	-9.134	+35.508
$[CuL(B+CH_2COH)]^+$		-10.2×10^{11}	238.730	191.575
$[R\text{-}C_2H_5O]$		-2.15×10^{11}	63.356	84.086
△(Reaction 2c)		-0.89	-12.080	+51.089

$[CuL(L-H)-CH_2O]^+$		-11.7×10^{11}	291.787	216.092
$[CH_2O]$		-0.72×10^{11}	18.481	52.221
△(Reaction 2d)		-6.04	-3.898	+43.741

Table 3S B3LYP/LANDL2DZ6-311+G(d) calculations fo potential structures of reactant and products and final reaction energies associated with the fragmentation pathway for the CID of $[CuL_2)]^{2+}$

Compound	**Structure**	E_{zpe} **(kcal mol^{-1})**	$E_{thermal}$ **(kcal mol^{-1})**	S **(kcal mol^{-1} K^{-1})**
$[CuL_2]^{2+}$		-12.4×10^{11}	324.026	224.526
$[Cu(L-H)]^+$		-6.82×10^{11}	151.792	139.830
$[L+H]^+$		-5.59×10^{11}	167.774	127.495
△(Reaction 3a)		-24.5	-4.46	+42.799
$[CuLB]^{2+}$		-9.30×10^{11}	230.960	176.684
[R-H]		-3.11×10^{11}	90.164	91.563

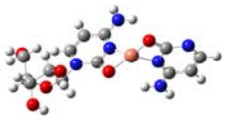
△(Reaction 3b)		-10.0	-2.902	+43.721
$[CuL(B-H)]^+$		-9.30×10^{11}	222.298	175.615
$[R]^+$		-3.12×10^{11}	97.869	93.439
△(Reaction 3c)		-7.18	-3.859	+44.528
$[CuL(R-2H)]^+$		-9.93×10^{11}	238.324	187.313
$[B+H]^+$		-2.48×10^{11}	80.075	81.932
△(Reaction 3d)		-79.2	-5.627	+44.716

Table 4S B3LYP/LANDL2DZ6-311+G(d) calculations fo potential structures of reactant and products and final reaction energies associated with the fragmentation pathway for the CID of $[CuL_3]^{2+}$

Compound	**Structure**	E_{zpe} **(kcal mol^{-1})**	$E_{thermal}$ **(kcal mol^{-1})**	S **(kcal mol^{-1} K^{-1})**
$[CuL_3]^{2+}$		-18.0×10^{11}	486.268	297.888

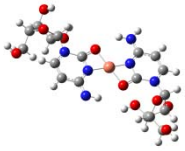
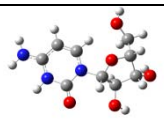
$[CuL(L-H)]^+$		-12.4×10^{11}	314.166	224.572
$[L+H]^+$		-5.59×10^{11}	167.774	127.495
△(Reaction 4)		-14.9	-4.328	+54.179

Table 6S B3LYP/LANDL2DZ6-311+G(d) calculations fo potential structures of reactant and products and final reaction energies associated with the fragmentation pathway for the CID of $[CuL_4]^{2+}$

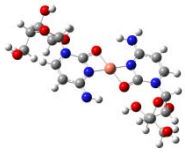
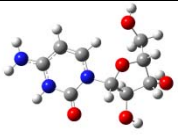
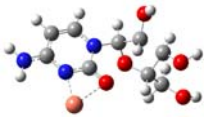
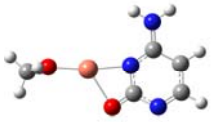
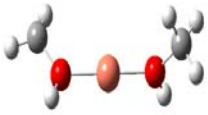
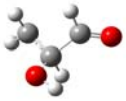
Compound	**Structure**	E_{zpe} **(kcal mol^{-1})**	$E_{thermal}$ **(kcal mol^{-1})**	S **(kcal mol^{-1} K^{-1})**
$[CuL_4]^{2+}$		-23.6×10^{11}	647.739	374.417
$[CuL(L-H)]^+$		-12.4×10^{11}	314.166	224.572
$[L_2+H]^+$		-11.2×10^{11}	329.695	211.133
△(Reaction 5a)		-12.1	-3.868	+51.288
$[L+H]^+$		-5.59×10^{11}	167.774	127.495
$[CuL_2(L-H)]^+$		-18.0×10^{11}	477.110	296.795
△(Reaction 5b)		-11.8	-3.0	+49.871

Table 5S B3LYP/LANDL2DZ6-311+G(d) calculations fo potential structures of reactant and products and final reaction energies associated with the fragmentation pathway for the CID of $[CuL(MeOH)]^{2+}$

Compound	**Structure**	E_{zpe} **(kcal mol^{-1})**	$E_{thermal}$ **(kcal mol^{-1})**	S **(kcal mol^{-1} K^{-1})**
$[CuL(MeOH)]^{2+}$		-7.55×10^{11}	197.002	166.221
$[CuL]^{2+}$		-6.82×10^{11}	160.313	140.570
[MeOH]		-0.73×10^{11}	34.260	56.683
△(Reaction 9a)		-44.3	-2.429	+31.032
$[CuB(MeOH)]^{+}$		-4.43×10^{11}	96.103	114.126
$[R]^{+}$		-3.12×10^{11}	97.869	93.439
△(Reaction 9b)		-28.3	-3.03	+41.344
$[Cu(CH_2OH)(MeOH)]$		-2.67×10^{11}	57.652	95.916
$[L\text{-}CH_2OH]^{+}$		-4.87×10^{11}	136.002	115.740
△(Reaction 9c)		+27.1	-3.348	+45.435
$[Cu(MeOH)(BCOH)]^{+}$		-5.15×10^{11}	111.770	129.262

$[C_3H_5O_2]^+$		-1.68×10^{11}	49.220	75.036
$[CH_2OH]^{\bullet}$		-0.72×10^{11}	6.969	54.453
△(Reaction 9d)		+9.72	-29.043	+92.53