Supporting Information for

Models for Dioxygen Activation by the Cu_B Site of PHM and DβM

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Table S1. O–O bond distances (Å) and ν(O–O) (cm^{-1}) for all 1:1 Cu-O_2 adducts stable under optimization.

ligand set	O_2 hapticity	multiplicity	O–O	ν(O–O)
$(N)_3$	η^1	singlet	1.256	1346
	η^2	singlet	1.307	1198
$(N)_3(OH)$	η^1	singlet	1.311	1161
	η^1	triplet	1.302	1180
$(N)_3(H_2O)$	η^1	singlet	1.280	1255
	$\eta^{2\,(a)}$	singlet	1.307	1198
	η^1	triplet	1.226	1404
$(N)_3(S)$	η^1	singlet	1.262	1318
$(N)_2(OH)$	η^1	singlet	1.290	1216
	η^2	singlet	1.347	1092
	η^1	triplet	1.282	1220
	η^2	triplet	1.300	1195
$(N)_2(H_2O)$	η^1	singlet	1.254	1352
	$\eta^{1\,(a)}$	singlet	1.244	1395
	η^2	singlet	1.321	1163
$(N)_2(S)$	η^1	singlet	1.253	1352
	η^2	singlet	1.306	1191
$(N)_2(H_2O)(S)$	η^1	singlet	1.263	1311
	$\eta^{1\,(a)}$	singlet	1.253	1352

[(a)] The aqua ligand is lost in formation of this 1:1 Cu-O_2 adduct.

Figure S1. Correlation between O–O bond length in the 1:1 Cu-O_2 adducts and computed ν(O–O) based upon data in Table S1. For the linear fit, $R^2 = 0.964$.

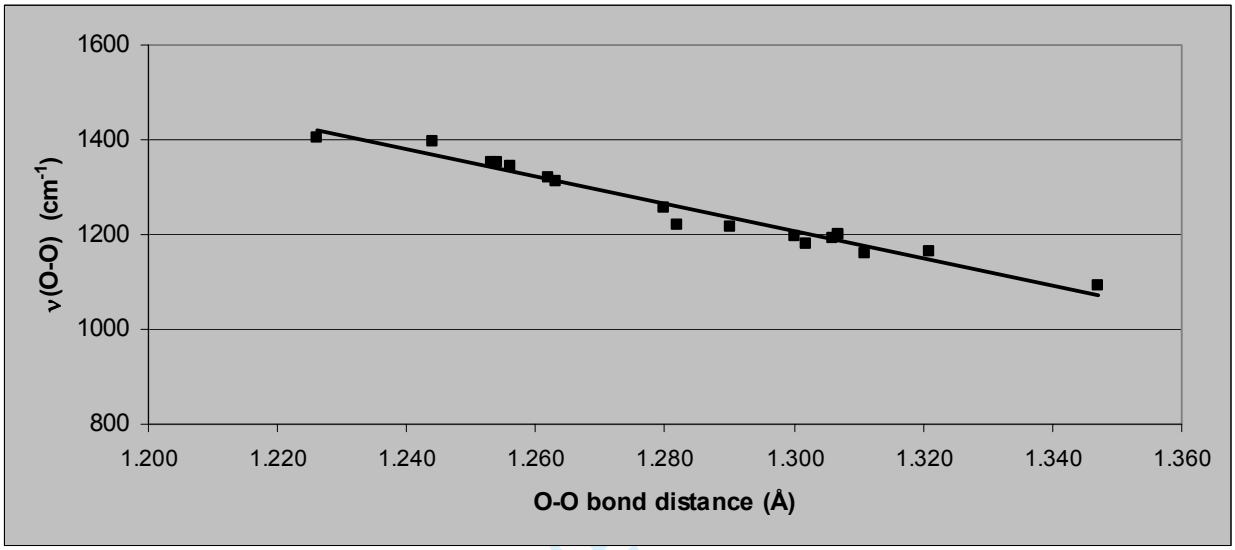
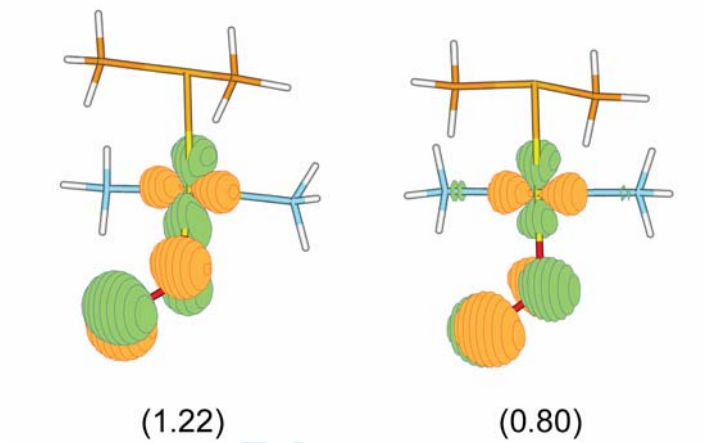


Figure S2. Partially occupied frontier orbitals in the CASSCF wave function for the singlet η^1 Cu-O_2 with the $(N)_2(S)$ ligand set. Occupation numbers are shown in parentheses. Orange is C, blue N, red O, white H, and yellow Cu.



Atomic Coordinates for Computed Structures.

1.) $[Cu(imid)_3]^+$

Cu	-8.5008461566	-.0001468272	-9.4613554533
C	-5.6101614402	.6214303534	-10.2687172553
N	-4.6924014799	.4186027802	-11.2437870482
C	-5.2700321486	-.3667068011	-12.2205117745
C	-6.5434721763	-.6108950793	-11.7862177212
N	-6.7474008804	.0101893483	-10.5663415794
H	-5.4155566199	1.1986715419	-9.3776553475
H	-4.7370098677	-.6701365896	-13.1069730261
H	-7.3237462801	-1.1797669110	-12.2672696398
C	-9.0436926337	.7245043886	-6.5789307984
N	-8.6274070552	.4663619299	-5.3169686326
C	-7.6004331768	-.4529780682	-5.3810201574
C	-7.4313562200	-.7202246970	-6.7109725243
N	-8.3370656855	.0205027349	-7.4525895340
H	-9.8424312946	1.4106979910	-6.8148248825
H	-7.0991922331	-.8212377442	-4.5006477704
H	-6.7228617711	-1.3835726836	-7.1817189905
C	-10.2357353444	.6422698785	-11.8734535052
C	-11.4490622165	.3766279084	-12.4444000918
N	-12.0905057893	-.4742373476	-11.5678611740
C	-11.2686838258	-.6948748337	-10.5146631635
N	-10.1317620362	-.0314924162	-10.6678585862
H	-9.4327489310	1.2578609700	-12.2474215450
H	-11.9009439066	.7049186914	-13.3663095823
H	-11.5278649313	-1.3249897482	-9.6777649377
H	-3.7495151340	.7810248245	-11.2519172780
H	-9.0050051431	.8793082971	-4.4759208267
H	-13.0123115280	-.8693007976	-11.6886259509

2.) $[Cu(imid)_3(OH)]$

Cu	-1.6618048510	.0443380782	-.5347122013
C	-1.3150754276	2.9219091675	.4495793359
C	-.4034384101	3.9415658757	.5068157279
N	.7948496713	3.3870504377	.1003380061
C	.5676998507	2.0738784709	-.1844465249
N	-.7005740798	1.7623357405	.0150820327
H	-2.3701217382	2.9342400022	.6735732259
H	-.4888896342	4.9785139158	.7908763506
H	1.3339070836	1.3992021798	-.5334185190
C	-.7182411484	-2.6889457835	-.6970451878
N	.0485512040	-3.7874527345	-.4561121200
C	.6639160973	-3.6217354058	.7734034279
C	.2297937109	-2.4030728725	1.2242087469
N	-.6275039892	-1.8334559572	.3082015879
H	-1.3119452129	-2.4632869872	-1.5895588097
H	1.3259955183	-4.3633398278	1.1915603853
H	.4739471465	-1.9063568433	2.1522867978
C	-4.6573642361	-.1743621541	-.4033504439
C	-5.8874985476	-.1638012219	.1969357250
N	-5.6885330117	.3879798192	1.4518998624
C	-4.3609519975	.6819931492	1.5593109326
N	-3.7150307829	.3570393294	.4594220636
H	-4.3063012296	-.5398151543	-1.3658360635
H	-6.8614511525	-.4873739900	-.1346718008
H	-3.9279897864	1.1213567014	2.4467228642
H	-6.3923000197	.5376727804	2.1584513647
H	1.6783990060	3.8672031180	.0221430171
H	.1504914787	-4.5775541013	-1.0740715905

O	-2.3550589804	-.9199290948	-2.1000099402
H	-2.1698746337	-.4183603855	-2.9034627059

3.) $[Cu(imid)_3(H_2O)]^+$

Cu	-1.4029854188	-.0193136375	-.1182397465
C	-1.5887871537	3.0010663272	-.0320683033
C	-.8570108584	4.1367784479	.1796885200
N	.4350412403	3.7068564553	.4043057621
C	.4488124351	2.3542203496	.3231686635
N	-.7642230283	1.8922298572	.0585995822
H	-2.6432646747	2.8983036608	-.2340575497
H	-1.1271926514	5.1802573100	.1927005009
H	1.3379533786	1.7588783025	.4621316574
C	-1.4826197934	-2.9548591478	.2255284560
N	-.7572648049	-4.0988011223	.2409725321
C	.5597141464	-3.7768450226	-.0169800124
C	.5772012061	-2.4190734539	-.1814870317
N	-.7024324169	-1.9141507017	-.0300993109
H	-2.5476615457	-2.9142677197	.3944445050
H	1.3382656292	-4.5213669558	-.0569374905
H	1.4169696873	-1.7771850510	-.3960119088
C	-4.5380467446	-.1254904845	-.5938487413
C	-5.7506459177	-.0185326025	.0320111427
N	-5.4613625734	.1639820997	1.3694950623
C	-4.1112586218	.1627653683	1.5092014258
N	-3.5202956626	-.0101697343	.3376516542
H	-4.3134417461	-.2624388308	-1.6401962686
H	-6.7629326469	-.0511495395	-.3376653292
H	-3.6136017739	.2935017618	2.4586029103
H	-6.1336884167	.2808128969	2.1139901030
H	1.2329820835	4.2946995383	.5990225302
H	-1.1201808550	-5.0253561335	.4136200461
O	-2.0208561257	-.0460233064	-2.5713807601
H	-1.7624897896	.7690123730	-3.0212652200
H	-1.5309276185	-.7414021648	-3.0291497146

4.) $[Cu(imid)_3(CH_3SCH_3)]^+$

Cu	-1.7483900000	-0.0079300000	0.0678100000
C	-1.7226500000	3.0837900000	0.3187200000
C	-0.8754500000	4.1573300000	0.2853500000
N	0.3943600000	3.6202700000	0.2276400000
C	0.2817200000	2.2698800000	0.2274200000
N	-0.9907700000	1.9094500000	0.2801900000
H	-2.8005800000	3.0736600000	0.3625700000
H	-1.0526600000	5.2205500000	0.2980600000
H	1.1270200000	1.6008000000	0.1806500000
C	-0.8993200000	-2.8513900000	0.8067800000
N	0.0173900000	-3.8180300000	0.5551800000
C	1.0044900000	-3.2753100000	-0.2402800000
C	0.6360400000	-1.9730000000	-0.4391800000
N	-0.5544000000	-1.7170100000	0.2197400000
H	-1.7837500000	-3.0088100000	1.4046900000
H	1.8533600000	-3.8476400000	-0.5779400000
H	1.1348500000	-1.2108800000	-1.0173100000
C	-4.6513500000	-0.7839600000	-0.6266500000
C	-5.9238100000	-0.8034800000	-0.1263100000
N	-5.8205700000	-0.3177700000	1.1604200000
C	-4.5180100000	-0.0233500000	1.3959500000
N	-3.7797700000	-0.2948200000	0.3300800000
H	-4.3008400000	-1.0740400000	-1.6037600000
H	-6.8649600000	-1.1075400000	-0.5550300000
H	-4.1572400000	0.3748700000	2.3319700000
H	-6.5813200000	-0.1965100000	1.8136300000

H	1.2597200000	4.1402000000	0.1939900000
H	-0.0168100000	-4.7684400000	0.8953300000
S	-1.2907100000	0.1520000000	-2.5906200000
C	-1.9702100000	1.5820200000	-3.5003400000
H	-1.3938700000	1.7680000000	-4.4094900000
H	-3.0217400000	1.4245500000	-3.7536900000
H	-1.8888500000	2.4451800000	-2.8384300000
C	-1.5999900000	-1.1819800000	-3.8008800000
H	-1.1868700000	-2.0995100000	-3.3769300000
H	-2.6693700000	-1.3165300000	-3.9828700000
H	-1.0924800000	-0.9667400000	-4.7443100000

5.) $[Cu(imid)_2(OH)]$

Cu	-8.4003341340	-0.0597325948	-9.8590698516
C	-5.5381603899	0.4437792721	-10.0922817751
N	-4.5267204854	0.4545523664	-10.9968831665
C	-5.0205390754	-0.0207598236	-12.1966019559
C	-6.3364876867	-0.3043424086	-11.9640972842
N	-6.6436981963	-0.0095290853	-10.6517875930
H	-5.4425427191	0.7683985021	-9.0675103083
H	-4.4086634841	-0.1107038233	-13.0783960463
H	-7.0853372887	-0.6932299311	-12.6354527720
C	-9.1822407349	0.1151415680	-7.0059773437
N	-9.0284521182	0.2418052538	-5.6593042518
C	-7.7391279082	-0.1361823710	-5.3364282172
C	-7.1629803462	-0.4802113559	-6.5310223283
N	-8.0650964997	-0.3202731514	-7.5657891683
H	-10.0778232421	0.3341311584	-7.5811175941
H	-7.3729287781	-0.1231780541	-4.3212851810
H	-6.1594089545	-0.8419199687	-6.7041053152
H	-3.5835078553	0.7630679326	-10.8203333540
H	-9.7371271415	0.5499539807	-5.0105619866
O	-10.2286011428	0.0575334530	-9.5580570613
H	-10.7009692392	0.4228303496	-10.3136658676

6.) $[Cu(imid)_2(H_2O)]^+$

Cu	-7.5821524346	-0.0717972019	-9.1328590376
C	-5.2293040276	0.3528957378	-10.8230516494
N	-4.8100779666	0.2517976802	-12.1026440525
C	-5.8701072261	-0.1787295535	-12.8747327138
C	-6.9204890242	-0.3237370951	-12.0129108081
N	-6.5103362247	0.0116627983	-10.7333513523
H	-4.5994641224	0.6785121276	-10.0101103700
H	-5.7846448739	-0.3309010948	-13.9382152290
H	-7.9343279346	-0.6271314330	-12.2153906494
C	-9.6573350785	0.2109754520	-7.1309873304
N	-9.8883978211	0.1539052842	-5.8027119538
C	-8.7140539552	-0.2048308303	-5.1707959355
C	-7.7912167239	-0.3558369832	-6.1666599576
N	-8.3905296238	-0.0920774900	-7.3886682189
H	-10.3946705468	0.4599546436	-7.8772617367
H	-8.6457610826	-0.3170828834	-4.1010975924
H	-6.7511711746	-0.6290782309	-6.0911436834
H	-3.8782944571	0.4607726730	-12.4331260089
H	-10.7726529291	0.3443696389	-5.3526466933
O	-9.7650137402	0.0971857350	-10.3295610844
H	-10.0497603199	0.8588494239	-10.8522792418
H	-10.3796946467	-0.6176929996	-10.5450838458

7.) $[Cu(imid)_2(CH_3SCH_3)]^+$

Cu	-7.8277568318	-0.2916722138	-9.3328765911
C	-5.3323021086	0.1536199389	-10.8330752432
N	-4.7740285148	-0.0163588543	-12.0520878112
C	-5.6975204362	-0.6307911794	-12.8725407791

C	-6.8101988029	-0.8144153193	-12.1005645711
N	-6.5734130969	-0.3178005275	-10.8291878166
H	-4.8234260750	0.6095638241	-9.9981664526
H	-5.4841036764	-0.8755305397	-13.9002887639
H	-7.7550420751	-1.2617426502	-12.3651858098
C	-8.8500576625	-1.2770194275	-6.7204836389
N	-9.3790174839	-0.8300163425	-5.5591800227
C	-9.3833528560	0.5490950114	-5.5850682155
C	-8.8454955655	0.8967039761	-6.7928529719
N	-8.5157501875	-0.2525657291	-7.4959478105
H	-8.7275946195	-2.3219586685	-6.9595486993
H	-9.7542157788	1.1416833864	-4.7644901902
H	-8.6768598812	1.8803214076	-7.2018817361
H	-3.8390838954	0.2640626131	-12.3135328620
H	-9.7018859153	-1.4116566676	-4.7985050597
S	-9.9189576547	0.8632440201	-10.4189271124
C	-11.5631209450	0.5480362151	-9.6889759061
H	-12.2364918590	1.3786419127	-9.9097884751
H	-11.9860289544	-0.3886059028	-10.0581931322
H	-11.4225496236	0.4834043926	-8.6086217533
C	-10.3300564102	0.9222009825	-12.1976287475
H	-9.3950726094	1.0829216690	-12.7372703410
H	-10.7867332724	-0.0136739659	-12.5269419862
H	-11.0033631551	1.7582326518	-12.3969251117

8.) $[Cu(imid)_2(CH_3SCH_3)]^+ \cdot H_2O$

H	4.7529480622	1.3399416144	-3.6595406793
H	2.7273477286	0.1495153527	-2.9877189442
H	5.1458266020	-0.0813622049	-3.2208142304
O	4.4422510487	0.5769403804	-3.1561902176
C	-1.4756091870	-1.0409686585	2.6647814639
C	-2.5263417985	0.4798282204	3.8839277150
C	-2.4904404353	0.8781142943	2.5772564499
C	1.1667006217	0.1922518014	-1.5587186639
C	-4.9856147599	0.4974347986	-1.0164659115
C	-3.2530881449	1.9428188062	-2.7043968479
C	0.7906578654	-0.5923759791	-3.5823689677
C	-0.3591289281	-0.6624484978	-2.8443143103
H	-0.9419146396	-1.9431458337	2.4085011175
H	-2.9371928432	0.9411764569	4.7674967280
H	-2.8838556511	1.7769373330	2.1284588868
H	-1.7293310417	-1.3081363308	4.7387660115
H	-5.8045323194	1.1506221239	-1.3245429601
H	-4.9055451980	-0.3515324597	-1.6988453909
H	-5.1800550191	0.1322393918	-0.0064441844
H	-2.3288701988	2.5177088564	-2.7857461727
H	-3.1945002714	1.0714693999	-3.3604338874
H	-4.0936983203	2.5758444797	-2.9953811975
H	1.6920312467	0.6163869864	-0.7168851265
H	1.0069064330	-0.8763620646	-4.5999329945
H	-1.3293604843	-1.0356315653	-3.1317436015
N	-1.8798702308	-0.7379792055	3.9187057250
N	-1.8355787825	-0.0807370299	1.8231077314
N	1.7435252102	-0.0476165643	-2.7528757728
N	-0.1145153096	-0.1677575526	-1.5752958693
S	-3.4239214344	1.4455195484	-0.9542397848
Cu	-1.3884045427	0.0337475993	-0.1014829875

9.) $[Cu(imid)_2(H_2O)(CH_3SCH_3)]^+$

C	2.7179831690	-1.6059750982	-3.4346369792

C	1.8794289504	-2.1755911077	-1.4651913806
N	2.7649500564	-2.5412220933	-2.4217622533
C	1.7829565900	-0.6883761256	-3.0427294658
N	1.2637009459	-1.0529024945	-1.8109227438
H	3.3353170465	-1.6770880359	-4.3155031170
H	1.7148534834	-2.7334008936	-0.5563505177
H	3.3568997918	-3.3596963409	-2.3961192257
H	1.4503596693	0.2009954906	-3.5552096397
C	-2.1423364490	-0.3600202139	-3.6919679130
C	-3.0293094913	1.7111873386	-2.0146310224
S	-1.4856936870	1.0487727459	-2.7305528149
H	-2.7849114398	-0.0000737433	-4.4976920955
H	-2.6968908542	-1.0448059052	-3.0468042655
H	-1.2863633148	-0.8839661025	-4.1203772942
H	-3.5063611553	0.9714998613	-1.3684364014
H	-3.7112290009	2.0172310787	-2.8103438522
H	-2.7587474577	2.5863208809	-1.4214320591
C	-2.1797924548	-0.6927024100	1.4204642854
C	-1.1533121895	1.2059350417	1.6658804750
N	-2.0355908828	1.0858077744	2.6854998271
C	-2.6990382882	-0.1165296140	2.5471192766
N	-1.2160298823	0.1399550343	0.8779958152
H	-2.4290484023	-1.6416355768	0.9722370448
H	-0.4944238484	2.0467521194	1.5142450639
H	-2.1747415513	1.7610001355	3.4239233171
H	-3.4544162092	-0.4421525428	3.2437939026
Cu	-0.1464523675	-0.0772165268	-0.7883925711
O	1.0129386682	2.1837239305	-0.3479071776
H	1.9607852161	2.0599585636	-0.2057580625
H	0.9546154766	2.7770407348	-1.1087272395

10.) $[Cu(imid)_2(H_2O)(CH_3SCH_3)]^+ \cdot H_2O$

O	-2.4956647512	2.8569365729	4.1822617954
H	-3.2188674717	3.4947305270	4.2160685200
H	3.4442619958	-3.4353535472	-3.1517282116
H	-2.0626516872	2.9027047475	5.0432627711
C	2.7510302836	-1.6521497756	-4.1012654777
C	-2.7969433036	1.6854615898	-2.5121736742
C	-1.9449764859	-0.8500234413	0.9441656794
C	-1.0349374890	1.1105067079	1.1491010974
C	2.0710072678	-2.2475606047	-2.0803496796
C	-2.5200091028	-0.2573472892	2.0357057357
C	1.8671598660	-0.7287769949	-3.6161980123
C	-1.9956408534	-0.3484227937	-4.2756348633
H	-2.6087216298	0.0894292069	-5.0660941325
H	-2.5935778550	-1.0389175886	-3.6764650444
H	-1.1631276324	-0.8918079574	-4.7263065082
H	-3.3405133537	0.9393320397	-1.9285390181
H	-3.4344965286	2.0878775219	-3.3021449607
H	-2.4877550881	2.4991850630	-1.8534396067
H	-2.1294151735	-1.8273238713	0.5261953053
H	-0.4202682725	1.9826559557	0.9876781447
H	-2.1360058241	1.6841640650	2.8689638496
H	-3.2737367548	-0.6017937175	2.7256345814
H	2.0803240314	2.0740346975	-0.8082219590
H	1.0300189649	2.6404845114	-1.7707347266
H	3.2921381071	-1.7139948161	-5.0318087496
H	1.9741198293	-2.8214621242	-1.1716210989
H	1.5070987227	0.1746327476	-4.0832914298
N	-1.9301233317	0.9811980741	2.1495416054

N	-1.0140788872	0.0143101386	0.3949342757
N	2.8678803287	-2.6069216349	-3.1135518123
N	1.4477328052	-1.1097623820	-2.3518272867
O	1.1262642277	2.1531462959	-0.9414822283
S	-1.2779605945	0.9659559129	-3.2279747873
Cu	0.0822049891	-0.2004102310	-1.2250443384

11.) $[Cu(imid)_3(O_2)]^+$ Singlet – End-on

O	-0.8787699181	2.3600892396	-0.1113089277
O	-1.7321466466	3.0045945883	-0.7693730633
C	2.7903272387	-0.0044920392	-1.0339557433
C	3.0118377686	-0.8227911117	-3.0796149269
C	1.6878529344	-0.6386624685	-2.7913055857
C	-3.3002623994	0.0996169749	-3.4218339224
C	-2.3727959993	0.8334334847	-2.7352860109
C	0.8829728231	-0.8358159942	1.9825255682
C	0.8777429535	-0.7079735071	3.3442340174
C	-0.2413612501	0.9694072875	2.4241051455
C	-2.1811689025	-1.2164213288	-2.0361246987
H	0.8252706991	-0.8261408728	-3.4108074965
H	3.5166960888	-1.1923863447	-3.9573961033
H	4.6989495692	-0.4106262927	-1.8337171139
H	-0.8201170977	1.8741595179	2.3252208675
H	1.3046189293	-1.3117243940	4.1287182945
H	1.3357290212	-1.6046445246	1.3760592705
H	3.0531933357	0.3708640044	-0.0567337250
H	-3.7115770713	-1.9918241824	-3.2605474589
H	-1.8743428103	-2.1063389436	-1.5081297788
H	-0.0344660672	0.8293792773	4.5157285472
H	-4.0219867752	0.3737716273	-4.1740034195
H	-2.1589870221	1.8896839826	-2.7847169272
N	-3.1621276260	-1.1961405782	-2.9674190066
N	0.1832794388	0.2167424288	1.4186671647
N	0.1613836206	0.4427150967	3.6028852426
N	1.5600392337	-0.1286652181	-1.5125439284
N	3.6954157819	-0.4154852806	-1.9517128911
N	-1.6818060992	0.0018101926	-1.8735067972
Cu	-0.1845634968	0.5405671401	-0.5917814621

12.) $[Cu(imid)_3(O_2)]^+$ Singlet – Side-on

O	-0.8787699181	2.3600892396	-0.1113089277
O	-1.7321466466	3.0045945883	-0.7693730633
C	2.7903272387	-0.0044920392	-1.0339557433
C	3.0118377686	-0.8227911117	-3.0796149269
C	1.6878529344	-0.6386624685	-2.7913055857
C	-3.3002623994	0.0996169749	-3.4218339224
C	-2.3727959993	0.8334334847	-2.7352860109
C	0.8829728231	-0.8358159942	1.9825255682
C	0.8777429535	-0.7079735071	3.3442340174
C	-0.2413612501	0.9694072875	2.4241051455
C	-2.1811689025	-1.2164213288	-2.0361246987
H	0.8252706991	-0.8261408728	-3.4108074965
H	3.5166960888	-1.1923863447	-3.9573961033
H	4.6989495692	-0.4106262927	-1.8337171139
H	-0.8201170977	1.8741595179	2.3252208675
H	1.3046189293	-1.3117243940	4.1287182945

H	1.3357290212	-1.6046445246	1.3760592705
H	3.0531933357	0.3708640044	-0.0567337250
H	-3.7115770713	-1.9918241824	-3.2605474589
H	-1.8743428103	-2.1063389436	-1.5081297788
H	-0.0344660672	0.8293792773	4.5157285472
H	-4.0219867752	0.3737716273	-4.1740034195
H	-2.1589870221	1.8896839826	-2.7847169272
N	-3.1621276260	-1.1961405782	-2.9674190066
N	0.1832794388	0.2167424288	1.4186671647
N	0.1613836206	0.4427150967	3.6028852426
N	1.5600392337	-0.1286652181	-1.5125439284
N	3.6954157819	-0.4154852806	-1.9517128911
N	-1.6818060992	0.0018101926	-1.8735067972
Cu	-0.1845634968	0.5405671401	-0.5917814621

13.) $[Cu(imid)_3(OH)(O_2)]$ Singlet – End-on

O	1.6080623753	-0.1822266070	2.1715774944
O	1.2114692419	0.7226490484	3.0332202547
C	2.5086680790	3.8119690049	-0.7327868634
C	1.8958348415	2.6201751907	-1.0079127954
C	2.4339012103	2.5533386844	1.0983106354
C	-3.2037670927	-0.5238440770	0.7151223615
C	-2.0348610498	-0.4403212133	0.0074839862
C	2.6029124010	-2.8267378367	0.9667424587
C	2.7480435868	-4.0650389647	0.4003612021
C	1.5906293397	-2.7368916775	-0.9495547947
C	-1.5008194177	-0.1614567394	2.0957684445
H	2.4870276335	2.2308442811	2.1312347623
H	2.7289809602	4.6728565463	-1.3430611227
H	3.3013743385	4.4765924136	1.1436313712
H	1.0049376988	-2.3487616215	-1.7728926974
H	3.2372343988	-4.9657193946	0.7360647654
H	2.9476911601	-2.4598605085	1.9213108580
H	1.4480169722	2.2448979941	-1.9152077354
H	1.3426852456	-0.0672269872	-2.1074236759
H	-3.4729476510	-0.3443868516	2.8336929130
H	2.0028701813	-4.7379237231	-1.4915476137
H	-0.9182251089	0.0319041641	2.9877207816
H	-1.8331453787	-0.5130660131	-1.0505780150
H	-4.2261972547	-0.6878772952	0.4142796393
N	-2.8472414157	-0.3429958270	2.0431273666
N	1.8880507946	-2.0165178674	0.1142459638
N	2.0973870197	-3.9911016242	-0.8205351382
N	2.8428020157	3.7534389170	0.6112802727
N	1.8624503707	1.8546561551	0.1365527045
N	-0.9935523534	-0.2180057585	0.8812116687
O	0.5163292104	-0.1274491307	-1.6089026984
Cu	1.0320051131	-0.0559055740	0.2948983143

14.) $[Cu(imid)_3(OH)(O_2)]$ Triplet – End-on

O	2.4488043638	-0.0097317474	2.8038903692
O	1.2139454731	-0.1054205111	2.4029562720
C	2.3635317541	3.7889109326	-0.7498240413
C	1.6570006626	2.6255824132	-0.8931219743
C	2.7542120825	2.4393720802	0.9690911134

C	-3.3491840275	-0.1256709348	0.3406594129
C	-2.0924139320	-0.1024855159	-0.2029045663
C	2.6503932612	-2.8487167321	1.1231378103
C	2.8820273983	-4.0583932790	0.5245019085
C	1.6589203715	-2.7684756963	-0.8045262987
C	-1.8230554571	-0.1662139979	1.9493748905
H	3.1407273516	2.0490162684	1.8990143076
H	2.4372466294	4.6748240286	-1.3599530174
H	3.6798375420	4.3358032893	0.8494834666
H	1.0814238842	-2.3812659204	-1.6348933055
H	3.4243942177	-4.9348715921	0.8417532589
H	2.9674153224	-2.4811577351	2.0869627836
H	0.9877913836	2.2865957321	-1.6699258315
H	1.3261916611	-0.0187186012	-2.0347025922
H	-3.8879198289	-0.1919008305	2.4137651116
H	2.2100341210	-4.7200498396	-1.3991572750
H	-1.3728115195	-0.1947547867	2.9301359058
H	-1.7506053325	-0.0678029822	-1.2278911339
H	-4.3328825040	-0.1186926550	-0.1010070779
N	1.8910479852	-2.0618391927	0.2850432590
N	2.2425824899	-3.9912683162	-0.7031214033
N	3.0574355534	3.6551468997	0.4416934087
N	1.9114372767	1.8007087549	0.1830983817
N	-1.1592630449	-0.1286993932	0.8124758297
N	-3.1627095730	-0.1661325828	1.7136721629
O	0.5128076409	-0.1915292492	-1.5423900939
Cu	0.9618921136	-0.1091438556	0.3752692265

15.) $[Cu(imid)_3(H_2O)(O_2)]^+$ Singlet – End-on

O	3.4098764200	-0.7788651693	-1.8908875886
O	3.3477245140	-0.0863694870	-0.8163859701
C	1.4981514796	4.0111156614	1.1304914677
C	-1.1868316000	-0.0546449867	1.6609297339
C	2.9158219407	2.5534229135	0.2507068749
C	-2.8127293111	-0.0214215766	0.1563411568
C	0.9320762119	-2.9972364123	0.6114584186
C	-1.5992095278	-0.1056334798	-0.4706604570
C	2.8931302463	-3.9810973514	0.9220621475
C	3.0802622868	-2.6520558659	0.6688305127
C	0.8947586402	2.7907581166	1.0065499971
H	0.8535676360	1.0785688003	-2.5548524823
H	-3.8209987538	0.0182181569	-0.2235428122
H	1.7668411488	-0.1637546605	-2.6236492474
H	-1.3663271507	-0.1582404138	-1.5222942018
H	-0.6939138559	-0.0477069381	2.6217040476
H	-3.2094548771	0.0707407273	2.2550924003
H	-0.1118196864	2.5049795382	1.2632718831
H	1.1432969792	4.9581796631	1.5040181194
H	3.4961597436	4.5492399884	0.5918337805
H	3.8155157388	2.1426935814	-0.1799210004
H	-0.1328726003	-2.8613083103	0.5114598820
H	1.0498404133	-5.0615676537	1.0100436718
H	3.5873837747	-4.7809890708	1.1213232345
H	3.9949762178	-2.0885657729	0.5926220527
N	-2.5319026491	0.0109016711	1.5077896833
N	1.8497162184	-2.0496196715	0.4785588423

N	1.5264536244	-4.1805555971	0.8807338557
N	1.7889320244	1.8884919462	0.4584529586
N	2.7794459254	3.8390028659	0.6463683610
N	-0.5918235849	-0.1227768975	0.4787455222
O	0.8913785839	0.1442607109	-2.3113475235
Cu	1.5000996704	-0.1144817203	-0.0086936770

16.) $[Cu(imid)_3(H_2O)(O_2)]^+$ Triplet – End-on

O	1.6413501088	-0.9258454466	3.1124962816
O	2.2388652449	-0.1742025621	2.3504479959
C	1.3683591179	4.0744452885	0.1781948476
C	-1.4024512081	-0.0710225305	1.6831171925
C	2.8819726465	2.5093307353	0.5768712339
C	-2.9753931172	0.2532794457	0.1605595626
C	1.0744864841	-3.0325864282	0.4156130795
C	-1.7621071782	0.0679946263	-0.4469024321
C	3.0118596415	-4.0435378069	0.0469479163
C	3.1191139495	-2.7103401264	-0.2352467632
C	0.8579684977	2.8419925514	-0.1233872570
H	1.3858826740	0.7849900188	-2.7698443614
H	-3.9631952599	0.4350718694	-0.2317644570
H	1.1524912231	-0.7297372972	-2.8288937239
H	-1.5213437793	0.0709964757	-1.4989326800
H	-0.9370480895	-0.1813347821	2.6510461062
H	-3.4124891037	0.2451392633	2.2536075316
H	-0.1227891748	2.5835449890	-0.4898171880
H	0.9470452386	5.0652575873	0.1210032142
H	3.3129899170	4.5454560527	0.9302573872
H	3.8115040253	2.0535970419	0.8810666615
H	0.0449184473	-2.8778855623	0.6983140259
H	1.2931291783	-5.1028222300	0.7464069543
H	3.7227777658	-4.8520601429	-0.0034324757
H	3.9807899061	-2.1593680945	-0.5783909190
N	-2.7291793271	0.1563888982	1.5148346172
N	1.9051444745	-2.0889776496	-0.0031878038
N	1.7070681315	-4.2282143935	0.4574688676
N	1.8118903827	1.8698123945	0.1270348211
N	2.6546529062	3.8439833811	0.6217253721
N	-0.7834733021	-0.1295031140	0.5138223136
O	0.8630362018	0.0738079530	-2.3776166172
Cu	1.4267079302	-0.1295787508	0.0692996709

17.) $[Cu(imid)_3(CH_3SCH_3)(O_2)]^+$ Singlet – End-on

O	0.8570698553	-0.4049941763	3.3152062994
O	1.9557722806	-0.2176936427	3.9061248239
C	0.5117455999	-1.4447365620	-2.2764450450
C	2.4332280815	2.2176632207	2.2006151727
C	0.5551169908	1.3483377681	-2.1809141900
C	1.3272139926	4.0183012175	1.5354159329
C	0.7071226518	2.8892999536	1.0745351735
C	-1.9388415465	0.1077748509	2.2515006012
C	-3.3648281486	-1.0793981103	1.0428045071
C	1.8056757471	-2.9645763874	2.1687968202
C	-2.0945033534	-1.2338046867	0.5585888917
C	3.3823068693	-3.7594194256	0.8302814866
C	2.9845905851	-2.5229007543	0.4013534442

H	-4.0000230203	0.1016952710	2.7068848864
H	1.1181020575	-2.8829424788	2.9955886992
H	4.1192351173	-4.4516548046	0.4565733389
H	3.3493453683	-1.9490716467	-0.4361480955
H	-0.5733443317	-1.3536663988	-2.1958622103
H	3.1650846891	1.6058203811	2.7045278983
H	0.8365601236	-2.3819039847	-1.8214025393
H	1.0948206512	5.0656823988	1.4304790207
H	0.9748961190	2.2447573947	-1.7231734266
H	-1.7629372212	-1.8413495260	-0.2678312186
H	-4.3124178984	-1.4912124705	0.7346839340
H	-1.5542159115	0.7568318389	3.0231647415
H	0.8048219471	-1.4339002868	-3.3281563795
H	3.0950991003	4.1483459285	2.7307097393
H	2.6735716901	-4.8510561435	2.5264120517
H	-0.1939758321	2.8046252173	0.4873874638
H	-0.5269518652	1.3300778455	-2.0308466067
H	0.7845879881	1.3500016536	-3.2482456095
N	-1.2122176427	-0.4877910607	1.3184742832
N	2.4219394352	3.5711053075	2.2469287695
N	-3.2460574487	-0.2227434310	2.1180137836
N	2.6219651061	-4.0217677826	1.9521474802
N	1.9984792879	-2.0376483498	1.2431579967
N	1.4078916752	1.7724519443	1.4939180815
S	1.3454668892	-0.0891534344	-1.3818465870
Cu	0.9077058996	-0.2462848817	1.2041694689

18.) [Cu(imid)$_2$(OH)(O$_2$)] Singlet – End-on

O	-1.7384279149	-0.7021171956	-4.0061035719
O	-2.0770306783	-1.1034568668	-2.8274363524
C	2.3802469880	-0.0691218150	-3.1912898677
C	1.0514159079	-0.3846486621	-3.1123282212
C	0.1342216967	-0.3777376622	1.8476016569
C	-1.9133860169	0.2953828262	1.6617113077
C	-0.3301579596	-0.2281114827	3.1261733707
C	1.5664086922	0.5971655971	-1.2427506483
H	0.1270019648	-0.3869754664	4.0900640617
H	1.1074589649	-0.7172792364	1.5249927614
H	-2.2812619694	0.3980690625	3.7360178814
H	1.5126209143	1.0372016476	-0.2594268439
H	-2.8648262253	0.5656596712	1.2202771447
H	3.5924386502	0.9225822577	-1.7320421744
H	3.1144456188	-0.2240553089	-3.9653457823
H	0.3774744367	-0.8333414867	-3.8310425787
H	-3.6416146361	0.0501345923	-1.5870159037
N	-1.6354924017	0.2026611618	2.9865067045
N	0.5597959281	0.0360121955	-1.8914064209
N	-0.8567934036	-0.0467958810	0.9448286908
N	2.6922005649	0.5522855089	-1.9955471295
O	-3.1001981629	0.3296016741	-0.8374824150
Cu	-1.3592137955	-0.1137992393	-1.2599108347

19.) [Cu(imid)$_2$(OH)(O$_2$)] Singlet – Side-on

O	-1.5971349223	-1.5256713060	-1.9349828865
O	-2.3220889483	-0.6707531942	-2.6820797581
C	2.5705126535	0.6829040475	-2.9126910962

C	1.5496386549	-0.1446078188	-2.5234375192
C	-0.6438468198	-1.0811140107	1.5556243603
C	-1.4885064160	0.9210944240	1.6170182535
C	-0.6533730101	-0.7088000759	2.8716233810
C	0.9179687674	1.8605622478	-2.0176266625
H	-0.3413025559	-1.2168081241	3.7701402572
H	-0.3089866406	-2.0046079126	1.1093344886
H	-1.3534829328	1.1307914842	3.7095503147
H	0.3062699214	2.6892992664	-1.6904114274
H	-1.9306756835	1.8510667895	1.2827192568
H	2.6610073983	2.8143326441	-2.7503336511
H	3.5245336115	0.4948763627	-3.3794898018
H	1.4667730895	-1.2178450582	-2.6093503125
H	-2.6894826581	2.2344771589	-1.6177209524
N	-1.1917989686	0.5655704883	2.8903563186
N	0.5365512396	0.6023905856	-1.9710201426
N	-1.1629425932	-0.0583998288	0.7924745342
N	2.1524884548	1.9601832803	-2.5823806670
O	-2.0188874026	1.9918496586	-0.9661712139
Cu	-1.5639919474	0.2063296406	-1.1886692518

20.) [Cu(imid)$_2$(OH)(O$_2$)] Triplet – Side-on

O	-2.1318325738	-0.7423469552	-2.6938122563
O	-1.6238440814	-1.9191700656	-2.7195712898
C	2.3915125704	-0.0599629693	-2.8500292178
C	1.1314454722	-0.5374315575	-2.6154298095
C	0.1919345107	0.0918967837	2.0076362870
C	-1.9111754308	0.6044453464	1.9136164026
C	-0.2114483606	0.2725304360	3.3033709656
C	1.3793354976	1.1883914088	-1.3261315132
H	0.3089336276	0.1993337415	4.2449786489
H	1.1689474771	-0.1821731084	1.6386237922
H	-2.1677200706	0.7940093566	3.9989356183
H	1.2087028989	1.9681464436	-0.5996405138
H	-2.8912749604	0.8128747895	1.4987111491
H	3.3460121042	1.6331506485	-1.9528884304
H	3.1782601509	-0.3881513524	-3.5096172427
H	0.6127578984	-1.3764065400	-3.0517983147
H	-3.7609185807	0.6229335274	-1.2527049514
N	-1.5535441211	0.6002165824	3.2226939739
N	0.5139371428	0.2485139615	-1.6632755690
N	-0.8713770726	0.3032913854	1.1537988828
N	2.5341979579	1.0386911803	-2.0221972096
O	-3.1423483108	0.8294777635	-0.5418247556
Cu	-1.4359782769	0.2012633040	-0.9888043687

21.) [Cu(imid)$_2$(OH)(O$_2$)] Triplet – End-on

O	0.5828228972	2.0144450861	0.1393608437
O	1.1066072012	0.8621498046	0.4351574490
C	0.8967780230	-1.2914848382	-4.2117862651
C	-0.0315002072	-1.0031719581	-3.2483409668
C	-0.8130541611	-1.1016872172	2.5984180237
C	-2.5504576046	-1.1111456263	1.2953416895
C	-1.8436074162	-1.6169051999	3.3375127321
C	1.9056061523	-0.5340288065	-2.3889722471
H	-1.9022395323	-1.9699517598	4.3544905808

H	0.2109746657	-0.9220009609	2.8867548137
H	-3.8705061798	-1.9300602829	2.7217584882
H	2.6857302909	-0.2100144819	-1.7166917070
H	-3.1539179482	-0.9561827825	0.4089175278
H	3.0252346469	-1.0758065906	-4.0977232618
H	0.8065091645	-1.6699154646	-5.2172403069
H	-1.1104213584	-1.0630311924	-3.2370379062
H	-2.4425137962	0.7804180682	-1.7023045705
N	-2.9399676857	-1.6169408450	2.4913690614
N	0.6145571387	-0.5360046000	-2.1227777537
N	-1.2677488965	-0.7961185669	1.3343366359
N	2.1258509089	-0.9881899191	-3.6493778158
O	-2.2102225205	-0.0793655305	-1.3275937406
Cu	-0.5206637116	0.0691724292	-0.4439295027

22.) $[Cu(imid)_2(H_2O)(O_2)]^+$ Singlet – Side-on

O	-1.8949210937	-2.3915741504	-0.3294089671
O	-1.2140869418	-2.3478236204	-1.4603533550
C	1.5089000130	0.9563429356	-1.2009269857
C	2.4317485556	-0.0005951719	-2.9753236247
C	1.4069170703	-0.7804316457	-2.5203829900
C	0.1976519738	-0.3327424548	2.4504524841
C	-1.6518989420	0.6898555982	1.9031190701
C	-0.2621998827	0.2790191554	3.5822046858
H	-3.2166541362	-0.5970677834	-0.9501929725
H	-2.8301359617	0.5983578027	-1.8451846850
H	1.0776896561	-0.9417199638	2.3157866355
H	0.1225208733	0.3127256046	4.5885024775
H	1.3188674462	1.6662877901	-0.4113480314
H	3.1291034429	1.8608825705	-2.1901394818
H	3.1146125191	-0.1210854627	-3.8005266220
H	1.0416069714	-1.7229449795	-2.8960778248
H	-2.4969489452	1.0575600031	1.3418677484
H	-2.0253327982	1.4634177272	3.8211583573
N	-0.6760245500	-0.0647893771	1.4100896166
N	-1.4284490582	0.9194850856	3.2130746070
N	0.8394161134	-0.1702410061	-1.4138721764
N	2.4782972444	1.0898396070	-2.1290416632
O	-2.6977893154	0.2232824991	-0.9639873338
Cu	-0.6845261766	-0.8885655719	-0.3890279745

23.) $[Cu(imid)_2(H_2O)(O_2)]^+$ Singlet – End-on

O	-1.0607018810	-2.3259308921	-0.6679509744
O	-1.6086410293	-2.3767445013	-1.7945136185
C	1.8736357242	0.6508414507	-1.7463774558
C	1.9093135323	-0.4659206607	-3.6582124745
C	0.9265282919	-0.9706482614	-2.8551232312
C	-0.2635435612	-0.4619823862	2.9011041062
C	-2.1558407837	0.1515679082	2.0055708682
C	-1.1057588047	-0.1615555276	3.9334790747
H	-2.7469926159	-0.6533082440	-1.4666567748
H	-2.6560772305	0.8700885448	-1.7086673359
H	0.7581156473	-0.8052032822	2.9381375409
H	-0.9724998270	-0.1859716257	5.0027487419

H	2.1335560431	1.3730977226	-0.9876962488
H	3.2638017735	1.1363700896	-3.2468597520
H	2.2404921565	-0.7398254733	-4.6466065435
H	0.2384131140	-1.7812121907	-3.0411513087
H	-2.9245584523	0.3867178677	1.2854115374
H	-3.1339824792	0.5069682777	3.8305343488
N	-0.9277215259	-0.2603506713	1.7015999994
N	-2.2944921103	0.2237703936	3.3441959865
N	0.9101946891	-0.2630898736	-1.6657711325
N	2.4951898568	0.5561991573	-2.9392626788
O	-2.5264382757	0.1897816572	-1.0352442458
Cu	-0.2918988831	-0.4763103314	-0.1413603081

24.) $[Cu(imid)_2(O_2)]^+$ Singlet – End-on

O	1.7732595724	0.0310335463	1.1329089442
O	2.6605016375	-0.8171128617	0.9327788401
C	2.0416483409	-0.1502581898	-1.9913405425
C	1.0310592567	0.1571580855	-3.9404939066
C	0.0983782933	0.1424359831	-2.9441570107
C	-0.7159293936	-0.0355273081	2.9104577345
C	-2.4899902480	-0.1731530022	1.6461794308
C	-1.7945507389	-0.0650860330	3.7458507172
H	0.3340798036	0.0233668126	3.1448412066
H	-1.8708473457	-0.0330143627	4.8207420282
H	2.8208629504	-0.3092143782	-1.2597844314
H	3.1484706178	-0.0717691636	-3.7708323556
H	0.9407167243	0.2807178551	-5.0075686049
H	-0.9715680075	0.2552797688	-3.0165881869
H	-3.1566224379	-0.2376320787	0.8003403830
H	-3.8648622222	-0.1942807819	3.2330318678
N	-1.1615975486	-0.1020600212	1.5993402963
N	-2.9021403580	-0.1521089469	2.9277153171
N	0.7402340444	-0.0530312641	-1.7293922578
N	2.2467335090	-0.0305088449	-3.3157452716
Cu	-0.0713961674	-0.0826332965	0.0154926185

25.) $[Cu(imid)_2(CH_3SCH_3)(O_2)]^+$ Singlet – End-on

O	2.0624842656	0.2653501856	1.2553616064
O	2.9982875140	-0.3306447799	0.6721623382
C	2.5656033491	1.0913123616	-1.8159861431
C	1.6353015601	0.5832749519	-3.7618584311
C	0.6902713878	0.5500010766	-2.7771650672
C	-1.7415626904	3.0121756821	-2.6377036128
C	-1.4117991323	2.1423222005	2.3453608959
C	-1.8583312439	1.8207020853	3.5955981711
C	-3.3184928107	1.3605826736	-1.0121494601
C	-0.4314653697	0.2744736595	2.8965360024
H	-0.3590259773	0.3166915697	-2.8533455821
H	1.5780551642	0.3891153538	-4.8207303008
H	3.3198060107	1.3276886458	-1.0821892932
H	-0.8406426210	3.6188644696	-2.7344376952
H	0.1943704603	-0.6036017587	2.8849578548
H	-2.5435080126	2.3175160669	4.2633961790
H	-1.6607665304	2.9929864000	1.7319640409
H	3.7145298153	1.0408087334	-3.5770543916
H	-1.3373011137	0.1262413869	4.7884070814
H	-2.6196020128	3.6376800483	-2.8097005857
H	-1.7117169762	2.2028987091	-3.3701213952
H	-4.1636708383	2.0067825736	-1.2586228230
H	-3.2343836017	0.5632312934	-1.7541530981
H	-3.4801173531	0.9224459979	-0.0261015782
N	-0.5206022948	1.1678132275	1.9177061024
N	-1.2280419030	0.6374919092	3.9234781534
N	1.2794058416	0.8719319343	-1.5655964706
N	2.8135109732	0.9306217491	-3.1327830493
S	-1.7845443949	2.3559410299	-0.9341520731
Cu	0.3735528621	1.0208337764	0.1873726698

26.) $[Cu(imid)_2(CH_3SCH_3)(O_2)]^+$ Singlet – Side-on

O	-1.9350851531	-1.5150775849	-0.8081856390
O	-0.8254790923	-2.1928138202	-0.6809652600
C	2.2110220593	0.9381373749	-1.3590525551
C	3.2048279621	-0.7285456649	-2.4329593378
C	1.9644008978	-1.1231636928	-2.0173175201
C	-3.2525705343	1.5617513797	-0.2286668989
C	-0.7182331093	-1.1895208123	2.3289870774
C	-2.3866046419	1.1645108840	-2.8744844289
C	-0.3972299631	0.4545290678	3.7771330549
C	-0.2593512606	0.9227461030	2.4981960356
H	-2.9596823098	1.7503174855	0.8046555840
H	-3.1511487811	1.8772319246	-3.1882013368
H	-2.7919694326	0.1537607901	-2.8160652906
H	-1.5525352838	1.1951196134	-3.5768447927
H	2.0526254164	1.9116273906	-0.9220842179
H	4.1500688799	1.1661890961	-2.1490470938
H	3.9803851530	-1.2435098501	-2.9767327911
H	1.4617767997	-2.0686084291	-2.1445179341
H	-0.9160832229	-2.1768398460	1.9380432404
H	-0.8482038612	-1.5383040398	4.4046346971
H	-0.3189644039	0.9387681911	4.7369904570
H	-0.0292646652	1.9252153877	2.1711301507
H	-3.9535573117	2.3297218825	-0.5598830087
H	-3.6935309046	0.5679679215	-0.3139707684
N	-0.4613312658	-0.1108318797	1.6017669093
N	-0.6875221317	-0.8881132590	3.6479998330
N	1.3522752184	-0.0730609367	-1.3514968754
N	3.3412809106	0.5772371652	-2.0066821411
S	-1.7373742791	1.6741901581	-1.2421338568
Cu	-0.4952588373	-0.2348785122	-0.5600959274

27.) $[Cu(imid)_2(CH_3SCH_3)(O_2)]^+ \cdot H_2O$ Singlet – End-on

H	-2.6819728547	-3.6021140772	4.7962128442
H	-4.0020738989	-3.0111992451	4.2670563112
O	-3.0427299563	-2.9530488806	4.1797571563
C	-0.5014665157	0.8293526347	2.3024836261
C	2.5582766671	0.4378028639	-2.5456631703
C	2.0628449930	-1.0752152797	-4.0869296574
C	1.0800036909	-1.0444449985	-3.1385414304
C	-3.2843806868	1.0390011856	-0.6251156207
C	-1.0852846644	-1.1275902867	1.5519900012
C	-2.5780232069	-0.2576738814	-3.0031388426
C	-1.2120631917	0.2117479045	3.2956787482
H	-3.0176273056	1.7753001900	0.1345082640
H	-3.5473288615	0.0645806103	-3.3902998029
H	-2.6820458912	-1.2308086792	-2.5166622511
H	-1.8781789791	-0.3320304632	-3.8369505300
H	3.0876955579	1.2058710115	-2.0041065473
H	3.8415956748	0.1036825550	-4.1769181993
H	2.1844248276	-1.6678009987	-4.9793448454
H	0.1798688041	-1.6349296467	-3.0769275147
H	-1.2127465245	-2.0021726792	0.9325843615
H	-2.1128272236	-1.7398818092	3.3047185628
H	-1.4865385170	0.5365028978	4.2865536387
H	-0.0298859468	1.7998591048	2.2890424647

H	-4.2132205086	1.3464692098	-1.1106778738
H	-3.4146992120	0.0627006926	-0.1526832746
N	-0.4291971844	-0.0184129929	1.2136036447
N	-1.5724926565	-1.0214905324	2.8024975156
N	1.3973223730	-0.0910897320	-2.1852953462
N	2.9862559586	-0.1297319628	-3.6928126146
O	1.7020673801	1.8214490533	-0.0598923753
O	1.9359443432	2.1714003608	1.1189891221
S	-1.9291967758	1.0057518944	-1.8507092686
Cu	0.3712863546	0.3523547728	-0.5537103032

28.) $[Cu(imid)_2(CH_3SCH_3)(O_2)]^+ \cdot H_2O$ Singlet – Side-on

H	-0.5005393366	0.4077420900	6.1684249824
H	0.0866230354	-1.0167540470	6.1380747580
O	-0.1588760283	-0.2723991904	5.5738472463
C	-1.7739662183	-0.7375811188	0.9065757181
C	1.6884095827	-0.8794225896	-3.0130874333
C	0.6392676404	-2.8031161524	-3.3412683071
C	0.0170470479	-2.1078120028	-2.3431115885
C	-1.3213231290	2.4371299220	-3.5324792367
C	-0.0345745507	0.0339039594	1.9686897730
C	-2.2419951160	3.0922370747	-0.9648360828
C	-1.9856238940	-0.9524514368	2.2410717880
H	-1.1737144557	1.6584703293	-4.2835305388
H	-2.9069123012	3.8143370379	-1.4429646362
H	-1.2756789617	3.5473068570	-0.7400975257
H	-2.7037723469	2.7413519198	-0.0399184656
H	2.4047194304	-0.0786854894	-3.1162370054
H	2.3592582967	-2.2330563989	-4.4744037649
H	0.4342125310	-3.7638535270	-3.7852736018
H	-0.8455032321	-2.3821921172	-1.7574566485
H	0.9130736672	0.4973972709	2.1969946719
H	-0.7024653509	-0.4464834617	3.9096847005
H	-2.8128166457	-1.4003294585	2.7681241156
H	-2.4125426251	-0.9582851954	0.0659516315
H	-2.0228919869	3.1767706480	-3.9234730913
H	-0.3640454909	2.9035165657	-3.2921881962
N	-0.5482933222	-0.1188234463	0.7499187529
N	-0.8759444332	-0.4617903219	2.8924561628
N	0.6797999517	-0.9103434390	-2.1504288601
N	1.6919431256	-2.0092635428	-3.7492378277
O	1.0439057414	2.2514048558	-0.3442711632
O	1.4225818522	1.9339814270	-1.5689866983
S	-2.0269107437	1.6336596974	-2.0482364187
Cu	0.2914833153	0.5737834550	-0.8822424888

29.) $[Cu(imid)_2(H_2O)(CH_3SCH_3)(O_2)]^+$ Singlet – End-on

O	-1.2433195713	-1.4750015971	-0.4732649565
O	-1.0639980506	-2.5556019815	0.1558115609
C	1.3697461611	-2.0314345743	-1.6353555823
C	2.3203185541	-0.1568267188	-2.1956571079
C	2.8975917202	-1.1280971099	-2.9651680286
C	-1.3507653664	0.4535870108	-3.6564794938
C	-3.1418134298	1.5980442430	-1.8028205666
C	-2.4400439730	0.4469488683	3.2037644797
C	-1.8582134987	-0.2509105419	2.1834891304

C	-1.0591383386	1.7760519246	2.0887163404
H	-0.3089268641	0.2985764481	-3.9417022649
H	0.6844964201	2.6790345643	-0.9643730030
H	1.9382253870	2.3983227314	-0.0824835385
H	-3.1565529038	0.1586021776	3.9555222693
H	-2.1476739932	2.4961976648	3.7401642688
H	3.6648351313	-1.0892692608	-3.7214256974
H	-0.4998089615	2.6496241644	1.7931592221
H	2.4764771180	-3.2239064630	-2.9685955203
H	2.5177331858	0.9026271930	-2.1871995097
H	-1.8649465399	0.9946376161	-4.4531370456
H	-1.8276496458	-0.5143946563	-3.4872441402
H	0.7337843152	-2.7690647572	-1.1653612167
H	-3.5915410186	0.6121733609	-1.6665487819
H	-3.6256463208	2.1244624039	-2.6277496873
H	-3.2587243677	2.1782694649	-0.8864323524
H	-1.9823251483	-1.2842435916	1.8995756084
N	2.2835234780	-2.3061517947	-2.5915754754
N	-1.9241873620	1.7264509659	3.1254774638
N	-0.9995187769	0.5900013166	1.4971139917
N	1.3682138412	-0.7297410332	-1.3691527740
O	0.9867858844	2.2442463827	-0.1516234102
S	-1.3521274009	1.4396063162	-2.1211264167
Cu	0.0368476905	0.1540652447	-0.1454394722

30.) $[Cu(imid)_2(H_2O)(CH_3SCH_3)(O_2)]^+ \cdot H_2O$ Singlet – End-on

H	4.0793020101	-4.1308704091	-2.8197881598
H	2.6973517562	-4.7391334275	-2.5452058964
O	3.2184199093	-3.9345310907	-2.4259899687
C	-1.4016669620	2.6196647235	2.1632918980
C	1.0164132576	-1.1377352745	-1.2721221124
C	1.7112424542	0.7640527316	-2.0531756587
C	2.5653123219	-0.1937717003	-2.5288032346
C	-2.0389237711	0.7731760393	-3.5655544859
C	-3.8740823845	1.9669096355	-1.8097419862
C	-2.5607211701	1.3262201176	3.5376903013
C	-2.2858183538	0.6422559039	2.3861211816
H	-1.0210371648	0.7789586960	-3.9591381996
H	0.1026939241	3.6315146213	-1.0671640342
H	1.2620869990	3.0884298879	-0.2019201547
H	-3.0915552092	1.0454798699	4.4326903372
H	-2.0124848405	3.3292365419	4.0480157046
H	3.4330794363	-0.1260023277	-3.1653814059
H	-0.8639383566	3.4667791888	1.7706597281
H	2.5243896477	-2.3191106559	-2.1891868963
H	1.7237512320	1.8272085783	-2.2281323904
H	-2.7419410386	0.9487453807	-4.3821098513
H	-2.2352974511	-0.1899779983	-3.0875656059
H	0.4333042204	-1.8835448205	-0.7516959530
H	-4.0388541056	0.9919119159	-1.3462121066
H	-4.5457356468	2.1065900877	-2.6588581098
H	-4.0524476444	2.7556632253	-1.0767563777
H	-2.5296300780	-0.3712489767	2.1086912756
N	2.1115428415	-1.3916689905	-2.0204573327
N	-1.9957881322	2.5760569180	3.3755156965
N	-1.5647061335	1.4619522573	1.5375627106

N	0.7430339235	0.1655935269	-1.2702776864
O	-1.9795467327	-0.6122626497	-0.4864714418
O	-1.7117709399	-1.5986437354	0.2652072738
O	0.2986424836	3.1156128056	-0.2730434044
S	-2.1370196843	2.1316039104	-2.3476643666
Cu	-0.8306124374	1.0196312635	-0.2897009473

31.) $[Cu(imid)_2(H_2O)(CH_3SCH_3)]^+$ – PHM

C	-1.5906585832	-0.8009199879	1.7661546935
C	0.9792032048	0.6879437474	-1.8416377684
C	3.3230752755	-0.8992488607	3.3564396243
C	2.8867096087	1.5990127217	-1.3483428242
C	-2.0188734214	0.9797214456	0.6022163314
C	1.6372905747	0.8481293202	-3.0305950656
C	-2.9535398646	-0.7126140861	1.6921064878
C	2.9087239077	-1.9641289085	0.7879193134
H	3.7908711501	-1.8410809880	3.6430522864
H	4.0688228716	-0.2261776163	2.9303035599
H	3.6404245083	-1.2595432903	0.3922565842
H	3.4008322599	-2.8785040994	1.1243145171
H	2.8741889128	-0.4428509571	4.2408359621
H	1.6584563276	2.7115968820	2.8826233404
H	0.0050143544	0.2647358798	-1.6527878455
H	0.9999220003	3.3138670348	1.6180462606
H	3.7284356006	2.0337917754	-0.8316747489
H	3.5681628845	1.6820304107	-3.3388490162
H	1.3749749756	0.6155467831	-4.0514543467
H	-0.9823400559	-1.5424390407	2.2593990042
H	-1.9353074587	1.8800879602	0.0155283769
H	-4.1093250209	0.7745096898	0.7048338967
H	-3.7467831554	-1.3294530066	2.0801333542
H	2.1875492627	-2.2056275056	0.0082645841
N	2.8420000000	1.4260000000	-2.6920000000
N	-3.2000000000	0.4230000000	0.9520000000
N	1.7680000000	1.1590000000	-0.8060000000
N	-1.0220000000	0.2600000000	1.0860000000
S	1.9630000000	-1.2200000000	2.1690000000
O	1.1060000000	2.4900000000	2.1140000000
Cu	0.9560000000	0.8250000000	1.2610000000

32.) $[Cu(imid)_2(CH_3SCH_3)(O_2)]^+$ Singlet – End-on – PHM

C	-1.6501180861	-0.7690815279	1.6785484869
C	0.7974724845	1.1316030257	-1.6680094818
C	3.5460615231	-0.3059210777	3.1503812875
C	2.8681829776	1.4153301786	-1.0947142401
C	-2.0984542877	1.1774459945	0.8330627678
C	1.5207108178	1.1105880559	-2.8272080473
C	2.7963117870	-1.8493371994	0.8952103759
C	-3.0021241109	-0.7379820873	1.4811433269
H	4.2425453658	0.1505791235	2.4437379707
H	1.9716910482	-2.2749509834	0.3197062638
H	3.2199912963	0.4397027856	3.8789951048
H	3.3934917776	-1.1954913730	0.2567557786
H	4.0228560918	-1.1349600428	3.6766640636
H	1.2334296063	0.9927179594	-3.8598298835
H	3.6268775273	1.3527335430	-3.0599547572

S23

H	3.7764470500	1.5854491440	-0.5362260009
H	-1.0482069001	-1.5602701720	2.0981582566
H	-2.0230499429	2.1854308386	0.4532845785
H	-4.1761692334	0.8596566596	0.6944343698
H	-3.7790988822	-1.4605694681	1.6726960932
H	-0.2659103071	1.0121842518	-1.5334475667
H	3.4074983692	-2.6584047062	1.2990707995
N	-3.2640000000	0.5020000000	0.9410000000
N	2.8310000000	1.2830000000	-2.4410000000
N	1.6460000000	1.3240000000	-0.5920000000
N	-1.0960000000	0.4300000000	1.2680000000
S	2.0560000000	-0.9180000000	2.2860000000
Cu	0.9690000000	0.8500000000	1.3660000000
O	0.9872862091	2.0922702882	2.9399376554
O	2.0814521098	2.5015717180	3.3848569788

Vibrational Frequencies. Imaginary frequencies attributable to numerical noise from the computation are denoted in parenthesis.

1.) $[Cu(imid)_3]^+$

(-1.37)	22.71	27.94	32.70	34.84	48.03
95.80	104.56	112.82	154.21	157.31	167.15
185.43	192.24	240.24	590.10	590.50	591.21
651.85	652.47	652.60	679.58	679.95	681.12
749.28	750.21	751.86	816.17	817.01	817.80
863.39	865.19	868.64	932.03	932.68	932.92
951.64	953.92	954.34	1088.83	1089.42	1091.32
1121.20	1122.60	1122.80	1155.39	1157.06	1159.39
1186.76	1187.52	1188.46	1291.30	1292.01	1292.92
1373.60	1375.12	1375.79	1462.31	1463.41	1463.71
1535.40	1537.21	1539.09	1586.90	1588.57	1589.68
3285.63	3287.27	3287.52	3288.87	3291.60	3292.35

2.) $[Cu(imid)_3(OH)]$

(-11.83)	16.83	30.85	38.23	53.87	57.74
61.11	71.14	85.22	94.77	114.09	140.17
149.25	160.19	177.37	193.98	219.93	301.00
429.73	500.34	518.01	535.27	642.92	644.44
645.33	669.31	676.43	679.39	686.48	709.11
723.78	724.80	790.95	795.74	843.41	871.29
900.95	909.34	924.65	941.69	942.11	944.60
994.06	999.49	1068.68	1079.12	1081.14	1095.67
1099.08	1104.26	1154.29	1157.04	1161.86	1165.55
1171.36	1172.93	1281.83	1282.08	1295.72	1366.53
1373.44	1376.36	1450.80	1451.08	1457.12	1496.16
1518.01	1520.20	1570.56	1578.20	1579.23	3077.15
3175.79	3257.07	3263.43	3282.02	3289.49	3289.98
3291.03	3301.34	3662.50	3666.96	3669.70	3828.47

3.) $[Cu(imid)_3(H_2O)]^+$

9.71	14.37	32.27	34.02	35.91	40.88
48.82	72.43	97.62	102.62	115.56	116.95
129.72	150.45	153.69	166.18	168.62	171.94
245.54	277.92	289.56	580.78	585.96	587.06
651.52	652.46	652.81	679.53	681.43	682.76
748.93	749.35	754.34	814.89	815.70	822.32
861.51	867.14	899.52	926.78	932.01	933.71
946.83	952.41	953.05	1086.68	1088.52	1090.18
1116.36	1119.10	1120.62	1155.41	1156.62	1159.91
1179.84	1185.51	1188.12	1288.92	1289.07	1290.87
1371.54	1374.06	1374.88	1459.06	1462.10	1462.18
1530.37	1533.41	1535.60	1582.43	1585.81	1587.54
1647.09	3281.99	3286.82	3287.99	3288.61	3292.51
3293.58	3307.47	3309.73	3310.09	3657.57	3658.13
3659.23	3802.46	3909.43			

4.) $[Cu(imid)_3(CH_3SCH_3)]^+$

(-3.89)	13.88	18.89	29.43	30.19	31.62
37.02	39.33	45.51	55.28	71.67	101.04
110.45	118.59	120.24	145.14	149.21	157.80
170.66	183.74	188.64	193.13	201.94	265.85
581.71	583.32	585.12	650.66	651.45	652.00
678.33	679.24	680.36	681.36	734.76	746.93
748.36	748.93	811.51	815.86	816.46	863.34
864.14	865.34	926.13	930.86	931.51	931.68
949.06	949.33	950.44	965.28	998.62	1063.17
1087.79	1088.00	1090.35	1117.43	1118.91	1120.91
1156.67	1157.19	1159.84	1182.83	1184.35	1185.19
1289.18	1290.64	1291.93	1361.40	1373.48	1375.12
1376.67	1386.22	1462.43	1462.73	1463.08	1476.68
1486.56	1491.07	1499.50	1533.23	1533.89	1535.77
1585.81	1586.17	1586.73	3054.54	3059.41	3140.07
3146.52	3158.69	3168.04	3284.10	3284.79	3288.74
3291.21	3292.34	3292.72	3308.26	3308.84	3311.80
3656.79	3657.42	3657.74			

5.) $[Cu(imid)_2(OH)]$

(-8.53)	29.88	42.25	64.53	81.25	96.42
141.73	155.82	186.38	215.55	239.52	252.41
535.40	538.89	549.86	643.83	647.17	671.14
684.98	719.53	728.32	740.82	812.96	841.43
862.66	913.95	935.70	939.33	941.10	957.02
1072.37	1083.80	1103.15	1114.09	1154.87	1160.30
1168.34	1192.90	1285.89	1288.80	1371.78	1385.51
1455.12	1463.07	1500.05	1536.21	1571.08	1592.51
3196.80	3253.76	3284.81	3291.34	3292.67	3314.22
3662.12	3678.86	3859.13			

6.) $[Cu(imid)_2(H_2O)]^+$

27.66	35.07	40.29	50.88	82.26	117.10
129.18	154.96	194.70	200.16	226.75	229.08
271.62	293.86	339.14	601.72	602.36	653.70
656.25	680.60	683.48	755.38	755.72	823.76
850.26	869.27	876.46	935.28	935.93	964.95
968.58	1089.75	1092.71	1122.42	1126.53	1157.41
1160.11	1200.26	1201.77	1291.74	1293.39	1371.93
1375.14	1466.23	1466.25	1543.56	1545.24	1591.94
1592.94	1635.18	3295.47	3298.93	3300.43	3306.33
3315.94	3318.63	3656.06	3657.93	3783.67	3900.08

7.) $[Cu(imid)_2(CH_3SCH_3)]^+$

(-8.05)	24.85	30.08	32.71	43.49	49.11
51.28	82.66	105.09	131.22	142.26	177.79
182.68	184.48	185.86	207.71	266.28	310.88
599.37	600.81	654.57	655.36	676.39	680.16
681.30	735.19	754.35	755.05	822.50	823.81
868.72	869.10	928.40	934.29	935.24	960.50
963.82	967.79	999.39	1065.37	1093.39	1093.69
1125.05	1126.38	1157.16	1159.71	1193.65	1197.43
1294.60	1295.70	1361.55	1372.49	1374.47	1386.38
1465.11	1465.40	1475.61	1485.61	1490.04	1498.72
1542.05	1542.91	1590.69	1591.96	3062.38	3065.53
3154.04	3159.36	3165.66	3166.76	3291.03	3292.13
3296.19	3297.43	3312.51	3313.81	3655.04	3655.63

8.) $[Cu(imid)_2(CH_3SCH_3)]^+ \cdot H_2O$

(-21.12) 13.61 21.10 24.35 37.11 39.25
50.69 61.77 73.81 87.21 114.78 116.24
124.57 142.61 162.83 167.34 181.20 187.21
198.90 210.76 222.04 263.37 300.47 336.51
596.20 633.42 653.50 672.90 675.74 680.74
732.08 756.07 756.68 821.65 825.31 855.24
877.34 928.02 934.79 935.47 959.25 967.96
968.62 983.32 1001.68 1064.59 1093.96 1101.61
1126.32 1128.85 1159.96 1183.33 1195.33 1217.87
1295.39 1298.21 1363.78 1374.66 1377.23 1388.49
1465.84 1473.56 1483.65 1487.60 1494.39 1496.82
1541.76 1548.46 1592.11 1596.30 1657.77 3062.33
3065.33 3153.42 3158.48 3166.14 3167.39 3285.61
3287.17 3291.98 3293.99 3306.01 3309.92 3310.21
3659.52 3811.01 3917.93

9.) $[Cu(imid)_2(H_2O)(CH_3SCH_3)]^+$

19.58 22.01 31.94 36.03 37.86 50.84
59.44 65.41 84.03 90.15 106.42 122.50
125.68 144.09 165.45 171.65 176.38 184.90
190.18 194.29 264.14 276.09 287.67 309.44
595.12 596.72 653.71 654.77 678.60 681.76
684.01 733.64 753.00 754.54 822.79 855.45
867.75 868.60 930.13 933.64 935.19 955.03
956.80 969.06 1002.92 1066.17 1088.76 1091.61
1121.99 1123.22 1157.19 1159.75 1189.19 1190.93
1291.89 1292.97 1363.32 1374.23 1374.79 1388.47
1463.07 1463.34 1474.34 1484.15 1486.74 1496.15
1533.22 1537.27 1586.52 1588.72 1649.50 3063.58
3066.57 3155.35 3160.74 3166.60 3169.00 3284.01
3286.89 3295.13 3299.24 3309.85 3310.54 3654.99
3657.36 3797.73 3904.32

10.) $[Cu(imid)_2(H_2O)(CH_3SCH_3)]^+ \cdot H_2O$

(-58.01) 7.46 24.86 27.02 30.66 34.76
45.14 54.45 55.71 70.31 72.56 79.46
84.59 100.30 110.30 114.93 126.67 144.61
160.48 168.31 175.97 184.38 188.57 192.11
210.72 264.58 287.65 295.14 299.47 307.99
592.39 634.78 653.39 675.54 678.37 680.84
732.95 754.86 756.57 824.00 850.05 857.10
870.41 930.33 934.27 935.48 951.64 956.83
965.15 967.95 1001.97 1066.49 1092.56 1097.01
1123.50 1128.54 1158.05 1181.85 1190.20 1209.79
1293.64 1296.74 1363.23 1372.85 1376.12 1388.59
1464.68 1474.59 1484.72 1487.58 1488.87 1497.09
1539.51 1543.31 1589.86 1593.76 1646.56 1651.94
3060.80 3063.81 3151.84 3157.44 3163.06 3165.04
3282.98 3284.72 3293.84 3295.81 3305.74 3308.15
3370.51 3660.46 3793.41 3818.68 3903.24 3927.36

11.) $[Cu(imid)_3(O_2)]^+$ Singlet – End-on

30.11 33.66 37.21 37.92 50.35 56.74
64.37 107.40 113.42 125.64 135.48 156.67
162.17 173.62 174.37 176.78 190.76 219.16
248.59 348.56 597.29 597.67 602.95 653.39
654.63 655.67 679.70 682.48 683.17 751.73
753.49 755.17 815.39 822.86 853.02 866.21
869.04 889.41 932.51 933.19 933.74 952.76
953.98 955.16 1087.51 1089.58 1091.92 1121.39

1122.00	1126.46	1157.35	1157.86	1160.89	1192.12
1193.20	1194.00	1289.55	1291.65	1293.75	1376.02
1376.29	1377.09	1402.79	1463.16	1463.60	1465.18
1535.09	1537.25	1539.67	1587.79	1588.33	1589.36
3285.77	3289.25	3290.54	3291.17	3291.84	3304.00
3310.20	3311.66	3311.94	3654.20	3654.44	3655.45

12.) $[Cu(imid)_3(O_2)]^+$ Singlet – Side-on

23.13	27.67	36.79	40.43	41.37	45.98
65.69	88.92	111.55	129.71	139.86	145.88
157.19	162.07	173.45	204.35	226.45	250.20
337.98	386.23	586.70	601.24	604.85	651.94
654.00	655.06	678.71	681.02	683.32	751.80
752.89	754.09	813.15	825.38	842.97	866.05
873.88	887.40	928.73	934.08	935.64	951.00
958.21	960.07	1087.84	1090.02	1091.88	1120.31
1122.52	1122.99	1154.86	1159.87	1162.94	1185.16
1200.03	1202.08	1247.68	1290.72	1294.56	1295.08
1373.84	1377.32	1379.39	1460.89	1466.05	1466.12
1535.51	1540.90	1544.80	1587.75	1590.40	1592.35
3283.62	3290.09	3290.77	3295.00	3298.36	3299.17
3310.18	3313.20	3316.65	3653.99	3654.62	3658.29

13.) $[Cu(imid)_3(OH)(O_2)]$ Singlet – End-on

20.39	25.37	60.41	66.15	75.12	77.36
96.35	102.31	104.91	121.12	126.03	144.34
154.24	168.11	169.25	177.79	189.93	206.97
209.85	224.08	250.29	384.84	391.80	448.45
533.25	541.79	543.86	645.73	646.59	647.63
676.24	678.16	683.56	723.97	724.93	725.71
741.25	863.66	878.20	891.77	898.82	904.16
919.71	924.86	926.71	932.39	945.70	947.27
947.44	1059.26	1073.22	1075.98	1095.18	1095.93
1098.55	1144.99	1157.74	1162.15	1184.90	1187.26
1189.36	1208.88	1264.52	1285.71	1290.75	1382.93
1383.85	1387.57	1455.58	1456.56	1458.24	1511.96
1521.08	1523.68	1580.92	1582.67	1583.53	3239.74
3247.53	3258.25	3279.16	3281.23	3283.22	3298.58
3300.04	3303.00	3670.62	3671.98	3672.59	3808.27

14.) $[Cu(imid)_3(OH)(O_2)]$ Triplet – End-on

20.45	23.28	60.62	62.32	66.52	73.87
80.15	91.91	104.18	113.38	119.79	124.72
127.49	150.95	162.28	168.85	178.58	190.86
195.45	221.89	225.03	352.48	401.57	434.37
526.53	537.88	539.83	646.69	647.02	648.98
676.99	679.32	685.18	724.47	726.23	729.78
741.15	831.73	854.92	879.63	916.80	920.20
921.74	922.90	924.75	928.06	945.34	946.69
947.46	1059.41	1072.47	1074.95	1094.52	1097.00
1099.75	1147.48	1153.07	1156.56	1181.87	1182.51
1183.73	1229.18	1268.01	1275.39	1278.54	1377.26
1378.22	1384.54	1455.10	1455.34	1456.98	1510.48
1520.97	1522.82	1579.47	1581.89	1582.92	3249.60
3270.26	3276.38	3280.58	3284.78	3288.63	3296.56
3299.33	3299.71	3669.44	3670.76	3671.88	3816.39

15.) $[Cu(imid)_3(H_2O)(O_2)]^+$ Singlet – End-on

27.64	35.59	38.12	44.87	53.58	58.18
75.90	92.79	104.62	125.58	132.40	135.39
157.56	160.07	170.14	176.12	189.01	200.67
205.09	229.40	241.68	264.07	354.08	384.82
441.16	591.80	597.25	598.77	651.14	653.34
657.83	676.76	680.70	686.58	717.52	749.20
751.27	761.22	819.73	823.07	839.74	865.41
879.74	908.92	928.80	932.32	933.79	949.60
951.77	956.34	1085.67	1086.48	1089.38	1119.85
1122.85	1123.14	1153.58	1157.40	1160.53	1186.05
1194.50	1196.92	1287.50	1288.76	1289.14	1307.31
1370.74	1375.62	1377.84	1460.02	1466.31	1468.18
1533.18	1537.85	1540.58	1584.23	1590.10	1592.70
1663.94	3284.08	3294.50	3296.28	3299.49	3302.58
3303.92	3312.04	3315.13	3322.45	3585.04	3652.86
3654.21	3660.07	3861.56			

16.) $[Cu(imid)_3(H_2O)(O_2)]^+$ Triplet – End-on

(-76.22)	13.03	22.78	32.76	37.16	40.03
44.66	45.79	50.72	54.82	60.97	78.19
106.61	110.91	119.57	124.23	125.67	140.11
156.06	159.41	165.00	181.30	190.92	260.89
275.02	303.16	586.52	589.19	590.74	651.85
653.34	654.90	681.11	682.51	686.35	750.06
751.16	758.22	819.73	826.39	830.20	864.02
872.39	895.28	924.76	932.15	934.84	945.58
952.70	955.15	1086.37	1088.64	1091.06	1116.16
1122.33	1122.84	1153.66	1157.52	1159.69	1179.03
1187.21	1191.96	1289.58	1289.83	1293.32	1369.16
1374.44	1377.56	1459.76	1463.23	1463.83	1526.25
1533.84	1536.26	1539.98	1579.92	1588.54	1588.98
1639.44	3284.36	3285.77	3286.01	3289.69	3293.59
3298.16	3305.58	3309.36	3311.34	3654.21	3656.05
3661.34	3802.32	3913.54			

17.) $[Cu(imid)_3(CH_3SCH_3)(O_2)]^+$ Singlet – End-on

7.33	21.92	28.61	34.73	39.75	50.86
59.50	61.26	70.14	78.92	85.14	105.46
109.81	116.66	127.17	142.12	145.92	152.91
157.83	163.05	169.50	175.10	185.03	195.60
201.84	210.25	218.74	272.77	314.22	588.86
590.65	592.31	652.27	653.20	653.26	677.56
680.26	681.72	682.50	734.35	747.99	749.56
751.34	816.88	830.78	843.94	861.08	862.47
871.62	931.78	932.56	933.10	933.69	948.84
950.00	951.19	966.31	1000.53	1067.02	1085.69
1087.05	1089.86	1119.23	1120.39	1123.46	1156.37
1158.10	1162.19	1186.37	1188.56	1189.94	1288.45
1288.85	1295.93	1360.49	1372.72	1376.98	1377.91
1379.07	1388.92	1462.72	1464.43	1465.30	1477.70
1487.15	1489.22	1497.43	1532.45	1534.26	1539.41
1584.96	1587.66	1588.48	3062.97	3065.83	3152.46
3157.43	3169.38	3174.91	3284.74	3285.68	3291.25
3294.73	3297.47	3304.83	3309.30	3310.15	3310.54
3656.46	3657.86	3658.96			

18.) $[Cu(imid)_2(OH)(O_2)]$ Singlet – End-on

25.94	40.10	44.78	70.87	78.62	96.36
112.61	138.58	149.60	172.73	179.47	194.29
204.32	244.59	247.11	388.03	394.83	549.60
550.16	562.28	647.01	648.63	679.16	682.05
728.14	740.07	820.61	854.00	858.30	899.05
924.40	926.62	942.95	943.77	958.29	1077.11
1087.07	1110.86	1118.77	1157.93	1166.81	1178.62
1191.45	1267.36	1285.25	1295.11	1378.22	1380.08
1461.91	1462.37	1514.80	1533.55	1580.39	1590.44
3240.53	3250.68	3265.84	3295.32	3296.99	3301.47
3672.11	3673.10	3841.15			

19.) $[Cu(imid)_2(OH)(O_2)]$ Singlet – Side-on

23.98	34.48	49.77	60.07	62.16	99.05
109.16	132.28	144.14	160.42	188.10	205.82
212.39	229.75	287.93	405.90	455.39	536.09
559.49	570.03	645.64	646.96	679.62	683.65
728.39	731.94	858.89	859.56	862.77	872.92
903.12	923.16	935.31	946.43	951.76	1069.19
1073.09	1100.39	1111.38	1137.75	1149.73	1156.55
1187.74	1197.69	1274.88	1281.07	1388.83	1390.10
1453.13	1463.15	1517.71	1524.99	1579.04	1588.50
3263.28	3273.20	3278.03	3283.34	3295.85	3303.40
3672.97	3675.70	3835.55			

20.) $[Cu(imid)_2(OH)(O_2)]$ Triplet – Side-on

9.95	36.76	46.29	51.76	58.91	80.90
100.72	109.18	127.70	147.99	169.32	178.46
198.27	216.95	230.13	303.84	327.41	523.66
549.21	560.52	646.47	647.84	678.04	683.46
724.78	735.88	804.43	813.93	848.90	896.57
921.63	924.95	931.02	943.52	950.32	1070.72
1084.18	1105.74	1113.61	1153.97	1159.70	1178.45
1189.03	1271.43	1281.48	1291.13	1378.65	1379.96

1458.99 1461.40 1509.44 1533.05 1578.02 1588.35
3231.57 3269.90 3289.94 3290.80 3297.41 3309.02
3669.78 3671.73 3849.54

21.) $[Cu(imid)_2(OH)(O_2)]$ Triplet – End-on

11.22 33.53 49.06 54.48 59.70 102.88
111.48 114.22 142.66 149.00 183.45 190.20
201.14 209.64 230.50 234.14 331.14 494.84
544.11 556.63 646.67 648.71 677.19 682.67
726.63 734.84 774.38 823.94 857.28 916.90
923.05 930.91 935.19 945.97 949.43 1065.39
1076.39 1097.39 1104.95 1150.92 1156.49 1186.96
1189.04 1245.25 1275.54 1278.00 1376.64 1386.51
1458.21 1459.20 1514.96 1529.16 1581.32 1584.56
3245.78 3273.12 3281.75 3287.57 3300.51 3302.64
3666.99 3672.31 3824.77

22.) $[Cu(imid)_2(H_2O)(O_2)]^+$ Singlet – Side-on

30.61 36.60 44.98 59.52 74.74 93.23
125.83 135.56 162.18 178.98 184.33 201.74
221.26 235.28 263.25 270.85 395.78 414.63
441.36 534.21 608.71 613.51 654.21 656.11
680.11 684.75 756.21 757.26 826.37 862.77
872.13 878.94 933.30 935.13 964.07 965.49
1089.27 1091.47 1127.35 1129.15 1156.29 1159.49
1203.22 1204.25 1210.69 1295.41 1296.51 1377.42
1377.70 1466.35 1467.03 1543.11 1547.91 1593.61
1596.16 1643.49 3291.47 3296.72 3300.71 3301.81
3314.46 3316.22 3652.23 3652.92 3758.06 3877.91

23.) $[Cu(imid)_2(H_2O)(O_2)]^+$ Singlet – End-on

30.61 36.60 44.98 59.52 74.74 93.23
125.83 135.56 162.18 178.98 184.33 201.74
221.26 235.28 263.25 270.85 395.78 414.63
441.36 534.21 608.71 613.51 654.21 656.11
680.11 684.75 756.21 757.26 826.37 862.77
872.13 878.94 933.30 935.13 964.07 965.49
1089.27 1091.47 1127.35 1129.15 1156.29 1159.49
1203.22 1204.25 1210.69 1295.41 1296.51 1377.42
1377.70 1466.35 1467.03 1543.11 1547.91 1593.61
1596.16 1643.49 3291.47 3296.72 3300.71 3301.81
3314.46 3316.22 3652.23 3652.92 3758.06 3877.91

24.) $[Cu(imid)_2(O_2)]^+$ Singlet – End-on

12.40 36.58 52.75 56.41 114.63 125.65
133.05 137.69 169.27 200.15 205.24 240.90
272.31 351.64 610.39 614.85 654.35 658.38
681.81 685.57 756.87 760.69 822.79 864.71
878.75 889.43 934.94 937.02 966.14 972.43
1095.94 1099.61 1130.90 1131.28 1159.21 1163.62
1209.49 1212.67 1296.45 1307.40 1370.15 1372.77
1453.17 1470.83 1472.77 1551.27 1553.43 1596.25
1597.44 3276.11 3292.79 3296.70 3301.75 3314.12
3319.83 3652.48 3652.90

25.) $[Cu(imid)_2(CH_3SCH_3)(O_2)]^+$ Singlet – Side-on

(-19.83)	22.20	38.03	46.73	50.22	57.96
70.73	91.37	99.30	103.40	126.60	127.49
144.01	160.75	170.68	182.73	184.36	190.08
211.47	227.50	267.97	274.63	342.62	603.29
608.38	655.29	656.57	674.60	680.56	683.11
728.69	754.30	759.55	829.02	843.37	874.06
883.00	927.44	935.00	935.65	959.61	965.82
968.31	1000.45	1062.70	1091.83	1093.33	1125.08
1131.40	1156.48	1162.27	1199.04	1202.55	1294.40
1298.80	1364.38	1373.34	1373.51	1387.86	1408.01
1468.41	1468.99	1471.68	1482.93	1486.30	1495.84
1543.30	1546.15	1594.21	1594.54	3063.42	3068.36
3152.50	3159.22	3170.13	3176.72	3295.99	3297.15
3304.62	3306.40	3314.45	3315.82	3654.20	3654.90

26.) $[Cu(imid)_2(CH_3SCH_3)(O_2)]^+$ Singlet – End-on

23.46	34.11	36.03	37.59	51.22	54.84
66.58	90.05	108.11	119.62	134.50	145.93
150.29	158.62	174.85	178.38	186.67	192.34
233.87	257.69	272.02	313.45	356.59	600.67
602.39	653.96	655.47	670.08	678.68	686.02
723.17	753.55	757.42	820.15	847.62	861.77
885.81	932.45	934.33	942.45	950.71	959.54
980.90	1013.52	1073.42	1088.77	1091.53	1121.20
1126.08	1156.34	1160.11	1190.88	1195.31	1240.51
1291.61	1294.85	1364.34	1373.34	1375.78	1388.24
1462.42	1464.48	1471.57	1477.41	1483.40	1489.90
1534.08	1543.16	1583.74	1593.42	3073.55	3076.41
3175.57	3178.10	3182.61	3185.25	3278.85	3287.46
3295.08	3297.23	3309.17	3313.65	3654.46	3654.83

27.) $[Cu(imid)_2(CH_3SCH_3)(O_2)]^+ \cdot H_2O$ Singlet – End-on

(-33.65)	20.52	23.80	31.88	34.20	37.40
45.30	63.17	72.78	83.85	98.57	103.25
110.40	123.54	125.11	134.25	143.21	158.90
171.38	176.09	182.04	185.59	200.83	216.72
225.16	270.22	285.47	323.50	342.08	603.73
633.63	653.63	671.19	676.54	680.39	728.92
754.79	761.93	816.68	853.00	866.46	886.62
929.07	934.03	936.14	961.40	966.30	967.53
981.57	1000.32	1064.60	1091.77	1103.04	1126.40
1135.94	1161.45	1181.12	1200.35	1220.24	1294.40
1297.40	1363.60	1375.47	1379.11	1388.12	1415.36
1469.82	1474.62	1485.78	1486.49	1490.03	1496.77
1545.18	1549.45	1594.24	1596.97	1654.09	3058.81
3063.21	3146.42	3153.12	3167.43	3170.53	3285.29
3288.76	3290.91	3303.28	3307.16	3311.84	3319.18
3659.60	3817.45	3924.03			

28.) $[Cu(imid)_2(CH_3SCH_3)(O_2)]^+ \cdot H_2O$ Singlet – Side-on

8.69	24.63	28.16	32.76	40.48	41.47
54.01	73.11	84.90	92.38	99.84	104.83
126.27	137.49	139.65	158.65	168.47	174.94
186.03	196.04	200.45	216.18	226.26	241.11
266.70	271.76	349.52	398.31	419.73	606.42

634.76	653.47	667.93	675.73	680.14	728.85
753.04	758.75	840.63	841.35	862.46	867.83
933.45	934.48	935.91	962.07	971.07	976.62
1001.06	1009.93	1069.83	1092.24	1101.57	1125.52
1129.32	1162.22	1185.96	1205.90	1208.40	1226.73
1296.68	1304.64	1361.71	1378.25	1381.03	1386.99
1468.27	1477.66	1487.48	1488.03	1494.40	1498.57
1545.15	1554.34	1592.97	1596.92	1657.62	3063.37
3066.49	3160.01	3162.89	3164.51	3167.49	3279.90
3289.18	3294.87	3295.25	3296.53	3309.57	3314.02
3655.29	3808.27	3915.71			

29.) $[Cu(imid)_2(H_2O)(CH_3SCH_3)(O_2)]^+$ Singlet – End-on

(-35.89)	31.38	34.02	41.93	53.64	57.60
69.79	79.11	91.70	106.15	123.41	125.65
127.79	140.04	143.30	162.81	167.99	177.65
182.02	188.60	191.28	209.07	235.87	264.58
281.07	292.00	317.42	369.60	491.16	599.02
608.17	654.18	657.06	679.98	681.61	687.20
736.63	754.30	759.25	846.70	858.74	902.19
904.54	931.44	933.18	936.97	953.70	959.71
969.54	1001.67	1067.84	1088.87	1092.98	1119.86
1132.98	1158.82	1164.27	1196.52	1199.29	1295.18
1304.06	1362.63	1366.41	1370.96	1381.65	1388.38
1465.81	1468.15	1473.47	1484.05	1486.39	1495.60
1539.10	1541.83	1588.15	1594.38	1613.76	3063.78
3067.06	3156.26	3161.32	3168.15	3171.11	3263.43
3290.00	3292.81	3303.53	3312.62	3312.72	3652.14
3659.03	3752.54	3885.41			

30.) $[Cu(imid)_2(H_2O)(CH_3SCH_3)(O_2)]^+ \cdot H_2O$ Singlet – End-on

(-28.97)	(-14.39)	27.80	37.86	40.59	44.63
51.58	64.78	74.27	80.03	89.13	100.39
102.19	117.23	123.54	127.82	138.08	145.40
150.46	166.46	173.33	178.08	185.91	194.08
196.38	211.28	219.64	227.54	257.01	268.92
270.04	349.36	358.96	361.02	398.14	595.27
636.06	652.84	673.56	677.62	680.59	731.64
754.66	757.28	838.41	849.42	865.15	895.87
897.92	933.50	936.41	937.81	956.37	960.39
975.55	1005.81	1071.86	1090.36	1097.05	1124.67
1127.87	1161.23	1187.80	1197.92	1223.41	1293.54
1306.51	1346.96	1364.37	1371.22	1380.17	1388.96
1466.25	1474.19	1483.47	1485.03	1494.57	1503.38
1538.20	1540.76	1591.02	1606.56	1629.41	1663.61
3061.08	3064.95	3155.79	3162.16	3167.10	3168.19
3278.44	3288.77	3290.50	3308.32	3310.80	3315.67
3327.59	3661.44	3791.29	3801.44	3904.15	3904.53