Electronic Supplementary Material for PCCP

Dissociations of Copper(II)-Containing Complexes of Aromatic Amino Acids: Radical Cations of Tryptophan, Tyrosine, and Phenylalanine

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Figure S1. CID spectra of $[Cu^{II}(4Cl\text{-}tpy)(Phe)]^{\bullet 2+}$ and $[Cu^{II}(4Cl\text{-}tpy)(^{15}N\text{-}Phe)]^{\bullet 2+}$

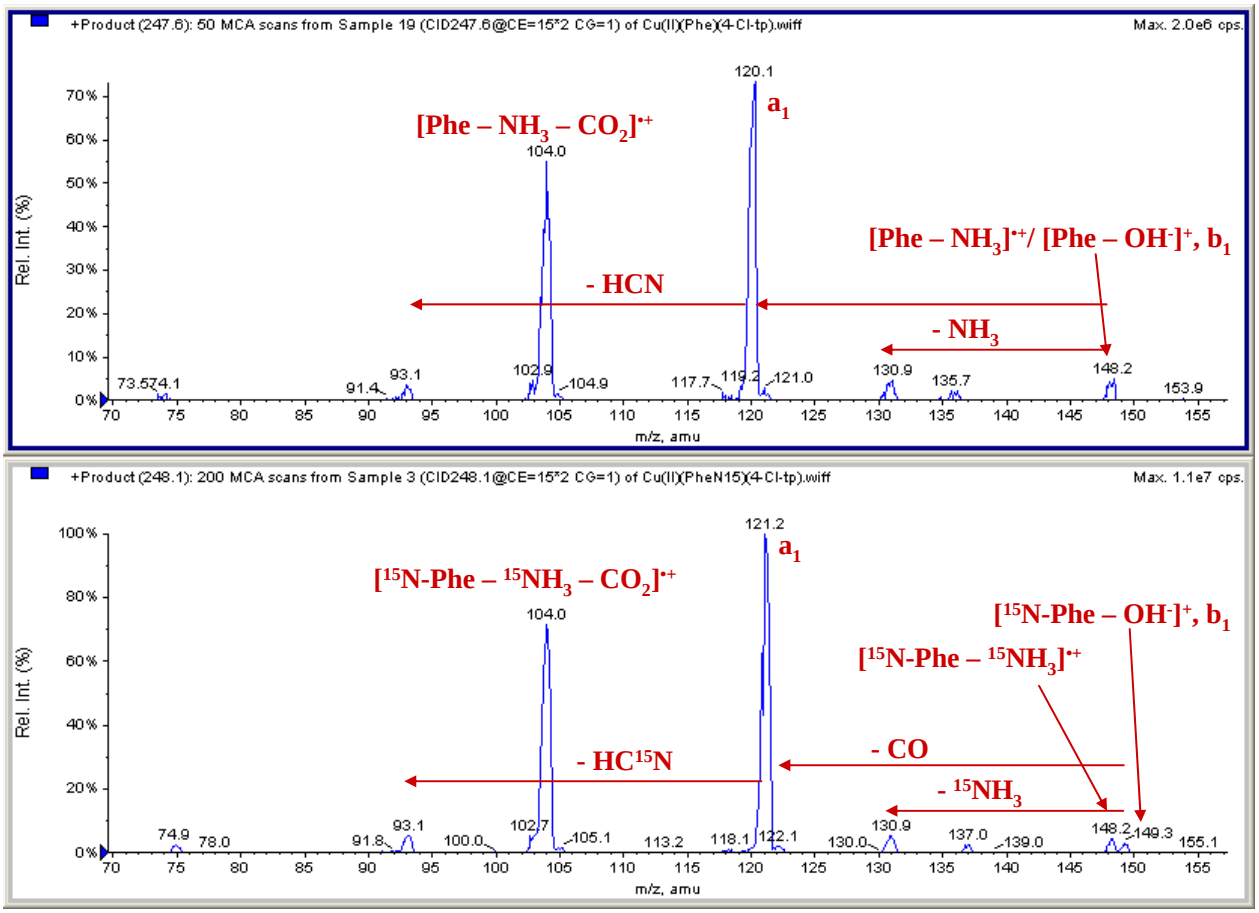

Figure S2. Potential-energy scan for (a) $[Cu^{II}(tpy)(Trp)]^{\bullet 2+}$ and (b) $[Cu^{II}(tpy)(Phe)]^{\bullet 2+}$ at the UB3LYP/6-31++G(d,p) level.

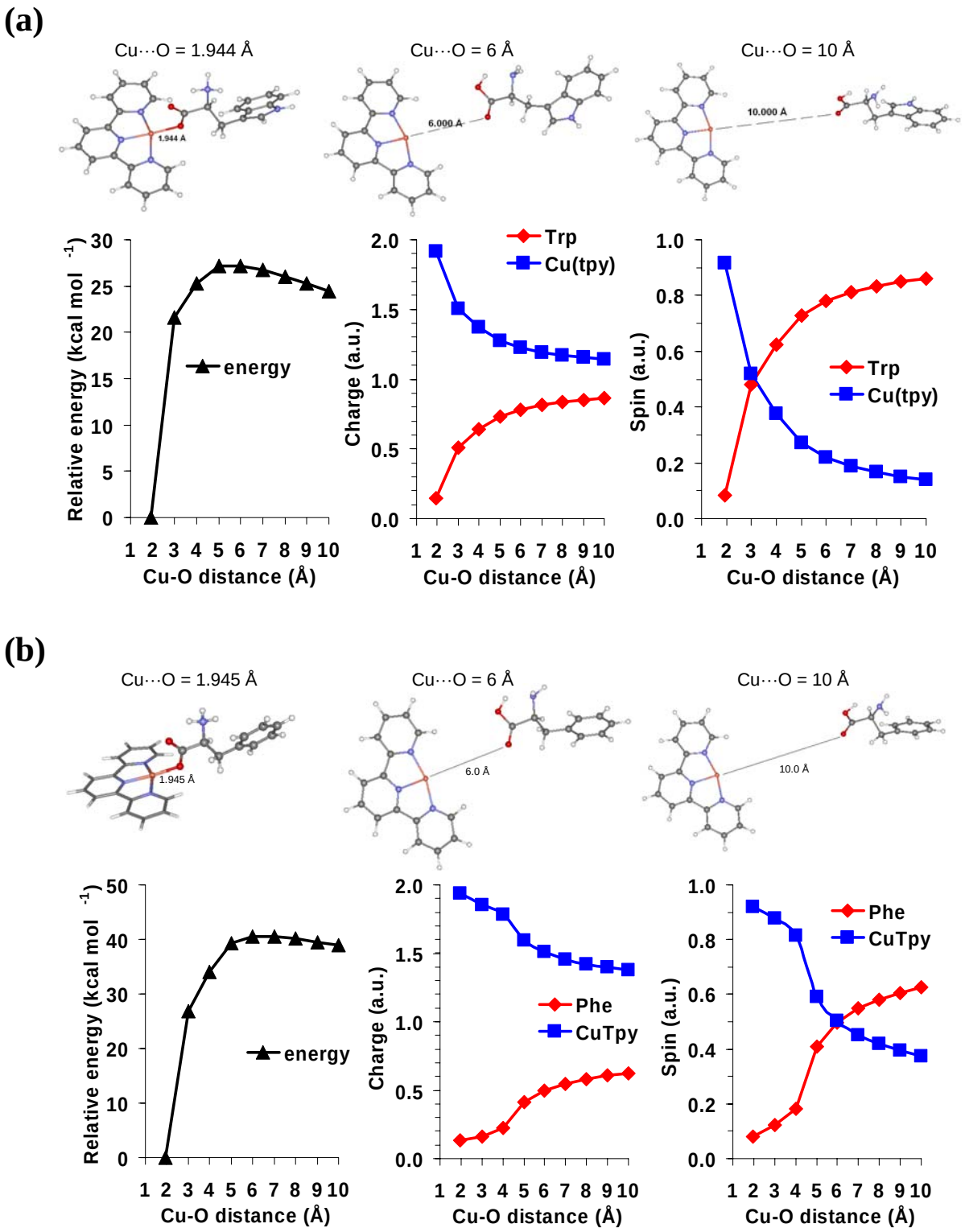

Figure S3. Possible reactions of the tyrosine radical cation. The relative energy $\Delta H°_0$ are evaluated at the UB3LYP/6-31++G(d,p) level and are in kcal mol^{-1}.

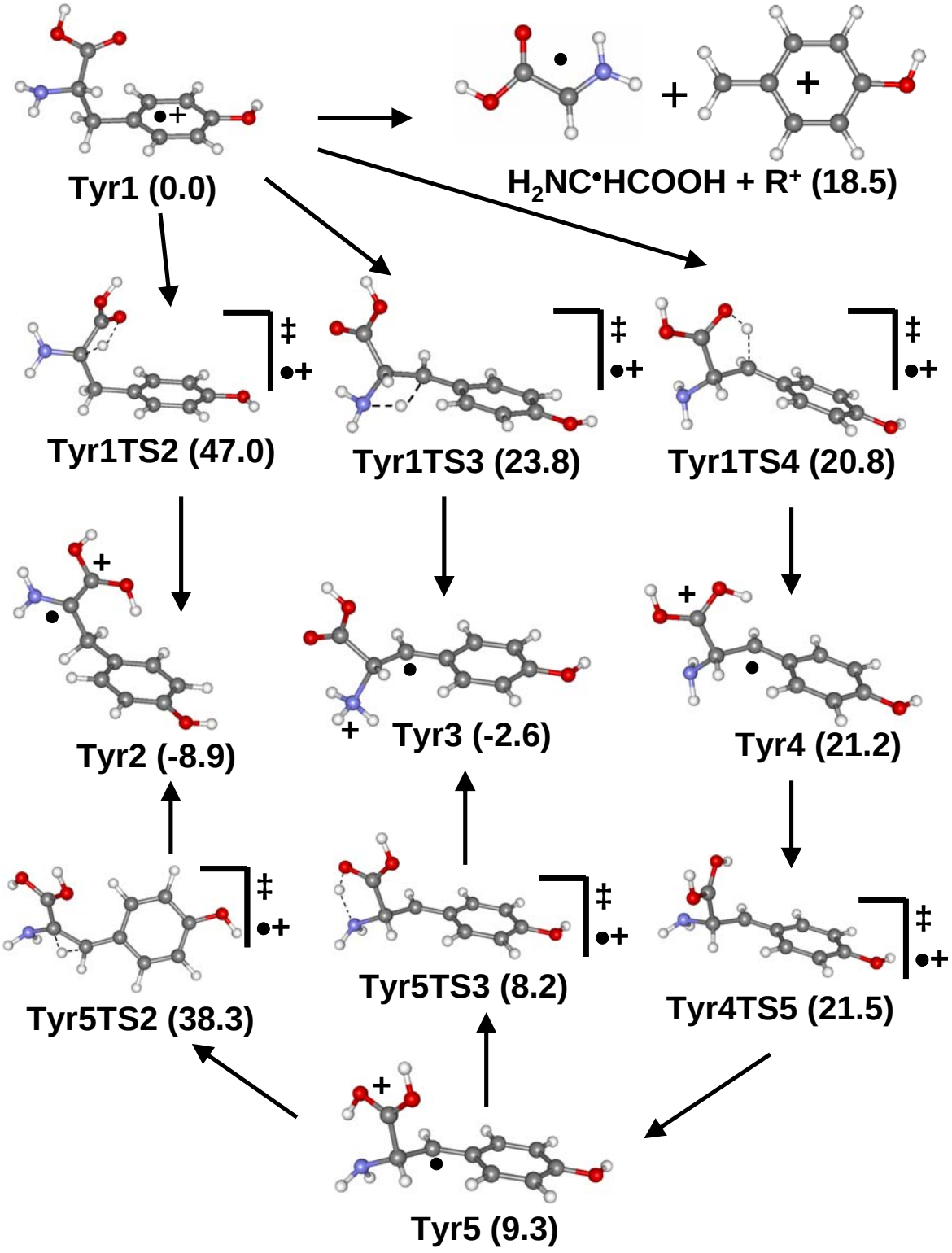

Figure S4. Possible reactions of the phenylalanine radical cation. The relative energy $\Delta H°_0$ are evaluated at the UB3LYP/6-31++G(d,p) level and are in kcal mol^{-1}.

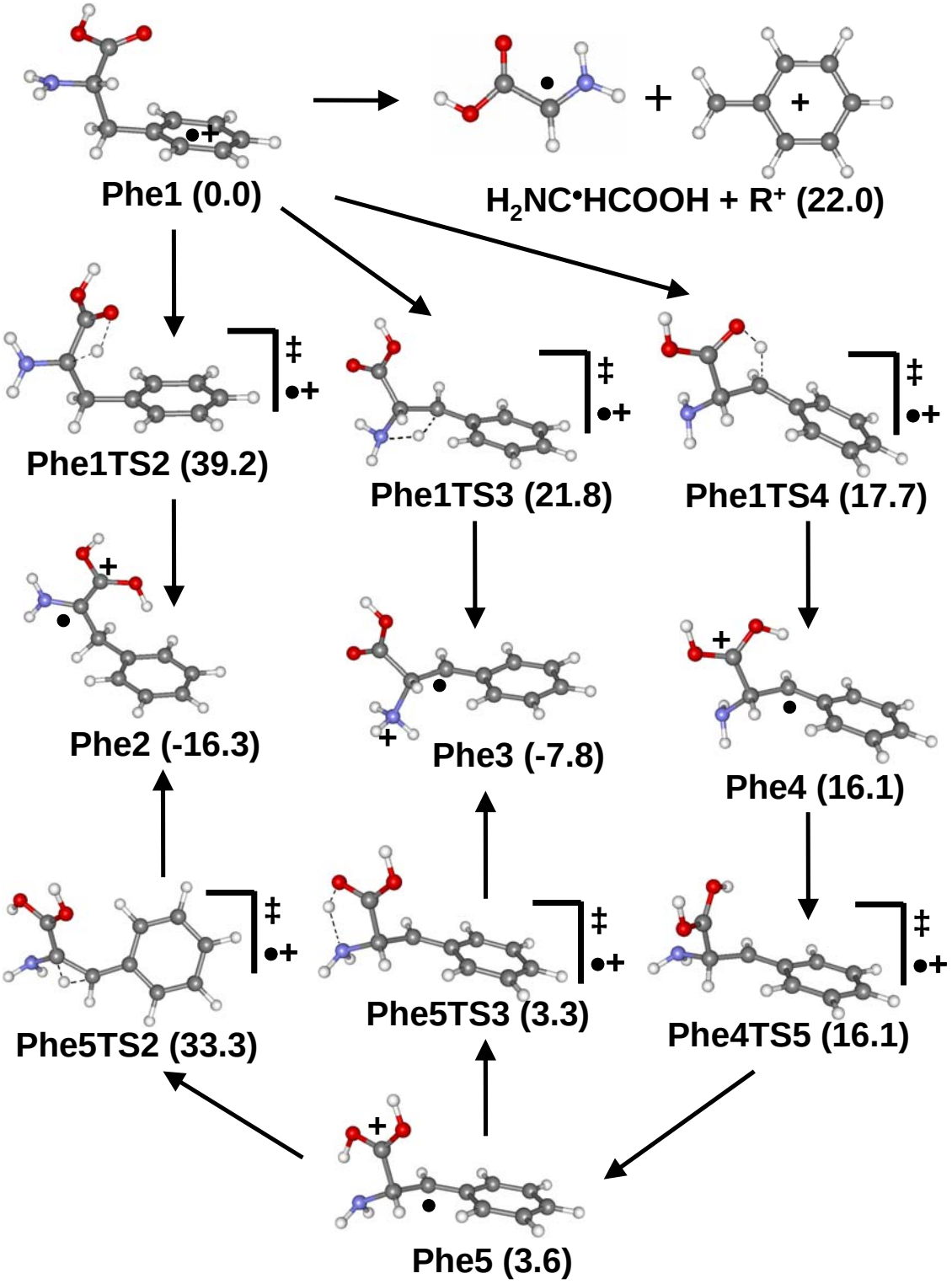

Table S1. Cartesian coordinates of the geometries optimized at the UB3LYP/6-31++G(d,p) level.

Column 1 Atomic Symbol	Column 2 X-coordinate	Column 3 Y-coordinate	Column 4 Z-coordinate	Column 5 NPA charge	Column 6 NPA spin
Optimized geometries for glycine as shown in Table 2					
	8				
NH=CH-COOH	E=-283.226040162	H0=-283.169737	H298=-283.164099	G298=-283.197378	
H	1.54118	-0.48904	0.00000	0.52761	
H	-0.67163	-2.63304	0.00000	0.38896	
H	-1.84628	-0.62581	0.00000	0.22082	
C	-0.75621	-0.71582	0.00000	0.01856	
C	0.00000	0.59544	0.00000	0.73906	
N	-0.08500	-1.79595	0.00000	-0.64185	
O	1.33442	0.46817	0.00000	-0.69829	
O	-0.57080	1.66206	0.00000	-0.55486	
	9				
Gly+	E=-283.561091106	H0=-283.491536	H298=-283.485630	G298=-283.519521	
H	-2.42971	-0.22174	0.00006	0.56113	
H	1.75502	1.03061	-0.00001	0.48689	
H	2.75684	-0.42046	0.00003	0.48341	
H	0.78146	-1.77065	0.00002	0.29025	
C	0.75154	-0.68215	0.00000	0.20656	
C	-0.55285	0.10842	-0.00005	0.73400	
N	1.82943	0.00456	0.00001	-0.59949	
O	-1.58532	-0.71456	0.00001	-0.65229	
O	-0.52240	1.31365	0.00002	-0.51047	
	9				
Gly•	E=-283.824840469	H0=-283.758260	H298=-283.751766	G298=-283.787098	
H	2.37956	-0.09890	0.00025	0.51476	-0.00188
H	-1.84066	1.02081	0.04582	0.43791	-0.00626
H	-2.76845	-0.44274	0.14180	0.42158	-0.00536
H	-0.73481	-1.75614	0.00763	0.23261	-0.01597
C	-0.71603	-0.67514	0.00673	-0.10475	0.52351
C	0.50171	0.07432	0.00200	0.67349	0.05357
N	-1.88899	0.01299	-0.03850	-0.78628	0.26352
O	1.62443	-0.70865	-0.00192	-0.72827	0.03468
O	0.55973	1.30752	0.00463	-0.66105	0.15421
Optimized geometries for phenylalanine as shown in Table 2 and Figure 5c					
	23				
Phe1	E=-554.541143971	H0=-554.353658	H298=-554.341028	G298=-554.393145	
H	-0.91293	0.50613	1.81491	0.27063	0.00176
H	-0.55389	2.07863	1.04324	0.27762	0.00716
H	-2.79217	-2.28425	0.04948	0.54450	0.00060
H	-3.53685	0.87213	0.74558	0.44492	-0.00837
H	-3.16739	2.26003	-0.21827	0.44210	-0.00862
H	1.26469	2.27635	-0.66955	0.25304	-0.00238
H	3.52003	1.48907	-1.31701	0.26862	0.00053
H	4.33063	-0.72963	-0.53356	0.26422	-0.00624
H	2.90302	-2.15231	0.92464	0.26850	0.00056
H	0.63931	-1.38194	1.56502	0.25463	-0.00233
H	-1.29866	1.21268	-1.17043	0.28949	0.00338
C	1.62123	1.30655	-0.33328	-0.18225	0.07796
C	2.88280	0.87067	-0.69387	-0.21481	-0.02321
C	3.34317	-0.38383	-0.24374	-0.09928	0.22324
C	2.53298	-1.19379	0.57673	-0.21245	-0.02216
C	1.26769	-0.76215	0.93233	-0.17445	0.07577
C	0.79120	0.50579	0.50120	0.01799	0.14127
C	-0.53660	0.99489	0.91397	-0.44609	0.06349
C	-1.69975	0.75166	-0.26727	-0.14350	0.04611
C	-1.79063	-0.76120	-0.50142	0.80353	0.00771
N	-2.92678	1.32221	0.07391	-0.69210	0.35130
O	-2.75945	-1.32776	0.23376	-0.71012	0.00480
O	-1.03816	-1.34398	-1.24119	-0.52475	0.06767
	23				
Phe2	E=-554.568977897	H0=-554.379670	H298=-554.367664	G298=-554.417707	
H	0.61803	-1.06890	1.94276	0.28581	0.01331
H	0.56179	-2.28657	0.68166	0.27656	0.00382
H	2.95092	2.19295	-0.76471	0.55588	-0.00215
H	0.04134	1.30150	0.34948	0.55318	-0.00186
H	3.64794	-0.97498	-0.48266	0.45886	-0.00732
H	2.78489	-2.35447	0.11262	0.45031	-0.00797
H	-1.28891	0.30195	2.26525	0.25654	0.00003

H	-3.44502	1.22605	1.47496	0.26248	-0.00006
H	-4.32441	0.76961	-0.84218	0.26208	-0.00004
H	-2.83088	-0.61425	-2.36666	0.26067	0.00002
H	-0.66638	-1.52213	-1.59664	0.24762	-0.00005
C	-1.60678	0.12512	1.23999	-0.27342	-0.00108
C	-2.83360	0.63793	0.79810	-0.20599	0.00305
C	-3.27162	0.37782	-0.50107	-0.20516	0.00113
C	-2.48623	-0.40003	-1.35997	-0.20259	0.00041
C	-1.26272	-0.90955	-0.92476	-0.22475	0.00099
C	-0.80912	-0.64946	0.37981	-0.11446	0.00484
C	0.52547	-1.20510	0.85670	-0.50174	-0.01016
C	1.73999	-0.58887	0.19855	0.16591	0.25822
C	1.84384	0.79268	-0.08686	0.70984	0.26926
N	2.79993	-1.36267	-0.08572	-0.69912	0.29150
O	0.91383	1.69866	0.10994	-0.65128	0.10241
O	2.98814	1.23693	-0.58203	-0.66724	0.08170

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Phe3	E=-554.555982645	H0=-554.366127	H298=-554.353790	H298=-554.405827	
H	2.71172	1.15714	-1.46625	0.48768	-0.00114
H	2.37290	2.39248	-0.41074	0.46869	0.00483
H	3.36569	-1.70009	1.49468	0.54510	-0.00024
H	1.20161	1.91876	-1.50366	0.47583	-0.00081
H	0.63258	-1.05272	-1.26928	0.24853	-0.01659
H	-1.60671	-1.70648	-1.63100	0.24843	-0.00623
H	-4.02476	-1.52894	-1.17235	0.26179	0.00267
H	-4.86444	0.12299	0.49221	0.25850	-0.00746
H	-3.26351	1.59478	1.69849	0.25902	0.00244
H	-0.86369	1.44026	1.27186	0.22551	-0.00599
H	1.15447	0.98836	0.99275	0.28849	0.00260
C	1.45170	0.48296	0.07297	-0.19229	-0.00463
C	0.34547	-0.29571	-0.54367	-0.21889	0.58587
C	2.70058	-0.37695	0.31420	0.80614	0.01114
C	-1.02691	-0.14665	-0.23144	-0.10071	-0.08875
C	-1.53613	0.79000	0.71999	-0.21154	0.19536
C	-2.89631	0.88000	0.96902	-0.22010	-0.08766
C	-3.80118	0.04797	0.28907	-0.16835	0.24992
C	-3.32719	-0.88296	-0.64914	-0.22332	-0.09567
C	-1.97051	-0.98241	-0.90768	-0.17578	0.20374
N	1.96087	1.59024	-0.90023	-0.79662	0.04547
O	3.65155	-0.34552	-0.44183	-0.59649	0.00632
O	2.57606	-1.13643	1.39246	-0.66961	0.00479

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Phe4	E=-554.515737225	H0=-554.328050	H298=-554.315742	G298=-554.367235	
H	1.18678	-1.01201	-1.40480	0.55818	0.01232
H	0.48987	1.33966	-1.30168	0.24631	-0.01513
H	4.23286	-1.28280	-0.25909	0.55766	0.00105
H	2.29461	2.36386	0.16056	0.40967	-0.00152
H	1.80856	2.05791	1.70784	0.42303	-0.00124
H	-1.79182	1.34267	-1.90435	0.24709	-0.00633
H	-4.14480	0.72348	-1.49981	0.26189	0.00271
H	-4.74775	-0.69138	0.46025	0.25874	-0.00765
H	-2.97370	-1.48106	2.01445	0.25984	0.00248
H	-0.63413	-0.89233	1.63877	0.22775	-0.00607
H	1.22213	-0.09007	1.34268	0.30080	0.00150
C	-2.05016	0.72050	-1.05208	-0.18075	0.20709
C	-3.37100	0.37410	-0.82386	-0.22292	-0.09712
C	-3.71188	-0.42222	0.28163	-0.16810	0.25652
C	-2.70908	-0.86806	1.15881	-0.21867	-0.08887
C	-1.38312	-0.53025	0.94049	-0.21191	0.19868
C	-1.00730	0.28050	-0.17560	-0.09834	-0.08508
C	0.32899	0.65606	-0.46776	-0.29292	0.57136
C	1.52379	0.46484	0.44096	-0.20369	-0.01838
C	2.50622	-0.50418	-0.21188	0.91289	0.01225
N	2.23319	1.65075	0.88188	-0.86755	0.04475
O	3.70804	-0.60584	0.21586	-0.58052	0.00024
O	2.12524	-1.26427	-1.17489	-0.61849	0.01641

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Phe5	E=-554.535230099	H0=-554.347427	H298=-554.335439	G298=-554.386033	
H	-2.33975	2.22466	-1.30875	0.55749	0.00042
H	-0.64951	-1.61875	-0.81730	0.24291	-0.01595
H	-3.48162	-0.71267	-0.24758	0.54597	-0.00069
H	-2.97794	-1.18993	1.91802	0.43988	0.00032
H	-2.16259	-2.25572	0.96018	0.44215	-0.00030
H	1.59651	-1.83038	-1.53046	0.24692	-0.00588

H	3.97235	-1.16828	-1.45006	0.26116	0.00254
H	0.74582	0.64338	0.08957	0.25813	-0.00695
H	3.05882	1.79362	1.54516	0.25902	0.00232
H	0.69589	1.16609	1.48360	0.23097	-0.00566
H	-1.22573	0.29273	1.55164	0.28715	0.01101
C	1.91704	-1.03823	-0.85985	-0.17164	0.19194
C	3.25020	-0.66744	-0.81343	-0.22665	-0.09059
C	3.66848	0.35388	0.05450	-0.16696	0.23244
C	2.73332	1.00266	0.87712	-0.22237	-0.08270
C	1.39592	0.64136	0.84119	-0.19874	0.18492
C	0.94500	-0.39884	-0.02749	-0.11167	-0.08953
C	-0.39176	-0.84643	-0.09509	-0.18269	0.56699
C	-1.55141	-0.28470	0.68153	-0.19127	-0.02605
C	-2.28675	0.62425	-0.29143	0.85769	0.07511
N	-2.55847	-1.31940	0.99949	-0.91347	0.01825
O	-3.36534	0.17026	-0.80033	-0.62750	0.02122
O	-1.80604	1.77623	-0.62375	-0.61646	0.01680

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Phe1TS2	E=-554.473930897	H0=-554.291158	H298=-554.279124	G298=-554.329746	
H	-0.84261	-0.72890	-1.97297	0.28378	0.02263
H	-0.63169	-2.17333	-0.97812	0.27279	0.00100
H	-2.06686	2.66368	0.24492	0.56031	0.00101
H	-3.82229	-0.87018	0.19105	0.44952	-0.00822
H	-3.00192	-2.18639	-0.55252	0.45200	-0.00890
H	1.05259	-2.13114	0.94811	0.24202	-0.00006
H	3.24724	-1.27282	1.69373	0.25700	-0.00026
H	4.22815	0.74726	0.62644	0.25815	0.00011
H	2.99954	1.90238	-1.19991	0.25600	-0.00025
H	0.79754	1.05527	-1.94671	0.24283	-0.00002
H	-1.21528	-0.52522	1.32876	0.41973	0.15193
C	1.46175	-1.23221	0.49156	-0.23211	-0.00213
C	2.70565	-0.75389	0.90924	-0.20624	0.00948
C	3.25767	0.38104	0.30717	-0.21000	-0.00388
C	2.56611	1.03263	-0.71628	-0.21089	0.00867
C	1.31869	0.55613	-1.13278	-0.23429	-0.00050
C	0.75629	-0.57564	-0.52781	-0.09885	0.00167
C	-0.60614	-1.07698	-0.95812	-0.47692	0.00843
C	-1.76055	-0.62311	-0.05434	-0.02231	0.28349
C	-1.75865	0.80145	0.42470	0.82708	0.00503
N	-2.96725	-1.23042	-0.21639	-0.69520	0.34829
O	-2.17535	1.82485	-0.24824	-0.61842	0.00108
O	-1.27699	0.80963	1.58222	-0.51601	0.18139

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Phe1TS3	E=-554.502555201	H0=-554.318940	H298=-554.307097	G298=-554.357559	
H	-0.66101	-0.86188	-1.34448	0.29272	0.00472
H	-0.70137	-1.74319	0.30071	0.38983	0.04691
H	-3.23027	2.04738	-1.12379	0.54161	-0.00013
H	-2.77748	-1.81546	0.70683	0.46763	-0.00383
H	-1.83198	-1.59117	2.09445	0.45442	-0.00172
H	0.81640	0.92294	1.68985	0.24385	-0.00384
H	3.20905	1.43732	1.87536	0.26785	0.00125
H	4.81433	0.58489	0.17929	0.26473	-0.00717
H	4.00968	-0.78737	-1.73667	0.26991	0.00187
H	1.60326	-1.32061	-1.94498	0.25744	-0.00466
H	-1.24501	0.56248	1.35380	0.28462	0.00020
C	1.50177	0.54119	0.94104	-0.18616	0.12712
C	2.84915	0.83442	1.04825	-0.21195	-0.04805
C	3.75796	0.35385	0.08456	-0.11734	0.24803
C	3.30516	-0.42343	-0.99636	-0.22339	-0.07005
C	1.95991	-0.72086	-1.11270	-0.15683	0.15382
C	1.01760	-0.23384	-0.15300	-0.02385	0.05062
C	-0.36480	-0.59194	-0.32683	-0.38257	0.28411
C	-1.53355	-0.11886	0.55273	-0.17311	-0.00917
C	-2.71306	0.46025	-0.22171	0.80441	-0.00151
N	-1.88672	-1.47201	1.08349	-0.80169	0.21744
O	-2.46827	1.71043	-0.61716	-0.68932	0.00084
O	-3.71665	-0.17742	-0.44917	-0.57279	0.01320

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Phe1TS4	E=-554.509482514	H0=-554.325527	H298=-554.313816	G298=-554.363397	
H	0.99515	-0.20608	-1.33879	0.46019	0.04881
H	0.49211	1.62860	-0.84411	0.26864	-0.00542
H	4.23158	-1.19051	-0.62399	0.55301	-0.00034
H	2.36756	2.20587	0.76101	0.41228	-0.00206
H	1.69955	1.61713	2.16968	0.42482	-0.00212

H	-1.77986	1.87330	-1.37200	0.25362	-0.00524
H	-0.61483	1.23111	-1.09431	0.26688	0.00209
H	-4.74286	-0.74194	0.30217	0.26239	-0.00751
H	-2.96250	-2.07309	1.41694	0.26510	0.00174
H	-0.60428	-1.46611	1.14742	0.23839	-0.00478
H	1.23406	-0.45220	1.31684	0.29154	0.00059
C	-2.03749	1.01250	-0.76448	-0.16556	0.17094
C	-3.36425	0.65315	-0.60955	-0.22275	-0.07796
C	-3.70194	-0.45977	0.18023	-0.13172	0.25689
C	-2.69407	-1.21290	0.81247	-0.21682	-0.06558
C	-1.36458	-0.86285	0.66153	-0.19314	0.15597
C	-0.99376	0.26995	-0.12694	-0.03379	0.01137
C	0.36636	0.66019	-0.35183	-0.40688	0.34870
C	1.54423	0.30428	0.58511	-0.17158	-0.00078
C	2.52386	-0.42934	-0.33806	0.87280	-0.00569
N	2.17137	1.37334	1.30721	-0.84284	0.08094
O	3.72229	-0.70589	0.05531	-0.60684	0.00394
O	2.06993	-0.75045	-1.46559	-0.57774	0.09551

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Phe4TS5	E=-554.515751093	H0=-554.328071	H298=-554.316415	G298=-554.365912	
H	1.82519	-0.59874	1.81853	0.56421	0.00579
H	0.45045	-2.07126	0.24549	0.24140	-0.01704
H	3.14897	2.13573	0.67453	0.55742	0.00154
H	2.27745	-2.31917	-1.06174	0.42404	0.00006
H	3.25523	-1.12864	-1.67363	0.42481	-0.00050
H	-1.85951	-2.21931	0.81415	0.24655	-0.00623
H	-4.13585	-1.27031	0.89981	0.26117	0.00269
H	-4.56713	1.02693	0.04070	0.25815	-0.00736
H	-2.70217	2.36941	-0.90963	0.25854	0.00244
H	-0.43415	1.45438	-1.01401	0.22846	-0.00598
H	1.34023	0.21244	-1.56215	0.27713	0.01425
C	-2.04312	-1.21464	0.44368	-0.17758	0.20357
C	-3.32093	-0.68234	0.49002	-0.22411	-0.09589
C	-3.56484	0.61267	0.00561	-0.17158	0.24631
C	-2.51048	1.37087	-0.52988	-0.21931	-0.08683
C	-1.22702	0.85019	-0.58198	-0.21567	0.19649
C	-0.95134	-0.46502	-0.09563	-0.10848	-0.09431
C	0.33256	-1.05558	-0.12833	-0.22979	0.60452
C	1.56894	-0.41001	-0.68723	-0.19121	-0.02308
C	2.20199	0.51661	0.35108	0.91503	0.03896
N	2.63706	-1.38199	-0.90980	-0.89101	0.00999
O	2.72365	1.62360	-0.04481	-0.60506	0.00140
O	2.27978	0.24463	1.60638	-0.62312	0.00922

23

Phe5TS2	E=-554.484935202	H0=-554.300615	H298=-554.288690	G298=-554.338318	
H	1.89863	-2.31138	1.09921	0.55227	-0.00140
H	0.27121	2.31743	0.13582	0.27730	-0.01111
H	3.63411	-0.38134	-0.84295	0.55548	-0.00092
H	3.39773	1.92041	0.03919	0.43482	-0.00076
H	2.34410	2.21585	-1.23041	0.43662	0.00182
H	-2.01761	2.24815	0.81356	0.24890	-0.00326
H	-4.25201	1.21240	0.62453	0.26235	0.00139
H	-4.48347	-1.08803	-0.29625	0.26014	-0.00370
H	-2.47210	-2.33514	-1.04982	0.25931	0.00143
H	-0.24123	-1.32628	-0.86434	0.23716	-0.00302
H	1.19812	1.06142	1.14577	0.39339	-0.01263
C	-2.11630	1.24177	0.41642	-0.17016	0.10490
C	-3.37240	0.66075	0.30967	-0.22429	-0.04981
C	-3.50128	-0.63462	-0.20841	-0.16652	0.12466
C	-2.36598	-1.34147	-0.62683	-0.22299	-0.04200
C	-1.10317	-0.77312	-0.51224	-0.18382	0.09794
C	-0.95384	0.53244	0.01554	-0.12403	-0.04922
C	0.30402	1.23142	0.08853	-0.23396	0.35656
C	1.69806	0.72355	0.03201	-0.12330	0.06106
C	2.12113	-0.63101	0.23784	0.72991	0.26237
N	2.69645	1.52326	-0.57886	-0.88837	0.03566
O	3.25968	-1.07314	-0.25450	-0.65827	0.07369
O	1.43856	-1.45867	0.99980	-0.65194	0.05634

23

Phe5TS3	E=-554.535214860	H0=-554.348345	H298=-554.337010	G298=-554.385926	
H	-2.39929	2.21564	-1.31546	0.55745	0.00044
H	-0.63646	-1.59921	-0.85081	0.24185	-0.01620
H	-3.47050	-0.73344	-0.14846	0.53698	-0.00074
H	-2.92807	-1.22129	1.92830	0.44346	0.00022

H	2.15996	-2.26211	0.90444	0.44532	-0.00034
H	0.96423	-1.80903	-1.55195	0.24655	-0.00597
H	3.98948	-1.14828	-1.45532	0.26087	0.00257
H	4.72572	0.64651	0.10664	0.25788	-0.00704
H	3.06498	1.78114	1.56813	0.25870	0.00236
H	0.70269	1.15565	1.49013	0.22998	-0.00576
H	-1.21627	0.29148	1.53493	0.28846	0.01016
C	1.93214	-1.02443	-0.87127	-0.17316	0.19486
C	3.26515	-0.65426	-0.81581	-0.22629	-0.09194
C	3.68065	0.35741	0.06466	-0.16865	0.23535
C	2.74226	0.99716	0.89054	-0.22211	-0.08420
C	1.40487	0.63658	0.84533	-0.20043	0.18804
C	0.95668	-0.39390	-0.03622	-0.11027	-0.09209
C	-0.38065	-0.83833	-0.11578	-0.18836	0.57736
C	-1.54049	-0.28292	0.66269	-0.19143	-0.02547
C	-2.31207	0.62251	-0.29109	0.85891	0.06553
N	-2.54504	-1.32394	0.99034	-0.90540	0.01941
O	-3.40851	0.16119	-0.73915	-0.62356	0.01905
O	-1.83681	1.76775	-0.65351	-0.61673	0.01439

14

R+	(Phe)	E=-270.677355392	H0=-270.560284	H298=-270.553677	G298=-270.588787
H	0.00000	0.92728	2.92333	0.25157	
H	0.00000	-0.92728	2.92333	0.25157	
H	0.00000	2.18166	0.80702	0.27154	
H	0.00000	2.16344	-1.68454	0.28332	
H	0.00000	0.00000	-2.89086	0.27683	
H	0.00000	-2.16344	-1.68454	0.28332	
H	0.00000	-2.18166	0.80702	0.27154	
C	0.00000	1.24667	0.25456	-0.07008	
C	0.00000	1.23608	-1.12224	-0.24623	
C	0.00000	0.00000	-1.80401	-0.03210	
C	0.00000	-1.23608	-1.12224	-0.24623	
C	0.00000	-1.24667	0.25456	-0.07008	
C	0.00000	0.00000	0.98386	-0.17634	
C	0.00000	0.00000	2.35537	-0.04863	

14

Rdot	(Phe)	E=-270.937950637	H0=-270.823393	H298=-270.816759	G298=-270.852430
H	0.00000	0.92850	2.96567	0.20643	-0.01967
H	0.00000	-0.92850	2.96567	0.20643	-0.01967
H	0.00000	2.16214	0.79329	0.23412	-0.00664
H	0.00000	2.15454	-1.67759	0.23902	0.00290
H	0.00000	0.00000	-2.92765	0.23700	-0.00737
H	0.00000	-2.15454	-1.67759	0.23902	0.00290
H	0.00000	-2.16214	0.79329	0.23412	-0.00664
C	0.00000	1.21945	0.25248	-0.20329	0.21593
C	0.00000	1.21322	-1.13495	-0.24207	-0.10050
C	0.00000	0.00000	-1.84196	-0.22901	0.24157
C	0.00000	-1.21322	-1.13495	-0.24207	-0.10050
C	0.00000	-1.21945	0.25248	-0.20329	0.21593
C	0.00000	0.00000	0.99643	-0.13489	-0.13809
C	0.00000	0.00000	2.40463	-0.34152	0.71984

15

Rdot+	(Phe)	E=-271.273600540	H0=-271.147923	H298=-271.140292	G298=-271.179797
H	-0.74308	2.17539	-0.01305	0.27711	-0.00301
H	1.74312	2.17164	0.00471	0.28365	-0.00027
H	2.97244	-0.00001	0.01690	0.27193	-0.01183
H	1.74310	-2.17165	0.00471	0.28365	-0.00027
H	-0.74310	-2.17537	-0.01305	0.27711	-0.00301
C	-0.18742	1.24281	-0.00821	0.17557	0.08733
C	1.18479	1.24140	0.00157	0.20084	-0.00554
C	1.88602	-0.00001	0.00704	0.00270	0.42048
C	1.18478	-1.24140	0.00157	0.20086	-0.00556
C	-0.18743	-1.24280	-0.00821	0.17555	0.08737
C	-0.91817	0.00001	-0.01687	0.20210	0.36438
C	-2.39627	0.00001	-0.00091	0.71954	0.01033
H	-2.73101	-0.00025	1.05455	0.31077	0.04235
H	-2.81969	0.89999	-0.45512	0.28166	0.00862
H	-2.81966	-0.89980	-0.45549	0.28167	0.00864

Optimized geometries for tyrosine as shown in Table 2 and Figure 5b

24

Tyr1	E=-629.781272623	H0=-629.588613	H298=-629.575050	G298=-629.629430	
H	4.53632	-1.26280	-0.05640	0.53212	-0.00306
H	-1.39925	0.55371	1.79870	0.26675	0.00291

H	3.11075	2.11393	0.98986	0.27484	0.00856
H	3.12155	-2.39572	-0.05856	0.53884	0.00031
H	-3.97871	0.78479	0.64401	0.43451	-0.00525
H	-3.59089	2.16150	-0.30128	0.43116	-0.00512
H	0.75569	2.37505	-0.66840	0.26016	-0.00061
H	3.08082	1.70293	-1.22873	0.28124	-0.00205
H	2.61006	-1.88826	1.14342	0.26444	-0.00156
H	0.29652	-1.23150	1.68431	0.26206	-0.00134
H	-1.69872	1.10616	-1.22229	0.28020	0.00169
C	1.15949	1.44262	-0.28467	-0.18827	0.00866
C	2.44769	1.08519	-0.60140	-0.22654	0.06172
C	2.97698	-0.13042	-0.08628	0.41448	0.16452
C	2.19219	-0.96574	0.75034	-0.26795	0.04265
C	0.90156	-0.59307	1.04862	-0.15944	0.03574
C	0.35017	0.62376	0.55464	0.04168	0.21963
C	-1.03153	1.02957	0.88633	-0.47174	0.02646
C	-2.11231	0.67520	-0.30827	-0.14160	0.04032
C	-2.11014	-0.84589	-0.48341	0.80666	0.00466
N	-3.39698	1.19616	-0.07421	-0.76351	0.23147
O	4.22753	-0.42183	-0.43188	-0.60392	0.12156
O	-3.17288	-1.43367	0.08621	-0.70411	0.00434
O	-1.21001	-1.43452	-1.03690	-0.56206	0.04380

24

Tyr2 E=-629.796182859 H0=-629.602826 H298=-629.589661 G298=-629.642301

H	-4.68576	0.88288	0.18850	0.51728	-0.00002
H	1.18045	-1.37678	1.74577	0.28494	0.01350
H	1.12066	-2.36993	0.30299	0.27470	0.00453
H	3.16831	2.43127	-0.47531	0.55523	-0.00211
H	0.37717	1.14537	0.55740	0.55254	-0.00166
H	4.07118	-0.69706	-0.74892	0.45831	-0.00728
H	3.31898	-2.20591	-0.34962	0.44985	-0.00791
H	-0.83489	-0.30455	2.40012	0.25652	0.00003
H	-3.09388	0.53897	1.89859	0.25598	-0.00010
H	-2.52173	-0.36802	-2.26896	0.27178	0.00006
H	-0.24511	-1.20741	-1.77902	0.24870	-0.00004
C	-1.18100	-0.30123	1.36915	-0.23754	-0.00108
C	-2.46694	0.17100	1.09104	-0.29133	0.00453
C	-2.94610	0.14873	-0.22487	0.34022	0.00102
C	-2.13025	-0.34705	-1.25765	-0.24990	-0.00075
C	-0.85503	-0.81210	-0.97030	-0.20816	0.00036
C	-0.35155	-0.79153	0.34684	-0.16130	0.00598
C	1.03441	-1.33563	0.65769	-0.49840	-0.01036
C	2.18014	-0.54776	0.06134	0.16518	0.25752
C	2.18664	0.86479	0.00136	0.70823	0.26925
N	3.26792	-1.19626	-0.38511	-0.70077	0.28920
O	-4.17748	0.58297	-0.57840	-0.67311	0.00087
O	1.20565	1.65440	0.37434	-0.65162	0.10296
O	3.27775	1.46385	-0.44887	-0.66734	0.08152

24

Tyr3 E=-629.786951729 H0=-629.592718 H298=-629.579283 G298=-629.633334

H	-5.22591	-0.47836	-0.07237	0.52030	-0.00180
H	1.11439	-1.12594	-1.21807	0.24810	-0.01494
H	1.66389	1.86697	-1.57735	0.47378	-0.00068
H	3.77873	-1.57791	1.66096	0.54343	-0.00024
H	3.15845	1.08306	-1.50838	0.48603	-0.00111
H	2.84514	2.36559	-0.50337	0.46563	0.00549
H	-0.48779	1.50423	1.12081	0.22896	-0.00497
H	-2.90770	1.65216	1.47072	0.27074	0.00136
H	-3.53983	-1.65108	-1.22559	0.25587	0.00173
H	-1.11853	-1.82112	-1.60165	0.25087	-0.00553
H	1.55556	1.04138	0.93829	0.28595	0.00243
C	-1.13378	0.81143	0.58985	-0.20532	0.15606
C	-2.49277	0.90697	0.80072	-0.25384	-0.05356
C	-3.37449	0.02045	0.14660	0.35991	0.19587
C	-2.86364	-0.96441	-0.72325	-0.29060	-0.06692
C	-1.50284	-1.05641	-0.93315	-0.16680	0.17586
C	-0.57896	-0.17378	-0.28797	-0.10383	-0.05658
C	0.80055	-0.32769	-0.55048	-0.25773	0.52634
C	1.87952	0.48626	0.05691	-0.18877	0.00043
C	3.12458	-0.34948	0.37755	0.80488	0.01148
N	2.41765	1.55210	-0.96042	-0.80046	0.04668
O	-4.68848	0.17228	0.40281	-0.65574	0.07107
O	4.08504	-0.37844	-0.36687	-0.59962	0.00670
O	2.98983	-1.02429	1.51133	-0.67175	0.00483

	24				
Tyr4	E=-629.746766153	H0=-629.554790	H298=-629.541428	G298=-629.595227	
H	-5.19769	-0.02697	-0.28878	0.52069	-0.00189
H	1.64157	-0.26916	-1.67076	0.55042	0.01768
H	1.00718	1.76526	-0.65705	0.24704	-0.01276
H	4.62649	-1.21658	-0.71052	0.55606	0.00070
H	2.78833	2.02446	1.13375	0.40778	-0.00138
H	2.21686	1.14441	2.40560	0.42087	-0.00112
H	-1.26053	2.12413	-1.23071	0.24974	-0.00552
H	-3.64267	1.53863	-1.11600	0.25622	0.00167
H	-2.68707	-1.96842	1.20228	0.27184	0.00128
H	-0.30328	-1.41533	1.09855	0.23186	-0.00490
H	1.60290	-0.65095	1.17977	0.29753	0.00102
C	-1.56437	1.22540	-0.70188	-0.17081	0.17556
C	-2.90372	0.90009	-0.63922	-0.28949	-0.06492
C	-3.31221	-0.25948	0.05168	0.36135	0.19979
C	-2.34976	-1.08282	0.67471	-0.25146	-0.05094
C	-1.01258	-0.75575	0.60784	-0.20439	0.15403
C	-0.55971	0.41471	-0.08176	-0.09523	-0.04499
C	0.79991	0.79757	-0.19871	-0.34560	0.50421
C	1.95105	0.21296	0.59377	-0.19758	-0.01481
C	2.93405	-0.43418	-0.37937	0.91004	0.01051
N	2.67402	1.08435	1.50238	-0.86977	0.04087
O	-4.59870	-0.64246	0.15902	-0.65358	0.07462
O	4.10694	-0.78494	-0.00188	-0.58429	0.00037
O	2.56598	-0.66647	-1.58529	-0.61924	0.02092

	24				
Tyr5	E=-629.766526742	H0=-629.573744	H298=-629.560661	G298=-629.613539	
H	-2.49028	2.26925	-1.33643	0.55461	0.00040
H	-1.18308	-1.67693	-0.71378	0.24521	-0.01343
H	-3.90116	-0.57548	-0.45430	0.55494	-0.00062
H	-3.58915	-0.97101	1.88279	0.43268	0.00059
H	-2.72272	-2.15050	1.12470	0.43576	0.00012
H	1.04818	-2.00305	-1.45587	0.25060	-0.00494
H	3.44263	-1.45061	-1.43391	0.25621	0.00157
H	2.71722	1.66173	1.46066	0.27188	0.00120
H	0.31962	1.13466	1.45809	0.23758	-0.00439
H	-1.66190	0.33166	1.59428	0.28065	0.01327
H	5.07511	-0.03877	-0.49767	0.52073	-0.00161
C	1.40640	-1.20132	-0.81681	-0.15696	0.15646
C	2.75108	-0.89513	-0.80609	-0.29558	-0.06052
C	3.22593	0.14340	0.02202	0.36789	0.17426
C	2.32710	0.86577	0.83579	-0.25781	-0.04659
C	0.98456	0.55595	0.82571	-0.18674	0.13858
C	0.46813	-0.49596	0.00330	-0.12005	-0.05225
C	-0.88236	-0.88881	-0.02666	-0.20046	0.47324
C	-2.01049	-0.24423	0.73118	-0.18478	-0.02597
C	-2.60655	0.67936	-0.30592	0.83521	0.11671
N	-3.08415	-1.20477	1.03070	-0.92234	0.01477
O	-3.64335	0.27480	-0.95308	-0.64088	0.03154
O	-2.05908	1.82123	-0.58351	-0.62509	0.02444
O	4.52140	0.50250	0.08427	-0.65325	0.06313

	24				
Tyr1TS2	E=-629.700441576	H0=-629.513660	H298=-629.553876	G298=-629.553876	
H	4.50813	1.15903	-0.17912	0.51458	-0.00009
H	-1.36647	-0.97639	-1.86723	0.28256	0.02590
H	-1.22865	-2.28126	-0.68455	0.27219	0.00067
H	-2.08405	2.77793	0.14242	0.55949	0.00084
H	-4.30660	-0.46552	0.19495	0.44874	-0.00790
H	-3.66023	-1.93722	-0.41531	0.45129	-0.00866
H	0.58297	-2.13403	1.12495	0.24380	0.00002
H	2.87730	-1.35500	1.64208	0.26842	-0.00042
H	2.65121	1.47223	-1.59262	0.24978	0.00004
H	0.36665	0.70863	-2.10990	0.24390	-0.00014
H	-1.68637	-0.41357	1.41716	0.42281	0.14511
C	1.01797	-1.32677	0.53971	-0.21191	-0.00391
C	2.30768	-0.90360	0.83709	-0.24992	0.01541
C	2.90072	0.11580	0.07388	0.33585	0.00277
C	2.19122	0.69797	-0.98432	-0.29783	-0.00190
C	0.89513	0.26495	-1.26906	-0.21189	0.00381
C	0.28778	-0.74600	-0.51136	-0.13226	0.00258
C	-1.11869	-1.19853	-0.81994	-0.47377	0.00787
C	-2.22280	-0.53344	0.02723	-0.02684	0.28931
C	-2.02772	0.90360	0.41849	0.82922	0.00424

N	-3.49025	-0.97283	-0.14721	-0.70280	0.33954
O	-0.16265	0.47789	0.41427	-0.67689	0.00339
O	-2.30250	1.93717	-0.30902	-0.61807	0.00122
O	-1.55293	0.91133	1.58066	-0.52046	0.18030

24

Tyr1TS3	E=-629.739219026	H0=-629.550734	H298=-629.537862	G298=-629.590662	
H	5.18761	0.05415	-0.50633	0.52801	-0.00243
H	-1.13579	-0.99950	-1.26915	0.28504	0.00405
H	-1.23872	-1.74028	0.48497	0.39590	0.05144
H	-3.56460	2.06172	-1.23896	0.53957	-0.00011
H	-3.28413	-1.68984	0.83476	0.46480	-0.00282
H	-2.38275	-1.37854	2.22433	0.45144	-0.00030
H	0.44261	0.95769	1.61248	0.24710	-0.00262
H	2.86045	1.39172	1.74536	0.27870	-0.00045
H	3.52473	-1.08307	-1.73401	0.26328	0.00029
H	1.11008	-1.53257	-1.88053	0.26028	-0.00354
H	-1.63682	0.65038	1.31439	0.28139	-0.00001
C	1.10174	0.50111	0.88239	-0.18586	0.07866
C	2.45048	0.75472	0.96929	-0.23927	0.00681
C	3.33791	0.18165	0.02437	0.39555	0.18154
C	2.84216	-0.64902	-1.00869	-0.28374	-0.02037
C	1.49091	-0.89627	-1.08730	-0.15376	0.11001
C	0.56843	-0.32555	-0.15302	-0.02718	0.09196
C	-0.82022	-0.66096	-0.27905	-0.41185	0.24776
C	-1.96290	-0.07241	0.56577	-0.17084	-0.00451
C	-3.11140	0.50790	-0.25109	0.80440	-0.00081
N	-2.38481	-1.36211	1.20467	-0.82733	0.15623
O	4.63318	0.47277	0.17085	-0.62648	0.09630
O	-2.82037	1.73020	-0.70359	-0.69134	0.00100
O	-4.13428	-0.10348	-0.46676	-0.57781	0.01191

24

Tyr1TS4	E=-629.744107963	H0=-629.555429	H298=-629.542621	G298=-629.594798	
H	-5.18686	0.00545	-0.21642	0.52479	-0.00223
H	1.47202	-0.05811	-1.39631	0.47562	0.04468
H	1.00382	1.75965	-0.64093	0.26315	-0.00554
H	4.58367	-1.28862	-0.72858	0.55210	-0.00024
H	2.88154	2.04127	1.01975	0.40820	-0.00144
H	2.18797	1.32294	2.34388	0.42081	-0.00146
H	-1.25051	2.14887	-1.18284	0.25542	-0.00442
H	-3.63967	1.58920	-1.02607	0.26000	0.00081
H	-2.66424	-2.02233	1.12819	0.27572	0.00036
H	-0.27167	-1.48987	0.97399	0.24053	-0.00365
H	1.61384	-0.59716	1.25648	0.28937	0.00063
C	-1.55499	1.23653	-0.67873	-0.16211	0.13917
C	-2.89472	0.92661	-0.59390	-0.28591	-0.03753
C	-3.29663	-0.25671	0.06542	0.38151	0.19239
C	-2.32763	-1.11916	0.63102	-0.24554	-0.02074
C	-0.99162	-0.80360	0.53987	-0.19437	0.11271
C	-0.54806	0.39079	-0.11234	-0.04513	0.03725
C	0.82599	0.74733	-0.26946	-0.42626	0.33762
C	1.96925	0.22239	0.61821	-0.17379	-0.00222
C	2.92392	-0.45794	-0.36942	0.87992	-0.00144
N	2.66626	1.15522	1.46646	-0.85833	0.05287
O	-4.57801	-0.62801	0.19337	-0.63799	0.08821
O	4.09375	-0.85711	-0.00103	-0.60406	0.00248
O	2.48093	-0.61679	-1.53988	-0.59367	0.07175
Tyr4TS5	E=-629.746369518	H0=-629.554373	H298=-629.541595	G298=-629.593649	
H	5.08617	-0.13195	0.35821	0.51987	-0.00175
H	-2.27008	0.55472	1.80356	0.56212	0.00658
H	-1.01465	2.07663	0.26076	0.24100	-0.01536
H	-3.45379	-2.26054	0.70591	0.55582	0.00154
H	-2.80537	2.19925	-1.13170	0.42260	0.00038
H	-3.71433	0.94117	-1.71235	0.42277	-0.00039
H	1.29113	2.39660	0.82004	0.24889	-0.00557
H	3.62634	1.63816	0.88645	0.25528	0.00182
H	2.48497	-2.10393	-0.92264	0.27043	0.00141
H	0.14290	-1.37365	-1.00416	0.23203	-0.00503
H	-1.72136	-0.27880	-1.54406	0.27372	0.01212
C	1.54282	1.40953	0.44292	-0.16793	0.17716
C	2.85658	0.98746	0.47996	-0.29205	-0.06939
C	3.19860	-0.28793	-0.01361	0.35810	0.19439
C	2.19771	-1.12885	-0.54433	-0.25354	-0.05453
C	0.88622	-0.70479	-0.58014	-0.20735	0.15920
C	0.50192	0.58459	-0.09003	-0.11204	-0.06396

C	-1.82061	1.07399	-0.11650	-0.26984	0.54338
C	2.08039	0.34641	-0.68653	-0.18730	-0.02070
C	-2.59978	-0.59534	0.35860	0.91018	0.04480
N	-3.12130	1.25152	-0.94947	-0.89165	0.01144
O	4.45758	-0.76955	-0.01080	-0.65710	0.06906
O	-3.05944	-1.73632	-0.02183	-0.60807	0.00237
O	-2.69385	-0.31023	1.61066	-0.62592	0.01101
	24				
Tyr5TS2	E=-629.716258979	H0=-629.527628	H298=-629.514585	G298=-629.566631	
H	2.16896	-2.37344	1.10578	0.55029	-0.00135
H	0.85871	2.35429	0.13093	0.27548	-0.00982
H	4.00498	-0.58456	-0.86979	0.55387	-0.00101
H	3.92633	1.74400	-0.01975	0.43314	-0.00078
H	2.88161	2.08052	-1.28476	0.43428	0.00172
H	-1.42889	2.49307	0.78637	0.25131	-0.00286
H	-3.73330	1.64898	0.64506	0.25678	0.00090
H	-2.27724	-2.09905	-0.90576	0.27147	0.00067
H	0.03708	-1.27381	-0.76731	0.24270	-0.00242
H	1.69680	1.04183	1.13381	0.38963	-0.00082
H	-5.06120	-0.20355	0.05840	0.52077	-0.00105
C	-1.60581	1.48411	0.42485	-0.15356	0.08956
C	-2.90330	1.01431	0.34723	-0.29804	-0.03524
C	-3.14229	-0.29167	-0.12308	0.37205	0.10230
C	-2.06480	-1.10716	-0.52240	-0.26227	-0.01947
C	-0.77023	-0.63484	-0.43352	-0.17062	0.07674
C	-0.49982	0.67502	0.04538	-0.13663	-0.02559
C	0.80400	1.26895	0.09375	-0.25487	0.30653
C	2.15614	0.65482	0.01168	-0.12211	0.04523
C	2.48645	-0.72006	0.22309	0.71622	0.27448
N	3.19805	1.37802	-0.62553	-0.89091	0.03107
O	3.59127	-1.24528	-0.27285	-0.66429	0.07415
O	1.75494	-1.49914	0.99731	-0.65964	0.05590
O	-4.37398	-0.82250	-0.22899	-0.65504	0.04116
	24				
Tyr5TS3	E=-629.766052616	H0=-629.575513	H298=-629.562971	G298=-629.614789	
H	5.13006	-0.01200	-0.47060	0.51966	-0.00164
H	-3.88444	-0.67393	-0.06055	0.52662	-0.00080
H	-1.13798	-1.60010	-0.83744	0.24112	-0.01458
H	-2.78036	2.22403	-1.37832	0.55505	0.00041
H	-2.66104	-2.17929	0.97446	0.44724	0.00000
H	-3.38569	-1.07951	1.97158	0.44484	0.00030
H	1.10597	-1.91576	-1.55533	0.24899	-0.00533
H	3.50114	-1.37535	-1.48258	0.25503	0.00175
H	2.75493	1.61575	1.53013	0.27062	0.00139
H	0.35741	1.10459	1.47508	0.23345	-0.00481
H	-1.61247	0.35182	1.52520	0.28574	0.00968
C	1.45904	-1.14322	-0.87853	-0.16292	0.16934
C	2.80528	-0.84334	-0.83927	-0.29411	-0.06650
C	3.27585	0.15609	0.03688	0.36137	0.18479
C	2.37017	0.84725	0.86859	-0.25691	-0.05345
C	1.02575	0.54535	0.82839	-0.19311	0.15157
C	0.51314	-0.46880	-0.04190	-0.11493	-0.06377
C	-0.84017	-0.85185	-0.10556	-0.22443	0.51985
C	-1.96418	-0.23064	0.66974	-0.18617	-0.02345
C	-2.72397	0.66609	-0.30186	0.84628	0.07344
N	-3.01020	-1.22486	1.03583	-0.89714	0.01948
O	4.57390	0.50605	0.12950	-0.65670	0.06482
O	-2.22072	1.78875	-0.70652	-0.62283	0.01531
O	-3.83338	0.21173	-0.71815	-0.62676	0.02226
	15				
R+	(Tyr)	E=-345.922816570	H0=-345.800891	H298=-345.793356	G298=-345.831421
H	-0.79676	3.11424	0.00000	0.53878	
H	0.93719	-3.37323	0.00000	0.24948	
H	-0.91607	-3.37606	0.00000	0.24837	
H	-2.17360	-1.25506	0.00000	0.27327	
H	-2.17662	1.21806	0.00000	0.27444	
H	2.16107	1.25296	0.00000	0.29202	
H	2.18941	-1.24001	0.00000	0.27356	
C	-1.23782	-0.70422	0.00000	-0.07725	
C	-1.24400	0.66110	0.00000	-0.30620	
C	0.00000	1.36061	0.00000	0.47463	
C	1.24734	0.66904	0.00000	-0.27450	
C	1.25041	-0.69485	0.00000	-0.08749	
C	0.00855	-1.44228	0.00000	-0.16877	

	0.00869	-2.80721	0.00000	-0.11248	
	0.07155	2.67575	0.00000	-0.59786	
	15				
Rdot	(Tyr)	E=-346.164016607	H0=-346.045490	H298=-346.037626	G298=-346.076719
H	-0.83459	3.11547	0.00000	0.50334	-0.00116
H	0.94985	-3.42500	0.00000	0.20669	-0.01927
H	-0.90723	-3.43520	0.00000	0.20597	-0.01925
H	-2.15147	-1.25602	0.00000	0.23580	-0.00675
H	-2.15661	1.20932	0.00000	0.23332	0.00259
H	2.14599	1.24440	0.00000	0.25163	0.00265
H	2.17160	-1.23520	0.00000	0.23636	-0.00628
C	-1.20727	-0.71849	0.00000	-0.18981	0.21523
C	-1.21222	0.66842	0.00000	-0.31151	-0.09268
C	0.00000	1.37705	0.00000	0.31020	0.20456
C	1.21947	0.67920	0.00000	-0.28102	-0.09435
C	1.22359	-0.70428	0.00000	-0.19055	0.19905
C	0.01105	-1.46275	0.00000	-0.14677	-0.13410
C	0.01828	-2.86956	0.00000	-0.36679	0.70447
O	0.05814	2.74559	0.00000	-0.69685	0.04528
	16				
Rdot+	(Tyr)	E=-346.523845458			
H	-3.20081	-0.76840	0.00949	0.54248	-0.00447
H	1.18023	-2.16674	-0.01426	0.27702	-0.00106
H	-1.29312	-2.17248	-0.00034	0.27397	-0.00290
H	-1.29575	2.17361	0.00031	0.29002	-0.00394
H	1.19879	2.17068	-0.01419	0.27860	0.00018
C	0.63302	-1.22909	-0.00958	-0.17523	0.02159
C	-0.73705	-1.23897	-0.00167	-0.25006	0.08188
C	-1.43532	0.00839	0.00206	0.44254	0.22212
C	-0.72378	1.25171	-0.00151	-0.19549	0.12243
C	0.64686	1.23629	-0.00915	-0.19948	-0.02410
C	1.36978	0.00355	-0.01347	0.15113	0.36191
O	-2.75011	0.09499	0.00794	-0.56740	0.17740
C	2.85664	-0.01481	0.00643	-0.71088	0.00002
H	3.20383	-0.20940	1.03495	0.29436	0.03290
H	3.25863	-0.82661	-0.60876	0.27749	0.01259
H	3.28816	0.93692	-0.30931	0.27092	0.00346

Optimized geometries for tryptophan as shown in Table 2 and Figure 5a

	27				
Trp1	E=-686.156485818	H0=-685.937176	H298=-685.923184	G298=-685.978498	
H	-2.15533	-2.60552	-0.69351	0.42180	-0.00013
H	-1.03646	-1.48552	-1.17661	0.40117	-0.00101
H	-2.94004	-1.40356	1.04768	0.27904	-0.00086
H	-1.74511	0.48562	2.08160	0.27164	0.00448
H	-0.84259	-1.03505	2.12321	0.28060	0.00974
H	-0.62168	2.62398	0.78394	0.27754	-0.00574
H	1.59985	3.02396	-0.26259	0.47148	-0.00299
H	3.88534	1.50327	-1.04383	0.26761	-0.00096
H	4.73288	-0.83969	-1.05166	0.26607	-0.00473
H	3.37679	-2.69809	-0.15814	0.26820	0.00160
H	1.10654	-2.27349	0.78365	0.27099	-0.00578
H	-4.47916	0.46559	-1.36940	0.53137	0.00081
C	-2.17847	-0.88661	0.45795	-0.15017	0.02809
C	-1.18571	-0.22849	1.46899	-0.48647	-0.00811
C	-2.88202	0.18963	-0.38155	0.80480	-0.00183
C	-0.01104	0.44486	0.85101	0.05488	0.30656
C	1.20708	-0.13624	0.39659	-0.13681	-0.05920
C	0.10236	1.84585	0.58960	0.13156	0.18272
C	2.01673	0.91090	-0.12556	0.15046	0.04342
C	3.27413	0.69798	-0.64926	-0.20633	0.03386
C	3.74574	-0.63566	-0.64984	-0.14789	0.15995
C	2.97602	-1.69047	-0.14210	-0.24931	-0.06120
C	1.70488	-1.45948	0.38974	-0.10175	0.19677
N	-1.52115	-1.87984	-0.37565	-0.86924	0.04683
N	1.28463	2.10488	0.02300	-0.50058	0.09683
O	-4.08682	-0.22060	-0.79948	-0.68990	0.00528
O	-2.39363	1.26432	-0.67918	-0.61075	0.03559
	27				
Trp2	E=-686.154272740	H0=-685.935662	H298=-685.921752	G298=-685.976077	
H	3.88560	-1.41274	-0.74257	0.45747	-0.00726
H	3.13314	-0.97837	-2.24176	0.44870	-0.00788
H	0.82738	1.01163	1.07151	0.54317	-0.00189
H	1.73263	1.65102	-1.61267	0.28654	0.01514

H	-1.15544	0.17095	-2.32500	0.27394	0.00521
H	-0.19585	3.13758	-0.49110	0.25800	0.00004
H	-2.48926	2.70857	0.41249	0.45818	0.00000
H	-4.21774	0.50964	0.89369	0.25536	0.00000
H	-4.28741	-1.96377	0.67379	0.25600	0.00001
H	-2.35412	-3.21791	-0.21962	0.25323	0.00000
H	-0.28580	-2.05372	-0.90834	0.23616	0.00000
H	3.31652	-0.62121	2.39215	0.55394	-0.00208
C	2.28487	-0.12308	-0.57901	0.16608	0.26986
C	1.27267	0.68344	-1.36646	-0.49567	-0.01117
C	2.38687	-0.04644	0.82848	0.70838	0.26019
C	-0.05213	0.91229	-0.68376	-0.21609	0.00333
C	-1.06308	-0.08426	-0.39206	-0.10954	0.00098
C	-0.60882	2.14522	-0.37426	-0.01005	-0.00121
C	-2.19111	0.61456	0.11148	0.14982	-0.00012
C	-3.36378	-0.03869	0.50846	-0.24369	0.00013
C	-3.39369	-1.42232	0.38136	-0.21426	0.00012
C	-2.28778	-2.13873	-0.12701	-0.23560	-0.00005
C	-1.12360	-1.48612	-0.51244	-0.21290	0.00006
N	3.16397	-0.89879	-1.23381	-0.70486	0.28819
N	-1.87735	1.96550	0.10772	-0.54415	0.00061
O	1.59616	0.65546	1.60228	-0.64954	0.10914
O	3.35991	-0.71845	1.42414	-0.66862	0.07862

27

Trp3 E=-686.145581095 H0=-685.926183 H298=-685.911891 G298=-685.967990

H	-3.41947	-0.47899	1.85782	0.48490	-0.00112
H	-3.61152	1.16904	1.89037	0.46268	0.00593
H	-2.28530	1.44257	-0.04637	0.28145	0.00127
H	-2.16808	0.50372	2.41935	0.47256	-0.00056
H	-1.02948	-1.36105	0.32249	0.25108	-0.01362
H	-0.23626	2.59638	-0.16898	0.23690	-0.00928
H	2.22017	2.87611	-0.37978	0.45775	-0.00407
H	4.57253	1.30610	-0.34797	0.25476	-0.00084
H	5.30904	-1.05979	-0.12330	0.25606	0.00014
H	3.66536	-2.87437	0.21500	0.25458	-0.00065
H	1.24227	-2.39007	0.34098	0.24378	-0.00011
H	-3.98807	-0.64919	-2.29107	0.54220	-0.00020
C	-2.33380	0.40169	0.27722	-0.18204	0.00194
C	-1.02108	-0.27713	0.25630	-0.29298	0.47727
C	-3.39611	-0.36625	-0.51570	0.80165	0.01316
C	0.20358	0.38383	0.09164	-0.10380	-0.02141
C	1.52141	-0.25290	0.06816	-0.10098	0.03126
C	0.45260	1.76706	-0.09485	0.00305	0.30350
C	2.48023	0.76573	-0.12564	0.14754	-0.01972
C	3.84936	0.51064	-0.19820	-0.24299	0.02541
C	4.25239	-0.81844	-0.07113	-0.20491	-0.00537
C	3.31621	-1.85130	0.12200	-0.23588	0.02058
C	1.95063	-1.58032	0.19387	-0.18233	0.00591
N	-2.92604	0.42072	1.73640	-0.80436	0.04407
N	1.79130	1.97588	-0.21887	-0.52354	0.13314
O	-3.33826	-0.09960	-1.81503	-0.67434	0.00501
O	-4.15931	-1.14445	0.02337	-0.60280	0.00837

27

Trp4 E=-686.106323026 H0=-685.889436 H298=-685.875255 G298=-685.930851

H	-2.67917	0.39689	2.62104	0.41878	-0.00096
H	-2.88471	-1.15797	2.11838	0.40654	-0.00112
H	-2.30925	1.24900	0.55448	0.29088	0.00092
H	-0.91374	-1.51050	0.54671	0.25336	-0.00996
H	-1.80708	-0.76271	-1.40301	0.53999	0.02413
H	-0.42440	2.47860	0.00831	0.23973	-0.00909
H	2.00097	2.93675	-0.23404	0.45914	-0.00428
H	4.45439	1.53144	-0.32756	0.25588	-0.00084
H	5.35722	-0.78369	-0.20076	0.25706	0.00002
H	3.84992	-2.71962	0.09722	0.25544	-0.00059
H	1.40118	-2.41066	0.27578	0.24347	-0.00032
H	-5.05051	-0.20699	-1.29713	0.55440	0.00036
C	-2.37044	0.15139	0.60586	-0.18777	-0.01147
C	-1.01601	-0.45609	0.28978	-0.39543	0.43781
C	-3.30978	-0.18407	-0.55418	0.90507	0.00783
C	0.16836	0.29033	0.14386	-0.08721	0.00465
C	1.52625	-0.25135	0.07275	-0.10556	0.02562
C	0.31927	1.69454	0.00778	0.00812	0.29757
C	2.40904	0.83771	-0.09739	0.14762	-0.01830
C	3.79042	0.68253	-0.19872	-0.24053	0.02599

C	4.28725	-0.61940	-0.12618	-0.20287	-0.00119
C	3.42884	-1.72113	0.04317	-0.23464	0.01844
C	2.04874	-1.54894	0.14387	-0.18061	0.01334
N	-3.01769	-0.18366	1.86150	-0.87280	0.03313
N	1.63587	2.00020	-0.13232	-0.51932	0.14108
O	-2.80407	-0.65404	-1.62978	-0.61925	0.02687
O	-4.57271	0.02787	-0.47613	-0.58946	0.00040
	27				
Trp5	E=-686.126455948	H0=-685.908201	H298=-685.894303	G298=-685.948903	
H	2.80196	-1.36688	-2.15336	0.43263	0.00041
H	4.06313	-0.31739	-1.98714	0.42834	0.00080
H	2.40049	1.12696	-1.14249	0.27244	0.01454
H	3.90082	-1.38439	0.21023	0.55655	-0.00071
H	1.05708	-1.56190	-0.38647	0.25052	-0.01148
H	0.44585	2.43085	-0.68325	0.24496	-0.00771
H	-1.97026	2.88517	-0.35876	0.45979	-0.00347
H	-4.37322	1.48469	0.14617	0.25580	-0.00073
H	-5.21753	-0.82654	0.52039	0.25705	0.00011
H	-3.67847	-2.75963	0.48764	0.25543	-0.00054
H	-1.25720	-2.45478	0.07959	0.24421	-0.00013
H	2.96137	0.86931	2.40483	0.55193	0.00060
C	2.44591	0.10602	-0.74636	-0.17814	-0.02552
C	1.08089	-0.48488	-0.53003	-0.21617	0.39473
C	2.97053	0.11158	0.66428	0.81315	0.15237
C	-0.09607	0.24732	-0.38790	-0.12548	-0.01326
C	-1.42900	-0.29816	-0.11592	-0.09246	0.02464
C	-0.27818	1.65010	-0.50113	0.03572	0.25394
C	-2.32907	0.78893	-0.09254	0.14292	-0.01685
C	-3.69631	0.63633	0.13325	-0.24011	0.02247
C	-4.16004	-0.66253	0.34120	-0.20629	-0.00408
C	-3.28320	-1.76281	0.32222	-0.23153	0.01717
C	-1.91809	-1.59324	0.09332	-0.18461	0.00663
N	3.32576	-0.80724	-1.48551	-0.92499	0.01283
N	-1.58713	1.95043	-0.32790	-0.51544	0.11393
O	2.64734	1.05557	1.49997	-0.63611	0.02950
O	3.70910	-0.87554	1.05932	-0.65009	0.03985
	27				
Trp1TS2	E=-686.060024014	H0=-685.847380	H298=-685.833384	G298=-685.888372	
H	-2.14826	2.52661	0.67021	0.44095	-0.00573
H	-1.59420	2.67000	-0.93874	0.43954	-0.00688
H	-3.54354	0.12966	-0.64705	0.43474	0.09809
H	-1.92826	-0.75277	-1.99632	0.27303	-0.00003
H	-1.11027	0.76855	-2.30344	0.27046	-0.00032
H	-0.52929	-2.76368	-0.97224	0.25162	-0.00192
H	1.72446	-3.03402	0.07779	0.45753	-0.00148
H	3.86847	-1.41663	0.96323	0.25556	-0.00078
H	4.57536	0.96596	1.06280	0.25671	-0.00047
H	3.11126	2.76053	0.20041	0.25370	-0.00014
H	0.90728	2.24122	-0.78519	0.23283	-0.00120
H	-2.58671	-0.73260	2.48583	0.55380	0.00025
C	-2.15909	0.75762	-0.43525	-0.07928	0.25922
C	-1.32147	0.02497	-1.52666	-0.46314	0.00368
C	-2.61057	-0.08686	0.70665	0.81852	0.00963
C	-0.08382	-0.56887	-0.93784	-0.11614	0.06777
C	1.09440	0.10092	-0.43861	-0.11114	-0.01008
C	0.11217	-1.92961	-0.72049	0.01145	0.06283
C	1.96144	-0.90903	0.05717	0.14623	-0.00465
C	3.21546	-0.62900	0.60023	-0.23177	0.02811
C	3.60542	0.70998	0.64937	-0.20984	0.01578
C	2.77021	1.73121	0.15990	-0.23868	0.00407
C	1.52256	1.44086	-0.38919	-0.18484	0.03520
N	-1.81541	2.05860	-0.16318	-0.74481	0.26617
N	1.32489	-2.13025	-0.13145	-0.52996	0.05178
O	-2.05363	-0.18828	1.87267	-0.61883	0.00005
O	-3.69050	-0.65103	0.36402	-0.56825	0.13105
	27				
Trp1TS3	E=-686.102979031	H0=-685.889112	H298=-685.875406	G298=-685.930266	
H	3.66671	0.60550	-1.95495	0.46329	-0.00241
H	2.55329	-0.63685	-1.87005	0.44997	0.00055
H	3.34865	1.13641	0.28035	0.27612	-0.00008
H	1.57275	2.56894	-0.07974	0.40061	0.05341
H	1.71100	1.22345	-1.62541	0.28284	0.00586
H	-0.74068	3.39445	0.34133	0.25118	-0.00687
H	-3.04352	2.46411	0.53462	0.46536	-0.00448

H	4.36029	0.00876	0.31246	0.26062	-0.00106
H	3.03885	-2.39765	-0.18418	0.26166	-0.00086
H	-1.65026	-3.19422	-0.68018	0.26091	-0.00015
H	0.26159	-1.66171	-0.66898	0.25157	-0.00178
H	2.16727	-1.36886	2.38729	0.53827	-0.00005
C	2.50705	0.58389	-0.14519	-0.16802	-0.00174
C	1.29819	1.53480	-0.28709	-0.43693	0.21693
C	2.38770	-0.72385	0.62068	0.80308	-0.00048
C	-0.09020	1.27100	-0.06340	-0.02997	0.13223
C	-0.93573	0.08328	-0.14221	-0.11205	-0.01375
C	-0.97936	2.34776	0.21080	0.05187	0.22381
C	-2.26543	0.50715	0.11144	0.14359	-0.00941
C	-3.35938	-0.34809	0.11046	-0.22629	0.03493
C	-3.11163	-1.69556	-0.17245	-0.19098	0.02812
C	-1.81325	-2.14642	-0.45108	-0.22817	0.00295
C	-0.72295	-1.27324	-0.44225	-0.15724	0.06314
N	2.74502	0.33611	-1.60988	-0.84031	0.11819
N	-2.23651	1.89187	0.32208	-0.49537	0.15105
O	2.21674	-0.51124	1.92696	-0.69362	0.00094
O	2.45907	-1.81157	0.08852	-0.58198	0.01100

27

Trp1TS4	E=-686.105798289	H0=-685.891357	H298=-685.877721	G298=-685.931977	
H	-2.60329	0.18583	2.66649	0.41813	-0.00105
H	-2.89696	-1.30732	2.02499	0.40626	-0.00110
H	-2.31374	1.22091	0.65815	0.28532	0.00058
H	-0.91651	-1.52647	0.45344	0.26210	-0.00508
H	-1.72643	-0.65196	-1.25521	0.49563	0.03939
H	-0.43679	2.46972	0.05431	0.24403	-0.00831
H	1.98809	2.94521	-0.12790	0.46151	-0.00441
H	4.44888	1.55092	-0.23487	0.25766	-0.00090
H	5.35696	-0.76615	-0.18679	0.25877	-0.00033
H	3.85192	-2.71584	0.00910	0.25742	-0.00042
H	1.39862	-2.42092	0.16028	0.24633	-0.00088
H	-5.05517	-0.14034	-1.30150	0.55198	-0.00015
C	-2.37823	0.12413	0.62496	-0.17453	-0.00466
C	-1.03263	-0.47142	0.19839	-0.44105	0.33989
C	-3.31857	-0.14706	-0.55482	0.88751	0.00121
C	0.16304	0.28002	0.11884	-0.05590	0.05890
C	1.52067	-0.25503	0.04632	-0.10926	0.00907
C	0.31181	1.69044	0.04017	0.02445	0.27167
C	2.40351	0.84148	-0.06605	0.14642	-0.01398
C	3.78539	0.69610	-0.15091	-0.23577	0.02832
C	4.28543	-0.60808	-0.12261	-0.19822	0.01031
C	3.42871	-1.71711	-0.01127	-0.23220	0.01258
C	2.04562	-1.55322	0.07441	-0.17147	0.03229
N	-2.98173	-0.30753	1.86582	-0.86827	0.03621
N	1.62484	2.00381	-0.06614	-0.50977	0.14676
O	-2.77374	-0.55839	-1.62125	-0.60641	0.05269
O	-4.58699	0.05850	-0.46658	-0.60068	0.00140

27

Trp4TS5	E=-686.104978887	H0=-685.887888	H298=-685.874248	G298=-685.928362	
H	3.92495	-0.74058	-1.99801	0.42052	0.00003
H	2.62884	-1.77555	-1.96600	0.42231	0.00075
H	2.36116	0.84550	-1.24632	0.26732	0.00835
H	0.86430	-1.70871	-0.43132	0.24204	-0.01398
H	2.28659	-1.35851	1.44467	0.56063	0.00760
H	0.54836	2.33389	-0.60157	0.23944	-0.00924
H	-1.83852	2.94717	-0.28099	0.45764	-0.00398
H	-4.33128	1.70007	0.19082	0.25474	-0.00080
H	-5.33243	-0.55723	0.49438	0.25601	0.00018
H	-3.92702	-2.58925	0.42037	0.25423	-0.00063
H	-1.48727	-2.43655	0.04321	0.24124	-0.00002
H	4.41199	1.08673	1.53751	0.55393	0.00166
C	2.37482	-0.13119	-0.74405	-0.18082	-0.01874
C	0.98864	-0.62815	-0.47227	-0.30418	0.48889
C	3.12710	0.06946	0.57004	0.90503	0.04886
C	-0.13950	0.18827	-0.33601	-0.11274	-0.02837
C	-1.50997	-0.26802	-0.09283	-0.09920	0.03383
C	-0.22460	1.60089	-0.41983	0.00526	0.30364
C	-2.33503	0.87747	-0.04880	0.14716	-0.01985
C	-3.71229	0.80893	0.16103	-0.24261	0.02412
C	-4.26430	-0.46043	0.32953	-0.20636	-0.00648
C	-3.46360	-1.61713	0.28811	-0.23571	0.02029
C	-2.08816	-1.53245	0.07734	-0.18669	0.00345

	3.19729	-1.13998	-1.41384	-0.89325	0.01459
	1.58755	1.99008	-0.24936	-0.52413	0.12958
O		2.99305	-0.69307	1.60007	-0.62908	0.01307
O		3.95844	1.05013	0.67018	-0.61272	0.00320
	27					
Trp5TS2	E=-686.076624365	H0=-685.862704	H298=-685.848835	G298=-685.902946	
H		2.73948	2.34402	-1.34593	0.43195	0.00157
H		3.66204	2.45220	0.04443	0.43162	-0.00039
H		1.73434	1.07719	1.05439	0.38631	0.01631
H		4.62488	0.26596	-0.64675	0.55280	-0.00098
H		0.62089	2.01444	-0.10781	0.27790	-0.00819
H		0.77830	-2.00054	-0.57033	0.25238	-0.00450
H		-1.55660	-2.82676	-0.65913	0.45932	-0.00253
H		-4.19514	-1.85698	-0.33945	0.25604	-0.00060
H		-5.42856	0.24662	0.16022	0.25740	0.00008
H		-4.21444	2.35955	0.57143	0.25555	-0.00039
H		-1.74668	2.44856	0.50299	0.24167	-0.00019
H		3.28074	-2.04185	1.16258	0.54777	-0.00113
C		2.38862	0.81133	-0.01581	-0.11882	0.02752
C		0.90809	0.96803	-0.04795	-0.27962	0.25051
C		3.11747	-0.38088	0.25763	0.70207	0.29020
C		-0.13314	0.01180	-0.11140	-0.12110	0.00659
C		-1.55204	0.33620	0.02134	-0.08886	0.01396
C		-0.07554	-1.36505	-0.39859	0.04471	0.15303
C		-2.27008	-0.85867	-0.20462	0.13541	-0.01355
C		-3.66259	-0.92791	-0.16241	-0.23786	0.01890
C		-4.34447	0.25480	0.11809	-0.21032	-0.00318
C		-3.65202	1.45822	0.35102	-0.22259	0.01260
C		-2.25998	1.51129	0.30862	-0.20788	0.00792
N		3.19574	1.82477	-0.60363	-0.89730	0.02098
N		-1.33188	-1.86284	-0.45392	-0.50243	0.08605
O		2.59634	-1.38296	0.95126	-0.67426	0.05358
O		4.38715	-0.50840	-0.09118	-0.67107	0.07583
	27					
Trp5TS3	E=-686.125069510	H0=-685.909604	H298=-685.896204	G298=-685.950130	
H		2.73416	-1.40561	-2.04602	0.44853	0.00043
H		3.86764	-0.20541	-2.14903	0.44478	0.00032
H		2.33881	1.16933	-1.04743	0.28024	0.01084
H		3.96921	-1.15935	-0.29147	0.52032	-0.00086
H		1.02427	-1.53669	-0.28375	0.24515	-0.01317
H		0.38408	2.45212	-0.63683	0.24015	-0.00866
H		-2.04271	2.88720	-0.35187	0.45791	-0.00371
H		-4.44002	1.46544	0.12097	0.25462	-0.00076
H		-5.26759	-0.85130	0.49373	0.25584	0.00020
H		-3.71017	-2.77053	0.49187	0.25411	-0.00063
H		-1.28642	-2.44360	0.11705	0.24237	0.00001
H		3.25588	0.68100	2.45752	0.55294	0.00059
C		2.39362	0.14119	-0.67827	-0.17999	-0.02217
C		1.04009	-0.46508	-0.46580	-0.25196	0.46590
C		3.10669	0.08467	0.66661	0.83219	0.08497
C		-0.14329	0.26456	-0.34586	-0.11925	-0.03145
C		-1.47555	-0.28956	-0.09110	-0.09494	0.03232
C		-0.33485	1.66381	-0.46703	0.01805	0.28447
C		-2.38563	0.78999	-0.08563	0.14565	-0.01921
C		-3.75478	0.62364	0.12134	-0.24254	0.02328
C		-4.20917	-0.67827	0.32866	-0.20736	-0.00732
C		-3.32198	-1.77078	0.32722	-0.23498	0.02008
C		-1.95587	-1.58844	0.11706	-0.18585	0.00162
N		3.27451	-0.73040	-1.50817	-0.89219	0.01773
N		-1.65290	1.95598	-0.31552	-0.52219	0.12080
O		2.77909	0.88960	1.63161	-0.63047	0.01697
O		3.97916	-0.82911	0.78437	-0.63112	0.02738
	18					
R+	(Trp)	E=-402.293916182	H0=-402.146316	H298=-402.138108	G298=-402.178018	
H		-3.07236	2.24813	0.00000	0.24791	
H		-1.39976	3.04282	0.00000	0.25133	
H		-3.24713	-0.46450	0.00000	0.27512	
H		-1.61997	-2.31896	0.00000	0.47891	
H		1.16264	-2.75352	0.00000	0.26746	
H		3.32004	-1.50028	0.00000	0.26888	
H		3.34848	0.96688	0.00000	0.26786	
H		1.24316	2.27567	0.00000	0.26151	
C		-1.99256	2.13329	0.00000	-0.16620	
C		-1.41467	0.90921	0.00000	-0.14873	

C	0.00000	0.49946	0.00000	-0.08885	
C	0.01648	-0.33021	0.00000	0.18317	
C	0.01648	-0.90768	0.00000	0.12488	
C	1.17754	-1.66848	0.00000	-0.21735	
C	2.38192	-0.95577	0.00000	-0.19206	
C	2.39641	0.44685	0.00000	-0.19967	
C	1.20978	1.19103	0.00000	-0.16196	
N	-1.33573	-1.34321	0.00000	-0.45220	

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Rdot	(Trp)	E=-402.516888425	H0=-402.373170	H298=-402.364446	G298=-402.405721
H	-2.84098	2.58008	0.00000	0.20825	-0.01863
H	-1.07004	3.13138	0.00000	0.20823	-0.01904
H	-3.26798	-0.23178	0.00000	0.23282	-0.01128
H	-1.75561	-2.24235	0.00000	0.43945	-0.00287
H	1.01203	-2.82821	0.00000	0.23753	-0.00069
H	3.22471	-1.69282	0.00000	0.23772	0.00065
H	3.38223	0.77862	0.00000	0.23775	-0.00093
H	1.33437	2.17962	0.00000	0.23915	0.00085
C	-1.78827	2.32010	0.00000	-0.40072	0.68607
C	-1.37349	0.98448	0.00000	-0.15927	-0.12910
C	0.00000	0.47436	0.00000	-0.09081	0.06229
C	-2.18986	-0.16228	0.00000	-0.01660	0.36782
C	-0.06554	-0.94118	0.00000	0.14728	-0.02084
C	1.07914	-1.74385	0.00000	-0.26506	0.01980
C	2.31517	-1.09936	0.00000	-0.23420	-0.02174
C	2.40439	0.30656	0.00000	-0.26465	0.03037
C	1.25519	1.09622	0.00000	-0.19185	-0.02737
N	-1.40559	-1.29783	0.00000	-0.56503	0.08464

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Rdot+	(Trp)	E=-402.899644297	H0=-402.742472	H298=-402.733282	G298=-402.777909
H	-3.21086	-0.46642	0.00000	0.27237	-0.00567
H	-1.62326	-2.38296	0.00000	0.47458	-0.00424
H	1.19967	-2.80363	0.00000	0.27105	-0.00185
H	3.34237	-1.52934	0.00000	0.27021	-0.00466
H	3.36671	0.93909	0.00000	0.27278	0.00152
H	1.23715	2.22679	0.00000	0.26485	-0.00641
C	-1.36377	0.84876	0.00000	0.08298	0.32370
C	0.00000	0.43480	0.00000	-0.13273	-0.06373
C	-2.13402	-0.35760	0.00000	0.09504	0.18181
C	0.02382	-0.98582	0.00000	0.13985	0.02067
C	1.19041	-1.71841	0.00000	-0.18742	0.06544
C	2.40411	-0.98429	0.00000	-0.13961	0.15763
C	2.41804	0.41380	0.00000	-0.23730	-0.05984
C	1.22233	1.14154	0.00000	-0.09475	0.22151
N	-1.31833	-1.41628	0.00000	-0.47177	0.14404
C	-1.91646	2.22899	0.00000	-0.69888	-0.00918
H	-1.57115	2.78490	0.88047	0.27753	0.01953
H	-1.57115	2.78490	-0.88047	0.27753	0.01953
H	-3.00792	2.23002	0.00000	0.26458	0.00022

Optimized geometries for the energy profile of [Phe - NH_3]$^{+}$ as shown in Figure 7

19

(I)	E=-497.876922919	H0=-497.730298	H298=-497.720004	G298=-497.766255	
H	0.96952	-0.38984	2.13349	0.29649	-0.00044
H	-1.21646	-2.31904	-0.34764	0.27043	0.00004
H	-3.42077	-1.35287	-0.94354	0.28368	-0.00002
H	-3.82074	1.07776	-0.64143	0.27797	0.00009
H	-2.05457	2.57066	0.25349	0.28483	-0.00001
H	0.16553	1.63988	0.84763	0.28701	-0.00069
H	1.16642	-1.77818	-0.65405	0.31037	0.00126
H	0.32281	-2.06264	1.70902	0.29212	0.00042
C	-1.40578	-1.25636	-0.22240	-0.06641	-0.00127
C	-2.63131	-0.72006	-0.55300	-0.24131	0.00057
C	-2.85231	0.66060	-0.37905	-0.04930	-0.00074
C	-1.85378	1.51244	0.12658	-0.24137	0.00049
C	-0.61787	0.99577	0.46004	-0.06157	0.00125
C	-0.36414	-0.41120	0.29969	-0.13775	-0.00025
C	0.64506	-1.08571	1.36606	-0.30906	0.00262
C	1.14601	-0.92589	0.01983	-0.26325	-0.00365
C	2.17381	0.12339	-0.29291	0.75198	-0.06034
O	2.87245	0.05234	-1.34655	-0.27229	0.64101
O	2.43381	1.10470	0.43331	-0.41254	0.41967

19

(ITSII)	E=-497.866297536	H0=-497.721978	H298=-497.711552	G298=-497.758047

H	-3.05697	-0.06301	2.10659	0.30379	0.00963
H	-1.19045	-2.34714	-0.16721	0.27049	-0.00035
H	-3.44377	-1.48661	-0.73583	0.28304	0.00012
H	-3.89093	0.95407	-0.64340	0.27728	-0.00116
H	-2.12147	2.55773	0.02605	0.28425	0.00072
H	0.14973	1.73039	0.58789	0.29075	-0.00119
H	1.21922	-1.82519	-0.47535	0.30891	-0.00505
H	0.36463	-1.81162	1.95575	0.29377	0.01329
C	-1.39949	-1.28140	-0.13173	-0.08090	0.00712
C	-2.65212	-0.80302	-0.44875	-0.23439	0.00526
C	-2.90078	0.58370	-0.39252	-0.05327	0.04019
C	-1.90126	1.49652	-0.01550	-0.24356	-0.01458
C	-0.63645	1.04088	0.30142	-0.06037	0.03887
C	-0.35030	-0.37005	0.24684	-0.14972	0.00096
C	0.68176	-0.89474	1.46504	-0.28912	-0.01548
C	1.10557	-0.91828	0.10552	-0.16078	0.43540
C	2.38459	0.28355	-0.35360	0.84969	-0.06818
O	2.87741	-0.29376	-1.30514	-0.37868	0.40500
O	2.36858	1.22731	0.39080	-0.51118	0.14942

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(II)	E=-309.308443022	H0=-309.177230	H298=-309.169473	G298=-309.208495	
H	-2.24005	-1.05532	1.18618	0.29252	0.02972
H	-0.52689	2.16208	-0.01815	0.27009	-0.00077
H	1.95453	2.17908	0.11382	0.28000	0.00032
H	3.20113	0.03567	0.11986	0.27513	-0.00129
H	2.01608	-2.13998	-0.00318	0.28068	0.00116
H	-0.46367	-2.18705	-0.16491	0.27323	-0.00201
H	-2.44104	0.71753	-1.44197	0.26447	-0.01102
H	-2.43084	0.77438	1.28902	0.28698	0.04053
C	0.03386	1.23182	-0.02089	-0.09204	0.02234
C	1.41510	1.24019	0.05126	-0.23409	0.00526
C	2.11681	0.02206	0.05596	-0.07375	0.04283
C	1.44931	-1.21528	-0.01314	-0.23964	-0.01406
C	0.07177	-1.24471	-0.09674	-0.07575	0.05469
C	-0.66816	-0.01326	-0.11770	-0.18423	-0.02165
C	-2.17593	-0.09463	0.67917	-0.32848	-0.05391
C	-2.08763	-0.00726	-0.71804	0.00489	0.90785

16

(IITSIII)	E=-309.307684872	H0=-309.177176	H298=-309.169819	G298=-309.208133	
H	-2.13521	-1.14284	1.15074	0.28387	0.02591
H	-0.48416	2.18128	-0.05841	0.26946	-0.00225
H	1.98439	2.16137	0.19138	0.27856	0.00099
H	3.20773	0.00157	0.22280	0.27367	-0.00373
H	1.99515	-2.15424	0.00149	0.27933	0.00206
H	-0.46893	-2.16599	-0.27638	0.27155	-0.00361
H	-2.49228	0.85799	-1.27950	0.26645	-0.01253
H	-2.59258	0.63323	1.37005	0.28214	0.03908
C	0.06214	1.24299	-0.05006	-0.13204	0.07433
C	1.43937	1.22938	0.08619	-0.22223	-0.02179
C	2.12826	0.00422	0.10491	-0.09070	0.12651
C	1.44429	-1.21999	-0.01675	-0.23105	-0.04425
C	0.07161	-1.23102	-0.16394	-0.11757	0.10623
C	-0.64789	0.01093	-0.21364	-0.13183	-0.00817
C	-2.25054	-0.16038	0.70020	-0.23525	-0.08741
C	-2.08292	0.06181	-0.66729	-0.04437	0.80861

16

(III)	E=-309.376457797	H0=-309.243642	H298=-309.235785	G298=-309.275287	
H	-2.44348	1.98546	0.00000	0.22769	-0.01240
H	2.15363	0.90380	0.00000	0.26872	-0.00276
H	2.73128	-1.50887	0.00000	0.27935	0.00045
H	0.91480	-3.21057	0.00000	0.27162	-0.00791
H	-1.47533	-2.52552	0.00000	0.27870	0.00085
H	-2.07531	-0.13795	0.00000	0.25998	-0.00328
H	0.59187	2.63125	0.00000	0.26802	0.00018
H	-1.61547	3.63753	0.00000	0.25148	-0.01272
C	1.37287	0.14936	0.00000	-0.13711	0.08507
C	1.69447	-1.19014	0.00000	-0.21708	-0.02490
C	0.66062	-2.15458	0.00000	-0.04845	0.27815
C	-0.69989	-1.76707	0.00000	-0.22412	-0.03942
C	-1.03197	-0.43126	0.00000	-0.13819	0.10355
C	0.00000	0.57108	0.00000	-0.00005	0.18377
C	-1.52075	2.55631	0.00000	-0.16213	0.45537
C	-0.27235	1.97045	0.00000	-0.17844	-0.00399

Optimized Geometries for $[Cu^{II}(tpy)]^{\bullet 2+}$, $[Cu^{I}(tpy)]^{+}$, $[Cu^{II}(tpy)(H_2O)]^{\bullet 2+}$, $[Cu^{II}(L)]^{\bullet 2+}$, $[Cu^{I}(L)]^{+}$, $[Cu^{II}(L)(solvent)]^{2+}$ as shown in Table 1

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$[Cu^{II}(tpy)]^{\bullet 2+}$	E=-2382.362199500	H0=-2382.131300	H298=-2382.116340	G298=-2382.173017
Cu	0.00000	-1.15762	0.00000	
N	-1.94301	-0.93841	0.00000	
N	0.00000	0.74206	0.00000	
N	1.94301	-0.93841	0.00000	
C	-2.87858	-1.90486	0.00000	
C	-4.24217	-1.61028	0.00000	
C	-4.63959	-0.27519	0.00000	
C	-3.66729	0.73264	0.00000	
C	-2.32282	0.38243	0.00000	
C	-1.19696	1.34814	0.00000	
C	-1.22314	2.74519	0.00000	
C	0.00000	3.42886	0.00000	
C	1.22314	2.74519	0.00000	
C	1.19696	1.34814	0.00000	
C	2.32282	0.38243	0.00000	
C	3.66729	0.73264	0.00000	
C	4.63959	-0.27519	0.00000	
C	4.24217	-1.61028	0.00000	
C	2.87858	-1.90486	0.00000	
H	-2.52764	-2.93216	0.00000	
H	-4.96453	-2.41903	0.00000	
H	-5.69293	-0.01340	0.00000	
H	-3.96286	1.77580	0.00001	
H	-2.15798	3.29382	0.00000	
H	0.00000	4.51438	0.00000	
H	2.15798	3.29382	0.00000	
H	3.96286	1.77580	0.00000	
H	5.69293	-0.01340	0.00000	
H	4.96453	-2.41903	0.00000	
H	2.52764	-2.93216	0.00000	

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$[Cu^{I}(tpy)]^{+}$	E=-2382.735769430	H0=-2382.506324	H298=-2382.490722	G298=-2382.549364
Cu	0.00000	-1.31556	-0.04594	
N	-2.00984	-0.94829	-0.04536	
N	0.00000	0.72602	0.10398	
N	2.00984	-0.94830	-0.04543	
C	-3.00469	-1.85052	-0.05302	
C	-4.35253	-1.49790	0.01782	
C	-4.68206	-0.14776	0.10103	
C	-3.65644	0.79912	0.10932	
C	-2.32844	0.37932	0.03545	
C	-1.17724	1.33743	0.03016	
C	-1.22031	2.73385	-0.07580	
C	0.00000	3.41897	-0.11656	
C	1.22031	2.73384	-0.07584	
C	1.17724	1.33743	0.03011	
C	2.32844	0.37932	0.03536	
C	3.65645	0.79912	0.10916	
C	4.68206	-0.14776	0.10083	
C	4.35253	-1.49790	0.01764	
C	3.00469	-1.85052	-0.05314	
H	-2.70737	-2.89135	-0.12301	
H	-5.11391	-2.26965	0.00625	
H	-5.71842	0.16841	0.16072	
H	-3.89101	1.85488	0.18137	
H	-2.15323	3.28170	-0.14177	
H	0.00000	4.50092	-0.20144	
H	2.15323	3.28169	-0.14185	
H	3.89102	1.85488	0.18120	
H	5.71843	0.16841	0.16047	
H	5.11391	-2.26965	0.00604	
H	2.70737	-2.89135	-0.12311	

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$[Cu^{II}(tpy)(H_2O)]^{\bullet 2+}$	E=-2458.845874050	H0=-2458.590271	H298=-2458.572132	G298=-2458.635590
O	-0.00057	-3.08650	0.00024	
H	0.00090	-3.65608	0.78528	
H	0.00114	-3.65636	-0.78461	
Cu	0.00001	-1.02682	0.00005	
N	-1.99659	-0.72299	-0.00002	
N	0.00008	0.90151	0.00002	
N	1.99651	-0.72302	-0.00002	

C	2.96108	-1.65660	-0.00010
C	4.31665	-1.32580	-0.00015
C	-4.67579	0.02049	-0.00010
C	-3.67327	0.99555	-0.00002
C	-2.33890	0.60017	0.00001
C	-1.18745	1.53182	0.00003
C	-1.21657	2.92824	0.00006
C	0.00012	3.61796	0.00006
C	1.21679	2.92820	0.00004
C	1.18759	1.53179	0.00002
C	2.33893	0.60010	-0.00001
C	3.67332	0.99540	-0.00004
C	4.67577	0.02030	-0.00010
C	4.31671	-1.32597	-0.00013
C	2.96187	-1.65666	-0.00009
H	-2.63652	-2.69058	-0.00013
H	-5.06313	-2.11236	-0.00021
H	-5.72062	0.31401	-0.00012
H	-3.93650	2.04698	0.00000
H	-2.15339	3.47264	0.00007
H	0.00013	4.70329	0.00009
H	2.15363	3.47256	0.00005
H	3.93663	2.04680	-0.00002
H	5.72061	0.31376	-0.00012
H	5.06298	-2.11257	-0.00018
H	2.63641	-2.69064	-0.00009

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$[Cu^{II}(tpy)(CH_3OH)]^{\bullet 2+}$ E=-2498.152449360 H0=-2497.867941 H298=-2497.848305 G298=-2497.916358

C	0.00570	-3.80898	0.91638
O	0.05928	-2.86330	-0.20696
H	0.67782	-4.64312	0.71015
H	0.34444	-3.26640	1.79789
H	-1.01705	-4.16229	1.05845
H	-0.10638	-3.32213	-1.04419
Cu	0.00071	-0.84071	-0.11068
N	2.00111	-0.52180	-0.10240
N	-0.00334	1.08778	0.01309
N	-2.00249	-0.53225	-0.10417
C	2.96829	-1.44906	-0.18409
C	4.32203	-1.11294	-0.17774
C	4.67630	0.23128	-0.08262
C	3.67069	1.19956	0.00105
C	2.33785	0.79853	-0.01221
C	1.18162	1.72155	0.06042
C	1.20768	3.11427	0.16473
C	-0.00998	3.79969	0.21515
C	-1.22447	3.10843	0.16129
C	-1.19118	1.71605	0.05734
C	-2.34321	0.78754	-0.01599
C	-3.67734	1.18526	-0.00210
C	-4.68127	0.21554	-0.08217
C	-4.32421	-1.12840	-0.17343
C	-2.97000	-1.46012	-0.18057
H	2.64210	-2.48006	-0.25829
H	5.07141	-1.89354	-0.24669
H	5.72000	0.52860	-0.07461
H	3.93029	2.24940	0.07307
H	2.14344	3.65880	0.20668
H	-0.01271	4.88192	0.29681
H	-2.16269	3.64886	0.20061
H	-3.93885	2.23469	0.06842
H	-5.72557	0.51075	-0.07354
H	-5.07172	-1.91113	-0.23828
H	-2.64741	-2.49272	-0.24909

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$[Cu^{II}(4Cl\text{-}tpy)]^{\bullet 2+}$ E=-2841.948733120 H0=-2841.727777 H298=-2841.711515 G298=-2841.771577

Cu	0.00000	-1.65642	0.00014
N	1.94453	-1.43374	0.00004
N	0.00000	0.23838	-0.00002
N	-1.94453	-1.43374	0.00020
C	2.88110	-2.39920	0.00009
C	4.24447	-2.10336	0.00001
C	4.64089	-0.76804	-0.00011
C	3.66765	0.23890	-0.00016

C	2.32375	-0.11271	-0.00008
C	1.19498	0.85077	-0.00012
C	1.22809	2.24259	-0.00025
C	0.00000	2.93214	-0.00026
C	-1.22809	2.24259	-0.00015
C	-1.19498	0.85077	-0.00003
C	-2.32375	-0.11271	0.00010
C	-3.66765	0.23890	0.00013
C	-4.64089	-0.76804	0.00026
C	-4.24447	-2.10336	0.00036
C	-2.88110	-2.39920	0.00032
H	2.53122	-3.42685	0.00018
H	4.96750	-2.91153	0.00006
H	5.69400	-0.50527	-0.00017
H	3.96275	1.28222	-0.00025
H	2.15970	2.79590	-0.00033
Cl	0.00000	4.64652	-0.00041
H	-2.15970	2.79590	-0.00016
H	-3.96275	1.28222	0.00006
H	-5.69400	-0.50527	0.00029
H	-4.96750	-2.91153	0.00046
H	-2.53122	-3.42685	0.00040

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$[Cu^{I}(4Cl\text{-}tpy)]^{+}$ E=-2842.324560360 H0=-2842.105035 H298=-2842.089029 G298=-2842.147921

Cu	0.00000	-1.82241	0.00015
N	2.01428	-1.44707	0.00004
N	0.00000	0.22119	0.00000
N	-2.01428	-1.44707	0.00020
C	3.01131	-2.34646	0.00007
C	4.35987	-1.98827	0.00000
C	4.68730	-0.63536	-0.00011
C	3.65904	0.30899	-0.00015
C	2.33129	-0.11691	-0.00008
C	1.17586	0.83780	-0.00011
C	1.22545	2.23596	-0.00025
C	0.00000	2.91681	-0.00026
C	-1.22545	2.23596	-0.00015
C	-1.17586	0.83780	-0.00002
C	-2.33129	-0.11691	0.00011
C	-3.65904	0.30899	0.00014
C	-4.68730	-0.63536	0.00027
C	-4.35987	-1.98827	0.00036
C	-3.01131	-2.34646	0.00032
H	2.71560	-3.39008	0.00016
H	5.12314	-2.75822	0.00004
H	5.72387	-0.31435	-0.00017
H	3.89409	1.36705	-0.00024
H	2.15261	2.79557	-0.00034
Cl	0.00000	4.65356	-0.00043
H	-2.15261	2.79557	-0.00017
H	-3.89409	1.36705	0.00007
H	-5.72387	-0.31435	0.00029
H	-5.12314	-2.75822	0.00045
H	-2.71560	-3.39008	0.00039

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$[Cu^{II}(4Cl\text{-}tpy)(H_2O)]^{\bullet 2+}$ E=-2918.432820950 H0=-2918.187144 H298=-2918.167707 G298=-2918.234520

O	-0.00053	-3.57210	0.00011
H	0.00019	-4.14177	-0.78490
H	0.00025	-4.14172	0.78516
Cu	-0.00008	-1.51501	0.00005
N	1.99860	-1.20751	-0.00003
N	0.00003	0.40873	-0.00001
N	-1.99870	-1.20729	0.00011
C	2.96503	-2.13993	-0.00004
C	4.31959	-1.80765	-0.00009
C	4.67734	-0.46110	-0.00015
C	3.67375	0.51293	-0.00014
C	2.34013	0.11577	-0.00009
C	1.18556	1.04467	-0.00007
C	1.22155	2.43648	-0.00012
C	0.00017	3.13014	-0.00010
C	-1.22128	2.43661	-0.00004
C	-1.18544	1.04480	0.00001
C	-2.34011	0.11602	0.00008

C	-4.37368	0.51330	0.00012
C	-4.08756	-0.46065	0.00019
C	-4.31974	-1.80722	0.00022
C	-2.96521	-2.13964	0.00018
H	2.64083	-3.17431	0.00000
H	5.06672	-2.59346	-0.00010
H	5.72184	-0.16642	-0.00019
H	3.93645	1.56452	-0.00018
H	2.15491	2.98593	-0.00018
Cl	0.00027	4.84686	-0.00016
H	-2.15458	2.98616	-0.00002
H	-3.93629	1.56492	0.00009
H	-5.72184	-0.16587	0.00022
H	-5.06693	-2.59297	0.00027
H	-2.64106	-3.17404	0.00020

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$[Cu^{II}(4Cl\text{-}tpy)(CH_3OH)]^{\bullet 2+}$ E=-2957.739454900 H0=-2957.464831 H298=-2957.443920 G298=-2957.515232

C	1.02631	-4.14528	0.97492
O	0.87675	-3.23165	-0.16675
H	1.83664	-4.84426	0.76360
H	1.28063	-3.52983	1.83679
H	0.09106	-4.67901	1.15231
H	0.80308	-3.73283	-0.99283
Cu	0.32015	-1.28761	-0.10465
N	2.18698	-0.49303	-0.10419
N	-0.14620	0.58156	-0.02627
N	-1.70229	-1.46546	-0.10373
C	3.34991	-1.16076	-0.16324
C	4.58251	-0.50746	-0.16027
C	4.60162	0.88411	-0.09358
C	3.39135	1.58259	-0.03527
C	2.19533	0.87101	-0.04327
C	0.84837	1.48730	0.00310
C	0.54656	2.84539	0.06485
C	-0.80560	3.22205	0.09262
C	-1.82208	2.25377	0.05753
C	-1.44972	0.91365	-0.00311
C	-2.34897	-0.26362	-0.05043
C	-3.73928	-0.19498	-0.04486
C	-4.48279	-1.37793	-0.09625
C	-3.81488	-2.59971	-0.15125
C	-2.42055	-2.59879	-0.15253
H	3.28302	-2.24129	-0.21692
H	5.49855	-1.08546	-0.21005
H	5.54268	1.42463	-0.08869
H	3.38977	2.66537	0.01338
H	1.31963	3.60337	0.09052
Cl	-1.22201	4.88627	0.16884
H	-2.86055	2.56038	0.07758
H	-4.24446	0.76300	-0.00194
H	-5.56738	-1.34011	-0.09341
H	-4.35375	-3.53970	-0.19288
H	-1.86134	-3.52654	-0.19330

Optimized geometries for the $[Cu^{II}(L)(Phe)]^{\bullet 2+}$ as shown in Table 1, Figure 4a and Figure 6.

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$[Cu^{II}(tpy)(Phe)]^{\bullet 2+}$ (1) E=-2937.306962520 H0=-2936.883468 H298=-2936.855783 G298=-2936.944656

C	-1.32869	-0.48758	0.47822
C	-2.83201	-0.80339	0.33598
C	-3.61935	0.33651	-0.36035
C	-5.11903	0.15035	-0.24984
C	-5.79310	-0.77525	-1.06278
C	-5.85016	0.87055	0.71097
C	-7.22778	0.66633	0.85881
C	-7.16686	-0.97551	-0.91673
C	-7.88546	-0.25948	0.04757
N	-3.34715	-0.99541	1.75061
O	-0.66233	-0.48506	-0.62132
O	-0.88296	-0.23674	1.60768
H	-2.65366	-0.52694	2.36754
H	-3.39116	-1.97990	2.02462
H	-4.29303	-0.59236	1.84948
H	-2.98092	-1.74079	-0.20322
H	-3.29089	0.34733	-1.40366

H	-5.27781	1.29503	0.08542
H	-5.25166	-1.32427	-1.82925
H	-5.35658	1.63234	1.31288
H	-7.78293	1.24126	1.59330
H	-7.67964	-1.68238	-1.56142
H	-8.95430	-0.41394	0.15415
Cu	1.22040	-0.08053	-0.34889
N	1.20454	1.96360	-0.43393
N	3.09188	0.28366	0.06326
N	1.95571	-1.98832	-0.35071
C	0.16761	2.74209	-0.76980
C	0.25560	4.13437	-0.77759
C	1.46332	4.72865	-0.41672
C	2.54811	3.91776	-0.07261
C	2.39381	2.53329	-0.09581
C	3.47519	1.56323	0.20483
C	4.78959	1.85328	0.57974
C	5.66925	0.78830	0.79234
C	5.24435	-0.53253	0.62406
C	3.91803	-0.75949	0.24817
C	3.27089	-2.06937	-0.00949
C	3.92295	-3.29895	0.05388
C	3.21159	-4.46198	-0.25372
C	1.86998	-4.36488	-0.61855
C	1.27613	-3.10282	-0.65167
H	-0.74589	2.22709	-1.04616
H	-0.60430	4.72966	-1.06325
H	1.56728	5.80877	-0.40826
H	3.49713	4.36423	0.20035
H	5.12838	2.87476	0.70382
H	6.69454	0.98924	1.08566
H	5.93403	-1.35286	0.78236
H	4.96963	-3.35657	0.32893
H	3.70517	-5.42759	-0.21449
H	1.28937	-5.24331	-0.87678
H	0.23778	-2.96474	-0.93316

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$[Cu^{II}(tpy)(Phe)]^{\bullet 2+}$ (1') E=-2937.294062080 H0=-2936.872588 H298=-2936.844945 G298=-2936.934428

C	-1.42015	-0.58575	0.57921
C	-2.92487	-0.85147	0.47705
C	-3.64630	0.38072	-0.14547
C	-5.14706	0.19386	-0.21541
C	-5.71596	-0.65014	-1.18171
C	-5.98830	0.84735	0.69685
C	-7.37296	0.65413	0.65175
C	-7.09748	-0.84165	-1.22888
C	-7.92822	-0.19301	-0.30880
N	-3.35222	-1.14047	1.85685
O	-0.68571	-0.40147	-0.41824
O	-0.96031	-0.54373	1.79175
H	-1.82002	-0.75927	2.34008
H	-3.60336	-2.11663	1.99222
H	-4.16311	-0.58551	2.12610
H	-3.07147	-1.71156	-0.18529
H	-3.22345	0.53886	-1.14308
H	-3.41106	1.26637	0.45838
H	-5.08242	-1.14678	-1.91387
H	-5.56858	1.53364	1.43008
H	-8.01355	1.17232	1.35838
H	-7.52722	-1.48856	-1.98725
H	-9.00271	-0.33993	-0.34905
Cu	1.24226	-0.05480	-0.27423
N	1.22045	1.98037	-0.31998
N	3.13291	0.28679	-0.00008
N	1.93417	-1.96972	-0.31826
C	0.16156	2.76866	-0.55556
C	0.25958	4.16013	-0.56590
C	1.50021	4.74424	-0.31848
C	2.60667	3.92409	-0.07935
C	2.44180	2.54135	-0.09106
C	3.53782	1.56342	0.11039
C	4.88201	1.83792	0.37381
C	5.76430	0.76238	0.51164
C	5.31281	-0.55429	0.38149

C	3.95078	-0.76758	0.11728
C	3.24285	-2.06769	-0.08000
C	3.90998	-3.30591	-0.05660
C	3.16135	-4.46214	-0.29430
C	1.79687	-4.34928	-0.55353
C	1.21960	-3.07950	-0.55435
H	-0.77955	2.26543	-0.74743
H	-0.61979	4.76182	-0.76615
H	1.61250	5.82359	-0.31646
H	3.58040	4.36282	0.10480
H	5.24143	2.85537	0.47025
H	6.81272	0.95187	0.71806
H	6.00475	-1.38163	0.48366
H	4.97420	-3.37601	0.13592
H	3.64331	-5.43433	-0.28253
H	1.18456	-5.22114	-0.75439
H	0.16398	-2.93795	-0.75805

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$[Cu^{II}(tpy)(Phe)]^{\bullet 2+}$ (2) E=-2937.291745890 H0=-2936.868508 H298=-2936.840991 G298=-2936.929415

C	-0.95441	-0.20575	2.30903
C	-2.00766	-0.04408	1.21685
C	-3.34608	-0.77463	1.48403
C	-4.34509	-0.54044	0.36712
C	-5.01248	0.69084	0.25917
C	-4.61222	-1.53945	-0.58061
C	-5.52009	-1.31255	-1.62072
C	-5.91913	0.91899	-0.77867
C	-6.17067	-0.08122	-1.72368
N	-1.38810	-0.43961	-0.08908
O	0.24190	-0.32070	2.06838
O	-1.46180	-0.16146	3.52951
H	-0.75120	-0.22211	4.19535
H	-1.95879	-0.04042	-0.83732
H	-1.52443	-1.44622	-0.19752
H	-2.20989	1.03271	1.16412
H	-3.73610	-0.41561	2.44087
H	-3.15172	-1.84764	1.60698
H	-4.85454	1.46299	1.00982
H	-4.14463	-2.51767	-0.48457
H	-5.73140	-2.10180	-2.33547
H	-6.44486	1.86700	-0.83773
H	-6.88486	0.09214	-2.52225
Cu	0.62296	-0.06317	-0.21421
N	1.38494	-1.99900	-0.47280
N	2.53660	0.31284	-0.23267
N	0.58811	2.00872	-0.42027
C	0.71814	-3.14635	-0.66506
C	1.34724	-4.38869	-0.72601
C	2.73140	-4.43987	-0.57444
C	3.43547	-3.25012	-0.38186
C	2.73967	-2.04192	-0.34166
C	3.39384	-0.72097	-0.19501
C	4.76475	-0.48186	-0.06294
C	5.20550	0.84043	0.01986
C	4.29332	1.89623	-0.04496
C	2.93541	1.59528	-0.17700
C	1.82516	2.56728	-0.30858
C	2.00314	3.94967	-0.36034
C	0.89359	4.77595	-0.54748
C	-0.36674	4.19660	-0.68460
C	-0.47210	2.80873	-0.61211
H	-0.35791	-3.07956	-0.78769
H	0.76003	-5.28510	-0.89075
H	3.25867	-5.38756	-0.61146
H	4.51328	-3.26947	-0.27273
H	5.47766	-1.29656	-0.02844
H	6.26511	1.04958	0.12513
H	4.64137	2.92083	0.00374
H	2.99242	4.38176	-0.26729
H	1.01634	5.85313	-0.59414
H	-1.25371	4.79850	-0.84763
H	-1.43804	2.32707	-0.72036

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$[Cu^{II}(tpy)(Phe)]^{\bullet 2+}$ (2') E=-2937.278239930 H0=-2936.855305 H298=-2936.827694 G298=-2936.916249

C	-3.79112	-1.28632	2.42835
C	-3.87643	-0.84289	1.27493
C	-3.25730	-1.52655	1.28799
C	-4.15995	-0.96921	0.20438
C	-4.81907	0.25804	0.39136
C	-4.34124	-1.65279	-1.00866
C	-5.15529	-1.12076	-2.01559
C	-5.63378	0.78891	-0.61194
C	-5.79879	0.10308	-1.82021
N	-1.16977	-1.01844	-0.04247
O	-1.34382	-1.86884	3.41133
O	0.31752	-0.88189	2.23432
H	0.82793	-1.13176	3.02733
H	-1.83450	-0.72529	-0.76747
H	-1.06759	-2.02258	-0.20235
H	-2.01388	0.23655	1.40863
H	-3.68996	-1.37354	2.28109
H	-3.12832	-2.60931	1.17288
H	-4.73212	0.77931	1.34274
H	-3.88729	-2.63158	-1.15244
H	-5.30294	-1.67294	-2.93852
H	-6.16168	1.72234	-0.44123
H	-6.44477	0.50816	-2.59256
Cu	0.63182	-0.10562	-0.21243
N	1.88556	-1.72691	-0.59586
N	2.36412	0.78571	-0.17848
N	0.01482	1.87520	-0.19996
C	1.54961	-2.99534	-0.87506
C	2.49258	-4.00435	-1.06466
C	3.84331	-3.68034	-0.95500
C	4.20294	-2.36064	-0.67365
C	3.20570	-1.40102	-0.50375
C	3.47610	0.03324	-0.24881
C	4.73034	0.63479	-0.11538
C	4.78831	2.01618	0.08448
C	3.61708	2.77613	0.13035
C	2.39183	2.11987	-0.01232
C	1.05036	2.74771	-0.04387
C	0.83345	4.12273	0.02954
C	-0.46823	4.61723	-0.07858
C	-1.51887	3.72148	-0.26575
C	-1.23265	2.35776	-0.31739
H	0.49198	-3.22042	-0.96186
H	2.16646	-5.01283	-1.29318
H	4.60806	-4.43788	-1.09239
H	5.24889	-2.08828	-0.59647
H	5.64280	0.05328	-0.16674
H	5.75134	2.50428	0.19445
H	3.66867	3.84912	0.26953
H	1.66458	4.80598	0.15838
H	-0.65249	5.68542	-0.02697
H	-2.54312	4.06065	-0.37185
H	-2.03300	1.63956	-0.46292

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$[Cu^{II}(tpy)(Phe)(H_2O)]^{\bullet 2+}$ (1+H2O) E=-3013.762123070 H0=-3013.313535 H298=-3013.283599 G298=-3013.376900

C	1.44552	-0.81928	-0.89303
C	2.80937	-1.01211	-0.19493
C	3.44353	0.34008	0.21858
C	4.87772	0.18863	0.68298
C	5.17331	-0.31658	1.95968
C	5.93838	0.50862	-0.18215
C	7.26739	0.32414	0.21929
C	6.49812	-0.49673	2.36063
C	7.54736	-0.18133	1.48963
N	3.71866	-1.71865	-1.18601
O	0.49152	-0.43922	-0.17698
O	1.43706	-1.03101	-2.14720
H	3.30966	-1.52974	-2.12144
H	3.73478	-2.73228	-1.05198
H	4.68601	-1.36701	-1.10582
H	2.70254	-1.65928	0.67742
H	2.80481	0.74947	1.00613
H	3.39272	1.03289	-0.62986
H	4.36715	-0.54991	2.65173

H	5.73067	0.95113	-1.15549
H	3.07644	0.59062	-0.45348
H	6.71384	-0.87398	3.35539
H	8.57628	-0.31736	1.80672
Cu	-1.59982	0.00092	-0.88130
N	-1.47532	2.04816	-0.87212
N	-2.64876	0.40067	0.71924
N	-2.35596	-1.87016	-0.47097
C	-0.86824	2.80961	-1.79120
C	-0.79189	4.19801	-1.66869
C	-1.36292	4.80318	-0.55077
C	-1.99816	4.00835	0.40704
C	-2.04342	2.62815	0.21876
C	-2.72019	1.67683	1.13253
C	-3.41524	1.98624	2.30520
C	-4.02645	0.94617	3.00938
C	-3.95424	-0.36839	2.54137
C	-3.24342	-0.61611	1.36399
C	-3.07567	-1.92236	0.68243
C	-3.61347	-3.12312	1.14439
C	-3.41060	-4.28961	0.40387
C	-2.67177	-4.22591	-0.77638
C	-2.15799	-2.99223	-1.17577
H	-0.44704	2.28388	-2.64125
H	-0.29953	4.78164	-2.43845
H	-1.32265	5.88016	-0.42393
H	-2.45358	4.46385	1.27864
H	-3.48948	3.00624	2.66260
H	-4.57295	1.16267	3.92155
H	-4.44554	-1.16816	3.08224
H	-4.18649	-3.15448	2.06365
H	-3.82721	-5.23148	0.74574
H	-2.49550	-5.10733	-1.38266
H	-1.57083	-2.89470	-2.08261
O	-0.90338	-0.21999	-2.76753
H	-1.38211	-0.56267	-3.53359
H	0.03735	-0.60473	-2.71176

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$[Cu^{II}(tpy)(Phe)(CH_3OH)]^{\bullet 2+}$ (1+CH3OH) E=-3053.064761370 H0=-3052.587805 H298=-3052.555908 G298=-3052.654493

C	-1.48299	-0.83351	0.78428
C	-2.86168	-1.00079	0.10629
C	-3.49992	0.36356	-0.25509
C	-4.94296	0.22964	-0.69680
C	-5.26386	-0.24517	-1.97903
C	-5.98643	0.53534	0.19381
C	-7.32332	0.36647	-0.18796
C	-6.59642	-0.40994	-2.36033
C	-7.62846	-0.10904	-1.46400
N	-3.75120	-1.73530	1.09504
O	-0.54804	-0.41942	0.06015
O	-1.44461	-1.10071	2.02514
H	-3.30453	-1.59024	2.02226
H	-3.78773	-2.74193	0.91956
H	-4.71509	-1.36804	1.06232
H	-2.77293	-1.62240	-0.78651
H	-2.87471	0.79484	-1.04181
H	-3.43138	1.03129	0.61208
H	-4.47125	-0.46692	-2.69030
H	-5.76007	0.95408	1.17327
H	-8.11897	0.62162	0.50497
H	-6.83163	-0.76376	-3.35928
H	-8.66353	-0.23294	-1.76567
Cu	1.55003	-0.00336	0.71753
N	1.43479	2.04900	0.76983
N	2.59123	0.44602	-0.88030
N	2.27152	-1.86906	0.21673
C	0.82191	2.78328	1.70670
C	0.74488	4.17448	1.62495
C	1.32122	4.81240	0.52797
C	1.95965	4.04592	-0.45031
C	2.00528	2.66059	-0.30178
C	2.67717	1.73583	-1.24606
C	3.37813	2.08266	-2.40461
C	3.98111	1.06435	-3.14648

C	3.89249	-0.26613	-2.72972
C	3.14783	-0.55083	-1.56351
C	2.98959	-1.88243	-0.93829
C	3.50278	-3.07119	-1.45650
C	3.27456	-4.26667	-0.77200
C	2.53246	-4.24340	0.40772
C	2.04507	-3.01918	0.86520
H	0.39474	2.23165	2.53723
H	0.24741	4.73522	2.40834
H	1.28055	5.89256	0.43219
H	2.41620	4.52669	-1.30762
H	3.46381	3.11474	-2.72254
H	4.53241	1.30989	-4.04836
H	4.37601	-1.05011	-3.29987
H	4.07510	-3.07135	-2.37673
H	3.67186	-5.19994	-1.15765
H	2.33382	-5.14909	0.96972
H	1.45562	-2.95199	1.77304
O	0.93985	-0.26954	2.62105
H	0.01540	-0.66417	2.59019
C	1.69263	-0.62931	3.80018
H	2.57923	0.00499	3.83465
H	1.08276	-0.44601	4.68787
H	1.99619	-1.68016	3.77286

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[Cu^{II}(4Cl-tpy)(Phe)]$^{\bullet 2+}$ (1) E=-3396.894375600 H0=-3396.480833 H298=-3396.451831 G298=-3396.544162

C	1.79373	0.47366	0.46610
C	3.31274	0.72888	0.38471
C	4.07918	-0.43320	-0.29790
C	5.58019	-0.30367	-0.13663
C	6.31217	0.60629	-0.91651
C	6.25420	-1.06032	0.83771
C	7.63288	-0.90702	1.03101
C	7.68677	0.75564	-0.72530
C	8.34846	0.00368	0.25221
N	3.78221	0.88115	1.81982
O	1.16917	0.51633	-0.65718
O	1.29520	0.22372	1.57341
H	3.05152	0.42820	2.40412
H	3.85010	1.85923	2.11154
H	4.70953	0.44380	1.94562
H	3.51970	1.66618	-0.13528
H	3.78534	-0.42132	-1.35154
H	3.73678	-1.38426	0.12746
H	5.81388	1.18300	-1.69259
H	5.71526	-1.81079	1.41442
H	8.14377	-1.50962	1.77537
H	8.24445	1.45075	-1.34502
H	9.41818	0.11845	0.39420
Cu	-0.73558	0.18683	-0.45373
N	-0.80448	-1.85755	-0.57361
N	-2.62966	-0.10552	-0.11103
N	-1.39603	2.12486	-0.44706
C	0.20930	-2.67430	-0.88811
C	0.06274	-4.06139	-0.92296
C	-1.18049	-4.60929	-0.61334
C	-2.24123	-3.75823	-0.29138
C	-2.02714	-2.38184	-0.28519
C	-3.07455	-1.36887	-0.00318
C	-4.40666	-1.61607	0.32331
C	-5.24958	-0.51462	0.52760
C	-4.76568	0.79458	0.39498
C	-3.42224	0.96525	0.06645
C	-2.71753	2.25384	-0.14748
C	-3.32282	3.50678	-0.08492
C	-2.55649	4.64517	-0.35020
C	-1.20856	4.50015	-0.67274
C	-0.66378	3.21593	-0.70737
H	1.15271	-2.19468	-1.12475
H	0.90601	-4.68831	-1.18998
H	-1.33037	-5.68394	-0.62735
H	-3.21697	-4.16850	-0.05857
H	-4.79706	-2.62128	0.42011
Cl	-6.90215	-0.77288	0.93889

H	-4.30015	1.63514	0.54674
H	-4.87585	3.60289	0.15645
H	-3.01294	5.62888	-0.31122
H	-0.58565	5.35857	-0.89758
H	0.37719	3.04123	-0.95709

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[Cu^{II}(4Cl-tpy)(Phe)]$^{\bullet 2+}$ (2) E=-3396.879002880 H0=-3396.465719 H298=-3396.436872 G298=-3396.529380

C	1.43552	0.14642	2.31174
C	2.46829	-0.09201	1.21370
C	3.84455	0.57354	1.46092
C	4.81785	0.28835	0.33325
C	5.41438	-0.97762	0.21333
C	5.13036	1.27531	-0.61300
C	6.01341	1.00328	-1.66359
C	6.29599	-1.25099	-0.83511
C	6.59336	-0.26181	-1.77845
N	1.86183	0.31093	-0.09652
O	0.24747	0.34136	2.08039
O	1.94873	0.07552	3.52817
H	1.25001	0.18847	4.19981
H	2.37324	-0.16942	-0.83943
H	2.09238	1.29395	-0.25091
H	2.61444	-1.17850	1.18129
H	4.22799	0.20023	2.41496
H	3.70377	1.65522	1.58124
H	5.22146	-1.74334	0.96238
H	4.71877	2.27755	-0.50797
H	6.26075	1.78285	-2.37740
H	6.76679	-2.22678	-0.90405
H	7.28841	-0.47099	-2.58526
Cu	-0.17795	0.11891	-0.18121
N	-0.76462	2.12287	-0.42723
N	-2.11439	-0.08401	-0.25384
N	-0.32915	-1.95288	-0.38319
C	0.00396	3.21197	-0.57133
C	-0.51381	4.50474	-0.63288
C	-1.89335	4.67283	-0.53479
C	-2.70298	3.54505	-0.39011
C	-2.11429	2.28152	-0.34458
C	-2.88262	1.01912	-0.23628
C	-4.26985	0.90967	-0.15195
C	-4.83023	-0.37266	-0.09066
C	-4.01195	-1.50942	-0.13165
C	-2.63354	-1.32408	-0.21722
C	-1.61474	-2.39590	-0.31274
C	-1.91778	-3.75598	-0.36783
C	-0.88346	-4.68200	-0.51432
C	0.42858	-4.22151	-0.60761
C	0.65834	-2.84856	-0.53508
H	1.07472	3.05641	-0.65018
H	0.15424	5.34969	-0.75666
H	-2.33608	5.66271	-0.57494
H	-3.77851	3.65622	-0.32016
H	-4.91316	1.78008	-0.13557
Cl	-6.53791	-0.55377	0.02169
H	-4.45661	-2.49587	-0.09917
H	-2.94491	-4.09597	-0.30790
H	-1.10338	-5.74352	-0.56285
H	1.26178	-4.90314	-0.73707
H	1.66780	-2.45908	-0.60934

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[Cu^{II}(tpy)(Phe)]$^{\bullet 2+}$ TS-1,2-hydride shift E=-2937.226364590 H0=-2936.812295 H298=-2936.782968

C	-1.27257	-0.27852	0.72497
C	-2.79062	-0.41870	0.82674
C	-3.65735	-0.13646	-0.25309
C	-5.11711	-0.17446	-0.25617
C	-5.88163	-0.49088	0.88771
C	-5.77385	0.13107	-1.46727
C	-7.16420	0.12397	-1.53393
C	-7.26923	-0.50048	0.81335
C	-7.91143	-0.19430	-0.39555
N	-2.91853	1.47391	2.47317
O	-0.80102	-0.11461	-0.47156
O	-0.60495	-0.34791	1.75553

H	-2.13996	1.23631	3.07780
H	-3.03852	1.51153	3.05061
H	-2.76472	2.41752	2.12361
H	-3.16906	-0.89475	1.72257
H	-3.12081	-1.29717	-0.19492
H	-3.17321	0.29084	-1.13083
H	-5.39975	-0.72014	1.83293
H	-5.19095	0.37342	-2.35181
H	-7.66420	0.36227	-2.46668
H	-7.85656	-0.74049	1.69349
H	-8.99573	-0.20205	-0.44555
Cu	1.14761	-0.04482	-0.31329
N	1.41511	1.98236	-0.41449
N	3.07601	0.05331	-0.02986
N	1.61217	-2.04150	-0.35627
C	0.47543	2.89716	-0.68737
C	0.75910	4.26248	-0.72897
C	2.06317	4.68148	-0.47058
C	3.04490	3.72759	-0.18994
C	2.69453	2.37892	-0.17443
C	3.64528	1.26623	0.06793
C	5.00888	1.36972	0.35300
C	5.74177	0.19212	0.52531
C	5.12460	-1.05550	0.40420
C	3.75735	-1.09468	0.11732
C	2.91875	-2.30222	-0.07903
C	3.39561	-3.61001	-0.01731
C	2.51389	-4.66716	-0.25664
C	1.18140	-4.38845	-0.55423
C	0.77020	-3.05594	-0.59075
H	-0.51972	2.51189	-0.88159
H	-0.02650	4.97241	-0.96207
H	2.31961	5.73569	-0.49204
H	4.06543	4.03654	0.00387
H	5.49565	2.33361	0.44025
H	6.80203	0.24739	0.74980
H	5.70030	-1.96448	0.52987
H	4.43688	-3.80930	0.20732
H	2.86872	-5.69180	-0.21551
H	0.46941	-5.18072	-0.75604
H	-0.25369	-2.78297	-0.82101

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$[Cu^{II}(tpy)(Phe)]^{\bullet 2+}$ TS-phenonium E=-2937.242643850 H0=-2936.825926 H298=-2936.796546 G298=-2936.889546

C	1.86615	-1.07108	0.35941
C	3.20202	-0.81416	1.05390
C	4.31554	-1.69937	0.89121
C	4.58153	-0.53346	-0.12560
C	4.29024	-0.71636	-1.50631
C	5.40869	0.55298	0.28082
C	5.95386	1.40269	-0.66694
C	4.84984	0.13724	-2.44485
C	5.67800	1.19093	-2.02816
N	2.10892	-1.87833	3.36167
O	0.96271	-0.18965	0.65010
O	1.75519	-2.05027	-0.37496
H	1.31606	-1.35924	3.73363
H	2.80573	-1.90943	4.10435
H	1.79502	-2.83774	3.22666
H	3.24194	-0.00620	1.77178
H	4.11457	-2.64353	0.39312
H	5.06377	-1.74169	1.67704
H	3.64359	-1.53300	-1.80890
H	5.63596	0.69052	1.33446
H	6.60305	2.21666	-0.36232
H	4.65377	-0.01412	-3.50103
H	6.11510	1.85278	-2.77015
Cu	-0.88296	-0.01882	0.14127
N	-0.76059	2.04442	0.29659
N	-2.76135	0.48547	-0.14447
N	-1.72169	-1.88553	-0.16760
C	0.35091	2.75134	0.53661
C	0.33915	4.14415	0.62126
C	-0.87034	4.81486	0.45035
C	-2.03047	4.07699	0.20304

C	-1.94606	2.68755	0.13213
C	-3.09835	1.78853	-0.11402
C	-4.42598	2.17201	-0.30002
C	-5.38257	1.17634	-0.51236
C	-5.00944	-0.16818	-0.53755
C	-3.66222	-0.49063	-0.34728
C	-3.07258	-1.84750	-0.34972
C	-3.81487	-3.01125	-0.53409
C	-3.16016	-4.24567	-0.53678
C	-1.78023	-4.27529	-0.36343
C	-1.09356	-3.07226	-0.18332
H	1.25513	2.16837	0.66593
H	1.25951	4.68218	0.81819
H	-0.91636	5.89743	0.50946
H	-2.97971	4.58241	0.06978
H	-4.71806	3.21489	-0.28008
H	-6.42234	1.45018	-0.65876
H	-5.75312	-0.93783	-0.70337
H	-4.88793	-2.96458	-0.67638
H	-3.72370	-5.16199	-0.67943
H	-1.22806	-5.20833	-0.37180
H	-0.01535	-3.03726	-0.08315

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$[Cu^{II}(tpy)(Phe)]^{\bullet 2+}$	TS-lactone	E=-2937.224633820	H0=-2936.809376	H298=-2936.779491	G298=-2936.875794
C	-1.50478	-0.19195	0.47901		
C	-2.94984	-0.21705	0.57372		
C	-3.81757	0.93213	0.21240		
C	-5.10491	0.54694	-0.49479		
C	-5.06140	-0.09085	-1.74354		
C	-6.34499	0.84578	0.08378		
C	-7.52987	0.51014	-0.57624		
C	-6.24694	-0.42757	-2.40025		
C	-7.48199	-0.12897	-1.81767		
N	-4.33499	-1.13360	3.08508		
O	-0.49664	0.11201	1.14944		
O	-1.67708	-0.64097	-0.68828		
H	-4.21679	-0.47948	3.85716		
H	-4.13850	-2.05629	3.47019		
H	-5.32898	-1.13133	2.85891		
H	-3.40692	-1.14525	0.90353		
H	-3.23946	1.68053	-0.34384		
H	-4.05128	1.39277	1.18759		
H	-4.10630	-0.31551	-2.21108		
H	-6.39116	1.35447	1.04381		
H	-8.48630	0.75279	-0.12404		
H	-6.20607	-0.91704	-3.36825		
H	-8.40224	-0.38712	-2.33186		
Cu	1.35242	0.02058	0.47961		
N	1.66943	-1.98836	0.38761		
N	3.13125	0.02022	-0.29563		
N	1.70304	2.02394	0.45580		
C	0.85149	-2.95756	0.82315		
C	1.16767	-4.31020	0.69839		
C	2.37432	-4.66127	0.09699		
C	3.23286	-3.65325	-0.35073		
C	2.85947	-2.32147	-0.18960		
C	3.69342	-1.16378	-0.59170		
C	4.94905	-1.19434	-1.20339		
C	5.58014	0.02097	-1.48412		
C	4.97164	1.23589	-1.15563		
C	3.71534	1.20474	-0.54571		
C	2.90110	2.36081	-0.10058		
C	3.29579	3.69218	-0.20354		
C	2.44907	4.69276	0.28276		
C	1.23315	4.33557	0.86212		
C	0.89459	2.98369	0.92840		
H	-0.07322	-2.63736	1.28930		
H	0.47851	-5.06161	1.06678		
H	2.65138	-5.70394	-0.01985		
H	4.17941	-3.90921	-0.81228		
H	5.43020	-2.13116	-1.45739		
H	6.55556	0.02120	-1.95983		
H	5.46991	2.17310	-1.37269		
H	4.24895	3.95339	-0.64837		

H -2.74267 5.73510 0.21249
H -0.56469 5.08198 1.25924
H -0.03617 2.64965 1.37342

Optimized geometries for the $[Cu^{II}(tpy)(Tyr)]^{2+}$ as shown in Table 1, Figure 4b

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$[Cu^{II}(tpy)(Tyr)]^{\bullet 2+}$ (1) E=-3012.533846330 H0=-3012.106236 H298=-3012.077418 G298=-3012.168685

C	-1.01395	-0.59931	0.34092
C	-2.52255	-0.86120	0.16638
C	-3.29705	0.40226	-0.29958
C	-4.79736	0.24388	-0.18232
C	-5.53276	-0.47497	-1.13866
C	-5.49093	0.78803	0.91613
C	-6.86592	0.61535	1.06398
C	-6.90856	-0.65027	-1.00653
C	-7.58251	-0.10855	0.10045
N	-3.02812	-1.28840	1.53073
O	-0.35008	-0.44667	-0.74979
O	-0.55727	-0.52183	1.49159
O	-8.91438	-0.23791	0.29783
H	-2.34350	-0.91493	2.21682
H	-3.05640	-2.30455	1.64295
H	-3.98020	-0.91790	1.68821
H	-2.69989	-1.68385	-0.52881
H	-2.99055	0.58641	-1.33354
H	-2.96349	1.26005	0.29699
H	-5.03433	-0.88712	-2.01314
H	-4.96140	1.39955	1.64539
H	-7.40157	1.05081	1.90058
H	-7.46064	-1.19623	-1.76699
H	-9.34389	-0.70961	-0.42983
Cu	1.52594	-0.06892	-0.39694
N	1.49595	1.97494	-0.45200
N	3.37471	0.30413	0.10188
N	2.27915	-1.97102	-0.39934
C	0.46690	2.74765	-0.82400
C	0.54463	4.14067	-0.81716
C	1.73215	4.74085	-0.40272
C	2.80836	3.93550	-0.02026
C	2.66595	2.55019	-0.06061
C	3.74068	1.58468	0.27669
C	5.03400	1.87982	0.71541
C	5.91107	0.81872	0.95648
C	5.50489	-0.50302	0.75301
C	4.19932	-0.73501	0.31269
C	3.57539	-2.04635	0.00873
C	4.23295	-3.27178	0.09419
C	3.54767	-4.43689	-0.26048
C	2.22618	-4.34565	-0.69390
C	1.62542	-3.08757	-0.74575
H	-0.43000	2.22635	-1.14034
H	-0.30751	4.73192	-1.13293
H	1.82740	5.82162	-0.38208
H	3.74195	4.38688	0.29465
H	5.35857	2.90217	0.86732
H	6.91992	1.02355	1.29982
H	6.19280	-1.32017	0.93370
H	5.26424	-3.32431	0.42311
H	4.04581	-5.39932	-0.20433
H	1.66658	-5.22559	-0.99050
H	0.60205	-2.95565	-1.08016

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$[Cu^{II}(tpy)(Tyr)]^{\bullet 2+}$ (2) E=-3012.518197100 H0=-3012.090904 H298=-3012.062242 G298=-3012.152790

C	0.73332	-0.70805	2.43190
C	1.77819	-0.83660	1.32860
C	3.05396	0.00367	1.64531
C	4.06003	-0.01995	0.51630
C	4.85030	-1.15462	0.27388
C	4.22827	1.09263	-0.32572
C	5.13674	1.07719	-1.38166
C	5.76548	-1.18615	-0.77672
C	5.91035	-0.06832	-1.61399
N	1.15901	-0.46921	0.01382
O	-0.41391	-0.31633	2.24828

	1.20579	-1.06714	3.61505
	0.74681	-0.02267	-2.65356
H	0.51824	-0.97222	4.30057
H	1.33004	-1.22006	-0.65457
H	1.68991	0.31130	-0.38187
H	2.07606	-1.88996	1.29321
H	3.47890	-0.39477	2.57096
H	2.75541	1.03695	1.86233
H	4.77656	-2.02150	0.92707
H	3.67716	2.01100	-0.12929
H	5.27963	1.94478	-2.01675
H	6.37944	-2.06896	-0.93459
H	7.31898	-0.82246	-2.70567
Cu	-0.87816	-0.05691	0.04311
N	-0.85638	2.02402	0.06666
N	-2.74622	0.31910	-0.41300
N	-1.58555	-1.99460	-0.27477
C	0.17421	2.83062	0.35751
C	0.05665	4.21843	0.40996
C	-1.18788	4.79026	0.15311
C	-2.26806	3.95697	-0.14200
C	-2.07611	2.57592	-0.17829
C	-3.15012	1.60030	-0.47167
C	-4.47674	1.90033	-0.79288
C	-5.35519	0.84617	-1.04995
C	-4.90797	-0.47534	-0.99164
C	-3.57008	-0.71303	-0.66611
C	-2.91319	-2.03649	-0.57078
C	-3.57566	-3.24918	-0.76347
C	-2.86350	-4.44398	-0.64944
C	-1.50499	-4.39480	-0.34151
C	-0.90993	-3.14777	-0.16150
H	1.12601	2.35298	0.55958
H	0.92224	4.82663	0.64753
H	-1.32062	5.86677	0.18459
H	-3.24500	4.38336	-0.33615
H	-4.82420	2.92474	-0.84747
H	-6.38989	1.05504	-1.30162
H	-5.58985	-1.29062	-1.20010
H	-4.63335	-3.26834	-0.99757
H	-3.36436	-5.39520	-0.79720
H	-0.91242	-5.29723	-0.24121
H	0.14382	-3.07743	0.08566

Optimized geometries for the $[Cu^{II}(tpy)(Trp)]^{2+}$ as shown in Table 1, Figure 4c

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$[Cu^{II}(tpy)(Trp)]^{\bullet 2+}$	(1)	E=-3068.891956050	H0=-3068.438945	H298=-3068.409345	G298=-3068.502269
C	-0.73754	-0.73032	0.13087	0.77059	-0.00373
C	-2.20221	-1.12042	-0.14820	-0.15151	0.00525
C	-2.98609	-0.00429	-0.89365	-0.46420	-0.00012
C	-4.46674	-0.24210	-0.91452	-0.17858	0.00008
C	-5.19849	-0.89896	-1.88318	-0.00009	0.00025
C	-5.40108	0.13066	0.12688	-0.13645	-0.00003
C	-6.67926	-0.34881	-0.27577	0.15148	0.00004
C	-5.29309	0.83786	1.34682	-0.26581	0.00017
C	-6.43385	1.01893	2.12238	-0.23324	-0.00003
C	-7.82821	-0.16299	0.50129	-0.23281	0.00007
C	-7.68601	0.51863	1.70522	-0.21881	0.00013
N	-2.82548	-1.38870	1.20977	-0.79432	0.00084
N	-6.51620	-0.96437	-1.50203	-0.54430	0.00005
O	0.01958	-0.65291	-0.90681	-0.82277	0.07929
O	-0.39791	-0.48919	1.29932	-0.69429	-0.00009
H	-2.20987	-0.91662	1.90007	0.48493	-0.00003
H	-2.84355	-2.38440	1.44203	0.46623	-0.00001
H	-3.79542	-1.03007	1.25890	0.48310	0.00018
H	-2.25373	-2.04573	-0.72501	0.27607	-0.00021
H	-2.57188	0.03600	-1.90506	0.28041	0.00001
H	-2.76553	0.96061	-0.41855	0.25064	0.00003
H	-4.87836	-1.31354	-2.82951	0.25063	-0.00001
H	-7.25891	-1.36423	-2.05705	0.45850	0.00000
H	-4.35092	1.28381	1.66164	0.23284	0.00000
H	-6.36755	1.57034	3.05474	0.25508	0.00000
H	-8.79708	-0.53051	0.17765	0.25941	0.00000
H	-8.55764	0.68104	2.33045	0.26015	-0.00001

C	1.82394	-0.10662	-0.43213	0.78801	0.59983
N	1.06585	1.92648	-0.59348	-0.56856	0.09868
N	3.59918	0.42557	0.17806	2.44127	0.08191
N	2.70693	-1.94536	-0.27992	-0.56488	0.09936
C	0.60322	2.60438	-1.07365	0.06391	-0.00743
C	0.57953	3.99846	-1.12461	-0.23402	0.00584
C	1.68624	4.70239	-0.65377	-0.14175	-0.00414
C	2.78572	3.99608	-0.15857	-0.21865	0.00284
C	2.74640	2.60343	-0.14541	0.14124	0.00065
C	3.85915	1.73630	0.31416	-0.80921	0.00994
C	5.09212	2.14660	0.82776	-0.29457	0.00631
C	6.02219	1.16584	1.18284	-0.13609	-0.00365
C	5.72732	-0.19028	1.01772	-0.28273	0.00611
C	4.47781	-0.53867	0.49865	-0.85170	0.01064
C	3.97271	-1.90540	0.21871	0.13660	0.00088
C	4.70769	-3.07349	0.40952	-0.21383	0.00285
C	4.13361	-4.30105	0.06790	-0.14211	-0.00419
C	2.84313	-4.32811	-0.45743	-0.23440	0.00592
C	2.15968	-3.12163	-0.61302	0.06348	-0.00750
H	-0.22801	2.00586	-1.42999	0.25219	0.00299
H	-0.28707	4.51067	-1.52717	0.27683	0.00047
H	1.70154	5.78722	-0.67531	0.27817	0.00011
H	3.65805	4.52852	0.20204	0.26831	0.00089
H	5.33098	3.19611	0.95040	0.26906	0.00139
H	6.98576	1.46052	1.58573	0.28207	0.00006
H	6.45654	-0.94468	1.28746	0.26918	0.00140
H	5.71455	-3.03512	0.80871	0.26841	0.00090
H	4.69381	-5.22019	0.20550	0.27822	0.00011
H	2.36954	-5.25967	-0.74604	0.27675	0.00047
H	1.15527	-3.08070	-1.02049	0.25376	0.00299

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$[Cu^{II}(tpy)(Trp)]^{\bullet 2+}$ (2) E=-3068.876614880 H0=-3068.423859 H298=-3068.394426 G298=-3068.486478

C	-0.27228	-0.76150	2.37094
C	-1.39401	-0.72619	1.34200
C	-2.58956	-1.67394	1.61527
C	-3.60701	-1.58982	0.51443
C	-4.00893	-2.61526	-0.31726
C	-4.34802	-0.41581	0.10906
C	-5.17067	-0.80494	-0.98463
C	-4.43050	0.91245	0.58041
C	-5.29272	1.80067	-0.05462
C	-6.03775	0.08682	-1.62729
C	-6.08198	1.39296	-1.15230
N	-0.79052	-0.94084	-0.01142
N	-4.93863	-2.14809	-1.21653
O	0.90799	-0.61554	2.07130
O	-0.70575	-0.91583	3.61169
H	0.04207	-0.88293	4.23739
H	-1.48637	-0.64789	-0.70143
H	-0.71894	-1.94964	-0.15808
H	-1.76900	0.30373	1.35818
H	-3.01690	-1.39461	2.58464
H	-2.22421	-2.70302	1.72214
H	-3.72448	-3.65908	-0.31191
H	-5.43381	-2.71852	-1.88629
H	-3.88333	1.23200	1.46453
H	-5.38912	2.81614	0.31724
H	-6.66500	-0.22927	-2.45509
H	-6.75321	2.10635	-1.61913
Cu	1.06205	-0.10597	-0.20818
N	2.24669	-1.78685	-0.61753
N	2.83082	0.71408	-0.25964
N	0.53008	1.90495	-0.28830
C	1.85950	-3.04516	-0.87002
C	2.75938	-4.09779	-1.02898
C	4.12188	-3.82918	-0.91446
C	4.53496	-2.52019	-0.66094
C	3.57729	-1.51552	-0.52269
C	3.90784	-0.08769	-0.30380
C	5.18757	0.46139	-0.18268
C	5.30637	1.84334	-0.02118
C	4.16970	2.65475	-0.00070
C	2.91720	2.04889	-0.12908
C	1.60462	2.73486	-0.17711

C	-1.45033	4.12057	-0.15878
C	-0.14112	4.66826	-0.27437
C	-0.92117	3.81398	-0.41140
C	-0.69563	2.43809	-0.41021
H	0.79323	-3.22476	-0.96130
H	2.39297	-5.09637	-1.23892
H	4.85463	-4.62152	-1.02736
H	5.59074	-2.29047	-0.58018
H	6.07315	-0.16154	-0.21366
H	6.28963	2.29133	0.07950
H	4.26793	3.72779	0.11014
H	2.31279	4.77019	-0.06759
H	0.03570	5.74493	-0.26681
H	-1.93108	4.19282	-0.52048
H	-1.52924	1.75148	-0.51627

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$[Cu^{II}(tpy)(Trp)]^{\bullet 2+}$ (TS-phenonium) E=-3068.839203900 H0=-3068.391701 H298=-3068.360969 G298=-3068.455414

C	-0.91814	-1.27400	-1.08079
C	-2.11302	-2.14922	-1.37941
C	-2.93353	-2.81774	-0.36966
C	-3.74310	-1.54225	-0.34949
C	-4.72923	-1.20774	-1.30116
C	-3.80951	-0.51459	0.68046
C	-4.84295	0.37390	0.29800
C	-3.15613	-0.30981	1.90476
C	-3.54474	0.77229	2.69350
C	-5.23999	1.46142	1.07671
C	-4.56933	1.64850	2.28480
N	-0.70087	-3.81674	-2.30372
N	-5.36215	-0.08594	-0.91793
O	-0.58439	-1.12327	0.16427
O	-0.29114	-0.78664	-2.03046
H	-0.11921	-3.27578	-2.94123
H	-1.22701	-4.49605	-2.85041
H	-0.09151	-4.33690	-1.67664
H	-2.45272	-2.11711	-2.40468
H	-2.43104	-2.99600	0.57916
H	-3.48025	-3.69616	-0.71159
H	-5.01194	-1.72777	-2.20706
H	-6.12595	0.34453	-1.42428
H	-2.36803	-0.97828	2.23147
H	-3.06007	0.93645	3.65062
H	-6.05014	2.11749	0.77397
H	-4.85704	2.47165	2.93061
Cu	1.04264	-0.04253	0.12017
N	2.36960	-1.52392	0.62525
N	2.72840	0.93649	-0.03943
N	0.32608	1.86292	-0.15895
C	2.05850	-2.76094	1.03435
C	3.03636	-3.70233	1.35732
C	4.37729	-3.33884	1.24089
C	4.70182	-2.04678	0.81985
C	3.67406	-1.15270	0.52422
C	3.87822	0.25931	0.11623
C	5.09836	0.90920	-0.08377
C	5.07893	2.26088	-0.43909
C	3.86801	2.94330	-0.57755
C	2.67981	2.23844	-0.36378
C	1.29848	2.77467	-0.43062
C	0.98461	4.10018	-0.72323
C	-0.35557	4.49517	-0.72586
C	-1.34174	3.55570	-0.43411
C	-0.95745	2.24248	-0.15868
H	0.99854	-2.98128	1.10611
H	2.74696	-4.69116	1.69521
H	5.16437	-4.04619	1.48125
H	5.73937	-1.74526	0.73567
H	6.04104	0.38802	0.03184
H	6.01396	2.78688	-0.60232
H	3.86051	3.99362	-0.84263
H	1.76547	4.81890	-0.94247
H	-0.61888	5.52391	-0.94924
H	-2.39144	3.82514	-0.41574
H	-1.68491	1.47351	0.07719

Optimized geometries of the potential energy scan for $[Cu^{II}(tpy)(Trp)]^{\bullet 2+}$ as shown in Figure S1a

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$[Cu^{II}(tpy)(Trp)]^{\bullet 2+}$	Cu-O=3.0	E=-3068.857549880			
C	1.46057	-0.52729	0.83265	0.83081	-0.00024
C	2.96166	-0.25739	1.09605	-0.16637	0.01021
C	3.59115	0.37120	-0.17920	-0.47237	-0.00435
C	5.03824	0.73326	-0.02321	-0.06135	0.13787
C	5.54675	1.86406	0.62814	0.03091	0.06300
C	6.17583	0.00169	-0.50084	-0.11925	-0.02329
C	7.33789	0.72272	-0.11105	0.14127	0.00223
C	6.33341	-1.19113	-1.24266	-0.16167	0.11552
C	7.62064	-1.62622	-1.55556	-0.24283	-0.03067
C	8.62479	0.29868	-0.41878	-0.20524	0.04835
C	8.74936	-0.89502	-1.14890	-0.17811	0.08285
N	3.58164	-1.53323	1.48321	-0.93247	0.00023
N	6.90372	1.85232	0.57731	-0.51392	0.06756
O	0.64487	0.35383	0.60557	-0.66225	0.01511
O	1.13918	-1.81446	0.86380	-0.72072	0.00221
H	2.00627	-2.26914	1.09608	0.54033	-0.00009
H	3.80027	-1.57782	2.47443	0.42657	0.00005
H	4.43789	-1.73013	0.97264	0.42319	0.00001
H	3.00851	0.47587	1.90922	0.26460	-0.00038
H	2.99647	1.25444	-0.43322	0.27711	0.00345
H	3.47733	-0.33200	-1.01262	0.25706	0.00060
H	5.01766	2.67500	1.11009	0.25351	-0.00199
H	7.50455	2.56974	0.96033	0.46430	-0.00194
H	5.47121	-1.75780	-1.58314	0.24446	-0.00332
H	7.75560	-2.53782	-2.12772	0.26276	0.00076
H	9.50318	0.85998	-0.11624	0.26385	-0.00135
H	9.74003	-1.25346	-1.40792	0.26449	-0.00241
Cu	-2.29580	-0.01753	0.14233	1.10998	0.32977
N	-2.40375	1.99699	0.06831	-0.56194	0.04636
N	-4.23034	0.17893	-0.21980	-0.54456	0.10219
N	-2.80856	-1.97047	0.11412	-0.56689	0.04289
C	-1.39631	2.86760	0.23650	0.05924	-0.00332
C	-1.58930	4.24850	0.17004	-0.24942	0.00304
C	-2.86942	4.73542	-0.08076	-0.14069	-0.00183
C	-3.92025	3.83099	-0.25694	-0.20172	0.00056
C	-3.66488	2.46445	-0.17740	0.17306	0.00026
C	-4.71257	1.41728	-0.34507	0.17054	-0.00520
C	-6.07633	1.59030	-0.60489	-0.15550	0.00500
C	-6.87143	0.44413	-0.72031	-0.17419	-0.00400
C	-6.32468	-0.83659	-0.58054	-0.21047	0.00505
C	-4.95323	-0.93810	-0.32140	0.18831	-0.00527
C	-4.13997	-2.17254	-0.12927	0.18580	0.00040
C	-4.67256	-3.45785	-0.18485	-0.22126	0.00044
C	-3.83386	-4.55803	0.01276	-0.14586	-0.00168
C	-2.48130	-4.34267	0.26150	-0.23841	0.00273
C	-2.00627	-3.03087	0.30421	0.05620	-0.00330
H	-0.42175	2.43125	0.42773	0.26676	0.00136
H	-0.74852	4.91770	0.31331	0.27176	0.00018
H	-3.05489	5.80302	-0.13910	0.27766	0.00006
H	-4.92333	4.19212	-0.45212	0.26667	0.00042
H	-6.51807	2.57360	-0.71572	0.26207	0.00071
H	-7.93249	0.55065	-0.92163	0.27674	0.00012
H	-6.95668	-1.71194	-0.67238	0.26902	0.00071
H	-5.72857	-3.60622	-0.37830	0.26576	0.00038
H	-4.23730	-5.56460	-0.02721	0.27530	0.00006
H	-1.79678	-5.16790	0.42194	0.27420	0.00020
H	-0.96116	-2.81245	0.49553	0.26440	0.00150

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$[Cu^{II}(tpy)(Trp)]^{\bullet 2+}$	Cu-O=4.0	E=-3068.851747060			
C	-1.80145	-0.28064	-0.44701	0.81925	0.00099
C	-3.31456	-0.47984	-0.72277	-0.17127	0.01203
C	-4.14718	0.54202	0.09712	-0.48390	-0.00448
C	-5.59026	0.60995	-0.29827	-0.02005	0.18530
C	-6.10086	1.26475	-1.43704	0.04565	0.09427
C	-6.72191	0.05229	0.37637	-0.12052	-0.03311
C	-7.87865	0.38260	-0.38247	0.14076	0.00708
C	-6.88239	-0.68369	1.57243	-0.13547	0.14825
C	-8.16511	-1.07338	1.95938	-0.24481	-0.04063
C	-9.15820	0.00243	-0.00910	-0.19891	0.05541
C	-9.28459	-0.73919	1.18204	-0.16551	0.10845

N	-3.64038	-1.89528	-0.52384	-0.92755	0.00327
N	-7.14183	1.12315	-1.48380	-0.50540	0.08750
O	-1.27347	0.80972	-0.36331	-0.62727	0.00600
O	-1.11954	-1.42577	-0.34794	-0.72405	0.00245
H	-1.81307	-2.13535	-0.43152	0.53640	-0.00004
H	-4.26197	-2.26705	-1.23770	0.42573	-0.00008
H	-4.06441	-2.08045	0.38330	0.41133	-0.00005
H	-3.43260	-0.25402	-1.78978	0.26880	-0.00050
H	-3.67183	1.52047	-0.02951	0.28811	0.00559
H	-4.06342	0.29294	1.16140	0.25561	0.00073
H	-5.57349	1.82874	-2.19479	0.25902	-0.00296
H	-8.04535	1.51950	-2.19513	0.46750	-0.00252
H	-6.02791	-0.93167	2.19500	0.24594	-0.00430
H	-8.30282	-1.63549	2.87667	0.26551	0.00101
H	-10.03284	0.26200	-0.59710	0.26632	-0.00154
H	-10.27242	-1.05063	1.50494	0.26654	-0.00317
Cu	2.60950	-0.09471	-0.04000	1.02330	0.23780
N	2.56835	1.91239	0.06018	-0.56325	0.03175
N	4.56117	0.24098	0.11785	-0.55138	0.07710
N	3.25982	-2.00082	-0.09532	-0.55682	0.02941
C	1.48664	2.70834	0.02334	0.05649	-0.00251
C	1.58456	4.09875	0.10827	-0.24108	0.00210
C	2.84422	4.67694	0.23449	-0.15021	-0.00127
C	3.97167	3.85160	0.27148	-0.22396	0.00030
C	3.81243	2.47139	0.18274	0.18581	0.00028
C	4.95527	1.50986	0.21239	0.18881	-0.00403
C	6.32374	1.78510	0.32161	-0.21093	0.00391
C	7.20886	0.70022	0.32582	-0.15505	-0.00308
C	6.74841	-0.61861	0.22376	-0.21644	0.00390
C	5.36747	-0.81917	0.11680	0.20596	-0.00408
C	4.62175	-2.10793	-0.00537	0.17119	0.00036
C	5.24531	-3.35338	-0.02969	-0.21743	0.00025
C	4.46991	-4.50951	-0.14745	-0.14798	-0.00122
C	3.08531	-4.39136	-0.23774	-0.24117	0.00195
C	2.52057	-3.11616	-0.20757	0.05654	-0.00238
H	0.52759	2.20952	-0.07792	0.27341	0.00111
H	0.68502	4.70284	0.07484	0.27137	0.00014
H	2.95614	5.75414	0.30321	0.27246	0.00004
H	4.96073	4.28409	0.36891	0.26396	0.00028
H	6.70275	2.79730	0.40046	0.26716	0.00053
H	8.27494	0.88513	0.40948	0.27588	0.00010
H	7.45207	-1.44280	0.22874	0.26698	0.00052
H	6.32433	-3.42659	0.04171	0.26521	0.00027
H	4.94542	-5.48470	-0.16784	0.27422	0.00004
H	2.44705	-5.26278	-0.33016	0.27322	0.00012
H	1.44706	-2.97317	-0.27436	0.25348	0.00106

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$[Cu^{II}(tpy)(Trp)]^{\bullet 2+}$ Cu-O=5.0 E=-3068.848683570

C	-2.49949	-0.64548	-0.36729	0.80630	0.00144
C	-4.03734	-0.80097	-0.53000	-0.17088	0.01542
C	-4.75094	0.47717	-0.00587	-0.49069	-0.00367
C	-6.17971	0.59819	-0.42765	0.00497	0.21507
C	-6.62379	1.00962	-1.70675	0.05871	0.11811
C	-7.36192	0.34666	0.33442	-0.12418	-0.03981
C	-8.47980	0.60795	-0.50546	0.14155	0.01159
C	-7.59436	-0.05717	1.66875	-0.12285	0.16579
C	-8.91064	-0.19786	2.11218	-0.24508	-0.04624
C	-9.78966	0.47377	-0.07939	-0.19653	0.05666
C	-9.98974	0.06036	1.25486	-0.15828	0.12276
N	-4.45518	-2.07543	0.05236	-0.92307	0.00913
N	-7.97147	1.00851	-1.74601	-0.50035	0.09889
O	-1.91538	0.40190	-0.53520	-0.59819	0.00895
O	-1.87179	-1.79004	-0.06990	-0.71681	0.00294
H	-2.58767	-2.46331	0.04373	0.53461	-0.00013
H	-5.19473	-2.53696	-0.46603	0.42238	-0.00016
H	-4.74183	-1.99823	1.02462	0.40827	-0.00013
H	-4.19095	-0.87025	-1.61432	0.26631	-0.00066
H	-4.17473	1.33309	-0.37423	0.29381	0.00703
H	-4.67846	0.49956	1.08731	0.25667	0.00087
H	-6.03889	1.31065	-2.56578	0.26237	-0.00370
H	-8.52870	1.28197	-2.54561	0.46936	-0.00288
H	-6.76784	-0.24299	2.34759	0.24926	-0.00482
H	-9.10403	-0.50411	3.13445	0.26729	0.00117
H	-10.63432	0.67758	-0.72981	0.26772	-0.00158

H	11.04428	-0.05254	1.62241	0.26771	-0.00360
C	3.05585	0.13171	-0.07074	0.96144	0.17316
N	3.46256	2.10921	0.02266	-0.55436	0.02194
N	5.04421	0.03813	0.09018	-0.55813	0.05561
N	3.28231	-1.87458	-0.10848	-0.55664	0.02193
C	2.59261	3.13143	-0.02070	0.05676	-0.00178
C	2.99344	4.46575	0.04987	-0.24171	0.00151
C	4.35167	4.74769	0.17033	-0.15053	-0.00095
C	5.26334	3.69035	0.21666	-0.21907	0.00023
C	4.79964	2.37860	0.14119	0.17055	0.00017
C	5.70504	1.18925	0.18456	0.20651	-0.00299
C	7.09945	1.16180	0.30970	-0.21709	0.00284
C	7.72588	-0.09047	0.32972	-0.15807	-0.00225
C	6.98930	-1.27741	0.22994	-0.21746	0.00283
C	5.59850	-1.17157	0.10731	0.20080	-0.00298
C	4.58995	-2.26941	-0.01170	0.18526	0.00016
C	4.93425	-3.61934	-0.02561	-0.22498	0.00023
C	3.93184	-4.58528	-0.14035	-0.15102	-0.00096
C	2.60494	-4.17561	-0.23892	-0.24292	0.00150
C	2.32361	-2.80916	-0.21901	0.05553	-0.00183
H	1.54451	2.86694	-0.11441	0.25237	0.00076
H	2.25113	5.25483	0.01031	0.27282	0.00008
H	4.70234	5.77298	0.22796	0.27265	0.00003
H	6.32442	3.89028	0.31045	0.26356	0.00020
H	7.69009	2.06685	0.39037	0.26542	0.00038
H	8.80563	-0.14243	0.42559	0.27435	0.00007
H	7.49658	-2.23487	0.24962	0.26525	0.00038
H	5.97281	-3.91983	0.05075	0.26353	0.00020
H	4.18956	-5.63931	-0.15281	0.27214	0.00004
H	1.79575	-4.89116	-0.33038	0.27101	0.00009
H	1.30337	-2.44733	-0.29932	0.25643	0.00082

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$[Cu^{II}(tpy)(Trp)]^{\bullet 2+}$	Cu-O=6.0	E=-3068.848638850			
C	-3.14779	-0.85616	-0.27103	0.80828	0.00166
C	-4.68772	-0.90723	-0.49021	-0.17015	0.01773
C	-5.34502	0.34492	0.16147	-0.49326	-0.00272
C	-6.73043	0.62444	-0.31751	0.01665	0.22841
C	-7.06024	1.22957	-1.55666	0.06490	0.13084
C	-7.97533	0.36145	0.33137	-0.12609	-0.04312
C	-9.01461	0.80737	-0.53135	0.14212	0.01382
C	-8.32302	-0.19770	1.58201	-0.11771	0.17267
C	-9.67326	-0.30499	1.92136	-0.24482	-0.04830
C	-10.35586	0.70849	-0.20872	-0.19601	0.05657
C	-10.67237	0.13733	1.04315	-0.15534	0.12814
N	-5.19435	-2.21036	-0.07070	-0.91957	0.01373
N	-8.39764	1.32959	-1.67528	-0.49813	0.10425
O	-2.51150	0.17339	-0.29765	-0.59373	0.01230
O	-2.58713	-2.05681	-0.09926	-0.70715	0.00375
H	-3.32922	-2.70748	-0.09325	0.53394	-0.00018
H	-5.95312	-2.56214	-0.64405	0.42126	-0.00023
H	-5.47884	-2.23975	0.90468	0.40765	-0.00021
H	-4.80981	-0.84419	-1.57886	0.26512	-0.00076
H	-4.68913	1.19401	-0.06183	0.29619	0.00769
H	-5.33899	0.22037	1.24988	0.25760	0.00086
H	-6.39882	1.59563	-2.33079	0.26369	-0.00409
H	-8.88081	1.74289	-2.46316	0.47008	-0.00304
H	-7.55775	-0.52783	2.27746	0.25111	-0.00503
H	-9.95526	-0.72938	2.87873	0.26820	0.00122
H	-11.13996	1.05314	-0.87535	0.26822	-0.00159
H	-11.71499	0.04677	1.32933	0.26820	-0.00376
Cu	3.48258	0.13127	-0.03429	0.93203	0.14017
N	3.87629	2.11781	0.05656	-0.55446	0.01770
N	5.48591	0.06373	0.06846	-0.55608	0.04476
N	3.74776	-1.87733	-0.08828	-0.55422	0.01768
C	2.99666	3.13269	0.04803	0.05574	-0.00146
C	3.38518	4.47060	0.11645	-0.24275	0.00121
C	4.74351	4.76574	0.19693	-0.15167	-0.00079
C	5.66584	3.71717	0.20693	-0.22537	0.00019
C	5.21324	2.40092	0.13617	0.19073	0.00012
C	6.13449	1.22268	0.14252	0.18579	-0.00243
C	7.53300	1.21546	0.21487	-0.21303	0.00232
C	8.17789	-0.02740	0.20476	-0.16277	-0.00185
C	7.45478	-1.22388	0.12530	-0.21826	0.00232
C	6.05886	-1.13668	0.05594	0.20036	-0.00244

C	5.49176	-2.24998	-0.03461	0.18582	0.00012
C	5.49176	-3.59388	-0.06389	-0.22569	0.00019
C	4.44452	-4.57792	-0.14942	-0.15202	-0.00079
C	3.10803	-4.19184	-0.20309	-0.24310	0.00121
C	2.80504	-2.83049	-0.16969	0.05572	-0.00148
H	1.94842	2.86049	-0.01563	0.24944	0.00062
H	2.63375	5.25193	0.10621	0.27196	0.00006
H	5.08582	5.79401	0.25161	0.27180	0.00002
H	6.72726	3.92701	0.26970	0.26278	0.00016
H	8.11354	2.12845	0.27710	0.26424	0.00030
H	9.26111	-0.06420	0.25953	0.27592	0.00006
H	7.97599	-2.17401	0.11899	0.26419	0.00030
H	6.47740	-3.87553	-0.02080	0.26273	0.00017
H	4.72084	-5.62702	-0.17319	0.27150	0.00003
H	2.30834	-4.92072	-0.26951	0.27134	0.00006
H	1.77564	-2.49002	-0.20901	0.25103	0.00063

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$[Cu^{II}(tpy)(Trp)]^{\bullet 2+}$	Cu-O=7.0	E=-3068.849264800			
C	-3.75368	-0.51129	0.86657	0.80699	0.00186
C	-5.29843	-0.71450	0.84080	-0.16932	0.01992
C	-5.91491	0.19507	-0.26608	-0.49481	-0.00199
C	-7.29049	-0.19963	-0.68234	0.02300	0.23576
C	-7.60230	-1.25553	-1.57821	0.06952	0.13834
C	-8.54387	0.36272	-0.29187	-0.12729	-0.04509
C	-9.56993	-0.36610	-0.95418	0.14269	0.01541
C	-8.90762	1.43705	0.55103	-0.11614	0.17498
C	-10.26149	1.73747	0.71484	-0.24472	-0.04910
C	-10.91433	-0.08001	-0.80318	-0.19607	0.05557
C	-11.24751	0.99333	0.05249	-0.15422	0.13046
N	-5.83295	-0.56542	2.18825	-0.91614	0.01854
N	-8.93621	-1.34759	-1.72908	-0.49711	0.10715
O	-3.09919	-0.33131	-0.13574	-0.58914	0.01578
O	-3.21538	-0.60010	2.08413	-0.69901	0.00451
H	-3.96331	-0.72457	2.71359	0.53367	-0.00023
H	-6.61049	-1.18095	2.39877	0.42093	-0.00031
H	-6.09046	0.38908	2.42329	0.40717	-0.00028
H	-5.43151	-1.76425	0.55084	0.26494	-0.00085
H	-5.23178	0.14746	-1.12171	0.29765	0.00759
H	-5.90841	1.23191	0.08760	0.25797	0.00117
H	-6.92853	-1.91524	-2.10897	0.26498	-0.00432
H	-9.40744	-2.01057	-2.33201	0.47052	-0.00314
H	-8.15138	2.03094	1.05442	0.25134	-0.00510
H	-10.55617	2.56070	1.35653	0.26841	0.00125
H	-11.68881	-0.64304	-1.31426	0.26852	-0.00156
H	-12.29313	1.24712	0.19205	0.26836	-0.00384
Cu	3.89211	0.01514	-0.09456	0.91461	0.11999
N	4.13020	2.03131	-0.14593	-0.55261	0.01517
N	5.90144	0.11471	-0.08273	-0.55680	0.03810
N	4.32588	-1.96765	-0.04256	-0.55318	0.01516
C	3.17268	2.97258	-0.17455	0.05537	-0.00129
C	3.45384	4.33868	-0.20643	-0.24347	0.00104
C	4.78593	4.74342	-0.20797	-0.15276	-0.00069
C	5.78910	3.77247	-0.17760	-0.22614	0.00018
C	5.44173	2.42272	-0.14695	0.18618	0.00009
C	6.45551	1.32342	-0.11329	0.20003	-0.00210
C	7.85162	1.43211	-0.11210	-0.21875	0.00198
C	8.59579	0.24648	-0.07923	-0.16384	-0.00159
C	7.97096	-1.00612	-0.04942	-0.21367	0.00198
C	6.57090	-1.03408	-0.05258	0.18542	-0.00209
C	5.66944	-2.22786	-0.02681	0.19116	0.00008
C	6.14780	-3.53673	0.01156	-0.22603	0.00018
C	5.24495	-4.60179	0.03467	-0.15268	-0.00069
C	3.87934	-4.33009	0.01937	-0.24350	0.00104
C	3.46518	-2.99879	-0.01922	0.05521	-0.00128
H	2.14832	2.61615	-0.17118	0.24812	0.00054
H	2.64189	5.05667	-0.22908	0.27124	0.00006
H	5.04626	5.79667	-0.23192	0.27115	0.00002
H	6.83175	4.06853	-0.17751	0.26227	0.00015
H	8.35746	2.39024	-0.13632	0.26352	0.00026
H	9.67968	0.29961	-0.07777	0.27519	0.00006
H	8.56767	-1.91044	-0.02552	0.26349	0.00025
H	7.21449	-3.72774	0.02381	0.26221	0.00014
H	5.60747	-5.62418	0.06468	0.27117	0.00003
H	3.14176	-5.12434	0.03675	0.27124	0.00006

H	24	-2.74509	-0.03252	0.24825	0.00053
[Cu^{II}(tpy)(Trp)]$^{\bullet 2+}$	Cu-O=8.0	E=-3068.850471460			
C	-4.34097	-0.48151	0.90577	0.80681	0.00192
C	-5.88607	-0.68700	0.87754	-0.16910	0.02124
C	-6.49577	0.21145	-0.24307	-0.49596	-0.00133
C	-7.85875	-0.20298	-0.67700	0.02724	0.24086
C	-8.13975	-1.26629	-1.57609	0.07215	0.14345
C	-9.12726	0.33825	-0.30645	-0.12819	-0.04645
C	-10.13052	-0.40891	-0.98303	0.14306	0.01646
C	-9.52209	1.40679	0.52935	-0.11471	0.17673
C	-10.88366	1.68372	0.67191	-0.24449	-0.04956
C	-11.48144	-0.14630	-0.85342	-0.19631	0.05487
C	-11.84622	0.92201	-0.00449	-0.15364	0.13170
N	-6.42803	-0.52538	2.21922	-0.91417	0.02151
N	-9.46849	-1.38083	-1.74686	-0.49628	0.10898
O	-3.68744	-0.30252	-0.09659	-0.58403	0.01843
O	-3.80426	-0.56745	2.12409	-0.69635	0.00506
H	-4.55057	-0.69070	2.75455	0.53322	-0.00026
H	-7.20971	-1.13476	2.43181	0.42067	-0.00034
H	-6.67684	0.43251	2.44947	0.40735	-0.00034
H	-6.01614	-1.73978	0.59723	0.26496	-0.00090
H	-5.79873	0.16500	-1.08769	0.29893	0.00779
H	-6.50486	1.25014	0.10491	0.25875	0.00117
H	-7.44673	-1.91536	-2.09516	0.26572	-0.00448
H	-9.91922	-2.05268	-2.35583	0.47079	-0.00319
H	-8.78387	2.01372	1.04374	0.25205	-0.00515
H	-11.20246	2.50225	1.30792	0.26859	0.00126
H	-12.23810	-0.72331	-1.37543	0.26859	-0.00155
H	-12.89817	1.15755	0.11851	0.26841	-0.00387
Cu	4.30830	-0.04190	-0.11143	0.90258	0.10632
N	4.45098	1.98470	-0.16039	-0.55179	0.01347
N	6.31460	0.15600	-0.07808	-0.55696	0.03362
N	4.84235	-2.00172	-0.05153	-0.55233	0.01347
C	3.45015	2.87918	-0.20374	0.05503	-0.00115
C	3.66592	4.25690	-0.23455	-0.24394	0.00092
C	4.97711	4.72495	-0.21961	-0.15351	-0.00062
C	6.02489	3.80316	-0.17493	-0.22673	0.00017
C	5.74212	2.43845	-0.14616	0.18648	0.00007
C	6.80865	1.39013	-0.09872	0.19981	-0.00187
C	8.19765	1.56834	-0.07486	-0.21932	0.00176
C	8.99891	0.42093	-0.02943	-0.16477	-0.00141
C	8.43612	-0.86108	-0.00827	-0.21407	0.00175
C	7.03915	-0.95792	-0.03457	0.18530	-0.00186
C	6.19700	-2.19456	-0.01953	0.19111	0.00007
C	6.73991	-3.47774	0.02472	-0.22646	0.00016
C	5.89168	-4.58680	0.03689	-0.15333	-0.00062
C	4.51461	-4.38397	0.00419	-0.24367	0.00092
C	4.03497	-3.07494	-0.03970	0.05501	-0.00115
H	2.44390	2.47409	-0.21454	0.24765	0.00048
H	2.82081	4.93501	-0.26937	0.27084	0.00005
H	5.18708	5.78932	-0.24242	0.27058	0.00002
H	7.05221	4.14818	-0.16285	0.26177	0.00013
H	8.65545	2.55046	-0.09035	0.26293	0.00023
H	10.07873	0.52740	-0.01009	0.27464	0.00006
H	9.07642	-1.73469	0.02735	0.26299	0.00022
H	7.81467	-3.61501	0.04947	0.26179	0.00013
H	6.30461	-5.58969	0.07131	0.27078	0.00002
H	3.81755	-5.21423	0.01204	0.27117	0.00005
H	2.96904	-2.87528	-0.06618	0.24744	0.00048

[Cu^{II}(tpy)(Trp)]$^{\bullet 2+}$	Cu-O=9.0	E=-3068.851703610			
C	-4.92338	-0.24451	0.98365	0.80661	0.00185
C	-6.46952	-0.44636	1.01002	-0.16882	0.02197
C	-7.08153	0.18318	-0.28068	-0.49679	-0.00059
C	-8.43768	-0.32856	-0.61868	0.03043	0.24431
C	-8.70494	-1.57615	-1.24515	0.07379	0.14772
C	-9.71210	0.27725	-0.40000	-0.12870	-0.04742
C	-10.70500	-0.61432	-0.89148	0.14336	0.01722
C	-10.11955	1.51061	0.15578	-0.11348	0.17794
C	-11.48362	1.80529	0.21490	-0.24434	-0.04986
C	-12.05799	-0.33670	-0.84140	-0.19659	0.05435
C	-12.43577	0.89969	-0.27217	-0.15318	0.13256
N	-7.00485	0.00999	2.28387	-0.91282	0.02340

		-1.73519	-1.39803	-0.49571	0.11039
		-0.28804	-0.03853	-0.57997	0.02075
O	-4.37752	-0.06908	2.18801	-0.69441	0.00545
H	-5.11709	-0.05097	2.83699	0.53296	-0.00030
H	-7.79024	-0.53072	2.62770	0.42032	-0.00036
H	-7.24295	0.99765	2.30056	0.40761	-0.00037
H	-6.60192	-1.53483	0.97109	0.26469	-0.00093
H	-6.37910	-0.03979	-1.09244	0.30047	0.00833
H	-7.10101	1.27224	-0.16647	0.25901	0.00095
H	-8.00364	-2.32507	-1.58920	0.26619	-0.00462
H	-10.47232	-2.53459	-1.83559	0.47095	-0.00324
H	-9.38932	2.22617	0.52012	0.25286	-0.00519
H	-11.81242	2.74886	0.63645	0.26871	0.00127
H	-12.80681	-1.02478	-1.22056	0.26861	-0.00153
H	-13.48985	1.15130	-0.21888	0.26839	-0.00390
Cu	4.71806	-0.04171	-0.10926	0.89398	0.09607
N	4.91686	1.98099	-0.18272	-0.55114	0.01220
N	6.73172	0.10393	-0.08491	-0.55710	0.03026
N	5.20335	-2.01469	-0.02788	-0.55166	0.01219
C	3.94073	2.90202	-0.23254	0.05484	-0.00106
C	4.19331	4.27302	-0.28028	-0.24415	0.00084
C	5.51669	4.70541	-0.27588	-0.15407	-0.00057
C	6.53915	3.75603	-0.22444	-0.22712	0.00016
C	6.21981	2.39984	-0.17876	0.18647	0.00005
C	7.25836	1.32394	-0.12315	0.19973	-0.00169
C	8.65173	1.46552	-0.10807	-0.21971	0.00158
C	9.42255	0.29791	-0.05238	-0.16548	-0.00128
C	8.82609	-0.96829	-0.01297	-0.21453	0.00158
C	7.42684	-1.02798	-0.03146	0.18514	-0.00168
C	6.55258	-2.24201	0.00207	0.19124	0.00006
C	7.06261	-3.53814	0.06068	-0.22690	0.00016
C	6.18640	-4.62484	0.08942	-0.15397	-0.00057
C	4.81488	-4.38710	0.05847	-0.24403	0.00083
C	4.36901	-3.06679	-0.00018	0.05478	-0.00106
H	2.92369	2.52472	-0.23399	0.24720	0.00044
H	3.36663	4.97326	-0.31961	0.27072	0.00004
H	5.75544	5.76333	-0.31186	0.27024	0.00002
H	7.57542	4.07345	-0.22008	0.26142	0.00012
H	9.13561	2.43474	-0.13799	0.26253	0.00019
H	10.50489	0.37596	-0.03951	0.27417	0.00005
H	9.44315	-1.85815	0.03008	0.26255	0.00020
H	8.13359	-3.70245	0.08389	0.26142	0.00012
H	6.57363	-5.63749	0.13510	0.27036	0.00002
H	4.09672	-5.19897	0.07875	0.27088	0.00004
H	3.30847	-2.84024	-0.02607	0.24712	0.00044

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$[Cu^{II}(tpy)(Trp)]^{\bullet 2+}$ Cu-O=10.0 E=-3068.852948860

C	-5.52088	-0.48095	0.94745	0.80654	0.00196
C	-7.07123	-0.65395	0.91736	-0.16859	0.02313
C	-7.65168	0.23318	-0.22973	-0.49726	-0.00029
C	-9.00740	-0.17800	-0.68317	0.03230	0.24668
C	-9.27642	-1.25089	-1.57661	0.07555	0.15003
C	-10.28048	0.37121	-0.34126	-0.12919	-0.04807
C	-11.27401	-0.37938	-1.02798	0.14358	0.01777
C	-10.68572	1.44901	0.47698	-0.11339	0.17805
C	-12.04880	1.73185	0.59255	-0.24425	-0.04985
C	-12.62582	-0.11123	-0.92533	-0.19684	0.05374
C	-13.00167	0.96685	-0.09349	-0.15323	0.13271
N	-7.61774	-0.44952	2.24934	-0.91125	0.02610
N	-10.60145	-1.36193	-1.77013	-0.49545	0.11125
O	-4.86420	-0.33129	-0.05682	-0.57699	0.02265
O	-4.98861	-0.56049	2.16761	-0.69257	0.00587
H	-5.73547	-0.65787	2.80047	0.53264	-0.00032
H	-8.41663	-1.03206	2.47228	0.42045	-0.00040
H	-7.83435	0.51971	2.46360	0.40770	-0.00042
H	-7.22232	-1.70982	0.66039	0.26511	-0.00099
H	-6.93741	0.16475	-1.05859	0.30069	0.00801
H	-7.65766	1.27710	0.10186	0.25959	0.00120
H	-8.57589	-1.90761	-2.07577	0.26682	-0.00469
H	-11.04366	-2.03841	-2.38035	0.47107	-0.00327
H	-9.95422	2.05786	0.99857	0.25281	-0.00520
H	-12.37600	2.55759	1.21484	0.26870	0.00127
H	-13.37516	-0.69084	-1.45493	0.26861	-0.00151
H	-14.05480	1.20719	0.00837	0.26835	-0.00391

C	5.13073	-0.01630	-0.10350	0.88823	0.08883
N	5.34985	2.00614	-0.14998	-0.54873	0.01129
N	7.14741	0.11116	-0.07033	-0.55744	0.02790
N	5.60007	-1.99491	-0.04617	-0.55097	0.01129
C	4.38269	2.93704	-0.19161	0.05489	-0.00099
C	4.64813	4.30613	-0.22120	-0.24430	0.00078
C	5.97547	4.72591	-0.20690	-0.15466	-0.00053
C	6.98870	3.76631	-0.16388	-0.22180	0.00015
C	6.65653	2.41267	-0.13618	0.17210	0.00005
C	7.68514	1.32663	-0.09032	0.20507	-0.00156
C	9.07966	1.45560	-0.06740	-0.21980	0.00146
C	9.83980	0.28052	-0.02376	-0.16324	-0.00118
C	9.23190	-0.98066	-0.00346	-0.21481	0.00146
C	7.83221	-1.02738	-0.02867	0.18528	-0.00155
C	6.94714	-2.23412	-0.01451	0.19122	0.00004
C	7.44605	-3.53525	0.02850	-0.22720	0.00015
C	6.56071	-4.61480	0.03958	-0.15439	-0.00053
C	5.19136	-4.36504	0.00705	-0.24418	0.00078
C	4.75697	-3.04030	-0.03544	0.05473	-0.00099
H	3.36214	2.56952	-0.20159	0.24699	0.00041
H	3.82815	5.01452	-0.25454	0.27061	0.00004
H	6.22430	5.78190	-0.22884	0.26995	0.00002
H	8.02787	4.07392	-0.15225	0.26114	0.00011
H	9.57241	2.42070	-0.08235	0.26223	0.00019
H	10.92274	0.34870	-0.00522	0.27127	0.00005
H	9.84084	-1.87649	0.03066	0.26222	0.00018
H	8.51553	-3.70884	0.05324	0.26112	0.00011
H	6.93923	-5.63122	0.07299	0.27006	0.00002
H	4.46626	-5.17095	0.01397	0.27075	0.00004
H	3.69846	-2.80460	-0.06211	0.24699	0.00041

Optimized geometries of the potential energy scan for $[Cu^{II}(tpy)(Phe)]^{\bullet 2+}$ as shown in Figure S1b

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$[Cu^{II}(tpy)(Phe)]^{\bullet 2+}$	Cu-O=3.0	E=-2937.264102290			
C	-2.08879	-0.86023	-0.54383	0.85394	-0.00198
C	-3.61436	-0.69907	-0.70125	-0.17748	0.00611
C	-4.20399	-0.06122	0.58621	-0.46190	-0.00028
C	-5.69685	0.16754	0.49517	-0.05685	0.02905
C	-6.21583	1.17754	-0.33692	-0.22479	0.01641
C	-6.58907	-0.62803	1.22962	-0.24333	-0.00411
C	-7.96823	-0.42749	1.13085	-0.20457	0.01513
C	-7.59118	1.38086	-0.43611	-0.21667	-0.00597
C	-8.47231	0.57581	0.29528	-0.19682	0.03420
N	-4.15206	-2.04107	-0.98193	-0.92805	0.00137
O	-1.31129	0.08141	-0.41167	-0.68728	0.03020
O	-1.69066	-2.12084	-0.54796	-0.72828	0.00236
H	-2.56584	-2.62236	-0.70424	0.54036	-0.00015
H	-4.47406	-2.13882	-1.94101	0.42956	-0.00003
H	-4.93632	-2.27393	-0.37720	0.43043	0.00038
H	-3.77946	-0.01650	-1.54206	0.27012	-0.00014
H	-3.67542	0.88290	0.75518	0.26570	0.00120
H	-3.97746	-0.71254	1.43911	0.24970	-0.00004
H	-5.53911	1.81664	-0.90006	0.23525	-0.00049
H	-6.20642	-1.39358	1.90101	0.24141	0.00005
H	-8.64745	-1.04545	1.70964	0.25699	-0.00043
H	-7.97798	2.16811	-1.07553	0.25564	0.00012
H	-9.54339	0.73446	0.22137	0.25837	-0.00093
Cu	1.67093	-0.00823	-0.09810	1.27376	0.52358
N	1.57328	1.96691	-0.11295	-0.57060	0.08318
N	3.55233	0.34197	0.11068	-0.53387	0.19277
N	2.27780	-1.89154	-0.02897	-0.57824	0.07624
C	0.46621	2.71694	-0.23654	0.06886	-0.00518
C	0.52457	4.11238	-0.23504	-0.22960	0.00570
C	1.76230	4.73542	-0.10123	-0.14744	-0.00290
C	2.91494	3.95203	0.02831	-0.18540	0.00053
C	2.79793	2.56702	0.01974	0.15665	0.00094
C	3.93810	1.62471	0.14875	0.18156	-0.00876
C	5.29863	1.90751	0.29814	-0.14863	0.00908
C	6.18803	0.83107	0.40174	-0.16077	-0.00698
C	5.73756	-0.49394	0.35735	-0.20763	0.00916
C	4.36631	-0.71772	0.20525	0.19818	-0.00890
C	3.63518	-2.00772	0.12722	0.14149	0.00115
C	4.24027	-3.25696	0.20120	-0.12401	0.00026
C	3.44831	-4.40743	0.11436	-0.16769	-0.00262

C	2.07132	-4.27644	-0.04530	-0.22952	0.00510
C	0.64765	-2.99658	-0.11381	0.06388	-0.00512
H	-0.46884	2.17519	-0.33698	0.27971	0.00230
H	-0.38943	4.68634	-0.33732	0.28186	0.00038
H	1.83860	5.81795	-0.09653	0.28505	0.00011
H	3.88615	4.42172	0.13419	0.27301	0.00073
H	5.66546	2.92660	0.33381	0.27020	0.00144
H	7.24893	1.02781	0.51874	0.28430	0.00020
H	6.44095	-1.31424	0.43911	0.27852	0.00142
H	5.31390	-3.34102	0.32455	0.26305	0.00066
H	3.90801	-5.38884	0.17096	0.28064	0.00010
H	1.42497	-5.14346	-0.11760	0.28257	0.00040
H	0.45052	-2.84258	-0.24025	0.27491	0.00243

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$[Cu^{II}(tpy)(Phe)]^{\bullet 2+}$	Cu-O=4.0	E=-2937.252846480			
C	2.17573	-0.61367	-0.42795	0.82193	-0.00022
C	3.61918	-0.11503	-0.60571	-0.17316	0.00600
C	4.47454	-0.55342	0.60896	-0.46855	-0.00135
C	5.94260	-0.23161	0.44140	-0.03009	0.06405
C	6.72729	-0.95876	-0.47773	-0.21741	0.02329
C	6.55568	0.77426	1.20535	-0.24116	-0.00365
C	7.91357	1.04795	1.06082	-0.20251	0.02111
C	8.08221	-0.68886	-0.62617	-0.21605	-0.00680
C	8.68139	0.31870	0.14101	-0.17528	0.07206
N	3.56318	1.35627	-0.78946	-0.93438	0.00022
O	1.88283	-1.78389	-0.32303	-0.60435	0.00194
O	1.27073	0.40090	-0.36384	-0.78219	0.00784
H	1.87280	1.20934	-0.50296	0.52835	-0.00015
H	3.85979	1.63900	-1.71957	0.42911	0.00006
H	4.16065	1.84312	-0.12555	0.42500	0.00000
H	4.00219	-0.59861	-1.50996	0.27619	-0.00015
H	4.32764	-1.62962	0.74386	0.28174	0.00226
H	4.08399	-0.06383	1.50946	0.24762	0.00003
H	6.27487	-1.75824	-1.05862	0.24339	-0.00073
H	5.97154	1.33206	1.93268	0.24077	-0.00001
H	8.37856	1.82001	1.66392	0.25800	-0.00062
H	8.67682	-1.26466	-1.32683	0.25959	0.00011
H	9.73957	0.52830	0.03185	0.25933	-0.00197
Cu	-1.67409	0.02998	-0.08176	1.24735	0.49049
N	-1.93592	-1.95043	-0.02567	-0.57701	0.07498
N	-3.60803	0.03354	0.06307	-0.53302	0.18012
N	-1.95712	2.01169	-0.09819	-0.57174	0.06872
C	-1.00279	-2.91658	-0.08007	0.06585	-0.00487
C	-1.34529	-4.27330	-0.01755	-0.22702	0.00522
C	-2.68304	-4.63167	0.09881	-0.13785	-0.00249
C	-3.65400	-3.62400	0.14977	-0.21283	0.00029
C	-3.26206	-2.29289	0.08808	0.17362	0.00100
C	-4.21408	-1.15828	0.14235	0.19490	-0.00846
C	-5.60917	-1.18989	0.26788	-0.20404	0.00891
C	-6.29761	0.02869	0.31254	-0.16236	-0.00652
C	-5.61584	1.25190	0.23772	-0.14953	0.00859
C	-4.22398	1.22290	0.11048	0.16905	-0.00811
C	-3.27632	2.36073	0.01708	0.17492	0.00095
C	-3.65961	3.69860	0.04100	-0.18824	0.00040
C	-2.68275	4.69450	-0.05677	-0.14662	-0.00246
C	-1.34440	4.32677	-0.18222	-0.23131	0.00444
C	-1.02311	2.96935	-0.20085	0.06574	-0.00465
H	0.03677	-2.60848	-0.18689	0.28516	0.00233
H	-0.55814	-5.01784	-0.06429	0.28291	0.00040
H	-2.97870	-5.67497	0.14759	0.28048	0.00012
H	-4.70334	-3.88334	0.23566	0.26917	0.00065
H	-6.15210	-2.12598	0.33200	0.27638	0.00132
H	-7.37891	0.02673	0.40943	0.28374	0.00022
H	-6.16362	2.18658	0.27999	0.26862	0.00136
H	-4.70568	3.96834	0.13419	0.27337	0.00059
H	-2.96832	5.74154	-0.03488	0.28576	0.00008
H	-0.55809	5.06892	-0.26595	0.28172	0.00036
H	-0.00175	2.62035	-0.29666	0.24924	0.00224

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$[Cu^{II}(tpy)(Phe)]^{\bullet 2+}$	Cu-O=5.0	E=-2937.244469090			
C	3.20663	-0.42998	0.07525	0.80919	0.00022
C	4.74108	-0.62586	0.19992	-0.17169	0.01486
C	5.48209	0.47938	-0.60065	-0.48290	0.00213
C	6.94591	0.58288	-0.27281	0.02898	0.13162

C	7.35644	1.12013	0.97529	-0.20444	0.05078
C	7.96262	0.15980	-1.18770	-0.22922	0.00246
C	9.28150	0.26192	-0.87123	-0.19428	0.03164
C	8.70458	1.22347	1.29503	-0.22227	-0.01527
C	9.67496	0.79222	0.37460	-0.13686	0.15310
N	5.06867	-2.01124	-0.14710	-0.92268	0.01304
O	2.66320	0.65178	0.11288	-0.59660	0.02033
O	2.52853	-1.58289	-0.03751	-0.73438	0.00422
H	3.23575	-2.28202	-0.07101	0.53486	-0.00035
H	5.77167	-2.41982	0.46005	0.42608	-0.00020
H	5.38566	-2.11144	-1.10837	0.41250	0.00006
H	4.95037	-0.49021	1.26821	0.27116	-0.00046
H	4.97556	1.42386	-0.36821	0.28903	0.00739
H	5.34140	0.29522	-1.67210	0.25149	-0.00007
H	6.60855	1.47144	1.67949	0.24857	-0.00159
H	7.63360	-0.23431	-2.15497	0.24954	-0.00029
H	10.03522	-0.06009	-1.58250	0.26273	-0.00099
H	9.00993	1.64440	2.24735	0.26320	0.00025
H	10.72949	0.87389	0.61834	0.26118	-0.00422
Cu	-2.31582	0.20428	0.01765	1.11871	0.36082
N	-2.89029	2.10923	-0.02102	-0.56923	0.04747
N	-4.23979	-0.10143	-0.00045	-0.54306	0.13420
N	-2.26599	-1.78398	0.05179	-0.56954	0.04759
C	-2.11199	3.20433	-0.03040	0.06301	-0.00315
C	-2.64155	4.49459	-0.06668	-0.23190	0.00338
C	-4.02528	4.64818	-0.09359	-0.15066	-0.00168
C	-4.83988	3.51152	-0.08240	-0.19119	0.00006
C	-4.25407	2.24996	-0.04586	0.17545	0.00091
C	-5.02784	0.97563	-0.03002	0.18969	-0.00652
C	-6.41399	0.78812	-0.04049	-0.20737	0.00677
C	-6.89617	-0.52697	-0.01823	-0.14590	-0.00508
C	-6.02769	-1.62552	0.01381	-0.20617	0.00675
C	-4.65201	-1.37066	0.02238	0.18983	-0.00654
C	-3.51989	-2.34052	0.05435	0.18601	0.00091
C	-3.68828	-3.72108	0.08479	-0.21697	0.00003
C	-2.56251	-4.55004	0.11372	-0.14005	-0.00167
C	-1.29492	-3.97480	0.10907	-0.23402	0.00334
C	-1.18579	-2.58363	0.07679	0.06126	-0.00328
H	-1.03963	3.03887	-0.00821	0.25921	0.00149
H	-1.97466	5.34927	-0.07301	0.28150	0.00022
H	-4.47149	5.63693	-0.12254	0.28289	0.00007
H	-5.91881	3.61397	-0.10233	0.27087	0.00041
H	-7.10503	1.62262	-0.06423	0.27471	0.00095
H	-7.96776	-0.69857	-0.02551	0.28148	0.00018
H	-6.42383	-2.63405	0.03116	0.27271	0.00096
H	-4.68307	-4.15140	0.08644	0.26908	0.00042
H	-2.68148	-5.62838	0.13855	0.27844	0.00006
H	-0.39703	-4.58169	0.12992	0.27783	0.00024
H	-0.21319	-2.10005	0.06622	0.26948	0.00164

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$[Cu^{II}(tpy)(Phe)]^{\bullet 2+}$ Cu-O=6.0 E=-2937.242487670

C	3.98391	-0.99859	0.09163	0.81192	0.00024
C	5.53533	-0.98705	0.23848	-0.16912	0.02116
C	6.12884	0.14179	-0.65569	-0.48423	0.00653
C	7.54096	0.50463	-0.30565	0.03770	0.14066
C	7.81241	1.23484	0.88391	-0.19892	0.06134
C	8.62172	0.13624	-1.13626	-0.22610	0.00740
C	9.92326	0.47834	-0.79604	-0.19345	0.03074
C	9.11149	1.57875	1.22639	-0.22442	-0.02030
C	10.17590	1.20014	0.39009	-0.12983	0.16953
N	6.04695	-2.33317	0.01255	-0.90988	0.03168
O	3.31705	0.01113	0.02804	-0.58646	0.04108
O	3.45265	-2.22286	0.08511	-0.70837	0.00759
H	4.22172	-2.84502	0.12740	0.53451	-0.00069
H	6.79385	-2.60186	0.64376	0.42591	-0.00045
H	6.35078	-2.49637	-0.94371	0.41252	-0.00020
H	5.70878	-0.73501	1.29184	0.27091	-0.00061
H	5.46961	1.00883	-0.52267	0.29092	0.00854
H	6.05598	-0.16391	-1.70552	0.25317	-0.00025
H	6.98653	1.54088	1.52083	0.24997	-0.00191
H	8.42873	-0.40715	-2.05685	0.25129	-0.00045
H	10.74895	0.19725	-1.44171	0.26366	-0.00097
H	9.30774	2.14485	2.13099	0.26383	0.00038
H	11.19459	1.46796	0.65224	0.26150	-0.00470

C	-2.69205	0.10991	-0.00502	1.07399	0.31019
N	-2.03851	2.08948	-0.04203	-0.56649	0.04011
N	-4.64363	0.11625	-0.00032	-0.54665	0.11273
N	-2.96871	-1.86785	0.03316	-0.56611	0.04004
C	-2.02155	3.05324	-0.06349	0.06121	-0.00278
C	-2.34478	4.41003	-0.08804	-0.23416	0.00286
C	-3.68827	4.77574	-0.09027	-0.14995	-0.00149
C	-4.66704	3.77796	-0.06822	-0.19309	0.00012
C	-4.28262	2.44043	-0.04443	0.17680	0.00070
C	-5.24930	1.30437	-0.02037	0.18870	-0.00558
C	-6.64795	1.34411	-0.01681	-0.20855	0.00573
C	-7.33591	0.12435	0.00782	-0.14881	-0.00431
C	-6.65515	-1.09949	0.02841	-0.20706	0.00572
C	-5.25624	-1.06818	0.02356	0.18875	-0.00559
C	-4.29642	-2.21019	0.04219	0.18773	0.00069
C	-4.68981	-3.54503	0.06731	-0.21818	0.00012
C	-3.71771	-4.54938	0.08371	-0.14121	-0.00149
C	-2.37202	-4.19244	0.07467	-0.23468	0.00284
C	-2.03922	-2.83786	0.04923	0.06137	-0.00280
H	-0.98714	2.72560	-0.06093	0.25542	0.00128
H	-1.55394	5.15128	-0.10487	0.27939	0.00017
H	-3.97738	5.82149	-0.10900	0.27811	0.00007
H	-5.71738	4.04565	-0.06982	0.26972	0.00036
H	-7.19609	2.27885	-0.03248	0.27288	0.00079
H	-8.42115	0.12762	0.01110	0.27997	0.00015
H	-7.20883	-2.03089	0.04755	0.27111	0.00080
H	-5.74194	-3.80546	0.07414	0.26817	0.00036
H	-4.01378	-5.59318	0.10332	0.27786	0.00006
H	-1.58592	-4.93877	0.08690	0.27897	0.00017
H	-1.00177	-2.51973	0.04135	0.25693	0.00131

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$[Cu^{II}(tpy)(Phe)]^{\bullet 2+}$	Cu-O=7.0	E=-2937.242351650			
C	4.67448	-0.87060	-0.80144	0.81111	-0.00004
C	6.22956	-0.89036	-0.65857	-0.16780	0.02478
C	6.72675	0.55276	-0.33572	-0.48493	0.00993
C	8.11014	0.59626	0.23449	0.04032	0.14318
C	8.34249	0.15586	1.56728	-0.19654	0.06613
C	9.20447	1.06810	-0.52438	-0.22398	0.01119
C	10.48059	1.09856	0.01951	-0.19404	0.02870
C	9.61648	0.18537	2.11342	-0.22500	-0.02268
C	10.69437	0.65372	1.34209	-0.12707	0.17647
N	6.81212	-1.53741	-1.82193	-0.90043	0.04588
O	3.95779	-0.19571	-0.09587	-0.57187	0.05631
O	4.20636	-1.69543	-1.73715	-0.69691	0.00973
H	4.99843	-2.09486	-2.17140	0.53430	-0.00093
H	7.60086	-2.14014	-1.61564	0.42612	-0.00062
H	7.06648	-0.89469	-2.56700	0.41321	-0.00047
H	6.41509	-1.53435	0.20977	0.27131	-0.00071
H	6.00374	0.95831	0.38412	0.29351	0.00932
H	6.65947	1.16150	-1.24415	0.25389	-0.00041
H	7.50457	-0.18960	2.16710	0.25105	-0.00205
H	9.03948	1.42178	-1.53805	0.25194	-0.00056
H	11.31632	1.46716	-0.56641	0.26394	-0.00092
H	9.78269	-0.14277	3.13416	0.26428	0.00044
H	11.69376	0.67974	1.76492	0.26154	-0.00490
Cu	-3.03565	0.07501	0.04039	1.04794	0.28007
N	-3.32320	2.05564	-0.06956	-0.56180	0.03589
N	-5.00453	0.08102	0.09820	-0.55116	0.10020
N	-3.32794	-1.90382	0.16779	-0.56394	0.03588
C	-2.39420	3.02215	-0.15681	0.06044	-0.00256
C	-2.72361	4.37570	-0.22765	-0.23573	0.00254
C	-4.06830	4.73632	-0.20714	-0.14256	-0.00138
C	-5.04059	3.73647	-0.11695	-0.21370	0.00014
C	-4.64923	2.40210	-0.04921	0.16915	0.00061
C	-5.61254	1.26630	0.04830	0.20826	-0.00508
C	-7.01070	1.30701	0.09121	-0.21274	0.00511
C	-7.69643	0.08947	0.18530	-0.15012	-0.00387
C	-7.01370	-1.13232	0.23567	-0.20775	0.00512
C	-5.61541	-1.10034	0.18840	0.18819	-0.00503
C	-4.65496	-2.24209	0.22649	0.18847	0.00059
C	-5.05011	-3.57408	0.31573	-0.21919	0.00015
C	-4.08049	-4.58012	0.34621	-0.14253	-0.00137
C	-2.73478	-4.22776	0.28662	-0.23580	0.00254
C	-2.40146	-2.87621	0.19786	0.06041	-0.00257

H	-1.85551	2.69918	-0.17018	0.25306	0.00116
H	-1.09855	5.11837	-0.29684	0.27836	0.00015
H	-4.36300	5.77931	-0.26052	0.27720	0.00006
H	-6.09189	3.99970	-0.10017	0.26742	0.00032
H	-7.56034	2.24025	0.05403	0.27008	0.00070
H	-8.78110	0.09290	0.22029	0.27896	0.00014
H	-7.56552	-2.06208	0.30943	0.27000	0.00070
H	-6.10221	-3.83052	0.36137	0.26739	0.00033
H	-4.37798	-5.62136	0.41567	0.27710	0.00006
H	-1.95002	-4.97534	0.30756	0.27822	0.00015
H	-1.36465	-2.56029	0.14902	0.25357	0.00116

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$[Cu^{II}(tpy)(Phe)]^{\bullet 2+}$	Cu-O=8.0	E=-2937.243018990			
C	-5.34257	-0.61767	1.13217	0.81097	-0.00019
C	-6.89624	-0.66129	0.95352	-0.16684	0.02740
C	-7.35080	0.63585	0.21174	-0.48477	0.01215
C	-8.70129	0.52030	-0.42021	0.04104	0.14356
C	-8.87027	-0.27447	-1.58864	-0.19463	0.06969
C	-9.82628	1.18662	0.11577	-0.22290	0.01302
C	-11.07052	1.06653	-0.48591	-0.19407	0.02789
C	-10.11244	-0.39553	-2.19216	-0.22568	-0.02460
C	-11.22129	0.27115	-1.64269	-0.12608	0.17950
N	-7.52398	-0.93617	2.23170	-0.89407	0.05617
O	-4.59910	-0.18349	0.28116	-0.56050	0.06824
O	-4.91296	-1.13935	2.27885	-0.69083	0.01133
H	-5.71919	-1.39053	2.78906	0.53387	-0.00111
H	-8.31290	-1.57130	2.18958	0.42673	-0.00076
H	-7.78220	-0.10552	2.75686	0.41407	-0.00065
H	-7.06983	-1.52611	0.30173	0.27201	-0.00077
H	-6.58414	0.81566	-0.55378	0.29496	0.00948
H	-7.31600	1.47572	0.91418	0.25466	-0.00050
H	-8.00741	-0.77493	-2.02014	0.25164	-0.00215
H	-9.70931	1.80846	0.99862	0.25233	-0.00061
H	-11.92985	1.58543	-0.07368	0.26401	-0.00090
H	-10.22975	-0.99467	-3.08907	0.26437	0.00051
H	-12.19635	0.18020	-2.11092	0.26149	-0.00499
Cu	3.38987	0.04607	-0.07043	1.02131	0.26077
N	3.68402	2.03070	0.00391	-0.56065	0.03305
N	5.36423	0.04906	-0.11207	-0.54993	0.09203
N	3.68647	-1.93761	-0.15836	-0.56064	0.03306
C	2.75800	3.00205	0.06426	0.05977	-0.00242
C	3.09056	4.35581	0.11143	-0.23646	0.00234
C	4.43646	4.71207	0.09535	-0.14348	-0.00130
C	5.40594	3.70762	0.03308	-0.21978	0.00014
C	5.01095	2.37315	-0.01184	0.18894	0.00048
C	5.97339	1.23384	-0.07891	0.18934	-0.00475
C	7.37208	1.27290	-0.10932	-0.20838	0.00470
C	8.05735	0.05323	-0.17360	-0.15161	-0.00358
C	7.37364	-1.16854	-0.20693	-0.20840	0.00470
C	5.97489	-1.13379	-0.17356	0.18934	-0.00475
C	5.01392	-2.27603	-0.19855	0.18895	0.00049
C	5.41082	-3.60933	-0.25903	-0.21980	0.00014
C	4.44267	-4.61679	-0.27931	-0.14354	-0.00130
C	3.09621	-4.26458	-0.23883	-0.23649	0.00234
C	2.76170	-2.91181	-0.17873	0.05982	-0.00242
H	1.72121	2.68273	0.07515	0.25200	0.00108
H	2.30557	5.10192	0.15934	0.27768	0.00014
H	4.73404	5.75500	0.13073	0.27651	0.00005
H	6.45819	3.96718	0.02003	0.26686	0.00030
H	7.92254	2.20606	-0.08473	0.26924	0.00064
H	9.14230	0.05493	-0.19838	0.27816	0.00014
H	7.92524	-2.09998	-0.25741	0.26922	0.00064
H	6.46350	-3.86555	-0.29027	0.26684	0.00030
H	4.74167	-5.65885	-0.32631	0.27646	0.00006
H	2.31218	-5.01308	-0.25299	0.27762	0.00014
H	1.72436	-2.59578	-0.14595	0.25216	0.00108

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$[Cu^{II}(tpy)(Phe)]^{\bullet 2+}$	Cu-O=9.0	E=-2937.243987900			
C	-5.98626	-0.62132	1.15463	0.81094	-0.00037
C	-7.54072	-0.65825	0.96497	-0.16614	0.02928
C	-7.97973	0.64139	0.21594	-0.48472	0.01370
C	-9.31959	0.52936	-0.43655	0.04160	0.14394
C	-9.47279	-0.26883	-1.60523	-0.19348	0.07182
C	-10.45068	1.20181	0.07933	-0.22207	0.01450

C	-11.85527	1.08466	-0.54199	-0.19431	0.02709
C	-10.66551	-0.38683	-2.22818	-0.22599	-0.02576
C	-11.82034	0.28595	-1.69856	-0.12534	0.18167
N	-8.18041	-0.92508	2.23679	-0.88991	0.06310
O	-5.23772	-0.19294	0.30591	-0.55146	0.07717
O	-5.56606	-1.13955	2.30548	-0.68739	0.01247
H	-6.37392	-1.38844	2.81284	0.53355	-0.00123
H	-8.96901	-1.56041	2.19461	0.42716	-0.00086
H	-8.43494	-0.09339	2.76189	0.41466	-0.00076
H	-7.71299	-1.52381	0.31398	0.27257	-0.00079
H	-7.19956	0.81631	-0.53747	0.29620	0.00970
H	-7.95235	1.48135	0.91846	0.25524	-0.00058
H	-8.60492	-0.77362	-2.02135	0.25221	-0.00221
H	-10.34536	1.82559	0.96225	0.25256	-0.00066
H	-12.54917	1.60815	-0.14545	0.26402	-0.00088
H	-10.81079	-0.98817	-3.12510	0.26452	0.00054
H	-12.78813	0.19717	-2.18204	0.26142	-0.00506
Cu	3.75136	0.04456	-0.06826	1.00918	0.24642
N	4.05264	2.03031	0.00938	-0.55975	0.03114
N	5.72964	0.04396	-0.10490	-0.55066	0.08617
N	4.04865	-1.94123	-0.15809	-0.55973	0.03117
C	3.13013	3.00498	0.06877	0.05940	-0.00232
C	3.46660	4.35768	0.11855	-0.23702	0.00220
C	4.81363	4.70964	0.10619	-0.14434	-0.00124
C	5.77976	3.70202	0.04493	-0.22041	0.00015
C	5.38054	2.36877	-0.00271	0.18914	0.00044
C	6.34093	1.22719	-0.06904	0.18917	-0.00448
C	7.73983	1.26426	-0.09644	-0.20893	0.00441
C	8.42318	0.04356	-0.16082	-0.15263	-0.00337
C	7.73739	-1.17694	-0.19719	-0.20893	0.00442
C	6.33856	-1.13941	-0.16670	0.18914	-0.00448
C	5.37581	-2.28055	-0.19540	0.18918	0.00044
C	5.77197	-3.61418	-0.25645	-0.22043	0.00015
C	4.80343	-4.62110	-0.28035	-0.14439	-0.00123
C	3.45708	-4.26817	-0.24282	-0.23707	0.00219
C	3.12383	-2.91517	-0.18195	0.05945	-0.00231
H	2.09233	2.68904	0.07668	0.25137	0.00103
H	2.68383	5.10618	0.16554	0.27722	0.00012
H	5.11460	5.75153	0.14368	0.27598	0.00005
H	6.83289	3.95805	0.03481	0.26635	0.00029
H	8.29198	2.19637	-0.06955	0.26864	0.00060
H	9.50817	0.04340	-0.18331	0.27755	0.00013
H	8.28761	-2.10919	-0.24780	0.26863	0.00060
H	6.82456	-3.87101	-0.28529	0.26636	0.00028
H	5.10201	-5.66326	-0.32782	0.27594	0.00005
H	2.67253	-5.01608	-0.25982	0.27719	0.00013
H	2.08723	-2.59696	-0.15114	0.25140	0.00102

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$[Cu^{II}(tpy)(Phe)]^{\bullet 2+}$ Cu-O=10.0 E=-2937.245035230

C	-6.63406	-0.63263	1.19888	0.81091	-0.00055
C	-8.18639	-0.67002	0.98337	-0.16560	0.03080
C	-8.60970	0.63325	0.23022	-0.48472	0.01504
C	-9.93415	0.52280	-0.45177	0.04174	0.14382
C	-10.06015	-0.26907	-1.62813	-0.19257	0.07351
C	-11.07773	1.19000	0.04331	-0.22147	0.01565
C	-12.29814	1.07385	-0.60534	-0.19452	0.02643
C	-11.27882	-0.38595	-2.27834	-0.22626	-0.02668
C	-12.40624	0.28144	-1.76913	-0.12500	0.18304
N	-8.84747	-0.93993	2.24184	-0.88635	0.06869
O	-5.87455	-0.19454	0.36552	-0.54442	0.08438
O	-6.23076	-1.16200	2.35012	-0.68443	0.01340
H	-7.04455	-1.41563	2.84454	0.53332	-0.00133
H	-9.63461	-1.57594	2.18694	0.42742	-0.00092
H	-9.10615	-0.11140	2.76971	0.41517	-0.00087
H	-8.34691	-1.53358	0.32676	0.27303	-0.00083
H	-7.81228	0.80965	-0.50474	0.29709	0.00979
H	-8.59696	1.47043	0.93635	0.25580	-0.00064
H	-9.18231	-0.76952	-2.02825	0.25262	-0.00226
H	-10.99283	1.80900	0.93178	0.25271	-0.00069
H	-13.17161	1.59334	-0.22480	0.26399	-0.00086
H	-11.36328	-0.98226	-3.18081	0.26458	0.00056
H	-13.36313	0.19342	-2.27401	0.26133	-0.00510
Cu	4.11329	0.01646	-0.08024	1.00001	0.23535
N	4.36380	2.01094	0.00514	-0.55894	0.02970

N	6.09678	0.06876	-0.09304	-0.55124	0.08168
N	4.46782	-1.96185	-0.17114	-0.55898	0.02970
C	3.41619	2.96174	0.05428	0.05911	-0.00223
C	3.71709	4.32261	0.10994	-0.23747	0.00209
C	5.05468	4.70897	0.11469	-0.14512	-0.00119
C	6.04678	3.72643	0.06417	-0.22091	0.00016
C	5.68247	2.38336	0.01004	0.18927	0.00039
C	6.67326	1.26727	-0.04592	0.18900	-0.00427
C	8.07098	1.34148	-0.05394	-0.20938	0.00420
C	8.78720	0.13946	-0.11195	-0.15343	-0.00321
C	8.13439	-1.09852	-0.16071	-0.20939	0.00419
C	6.73467	-1.09762	-0.14934	0.18905	-0.00427
C	5.80334	-2.26431	-0.19387	0.18925	0.00040
C	6.23745	-3.58618	-0.25557	-0.22089	0.00015
C	5.29801	-4.61967	-0.29506	-0.14507	-0.00119
C	3.94206	-4.30429	-0.27206	-0.23743	0.00209
C	3.57047	-2.96136	-0.20978	0.05911	-0.00223
H	2.38680	2.61935	0.04843	0.25100	0.00099
H	2.91482	5.05069	0.14810	0.27679	0.00012
H	5.32844	5.75814	0.15706	0.27551	0.00005
H	7.09303	4.00948	0.06711	0.26595	0.00027
H	8.59796	2.28768	-0.01691	0.26813	0.00057
H	9.87203	0.16802	-0.11945	0.27705	0.00012
H	8.70959	-2.01586	-0.20573	0.26813	0.00057
H	7.29713	-3.81301	-0.27312	0.26592	0.00028
H	5.62605	-5.65290	-0.34323	0.27554	0.00004
H	3.17886	-5.07361	-0.30134	0.27683	0.00013
H	2.52447	-2.67425	-0.19022	0.25103	0.00099