

Supporting information

Non-radiative deactivation in phenol-pyridine complex: Theoretical study

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Excited state minimum geometries of complexes computed at RICC2/aug-cc-pVDZ level of theory

A1) Optimized geometry of Pl conformer of PhOH-Py complex in it's ground state.

3.30411998112754	1.50655513190764	0.00000000000000	c
3.47728002451601	-1.15570421852682	0.00000000000000	c
5.87519276250998	-2.31640957750220	0.00000000000000	c
8.07239000265813	-0.82554004084668	0.00000000000000	c
7.90953306686495	1.83150882038002	0.00000000000000	c
5.51417879352451	2.98487973785200	0.00000000000000	c
1.39631485778605	-2.68751862617761	0.00000000000000	o
-3.28914201267009	-0.32032672115505	0.00000000000000	n
-4.14900573135674	2.08466324452272	0.00000000000000	c
-6.73084622583976	2.70109854341839	0.00000000000000	c
-8.51414127827387	0.73404273753365	0.00000000000000	c
-7.63411949184136	-1.77087999185743	0.00000000000000	c
-5.01546145508442	-2.20530524459169	0.00000000000000	c
-7.31945818279146	4.68065098871082	0.00000000000000	h
-2.71088695241890	3.57057561704040	0.00000000000000	h
-4.25216396972842	-4.12756975847586	0.00000000000000	h
-8.94511335803477	-3.36689383574178	0.00000000000000	h
-10.53967676381905	1.14339511613477	0.00000000000000	h
-0.14667614369122	-1.62667621832052	0.00000000000000	h
1.44258837689414	2.40550415918564	0.00000000000000	h
5.35599642129077	5.04696612400334	0.00000000000000	h
9.62400833362227	2.98465159162553	0.00000000000000	h
9.92326686324762	-1.74818039310907	0.00000000000000	h
5.97765476106584	-4.38024063912939	0.00000000000000	h

A2) Optimized geometry of Pe conformer of PhOH-Py complex in it's ground state.

-5.95855839534048	1.96130956107107	0.00000000000000	c
-6.48094888032386	3.96077401441344	0.00000000000000	h
-7.80458061226167	0.05295051342221	0.00000000000000	c
-9.80502645857868	0.57791263126260	0.00000000000000	h
-7.10121626603339	-2.51458007262531	0.00000000000000	c
-8.54277115605477	-3.99498740111001	0.00000000000000	h
-4.51986300657963	-3.15011260936486	0.00000000000000	c
-3.94182677696218	-5.13615611563759	0.00000000000000	h
-2.65459602878477	-1.25361795914615	0.00000000000000	c
-0.65091674840901	-1.75858381740781	0.00000000000000	h
-3.37236334755361	1.31848671452847	0.00000000000000	c
-1.66068246830408	3.25782648302508	0.00000000000000	o
0.07689839418621	2.55590037623582	0.00000000000000	h
3.19382876247385	1.25244569759183	0.00000000000000	n
4.33373787852296	0.59495814493630	-2.19077397975117	c
4.33373787852296	0.59495814493630	2.19077397975117	c
3.35250210596763	1.15218794648011	3.92403786603767	h
3.35250210596763	1.15218794648011	-3.92403786603767	h
6.63224637518721	-0.73020343294036	-2.28225691978372	c
6.63224637518721	-0.73020343294036	2.28225691978372	c
7.47083139105818	-1.21818583084232	4.10579733597807	h
7.47083139105818	-1.21818583084232	-4.10579733597807	h
7.80752696661875	-1.40940596147583	0.00000000000000	c
9.59653987118560	-2.44375355507750	0.00000000000000	h

B1) Optimized geometry of Pl conformer of PhOH-Py complex in it's A'(1 $\pi\pi^*$ (LE)) singlet excited state.

3.14374562665133	1.59962739637671	0.00000000000000	c
3.38681723656008	-1.12486852343661	0.00000000000000	c
5.76890998218161	-2.41428786507331	0.00000000000000	c
8.04676896415762	-0.91684237328027	0.00000000000000	c
7.82766370479000	1.78061074371677	0.00000000000000	c
5.43492563987092	3.06260268285676	0.00000000000000	c
1.30464190392050	-2.59397643963313	0.00000000000000	o
-3.18716634576909	-0.37301123947266	0.00000000000000	n
-4.00993404581344	2.05373346635033	0.00000000000000	c
-6.58245703108567	2.70642948142885	0.00000000000000	c
-8.39665517589222	0.75857869569395	0.00000000000000	c
-7.55942879679058	-1.76457686101055	0.00000000000000	c
-4.94622630391549	-2.23921185361852	0.00000000000000	c
-7.14357407897516	4.69432560428278	0.00000000000000	h
-2.54464267340633	3.51314483562529	0.00000000000000	h
-4.20635833949747	-4.17161654006538	0.00000000000000	h
-8.89646488747775	-3.33949896833123	0.00000000000000	h
-10.41636832520073	1.19940473981497	0.00000000000000	h
-0.29080530742960	-1.49016702922950	0.00000000000000	h
1.27238288911131	2.46643627698548	0.00000000000000	h
5.37424975856505	5.12740619410654	0.00000000000000	h
9.55597533149564	2.92079428383094	0.00000000000000	h
9.90729161545986	-1.81188702269189	0.00000000000000	h
5.77622736978663	-4.47909916074000	0.00000000000000	h

B2) Optimized geometry of PhO•...HPy• bi-radical (Pl conformer) in it's A'(1 $\pi\pi^*$ (CT)) singlet excited state computed at RICC2/aug-cc-pVDZ level of theory.

-5.93543398146233	-2.37929996396748	0.00000000000000	c
-4.12560853843348	-0.42317052941927	0.00000000000000	n
-4.91873532651140	2.11977667116397	0.00000000000000	c
-7.45905609798168	2.70347150584499	0.00000000000000	c
-9.35643626636460	0.76085374113825	0.00000000000000	c
-8.47889501617343	-1.81014159420635	0.00000000000000	c
2.08484180513922	-2.44594653501562	0.00000000000000	o
4.15206711208503	-1.10499101146958	0.00000000000000	c
4.06007750088885	1.61432130814601	0.00000000000000	c
6.29700845569903	3.00760686784667	0.00000000000000	c
8.65368852572490	1.72618298445750	0.00000000000000	c
8.79223441315550	-0.94465547496909	0.00000000000000	c
6.56310270415600	-2.36262416802979	0.00000000000000	c
-7.99305269275186	4.70284136134456	0.00000000000000	h
-3.42490976820725	3.54138104567647	0.00000000000000	h
-5.19002235298660	-4.30215468525045	0.00000000000000	h
-9.82183692620701	-3.38467875259917	0.00000000000000	h
-11.37019312037468	1.21671801811004	0.00000000000000	h
-2.25203304068533	-0.85832870413370	0.00000000000000	h
2.19819554452900	2.51080303555424	0.00000000000000	h
6.24960479986461	5.07434117336039	0.00000000000000	h
10.40308669869924	2.83088665228855	0.00000000000000	h
10.63464509815068	-1.88285396767993	0.00000000000000	h
6.56645382755281	-4.43119257398512	0.00000000000000	h

B3) Optimized geometry of PhO•...HPy• bi-radical (Pl conformer) in it's A"($^1\pi\sigma^*$) singlet excited state computed at RICC2/aug-cc-pVDZ level of theory.

4.16546511652912	2.01415566340502	0.00000000000000	c
3.57495903075754	-0.64065206716822	0.00000000000000	c
5.58630949227577	-2.46853759850701	0.00000000000000	c
8.09821520236761	-1.65583428350469	0.00000000000000	c
8.64184443690465	0.96565988386976	0.00000000000000	c
6.68333725507544	2.79628693918977	0.00000000000000	c
1.23025748314644	-1.42336305422277	0.00000000000000	o
-3.70338257967563	0.23618750277790	0.00000000000000	n
-5.04524703158602	2.41935481005819	0.00000000000000	c
-7.68518241691950	2.32920461773743	0.00000000000000	c
-8.89991892029876	-0.03131944511281	0.00000000000000	c
-7.44303546732834	-2.26632352089638	0.00000000000000	c
-4.81428941194170	-2.08093631980581	0.00000000000000	c
-8.75096966309441	4.10263985914066	0.00000000000000	h
-3.94628067731024	4.17604848548113	0.00000000000000	h
-3.52852335548195	-3.69574546727467	0.00000000000000	h
-8.33246457483546	-4.13179536406841	0.00000000000000	h
-10.96890076504697	-0.13881960210393	0.00000000000000	h
-1.72513509843487	0.27343856296895	0.00000000000000	h
2.59915940799975	3.36646405896048	0.00000000000000	h
7.14905430969433	4.81079653808454	0.00000000000000	h
10.61407052901374	1.59275651858665	0.00000000000000	h
9.64355014225379	-3.02968614399327	0.00000000000000	h
5.07116009815215	-4.47219862030544	0.00000000000000	h

C1) Optimized geometry of PhO•...HPy• bi-radical (Pe conformer) in it's A" singlet excited state computed at RICC2/aug-cc-pVDZ level of theory.

-1.79006211086663	-0.77049011337995	0.00000000000000	c
0.27234518698727	-0.79800688402697	0.00000000000000	h
-3.19183168916300	-3.00425807665567	0.00000000000000	c
-2.22001986518086	-4.82759531557001	0.00000000000000	h
-5.87337587119463	-2.90304475849248	0.00000000000000	c
-6.94853924597689	-4.67065949688888	0.00000000000000	h
-7.18442454369264	-0.58009552521256	0.00000000000000	c
-9.25143625481466	-0.54651842464333	0.00000000000000	h
-5.80409157477780	1.67694745615452	0.00000000000000	c
-6.71951305866069	3.53159977940594	0.00000000000000	h
-3.10703211965954	1.59187524708890	0.00000000000000	c
-1.83771721117224	3.82026142430042	0.00000000000000	o
2.33513951931536	3.54874797341607	0.00000000000000	h
3.94544559614401	2.46699638965495	0.00000000000000	n
4.40571288756171	1.12771962715304	2.30205636825320	c
4.14515999049930	2.22761816685620	4.03099943913537	h
5.14736484634867	-1.36934112604795	2.30854434659079	c
5.52321645591279	-2.26134097659050	4.13966199282045	h
5.45164967105113	-2.77349294583366	0.00000000000000	c
6.05501392807683	-4.74771629019984	0.00000000000000	h
5.14736484634867	-1.36934112604795	-2.30854434659079	c
5.52321645591279	-2.26134097659050	-4.13966199282045	h
4.40571288756171	1.12771962715304	-2.30205636825320	c
4.14515999049930	2.22761816685620	-4.03099943913537	h

C2) Optimized geometry of PhO•...HPy• bi-radical (Pe conformer) in it's A' singlet excited state computed at RICC2/aug-cc-pVDZ level of theory.

6.92332023924659	-1.93151850627933	0.00000000000000	c
6.04283627889931	-1.00312202895166	-2.33626170865067	c
4.12798036055996	0.97108482189481	-2.28699710103771	c
3.32223364324685	1.82764580486018	0.00000000000000	n
4.12798036055996	0.97108482189481	2.28699710103771	c
6.04283627889931	-1.00312202895166	2.33626170865067	c
-1.88840719257720	3.53497401749324	0.00000000000000	o
-3.26564979518873	1.48796352901639	0.00000000000000	c
-5.97745522692653	1.72095011344395	0.00000000000000	c
-7.49692919264654	-0.43967943185510	0.00000000000000	c
-6.35016923617396	-2.85592922762067	0.00000000000000	c
-3.68033879152340	-3.13155111813520	0.00000000000000	c
-2.13677912882863	-0.99654595766833	0.00000000000000	c
-6.77381657866890	3.63029822565585	0.00000000000000	h
-9.55806071620407	-0.27328053304744	0.00000000000000	h
-7.54253938561345	-4.54704368154962	0.00000000000000	h
-2.83927384707706	-5.02037157917223	0.00000000000000	h
-0.07702141983743	-1.14943388512245	0.00000000000000	h
1.78596219810988	3.03007565337533	0.00000000000000	h
3.25915150020115	1.84405973713259	3.93996441946992	h
3.25915150020115	1.84405973713259	-3.93996441946992	h
6.75435047513948	-1.71634687837982	4.13709758768842	h
6.75435047513948	-1.71634687837982	-4.13709758768842	h
8.35738874938047	-3.42875417508834	0.00000000000000	h

D1) Optimized geometry structure of Pl conformer of PhOH-Py complex in it's A'(³ππ*) triplet excited state computed at RICC2/aug-cc-pVDZ level of theory.

3.25767914853403	1.61467400067765	0.00000000000000	c
3.36332717299008	-1.01146690503881	0.00000000000000	c
5.85059799356882	-2.39984096621371	0.00000000000000	c
8.12423128016269	-0.93042522885261	0.00000000000000	c
8.01925897860864	1.68660552335835	0.00000000000000	c
5.52824139631276	3.06076815450812	0.00000000000000	c
1.34259902928692	-2.59310828942787	0.00000000000000	o
-3.28458057968361	-0.38793057298050	0.00000000000000	n
-4.09895956711560	2.03980246745123	0.00000000000000	c
-6.67007409142744	2.70670738842402	0.00000000000000	c
-8.49055575602540	0.76833847414005	0.00000000000000	c
-7.66383156235762	-1.75932637499092	0.00000000000000	c
-5.05248991518809	-2.24341265441013	0.00000000000000	c
-7.22261467023911	4.69712761086014	0.00000000000000	h
-2.62777499536733	3.49371527768996	0.00000000000000	h
-4.32331959544953	-4.17992254416187	0.00000000000000	h
-9.00813070126409	-3.32812119789277	0.00000000000000	h
-10.50847576039676	1.21755591658985	0.00000000000000	h
-0.26328267605846	-1.56559641058876	0.00000000000000	h
1.41843669673376	2.56089627907388	0.00000000000000	h
5.48972517437576	5.12277366839063	0.00000000000000	h
9.76674627091484	2.79183902165747	0.00000000000000	h
9.95594714067246	-1.89076143948355	0.00000000000000	h
5.82675431671567	-4.46170401783672	0.00000000000000	h

D2) Optimized geometry of Pe conformer of PhOH-Py complex in it's A'(3ππ*) triplet excited state computed at RICC2/aug-cc-pVDZ level of theory.

-5.94586596091166	2.01696942953437	0.00000000000000	c
-6.38340974259825	4.03229397825873	0.00000000000000	h
-7.83637124321260	0.07669794138873	0.00000000000000	c
-9.83655320731531	0.60451760737607	0.00000000000000	h
-7.14763194089078	-2.44825710581571	0.00000000000000	c
-8.60219014721145	-3.91804525497465	0.00000000000000	h
-4.41264443563528	-3.22591170571093	0.00000000000000	c
-3.91240322524899	-5.22725517533294	0.00000000000000	h
-2.51471767006612	-1.31335104361738	0.00000000000000	c
-0.51278904193382	-1.83084047776649	0.00000000000000	h
-3.21005483380870	1.22263025089526	0.00000000000000	c
-1.60616072158962	3.23045083306671	0.00000000000000	o
0.18998880982371	2.59261287399209	0.00000000000000	h
3.18917773641699	1.37886292083861	0.00000000000000	n
4.29757172661003	0.66279207964738	-2.19631620911621	c
4.29757172661003	0.66279207964738	2.19631620911621	c
3.33462288274828	1.25856184019878	3.92797344822697	h
3.33462288274828	1.25856184019878	-3.92797344822697	h
6.53516946965484	-0.76551260071111	-2.28884783941418	c
6.53516946965484	-0.76551260071111	2.28884783941418	c
7.35121498910322	-1.29528380901903	4.11157905654354	h
7.35121498910322	-1.29528380901903	-4.11157905654354	h
7.67698754791047	-1.49465001708386	0.00000000000000	c
9.41666236514769	-2.61152376941506	0.00000000000000	h