The optimized atomic coordinate of ph conformer in ground state

25

Energy = -841.6569271312

N	0.0729428	-0.8219140	-0.0307217
C	0.9040627	-1.9197956	0.0417211
C	2.2088467	-1.5120669	0.0834540
C	3.1981086	0.9086010	0.0443259
C	2.8280045	2.2414936	-0.0162650
C	1.4738609	2.6167422	-0.0874132
C	0.4661208	1.6654798	-0.0984048
C	2.2020407	-0.0787495	0.0351261
C	0.8399154	0.3219082	-0.0364683
H	-0.9399663	-0.8536548	-0.0685203
H	0.4904293	-2.9154461	0.0571343
H	3.0717661	-2.1557454	0.1411699
H	4.2445689	0.6309616	0.0981725
H	3.5899883	3.0116288	-0.0095547
H	1.2152793	3.6678798	-0.1351144
H	-0.5761488	1.9583906	-0.1544738
S	-3.4818414	-0.7168272	-0.0683520
C	-3.7237781	0.3318412	1.4136498
C	-3.7798792	0.5202756	-1.3854762
H	-4.7327191	0.7439323	1.4285876
H	-3.5911134	-0.3113619	2.2824940
H	-2.9907380	1.1376279	1.4530766
H	-3.0488332	1.3277703	-1.3440317
H	-3.6813880	0.0008206	-2.3375993
H	-4.7881248	0.9264751	-1.3059886

The optimized atomic coordinate of ph conformer in the S_1 state

25

Energy = -841.6443768547

N	-0.0079904	-0.9037564	-0.0227847
C	0.7851869	-1.9762599	0.0044953
C	2.1296988	-1.4995344	0.0329365
C	3.1168180	0.9231424	0.0358273
C	2.6739326	2.2788707	0.0073506
C	1.3357590	2.6143109	-0.0260033
C	0.2869229	1.6278798	-0.0338881
C	2.0932217	-0.0636871	0.0208572
C	0.7502157	0.2963224	-0.0135683
H	-1.0321622	-0.9346459	-0.0419920
H	0.4018478	-2.9824347	0.0040823
H	3.0051135	-2.1298731	0.0585838

H	4.1643878	0.6609659	0.0614837
H	3.4117168	3.0726467	0.0118246
H	1.0572446	3.6617245	-0.0475425
H	-0.7578519	1.8961474	-0.0669681
S	-3.4163297	-0.7177049	-0.0248391
C	-3.5171774	0.4235686	1.4078846
C	-3.5722534	0.4802659	-1.4052278
H	-4.4732602	0.9466174	1.4070265
H	-3.4499160	-0.1897794	2.3054145
H	-2.6945449	1.1396107	1.4033090
H	-2.7424077	1.1876770	-1.4126253
H	-3.5556989	-0.0978524	-2.3281051
H	-4.5210665	1.0120419	-1.3370037

The optimized atomic coordinate of ph conformer in the S_2 state

25

Energy = -841.6526289043

N	0.0477907	-0.7990355	-0.0333215
C	0.8671919	-1.9232502	0.0401208
C	2.1909887	-1.5075097	0.0814477
C	3.2344275	0.8813374	0.0463065
C	2.8431377	2.2417647	-0.0151492
C	1.4706008	2.6382763	-0.0861577
C	0.4266438	1.6953143	-0.0979800
C	2.2102280	-0.0933993	0.0348903
C	0.8151547	0.3347621	-0.0385715
H	-0.9680925	-0.8213478	-0.0678402
H	0.4440831	-2.9133488	0.0545610
H	3.0462966	-2.1618425	0.1387855
H	4.2773413	0.6020001	0.0993400
H	3.6017186	3.0139770	-0.0087840
H	1.2373090	3.6940834	-0.1324415
H	-0.6109062	1.9940180	-0.1546053
S	-3.4416808	-0.7226017	-0.0647735
C	-3.7069632	0.3239685	1.4160484
C	-3.7630420	0.5050497	-1.3868315
H	-4.7306580	0.6970542	1.4417296
H	-3.5393705	-0.3105318	2.2851836
H	-3.0034020	1.1564664	1.4435251
H	-3.0611939	1.3375909	-1.3340129
H	-3.6296595	-0.0107652	-2.3366088
H	-4.7865363	0.8742337	-1.3243327

The optimized atomic coordinate of py conformer in ground state

25

Energy = -841.6567128168

N	0.1018544	0.5445987	-0.0040749
C	0.3413577	1.9026347	-0.0034443
C	1.6887635	2.1368696	-0.0011676
C	3.6732304	0.4333565	0.0019199
C	3.9494761	-0.9232641	0.0022017
C	2.9138858	-1.8764101	0.0004254
C	1.5829504	-1.4912625	-0.0016887
C	2.3360220	0.8569457	-0.0002254
C	1.3065619	-0.1229413	-0.0020302
H	-0.8144306	0.1103854	-0.0048042
H	-0.4792573	2.6022871	-0.0047485
H	2.1629361	3.1051427	-0.0003200
H	4.4787324	1.1590092	0.0033191
H	4.9788600	-1.2613528	0.0038052
H	3.1622489	-2.9310730	0.0006832
H	0.7864192	-2.2262184	-0.0030458
S	-3.1673362	-0.8062079	0.0016321
C	-3.8971923	0.1176380	1.4036118
C	-3.9050953	0.1110573	-1.4005066
H	-4.9832838	0.0281628	1.3983619
H	-3.5084791	-0.3304958	2.3169666
H	-3.6100275	1.1687312	1.3730683
H	-3.6173617	1.1621716	-1.3768146
H	-3.5219278	-0.3417325	-2.3139084
H	-4.9911676	0.0220480	-1.3884448

The optimized atomic coordinate of py conformer in the S_1 state

25

Energy = -841.6450163237

N	0.0902109	0.5744698	-0.0037045
C	0.2765305	1.8992741	-0.0034566
C	1.6877216	2.1177023	-0.0013420
C	3.7074059	0.4545323	0.0018856
C	3.9617138	-0.9502081	0.0021849
C	2.9423090	-1.8802800	0.0005284
C	1.5508099	-1.5067482	-0.0015606
C	2.3373210	0.8407479	-0.0002792
C	1.3259435	-0.1187931	-0.0018457
H	-0.8259037	0.1210659	-0.0042574
H	-0.5387946	2.6019401	-0.0046064
H	2.1583963	3.0888343	-0.0006817

H	4.5059092	1.1823366	0.0033111
H	4.9881909	-1.2978008	0.0037906
H	3.1913520	-2.9352141	0.0007990
H	0.7551323	-2.2360366	-0.0031132
S	-3.1076111	-0.7515351	0.0012279
C	-3.8889344	0.1270296	1.4063579
C	-3.8969532	0.1205122	-1.4034702
H	-4.9712853	0.0036613	1.3766147
H	-3.5056534	-0.3298725	2.3176126
H	-3.6350102	1.1871766	1.4037408
H	-3.6427541	1.1805846	-1.4074395
H	-3.5191666	-0.3408838	-2.3147555
H	-4.9791397	-0.0024162	-1.3667699

The optimized atomic coordinate of py conformer in the S_2 state

25

Energy = -841.6523919959

N	0.0956011	0.5385815	-0.0038450
C	0.3244725	1.9111969	-0.0032864
C	1.6968433	2.1352986	-0.0012562
C	3.7001525	0.4687308	0.0018207
C	3.9612559	-0.9248611	0.0022174
C	2.9106026	-1.8954107	0.0004779
C	1.5546248	-1.5213167	-0.0016748
C	2.3478035	0.8801550	-0.0003521
C	1.2924869	-0.1312367	-0.0020185
H	-0.8227975	0.1042583	-0.0039671
H	-0.4959785	2.6091161	-0.0046401
H	2.1682758	3.1052690	-0.0005588
H	4.5067973	1.1885087	0.0031937
H	4.9854752	-1.2749706	0.0038909
H	3.1738503	-2.9452457	0.0008093
H	0.7588250	-2.2529820	-0.0031486
S	-3.1450683	-0.7834057	0.0013806
C	-3.8957204	0.1216213	1.4067249
C	-3.9037554	0.1151020	-1.4038241
H	-4.9806272	0.0170515	1.3955431
H	-3.5054521	-0.3312793	2.3170662
H	-3.6223270	1.1769057	1.3892594
H	-3.6299964	1.1703768	-1.3930307
H	-3.5189998	-0.3422888	-2.3142683
H	-4.9886034	0.0109041	-1.3857423

Calculated electronic excitation energy (cm^{-1}) (in TD-BP86 and RICC2 method) of isolated indole, indole-H_2O and indole-Me_2S (py and ph), also that of the corresponding experiment results (EX).

	indole		Indole-H_2O		Indole-Me_2S(py)		Indole-Me_2S(ph)	
	TD-BP86	RICC2	TD-BP86	RICC2	TD-BP86	RICC2	TD-BP86	RICC2
S_1	35536(0.014)	39222	32085(0.000)	39003	34186(0.000)	39003	34306(0.014)	38783
EX	35241		35109		35071		35071	
S_2	37349(0.044)	41197	34890(0.052)	40429	35249(0.062)	40693	35196(0.044)	40188
S_3	44688(0.000)	50196	35851(0.000)	49362	37253(0.019)	48704	37160(0.018)	48770
S_4	45597(0.154)	51448	37181(0.016)	5.943	37993(0.002)	51009	38198(0.000)	50218
S_5	47545(0.403)	53335	45569(0.192)	53028	38704(0.000)	52677	38505(0.002)	52721
S_6	48227(0.000)	54169	46444(0.000)	53269	38802(0.000)	52874	39295(0.000)	54059