Electronic Supplementary Information (ESI)

A new mechanism study of second generation TADF material based on the path integral approach incorporating Herzberg-Teller and the Duschinsky rotation effects

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Table S1. Coordinate of the optimized geometric structure for compound 1 at the B3LYP or ω*B97X-D3 /def2-SVP level.

B3LYP/def2-SVP def/J				ω*B97X-D3/def2-SVP (ω=0.04101)			
S_0 state				S_0 state			
N	5.25004153309439	2.62294459248650	14.47984916608796	N	5.37247900	2.59948600	14.50137000
N	8.39230134379723	7.08561777249319	5.32027884814828	N	8.01178700	6.98179600	5.12814900
C	7.27464918047498	2.92276073513438	11.33913345365884	C	7.32557000	3.00373500	11.33463800
C	6.23490510065656	3.02385156191450	12.27958893573522	C	6.31458100	3.07804900	12.30790700
H	5.36096394087904	3.63398619741712	12.05818068243367	H	5.41891100	3.67231400	12.12676500
C	8.01774082299643	3.79399942859994	8.87495459853035	C	7.93577400	3.81287300	8.80716600
C	6.29875728667216	2.42168309240385	13.53210501271342	C	6.41770500	2.44752800	13.54217500
C	7.96542410309964	4.91480890510241	8.02648131355040	C	7.79943700	4.89581300	7.92002600
H	7.41280764552522	5.79894381701349	8.34111171374353	H	7.22750600	5.77182300	8.22531000
C	7.15320257636362	3.90697451704784	10.14977609398503	C	7.12954500	3.94942200	10.12191400
C	8.58227406052150	4.94583274386630	6.77477698962086	C	8.35707300	4.90301900	6.64326000
C	5.06407708481924	3.90073015526074	15.05122354656799	C	5.35968900	3.74209900	15.31372300
C	4.20136666861854	1.68285912651369	14.53282491126898	C	4.35362100	1.64030000	14.55923300
C	7.31692955347611	5.30268904405100	10.78600786071757	C	7.28601100	5.37050500	10.68917200
N	10.46687798386072	3.72304445035265	4.01961674098159	N	10.17959800	3.65498500	3.85676200
C	8.74146748181228	2.66653224144440	8.43700510371303	C	8.68632800	2.70205400	8.37689300
C	5.69468632543763	3.98274505754280	9.66017299302943	C	5.65161100	3.97261400	9.70090900
C	7.40219483340835	1.62945041058237	13.85646660097657	C	7.55242900	1.69073000	13.83538900
H	7.45467139263963	1.14581367481024	14.83326775704507	H	7.64162600	1.19393500	14.80241200
C	8.48442736794096	6.12340203778399	5.96251648814544	C	8.17264100	6.04777100	5.79551400
C	9.29225030514813	3.80418669462596	6.33048328828779	C	9.09243000	3.77834000	6.20950400
C	8.37512087939790	2.10290234548248	11.65710582632252	C	8.45742000	2.21786100	11.62261200
C	8.40703289991203	1.46165684256948	12.90934281099445	C	8.54292200	1.57384400	12.86908100
H	9.25938587676623	0.81788936001571	13.14183589720771	H	9.42211500	0.96039300	13.07996800
C	3.24393492337777	1.77882419002946	15.56782867883288	C	3.31237700	1.75225000	15.50308300
C	4.08606214578088	0.67444746792062	13.55920212102052	C	4.36366700	0.55154100	13.66332800
H	4.82783748004429	0.60322435113477	12.76417727419216	H	5.15913100	0.46943100	12.92377300
C	9.36040071595718	2.69573576764559	7.17686074321653	C	9.24465000	2.70808800	7.08914000
H	9.92401066954278	1.82188512037652	6.84525143642353	H	9.82929100	1.84647900	6.76242800
C	6.11892427022133	6.03987803864190	10.69392123910123	C	6.07261700	6.07665700	10.62417300
C	4.96418838135298	3.01001789581098	8.98914465974192	C	4.91680200	2.95455900	9.10571400
H	5.41373562695359	2.04497610193167	8.74234053037007	H	5.37834600	1.99102700	8.87892000
C	4.10650006527354	4.04691767009012	16.08288596546544	C	4.34654600	3.92779300	16.27628800
C	3.50093230356175	2.78098207963538	16.69367408334186	C	3.22761900	2.90676300	16.50660500
C	5.79666028552538	5.02065820265176	14.61522634658162	C	6.36910400	4.71658500	15.17206600
H	6.56353668514542	4.91642356399758	13.84972113604136	H	7.15362500	4.58090300	14.42911100
C	3.01900367924331	−0.22229177047201	13.59655747798591	C	3.37168300	−0.42087200	13.70632600
H	2.94377627229233	−0.99965795434922	12.83158222038561	H	3.40710000	−1.25317800	13.00025900

C	5.12088905142780	5.23032782672764	9.97988655901641
C	9.49063438796735	1.81478111473254	10.68542726544938
H	10.09187948682064	0.98355786528892	11.08232871313152
H	10.17822236296751	2.67416585563965	10.59290091764056
C	8.95755559634545	1.44649337199259	9.29242418668183
H	9.66843655791010	0.78230814575301	8.77955510256293
H	8.02128160600290	0.87352665624909	9.40615317201773
C	8.42852192934681	5.82261896761917	11.43813503062959
H	9.34998860956972	5.24100493068905	11.52081083880165
C	9.93851776899764	3.77381069532332	5.05179879872850
C	2.16970307789002	0.88239808240908	15.56366522293798
H	1.41505175478398	0.94647126223545	16.34817999663110
C	2.04714715627331	−0.11543637442183	14.59237597091754
H	1.20181495108202	−0.80692375896656	14.62183283640785
C	6.03465724018948	7.31760731808926	11.25479318023695
H	5.10880000563941	7.89405302153142	11.19274366233609
C	4.56332946492851	2.16297839436489	17.64480967167421
H	4.18698458372595	1.22181399492448	18.07643354196864
H	4.79640266529434	2.86368447135394	18.46217151581813
H	5.49639319593752	1.94429873203253	17.10547876971627
C	5.53843747588000	6.28373706632643	15.14627199167969
H	6.11385477115238	7.13774668561915	14.78131438351803
C	2.23729011448699	3.07516710194719	17.51072000862596
H	1.44524772410245	3.52124817897233	16.89012569482655
H	2.46042037506790	3.76252845846056	18.33873121000472
H	1.84520588854603	2.15533188853386	17.96717450771257
C	3.85120351927811	5.33096155339105	16.57700514116930
H	3.10445761856892	5.46454233186144	17.36012442584151
C	3.63693025913588	3.28830112632268	8.63687090321045
H	3.04623776433953	2.53406550706593	8.11159350669221
C	8.34210065480102	7.10405087529351	11.99928254045871
H	9.20605283141260	7.52839803746790	12.51599964124871
C	3.79644986850155	5.50610232209844	9.62765883240638
H	3.34171165479080	6.46812303673668	9.87522731626732
C	4.54866940270633	6.45056724270956	16.11512388396264
H	4.33048966122980	7.43923639280686	16.52524139528485
C	7.15518967429849	7.84404361402249	11.90585307505419
H	7.10458301971335	8.84098022143972	12.34965284218042
C	3.06018010618129	4.52579857638749	8.95399816033711
H	2.02371341111453	4.72570067940861	8.67254404004644
	S_1 state		
N	5.31174394249173	2.64013504137362	14.45360066991558
N	9.29847136529176	7.64863356327040	6.02102183587577

C	5.06115700	5.21348900	9.99584900
C	9.55497900	1.96333200	10.62154900
H	10.21499500	1.17945600	11.01842600
H	10.18966400	2.85520300	10.48438500
C	8.99713800	1.52378900	9.26196500
H	9.72671900	0.88374900	8.74673500
H	8.09916600	0.90364900	9.41964700
C	8.42158400	5.95034600	11.24192700
H	9.36168200	5.39719300	11.29657000
C	9.68837300	3.72453100	4.90452500
C	2.33103100	0.75223100	15.52002600
H	1.52284000	0.81974500	16.25141200
C	2.34353100	−0.32919700	14.64316800
H	1.55973600	−1.08682300	14.69157800
C	5.98925800	7.38023000	11.11759000
H	5.05056900	7.93564200	11.07389600
C	3.36296300	2.33459400	17.93826600
H	2.56918300	1.60277000	18.15034200
H	3.29342100	3.13227100	18.69289700
H	4.33293600	1.83135400	18.06260300
C	6.37866800	5.85804900	15.96452000
H	7.17136700	6.59616100	15.82671100
C	1.85974400	3.61221800	16.34814700
H	1.75236500	4.02209600	15.33330200
H	1.75048500	4.43934300	17.06428500
H	1.02711200	2.91637100	16.52557500
C	4.39062400	5.08786500	17.06118900
H	3.61682100	5.24267100	17.81610600
C	3.57066500	3.18518900	8.80591300
H	2.97685400	2.39637500	8.34036400
C	8.33708400	7.25717000	11.73279500
H	9.21956800	7.72964800	12.16845700
C	3.71690500	5.44247700	9.69517200
H	3.24855700	6.40184700	9.92306100
C	5.38413400	6.05314200	16.92158700
H	5.38011800	6.94302700	17.55313500
C	7.13046800	7.96394900	11.67194800
H	7.08091400	8.98214600	12.06239800
C	2.97755400	4.41880500	9.09831200
H	1.92540200	4.58208100	8.85750200
	S_1 state		
N	5.33615000	2.53379800	14.41795000
N	7.77029900	6.91388800	5.04350900

C	7.20781475534315	2.92725325713909	11.22340109968222
C	6.22583336915707	3.06182618886925	12.22386986356375
H	5.39117394894899	3.74347879531638	12.06442478419839
C	8.07496154133743	3.95473475905035	8.89313273307436
C	6.31920599483358	2.39714733590578	13.43310588648460
C	8.29180983584937	5.16200774856454	8.23979766087541
H	7.90966749940252	6.08712171116942	8.67065636996487
C	7.06206361967505	3.93999929330323	10.05338805967173
C	8.96599136634206	5.28452931166263	7.00781869677720
C	5.36330529559834	3.82437224371101	15.17488417989080
C	4.32937024966945	1.68577299407346	14.65656218493924
C	7.00158785097017	5.31235973285510	10.74996164588695
N	10.64709829956776	4.04738242483484	4.07351617128274
C	8.57775904965669	2.75132567621878	8.25749447056307
C	5.63510973402206	3.85303771250907	9.48135081305433
C	7.37653129968529	1.52667624484819	13.69913201218837
H	7.45766705048617	1.01264366031359	14.65848252756826
C	9.15865671646726	6.57136514860173	6.45510006063421
C	9.43370416487375	4.06822749556716	6.34955396928449
C	8.23582922093484	1.98577937305810	11.44038292451710
C	8.29972612442750	1.31778021768427	12.68225148767608
H	9.11179588572216	0.60499298687153	12.84405647922522
C	3.40279488171042	1.82070570007170	15.72709528275742
C	4.24916815454744	0.57677851599393	13.77161113561943
H	4.94724492204611	0.50709358340715	12.94110707047584
C	9.22388580615860	2.84644640233214	7.04272717395773
H	9.62854715851616	1.93607849238311	6.59173070863060
C	5.73771274370028	5.91286759328820	10.58760933652191
C	5.06883053678799	2.83568397816669	8.71949674281611
H	5.64853487731909	1.94709967446788	8.46283948417876
C	4.45634304557177	4.04740434929194	16.24900771862113
C	3.45987157174736	2.98937257880875	16.69821266625396
C	6.31828062041101	4.81640228496989	14.82293120819013
H	6.99955755126477	4.64775421397907	13.99389054818741
C	3.28232773825840	−0.39213995167451	13.95761329280093
H	3.22239715527697	−1.23628858317490	13.26886488554067
C	4.89434579176485	5.01741753937225	9.78141108855137
C	9.23315411682677	1.58766195107981	10.38143310258566
H	9.70010915989106	0.64193158418562	10.69806954853362
H	10.04398223126823	2.33239328060778	10.31575155565581
C	8.58768386744787	1.43861332080297	8.99303702060351
H	9.15619313137379	0.70354040011939	8.40438260664750
H	7.57562831192933	1.00833191468774	9.12316478514409
C	8.00024771011068	5.94010831428803	11.48644032264590

C	7.19464200	2.83571100	11.18332800
C	6.17340100	2.84354300	12.17517000
H	5.19398400	3.26909500	11.95037900
C	7.81856900	3.77867900	8.75422300
C	6.40427600	2.39250200	13.45225100
C	7.64989100	4.85369000	7.86422600
H	7.07619900	5.72405000	8.18559600
C	7.08008100	3.93152600	10.10144200
C	8.17572400	4.85677200	6.57364800
C	5.19072000	3.75271100	15.05485700
C	4.50298600	1.45851900	14.67212100
C	7.45784900	5.24934600	10.79209000
N	9.93119800	3.59049900	3.75165900
C	8.58211700	2.67506900	8.32545500
C	5.60457600	4.20330100	9.78277800
C	7.64134100	1.85994400	13.88796200
H	7.80784100	1.53059600	14.91123500
C	7.95807700	5.98958300	5.71794300
C	8.91198900	3.73378800	6.13394900
C	8.45478300	2.23402300	11.58987000
C	8.63846900	1.76856200	12.87536300
H	9.58609000	1.28046600	13.12350100
C	3.42339500	1.57761900	15.58226500
C	4.74467100	0.23830600	13.99206700
H	5.58109700	0.18017700	13.29972600
C	9.10514900	2.67618200	7.02215800
H	9.69739700	1.82169900	6.68976300
C	6.32759900	6.07684000	10.96657000
C	4.71827000	3.38225000	9.09540200
H	5.05258500	2.42001200	8.70104900
C	4.12822700	3.96568900	15.97170800
C	3.11752600	2.87865900	16.31066900
C	6.11690700	4.79098900	14.76755100
H	6.92744800	4.60689000	14.06698800
C	3.92571700	−0.85382100	14.21746700
H	4.11758200	−1.79040200	13.69294100
C	5.18495300	5.44212100	10.29964300
C	9.53289500	1.99727200	10.56297300
H	10.24044000	1.24802400	10.94792500
H	10.13098300	2.90925000	10.37577900
C	8.94855300	1.52039600	9.22403800
H	9.67854500	0.89104200	8.69494300
H	8.06576200	0.89082300	9.42086200
C	8.68925700	5.62659300	11.32815000

H	8.98465177474023	5.47599230307920	11.58378466624277
C	10.09174960400017	4.07314080869647	5.10535922038844
C	2.44976136084223	0.81244154844470	15.89000211371543
H	1.73707386186251	0.87864327806945	16.71248209694812
C	2.37988824847470	−0.28253087780784	15.02764567629344
H	1.61754411058243	−1.04784484260627	15.18449026447814
C	5.47002504731202	7.15750152930399	11.16871290019796
H	4.49588135964921	7.63561593775608	11.03900245246435
C	3.92376201984355	2.44742247261740	18.08117282298965
H	3.22446455556881	1.68215320368861	18.44805673660369
H	3.96584953470116	3.26293664093241	18.81765785414162
H	4.92390165417689	1.99534676886046	18.00859995191421
C	6.36001214271244	6.01446699147144	15.50824480430778
H	7.07800260152696	6.77683583818281	15.20504592193326
C	2.05114884926514	3.62104557211205	16.83021672234401
H	1.70753138251514	4.01587870078407	15.86310369050869
H	2.05572786184658	4.44251285397271	17.55898628216933
H	1.31995188877983	2.88085141921270	17.18130451685843
C	4.54663770557605	5.26255634985942	16.93155864423841
H	3.87560338853238	5.45671461699208	17.76854281136782
C	3.75281836421368	2.98394527419952	8.26156559847624
H	3.30200825976696	2.19659234457023	7.65205177479156
C	7.73238308389250	7.18795086701525	12.06610818109406
H	8.51608306751296	7.70612007529549	12.62526356859604
C	3.58227289988421	5.16448969657021	9.32280123974246
H	3.01068808137580	6.06946527988086	9.54485817918178
C	5.47412450894686	6.24223002450614	16.57278743684526
H	5.50611270161825	7.18440913162930	17.12268950025038
C	6.47541828980618	7.79009371917599	11.90797607635417
H	6.28471310839546	8.76961911112553	12.35362567688213
C	3.01459301662829	4.13727986438589	8.56061706629174
H	1.99359340076620	4.23978044379676	8.18521067967213

H	9.56821100	4.99176900	11.20196500
C	9.47036800	3.66947000	4.81287400
C	2.61662800	0.45389700	15.77805200
H	1.77130400	0.51310300	16.46524600
C	2.85605700	−0.74833700	15.11332100
H	2.20312700	−1.60388700	15.29317200
C	6.42219200	7.27351200	11.67990600
H	5.54698500	7.91377600	11.81237600
C	3.15536100	2.61911500	17.83802800
H	2.42143300	1.85341600	18.12514300
H	2.91624500	3.53387600	18.39770800
H	4.15176500	2.27535400	18.15011700
C	5.97863000	6.02782700	15.37098700
H	6.69078400	6.81835400	15.13505300
C	1.70780200	3.36281800	15.88223700
H	1.67337900	3.55016300	14.79960700
H	1.43944300	4.29365400	16.40109500
H	0.94428100	2.61091900	16.12621700
C	4.02223700	5.22941900	16.55517300
H	3.21083400	5.43130300	17.25600700
C	3.39641800	3.80578100	8.92585300
H	2.68847300	3.17365400	8.38567400
C	8.78333600	6.82722900	12.03548900
H	9.74659600	7.13533400	12.44817800
C	3.86314600	5.86417200	10.13140900
H	3.52977800	6.82664900	10.52556100
C	4.92601900	6.25238300	16.26447000
H	4.80661000	7.22754100	16.73940700
C	7.65785000	7.64645500	12.21473100
H	7.75254700	8.58588000	12.76379500
C	2.97368000	5.03800300	9.44066800
H	1.93996900	5.35862700	9.29423500

T_1 state

N	5.31751264960061	2.54845598632405	14.41828607721010
N	8.46423093913802	7.39143881269638	5.51078958511113
C	7.23110173738202	2.87902800383887	11.22277024917782
C	6.21114501935292	2.94972327077176	12.19504658903090
H	5.32727193358971	3.55915224226191	12.01651042742567
C	7.95809691833526	3.87328987484523	8.81561205635296
C	6.34168068267971	2.32921940168364	13.42699816071608
C	7.95381094052426	5.04826642189700	8.04566638710936
H	7.44248026172441	5.93325990403515	8.42377814988834
C	7.08440378641439	3.91848614065935	10.08343229131421

T_1 state

N	5.60355900	2.58776000	14.64388100
N	7.49889200	6.82490100	5.02869600
C	7.40021700	3.05232500	11.39733600
C	6.42932800	3.09003700	12.41366200
H	5.48358500	3.60743000	12.25288800
C	7.83386800	3.80286500	8.81511100
C	6.62863900	2.49380100	13.65085400
C	7.56943500	4.83433100	7.89634300
H	6.92768300	5.66476700	8.18941400
C	7.05361300	3.90431700	10.14909500

C	8.56447751153080	5.14050925383032	6.79299682908017
C	5.29666214976142	3.77451117493905	15.06240746971193
C	4.41215539594993	1.53421511129992	14.66425924407696
C	7.22906646647371	5.27690942749227	10.80489049192301
N	10.38624414031517	4.01094029609869	3.94478991755987
C	8.63089291524924	2.74005882114681	8.28937511859789
C	5.61825397838958	3.99956662727626	9.61896145119020
C	7.46013248832281	1.55583664309630	13.73143050723747
H	7.55692677502880	1.07719529769673	14.70703742875220
C	8.51628411364834	6.37698422863440	6.07564664227755
C	9.22099994472351	3.99425912576918	6.25703881983685
C	8.34013581298061	2.05230868455859	11.49332555390411
C	8.42696541180363	1.39998389455946	12.73867130499759
H	9.28932004677358	0.75699240359857	12.93090821100612
C	3.42398166173025	1.68888760049143	15.70641394990989
C	4.44441508101213	0.33678785857416	13.88810840718674
H	5.16766933351682	0.24770542481824	13.07916368189463
C	9.24037497570051	2.82524629711004	7.03596080358228
H	9.76785908007313	1.95268611541006	6.64499604156524
C	6.00832148801325	5.98448742653718	10.79772609144794
C	4.90064396621679	3.06772088315650	8.87808068454275
H	5.37090502124349	2.13693395439883	8.55096822148132
C	4.30159625585329	4.02863393981716	16.07632142814872
C	3.30051312439241	2.97158995866112	16.50791776828049
C	6.24420574314121	4.78750611267129	14.72881592657471
H	6.99975339448480	4.59651004349490	13.96985747293560
C	3.57107809980514	-0.69339437250281	14.14736495717708
H	3.60497570157419	-1.60053132004503	13.54101429391178
C	5.02149122911974	5.21033021434437	10.03399585450479
C	9.40891876676116	1.76295219655238	10.47037524160652
H	9.99323760371261	0.89709372923509	10.81620206078580
H	10.12081533969956	2.60272814358446	10.38729417168098
C	8.81084898062289	1.47471134405267	9.08256566655306
H	9.47194391340884	0.79798708723931	8.52190132636396
H	7.85153979871584	0.94260934940708	9.21256127712864
C	8.34499056821410	5.78176249074964	11.46028456082602
H	9.28611414677287	5.22608728761925	11.46220194916164
C	9.85817763416801	4.01809046920517	4.98172890947386
C	2.56748245716881	0.61170637980795	15.94450047835969
H	1.82064032818535	0.69649059564003	16.73667976538154
C	2.62113399520598	-0.56900300372898	15.20311150465531
H	1.93098291585634	-1.38559492926475	15.42333547776145
C	5.90448385532610	7.20939596456366	11.46581113501089
H	4.96173217712140	7.76168764843533	11.47487015615616

C	8.08450500	4.84511300	6.60151400
C	5.73089100	3.54865400	15.62422000
C	4.46515000	1.76673700	14.53061100
C	7.03231400	5.36284800	10.63455000
N	9.93102700	3.66975500	3.79942600
C	8.66958300	2.74950000	8.39609700
C	5.57479100	3.70693100	9.77604700
C	7.82668700	1.83509300	13.92431100
H	7.98844800	1.37323200	14.89896800
C	7.76721300	5.93543300	5.72188400
C	8.90859700	3.77864600	6.18169400
C	8.60199000	2.37112400	11.66304500
C	8.78774700	1.77674500	12.92493800
H	9.72102300	1.24245500	13.11718000
C	3.31452400	2.01841100	15.31748300
C	4.46640800	0.70065100	13.61020300
H	5.35915800	0.49758900	13.01957800
C	9.18623000	2.75976700	7.09145100
H	9.83805400	1.94398500	6.77443600
C	5.73648600	5.90165100	10.56002800
C	4.96524400	2.56501900	9.27101500
H	5.54348400	1.65681600	9.08768000
C	4.72792600	3.46416400	16.73573600
C	3.30545600	3.17987300	16.31497600
C	6.74956500	4.50477600	15.64702200
H	7.43227800	4.59677300	14.80027700
C	3.33775500	-0.09399200	13.44425800
H	3.36151100	-0.91572600	12.72572300
C	4.83317900	4.87660700	10.01545000
C	9.67935400	2.17188500	10.62834000
H	10.41819100	1.46204200	11.02551300
H	10.22933700	3.10862400	10.43618700
C	9.11228600	1.63577800	9.30789200
H	9.87497500	1.04062600	8.78690400
H	8.27750200	0.94805900	9.52221400
C	8.09323000	6.11707600	11.12103400
H	9.09786800	5.69333600	11.18379600
C	9.46740400	3.73223300	4.86011300
C	2.19505000	1.20822700	15.11465200
H	1.29293800	1.39421700	15.69852900
C	2.18937600	0.15951300	14.19274800
H	1.29746500	-0.45747800	14.07143900
C	5.49413200	7.21292100	10.97459700
H	4.49101500	7.64016900	10.92070500

C	3.54123306710352	2.64850701242653	18.00904565313641
H	2.81809976096475	1.90241377858476	18.37059998299845
H	3.43332017814112	3.55311921848374	18.62552187417477
H	4.55476120897493	2.24800009727576	18.15971602497224
C	6.20335268093127	6.01948467787621	15.34105830835095
H	6.92677765581529	6.78382544113754	15.05435082099558
C	1.86454485190529	3.53423416390205	16.32049138484443
H	1.67695976566055	3.76621478865726	15.26169483201496
H	1.72330896982482	4.45442344124814	16.90602559080525
H	1.11110683710448	2.80561430387077	16.65313017512467
C	4.30484639246975	5.29097980555457	16.67893893335732
H	3.56320788591742	5.50908022269391	17.45011591558216
C	3.56656722931801	3.34754008107 20	8.55398969738791
H	2.98795331120135	2.62197693176631	7.97365653683179
C	8.24290802129260	7.01657313914132	12.11720653895911
H	9.11467157967016	7.43422850709459	12.62669754910966
C	3.68964083017077	5.48640120064887	9.70552127341366
H	3.22055804723698	6.42248833289190	10.01857580571101
C	5.21824859863170	6.28478163796725	16.33335269546263
H	5.17768544691014	7.25889286233686	16.82474978832229
C	7.02914386406888	7.71891280506066	12.12313316704532
H	6.96187851649232	8.67721355193292	12.64388212933882
C	2.96782567239243	4.54566265831686	8.96480300742169
H	1.92801797129144	4.74931847397797	8.69788308709961

C	2.41444000	2.88879100	17.53165300
H	1.36586000	2.74019000	17.23964300
H	2.42661200	3.74001300	18.22648400
H	2.75631500	1.99309000	18.07087200
C	6.93991600	5.28836500	16.78190700
H	7.72418100	6.04429000	16.81257200
C	2.75983000	4.43855300	15.57271100
H	3.38754000	4.68936500	14.70436500
H	2.75653400	5.30391400	16.25274800
H	1.73429700	4.26207100	15.21348600
C	5.09766500	4.13722500	17.96085900
H	4.52262600	3.96047100	18.87272000
C	3.59265200	2.59763100	9.00625700
H	3.09603000	1.70889900	8.61248200
C	7.84898400	7.43041100	11.53462000
H	8.66997600	8.03811100	11.91967600
C	3.46278800	4.90791500	9.74921600
H	2.87772400	5.81063700	9.93502500
C	6.13483500	5.01734700	17.98280100
H	6.39726100	5.52432500	18.91520700
C	6.56034900	7.97194400	11.46198400
H	6.38701500	8.99816000	11.79122400
C	2.84946400	3.75963800	9.24323800
H	1.77864000	3.76775200	9.03140700

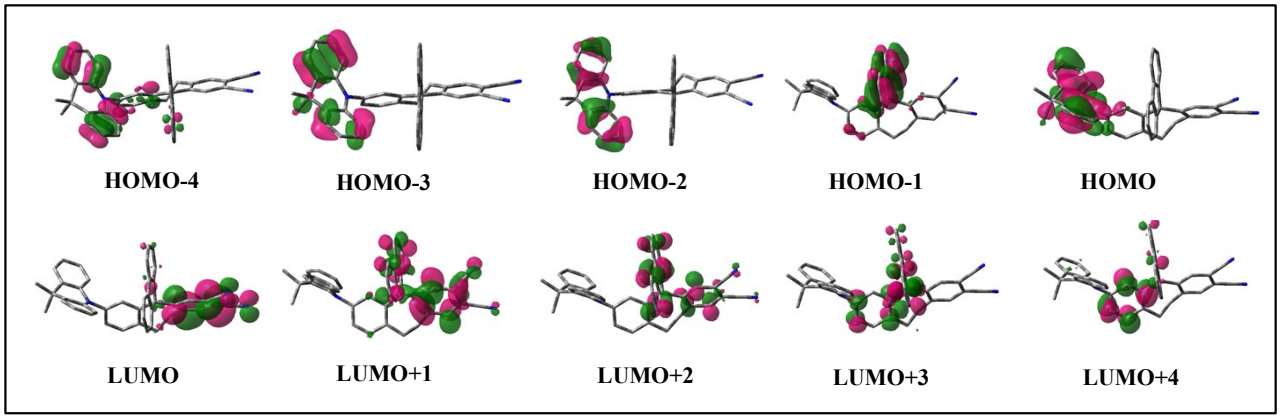

Figure S1. Selected molecular orbitals of compound 1 (contour plots drawn at an iso-value of 0.05) calculated in the S_0 optimized geometry at the B3LYP/def2-SVP//def2/J theory level.

Table S2. Calculated spin-orbital coupling matrix elements (Re, Im in cm^{-1}) between T_m and S_n states at the T_1 structure for compound 1 at the TD-B3LYP level.

CALCULATED SOCME BETWEEN TRIPLETS AND SINGLETS

Root		<T|HSO|S> (Re, Im) cm-1		
T	S	Z	X	Y
1	0	(0.00 , 0.05)	(0.00 , -0.18)	(-0.00 , -0.11)
1	1	(0.00 , 0.00)	(0.00 , -0.00)	(-0.00 , 0.00)
1	2	(0.00 , 0.13)	(0.00 , 0.01)	(-0.00 , 0.35)
1	3	(0.00 , 0.03)	(0.00 , -0.17)	(-0.00 , -0.48)
1	4	(0.00 , -0.27)	(0.00 , 0.02)	(-0.00 , -0.25)
1	5	(0.00 , -0.14)	(0.00 , -0.34)	(-0.00 , -0.51)
2	0	(0.00 , 0.40)	(0.00 , 0.57)	(-0.00 , 0.50)
2	1	(0.00 , -0.14)	(0.00 , 0.01)	(-0.00 , -0.32)
2	2	(0.00 , 0.03)	(0.00 , -0.03)	(-0.00 , -0.01)
2	3	(0.00 , -0.03)	(0.00 , 0.13)	(-0.00 , 0.33)
2	4	(0.00 , 0.13)	(0.00 , -0.11)	(-0.00 , -0.08)
2	5	(0.00 , -0.22)	(0.00 , 0.51)	(-0.00 , -0.10)
3	0	(0.00 , -0.70)	(0.00 , -0.05)	(-0.00 , -0.20)
3	1	(0.00 , 0.05)	(0.00 , -0.04)	(-0.00 , -0.01)
3	2	(0.00 , -0.07)	(0.00 , 0.07)	(-0.00 , -0.01)
3	3	(0.00 , 0.11)	(0.00 , -0.30)	(-0.00 , 0.12)
3	4	(0.00 , -0.20)	(0.00 , -0.17)	(-0.00 , 0.47)
3	5	(0.00 , -0.16)	(0.00 , -0.34)	(-0.00 , 0.40)
4	0	(0.00 , 0.06)	(0.00 , 0.34)	(-0.00 , 0.14)
4	1	(0.00 , -0.04)	(0.00 , 0.19)	(-0.00 , 0.49)
4	2	(0.00 , 0.04)	(0.00 , -0.11)	(-0.00 , -0.36)
4	3	(0.00 , -0.02)	(0.00 , 0.06)	(-0.00 , -0.02)
4	4	(0.00 , -0.30)	(0.00 , 0.67)	(-0.00 , 0.14)
4	5	(0.00 , -0.12)	(0.00 , -0.08)	(-0.00 , 0.20)
5	0	(0.00 , 1.01)	(0.00 , 0.01)	(-0.00 , -0.20)
5	1	(0.00 , -0.10)	(0.00 , -0.02)	(-0.00 , -0.06)
5	2	(0.00 , 0.02)	(0.00 , -0.05)	(-0.00 , -0.03)
5	3	(0.00 , -0.16)	(0.00 , 0.25)	(-0.00 , 0.14)
5	4	(0.00 , -0.12)	(0.00 , 0.01)	(-0.00 , 0.12)
5	5	(0.00 , 0.05)	(0.00 , 0.14)	(-0.00 , 0.14)

Table S3. Calculated spin-orbital coupling matrix elements (Re, Im in cm^{-1}) between T_m and S_n states at the T_1 structure for compound 1 at the TD-ω*B97X-D3 level.

CALCULATED SOCME BETWEEN TRIPLETS AND SINGLETS

Root		<T|HSO|S> (Re, Im) cm-1		
T	S	Z	X	Y
1	0	(0.00 , 0.06)	(0.00 , -0.17)	(-0.00 , -0.09)
1	1	(0.00 , -0.00)	(0.00 , -0.00)	(-0.00 , 0.00)
1	2	(0.00 , 0.14)	(0.00 , 0.01)	(-0.00 , 0.36)
1	3	(0.00 , 0.01)	(0.00 , -0.15)	(-0.00 , -0.49)
1	4	(0.00 , -0.26)	(0.00 , 0.01)	(-0.00 , -0.21)
1	5	(0.00 , -0.13)	(0.00 , -0.33)	(-0.00 , -0.46)
2	0	(0.00 , 0.42)	(0.00 , 0.53)	(-0.00 , 0.50)
2	1	(0.00 , -0.15)	(0.00 , 0.00)	(-0.00 , -0.34)
2	2	(0.00 , 0.02)	(0.00 , -0.03)	(-0.00 , -0.01)
2	3	(0.00 , -0.03)	(0.00 , 0.11)	(-0.00 , 0.32)
2	4	(0.00 , 0.15)	(0.00 , -0.14)	(-0.00 , -0.10)
2	5	(0.00 , -0.18)	(0.00 , 0.50)	(-0.00 , -0.11)
3	0	(0.00 , -0.70)	(0.00 , -0.07)	(-0.00 , -0.21)
3	1	(0.00 , 0.05)	(0.00 , -0.04)	(-0.00 , 0.01)
3	2	(0.00 , -0.07)	(0.00 , 0.11)	(-0.00 , -0.04)
3	3	(0.00 , 0.08)	(0.00 , -0.32)	(-0.00 , 0.15)
3	4	(0.00 , -0.23)	(0.00 , -0.14)	(-0.00 , 0.46)
3	5	(0.00 , -0.19)	(0.00 , -0.32)	(-0.00 , 0.40)
4	0	(0.00 , -0.07)	(0.00 , 0.42)	(-0.00 , 0.15)
4	1	(0.00 , -0.02)	(0.00 , 0.17)	(-0.00 , 0.51)
4	2	(0.00 , 0.05)	(0.00 , -0.10)	(-0.00 , -0.35)
4	3	(0.00 , -0.01)	(0.00 , 0.06)	(-0.00 , -0.04)
4	4	(0.00 , -0.25)	(0.00 , 0.67)	(-0.00 , 0.10)
4	5	(0.00 , -0.11)	(0.00 , -0.10)	(-0.00 , 0.14)
5	0	(0.00 , -1.60)	(0.00 , 0.52)	(-0.00 , -0.30)
5	1	(0.00 , 0.23)	(0.00 , 0.02)	(-0.00 , 0.21)
5	2	(0.00 , -0.10)	(0.00 , 0.18)	(-0.00 , 0.01)
5	3	(0.00 , 0.34)	(0.00 , -0.55)	(-0.00 , -0.28)
5	4	(0.00 , 0.23)	(0.00 , -0.00)	(-0.00 , -0.24)
5	5	(0.00 , -0.12)	(0.00 , -0.32)	(-0.00 , -0.30)

Table S4. Calculated Huang-Rhys factors and reorganization energy versus the normal vibration mode between T_1 and S_0 about the S_0 potential energy surface.

Vibrational Frequency (cm^{-1})	Reorganization energy (cm^{-1})	Huang-Rhys factor
8.71	0	0
20.64	0	0
28.05	0.02	7.13012E-4
29.41	0	0

39.69	0.01	2.51953E-4
45.24	0.01	2.21043E-4
54.55	0.01	1.83318E-4
59.42	0	0
69.02	0.03	4.34657E-4
82.02	0.1	0.00122
94.43	0.01	1.05899E-4
105.91	0.12	0.00113
117.06	0.02	1.70853E-4
123.36	0	0
126.04	0.39	0.00309
127.7	0.26	0.00204
134.3	1.25	0.00931
148.86	0.31	0.00208
155.26	0.01	6.44081E-5
180.17	0.28	0.00155
183.87	0.21	0.00114
202.93	0.28	0.00138
222	0.39	0.00176
244.42	6.57	0.02688
253.25	2.26	0.00892
260.09	11.47	0.0441
262.7	0.03	1.14199E-4
269.42	0.29	0.00108
290.71	0.09	3.09587E-4
299.81	0.16	5.33671E-4
308.16	1.19	0.00386
319.75	0.01	3.12744E-5
322.72	0.02	6.19732E-5
336.54	0	0
350.02	0.38	0.00109
363.62	6.58	0.0181
375.08	20.6	0.05492
380.18	0	0
400.86	3.91	0.00975
413.19	60.35	0.14606
417.61	3.7	0.00886
425.14	0.4	9.40867E-4
435.16	0.04	9.19202E-5
441.22	0	0
443.5	0.1	2.25479E-4
450.93	0.11	2.4394E-4
474.9	0.58	0.00122
481.43	4.21	0.00874

486.07	1.59	0.00327
487.4	0.29	5.94994E-4
513.52	0.9	0.00175
514.24	1.62	0.00315
523.02	2.62	0.00501
529.56	3.84	0.00725
534.46	0.3	5.61314E-4
559.2	74.93	0.13399
567.17	4.75	0.00837
571.6	9.93	0.01737
578.78	0.07	1.20944E-4
583.16	1.9	0.00326
594.85	0.07	1.17677E-4
598.98	0.13	2.17036E-4
611.52	0.09	1.47174E-4
627.54	12.54	0.01998
635.31	0.75	0.00118
645.09	1.65	0.00256
657.17	0.04	6.08671E-5
678.86	5.08	0.00748
682.43	53.24	0.07802
690.95	0	0
697.79	0.42	6.019E-4
723.05	2.29	0.00317
731.66	0.02	2.73351E-5
742.19	16.27	0.02192
747.38	51.04	0.06829
763.6	0.37	4.84547E-4
765.79	1.26	0.00165
768.39	5.8	0.00755
769.88	2.59	0.00336
773.44	7.2	0.00931
774.74	0.58	7.48638E-4
779.35	0	0
783.36	0.04	5.10621E-5
788.68	0.01	1.26794E-5
789.09	0.59	7.47697E-4
813.17	1.45	0.00178
826.31	1.79	0.00217
827.37	1.31	0.00158
851.99	1.74	0.00204
880.42	2.28	0.00259
882.86	5.43	0.00615
887.81	0.04	4.50547E-5

905.35	2.72	0.003
911.82	0.57	6.25123E-4
912.6	23.83	0.02611
917.8	15.23	0.01659
932.34	6.1	0.00654
933.98	2.02	0.00216
939	0.04	4.25985E-5
946	1.55	0.00164
954.35	3.69	0.00387
964.3	0.22	2.28145E-4
965.68	0.12	1.24265E-4
969.08	0.09	9.28716E-5
970.12	4.89	0.00504
976.72	0.15	1.53575E-4
978.42	1.34	0.00137
979.84	0.18	1.83703E-4
997.34	0.02	2.00533E-5
1006.64	0.02	1.98681E-5
1010.73	0.11	1.08832E-4
1016.63	0.1	9.83642E-5
1020.43	7.76	0.0076
1021.26	0.84	8.22513E-4
1022.58	0.45	4.40063E-4
1028.23	0.32	3.11214E-4
1046.37	1.78	0.0017
1051.93	99.48	0.09457
1054.73	1.23	0.00117
1071.16	0.24	2.24056E-4
1076.48	0.05	4.64477E-5
1097.44	0.3	2.73363E-4
1102.33	0.25	2.26792E-4
1107.87	1.24	0.00112
1118.45	105.95	0.09473
1123.73	13.7	0.01219
1131.58	2.21	0.00195
1134.62	0.4	3.52541E-4
1149.09	3.4	0.00296
1166.81	0.24	2.05689E-4
1168.51	8.15	0.00697
1171.51	3.85	0.00329
1174.49	2.88	0.00245
1175.49	0.71	6.04003E-4
1177.47	38.67	0.03284
1179.08	18.48	0.01567

1183.91	10.14	0.00856
1194.92	0.22	1.84113E-4
1206.01	0.03	2.48754E-5
1216.93	0.09	7.39566E-5
1221.67	6.74	0.00552
1237.39	4.04	0.00326
1239.7	26.02	0.02099
1244.49	13.77	0.01106
1250.59	0.5	3.99811E-4
1271.39	1.22	9.5958E-4
1280.93	2.01	0.00157
1291.53	0.54	4.18109E-4
1299.01	4.73	0.00364
1299.56	10.6	0.00816
1300.26	0.02	1.53815E-5
1310.26	1.36	0.00104
1320.98	0.26	1.96824E-4
1344.87	2.49	0.00185
1348.93	44	0.03262
1352.56	7.07	0.00523
1357.04	10.34	0.00762
1359.95	3.92	0.00288
1361.59	0.59	4.33317E-4
1367.06	0.39	2.85284E-4
1372.41	0.72	5.24625E-4
1375.78	0.01	7.2686E-6
1378.85	21.41	0.01553
1402.84	4.38	0.00312
1404.26	11.8	0.0084
1425.37	0.11	7.71729E-5
1440.12	0.44	3.0553E-4
1455.49	2.19	0.0015
1456.88	0.66	4.53023E-4
1459.9	0	0
1463.91	0.31	2.11762E-4
1476.99	0.11	7.44758E-5
1478.92	0.03	2.02851E-5
1484.06	1.71	0.00115
1488.49	1.6	0.00107
1491.77	8.18	0.00548
1496.26	0.59	3.94316E-4
1511.5	0	0
1512.66	11.5	0.0076
1520.45	36.54	0.02403

1538.16	2.29	0.00149
1538.56	1.11	7.21454E-4
1548.23	4.14	0.00267
1592.96	0.41	2.57382E-4
1624.28	2.75	0.00169
1627.99	0.04	2.45702E-5
1637.47	0.01	6.10698E-6
1638.65	103.21	0.06298
1645.39	0.56	3.40345E-4
1647.95	6.6	0.004
1653.58	53.27	0.03221
1660.02	15.03	0.00905
1662.49	2.52	0.00152
1663.55	7.61	0.00457
1672.06	0.75	4.48548E-4
2366.74	11.85	0.00501
2368.52	0.27	1.13995E-4
3021.76	0.01	3.30933E-6
3025.71	0.07	2.31351E-5
3031.52	0.25	8.24669E-5
3042.93	0.02	6.57261E-6
3087.64	0.03	9.71616E-6
3095	0	0
3110.36	0.01	3.21506E-6
3124.91	0.01	3.20009E-6
3125.09	0.05	1.59995E-5
3128.8	0.67	2.1414E-4
3169.38	0	0
3171.95	0	0
3172.62	0	0
3172.97	0.02	6.30324E-6
3176.59	0	0
3179.27	0.01	3.14538E-6
3181.17	0.18	5.6583E-5
3186.77	0	0
3189.36	0.01	3.13543E-6
3190.77	0.01	3.13404E-6
3191.96	0.1	3.13287E-5
3197.18	0.03	9.38327E-6
3199.29	0.02	6.25139E-6
3200.09	0.04	1.24996E-5
3203.06	0.24	7.49283E-5
3205.9	0.38	1.18531E-4
3208.77	0.88	2.74248E-4

3212.16	0	0
3217.32	0.03	9.32453E-6
3221.02	0.17	5.27783E-5
3222.08	0.24	7.4486E-5