Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information: Non-adiabatic dynamics simulations of the S_1 excited-state relaxation of diacetyl phenylenediamine

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1. Active space of calculations

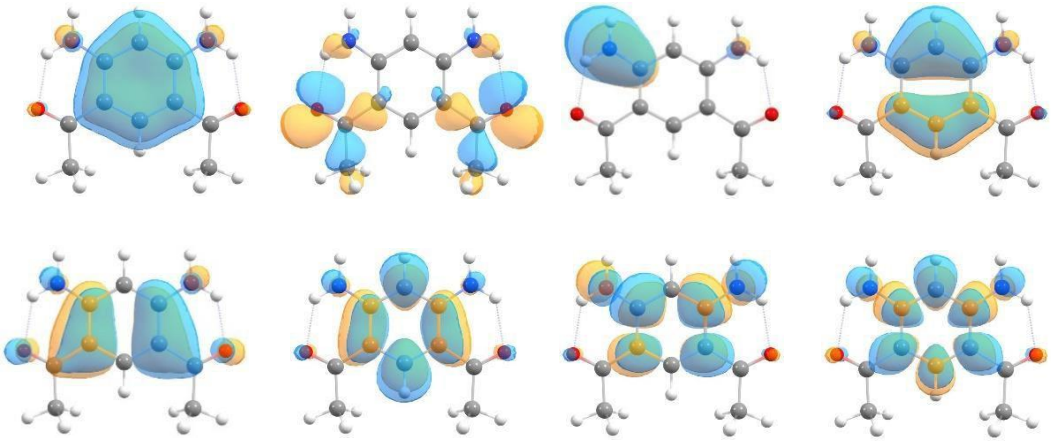

Figure S1. The active space (10e,8o) of *m*-DAPA used in the CAS(10,8)/6-31G* calculations.

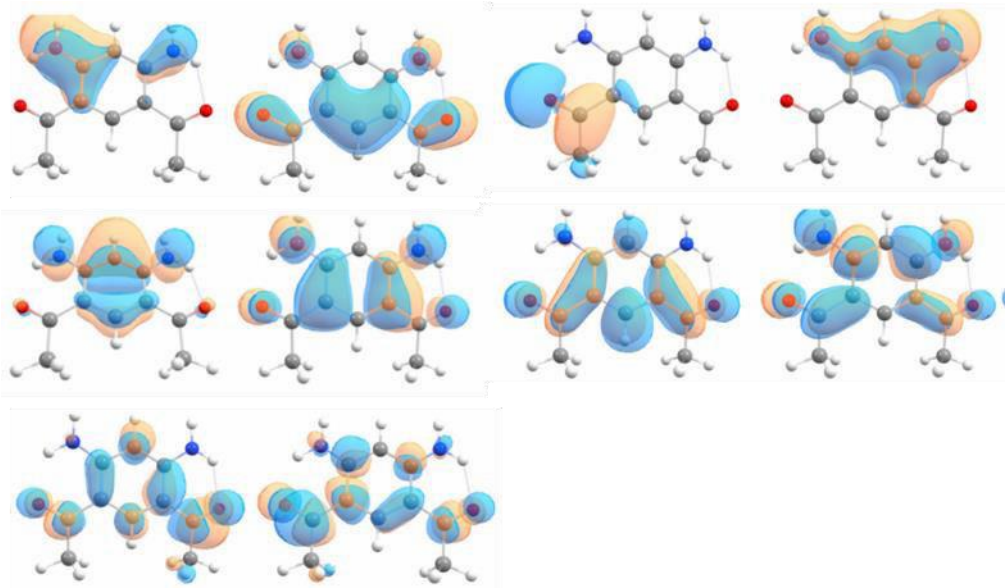

Figure S2. The active space (12e,10o) of *m*-DAPA used in the MS-CASPT2//CAS(12,10) /def2-TZVP calculations.

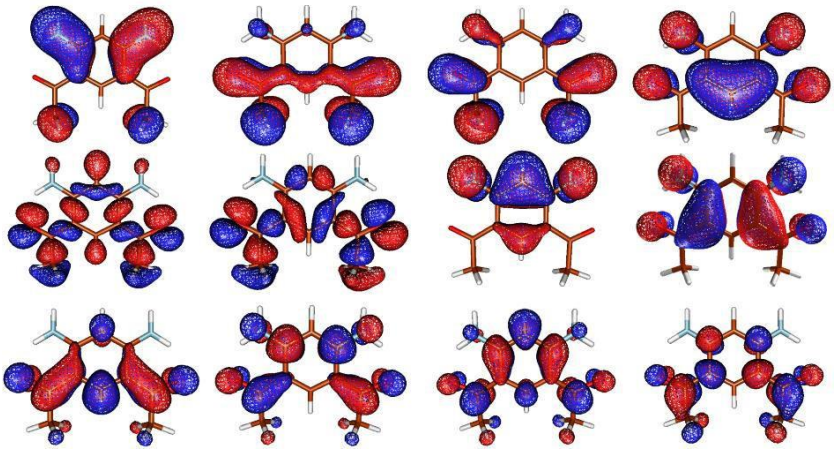

Figure S3. The active space (16e,12o) of *m*-DAPA used in the OM2/MRCI calculations.

2. Selected dihedral angles of structures from CAS(10,8)/6-31G* and OM2/MRCI optimizations and relative energies from OM2/MRCI and single point MS-CASPT2 calculations.

Table S1. Two Selected Dihedral Angles of Structures from CAS(10,8)/6-31G* and OM2/MRCI Optimizations and Relative Energies from OM2/MRCI and Single Point MS-CASPT2 Calculations.

Structures	**C4C3C11O12 (Degree)**	**C6C1C10O9 (Degree)**	**∆E (kcal/mol)**
	CAS(10,8)/6-31G*		
S0-KETO	0.018	-0.024	0.0
S0-1PT	-2.689	26.868	42.1
S1-KETO	4.112	-4.112	84.0
S1-1PT	0.030	0.038	70.3
S1S0-1PT	2.360	96.038	71.3
	OM2/MRCI		
S0-KETO	4.861	8.315	0.0
S0-1PT	-2.697	32.473	44.6
S1-KETO	0.018	0.016	87.2
S1-1PT	4.053	-24.405	74.1
S1S0-1PT	-0.153	88.009	82.8

3. Optimized structures of *m*-DAPA obtained from OM2/MRCI method.

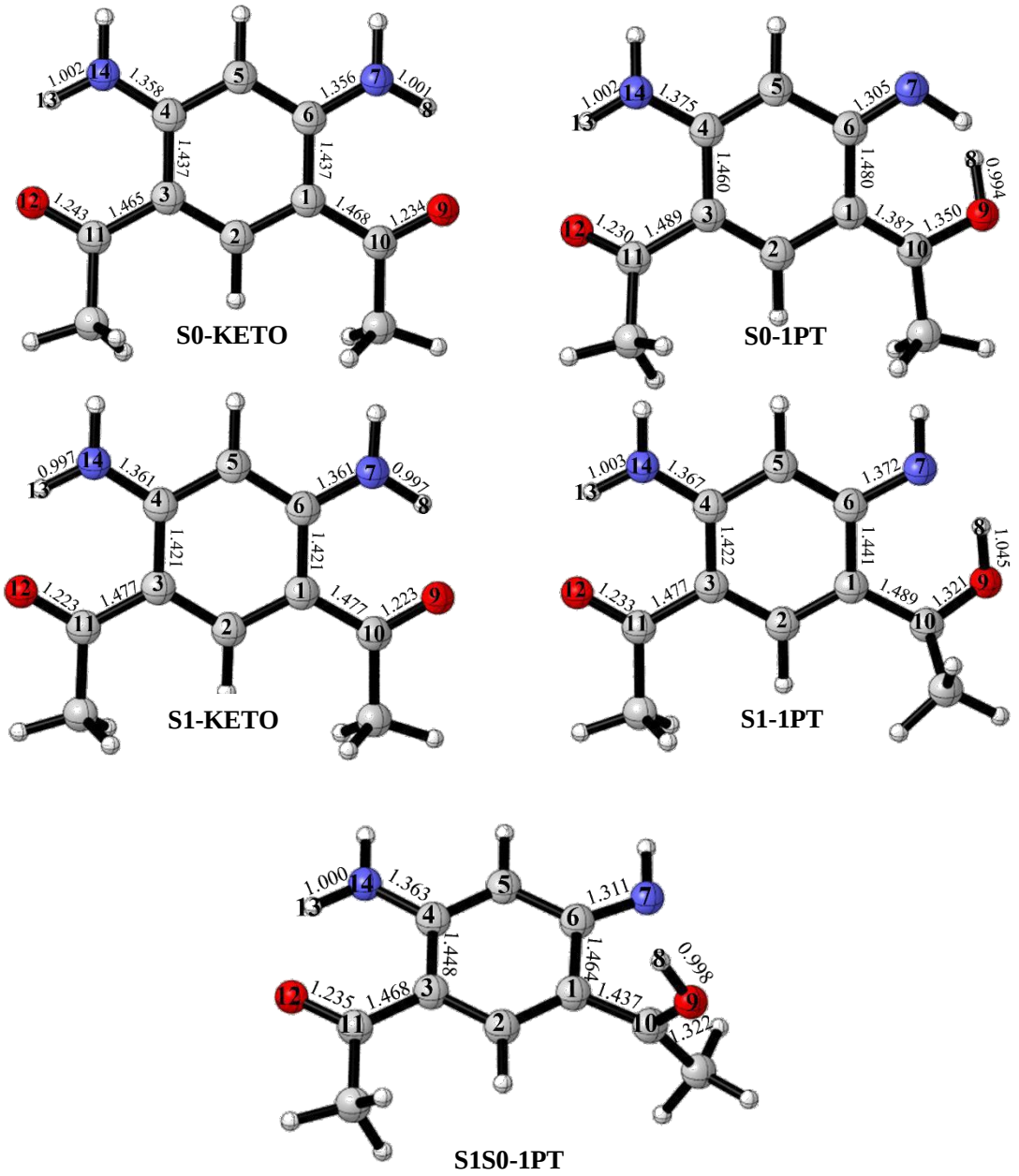

Figure S4. Structures of S_0, S_1 and CI calculated by OM2/MRCI method.

4. Optimized structures of *m*-DAPA calculated by CASSCF.

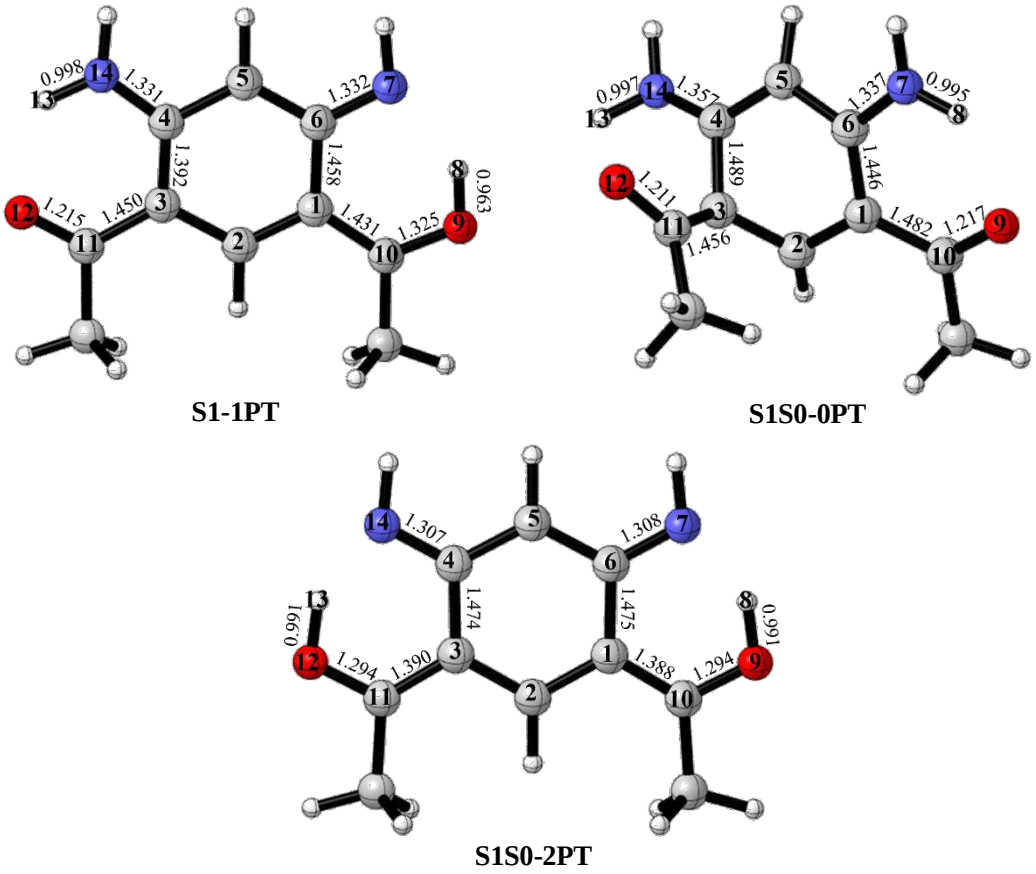

Figure S5. Structures of S1-1PT, S1S0-0PT and S1S0-2PT calculated at CAS(10,8)/6-31G* level.

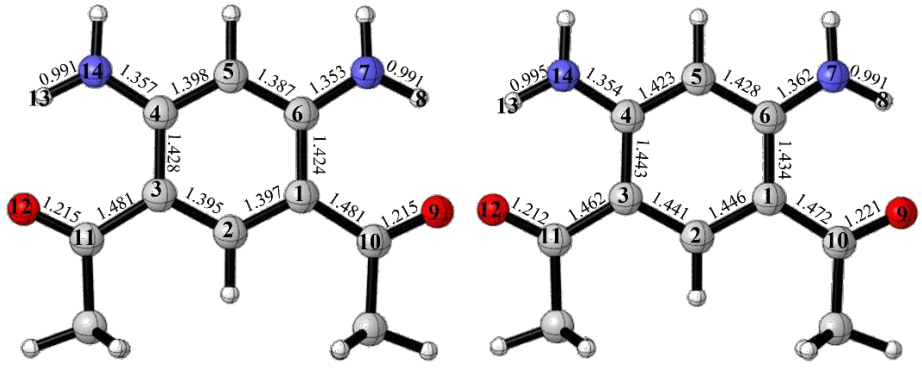

Figure S6. Structures of S0-KETO and S1-KETO calculated at CAS(12,10)/6-31G* level.

5. The deactivation pathways of *m*-DAPA.

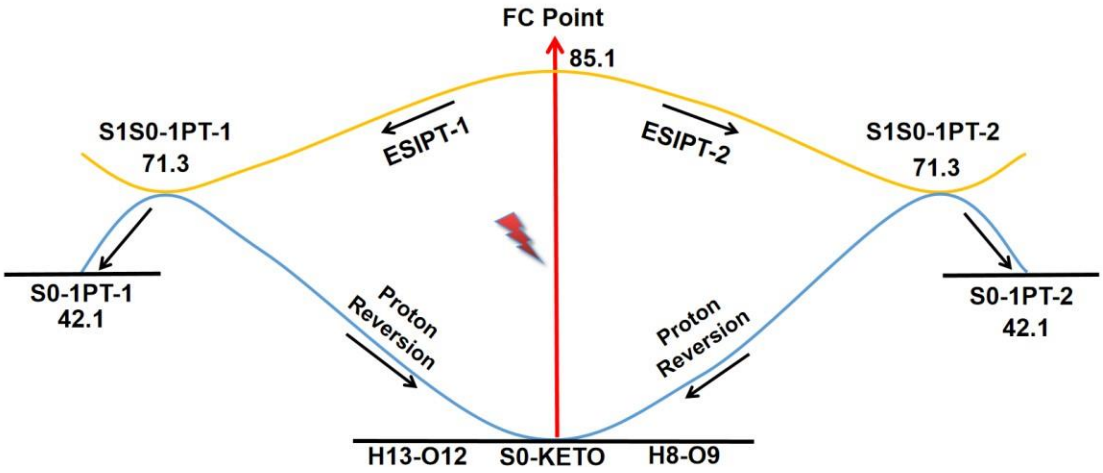

Figure S7. The deactivation pathways of *m*-DAPA.

6. Optimized conical intersection structure of *o*-DAPA calculated by CASSCF.

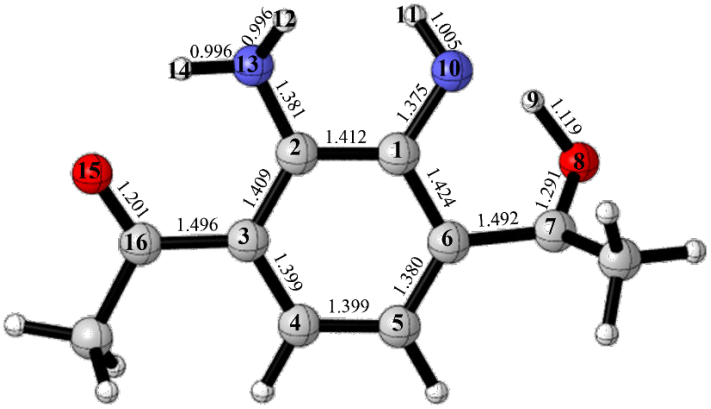

Figure S8. Structure of CI point of *o*-DAPA calculated by CASSCF method.

7. Minimum-energy reaction paths with proton transfer reaction coordinates of *o*-DAPA computed at MS-CASPT2//CAS(12,10)/def2-TZVP level.

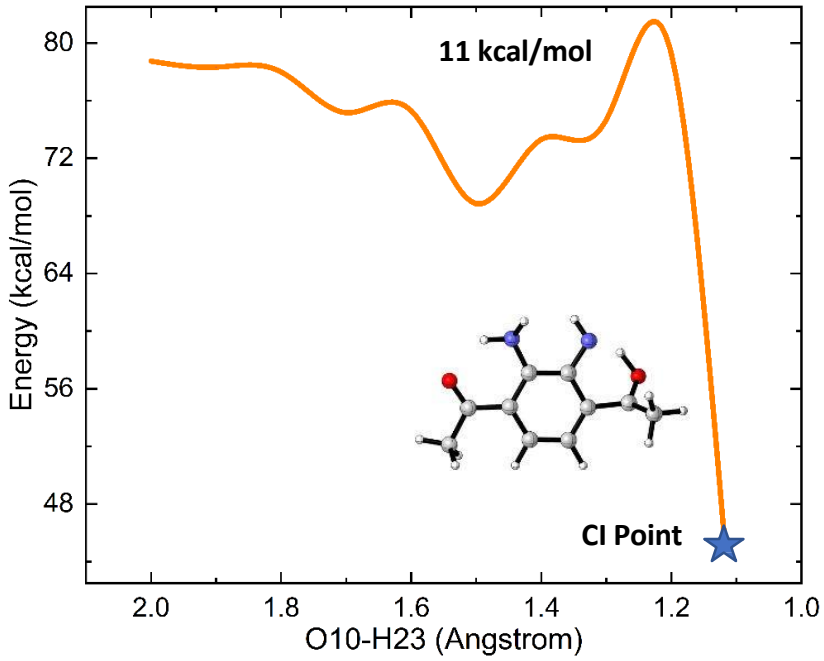

Figure S9. Minimum-energy reaction paths with proton transfer reaction coordinates computed of *o*-DAPA at MS-CASPT2//CAS(12,10)/def2-TZVP level.

8. Non-adiabatic dynamics simulation results of *o*-DAPA.

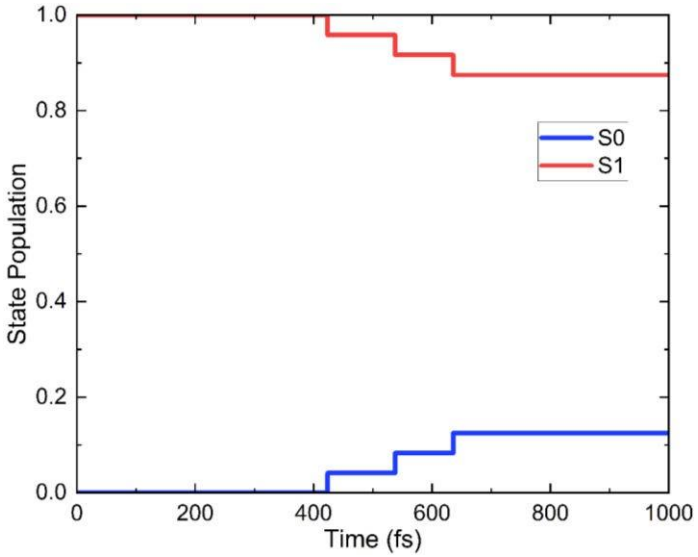

Figure S10. Time dependent S_1 and S_0 state population of *o*-DAPA.

The same dynamics calculation method as for *m*-DAPA was used to perform the dynamics simulations for *o*-DAPA. In the surface-hopping dynamics of *o*-DAPA, a total of 24 trajectories were simulated, of which only 3 successfully returned to the ground state via the surface hopping structures at the end of 1 ps simulation time. All 3 trajectories went through the single proton transfer process.

9. Cartesian coordinates of all optimized structures calculated by CASSCF.

Table S2. Cartesian coordinates of the Optimized Geometry of *m*-DAPA at S0-KETO calculated by CASSCF.

Atom	x	y	z
C	1.227574000	0.107304000	0.000519000
C	0.000001000	0.761475000	0.000042000
C	-1.227575000	0.107309000	0.000403000
C	-1.228566000	-1.313378000	0.001243000
C	-0.000004000	-1.974224000	0.001691000
C	1.228559000	-1.313383000	0.001358000
H	0.000003000	1.828677000	-0.000495000
H	-0.000007000	-3.046874000	0.002145000
N	-2.382961000	-2.033395000	0.001490000
H	-3.254362000	-1.548787000	0.001301000
H	-2.356125000	-3.027726000	0.002779000
N	2.382953000	-2.033403000	0.001724000
H	2.356114000	-3.027734000	0.002977000
H	3.254354000	-1.548797000	0.001607000
C	-2.492538000	0.870753000	0.000040000
C	2.492540000	0.870742000	0.000260000
O	-3.591011000	0.332025000	0.000851000
O	3.591010000	0.332009000	0.000931000
C	-2.416934000	2.388795000	-0.001191000
H	-1.900680000	2.752654000	0.879493000
H	-1.900566000	2.751311000	-0.882346000
H	-3.427811000	2.768014000	-0.001521000
C	2.416943000	2.388784000	-0.001121000
H	1.900589000	2.751217000	-0.882319000
H	1.900678000	2.752730000	0.879520000
H	3.427822000	2.767998000	-0.001476000

Table S3. Cartesian coordinates of the Optimized Geometry of *m*-DAPA at S0-1PT calculated by CASSCF.

Atom	x	y	z
C	-1.225982000	0.126969000	0.079674000
C	-0.066762000	0.814928000	0.226338000
C	1.247763000	0.179661000	0.119502000
C	1.258727000	-1.305391000	0.251537000
C	0.011666000	-1.980617000	-0.103556000
C	-1.179173000	-1.337980000	-0.152616000
H	-0.105304000	1.876265000	0.360578000
H	0.057011000	-3.052839000	-0.167999000
N	2.239784000	-2.025032000	0.673371000
H	3.427432000	-0.615701000	-0.702170000
H	2.998475000	-1.461026000	1.014242000
N	-2.380645000	-2.031775000	-0.270337000
H	-2.269666000	-2.969057000	-0.591770000
H	-3.098780000	-1.543920000	-0.758389000
C	2.339939000	0.881644000	-0.235064000
C	-2.519065000	0.883093000	0.041097000
O	3.517261000	0.318596000	-0.551794000
O	-3.448428000	0.498725000	-0.608662000
C	2.457237000	2.369219000	-0.386325000
H	1.621739000	2.913428000	0.023433000
H	3.363169000	2.694038000	0.112334000
H	2.559187000	2.617391000	-1.437931000
C	-2.633446000	2.180343000	0.818233000
H	-3.679461000	2.444916000	0.880337000
H	-2.213126000	2.091905000	1.812722000
H	-2.111180000	2.979294000	0.300766000

Table S4. Cartesian coordinates of the Optimized Geometry of *m*-DAPA at S1-KETO calculated by CASSCF.

Atom	x	y	z
C	1.269285320	0.114540870	-0.016571430
C	0.000018180	0.801221030	-0.023238730
C	-1.269302090	0.114642740	-0.016521130
C	-1.251601460	-1.323131350	-0.040691810
C	-0.000091090	-2.009118290	-0.063845610
C	1.251474370	-1.323228970	-0.040672700
H	0.000062310	1.867536640	0.009849170
H	-0.000132560	-3.079175290	-0.164365730
N	-2.396140240	-2.065876640	-0.139405440
H	-3.254025710	-1.604937240	0.065584630
H	-2.338475270	-3.021697300	0.130187130
N	2.395959180	-2.066061780	-0.139398290
H	2.338203230	-3.021886850	0.130160210
H	3.253864100	-1.605204700	0.065698030
C	-2.524222310	0.882260830	0.052565560
C	2.524259080	0.882065680	0.052579880
O	-3.600957430	0.349770440	0.165659520
O	3.600945830	0.349504410	0.165790870
C	-2.468093880	2.397660570	-0.012939560
H	-1.945111000	2.806535030	0.845773400
H	-1.959229130	2.738803680	-0.908112990
H	-3.482587710	2.768882260	-0.014938700
C	2.468286000	2.397441140	-0.013601290
H	1.959261950	2.738304890	-0.908786990
H	1.945531920	2.806690130	0.845076720
H	3.482817390	2.768559080	-0.015925720

Table S5. Cartesian coordinates of the Optimized Geometry of *m*-DAPA at S1-1PT calculated by CASSCF.

Atom	x	y	z
C	1.28600402	0.01663237	-0.01621572
C	0.07807750	0.69827308	-0.00372978
C	-1.24620106	0.08314134	-0.02154748
C	-1.26045828	-1.30816726	-0.05405212
C	-0.00730012	-2.05265725	-0.06821153
C	1.25020435	-1.44048662	-0.05052309
H	0.11201541	1.76762585	0.02121903
H	-0.06524380	-3.12664052	-0.09341122
N	-2.37530350	-2.03453775	-0.07385820
H	-3.25530554	-1.56347504	-0.06491220
H	-2.33738884	-3.02633262	-0.09649998
N	2.40079808	-2.11191166	-0.06338714
H	2.24947631	-3.10466718	-0.08731431
H	3.62952785	-0.77659790	-0.02944900
C	-2.47130290	0.85831240	-0.00724870
C	2.51820796	0.74339653	0.00412561
O	-3.57438392	0.34805738	-0.02203652
O	3.71844446	0.18249074	-0.00657211
C	-2.38198696	2.37362006	0.02764271
H	-1.85791370	2.71656778	0.91443145
H	-1.85292565	2.75667162	-0.83955105
H	-3.38637978	2.77176149	0.03390446
C	2.58639697	2.24189746	0.03973177
H	3.62493859	2.54119472	0.05150029
H	2.11090518	2.68803672	-0.82920357
H	2.10284216	2.64684632	0.92420121

Table S6. Cartesian coordinates of the Optimized Geometry of *m*-DAPA at S1S0-0PT calculated by CASSCF.

Atom	x	y	z
C	-1.08021140	0.25151518	-0.22908096
C	-0.00115259	0.71776876	-0.99437784
C	1.26146113	0.13063151	-0.52129154
C	1.29759061	-1.35189581	-0.65883367
C	0.21493470	-1.91845638	-0.08625031
C	-0.87195397	-1.05394304	0.35619524
H	-0.10740675	1.26499980	-1.91415826
H	0.07275008	-2.98436942	-0.01605821
N	2.30729286	-1.98368327	-1.30825767
H	3.18889382	-1.52143483	-1.26137094
H	2.37095277	-2.97198850	-1.18951420
N	-1.75603513	-1.58432619	1.20800752
H	-1.62069384	-2.50309342	1.56035516
H	-2.58736855	-1.09132940	1.44420844
C	1.95887878	0.62598161	0.65736538
C	-2.39663638	0.93020034	-0.18470735
O	2.83032833	-0.04239067	1.16864776
O	-3.29795747	0.56431921	0.54608833
C	1.70263430	2.03403304	1.15632449
H	2.38212073	2.71672312	0.65355009
H	0.69204704	2.37382017	0.97503656
H	1.91856224	2.06780074	2.21618116
C	-2.60724434	2.13489413	-1.07803105
H	-1.91274824	2.92946991	-0.82851623
H	-2.45308341	1.87727306	-2.12069429
H	-3.61920895	2.49202097	-0.94658669

Table S7. Cartesian coordinates of the Optimized Geometry of *m*-DAPA at S1S0-1PT calculated by CASSCF.

Atom	x	y	z
C	1.148994660	-0.167569720	-0.055626060
C	1.185262010	1.282102240	-0.233477260
C	-0.106881540	1.883604210	-0.209980840
C	-1.283780890	1.166538500	-0.110033410
C	-1.274145980	-0.278374290	0.013289760
C	-0.016979920	-0.894131330	0.036330940
H	-0.162640670	2.957920760	-0.254075070
H	0.039224710	-1.961562990	0.143389560
N	-2.464604720	1.824565050	-0.077071800
H	-3.311964540	1.305823850	-0.068619760
H	-2.483123590	2.800690160	-0.252134560
N	2.370174570	1.796891390	-0.412706330
H	2.330305420	2.796892120	-0.486359990
H	2.447834520	-0.652151780	1.851462260
C	2.462967230	-0.724601890	0.014624860
O	3.007577400	-0.947858910	1.135470330
C	-2.494098290	-1.059924090	0.139750660
O	-3.605992920	-0.578300290	0.110968350
C	3.284239040	-1.069329530	-1.158736860
H	4.167793710	-1.627957670	-0.893196490
H	2.678850820	-1.573252780	-1.897891460
H	3.556579120	-0.095622070	-1.562473390
C	-2.395669710	-2.572032920	0.292867480
H	-3.398902190	-2.962911860	0.367132210
H	-1.900398760	-3.034655920	-0.554160030
H	-1.848198950	-2.841718600	1.189594580

Table S8. Cartesian coordinates of the Optimized Geometry of *m*-DAPA at S1S0-2PT calculated by CASSCF.

Atom	x	y	z
C	1.26337030	1.30951182	-0.00117628
C	-0.00050787	1.97851752	-0.00165645
C	1.23740434	-0.16519979	0.00041033
C	0.00222344	-0.85186396	0.00133572
N	2.41170846	1.93585545	-0.00207367
C	2.43136074	-0.87287629	0.00116419
O	3.58401233	-0.28453851	0.00104045
C	2.52823072	-2.37281404	0.00365185
C	-1.23794096	-0.16287480	0.00062832
C	-1.26288831	1.31072010	0.00074931
C	-2.43233529	-0.87290404	-0.00226353
C	-2.52834522	-2.37286662	-0.00605745
O	-3.58320190	-0.28205301	-0.00058188
N	-2.41237539	1.93367930	0.00381356
H	0.00017342	3.05495630	-0.00175382
H	0.00071243	-1.92124784	0.00438592
H	3.45540064	0.69785388	-0.00007077
H	2.31084965	2.93260006	-0.00522735
H	2.05333702	-2.79009339	0.88463744
H	2.04289918	-2.79345966	-0.86991779
H	3.57025481	-2.65799343	-0.00191934
H	-2.06930488	-2.79121121	0.88306182
H	-3.57022202	-2.65756767	-0.02980681
H	-2.02751664	-2.79300853	-0.87094751
H	-2.31298745	2.93074939	0.00443955
H	-3.45420743	0.70022846	0.00193541

10. Cartesian coordinates of all optimized structures calculated by OM2/MRCI.

Table S9. Cartesian coordinates of the Optimized Geometry of *m*-DAPA at S0-KETO calculated by OM2/MRCI.

Atom	x	y	z
C	-1.217206826	0.143374617	0.134377010
C	-0.001461710	0.814159065	0.034097846
C	1.220163459	0.142922073	-0.089194523
C	1.211998754	-1.292805634	-0.145621686
C	-0.003827751	-1.991014748	-0.032837904
C	-1.220564586	-1.293364447	0.125534135
H	0.001722517	1.912744613	0.058047611
H	-0.007193018	-3.075724331	-0.046454609
N	2.368892766	-1.989242761	-0.285966630
H	3.252955190	-1.521106781	-0.343096351
H	2.371878552	-2.984911258	-0.263652248
N	-2.377464950	-1.990911667	0.246787121
H	-2.383707703	-2.983733789	0.175668081
H	-3.258872691	-1.525432961	0.342508998
C	2.494619336	0.865296437	-0.113676971
C	-2.493945027	0.866260503	0.178033376
O	3.572360699	0.266782916	-0.272381729
O	-3.563584790	0.278058740	0.359307066
C	2.526200963	2.353466591	0.107661284
H	1.943820432	2.861881136	-0.670677092
H	2.113534377	2.591843913	1.095656576
H	3.566042207	2.689964104	0.059667044
C	-2.526335112	2.348353723	-0.105324060
H	-1.926237916	2.884292464	0.638349867
H	-2.136593476	2.541042600	-1.110159875
H	-3.563501944	2.689114504	-0.044905412

Table S10. Cartesian coordinates of the Optimized Geometry of *m*-DAPA at S0-1PT calculated by OM2/MRCI.

Atom	x	y	z
C	-1.230030000	0.113860000	0.170100000
C	0.045800000	0.778070000	0.209090000
C	1.207690000	0.080920000	0.022740000
C	1.179580000	-1.359280000	-0.214790000
C	-0.014660000	-2.041970000	-0.143430000
C	-1.249560000	-1.365380000	0.199730000
H	0.061970000	1.866320000	0.345330000
H	-0.066540000	-3.115710000	-0.285270000
N	2.357450000	-2.026690000	-0.453840000
H	2.296560000	-2.916770000	-0.909640000
H	3.179800000	-1.503900000	-0.687380000
N	-2.266230000	-2.088570000	0.582240000
H	-3.080870000	-1.560180000	0.935490000
H	-3.549290000	-0.539920000	-0.600650000
C	2.505480000	0.807290000	-0.042630000
C	-2.379790000	0.875420000	0.020860000
O	3.395430000	0.446940000	-0.810920000
O	-3.609850000	0.350320000	-0.163080000
C	2.689080000	2.047240000	0.791220000
H	3.758240000	2.244520000	0.893370000
H	2.217010000	2.893250000	0.273670000
H	2.240610000	1.920330000	1.779560000
C	-2.504890000	2.359410000	0.170480000
H	-2.153350000	2.834410000	-0.753310000
H	-3.556690000	2.614830000	0.331610000
H	-1.908200000	2.711720000	1.023330000

Table S11. Cartesian coordinates of the Optimized Geometry of *m*-DAPA at S1-KETO calculated by OM2/MRCI.

Atom	x	y	z
C	1.238360000	0.160440000	0.001000000
C	0.000370000	0.835830000	0.001560000
C	-1.237560000	0.128710000	0.001810000
C	-1.238210000	-1.304210000	0.001570000
C	-0.004310000	-2.013850000	0.000790000
C	1.219130000	-1.296210000	0.000440000
H	-0.009370000	1.926000000	0.001840000
H	-0.002320000	-3.106290000	0.000470000
N	-2.398170000	-2.006430000	0.002010000
H	-3.287250000	-1.540880000	0.002540000
H	-2.394170000	-3.003560000	0.001770000
N	2.389160000	-1.959920000	-0.000410000
H	2.421850000	-2.962970000	-0.000890000
H	3.267540000	-1.428950000	-0.000570000
C	-2.506140000	0.850120000	0.002300000
C	2.513670000	0.849720000	0.000980000
O	-3.590320000	0.247890000	0.002840000
O	3.589750000	0.204530000	0.000180000
C	-2.525000000	2.360650000	0.002070000
H	-2.022250000	2.737750000	0.899040000
H	-2.022420000	2.737500000	-0.895110000
H	-3.567330000	2.693620000	0.002130000
C	2.561530000	2.354630000	0.001990000
H	2.064760000	2.748700000	-0.895650000
H	2.064770000	2.747510000	0.900160000
H	3.611730000	2.664410000	0.002180000

Table S12. Cartesian coordinates of the Optimized Geometry of *m*-DAPA at S1-1PT calculated by OM2/MRCI.

Atom	x	y	z
C	1.185795409	0.190101298	0.233601776
C	-0.042058654	0.824125352	0.278386672
C	-1.246979038	0.129535481	0.049205363
C	-1.198277659	-1.265794100	-0.220931603
C	0.051360672	-1.941719697	-0.237650827
C	1.240485016	-1.223894840	-0.037846578
H	-0.080531442	1.888211795	0.526694605
H	0.094203640	-3.000666193	-0.502438972
N	-2.331272591	-1.989980500	-0.466322449
H	-3.238303408	-1.567343159	-0.402018903
H	-2.285241331	-2.968461050	-0.652068227
N	2.469125192	-1.833186979	-0.071810432
H	2.440624802	-2.787097134	0.327509456
H	3.445316524	-0.794493864	0.624148410
C	-2.550300518	0.824387880	0.071204911
C	2.463729994	0.898107899	0.520246171
O	-3.601819671	0.195089071	-0.068395166
O	3.469758290	0.183040966	0.991673848
C	-2.596320372	2.323404381	0.233090400
H	-2.208531068	2.596985163	1.219838806
H	-1.997726091	2.805538521	-0.547014627
H	-3.637343515	2.649305107	0.149678059
C	2.862911201	1.992527331	-0.434132505
H	3.089023080	1.556083321	-1.415513339
H	2.046188476	2.716947860	-0.542187234
H	3.751927849	2.488298130	-0.037914826

Table S13. Cartesian coordinates of the Optimized Geometry of *m*-DAPA at S1S0-1PT calculated by OM2/MRCI.

Atom	x	y	z
C	1.154822871	-0.210671838	-0.023967192
C	1.170120973	1.241343167	-0.207940959
C	-0.111334649	1.872189100	-0.221630921
C	-1.291320495	1.141682900	-0.102892454
C	-1.258720637	-0.299002806	0.039024460
C	-0.030164111	-0.937818750	0.065484487
H	-0.139587568	2.955524988	-0.336824355
H	0.026825659	-2.032939505	0.166527287
N	-2.489062053	1.792679493	-0.115543376
H	-3.355472758	1.296325642	-0.054760839
H	-2.528324676	2.779827823	-0.241243690
N	2.353174229	1.793416588	-0.332966684
H	2.312263065	2.815564182	-0.454873535
H	2.612395242	-0.509364822	1.891818878
C	2.470434382	-0.788594346	-0.009932104
O	3.139174665	-0.873510419	1.126990831
C	-2.508282726	-1.062631126	0.142680967
O	-3.615131965	-0.514728190	0.116080047
C	3.322409243	-1.056466575	-1.192267338
H	4.184920419	-1.676105640	-0.931566280
H	2.727525645	-1.525765797	-1.982059476
H	3.657025242	-0.063918874	-1.523110384
C	-2.468630662	-2.568211292	0.286557024
H	-3.496533226	-2.937241856	0.346723268
H	-1.974362654	-3.015006294	-0.584151386
H	-1.931743277	-2.843504477	1.202182196

11. Cartesian coordinates of all optimized structures calculated by B3LYP/6-31G* and CAM-B3LYP methods.

Table S14. Cartesian coordinates of the Optimized Geometry of *m*-DAPA at S0-KETO calculated by B3LYP.

Atom	x	y	z
C	1.232076000	-0.099714000	-0.002112000
C	-0.000209000	-0.746389000	-0.000324000
C	-1.232572000	-0.099845000	0.004320000
C	-1.224174000	1.339243000	0.007889000
C	-0.000347000	2.011262000	0.006124000
C	1.223499000	1.339377000	0.001518000
H	-0.000176000	-1.828509000	-0.003416000
H	-0.000409000	3.098295000	0.009647000
N	-2.380736000	2.032153000	0.014553000
H	-3.249327000	1.511675000	0.008168000
H	-2.374653000	3.039369000	0.007017000
N	2.380044000	2.032408000	0.002009000
H	2.373857000	3.039626000	-0.005066000
H	3.248652000	1.512040000	-0.008425000
C	-2.479826000	-0.866876000	0.003688000
C	2.479405000	-0.866619000	-0.009230000
O	-3.589917000	-0.328437000	0.004650000
O	3.589423000	-0.328076000	-0.013530000
C	-2.422249000	-2.382288000	0.001309000
H	-1.903357000	-2.761301000	-0.884145000
H	-1.899421000	-2.764071000	0.883230000
H	-3.444983000	-2.759072000	0.002871000
C	2.421945000	-2.382040000	-0.011887000
H	1.903753000	-2.764268000	0.872568000
H	1.898488000	-2.760696000	-0.894805000
H	3.444709000	-2.758729000	-0.015781000

Table S15. Cartesian coordinates of the Optimized Geometry of *m*-DAPA at S1-KETO calculated by TD-CAM-B3LYP.

Atom	x	y	z
C	1.234999000	0.106883000	-0.169050000
C	0.000057000	0.760413000	-0.425277000
C	-1.234999000	0.106761000	-0.168929000
C	-1.218402000	-1.339013000	-0.047006000
C	-0.000176000	-2.022831000	0.002583000
C	1.218000000	-1.339165000	-0.047706000
H	-0.000020000	1.816093000	-0.649933000
H	-0.000187000	-3.106022000	0.075605000
N	-2.382786000	-2.001939000	0.022021000
H	-3.237744000	-1.446042000	0.000034000
H	-2.399757000	-2.992307000	0.215553000
N	2.382451000	-2.001952000	0.019774000
H	2.399777000	-2.992377000	0.213116000
H	3.237262000	-1.445576000	-0.001924000
C	-2.477260000	0.863314000	-0.007837000
C	2.477294000	0.863076000	-0.007549000
O	-3.604579000	0.319457000	-0.023591000
O	3.604746000	0.319020000	-0.023722000
C	-2.386591000	2.362746000	0.110691000
H	-1.626919000	2.662124000	0.841810000
H	-2.109304000	2.822796000	-0.846719000
H	-3.361339000	2.751009000	0.409391000
C	2.386866000	2.362445000	0.111441000
H	2.110514000	2.823019000	-0.846009000
H	1.626652000	2.661754000	0.842042000
H	3.361444000	2.750415000	0.411100000

12. Cartesian coordinates of optimized CI structure of *o*-DAPA calculated by CASSCF method.

Table S16. Cartesian coordinates of the Optimized Geometry of *o*-DAPA at CI point calculated by CASSCF.

Atom	x	y	z
C	-1.06040305	-1.07276230	0.94425135
C	0.11419755	-0.76495990	1.63859432
C	1.05684826	0.05811776	1.05634128
C	0.86556104	0.53254788	-0.27257468
C	-0.34152810	0.25597113	-0.95169821
C	-1.30794937	-0.56300586	-0.33511856
H	-1.78407196	-1.70353843	1.41998709
H	0.28574991	-1.18236038	2.61359586
C	-2.59798775	-0.89224968	-1.01736235
O	-2.89088927	-0.43623583	-2.08874329
C	2.39364866	0.39601970	1.62668481
O	3.34797185	0.19615060	0.78057600
C	-3.57483638	-1.83151989	-0.33658047
H	-4.41835504	-1.96828362	-0.99714042
H	-3.11882690	-2.79383883	-0.13206079
H	-3.92305677	-1.41904663	0.60416373
C	2.55019207	1.42969937	2.70101696
H	1.90138026	1.22025870	3.54469403
H	3.57910682	1.45831122	3.03735187
H	2.28742813	2.41698406	2.32031807
N	-0.48984206	0.80720490	-2.20931402
H	-0.13497402	1.73331552	-2.30292773
H	-1.39463573	0.69141041	-2.60912579
N	1.90317276	1.22354698	-0.85361639
H	1.90124377	1.09876627	-1.85111911
H	2.97828369	0.69885776	-0.14794737