Supporting Information (SI) For:

Simultaneously Improving the Efficiencies of Photo- and Thermal Isomerization of an Oxindole-Based Light-Driven Molecular Rotary Motor by a Structural Redesign

Jianzheng Ma[1], Di Zhao[1], Le Yu[2], Chenwei Jiang[1,*], Zhenggang Lan[3,*], and Fuli Li[1]

[1]Ministry of Education Key Laboratory for Nonequilibrium Synthesis and Modulation of Condensed Matter, Shaanxi Province Key Laboratory of Quantum Information and Quantum Optoelectronic Devices, School of Physics, Xi'an Jiaotong University, Xi'an 710049, China

[2]Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of Ministry of Education, College of Chemistry & Materials Science, Shaanxi Key Laboratory of Physico-Inorganic Chemistry, Northwest University, Xi'an, Shaanxi, 710127, China

[3]SCNU Environmental Research Institute, Guangdong Provincial Key Laboratory of Chemical Pollution and Environmental Safety & MOE Key Laboratory of Environmental Theoretical Chemistry, South China Normal University, Guangzhou 510006, China; School of Environment, South China Normal University, Guangzhou 510006, China

**Corresponding authors. Email: jiangcw@xjtu.edu.cn (C.J.); zhenggang.lan@m.scnu.edu.cn (Z. L.).*

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1. Details for generation of wavefunctions and multireference configurations in the OM2/MRCI calculations

In the standard OM2/MRCI implementation, the molecular orbitals are generated from the Hartree-Fork calculations with the OM2 Hamiltonian. Then all of these orbitals are frozen and several references are built. From each reference, different configurations are generated by electronic excitations. Then all configurations are combined to define the total wavefunctions and only the configuration interaction vectors are solved without the further optimization of the molecular orbitals. In the current work, the ROHF calculations were made to obtain all molecular orbitals. Next, we selected three references, including the closed-shell ground-state configuration and single and double excitations from the highest occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbital (LUMO). Then all configurations in MRCI wavefunctions were generated by the single or double excitations of these references.

2. Active space orbitals for *ZP*-DDIYM and *ZP*-DDPYM

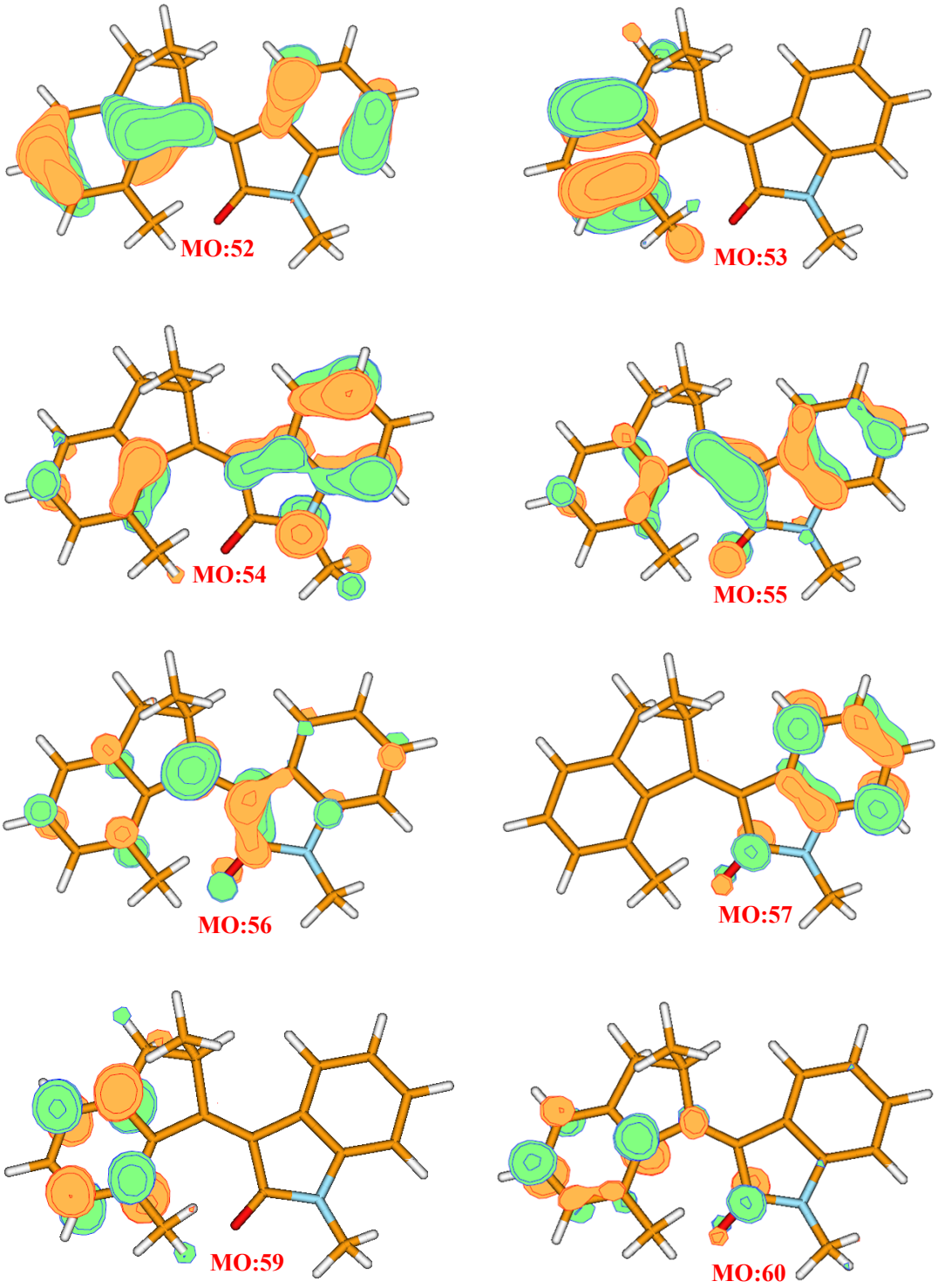


Figure S1: Active space orbitals for the *ZP* conformer of DDIYM calculated with the OM2/MRCI method implemented in MNDO99[S1] program.

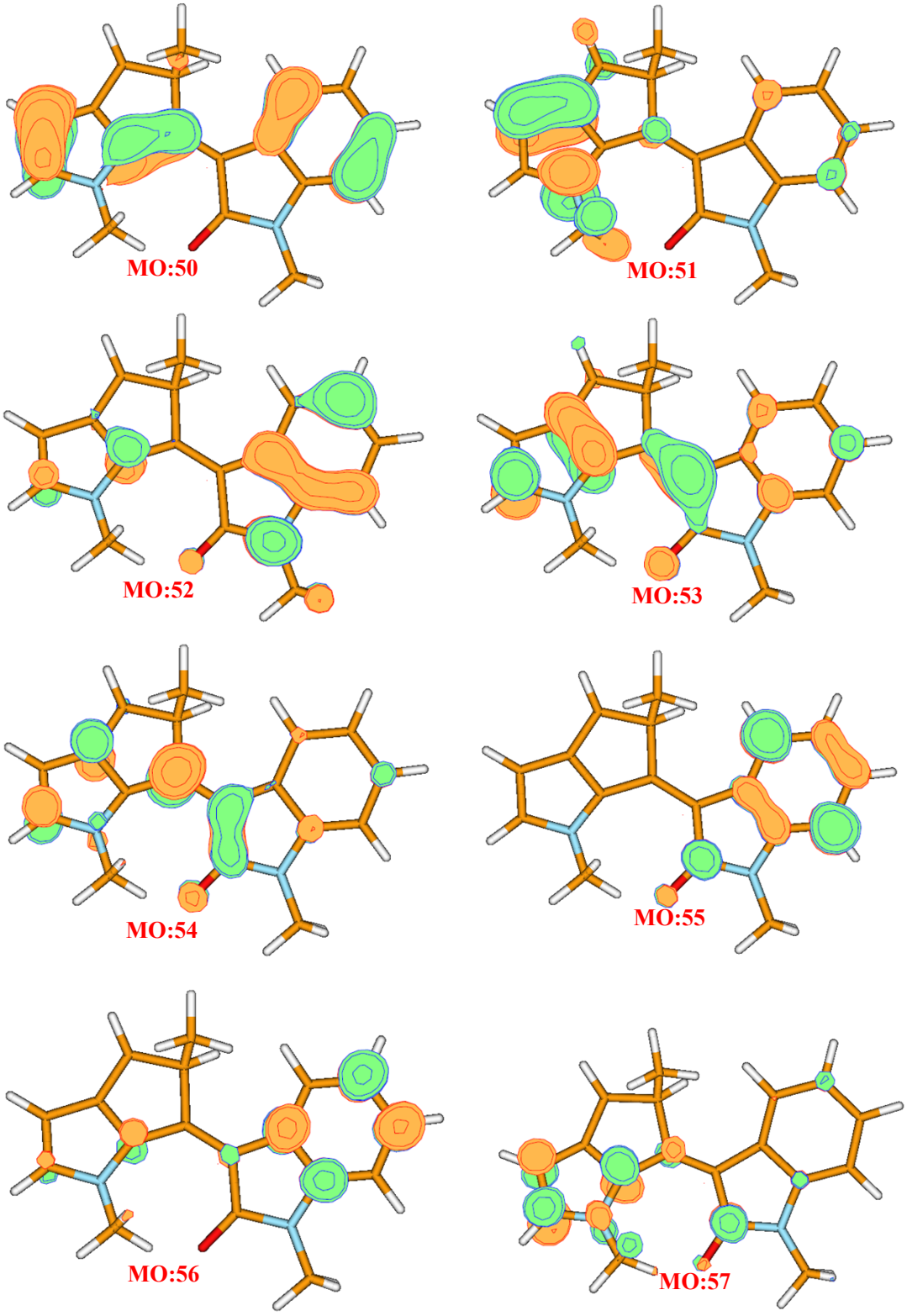


Figure S2: Active space orbitals of the *ZP* conformer of DDPYM calculated with the OM2/MRCI method implemented in MNDO99[S1] program.

3. Optimized local minima geometries in the ground state of DDIYM and DDPYM

(1) Optimized local minima geometries for DDIYM

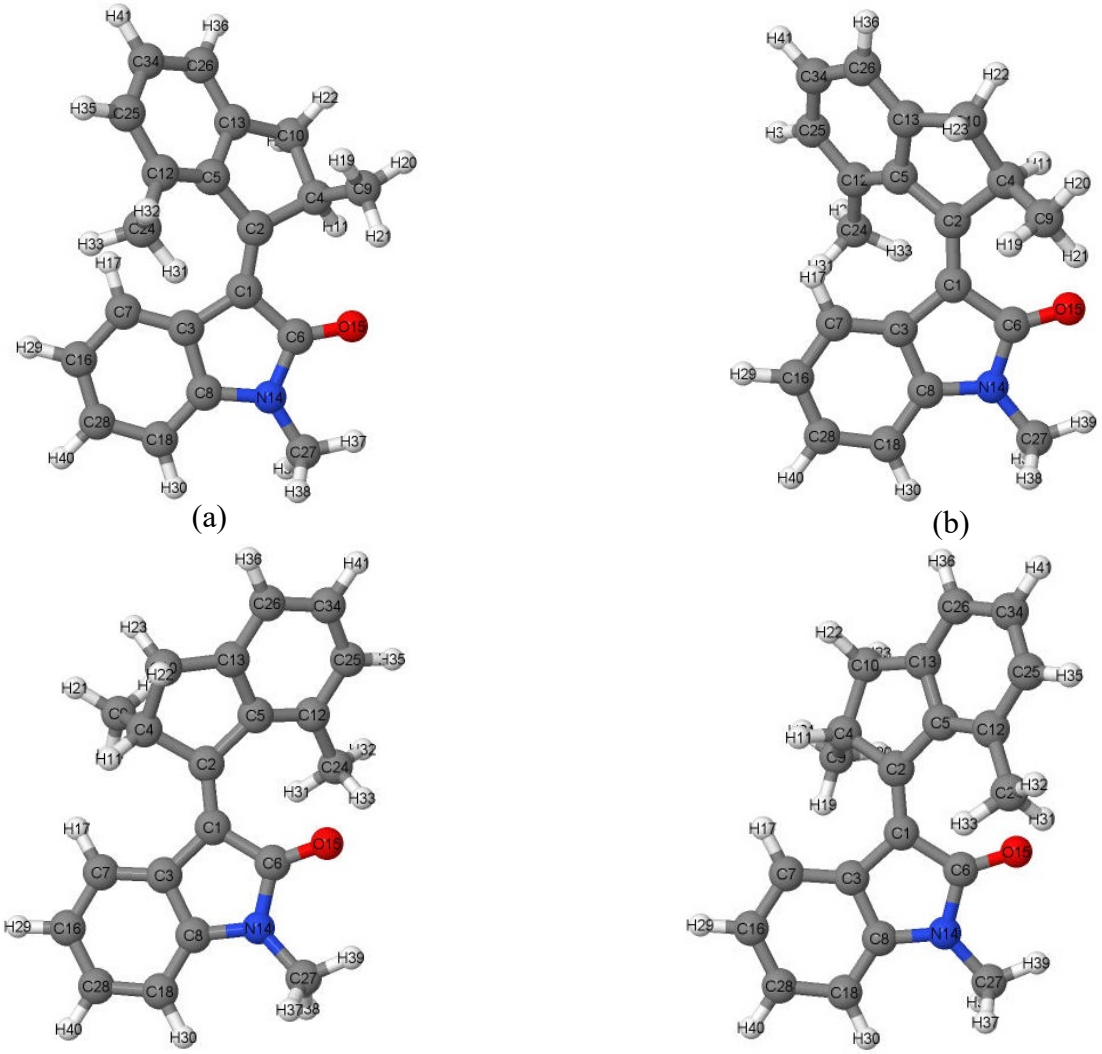


Figure S3. Optimized ground state geometries of (a) *EP*, (b) *EM*, (c) *ZP* and (d) *ZM* isomers for DDIYM calculated with the OM2/MRCI method implemented in MNDO99[S1] program. All atoms are labelled.

Table S1. Optimized geometrical parameters of ground state DDIYM, obtained from different methods. OM2/MRCI is implemented in MNDO99[S1] program; while B3LYP-D3/6-31G(d,p) and ωB97X-D/6-31G(d,p) are both implemented in Gaussian 09[S2] program. The lengths are in angstroms; the dihedral angles and bond angles are in degrees.

		B3LYP-D3/6-31G(d,p)	ωB97X-D/6-31G(d,p)	OM2/MRCI
EP	C1-C2	1.36	1.35	1.36
	C5-C2-C1	129.2	129.1	129.4
	C2-C1-C3	131.9	131.9	132.4
	C5-C2-C1-C3	14.4	12.1	11.6
	C5-C2-C1-C6	-168.1	-169.6	-172.0
	C1-C6-C3-C2	1.0	0.7	1.4
EM	C1-C2	1.37	1.36	1.36
	C5-C2-C1	126.9	126.5	126.3
	C2-C1-C3	130.1	129.9	129.0
	C5-C2-C1-C3	-25.1	-23.2	-22.7
	C5-C2-C1-C6	153.8	155.7	159.3
	C1-C6-C3-C2	0.4	0.5	-0.8
ZP	C1-C2	1.36	1.36	1.36
	C5-C2-C1	129.9	130.0	128.7
	C2-C1-C3	129.1	128.7	128.2
	C5-C2-C1-C3	-174.3	-175.8	-174.1
	C5-C2-C1-C6	16.6	15.7	13.1
	C1-C6-C3-C2	-4.3	-4.6	-2.8
ZM	C1-C2	1.37	1.36	1.37
	C5-C2-C1	128.1	128.1	128.5
	C2-C1-C3	129.6	129.4	127.5
	C5-C2-C1-C3	157.0	158.0	158.9
	C5-C2-C1-C6	-32.1	-31.4	-26.6
	C1-C6-C3-C2	3.6	3.8	2.2

(2) Optimized local minima geometries for DDPYM

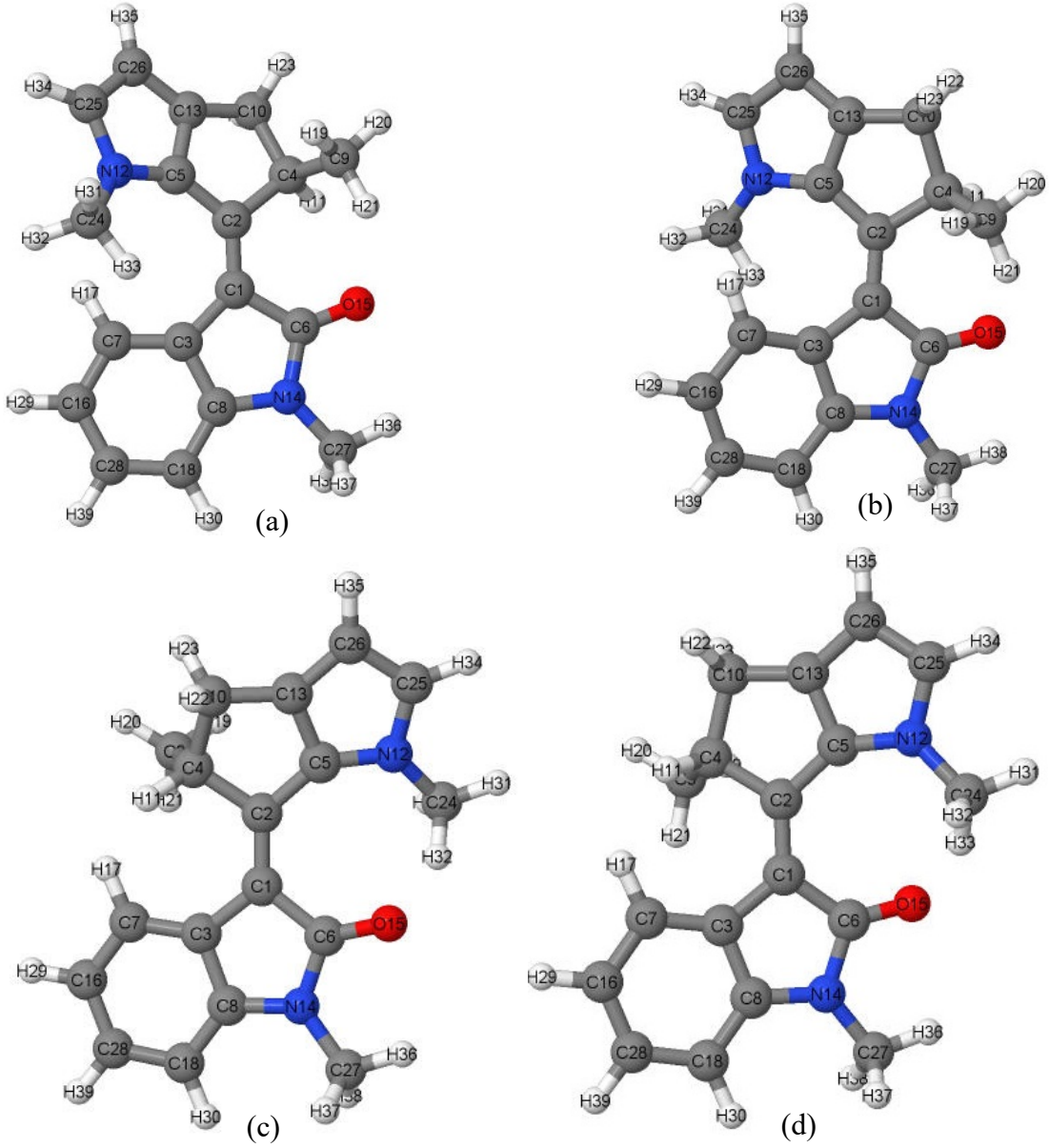
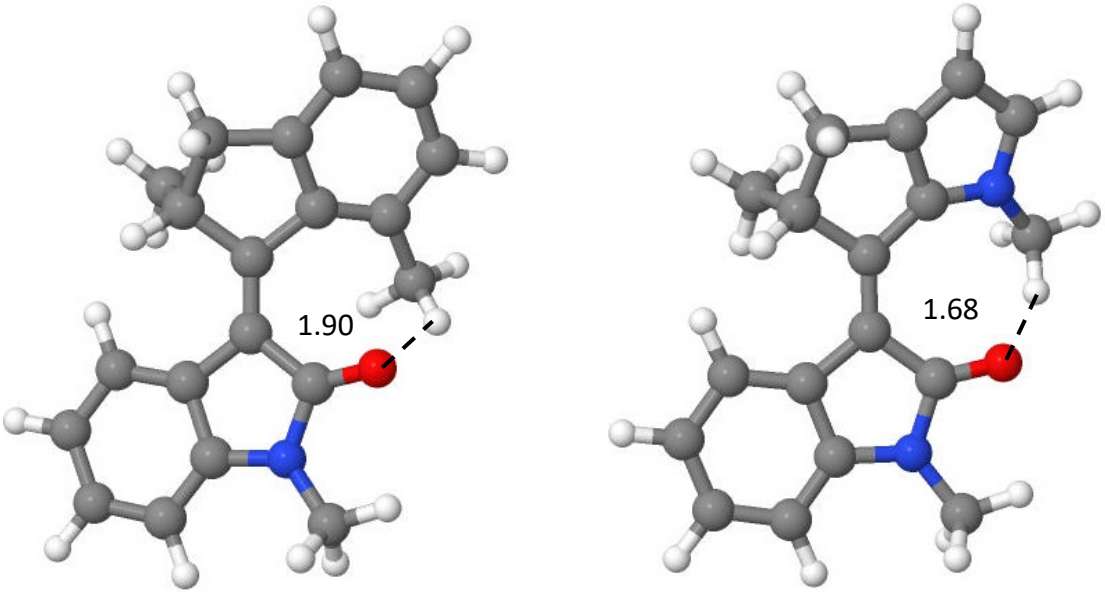


Figure S4. Optimized ground state geometries of (a) *EP*, (b) *EM*, (c) *ZP* and (d) *ZM* isomers for DDPYM calculated with the OM2/MRCI method implemented in MNDO99[S1] program. All atoms are labelled.

Table S2. Optimized geometrical parameters of ground state DDPYM, obtained from different methods. OM2/MRCI is implemented in MNDO99[S1] program; while B3LYP-D3/6-31G(d,p) and ωB97X-D/6-31G(d,p) are both implemented in Gaussian 09[S2] program. The lengths are in angstroms; the dihedral angles and bond angles are in degrees.

		B3LYP-D3/6-31G(d,p)	ωB97X-D/6-31G(d,p)	OM2/MRCI
EP	C1-C2	1.37	1.36	1.36
	C5-C2-C1	130.9	130.9	130.3
	C2-C1-C3	131.3	131.4	132.3
	C5-C2-C1-C3	13.3	11.9	7.9
	C5-C2-C1-C6	-169.2	-170.3	-170.4
	C1-C6-C3-C2	1.0	0.9	-0.7
EM	C1-C2	1.38	1.37	1.36
	C5-C2-C1	130.4	130.0	128.5
	C2-C1-C3	131.0	130.7	130.6
	C5-C2-C1-C3	-23.9	-22.6	-17.2
	C5-C2-C1-C6	153.3	153.9	159.1
	C1-C6-C3-C2	1.2	1.4	1.5
ZP	C1-C2	1.37	1.36	1.36
	C5-C2-C1	132.2	132.4	131.8
	C2-C1-C3	129.6	129.4	128.4
	C5-C2-C1-C3	-175.8	-176.3	-177.2
	C5-C2-C1-C6	14.1	13.5	7.0
	C1-C6-C3-C2	-4.0	-3.9	-1.7
ZM	C1-C2	1.38	1.37	1.37
	C5-C2-C1	130.8	131.0	131.6
	C2-C1-C3	129.5	129.3	127.6
	C5-C2-C1-C3	160.0	161.1	163.8
	C5-C2-C1-C6	-28.1	-27.0	-19.4
	C1-C6-C3-C2	3.3	3.3	1.2

4. Hydrogen bond length in fjord region of *ZP*-DDIYM and *ZP*-DDPYM



(a) (b)

Figure S5. Hydrogen bond length in fjord region of ground state (a) *ZP*-DDIYM and (b) *ZP*-DDPYM. The geometries was optimized based on the OM2/MRCI method implemented in MNDO99[S1] program. The unit is angstroms.

5. Optimized geometries of conical intersection in the photoisomerization processes of DDIYM and DDPYM

(1) Optimized conical intersections for DDIYM

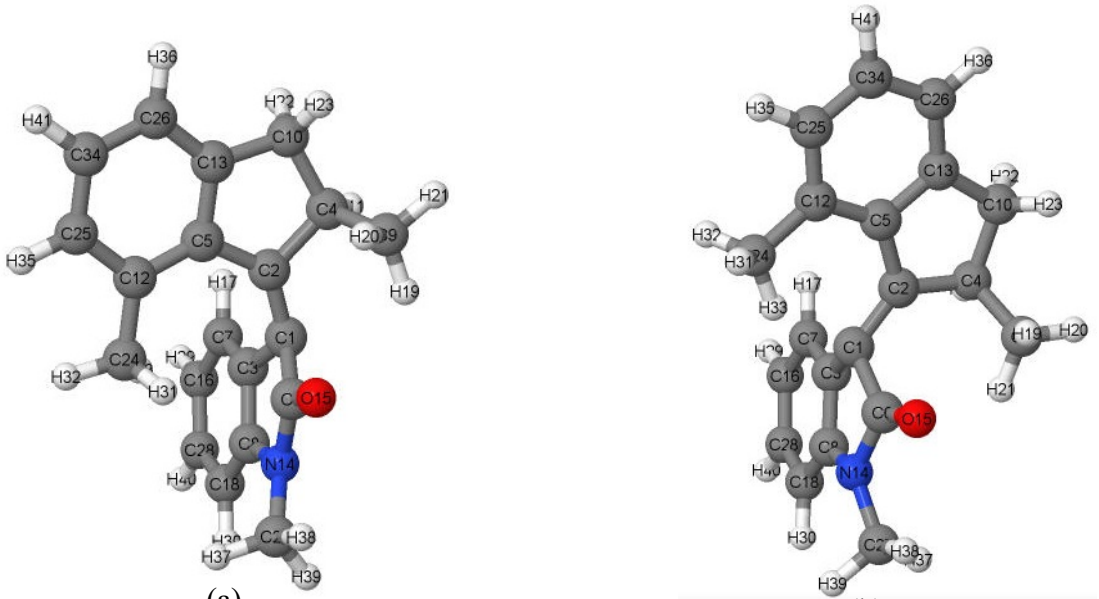


Figure S6. Optimized geometries of two S_1/S_0 conical intersections (a) *E*CI(1) and (b) *E*CI(2) in the *EP*→*ZM* photoisomerization process of DDIYM calculated with the OM2/MRCI method implemented in MNDO99[S1] program.

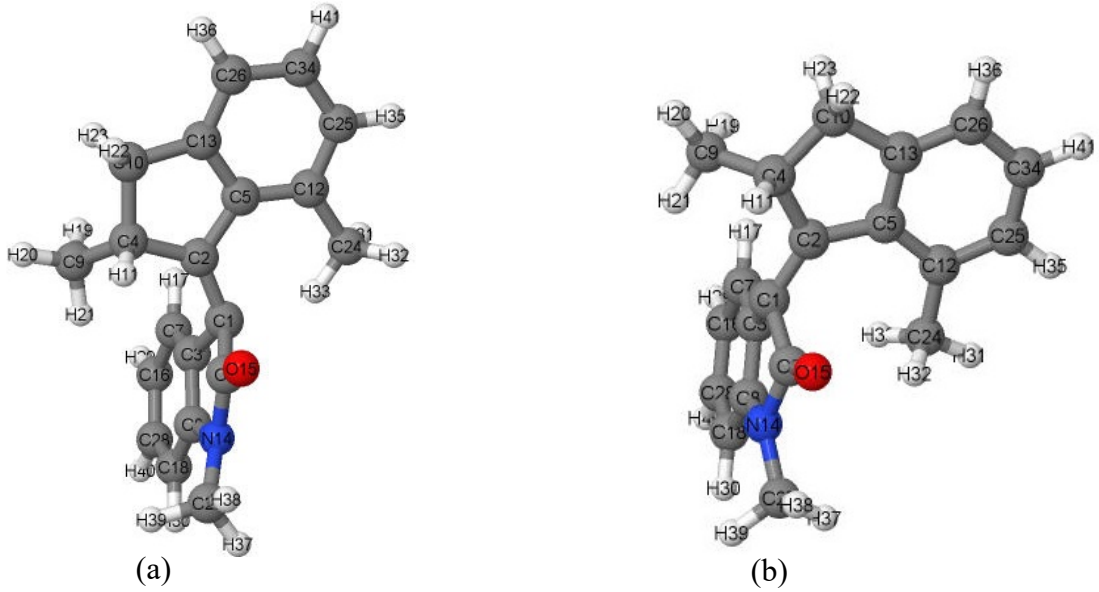


Figure S7. Optimized geometries of two S_1/S_0 conical intersections (a) *Z*CI(1) and (b) *Z*CI(2) in the *ZP*→*EM* photoisomerization process of DDIYM calculated with the OM2/MRCI method implemented in MNDO99[S1] program.

Table S3. Optimized geometrical parameters of four S_1/S_0 conical intersections (*E*CI(1) and *E*CI(2) in the *EP*→*ZM* photoisomerization process of DDIYM, together with ZCI(1) and ZCI(2) in the ZP→EM photoisomerization process) obtained from different methods. OM2/MRCI is implemented in MNDO99[S1] program; while CASSCF(12,12)/6-31G(d) is implemented in MOLPRO[S3,S4] program. The lengths are in angstroms; the dihedral angles and bond angles are in degrees.

		OM2/MRCI	CASSCF(12,12)/6-31G(d)
*E*CI(1)	C1-C2	1.38	1.43
	C5-C2-C1	131.7	129.4
	C2-C1-C3	123.0	137.1
	C5-C2-C1-C3	66.0	69.7
	C5-C2-C1-C6	-65.4	-76.8
	C1-C6-C3-C2	-21.8	-14.8
*E*CI(2)	C1-C2	1.40	1.44
	C5-C2-C1	123.4	126.6
	C2-C1-C3	117.6	137.7
	C5-C2-C1-C3	120.2	119.5
	C5-C2-C1-C6	-117.8	-98.4
	C1-C6-C3-C2	27.0	16.7
*Z*CI(1)	C1-C2	1.40	1.43
	C5-C2-C1	123.8	128.5
	C2-C1-C3	121.1	130.7
	C5-C2-C1-C3	-123.5	-106.1
	C5-C2-C1-C6	113.7	104.4
	C1-C6-C3-C2	-26.4	-14.1
*Z*CI(2)	C1-C2	1.37	1.43
	C5-C2-C1	131.8	129.4
	C2-C1-C3	125.3	131.6
	C5-C2-C1-C3	-67.0	-72.5
	C5-C2-C1-C6	64.7	74.7
	C1-C6-C3-C2	21.5	15.1

(2) Optimized S_1/S_0 conical intersections of DDPYM

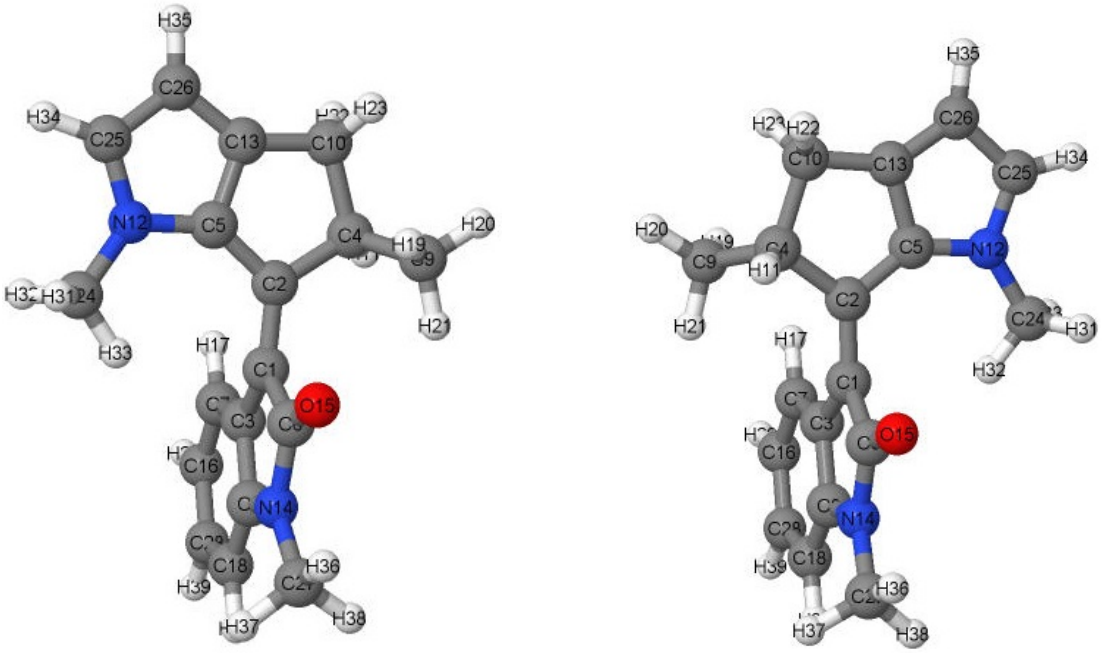


Figure S8. Optimized geometries of S_0/S_1 conical intersections (a) *E*CI in the *EP*→*ZM* photoisomerization process and (b) *Z*CI in the *ZP*→*EM* photoisomerization process of DDPYM calculated with the OM2/MRCI method implemented in MNDO99[S1] program.

Table S4. Optimized geometrical parameters of S_0/S_1 conical intersections (a) *E*CI in the *EP*→*ZM* photoisomerization process and (b) *Z*CI in the *ZP*→*EM* photoisomerization process of DDPYM, obtained from different methods. OM2/MRCI is implemented in MNDO99[S1] program; while CASSCF(10,9)/6-31G(d) is implemented in MOLPRO[S3,S4] program. The lengths are in angstroms; the dihedral angles and bond angles are in degrees.

		OM2/MRCI	CASSCF(10,9)/6-31G(d)
*E*CI	C1-C2	1.40	1.45
	C5-C2-C1	126.0	127.9
	C2-C1-C3	128.7	128.6
	C5-C2-C1-C3	94.3	89.2
	C5-C2-C1-C6	-94.1	-90.2
	C1-C6-C3-C2	3.5	-0.3
*Z*CI	C1-C2	1.40	1.45
	C5-C2-C1	126.1	127.9
	C2-C1-C3	129.1	129.6
	C5-C2-C1-C3	-95.1	-92.6
	C5-C2-C1-C6	93.2	87.7
	C1-C6-C3-C2	-3.5	-0.2

6. Time-dependent evolution of geometrical parameters in a typical trajectory of DDIYM and DDPYM

In order to explore the reaction dynamics of LDMRMs DDIYM and DDPYM in detail, time dependent evolution of geometrical parameters in a typical trajectory for both *EP*→*ZP* and *ZP*→*EP* photoisomerization processes are presented in the following.

(1) Typical trajectories for DDIYM

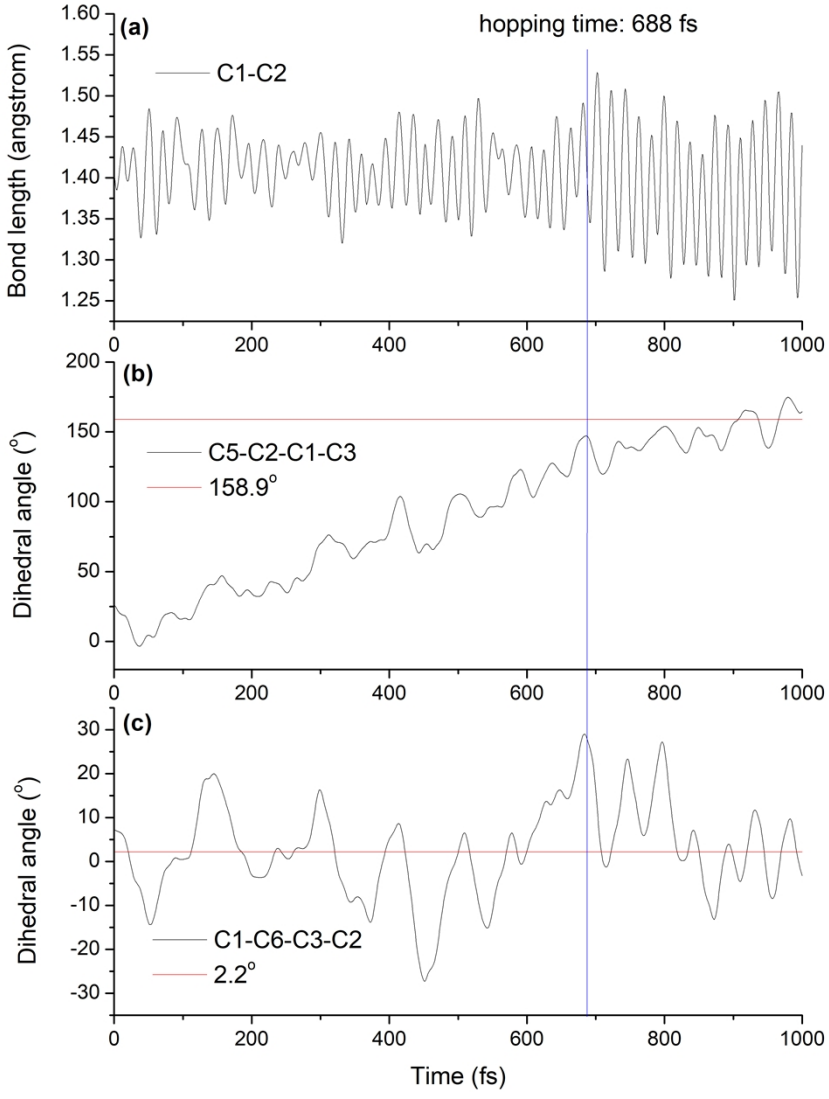


Figure S9. Time dependence of (a) central bond length C1-C2, (b) central dihedral angle C5−C2−C1−C3, and (c) pyramid dihedral angle C1−C6−C3−C2 in a representative trajectory of *EP*→*ZM* photoisomerization process for DDIYM. The correponding geometrical parameters of reaction product *ZM* isomer are also shown in the figure with red lines.

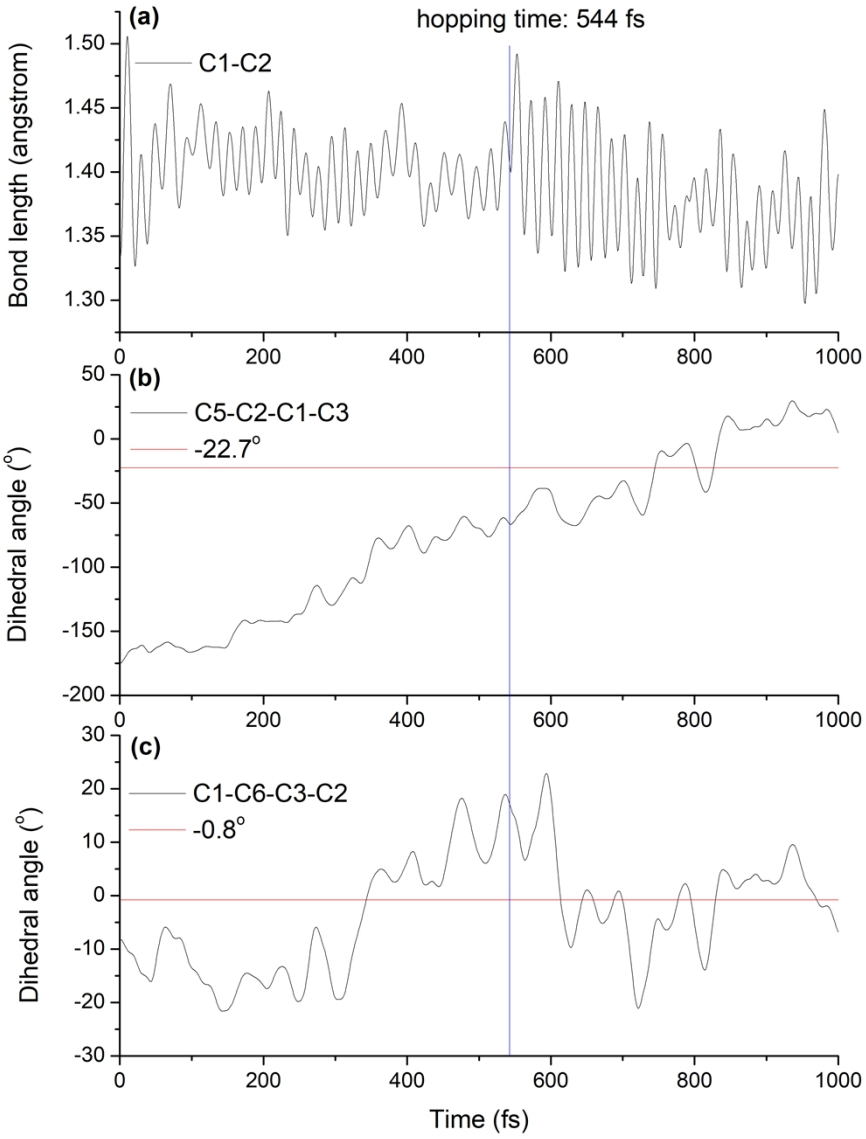


Figure S10. Time dependence of (a) central bond length C1-C2, (b) central dihedral angle C5−C2−C1−C3, and (c) pyramid dihedral angle C1−C6−C3−C2 in a representative trajectory of *ZP*→*EM* photoisomerization process for DDIYM. The correponding geometrical parameters of reaction product *EM* isomer is also shown in the figure with red lines.

(2) Typical trajectories of DDPYM

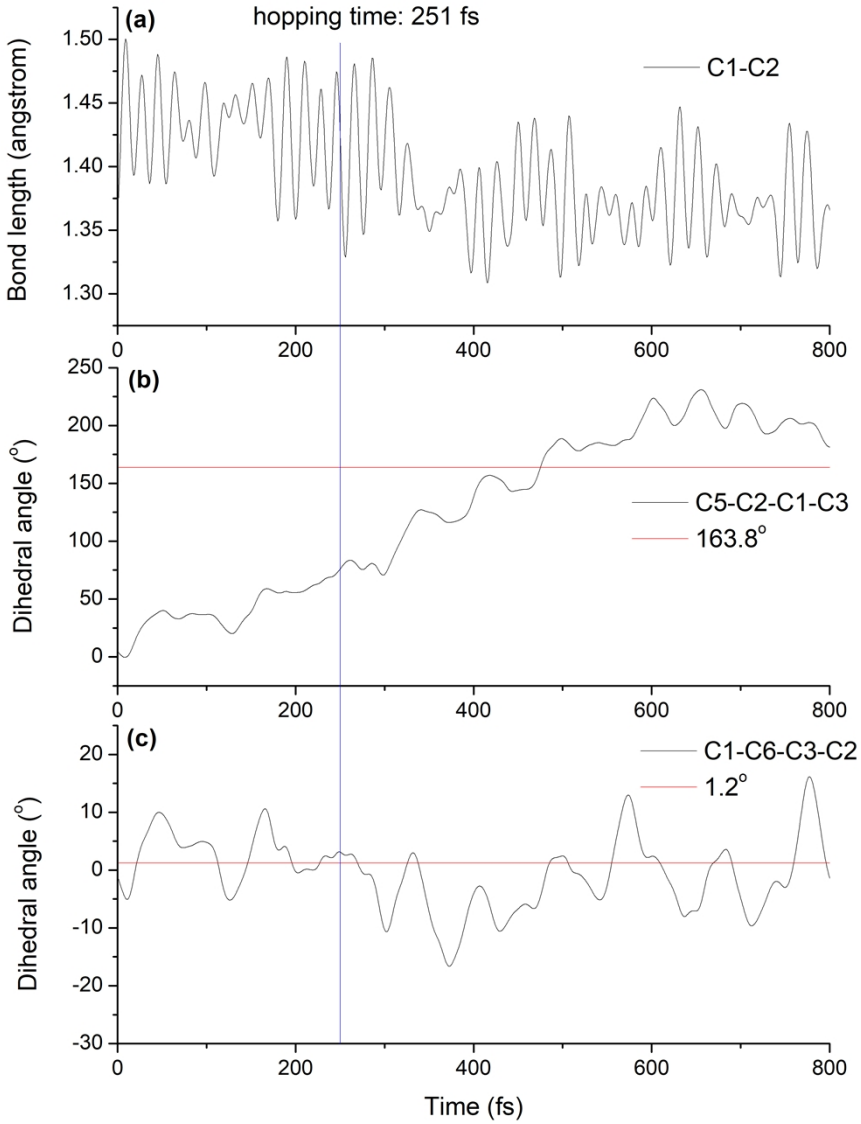


Figure S11. Time dependence of (a) central bond length C1-C2, (b) central dihedral angle C5−C2−C1−C3, and (c) pyramid dihedral angle C1−C6−C3−C2 in a representative trajectory of *EP*→*ZM* photoisomerization process for DDPYM. The correponding geometrical parameters of reaction product *ZM* isomer is also shown in the figure with red lines.

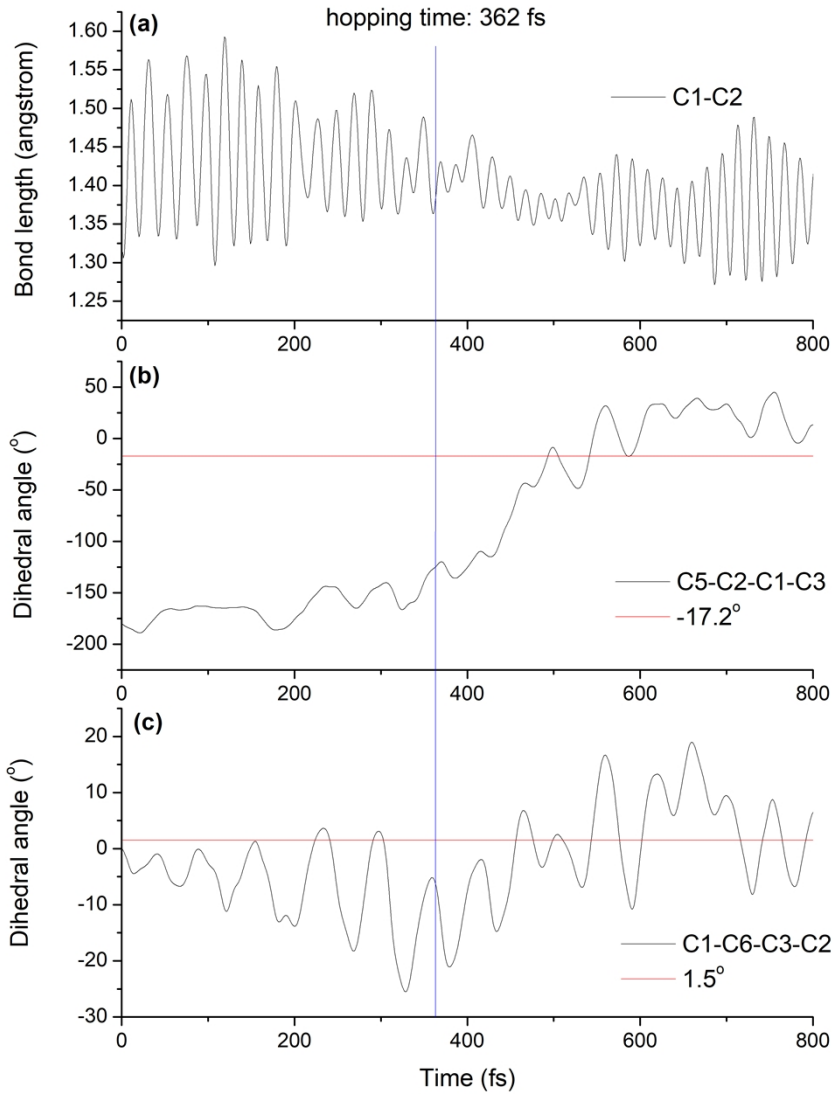


Figure S12. Time dependence of (a) central bond length C1-C2, (b) central dihedral angle C5−C2−C1−C3, and (c) pyramid dihedral angle C1−C6−C3−C2 in a representative trajectory of *ZP*→*EM* photoisomerization process for DDPYM. The correponding geometrical parameters of reaction product *EM* isomer is also shown in the figure with red lines.

7. Absorption spectra of different isomers of DDIYM and DDPYM

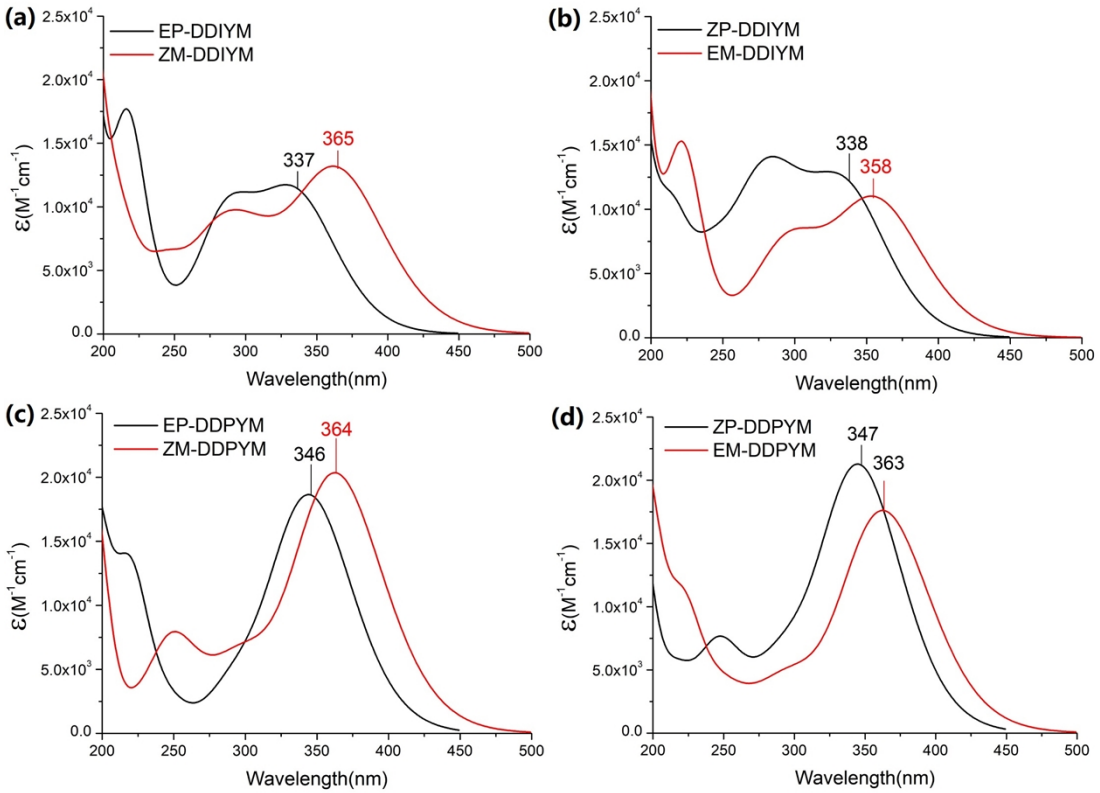
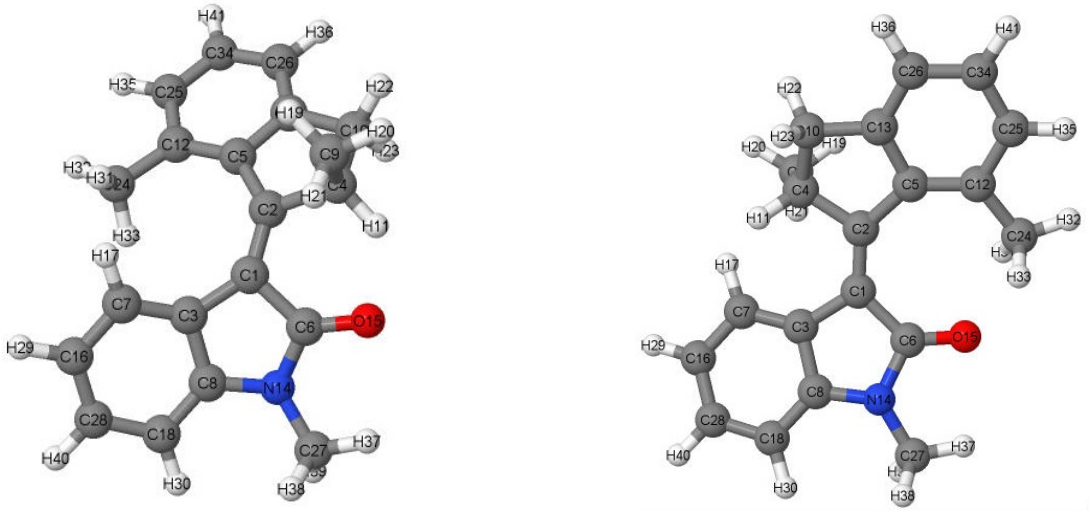


Figure S13. Simulated absorption spectra and their maxima calculated at the TD-ωB97X-D/6-31G(d,p) level of theory for (a) EP and ZM isomers for DDIYM; (b)ZP and EM isomers for DDIYM; (c)EP and ZM isomers of DDPYM; (d)ZP and EM isomers of DDPYM.

8. Transition state geometries and energy barriers in the ground state of DDIYM and DDPYM

(1) Transition state geometries in the ground state for DDIYM



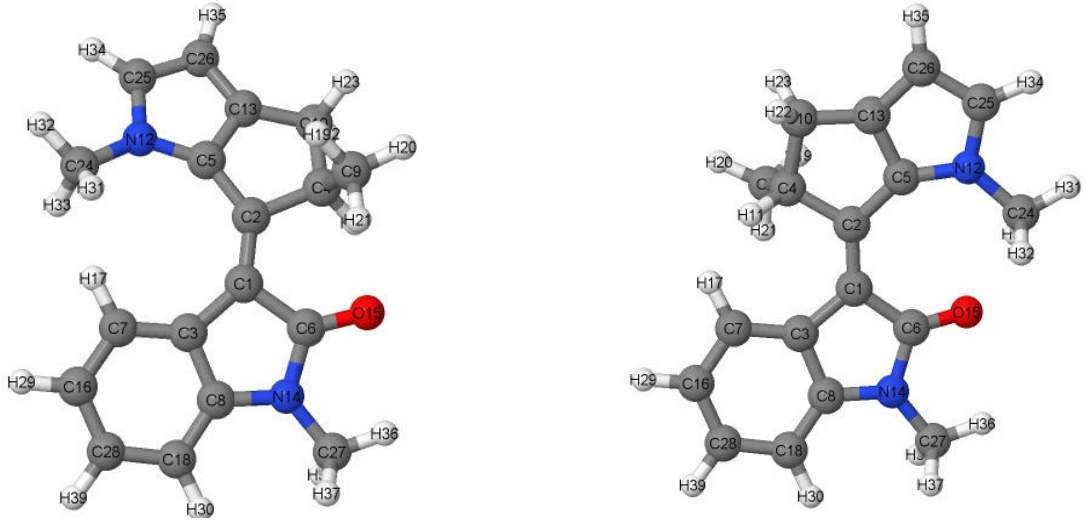
(a) (b)

Figure S14. Optimized transition state geometries of (a) *EM-EP-TS* and (b) *ZM-ZP-TS* for ground state DDIYM calculated with the OM2/MRCI method implemented in MNDO99[S1] program. All atoms are labelled.

Table S5. Optimized transition state geometrical parameters of DDIYM, obtained from different methods. The OM2/MRCI method is implemented in MNDO99[S1] program; while B3LYP-D3/6-31G(d,p) and ωB97X-D/6-31G(d,p) method are all implemented in Gaussian 09[S2] program. The lengths are in angstroms; the dihedral angles and bond angles are in degrees.

		OM2/MRCI	B3LYP-D3/6-31G(d,p)	ωB97X-D/6-31G(d,p)
EM-EP-TS	C1-C2	1.37	1.38	1.37
	C5-C2-C1	133.4	134.9	135.2
	C2-C1-C3	137.0	135.8	135.9
	C5-C2-C1-C3	-24.0	-20.1	-16.5
	C5-C2-C1-C6	141.3	141.8	144.2
	C1-C6-C3-C2	5.5	6.8	7.1
ZM-ZP-TS	C1-C2	1.37	1.38	1.37
	C5-C2-C1	135.7	138.2	138.1
	C2-C1-C3	126.0	126.3	126.1
	C5-C2-C1-C3	167.5	163.7	163.8
	C5-C2-C1-C6	-3.7	-8.1	-6.9
	C1-C6-C3-C2	-3.3	-3.1	-3.5

(2) Transition state geometries in the ground state for DDPYM



(a) (b)

Figure S15. Optimized transition state geometries of (a) *EM-EP-TS* and (b) *ZM-ZP-TS* for ground state DDPYM calculated with the OM2/MRCI method implemented in MNDO99[S1] program. All atoms are labelled.

Table S6. Optimized transition state geometrical parameters of LDMRM DDPYM, obtained from different methods. The OM2/MRCI method is implemented in MNDO99[S1] program; while B3LYP-D3/6-31G(d,p) and ωB97X-D/6-31G(d,p) method are both implemented in Gaussian 09[S2] program. The lengths are in angstroms; the dihedral angles and bond angles are in degrees.

		OM2/MRCI	B3LYP-D3/6-31G(d,p)	ωB97X-D/6-31G(d,p)
EM-EP-TS	C1-C2	1.37	1.38	1.37
	C5-C2-C1	136.1	137.4	137.2
	C2-C1-C3	137.2	135.4	135.3
	C5-C2-C1-C3	0.0	-2.5	-2.2
	C5-C2-C1-C6	171.5	167.0	166.1
	C1-C6-C3-C2	3.1	4.0	4.4
ZM-ZP-TS	C1-C2	1.36	1.38	1.37
	C5-C2-C1	133.3	136.7	136.5
	C2-C1-C3	127.8	128.7	128.5
	C5-C2-C1-C3	168.9	169.5	169.0
	C5-C2-C1-C6	-9.1	-9.8	-9.8
	C1-C6-C3-C2	-0.8	-0.3	-0.5

(3) Energy barriers in the ground state for DDIYM and DDPYM

Table S7. Energy barriers from EM to EP isomers and from ZM to ZP isomers in the ground state for DDIYM and DDPYM, obtained from the OM2/MRCI, B3LYP-D3/6-31G(d,p) and ωB97X-D/6-31G(d,p) methods. The energy unit is kcal/mol. The OM2/MRCI method is implemented in MNDO99[S1] program; while B3LYP-D3/6-31G(d,p) and ωB97X-D/6-31G(d,p) method are both implemented in Gaussian 09[S2] program.

		OM2/MRCI	B3LYP-D3/6-31G(d,p)	ωB97X-D/6-31G(d,p)
DDIYM	*EM→EP*	10.4	15.2	14.7
	ZM→ZP	7.3	11.7	11.1
DDPYM	*EM→EP*	5.3	8.2	7.8
	ZM→ZP	1.3	2.2	1.9

9. Schematic representation of the potential energy profile of the S_0 and S_1 states of DDIYM

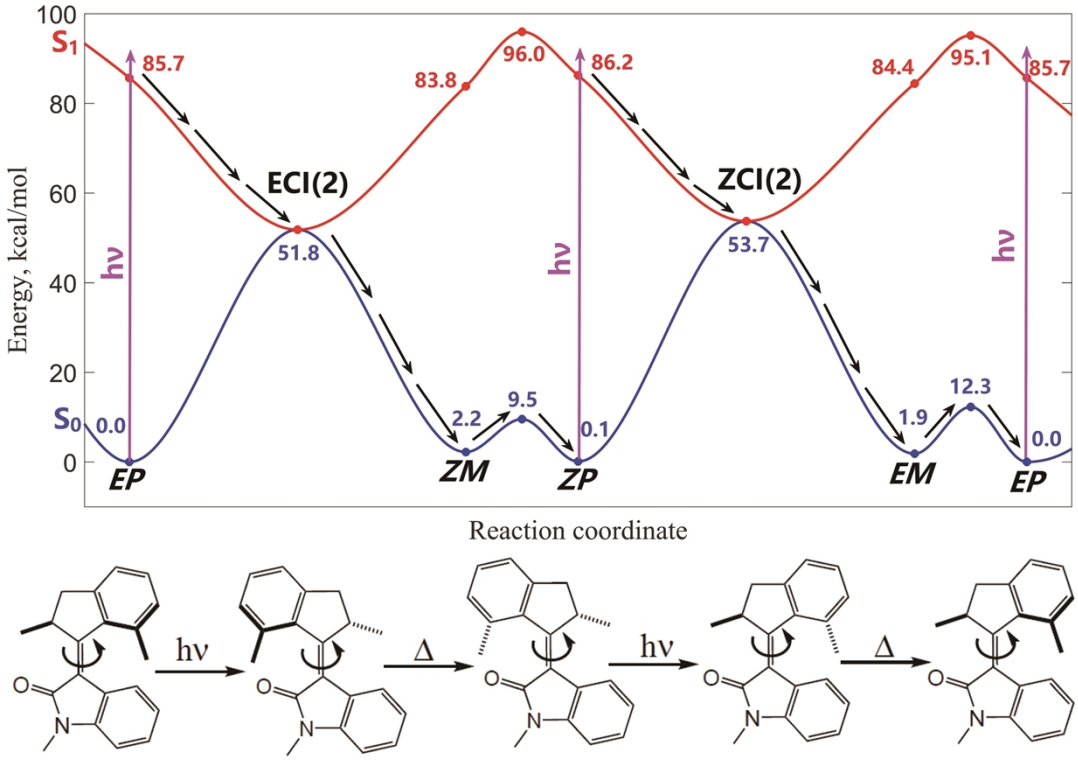


Figure S16. Schematic representation of the potential energy profile of the S_0 (blue) and S_1(red) states of DDIYM along the rotational reaction coordinate, as obtained from OM2/MRCI method. The S_0 energy profile is constructed from the energies of the local minima geometries, CIs and transition states optimized in the ground electronic state. The S_1 energy profile is obtained from the corresponding first excitation energies for local minima geometries, CIs and transition states optimized in the S_0 state. The vertical arrows (magenta) show the vertical excitation at the Franck-Condon region.

10. Cartesian coordinates for several structures of DDIYM and DDPYM optimized with the OM2/MRCI method

Unit of the Cartesian coordinate below is angstrom.

(1) Cartesian coordinates for DDIYM

① Four ground state local minima geometries

EM-DDIYM				*EP*-DDIYM			
C	-0.56330457	0.56396897	0.12080637	C	1.69364295	0.54719034	0.00316350
C	0.77096730	0.84610469	0.07229342	C	0.47567585	1.15160988	0.00668170
C	-1.25395342	-0.68282487	-0.20760825	C	2.10863966	-0.83413172	-0.24431070
C	1.39456347	2.21225895	-0.14868952	C	0.29055368	2.65147163	-0.14612759
C	1.86788053	-0.12788583	0.12749659	C	-0.86343272	0.54995239	-0.02054081
C	-1.63566333	1.53141816	0.49746947	C	2.96019408	1.31715989	0.20987143
C	-0.83607204	-1.83102302	-0.86623853	C	1.43996482	-1.93693765	-0.74285623
C	-2.65292254	-0.46378987	0.01235533	C	3.53588177	-0.87371852	-0.10533901
C	0.55379222	3.11481298	-1.03176569	C	0.14284829	3.29253265	1.22339715
C	2.74604753	1.88566913	-0.82951602	C	-1.01511762	2.75511062	-0.96594102
H	1.56389385	2.70196891	0.84811549	H	1.15649116	3.11147482	-0.68281190
C	1.95620640	-1.36942659	0.76306475	C	-1.36936839	-0.61620389	0.55249329
C	3.02194365	0.46712892	-0.42786363	C	-1.73350507	1.47610655	-0.64116805
N	-2.86303174	0.83334485	0.51371760	N	4.02884197	0.40004111	0.23168743
O	-1.54186886	2.70621768	0.88177482	O	3.10681208	2.53167782	0.40670480
C	-1.79575620	-2.79749792	-1.20529463	C	2.17226037	-3.10759586	-1.00498020
H	0.21383819	-1.97158092	-1.14021576	H	0.36599018	-1.90280170	-0.94391729
C	-3.60616208	-1.41897640	-0.34014599	C	4.26327751	-2.03538995	-0.37839852
H	0.25012034	2.58175501	-1.94631109	H	-0.67258630	2.81742647	1.79045361
H	1.15180218	3.99604797	-1.31782271	H	-0.08174109	4.36473896	1.10784410
H	-0.33281918	3.44987241	-0.49275618	H	1.08349545	3.18595544	1.77558260
H	3.55629535	2.56007798	-0.48429545	H	-1.62260597	3.63551403	-0.67282753
H	2.65749478	1.95846824	-1.93420985	H	-0.79583901	2.80780488	-2.05345721
C	0.85884179	-1.94425909	1.59770821	C	-0.57467612	-1.50094163	1.45967962
C	3.18177937	-2.06135241	0.67131493	C	-2.73320842	-0.90631647	0.34567962
C	4.22625734	-0.22552370	-0.51541843	C	-3.07892640	1.17818708	-0.84065788
C	-4.13351112	1.43445078	0.77989926	C	5.40891084	0.76467199	0.33792424
C	-3.14775795	-2.60220540	-0.92238721	C	3.55309439	-3.15360018	-0.80309149
H	-1.47463654	-3.72212875	-1.69383854	H	1.64940661	-3.99511508	-1.37115459
H	-4.66905497	-1.24244442	-0.16443975	H	5.34859274	-2.05505813	-0.25964553
H	0.25566710	-2.64526789	1.00690767	H	0.44369921	-1.12076016	1.58829490
H	1.29547311	-2.47794167	2.45654410	H	-1.07399212	-1.52178079	2.44043262
H	0.20733674	-1.14303881	1.96842652	H	-0.53127423	-2.52297124	1.05812053
C	4.27957137	-1.51199036	0.01713209	C	-3.55837247	-0.04010560	-0.36677668
H	3.27108210	-3.04561974	1.13798891	H	-3.15158570	-1.82486479	0.76431687
H	5.10711250	0.23340150	-0.97005181	H	-3.74168358	1.88746437	-1.34247926
H	-4.68302125	0.86694773	1.56994487	H	5.49273370	1.84756703	0.54754189
H	-4.77393242	1.45039913	-0.13872885	H	5.90478896	0.19983939	1.16431927
H	-3.98648383	2.47455006	1.12666396	H	5.95925329	0.54055945	-0.61067177
H	-3.87043204	-3.38717996	-1.17717202	H	4.09323072	-4.08900510	-0.99806390
H	5.21593645	-2.08157863	-0.03879080	H	-4.61261609	-0.30328546	-0.51948563

ZM-DDIYM				*ZP*-DDIYM			
C	-0.50193320	-0.01613759	-0.06440327	C	0.57509079	-0.02546923	-0.03813928
C	0.70323174	0.62897322	0.01576771	C	-0.63115932	0.60750892	-0.04092225
C	-1.83001728	0.53901053	0.20925890	C	1.91424118	0.57259860	0.02597642
C	0.84592998	2.13219185	-0.14602933	C	-0.81596786	2.09033284	-0.31224774
C	2.03826037	0.04931017	0.16493280	C	-1.97716276	0.02139188	0.01302078

C	-0.74015958	-1.39884001	-0.55920651	C	0.80294227	-1.48556686	-0.25150364
C	-2.26004117	1.72282707	0.79616034	C	2.37371409	1.86282811	0.22772409
C	-2.78610674	-0.49575377	-0.04826972	C	2.86319441	-0.49444191	-0.08813779
C	0.04394275	2.60368817	-1.35178845	C	-0.96151723	2.84085400	1.00206044
C	2.34979375	2.37639682	-0.38998618	C	-2.13364860	2.13738058	-1.11540058
H	0.50463814	2.66024309	0.78651252	H	0.03420837	2.50759946	-0.91432688
C	2.46231342	-1.20197953	0.64310812	C	-2.47587320	-1.10996485	0.66815126
C	2.99496007	1.05438840	-0.09128483	C	-2.85696046	0.90741701	-0.64229256
N	-2.13313359	-1.63818522	-0.53826105	N	2.19505255	-1.71687557	-0.25693464
O	0.04589058	-2.20962685	-1.07199604	O	-0.00405985	-2.38844585	-0.51671965
C	-3.62604893	1.89318294	1.05979861	C	3.75750773	2.09037763	0.28524781
H	-1.55080721	2.51461136	1.06230680	H	1.68520938	2.70573314	0.34157907
C	-4.14358167	-0.33093295	0.22211758	C	4.24004714	-0.27123654	-0.02020875
H	-1.02573846	2.40828525	-1.21873336	H	-0.05260057	2.72659084	1.61093142
H	0.38315615	2.07755901	-2.25617797	H	-1.81565563	2.44684232	1.56994791
H	0.19485509	3.68676268	-1.48996984	H	-1.12717461	3.91178597	0.80614538
H	2.75727523	3.16010591	0.28080973	H	-1.93432224	2.06767793	-2.20387231
H	2.54312221	2.66356049	-1.44329483	H	-2.71953686	3.05475580	-0.90544778
C	1.53928332	-2.26469424	1.12801971	C	-1.64624980	-1.99756063	1.53034835
C	3.85181824	-1.44053244	0.69806294	C	-3.85657395	-1.37550206	0.53533856
C	4.36153633	0.81053393	-0.02771702	C	-4.21415708	0.63188405	-0.77084632
C	-2.76343100	-2.81988807	-1.03972841	C	2.80458822	-2.97816678	-0.55012724
C	-4.54923146	0.89217137	0.76156618	C	4.66847966	1.04039423	0.16127452
H	-3.97376794	2.83444649	1.49586791	H	4.12556800	3.11043689	0.42864464
H	-4.85805048	-1.13087344	0.01975854	H	4.94513823	-1.10019409	-0.10394410
H	1.20439474	-2.85903464	0.27355894	H	-0.83921242	-1.41815001	2.00402213
H	2.05792018	-2.91152307	1.85587278	H	-2.27087826	-2.44797158	2.31989654
H	0.66554801	-1.80982773	1.61957595	H	-1.20829154	-2.78106519	0.90615889
C	4.77878608	-0.47178954	0.34623871	C	-4.69524058	-0.54549034	-0.19101502
H	4.20182436	-2.42270605	1.03224979	H	-4.26888378	-2.26447882	1.02195463
H	5.08694202	1.59619518	-0.24838652	H	-4.88185621	1.31531627	-1.29883988
H	-3.33078168	-3.34548482	-0.23036150	H	3.45227170	-2.90827207	-1.45868933
H	-3.48372362	-2.57400867	-1.85837033	H	3.44331602	-3.31905419	0.30254543
H	-1.99525889	-3.50895788	-1.43861347	H	2.02096252	-3.73747543	-0.73204170
H	-5.61443251	1.06295563	0.95926688	H	5.74378219	1.25144173	0.21475045
H	5.85165126	-0.69592244	0.39769318	H	-5.75961138	-0.79578612	-0.28767063

② Two transition state geometries at ground state

EM-EP-TS-DDIYM				*ZM-ZP-TS*-DDIYM			
C	-0.56474829	-0.46989403	0.29227521	C	-0.57132953	0.15135079	0.13131335
C	0.79618567	-0.62429139	0.29822943	C	0.65959493	-0.44597640	0.09706486
C	-1.51863190	0.64273300	0.35806348	C	-1.88125753	-0.54157999	0.02066605
C	1.36778073	-2.01591319	0.53191841	C	0.71298922	-1.97169044	0.11912617
C	1.92146010	0.26380695	-0.06328513	C	2.06432531	0.01912421	-0.04151534
C	-1.40723503	-1.63826651	-0.13735656	C	-0.94889240	1.60102740	0.10531495
C	-1.57505718	1.80432986	1.12049293	C	-2.32253310	-1.84483285	0.18312178
C	-2.71974410	0.21802235	-0.29783041	C	-2.86156949	0.44258829	-0.32801004
C	1.58794248	-2.12388016	2.03921961	C	0.66337442	-2.42635906	1.57146849
C	2.70800078	-2.03231415	-0.20979756	C	2.04500434	-2.36601993	-0.52173542
H	0.70510372	-2.83258864	0.18545025	H	-0.12473415	-2.41550395	-0.48045355
C	2.09682070	1.64936083	-0.22026576	C	2.74959412	1.23554887	0.13094502
C	3.01459699	-0.57897134	-0.40239196	C	2.84577352	-1.10814589	-0.40168539
N	-2.59946469	-1.12393976	-0.70295168	N	-2.28351517	1.71981186	-0.34455379
O	-1.13380544	-2.84342603	-0.21844615	O	-0.33569045	2.62005660	0.43530643
C	-2.69873675	2.63001935	1.02546392	C	-3.67618802	-2.15979066	-0.03665430
H	-0.76216348	2.06377626	1.80742538	H	-1.66784772	-2.65731009	0.51177410
C	-3.84342984	1.03140669	-0.39566111	C	-4.20734087	0.13991679	-0.54614965
H	2.24169573	-1.31418059	2.39865598	H	1.54503705	-2.05086312	2.11008949
H	2.05976362	-3.09149411	2.27147215	H	0.65762019	-3.52710384	1.62226284
H	0.62420220	-2.06567484	2.56406919	H	-0.23762242	-2.04015897	2.06865502
H	3.50613474	-2.54128538	0.36656214	H	2.53376493	-3.20974290	0.00631298
H	2.60574597	-2.52363779	-1.20059776	H	1.91870305	-2.63108515	-1.59215110
C	1.06431932	2.67067984	0.11415681	C	2.15345205	2.54097960	0.53016678
C	3.33007001	2.13328669	-0.69278681	C	4.14569415	1.26442473	-0.08392757

C	4.22670696	-0.09543744	-0.88486489	C	4.22167783	-1.07227758	-0.61078460
C	-3.70661574	-1.96144308	-1.06033079	C	-3.02119137	2.94383176	-0.23318749
C	-3.79519392	2.27584514	0.23991288	C	-4.59784208	-1.18651062	-0.40792565
H	-2.72642826	3.56518470	1.59427090	H	-4.00607080	-3.19249589	0.10416621
H	-4.72896519	0.70490949	-0.94359582	H	-4.91644478	0.92569906	-0.81383072
H	0.90573605	2.66031139	1.20551019	H	1.49109216	2.41117905	1.38961956
H	1.40816604	3.67916073	-0.16984507	H	2.94914278	3.26104024	0.79915046
H	0.13284625	2.45201775	-0.41402399	H	1.58508353	2.94999688	-0.31196126
C	4.37830161	1.28137562	-1.03450566	C	4.87711144	0.14496712	-0.45013728
H	3.46509002	3.21572914	-0.81470621	H	4.67095467	2.21901164	0.04505326
H	5.03615330	-0.78259816	-1.14124666	H	4.76753873	-1.97933605	-0.88114789
H	-3.41328048	-3.02353311	-0.96394854	H	-2.32679370	3.77643796	-0.01530528
H	-4.59120421	-1.77045667	-0.40453507	H	-3.55812000	3.16448734	-1.18588217
H	-4.01441595	-1.77301737	-2.11661412	H	-3.77957704	2.88685405	0.58637753
H	-4.64711475	2.95886545	0.15186580	H	-5.64432343	-1.46379695	-0.58262321
H	5.31607945	1.69357749	-1.42451572	H	5.96028272	0.21500429	-0.60385214

③ Four different S_1 /S_0 CIs

*E*CI(1)-DDIYM				*E*CI(2)-DDIYM			
C	-0.40199978	0.85450789	0.12558310	C	0.53559336	0.45019094	-0.01544494
C	-1.56680035	0.45550900	-0.48943964	C	-0.36187710	1.24816921	-0.72795081
C	0.59513357	1.73547499	-0.52764565	C	1.58874290	-0.26269164	-0.78814010
C	-2.91930889	0.82571977	0.09382797	C	-0.07565066	2.47650706	-1.59263855
C	-1.80851043	-0.39255537	-1.64847086	C	-1.78615960	1.03177325	-0.72890905
C	0.38252308	-0.18804315	0.75536950	C	1.30064339	1.15292030	1.03005492
C	0.45450442	2.81207718	-1.38279051	C	1.52429483	-0.99492110	-1.95832848
C	1.87623283	1.39289678	0.01567610	C	2.78608371	-0.25356619	-0.00220703
C	-2.97314495	0.02242726	1.39089161	C	0.64440623	3.51500750	-0.75160316
C	-3.98168022	0.37971243	-0.91738878	C	-1.43443197	2.98022473	-2.10863258
H	-2.95044620	1.90973158	0.31551842	H	0.58038523	2.14083071	-2.43066192
C	-0.89616758	-1.11340094	-2.44901443	C	-2.51743243	0.03589996	-0.04222377
C	-3.20614901	-0.45619217	-1.89791567	C	-2.43074615	2.02674889	-1.51273486
N	1.72064682	0.28965776	0.86368163	N	2.57404731	0.52496528	1.14180785
O	-0.04491477	-1.22388239	1.32516754	O	0.87283698	1.98440242	1.85760260
C	1.61106409	3.53497255	-1.71141629	C	2.67479233	-1.68753982	-2.36468657
H	-0.51456886	3.11329560	-1.78609693	H	0.60999117	-1.04987366	-2.55428308
C	3.00541145	2.12927637	-0.30819225	C	3.91370767	-0.95678732	-0.40950528
H	-2.09661021	0.25154937	1.99361481	H	0.05023520	3.77768327	0.13043451
H	-2.99113188	-1.05597668	1.18349898	H	0.81766500	4.41542446	-1.36125475
H	-3.88900338	0.30235467	1.93191327	H	1.60750234	3.11843629	-0.41500120
H	-4.42815351	1.24458795	-1.44164716	H	-1.49192954	2.94829323	-3.21287894
H	-4.77997454	-0.22209675	-0.44970160	H	-1.64702279	4.00617186	-1.75722638
C	0.56555775	-1.10763056	-2.17658601	C	-1.82132810	-0.98385012	0.78707100
C	-1.43072382	-1.86703558	-3.50790467	C	-3.91605344	0.07395722	-0.18618054
C	-3.71488085	-1.21110610	-2.94527059	C	-3.81052301	2.03695047	-1.64501091
C	2.77734986	-0.54319192	1.34479482	C	3.61288958	1.06611814	1.96436711
C	2.85639951	3.20573376	-1.19412522	C	3.84166092	-1.66848012	-1.61104293
H	1.51942761	4.39160182	-2.39467796	H	2.64343739	-2.26472140	-3.29823847
H	3.97835525	1.87877461	0.12443588	H	4.82068374	-0.95656109	0.20018823
H	0.73597811	-1.61069509	-1.22166166	H	-2.23675772	-0.95706907	1.80434026
H	1.10855670	-1.63859792	-2.97291256	H	-2.00890438	-1.97764619	0.35344762
H	0.92622511	-0.07861724	-2.11373708	H	-0.75438425	-0.75156092	0.78955655
C	-2.80306057	-1.91076089	-3.74427254	C	-4.53698952	1.04537036	-0.96883548
H	-0.75459278	-2.43222555	-4.15289181	H	-4.52319594	-0.67173136	0.33050147
H	-4.78501231	-1.26234321	-3.14025769	H	-4.31928849	2.79031785	-2.24513501
H	3.40833629	-0.93924890	0.50412946	H	4.36301047	1.63998418	1.35925640
H	2.35185047	-1.39850800	1.90228681	H	3.17240103	1.74444125	2.71867549
H	3.44770664	0.03323718	2.02722147	H	4.15644523	0.24695629	2.49163209
H	3.73526677	3.79550353	-1.47027246	H	4.71983795	-2.22525676	-1.95543381
H	-3.18350635	-2.51488093	-4.57867012	H	-5.63221553	1.04205506	-1.05812582

*Z*CI(1)-DDIYM				*Z*CI(2)-DDIYM			
C	0.65378581	0.21134313	-0.14378377	C	0.58121907	-0.38769206	0.53648127

C	-0.08203230	1.10997533	-0.91993060	C	-0.57934883	-0.68474438	1.21084760
C	1.85923320	0.65020345	0.60170571	C	1.79547655	0.20265570	1.14311563
C	0.37450788	1.88078693	-2.15663823	C	-1.88923993	-0.01179721	0.82393203
C	-1.48930819	1.35893869	-0.74046512	C	-0.87757523	-1.66775841	2.24202143
C	1.13669121	-0.94126279	-0.92489290	C	1.07294916	-1.45820710	-0.31038709
C	2.07882229	1.73817522	1.42808040	C	1.96270810	1.15500194	2.13147370
C	2.82076715	-0.40829212	0.53283765	C	2.91689201	-0.28178201	0.39403365
C	1.58297127	2.73563424	-1.83509694	C	-1.70419406	1.49102799	0.85493672
C	-0.83437023	2.70130822	-2.63745989	C	-2.96769218	-0.53786769	1.77753670
H	0.64452796	1.09270377	-2.90004378	H	-2.06057557	-0.35538479	-0.22150595
C	-2.36005664	0.79998690	0.22143663	C	-0.03148848	-2.61399833	2.86037392
C	-1.95322927	2.26164452	-1.73588616	C	-2.26223811	-1.61274438	2.55714033
N	2.33870039	-1.40452281	-0.32743953	N	2.45603293	-1.21033991	-0.54749240
O	0.53454104	-1.54309553	-1.83971013	O	0.38451774	-2.30521545	-0.93332499
C	3.28217562	1.78736786	2.14480215	C	3.26584549	1.60867248	2.37978065
H	1.34207899	2.53877744	1.52854811	H	1.12086677	1.56027313	2.69634026
C	4.00135871	-0.35661301	1.26269826	C	4.19591359	0.18966317	0.64433968
H	1.31124582	3.53311729	-1.12725875	H	-1.61448256	1.84817778	1.89385007
H	1.96058487	3.19610710	-2.75949385	H	-2.57434005	1.97596554	0.38979207
H	2.36884708	2.11886931	-1.39005720	H	-0.79801432	1.73832858	0.30281582
H	-1.08631927	2.48227721	-3.69074132	H	-3.83100619	-0.96503904	1.23775455
H	-0.66318144	3.78754574	-2.51581901	H	-3.31579887	0.25111396	2.46832791
C	-1.85328804	-0.15677701	1.24182822	C	1.40901618	-2.72996791	2.51006119
C	-3.70963640	1.18781131	0.14713230	C	-0.61505018	-3.47422807	3.80561453
C	-3.28953142	2.62716927	-1.78807416	C	-2.82158798	-2.47707438	3.48755010
C	3.14353780	-2.41635695	-0.94263591	C	3.27024534	-2.15087874	-1.25106743
C	4.22336229	0.76849342	2.06485249	C	4.35867149	1.14045959	1.66229523
H	3.47780687	2.65239088	2.79309022	H	3.41959194	2.36300453	3.16531206
H	4.72490521	-1.17395320	1.21377264	H	5.04727105	-0.16524193	0.05611424
H	-2.00129914	0.28038787	2.24059392	H	1.92263135	-3.40801079	3.20794258
H	-2.43340084	-1.08761275	1.17219709	H	1.47591604	-3.13225770	1.49593601
H	-0.79534426	-0.34086717	1.04509545	H	1.88343578	-1.74717473	2.54065624
C	-4.15375022	2.07714600	-0.83004154	C	-1.97371896	-3.40320757	4.10598238
H	-4.42137767	0.77551501	0.86489860	H	0.00917334	-4.21761164	4.30576192
H	-3.66193523	3.31510052	-2.54630657	H	-3.88261632	-2.44052248	3.72973566
H	3.52451734	-3.12911518	-0.17343037	H	3.89420002	-2.76663642	-0.54867179
H	2.53721807	-2.97637355	-1.67858561	H	2.62791628	-2.82936684	-1.84289022
H	4.02936434	-1.97455644	-1.46892176	H	3.96677222	-1.61995683	-1.94379299
H	5.15031697	0.83733854	2.64346545	H	5.36015219	1.51965689	1.88379600
H	-5.21598373	2.35716771	-0.85630756	H	-2.39519040	-4.09660879	4.84598905

(2) Cartesian coordinates for DDPYM

① Four ground state local minima geometries

EM-DDPYM				*EP*-DDPYM			
C	0.38611437	0.86953741	-0.63940464	C	0.43732512	0.51577790	-0.12233461
C	-0.92202969	0.85470120	-0.25869627	C	-0.91456737	0.64836992	-0.14830423
C	1.18738722	1.92918097	-1.24237191	C	1.31013220	-0.65288922	-0.17773801
C	-1.75835302	-0.40482062	-0.02359872	C	-1.64138564	1.97709175	-0.37385783
C	-1.80201205	1.97157994	-0.03239994	C	-1.94953523	-0.35166381	-0.08974446
C	1.32968333	-0.26941595	-0.42198879	C	1.35440085	1.69134380	0.01675852
C	0.84068197	3.10074953	-1.91064827	C	1.09239697	-1.97615301	-0.54722157
C	2.54405839	1.46340048	-1.30185075	C	2.65538339	-0.19250600	0.02001495
C	-1.55125932	-1.39818321	-1.15317472	C	-1.83167500	2.67467628	0.96034282
C	-3.24282814	0.05470384	0.02760461	C	-3.01074600	1.59508250	-1.00036537
H	-1.45380021	-0.86210646	0.95381446	H	-1.04241186	2.62723385	-1.06161429
N	-1.75704060	3.33919476	0.20957244	N	-2.18229937	-1.63634676	0.38061971
C	-3.14264292	1.53039012	0.14396590	C	-3.17416647	0.17787532	-0.58439688
N	2.62653185	0.17974153	-0.74955867	N	2.66322376	1.19912371	0.18525459
O	1.12440018	-1.37999178	0.08507195	O	1.07938185	2.89661370	0.06881580
C	1.85497353	3.85147753	-2.51572188	C	2.18847645	-2.84535758	-0.60217223
H	-0.20423224	3.41237842	-1.98569774	H	0.09498425	-2.32245079	-0.82728711
C	3.55019562	2.21260828	-1.91069237	C	3.74415395	-1.06152791	-0.03751622

H	-1.70790530	-0.91137427	-2.12859096	H	-2.36763715	2.02043904	1.66546442
H	-2.27622523	-2.22203051	-1.04728256	H	-2.41782751	3.59647258	0.81703424
H	-0.54315404	-1.81552314	-1.11093952	H	-0.85477181	2.94274368	1.37686942
H	-3.77930271	-0.37936569	0.89851793	H	-2.97394304	1.67636046	-2.11016704
H	-3.77989151	-0.22758755	-0.90509040	H	-3.83670837	2.23027877	-0.61705337
C	-0.59826902	4.14310443	0.49990263	C	-1.35014925	-2.39894467	1.27399140
C	-3.05360938	3.75116196	0.48241664	C	-3.52161454	-1.92098280	0.14776879
C	-3.93540251	2.65593700	0.42474504	C	-4.15285009	-0.82656841	-0.47509943
C	3.81170845	-0.62121300	-0.65000527	C	3.82637199	2.02141152	0.35378703
C	3.18412176	3.43186294	-2.49044048	C	3.48108139	-2.40504015	-0.32369072
H	1.59692050	4.78633412	-3.02534075	H	2.02553201	-3.89394499	-0.87499492
H	4.58015366	1.85307193	-1.94127254	H	4.76155656	-0.70125313	0.12392590
H	-0.66822271	4.54831021	1.53123919	H	-1.86318287	-2.53121106	2.24996888
H	-0.52633532	5.00175095	-0.20718066	H	-1.14007646	-3.40911661	0.85225192
H	0.32194995	3.54113918	0.42604763	H	-0.39423276	-1.87890070	1.45397180
H	-3.31365470	4.78649170	0.68106245	H	-3.97357513	-2.87500262	0.40174543
H	-5.00044572	2.69093752	0.59044722	H	-5.18521416	-0.78062358	-0.77588178
H	4.57675062	-0.11882376	-0.01130937	H	3.52289273	3.08372247	0.40259402
H	4.26018992	-0.79810296	-1.65769416	H	4.36377937	1.75839171	1.29590617
H	3.55839421	-1.59837881	-0.19850408	H	4.53393123	1.89113934	-0.50039123
H	3.95671666	4.05464742	-2.95636435	H	4.31378852	-3.11736607	-0.35424606

ZM-DDPYM				*ZP*-DDPYM			
C	-0.37082672	0.05846486	0.08414959	C	0.49728230	0.84979845	0.02786747
C	0.85963030	-0.53362348	0.01171923	C	-0.86383350	0.89822388	-0.04056033
C	-1.68374558	-0.58135862	-0.06804085	C	1.46328795	0.74009208	-1.07532974
C	1.04505416	-2.04695547	0.17858907	C	-1.64592390	0.67338970	-1.34064620
C	2.17296556	0.01775139	-0.15684680	C	-1.87013649	1.05578367	0.97450673
C	-0.67406534	1.48086018	0.39874088	C	1.32828722	0.80951408	1.26632050
C	-2.09569388	-1.85956053	-0.43662734	C	1.35323497	0.71312128	-2.46232380
C	-2.68402811	0.43532531	0.09203221	C	2.77636885	0.68941921	-0.49839067
C	0.48120498	-2.44824032	1.53311608	C	-1.79173383	2.00988183	-2.04929872
C	2.56098266	-2.35507877	0.12155063	C	-3.03837516	0.13824580	-0.92426592
H	0.51667359	-2.58809585	-0.65552340	H	-1.11948648	-0.07656838	-1.99330719
N	2.83500776	1.20435955	-0.45545156	N	-2.07012557	1.53681959	2.26159673
C	3.15913610	-1.01936950	-0.10090230	C	-3.13932733	0.62031621	0.47331950
N	-2.06887020	1.65495699	0.39398543	N	2.68085061	0.72845808	0.89699514
O	0.07422966	2.41401041	0.73970735	O	0.99860898	0.76910305	2.46330124
C	-3.46092371	-2.11500078	-0.60453125	C	2.51504671	0.63112970	-3.23842785
H	-1.37355033	-2.66296993	-0.61270342	H	0.38124214	0.75037039	-2.96169370
C	-4.04497971	0.18110707	-0.07463104	C	3.93529221	0.61452573	-1.27097625
H	1.02868223	-1.92987533	2.33363324	H	-2.36864571	2.70283265	-1.42126113
H	0.59072994	-3.53600269	1.67287743	H	-2.32004930	1.87379151	-3.00632843
H	-0.58070444	-2.18587806	1.61366424	H	-0.80725362	2.45723139	-2.24803322
H	2.81231808	-3.04326152	-0.71581156	H	-3.06107565	-0.97431297	-0.95860127
H	2.92320312	-2.80194920	1.07298137	H	-3.85316885	0.53792430	-1.56448238
C	2.28045833	2.49706378	-0.77750080	C	-1.14846599	2.26372865	3.10210978
C	4.17927155	0.92270126	-0.55317731	C	-3.40786211	1.38857635	2.56067877
C	4.41726695	-0.44939108	-0.33079157	C	-4.09592438	0.80164967	1.47520503
C	-2.73525442	2.88363542	0.71756133	C	3.76968784	0.61241998	1.82486366
C	-4.41923167	-1.12117484	-0.41367124	C	3.78118175	0.58299426	-2.65801703
H	-3.78288900	-3.12325004	-0.88745821	H	2.42421989	0.60520512	-4.33017604
H	-4.78412440	0.97377001	0.05403590	H	4.92062960	0.58113822	-0.80284529
H	3.07723203	3.27054188	-0.72728424	H	-1.56662443	2.35280151	4.12772355
H	1.88238873	2.48211300	-1.81848673	H	-0.18031421	1.74656949	3.14394642
H	1.47081901	2.75467238	-0.08025547	H	-1.00783331	3.29238556	2.69767492
H	4.93061725	1.68390552	-0.74847620	H	-3.83404534	1.67606849	3.51850194
H	5.37684412	-0.93854708	-0.33463832	H	-5.14521117	0.55926321	1.45040229
H	-1.98401285	3.65372434	0.97377173	H	3.37463766	0.60037402	2.85773423
H	-3.34035540	3.24664441	-0.14852318	H	4.33984776	-0.33007160	1.64957349
H	-3.41779496	2.74610044	1.58853402	H	4.47257944	1.47329190	1.71913782
H	-5.48168827	-1.36098901	-0.53409523	H	4.66944455	0.51878676	-3.29669404

② Two transition state geometries at ground state

EM-EP-TS-DDPYM				*ZM-ZP-TS*-DDPYM			
C	-0.44164071	-0.39200982	0.09434349	C	-0.38322781	0.08433324	0.03889728
C	0.91824653	-0.52653310	0.05554172	C	0.83794095	-0.52328392	-0.00201357
C	-1.41655599	0.70400383	0.06389390	C	-1.71038493	-0.54616958	-0.08879357
C	1.52532322	-1.94366702	0.01785902	C	0.96357376	-2.05250939	0.06651982
C	2.05824110	0.37186743	-0.03516473	C	2.18795128	-0.02417395	-0.09473510
C	-1.29142814	-1.63555743	-0.00073071	C	-0.67662522	1.54235597	0.18190733
C	-1.34622833	2.08204963	0.22227166	C	-2.16353139	-1.85647536	-0.21579027
C	-2.72194246	0.13329149	-0.13032150	C	-2.68748939	0.50429572	-0.13575149
C	1.60376426	-2.41325949	1.46321016	C	0.61367878	-2.47314560	1.48631818
C	2.93802903	-1.82226407	-0.58845274	C	2.42429238	-2.43456716	-0.25369984
H	0.90877100	-2.64209439	-0.58833067	H	0.27733554	-2.53074757	-0.68619275
N	2.46218435	1.71002586	0.02807451	N	2.94651086	1.14180310	-0.13678744
C	3.20054476	-0.37239826	-0.46473523	C	3.10256557	-1.12038145	-0.22172491
N	-2.63068017	-1.25827655	-0.19002134	N	-2.05881006	1.74376459	0.01939483
O	-0.97719600	-2.83265985	0.04024496	O	0.06877680	2.49613246	0.44046289
C	-2.51246691	2.85589519	0.18323642	C	-3.53022937	-2.09976281	-0.39810105
H	-0.39415191	2.57293512	0.39815276	H	-1.48146536	-2.71081775	-0.18401014
C	-3.88572532	0.89894900	-0.19198164	C	-4.04905926	0.26561378	-0.31919001
H	2.19309669	-1.71094002	2.07448626	H	1.35718553	-2.06782248	2.18775009
H	2.08279476	-3.40548710	1.49757810	H	0.61581610	-3.57276889	1.56274093
H	0.59378422	-2.50119863	1.88251943	H	-0.37643591	-2.09850126	1.77700925
H	2.94538685	-2.13179946	-1.65760808	H	2.51500741	-2.89141893	-1.26491273
H	3.69095647	-2.42214146	-0.03494791	H	2.84840927	-3.13621939	0.49589327
C	1.81113051	2.87114771	0.56655267	C	2.54415623	2.52996694	-0.10195462
C	3.79765452	1.77815043	-0.33675593	C	4.27163893	0.78351811	-0.26734613
C	4.28087785	0.50187229	-0.66699055	C	4.40460733	-0.61628830	-0.32953187
C	-3.70592693	-2.17610552	-0.43153357	C	-2.71706217	3.00760282	0.18607116
C	-3.76029215	2.28182364	-0.03827221	C	-4.45834225	-1.06299826	-0.44869982
H	-2.43605485	3.93996569	0.32275720	H	-3.87533648	-3.13480255	-0.49800075
H	-4.85723577	0.42708701	-0.34953603	H	-4.76165853	1.09113277	-0.36108020
H	1.22909796	2.60508049	1.47060291	H	3.44548403	3.18295957	-0.13289043
H	2.56494576	3.62794829	0.86718862	H	1.91160389	2.76386482	-0.98188655
H	1.15295292	3.34582659	-0.20144576	H	1.96696690	2.74815580	0.81029448
H	4.36152449	2.70784634	-0.34556355	H	5.08059689	1.51018247	-0.29570875
H	5.27918135	0.25767192	-0.98356138	H	5.32386866	-1.16757004	-0.42675339
H	-3.33188586	-3.21310973	-0.33747405	H	-1.96037693	3.80831212	0.28269820
H	-4.53044348	-2.02318980	0.30548852	H	-3.36844682	3.23287959	-0.69226762
H	-4.12389270	-2.03641216	-1.45841250	H	-3.35398254	3.00572437	1.10279419
H	-4.65318928	2.91473939	-0.08894144	H	-5.52188014	-1.28939993	-0.58430073

③ Two different S_1 /S_0 CIs

*E*CI-DDPYM				*Z*CI-DDPYM			
C	0.58966701	-0.32482539	0.46980547	C	0.95735588	1.36266930	0.83544622
C	-0.77335904	-0.59532698	0.64626241	C	-0.25579804	1.77406612	1.40269422
C	1.51886259	-0.93162791	-0.45252071	C	1.64659643	1.88534918	-0.31915227
C	-1.93999648	0.01717748	-0.12362822	C	-1.65593204	1.30950997	1.01158562
C	-1.32564979	-1.48198443	1.58774415	C	-0.40834656	2.67466926	2.47167925
C	1.27846478	0.78685269	1.11058346	C	1.66764494	0.16280969	1.25712122
C	1.41518593	-2.00085394	-1.33394235	C	1.42142263	2.98506066	-1.13851179
C	2.76646842	-0.22132413	-0.32195720	C	2.78847367	1.03565098	-0.54873762
C	-1.91481889	1.51948149	0.09358535	C	-1.88510273	1.57507399	-0.46402056
C	-3.24385806	-0.62719481	0.42380130	C	-2.66531163	2.07937989	1.90742739
H	-1.80850493	-0.21918589	-1.21481784	H	-1.70622836	0.20723048	1.21730164
N	-0.90918028	-2.35300617	2.58911832	N	0.37515847	3.45332487	3.31694647
C	-2.76089115	-1.55093354	1.48515432	C	-1.79436085	2.89145754	2.79912207
N	2.61324366	0.78679675	0.63299260	N	2.79915350	0.02450158	0.41511864
O	0.86258328	1.58689700	1.97121815	O	1.42166536	-0.60897392	2.20412185
C	2.54494059	-2.34849377	-2.08110311	C	2.32287945	3.22436197	-2.18017035
H	0.47803114	-2.55344137	-1.44277921	H	0.56279742	3.64218651	-0.97529065

C	3.88251278	-0.58148457	-1.07057556	C	3.67814792	1.28899982	-1.58816577
H	-1.99328010	1.75214151	1.16280389	H	-1.85541941	2.65660945	-0.66922522
H	-2.75395822	1.98800132	-0.44533856	H	-2.86878165	1.18336044	-0.76599837
H	-0.97113684	1.93253896	-0.28134794	H	-1.10502599	1.08161140	-1.05501429
H	-3.78245474	-1.18943832	-0.36748503	H	-3.29222761	1.38534690	2.50353305
H	-3.92287476	0.13429725	0.85780231	H	-3.32242973	2.73991122	1.30425894
C	0.45801500	-2.53490528	3.01546441	C	1.81834595	3.47887791	3.32247563
C	-2.03201125	-2.94662803	3.09987508	C	-0.47750161	4.12996104	4.14758438
C	-3.20040153	-2.47357207	2.43049511	C	-1.83479520	3.80635014	3.84769811
C	3.57451835	1.78601674	0.98101678	C	3.69457229	-1.08835058	0.47581683
C	3.74898648	-1.65533526	-1.95281890	C	3.42411068	2.39605677	-2.39987114
H	2.48188530	-3.18652801	-2.78667788	H	2.15945251	4.08460145	-2.84149181
H	4.82590620	-0.04044302	-0.96751206	H	4.54206927	0.64227959	-1.75761315
H	0.58442055	-2.17991594	4.06051756	H	2.20573090	3.06739723	4.27882119
H	0.73919424	-3.60955942	2.96628158	H	2.19978561	2.86529342	2.49005732
H	1.12737473	-1.95574746	2.35874049	H	2.18781021	4.52139027	3.20607668
H	-2.01303149	-3.68368723	3.89984784	H	-0.14497315	4.82431576	4.91618693
H	-4.20766450	-2.78374840	2.64687286	H	-2.69455500	4.20287961	4.35878262
H	3.14272517	2.46755916	1.73664008	H	3.41937285	-1.73863533	1.32620651
H	4.49502753	1.31776502	1.40326591	H	3.65067388	-1.68799499	-0.46439187
H	3.87207488	2.38314922	0.08623122	H	4.74596332	-0.74151419	0.61356688
H	4.61129002	-1.95817680	-2.55743916	H	4.10699843	2.61724714	-3.22790804

11. Cartesian coordinates for several structures of DDIYM and DDPYM optimized with the B3LYP-D3/6-31G(d,p) method

Unit of the Cartesian coordinate below is angstrom.

(1) Cartesian coordinates for DDIYM

① Four ground state local minima geometries

EM-DDIYM				*EP*-DDIYM			
C	0.76680500	-0.84563800	-0.05120400	C	-0.72297700	0.77658200	-0.07822600
C	-0.57308000	-0.56189200	-0.06904300	C	0.61968500	0.54635700	-0.04911100
C	-1.28070400	0.66689700	0.29275400	C	1.40554400	-0.68070300	-0.19235300
C	-2.66123500	0.44025100	0.07903000	C	2.76956100	-0.32201900	-0.06617300
N	-2.84435600	-0.84100800	-0.43562400	N	2.87186800	1.05198000	0.15196400
C	-1.63137700	-1.52690600	-0.51807000	C	1.61730600	1.65832900	0.10572200
C	1.87260400	0.11466500	-0.15420900	C	-1.83129500	-0.18251100	0.01465100
C	3.03714800	-0.46106000	0.40343300	C	-2.92741700	0.34148200	-0.70912900
C	2.74258300	-1.85061000	0.88839400	C	-2.58640700	1.70940700	-1.24791000
C	1.38805600	-2.22417100	0.20899100	C	-1.34749200	2.13169300	-0.40260900
C	-0.88356000	1.84856500	0.91981800	C	1.08784900	-1.98653600	-0.56459100
C	-1.84544500	2.80881700	1.25365600	C	2.11223400	-2.92812900	-0.72075700
C	-3.19865700	2.58426900	0.98577800	C	3.44737000	-2.56579100	-0.52737600
C	-3.62755700	1.38447300	0.40404200	C	3.79636500	-1.24650500	-0.21040300
C	1.95892700	1.34105100	-0.85989900	C	-1.98155700	-1.34855500	0.79701400
C	3.19374300	2.00564100	-0.83111600	C	-3.20036700	-2.03483900	0.68585000
C	4.31182700	1.47494100	-0.18642900	C	-4.24154700	-1.57029100	-0.11885400
C	4.24854200	0.21375100	0.41305500	C	-4.12278300	-0.35547200	-0.80286700
C	0.59745000	-3.20963700	1.07306700	C	-1.74610700	2.89623900	0.87110100
O	-1.51697100	-2.65451200	-0.98578000	O	1.43018800	2.86381400	0.23139500
H	-3.93272800	3.34128900	1.24511000	H	4.23052900	-3.30901500	-0.64386700
H	2.60847600	-1.86164800	1.97885200	H	-3.42044400	2.41355600	-1.16048700
H	3.54236900	-2.56147100	0.65761100	H	-2.31414600	1.65510800	-2.31027600
H	1.60621700	-2.68907300	-0.76315400	H	-0.65307100	2.75033700	-0.97163900
H	-0.26979500	-3.60304300	0.54822700	H	-0.85354000	3.13045100	1.45447500
H	0.26107800	-2.72172200	1.99479000	H	-2.43384600	2.30440100	1.48483400
H	1.24701500	-4.04584600	1.35434000	H	-2.24309600	3.83590000	0.60788300
H	0.16358100	2.01991400	1.14621400	H	0.05700200	-2.26534000	-0.75069500
H	-1.53536100	3.73464600	1.72802300	H	1.86408900	-3.94738600	-0.99990800
H	-4.68040600	1.19294100	0.22514700	H	4.83482900	-0.95234700	-0.10012000
H	5.13204700	-0.23748100	0.85544200	H	-4.95741800	0.04579000	-1.37066400
C	-4.10938900	-1.41297900	-0.83630400	C	4.10652900	1.78748100	0.30454400
H	-4.57718500	-0.81010300	-1.62259000	H	4.74481700	1.66876400	-0.57879800
H	-3.90804100	-2.41469900	-1.21788700	H	3.84641000	2.83983400	0.42540800
H	-4.79757400	-1.47767500	0.01443200	H	4.65821900	1.44374100	1.18644700
C	0.85322100	1.89976500	-1.71824100	C	-0.96703000	-1.80175100	1.81780000
H	1.27797700	2.43545800	-2.57213300	H	-0.34953700	-2.63072900	1.45700700
H	0.20059300	1.10714100	-2.09133100	H	-0.28502500	-0.99336300	2.08778700
H	0.21307400	2.59905300	-1.17065900	H	-1.47849000	-2.14344100	2.72295900
H	5.24798300	2.02591100	-0.19589500	H	-5.16971900	-2.13239500	-0.17067700
H	3.28753400	2.94839700	-1.36394100	H	-3.34691300	-2.93504000	1.27750300

ZM-DDIYM				*ZP*-DDIYM			
C	0.70504100	-0.62498300	0.01660500	C	0.63343100	-0.57673100	-0.03125300
C	-0.51626800	0.00091400	0.04710400	C	-0.58739200	0.03253300	-0.01218900
C	-1.84363700	-0.52784400	-0.26353600	C	-1.92303600	-0.57154400	0.06489700
C	-2.78992000	0.47008100	0.07405100	C	-2.86575700	0.46917900	-0.12377300
N	-2.12790300	1.56530400	0.61879200	N	-2.19577000	1.66956100	-0.34315000

C	-0.74328300	1.37027800	0.61312000	C	-0.81254500	1.48874500	-0.30143700
C	2.02920200	-0.01689000	-0.12199300	C	1.97970900	0.01012000	0.00468400
C	3.01306600	-0.96055000	0.26050700	C	2.84942500	-0.85354500	-0.70302200
C	2.37750200	-2.25369300	0.67924000	C	2.10016200	-2.07174600	-1.18381000
C	0.89760900	-2.13647300	0.21129100	C	0.82400500	-2.06758500	-0.29334200
C	-2.28722700	-1.67369100	-0.92686900	C	-2.39730800	-1.85611600	0.33723800
C	-3.65333200	-1.84328100	-1.17651400	C	-3.77717200	-2.09078400	0.38308200
C	-4.57349000	-0.86395300	-0.79148000	C	-4.68469400	-1.05040900	0.17531900
C	-4.14964300	0.31731000	-0.17019000	C	-4.23697700	0.25261500	-0.07565100
C	2.42913100	1.20446800	-0.72649400	C	2.49664700	1.11650100	0.71432200
C	3.80532100	1.46537300	-0.78453900	C	3.86615400	1.38080800	0.56469400
C	4.76069700	0.56488000	-0.31388600	C	4.69927600	0.58040000	-0.21684500
C	4.36788000	-0.67725800	0.19045400	C	4.19818600	-0.56634900	-0.84175300
C	-0.03762200	-2.80402400	1.22892000	C	1.05130900	-2.85976300	1.00784000
O	0.05505800	2.16142300	1.10081200	O	-0.00521400	2.37266400	-0.55757700
H	-5.63122400	-1.01088800	-0.98845200	H	-5.75173200	-1.24801600	0.21518700
H	2.40464700	-2.36356000	1.77150400	H	2.68328300	-2.99340200	-1.08526700
H	2.88813600	-3.12750800	0.26123600	H	1.81924800	-1.97061300	-2.24005800
H	0.80236400	-2.63730700	-0.76367000	H	-0.03330600	-2.48026200	-0.83117800
H	-1.08151600	-2.81777500	0.92039400	H	0.20517100	-2.75865400	1.69354800
H	0.01927800	-2.27738000	2.18705700	H	1.94457000	-2.49243100	1.52281600
H	0.28071100	-3.83900800	1.39292300	H	1.19394200	-3.92313300	0.78916100
H	-1.57908100	-2.42789400	-1.25348400	H	-1.71388100	-2.67531600	0.52180600
H	-3.99919200	-2.74136000	-1.67859200	H	-4.14162800	-3.09260400	0.58761800
H	-4.85787500	1.09235700	0.10348800	H	-4.93754300	1.06719100	-0.22612000
H	5.10487000	-1.41284300	0.49985200	H	4.85386100	-1.22946900	-1.39885000
C	-2.75928800	2.75228500	1.14803600	C	-2.82145500	2.93280500	-0.66073600
H	-3.44405500	2.49857500	1.96500500	H	-3.46343000	3.26903400	0.16139900
H	-1.96792800	3.40053400	1.52641900	H	-2.02458700	3.65993000	-0.82143900
H	-3.32160500	3.27874500	0.36808600	H	-3.42797300	2.85065700	-1.56988100
C	1.49237700	2.17724500	-1.38729200	C	1.69308200	1.94042200	1.68351100
H	1.99418600	2.67729700	-2.22093900	H	1.32238900	2.85110000	1.20688700
H	0.59862300	1.67504200	-1.76909900	H	0.81839000	1.39155800	2.04211100
H	1.14899300	2.93248600	-0.67555800	H	2.30878400	2.21684900	2.54531700
H	5.81545000	0.81571300	-0.38301800	H	5.75399700	0.82675200	-0.30139200
H	4.13538100	2.39508600	-1.24039900	H	4.29223500	2.22524900	1.10034500

② Two transition state geometries at ground state

EM-EP-TS-DDIYM				*ZM-ZP-TS*-DDIYM			
C	0.73908300	-0.59491000	0.39677400	C	0.65966000	-0.41819400	0.11516400
C	-0.63217700	-0.47652500	0.35700700	C	-0.59746800	0.14132500	0.19307100
C	-1.59699800	0.63928300	0.26275400	C	-1.89943100	-0.57766500	0.03134500
C	-2.76599900	0.14633800	-0.36859800	C	-2.88047700	0.40233700	-0.27193500
N	-2.63076000	-1.21771500	-0.59668500	N	-2.31979800	1.67142900	-0.18850400
C	-1.47011200	-1.70771200	-0.00106800	C	-1.01193500	1.59142800	0.28585100
C	1.89577000	0.28661500	0.00005300	C	2.08671700	0.04193000	-0.05704600
C	2.90224000	-0.58186300	-0.50341600	C	2.86223900	-1.10826600	-0.38146900
C	2.54987200	-2.02798900	-0.31346000	C	2.04059000	-2.35128400	-0.49386900
C	1.36969100	-1.96753600	0.66189800	C	0.71320000	-1.95223500	0.14689400
C	-1.68363300	1.90605800	0.83963800	C	-2.34933400	-1.90221800	0.11918900
C	-2.81024900	2.70996900	0.62825100	C	-3.68720300	-2.22313600	-0.14996500
C	-3.89162900	2.23831300	-0.11583700	C	-4.60587500	-1.23663100	-0.49771300
C	-3.89366200	0.92540400	-0.59865300	C	-4.20721100	0.10309800	-0.55038000
C	2.17027800	1.67879200	-0.01173300	C	2.79275000	1.28611700	0.01042700
C	3.35997400	2.11679700	-0.61127000	C	4.17890800	1.26989000	-0.21299000
C	4.29475600	1.24754300	-1.16940600	C	4.90538500	0.12127800	-0.51383200
C	4.07227300	-0.12255900	-1.09514000	C	4.23251200	-1.08781600	-0.60661500
C	1.82664300	-2.02757800	2.13473300	C	0.62489400	-2.44245800	1.60642700
O	-1.24652300	-2.90883900	0.08809400	O	-0.43658200	2.55880000	0.75641100
H	-4.75758200	2.87212300	-0.28171500	H	-5.63844900	-1.49938000	-0.70671200
H	3.39562800	-2.61374300	0.06308200	H	2.51022200	-3.21140600	-0.00396700
H	2.23886900	-2.48060300	-1.26430700	H	1.90614400	-2.62036900	-1.54982300
H	0.66142300	-2.77256600	0.49509200	H	-0.10859600	-2.36879300	-0.43257800
H	0.97482300	-1.90019700	2.80902800	H	-0.26570500	-2.05629900	2.10834000

H	2.56242800	-1.24717000	2.35857800	H	1.50130000	-2.10104900	2.16718900
H	2.28469400	-3.00030500	2.34200300	H	0.60106000	-3.53710300	1.64357200
H	-0.90621700	2.26196400	1.49366800	H	-1.70262900	-2.70526400	0.43809300
H	-2.84633800	3.70069200	1.07044400	H	-4.00544900	-3.25787600	-0.07055700
H	-4.76005200	0.51488900	-1.10601300	H	-4.91419200	0.89098100	-0.78649800
H	4.80148700	-0.83257400	-1.47494100	H	4.75357000	-2.01000400	-0.84763700
C	-3.68928000	-2.07863000	-1.07845000	C	-3.08343500	2.90029000	-0.16055000
H	-3.96902600	-1.80294500	-2.10024300	H	-3.85504300	2.86739900	0.61845300
H	-3.31482400	-3.10202400	-1.06412400	H	-2.39129900	3.71422900	0.05498800
H	-4.57685200	-2.00714700	-0.43791000	H	-3.56620400	3.07306200	-1.12772300
C	1.33088900	2.74162100	0.64393300	C	2.22390200	2.64822100	0.29999100
H	0.45891700	3.00584200	0.04328300	H	1.50566600	2.95824600	-0.45934700
H	0.98668400	2.41537900	1.62802100	H	1.69193800	2.67766800	1.24810900
H	1.92043500	3.65072900	0.78913600	H	3.03078300	3.38516700	0.32341900
H	5.20062700	1.64018100	-1.62196300	H	5.97809500	0.17953000	-0.67392300
H	3.56600400	3.18362100	-0.61712400	H	4.70970600	2.21478600	-0.14713000

(2) Cartesian coordinates for DDPYM

① Four ground state local minima geometries

EM-DDPYM				*EP*-DDPYM			
C	-0.98678700	0.64481400	0.01947800	C	-0.92973900	0.64184600	-0.11585800
C	0.38349200	0.52862200	-0.02096800	C	0.43377800	0.52974800	-0.06324300
C	1.27187100	1.64429200	-0.44809100	C	1.33282000	1.71408900	0.05972200
C	-3.23861400	1.60780000	0.44549600	C	-3.01652400	1.47100300	-1.10268800
C	-1.72576700	1.97903000	0.25084200	C	-1.68954600	1.94786300	-0.40987600
C	-1.18504400	2.76485500	1.45440600	C	-1.98678900	2.72012400	0.88773500
O	0.99489600	2.79797000	-0.76879600	O	1.05914200	2.91001400	0.11917700
H	-3.54936200	1.82576200	1.47525700	H	-3.86824800	2.10958000	-0.84505000
H	-3.89767600	2.19045100	-0.20846800	H	-2.90785000	1.50110100	-2.19454700
H	-1.59295600	2.59505800	-0.64617400	H	-1.09247400	2.58791700	-1.06159400
H	-0.15390900	3.07519100	1.29247900	H	-1.05486900	2.99833400	1.38163000
H	-1.24011000	2.15757100	2.36471600	H	-2.59254700	2.10955500	1.56655000
H	-1.78977200	3.66470800	1.61054600	H	-2.54275700	3.63604300	0.66144600
C	-3.46254000	-1.97932900	-0.51816600	C	-3.43298100	-1.99890000	0.21634800
C	-3.28522900	0.14785400	0.13405800	C	-3.15416100	0.06652900	-0.59528800
C	-2.00579800	-0.35084200	-0.10379400	C	-1.95833600	-0.35577900	-0.02719000
H	-5.28747700	-0.85893700	-0.00998400	H	-5.11272200	-1.01746900	-0.81095600
C	-1.13140300	-2.46729600	-1.24580400	C	-1.33327600	-2.25380100	1.53808200
H	-1.59413600	-2.90207400	-2.13488100	H	-1.10460900	-3.29273800	1.28595800
H	-0.30814000	-1.82590600	-1.55422900	H	-0.39712700	-1.71156800	1.64801700
H	-0.72644400	-3.26779300	-0.62220500	H	-1.87391300	-2.22329900	2.48905900
H	-3.79120300	-2.95540500	-0.84808100	H	-3.80882500	-2.94829600	0.57260900
N	2.56408500	1.10647400	-0.51621300	N	2.63361000	1.20897000	0.15007400
C	3.72272800	1.87611100	-0.90555100	C	3.80372200	2.04642000	0.27734500
H	4.22376000	1.42063500	-1.76706100	H	4.45651500	1.94586600	-0.59790500
H	3.37423800	2.87437900	-1.17393200	H	3.45844900	3.07823200	0.35502300
H	4.44083800	1.95030700	-0.08021200	H	4.37590300	1.78375100	1.17415000
C	2.15015200	-2.68360600	1.10503600	C	2.19949400	-2.84561800	-0.57883600
C	3.43967800	-2.29521600	0.72969800	C	3.49942500	-2.37594200	-0.37516100
C	3.67416100	-1.03793800	0.15722800	C	3.73911700	-1.02243700	-0.10494300
C	2.58091900	-0.20673700	-0.05647000	C	2.64272300	-0.17340800	-0.01619800
C	1.25666500	-0.60766200	0.25242500	C	1.31075000	-0.63846600	-0.15506400
C	1.05829800	-1.83689000	0.88240100	C	1.10374000	-1.97959900	-0.48170400
H	1.99425500	-3.64541200	1.58415800	H	2.03528400	-3.89046200	-0.82412500
H	4.27702200	-2.96425900	0.90421300	H	4.33905300	-3.06075900	-0.44791300
H	4.67936600	-0.71581100	-0.09450700	H	4.74951300	-0.64475600	0.01261500
H	0.06494500	-2.12312400	1.21245300	H	0.10331800	-2.34482900	-0.68360800
N	-2.12372800	-1.66814700	-0.53230400	N	-2.13201900	-1.63167200	0.48527300
C	-4.21093400	-0.88576000	-0.10123800	C	-4.08861200	-0.98324000	-0.46688400

ZM-DDPYM				*ZP*-DDPYM			
C	0.87767500	-0.55276000	0.02154200	C	0.81784400	-0.52256200	-0.07457800
C	-0.36782400	0.03819600	0.01815000	C	-0.42595700	0.05203800	-0.01321100
C	-0.62820600	1.43184100	0.46607300	C	-0.67537900	1.50870100	-0.20333100
C	2.64504500	-2.27425700	0.37746500	C	2.42561900	-2.11575400	-1.03024400
C	1.09750900	-2.06763700	0.23049800	C	1.04333400	-2.02641300	-0.29931700
C	0.34763800	-2.61023000	1.45685000	C	1.09558800	-2.77958000	1.04433400
O	0.14703000	2.27619200	0.91099800	O	0.11891300	2.42277100	-0.40791700
H	2.88474700	-2.61369700	1.39309200	H	2.98498500	-3.01420100	-0.74721100
H	3.02846900	-3.04116800	-0.30565800	H	2.27951300	-2.15356500	-2.11737900
H	0.75538400	-2.59902100	-0.66708000	H	0.24320500	-2.43704900	-0.92169500
H	-0.73136300	-2.47382400	1.38077600	H	0.19702800	-2.60757200	1.64246600
H	0.68990800	-2.09357800	2.35947600	H	1.95689500	-2.43727600	1.62708600
H	0.55157000	-3.67924700	1.57907000	H	1.19931900	-3.85693600	0.87810000
C	4.12184100	1.00749700	-0.54105000	C	4.14276400	0.98428000	0.11444200
C	3.20200800	-0.92227100	0.08197300	C	3.08261300	-0.84184300	-0.59785700
C	2.18199200	0.01716700	-0.10297500	C	2.14240200	0.03673500	-0.05325400
H	5.42580800	-0.71928400	-0.11911600	H	5.30121200	-0.62234000	-0.85279300
C	2.12429600	2.39457700	-1.06467700	C	2.31566400	2.22498300	1.26388500
H	1.22100700	2.09765800	-1.59986800	H	2.05404300	3.11089900	0.68723300
H	1.83534500	3.08836100	-0.27773800	H	1.41728500	1.88123300	1.77409700
H	2.81461500	2.86472000	-1.76849200	H	3.08237700	2.45891000	2.00705500
H	4.77781400	1.80834300	-0.85335900	H	4.86097700	1.73474200	0.41455000
N	-2.01411200	1.61021300	0.41669000	N	-2.06021600	1.67744000	-0.20346200
C	-2.67508300	2.81829800	0.85180600	C	-2.70596800	2.94833400	-0.43571900
H	-3.34539600	2.61675300	1.69544200	H	-3.34538000	3.22374400	0.41080900
H	-1.89987100	3.51855800	1.16568900	H	-1.92071500	3.69546100	-0.55768100
H	-3.26034800	3.26050500	0.03722200	H	-3.32033300	2.91508300	-1.34298400
C	-3.47231600	-2.01644200	-0.95197200	C	-3.58540000	-2.14698300	0.23467200
C	-4.41151900	-1.01475400	-0.69461000	C	-4.50952600	-1.10694000	0.12536800
C	-4.00709800	0.24174400	-0.22651300	C	-4.07819900	0.21733800	-0.02186100
C	-2.65014000	0.45063200	-0.01408300	C	-2.71065700	0.45494600	-0.06118700
C	-1.67797300	-0.55623700	-0.24386800	C	-1.74761500	-0.58211200	0.04191400
C	-2.10777800	-1.79138400	-0.73595600	C	-2.20853300	-1.89202800	0.19832200
H	-3.80143500	-2.98198600	-1.32366500	H	-3.93373600	-3.16864400	0.35124500
H	-5.46696900	-1.20664300	-0.86301900	H	-5.57355300	-1.32153200	0.15624600
H	-4.72953100	1.02911700	-0.03777500	H	-4.78893300	1.03299900	-0.10507600
H	-1.39611400	-2.58062300	-0.95027500	H	-1.51951800	-2.72075600	0.29368800
N	2.76798000	1.20657900	-0.51557200	N	2.81382400	1.15834100	0.40205700
C	4.43210800	-0.29765000	-0.16874300	C	4.34786500	-0.23744500	-0.51980900

② Two transition state geometries at ground state

EM-EP-TS-DDPYM				*ZM-ZP-TS*-DDPYM			
C	0.92322200	-0.53676600	0.06290100	C	0.84013200	-0.47032400	-0.00786300
C	-0.45480300	-0.42408700	0.11960100	C	-0.41684700	0.09838600	0.02031500
C	-1.31718100	-1.66225000	-0.01704100	C	-0.71982800	1.54710200	0.17039200
C	2.96936500	-1.81443000	-0.56184400	C	2.40790600	-2.39046500	-0.30887500
C	1.56376500	-1.95283600	0.06935900	C	0.95225400	-2.01003000	0.06067300
C	1.64043600	-2.48299500	1.51266400	C	0.60064800	-2.50313100	1.47749600
O	-1.03828300	-2.85675800	0.05737300	O	0.02896000	2.49324000	0.39601400
H	3.72197100	-2.41070000	-0.03355600	H	2.82610900	-3.12967500	0.38412300
H	2.96924800	-2.15427600	-1.60577700	H	2.46765300	-2.83060800	-1.31259200
H	0.94649700	-2.64266200	-0.50066000	H	0.26698800	-2.45248100	-0.66463100
H	0.64323600	-2.54812900	1.95000600	H	-0.38753700	-2.16557500	1.79564600
H	2.26460800	-1.82838300	2.13187100	H	1.33736600	-2.11890500	2.19088600
H	2.08049500	-3.48568400	1.52012900	H	0.62388500	-3.59734400	1.51850800
C	3.78196300	1.78446200	-0.38306400	C	4.30314900	0.77645900	-0.29371300
C	3.21598100	-0.35458100	-0.46523000	C	3.10077600	-1.07799700	-0.25170500
C	2.07187800	0.35861100	-0.07952300	C	2.21341900	0.00202600	-0.08977200
H	5.29427100	0.30229200	-0.97797400	H	5.32052300	-1.16494300	-0.51786200
C	1.77346300	2.88962400	0.46161400	C	2.67723300	2.58357600	-0.01484400
H	2.51711600	3.67256500	0.61851300	H	1.97128200	2.88757600	-0.78362500
H	1.03411600	3.25590700	-0.25281500	H	2.23495900	2.80878400	0.95218600

H	1.29699700	2.68714200	1.42297400	H	3.61213100	3.13448400	-0.13463300
H	4.27887400	2.74463900	-0.38222700	H	5.07910600	1.52749200	-0.34079300
N	-2.61171100	-1.22668600	-0.28339000	N	-2.09873900	1.69412600	0.05903800
C	-3.72903300	-2.12507300	-0.46496700	C	-2.77654500	2.96258000	0.18949400
H	-4.21969500	-1.94263000	-1.42732100	H	-3.46528200	2.95188200	1.04230500
H	-3.33803800	-3.14243600	-0.44119300	H	-2.01359400	3.72532000	0.34848100
H	-4.46771400	-1.99902800	0.33558800	H	-3.34529900	3.19677400	-0.71759800
C	-2.51508000	2.85751000	0.27760600	C	-3.56969500	-2.13995500	-0.37409500
C	-3.74545800	2.30050800	-0.06727000	C	-4.50285600	-1.10455500	-0.37036600
C	-3.85267100	0.92334700	-0.28582500	C	-4.07928700	0.22120800	-0.22936500
C	-2.70196100	0.15152800	-0.18078800	C	-2.71801000	0.46158700	-0.09846400
C	-1.42050900	0.69237100	0.10542000	C	-1.73578000	-0.56467100	-0.10322100
C	-1.36917500	2.05842400	0.37472900	C	-2.19977800	-1.87940200	-0.23998700
H	-2.43996400	3.91987200	0.48941300	H	-3.90263700	-3.16838200	-0.47529700
H	-4.62839400	2.92791900	-0.14347700	H	-5.56161600	-1.32308600	-0.47163800
H	-4.80779600	0.46364400	-0.51670500	H	-4.79017200	1.04085700	-0.22046200
H	-0.45628000	2.51289300	0.70288500	H	-1.52565300	-2.72347600	-0.23016100
N	2.45569200	1.70585100	-0.02933200	N	2.99871600	1.16150600	-0.12867300
C	4.28393800	0.53112700	-0.67161000	C	4.40981800	-0.60139900	-0.37668500

12. Cartesian coordinates for several structures of DDIYM and DDPYM optimized with the ωB97X-D/6-31G(d,p) method

Unit of the Cartesian coordinate below is angstrom.

(1) Cartesian coordinates for DDIYM

① Four ground state local minima geometries

EM-DDIYM				*EP*-DDIYM			
C	0.75586500	0.85984500	0.06839600	C	-0.71456300	0.78713900	-0.06287900
C	-0.57243400	0.56947900	0.07461600	C	0.61866700	0.55564300	-0.05107700
C	-1.26473100	-0.67437200	-0.28060200	C	1.39937100	-0.67821400	-0.18901400
C	-2.64166400	-0.45538400	-0.09193000	C	2.75695100	-0.32457900	-0.07064700
N	-2.84509200	0.82918800	0.40001100	N	2.86765500	1.04839200	0.13420400
C	-1.64852300	1.52456500	0.49629000	C	1.62450600	1.65963000	0.08861400
C	1.86408900	-0.10643100	0.15901300	C	-1.82529600	-0.17755700	0.01669300
C	3.01244500	0.46279000	-0.41824300	C	-2.90771800	0.35176400	-0.70947400
C	2.71496300	1.85483500	-0.88868400	C	-2.56714900	1.72739500	-1.22210800
C	1.38564700	2.23169100	-0.17575000	C	-1.34526100	2.13974500	-0.35941700
C	-0.84970200	-1.85534800	-0.88489800	C	1.07451400	-1.98127300	-0.54377500
C	-1.79705800	-2.82507800	-1.21696200	C	2.09143300	-2.92691400	-0.68833200
C	-3.15052300	-2.60814300	-0.97087800	C	3.42377400	-2.56871000	-0.50192400
C	-3.59524600	-1.40789200	-0.41387800	C	3.77789000	-1.25115000	-0.20431000
C	1.95465200	-1.32245100	0.86534100	C	-1.97909000	-1.34606400	0.78074500
C	3.18201300	-1.99282300	0.81612200	C	-3.19079500	-2.03416000	0.64660200
C	4.28596800	-1.47089700	0.15045900	C	-4.22025500	-1.56401600	-0.16146000
C	4.21821200	-0.21507100	-0.44950600	C	-4.09814600	-0.34371700	-0.82552800
C	0.59602700	3.24033900	-1.00516100	C	-1.75921000	2.86668700	0.92468700
O	-1.55520900	2.65051600	0.95756900	O	1.44721400	2.86183800	0.20272400
H	-3.87481600	-3.37335300	-1.23073200	H	4.20273700	-3.31675400	-0.60905500
H	2.55490800	1.87368500	-1.97451200	H	-3.40377600	2.42652300	-1.12820200
H	3.52208300	2.55927800	-0.66817500	H	-2.28560300	1.68968600	-2.28141800
H	1.62980000	2.67358600	0.79969000	H	-0.65172500	2.77553800	-0.90912000
H	-0.24889200	3.64506200	-0.45323100	H	-0.87280900	3.10291400	1.51669400
H	0.22433200	2.77015300	-1.92209900	H	-2.43810700	2.25182000	1.52490800
H	1.25758200	4.06324700	-1.29475600	H	-2.26897100	3.80362500	0.68082200
H	0.20163000	-2.02367900	-1.09454100	H	0.04171300	-2.25802200	-0.72370800
H	-1.47367900	-3.75385700	-1.67476100	H	1.83992000	-3.94862500	-0.95226300
H	-4.65175500	-1.22291300	-0.25165200	H	4.81791600	-0.96180600	-0.09725700
H	5.09575200	0.23120800	-0.90702600	H	-4.92778100	0.06323400	-1.39539700
C	-4.11721600	1.38732900	0.77850700	C	4.10425700	1.77374300	0.26974600
H	-4.58175200	0.79436400	1.57314200	H	4.72804500	1.65503600	-0.62280000
H	-3.93248900	2.39800400	1.14347800	H	3.85164700	2.82692000	0.39615700
H	-4.79814300	1.42815900	-0.07835000	H	4.66401100	1.42710600	1.14422000
C	0.86475900	-1.87277700	1.74552000	C	-0.97913400	-1.81282700	1.80666900
H	1.30750100	-2.36314700	2.61636700	H	-0.41731300	-2.68961700	1.47105900
H	0.19432000	-1.08392500	2.09257900	H	-0.25273100	-1.03454300	2.04481300
H	0.24553100	-2.60925600	1.22457900	H	-1.50193000	-2.08994700	2.72653000
H	5.21949200	-2.02513000	0.14467000	H	-5.14572900	-2.12730600	-0.23127000
H	3.28063500	-2.93517100	1.34806600	H	-3.33928800	-2.94461100	1.22118300

ZM-DDIYM				*ZP*-DDIYM			
C	0.69801700	0.62079200	-0.01013900	C	-0.62479500	0.56916500	-0.01257500
C	-0.51098100	-0.00754400	-0.03858900	C	0.58465800	-0.04206700	0.01015900
C	-1.84286900	0.52365200	0.26359900	C	1.92161800	0.56582200	0.07627600
C	-2.77991900	-0.46953900	-0.07814400	C	2.85768500	-0.46685500	-0.12834700
N	-2.11661900	-1.56549900	-0.61332300	N	2.19009400	-1.66806300	-0.33557400

C	-0.73910800	-1.37787100	-0.59663500	C	0.81427500	-1.49639600	-0.27288100
C	2.03004200	0.01695300	0.11855000	C	-1.97844400	-0.01026800	0.00505800
C	2.99855700	0.95992800	-0.27445700	C	-2.82144400	0.85238100	-0.72045700
C	2.35487600	2.25024300	-0.68176000	C	-2.05735200	2.06490700	-1.18507200
C	0.88632500	2.12922600	-0.19795600	C	-0.80845000	2.05722500	-0.26804300
C	-2.28589000	1.66194300	0.92843000	C	2.39240300	1.84518700	0.35065800
C	-3.65005800	1.83248600	1.16616200	C	3.76838700	2.08317000	0.37486700
C	-4.56454100	0.85930500	0.76980200	C	4.67166600	1.05046100	0.14483400
C	-4.13829900	-0.31760900	0.15237100	C	4.22524800	-0.24873000	-0.10399100
C	2.43489300	-1.19167400	0.72617200	C	-2.51159400	-1.10214400	0.71034000
C	3.80905800	-1.44740200	0.77603500	C	-3.87643700	-1.35828600	0.53745400
C	4.75294000	-0.54890300	0.29223400	C	-4.68533500	-0.55984400	-0.26325400
C	4.35258300	0.68428800	-0.21546300	C	-4.16655000	0.57592900	-0.88335600
C	-0.05477700	2.79415100	-1.20526400	C	-1.06484300	2.83449300	1.02975700
O	0.05492900	-2.17046700	-1.07447800	O	0.01234200	-2.38270600	-0.50964300
H	-5.62309800	1.00785200	0.95713100	H	5.73803700	1.25078900	0.16787000
H	2.37011800	2.36449900	-1.77279900	H	-2.63788200	2.98843500	-1.09720400
H	2.86582300	3.12176800	-0.26206100	H	-1.75492500	1.95972300	-2.23360700
H	0.79924500	2.62549800	0.77891500	H	0.05965900	2.47229400	-0.78506100
H	-1.09573600	2.81569500	-0.88747300	H	-0.23503200	2.72589200	1.73392600
H	-0.00910800	2.26407700	-2.16152400	H	-1.96985100	2.46386000	1.52080000
H	0.26721900	3.82625800	-1.37550700	H	-1.20122100	3.89925700	0.81818100
H	-1.57984700	2.41317600	1.26685700	H	1.70961900	2.66054800	0.55714500
H	-3.99932800	2.72819600	1.66852900	H	4.13395800	3.08372800	0.57975200
H	-4.84583600	-1.09045400	-0.12841500	H	4.92690800	-1.05917300	-0.27010300
H	5.08370300	1.42096600	-0.53377300	H	-4.80660200	1.23927800	-1.45692400
C	-2.74530500	-2.74685900	-1.14437100	C	2.81530500	-2.92287200	-0.66385600
H	-3.42476200	-2.49114700	-1.96390400	H	3.49654900	-3.23955100	0.13263600
H	-1.95224800	-3.39423900	-1.51991800	H	2.02147600	-3.66164200	-0.77786200
H	-3.30852100	-3.27473200	-0.36715400	H	3.37545800	-2.84709500	-1.60194500
C	1.50707000	-2.16164700	1.39793000	C	-1.73040500	-1.92406000	1.69524100
H	2.01603200	-2.64767800	2.23454000	H	-1.35012200	-2.83270100	1.22442000
H	0.61279100	-1.66078300	1.77947300	H	-0.86575100	-1.37354700	2.07486900
H	1.16992600	-2.92460000	0.69299500	H	-2.36606500	-2.19919000	2.54172300
H	5.80885200	-0.79319900	0.35675900	H	-5.73934800	-0.79863200	-0.36737100
H	4.14600100	-2.37243500	1.23536700	H	-4.31783100	-2.19749900	1.06803100

② Two transition state geometries at ground state

EM-EP-TS-DDIYM				*ZM-ZP-TS*-DDIYM			
C	0.73653100	-0.60303300	0.37321600	C	0.65337900	-0.41847900	0.11640700
C	-0.62538200	-0.47704700	0.36094600	C	-0.59123900	0.14109500	0.20694600
C	-1.58969900	0.64367000	0.26674000	C	-1.89478500	-0.57627900	0.04292900
C	-2.74184300	0.15647300	-0.38279900	C	-2.86142100	0.40017900	-0.28107800
N	-2.60941400	-1.20653200	-0.60860900	N	-2.29865300	1.66740300	-0.20547400
C	-1.47406600	-1.69887000	0.01781000	C	-1.00886700	1.58782200	0.29738900
C	1.89820600	0.28664500	-0.00303000	C	2.08378900	0.04096000	-0.05660200
C	2.90820800	-0.56732200	-0.50006800	C	2.85051400	-1.10227700	-0.38843800
C	2.55943200	-2.01494800	-0.34535800	C	2.02705700	-2.34098500	-0.51411900
C	1.36139200	-1.98027500	0.59993100	C	0.70610600	-1.94767800	0.13324700
C	-1.68895200	1.89515600	0.86194700	C	-2.34541400	-1.89283000	0.14703700
C	-2.80995400	2.69801100	0.64078500	C	-3.67893400	-2.21099900	-0.12780600
C	-3.87111000	2.23665600	-0.12930600	C	-4.58603600	-1.22874100	-0.49766000
C	-3.86323700	0.93350500	-0.62582800	C	-4.18321000	0.10495200	-0.56627800
C	2.16128100	1.67518800	-0.00005800	C	2.78139300	1.28013500	0.01581500
C	3.35874300	2.12521800	-0.56391300	C	4.16456500	1.26784800	-0.20040100
C	4.30739900	1.26831400	-1.10747300	C	4.88902100	0.12350200	-0.50265600
C	4.08756600	-0.09821300	-1.05878100	C	4.21892400	-1.08129600	-0.60833000
C	1.77970100	-2.09376800	2.07461700	C	0.62518600	-2.44830700	1.58383200
O	-1.27412200	-2.89460600	0.14576600	O	-0.44636400	2.54675600	0.78581800
H	-4.73437100	2.87100200	-0.30262800	H	-5.61772400	-1.48916900	-0.71028000
H	3.39771600	-2.60023200	0.04585400	H	2.49432200	-3.20602700	-0.03274800
H	2.27859600	-2.45059100	-1.31174600	H	1.89035300	-2.59331300	-1.57231400
H	0.65451300	-2.77636000	0.39015000	H	-0.11906500	-2.35468600	-0.44823700
H	0.90906500	-2.00063500	2.72896600	H	-0.25509400	-2.05456900	2.09787900

H	2.50336800	-1.31820300	2.34793800	H	1.51070800	-2.12398100	2.13986100
H	2.24007100	-3.06984700	2.25491600	H	0.58673500	-3.54221600	1.61099700
H	-0.92616400	2.24223300	1.53885800	H	-1.70227500	-2.69285400	0.48339300
H	-2.85850200	3.68036700	1.09827900	H	-4.00311000	-3.24201800	-0.03466800
H	-4.72120800	0.52785800	-1.15069500	H	-4.88642600	0.89039500	-0.82063300
H	4.82501300	-0.80107500	-1.43448500	H	4.74061400	-2.00107600	-0.85477900
C	-3.67107100	-2.06256800	-1.07648100	C	-3.06134600	2.89093000	-0.17904700
H	-3.92239500	-1.82771700	-2.11489300	H	-3.84054700	2.85362100	0.59095300
H	-3.31385500	-3.08998100	-1.01099500	H	-2.37054500	3.70160500	0.05139500
H	-4.56873400	-1.95096200	-0.45756500	H	-3.52940900	3.07129200	-1.15105900
C	1.29185600	2.72573900	0.62697700	C	2.20269700	2.63698600	0.29544700
H	0.40420500	2.93072600	0.02805000	H	1.47473100	2.92889400	-0.46071700
H	0.97771600	2.42086300	1.62766500	H	1.68253600	2.67158500	1.24943300
H	1.84697700	3.66082400	0.73045500	H	3.00240600	3.38098600	0.30070100
H	5.22051100	1.66991400	-1.53523100	H	5.96163500	0.18327100	-0.65785600
H	3.55634400	3.19320000	-0.55801100	H	4.69335600	2.21316000	-0.12935200

(2) Cartesian coordinates for DDPYM

① Four ground state local minima geometries

EM-DDPYM				*EP*-DDPYM			
C	-0.98155500	0.65705300	0.01461800	C	-0.92157200	0.64658400	-0.10661300
C	0.37910600	0.54083400	-0.01651500	C	0.43203800	0.53108800	-0.06190700
C	1.28090400	1.64588300	-0.43679100	C	1.33636500	1.71059700	0.05082700
C	-3.22925800	1.59083400	0.46745600	C	-2.99252500	1.48318500	-1.09452000
C	-1.73296900	1.97973100	0.23284800	C	-1.67978500	1.94950200	-0.38480800
C	-1.18458800	2.79950300	1.40315600	C	-1.98708000	2.69350400	0.92090200
O	1.01881600	2.79582100	-0.76066400	O	1.06795000	2.90179200	0.10479300
H	-3.50694400	1.79298300	1.50867700	H	-3.84527800	2.11692600	-0.83155600
H	-3.91084000	2.17165200	-0.16190400	H	-2.87425900	1.52719900	-2.18335300
H	-1.63451100	2.57494800	-0.68229700	H	-1.07775700	2.60128100	-1.01933100
H	-0.16732500	3.13512400	1.20734300	H	-1.05894000	2.95750200	1.43013200
H	-1.19995300	2.20836800	2.32494300	H	-2.60263200	2.07300300	1.58101000
H	-1.81031700	3.68417100	1.55742000	H	-2.53411500	3.61658000	0.70697200
C	-3.43312000	-1.97947600	-0.52067100	C	-3.42779500	-1.98562000	0.18992700
C	-3.26654900	0.13504400	0.14646200	C	-3.13401600	0.07506800	-0.60501100
C	-1.99615900	-0.35128900	-0.10299700	C	-1.95608800	-0.35310300	-0.02866400
H	-5.26115400	-0.88533100	0.01021700	H	-5.09227100	-1.00231900	-0.84759900
C	-1.11132000	-2.44006400	-1.26310000	C	-1.35157300	-2.25195000	1.52625300
H	-1.57932200	-2.88335700	-2.14404900	H	-1.15472500	-3.29950400	1.28538100
H	-0.30360900	-1.78535100	-1.58622400	H	-0.39922600	-1.73564200	1.62632000
H	-0.68523600	-3.23143200	-0.64292600	H	-1.88480900	-2.19414600	2.47910900
H	-3.75530100	-2.95588800	-0.85552000	H	-3.80918500	-2.93600700	0.53703400
N	2.55928100	1.09750700	-0.50118300	N	2.62716800	1.20395400	0.14097500
C	3.72137500	1.85138300	-0.89302300	C	3.79631700	2.03602600	0.25666800
H	4.20385300	1.40046500	-1.76630800	H	4.44098100	1.93400500	-0.62323100
H	3.38332900	2.85712800	-1.14535100	H	3.45150000	3.06770700	0.33415600
H	4.44813000	1.90654700	-0.07516500	H	4.37185900	1.77677300	1.15122200
C	2.11340600	-2.68204600	1.10448800	C	2.19049000	-2.84330000	-0.55781800
C	3.40193000	-2.30446100	0.73275800	C	3.48604600	-2.37344600	-0.36072400
C	3.64719800	-1.05207200	0.16540400	C	3.72645400	-1.02263100	-0.10192500
C	2.56287600	-0.21531300	-0.04684000	C	2.63225900	-0.17697300	-0.01728000
C	1.24303900	-0.60573900	0.25561900	C	1.30771900	-0.64127200	-0.14890400
C	1.03208600	-1.82777000	0.88284700	C	1.09801500	-1.97840700	-0.46603300
H	1.94996600	-3.64239300	1.58231400	H	2.02605100	-3.88952200	-0.79337100
H	4.23246900	-2.98068000	0.90823300	H	4.32407600	-3.05959800	-0.42988000
H	4.65594800	-0.73846300	-0.08229200	H	4.73695300	-0.64438600	0.01169800
H	0.03582700	-2.10609300	1.21244300	H	0.09700100	-2.34603100	-0.66314500
N	-2.10327400	-1.65843300	-0.54122400	N	-2.13506300	-1.62414800	0.47386000
C	-4.18600000	-0.90244900	-0.09028400	C	-4.07252900	-0.97165500	-0.49266200

ZM-DDPYM				*ZP*-DDPYM			
C	0.86995500	-0.54763600	0.01647600	C	0.81094400	-0.51592800	-0.07338300
C	-0.36464800	0.04322500	0.01325600	C	-0.42271100	0.05726000	-0.01254100
C	-0.62728600	1.43763700	0.44906000	C	-0.67779900	1.51104700	-0.19622900
C	2.61883200	-2.27975900	0.35919100	C	2.40168600	-2.11426900	-1.02560800
C	1.08089000	-2.05994400	0.21443700	C	1.03191600	-2.01594200	-0.28867400
C	0.33381100	-2.59562200	1.44020800	C	1.09027100	-2.75429600	1.05684300
O	0.14396600	2.28198200	0.88451900	O	0.11048700	2.42387600	-0.39325100
H	2.85465300	-2.63780300	1.36795900	H	2.95799800	-3.01140000	-0.73573600
H	2.99606300	-3.03253000	-0.34067900	H	2.25061700	-2.15792800	-2.11030500
H	0.73250200	-2.58361200	-0.68422100	H	0.22767200	-2.42772500	-0.90422700
H	-0.74421500	-2.44826000	1.37122300	H	0.19674500	-2.57177300	1.65943700
H	0.68786000	-2.08399600	2.34052000	H	1.95757600	-2.41178100	1.62991300
H	0.52758600	-3.66606000	1.55915700	H	1.18743800	-3.83256200	0.89835400
C	4.12396000	0.98673400	-0.51602800	C	4.13988500	0.96561000	0.10349100
C	3.18444400	-0.92926600	0.08720600	C	3.06459400	-0.84290000	-0.60390900
C	2.18343900	0.01596600	-0.09650200	C	2.14266700	0.03841200	-0.05821600
H	5.40970600	-0.74807100	-0.09626700	H	5.28254200	-0.64368000	-0.86609900
C	2.15296900	2.38614400	-1.05119900	C	2.33305400	2.21644700	1.25265900
H	1.27443600	2.09489900	-1.62957800	H	2.02173900	3.08093000	0.66984200
H	1.83189500	3.06605000	-0.26555500	H	1.47055600	1.85966700	1.81468400
H	2.86908600	2.86723200	-1.71973900	H	3.12569300	2.48463400	1.95435600
H	4.78856400	1.78351000	-0.81978400	H	4.86398200	1.71090800	0.40132300
N	-2.00516100	1.61240300	0.40338700	N	-2.05528000	1.67372000	-0.20024000
C	-2.66473800	2.81762100	0.83204200	C	-2.70190900	2.93925500	-0.42766500
H	-3.35216900	2.61294400	1.65967000	H	-3.35051800	3.20474200	0.41382900
H	-1.89125600	3.50911900	1.16773300	H	-1.91774800	3.68974300	-0.53249800
H	-3.22670600	3.27202900	0.00892900	H	-3.30211600	2.91347700	-1.34364900
C	-3.47173300	-2.00960800	-0.93065600	C	-3.57467900	-2.14111900	0.23097100
C	-4.40431700	-1.00828200	-0.67502800	C	-4.49538700	-1.10501900	0.11883700
C	-3.99652900	0.24608800	-0.21818500	C	-4.06628400	0.21537500	-0.02786800
C	-2.64149200	0.45150300	-0.01526900	C	-2.70231800	0.45137800	-0.06352800
C	-1.67892800	-0.55391300	-0.23979400	C	-1.74555800	-0.58036400	0.03970000
C	-2.10971200	-1.78596000	-0.72292500	C	-2.20177100	-1.88584900	0.19672900
H	-3.80435000	-2.97513700	-1.29723900	H	-3.92309700	-3.16175700	0.34964400
H	-5.46016000	-1.19847000	-0.83830300	H	-5.55876500	-1.31958900	0.14947500
H	-4.71743400	1.03525600	-0.03194200	H	-4.77879900	1.02924100	-0.11149700
H	-1.40080300	-2.57779400	-0.93791000	H	-1.51166800	-2.71414600	0.29616700
N	2.77808000	1.19658100	-0.49817900	N	2.81952100	1.14859200	0.39520600
C	4.42151400	-0.31626800	-0.15072000	C	4.33449500	-0.25046200	-0.53023600

② Two transition state geometries at ground state

EM-*EP*-*TS*-DDPYM				*ZM*-*ZP*-*TS*-DDPYM			
C	0.91561300	-0.54124200	0.07945700	C	0.83528000	-0.47147900	0.00005000
C	-0.45131400	-0.42959900	0.14125600	C	-0.41074400	0.09649900	0.03406800
C	-1.31444800	-1.66241100	0.00015600	C	-0.71522300	1.54205500	0.18930200
C	2.94355900	-1.80656200	-0.58289800	C	2.40071500	-2.38488900	-0.29640400
C	1.56087800	-1.94684700	0.08386800	C	0.94781500	-2.00531500	0.06051900
C	1.67979200	-2.45523000	1.52676400	C	0.58676300	-2.50160400	1.46835600
O	-1.04146300	-2.85097500	0.08945000	O	0.02842300	2.48018300	0.43273600
H	3.70870700	-2.40054400	-0.07251600	H	2.81283100	-3.11324000	0.41017800
H	2.91487800	-2.14211300	-1.62613400	H	2.46968500	-2.83282600	-1.29414000
H	0.93149600	-2.64566600	-0.46067700	H	0.26789500	-2.43995700	-0.67440200
H	0.69569100	-2.52410800	1.99267600	H	-0.40041100	-2.16019500	1.78570300
H	2.31378200	-1.78838800	2.12174800	H	1.32272600	-2.12570400	2.18646200
H	2.12877700	-3.45291100	1.53428300	H	0.60384500	-3.59543700	1.50350200
C	3.75153800	1.78400000	-0.40772100	C	4.28474900	0.77714200	-0.30501400
C	3.18879300	-0.34775500	-0.48808500	C	3.09023900	-1.07229000	-0.24572200
C	2.06348400	0.35981700	-0.07668400	C	2.21164700	0.00113400	-0.08500800
H	5.25450300	0.31643800	-1.04100700	H	5.30905100	-1.15465000	-0.52307400
C	1.76546900	2.87379300	0.48214200	C	2.65803500	2.57278700	-0.04081800
H	2.51213000	3.65347000	0.63729100	H	1.94261500	2.85968400	-0.80709400
H	1.02020600	3.24675200	-0.22182400	H	2.22521100	2.80998300	0.92688300

H	1.30394300	2.66199700	1.44818200	H	3.58813100	3.12569100	-0.18117900
H	4.24498700	2.74574300	-0.41159400	H	5.05681900	1.53125000	-0.36187400
N	-2.59433400	-1.22587100	-0.29637300	N	-2.08467800	1.68975800	0.06122200
C	-3.70669000	-2.12060800	-0.48534900	C	-2.75951700	2.95405900	0.19177800
H	-4.17799100	-1.95316300	-1.45900000	H	-3.46445200	2.93645500	1.02986600
H	-3.31510100	-3.13680300	-0.43989900	H	-1.99639800	3.71058700	0.37607800
H	-4.45776500	-1.98483000	0.30089200	H	-3.30483800	3.20236100	-0.72489700
C	-2.51061300	2.84372900	0.29160100	C	-3.55923800	-2.12985800	-0.38030200
C	-3.72868500	2.29007200	-0.08164600	C	-4.48515400	-1.09459600	-0.38862900
C	-3.83160800	0.91881400	-0.31229400	C	-4.06069700	0.22616000	-0.24607200
C	-2.68472900	0.15050100	-0.19307300	C	-2.70364000	0.46009100	-0.10286400
C	-1.41696400	0.68941800	0.11671600	C	-1.73153300	-0.56475500	-0.09731800
C	-1.36934500	2.04616100	0.40296700	C	-2.19364800	-1.87409100	-0.23362100
H	-2.44062900	3.90340700	0.51436200	H	-3.89487400	-3.15648500	-0.48319600
H	-4.61020300	2.91708600	-0.16758600	H	-5.54274000	-1.30913500	-0.50240000
H	-4.78309800	0.46131700	-0.56113900	H	-4.77057300	1.04653400	-0.24578000
H	-0.46306700	2.49577300	0.75863600	H	-1.52258000	-2.72102800	-0.21311700
N	2.43992700	1.69995700	-0.02728100	N	2.98648800	1.15703800	-0.13563300
C	4.25048500	0.53990300	-0.71329600	C	4.39715000	-0.59487200	-0.38038800

13. Cartesian coordinates for S_1/S_0 conical intersections of DDIYM and DDPYM optimized with the CASSCF method

Unit of the Cartesian coordinate below is angstrom.

(1) Four different S_1/S_0 CIs for DDIYM

Four S_1/S_0 conical intersections for molecular motor DDIYM were obtained from CASSCF(12,12)/6-31G(d) method implemented in MOLPRO[S3,S4] program. According to the characteristic dihedral angles C5-C2-C1-C3, the four CIs are named ECI(1), ECI(2), ZCI(1) and ZCI(2), respectively. The conical intersections of *E*CI(1) and *E*CI(2) for DDIYM are same as the geometries obtained by Pooler et al.[S5].

*E*CI(1)-DDIYM				*E*CI(2)-DDIYM			
C	0.27004864	1.11525526	-0.60342782	C	0.83906308	1.51029141	-1.28324206
C	1.57301905	0.54790330	-0.42213967	C	1.50532508	0.43926516	-0.59740732
C	2.33435370	-0.55995008	-0.96606145	C	2.36990107	-0.67249570	-0.93229268
C	3.23609296	-0.90733631	0.05631963	C	3.18893661	-0.83683981	0.19755152
N	2.96532239	-0.12733836	1.16527345	N	2.89885755	0.16568087	1.10508777
C	1.89249055	0.71946533	0.88469354	C	1.91927755	0.99703470	0.57932246
C	-1.01010222	0.58708497	-0.23996545	C	-0.57491351	1.74503197	-1.33130696
C	-2.00350669	1.46624957	-0.69961988	C	-0.80377783	3.03509147	-1.83485170
C	-1.41985997	2.72561448	-1.26085657	C	0.48546634	3.71550821	-2.18491122
C	0.07478190	2.41814821	-1.28946207	C	1.52361152	2.60371779	-2.02323296
C	2.38898677	-1.25631253	-2.17060409	C	2.51002732	-1.55110804	-2.00078585
C	3.34708258	-2.26131105	-2.34178584	C	3.45036949	-2.57983115	-1.92932095
C	4.25469732	-2.57069747	-1.33232199	C	4.24378927	-2.74981353	-0.79080181
C	4.20455415	-1.88213029	-0.11815346	C	4.11399241	-1.88252165	0.28857722
C	-1.31412377	-0.65375619	0.39514205	C	-1.62697751	0.89168032	-0.89428246
C	-2.66480869	-0.95786653	0.47855723	C	-2.90764237	1.41145073	-1.03815428
C	-3.65673118	-0.09456336	-0.02225090	C	-3.13724958	2.69848756	-1.55587552
C	-3.35292254	1.12082307	-0.61190648	C	-2.10171012	3.52414252	-1.96873349
C	1.03055770	3.52599341	-0.83672140	C	2.93476922	2.99787113	-1.61229723
O	1.29142225	1.43921362	1.73865698	O	1.52921141	2.09756181	1.06465758
H	4.99268366	-3.33849583	-1.48312546	H	4.95803380	-3.55345294	-0.75041099
H	-1.64239055	3.55878716	-0.60387717	H	0.68882229	4.50011847	-1.46462001
H	-1.82443881	2.96143353	-2.23842106	H	0.46826092	4.16090051	-3.17292874
H	0.37579224	2.09116593	-2.29420573	H	1.58391682	2.04089370	-2.97219163
H	2.04945088	3.19410971	-0.93685799	H	3.59210286	2.14168390	-1.63400303
H	0.84933087	3.77204583	0.19962500	H	2.91912267	3.40192305	-0.61131035
H	0.86418903	4.40294867	-1.45332347	H	3.31057955	3.74237052	-2.30587220
H	1.71459937	-1.02222315	-2.97902700	H	1.89823422	-1.45113231	-2.88314544
H	3.38636944	-2.79587906	-3.27606632	H	3.56107030	-3.25438423	-2.76111859
H	4.89911683	-2.11447283	0.67062406	H	4.72260006	-2.00488768	1.16773631
H	-4.12378398	1.77417151	-0.97486310	H	-2.29430348	4.50399499	-2.36329658
C	3.69716938	-0.10491524	2.39832039	C	3.52861936	0.38295792	2.37441308
H	4.72826156	0.20478206	2.24769569	H	4.60178484	0.52355017	2.26673482
H	3.20760407	0.60190399	3.05215469	H	3.09749931	1.27684897	2.80155570
H	3.70303667	-1.08197913	2.87437030	H	3.35790663	-0.45238753	3.04971930
H	-2.97008985	-1.87431877	0.94740576	H	-3.75145077	0.81832671	-0.73990779
H	-4.68670450	-0.39086204	0.06954716	H	-4.15119189	3.04862017	-1.62931514
C	-0.29330189	-1.56473687	1.02066975	C	-1.43212877	-0.48716052	-0.31399895
H	0.43545891	-1.90726568	0.30207619	H	-0.84526916	-1.11929906	-0.96345477
H	0.23099287	-1.02709201	1.79823477	H	-0.90204982	-0.42753953	0.62490169
H	-0.79443623	-2.42125306	1.45441956	H	-2.39930006	-0.94826780	-0.15382711
*Z*CI(1)-DDIYM				*Z*CI(2)-DDIYM			
C	-0.41096416	-0.32778130	-0.78221617	C	0.81256116	-0.03387378	-0.86494103
C	-0.13150772	0.17106508	0.53387749	C	0.71018439	-0.20945828	0.55341807
C	-1.08693100	1.04090195	1.02178557	C	0.33797143	-1.48398290	0.89072340

C	-1.53207975	-1.52913444	-2.54664314	C	1.84534669	0.18785539	-3.03557810
C	-1.54425068	-1.17552487	-1.06707672	C	2.08612303	-0.12486231	-1.56395471
C	-2.04434946	-2.19413410	-0.05428022	C	3.35252137	0.39154340	-0.89714154
O	-2.03021907	1.60770796	0.42893484	O	0.32121609	-2.52309862	0.18560299
H	-1.30074429	-2.58004566	-2.68376950	H	2.31548591	1.12556914	-3.31137371
H	-2.47869083	-1.33474522	-3.03776981	H	2.22374106	-0.57681117	-3.70577244
H	-2.13577416	-0.21831386	-0.91168634	H	2.01944523	-1.23069929	-1.38882459
H	-2.01348138	-1.78759657	0.94372811	H	3.36336538	0.10579506	0.14210858
H	-1.43225533	-3.08819468	-0.08863963	H	3.40311573	1.47275485	-0.97031003
H	-3.06408236	-2.47139098	-0.29309011	H	4.22018268	-0.01992061	-1.39966413
C	1.00829205	0.38825525	-4.65434587	C	-1.80083892	0.50674898	-4.04527490
C	-0.43277308	-0.65801058	-3.08186169	C	0.35129400	0.28266771	-3.11044724
C	0.19956013	0.05357017	-2.04179060	C	-0.23075434	0.08889469	-1.84585193
H	-0.52835482	-1.01665099	-5.20348875	H	-0.00221665	0.63642161	-5.20151375
C	2.02242514	1.75140361	-1.24714376	C	-2.31996398	-0.26151469	-0.34927323
H	2.01754187	2.79779129	-1.53309848	H	-2.04695805	-1.26130003	-0.03952472
H	1.59735935	1.64740964	-0.26637839	H	-2.02823234	0.42147859	0.43441151
H	3.05653239	1.42068079	-1.22790908	H	-3.39391228	-0.21083442	-0.48281963
H	1.34378003	0.53558954	-5.66494987	H	-2.44202436	0.67725966	-4.89170442
N	-0.87033152	1.13410078	2.39893873	N	-0.11543006	-1.44220290	2.21224047
C	-1.62690437	1.99495114	3.26245963	C	-0.44063180	-2.61188243	2.97582059
H	-0.98631145	2.71253201	3.76841835	H	-1.46827407	-2.58152241	3.32995703
H	-2.34022923	2.52535430	2.65079611	H	-0.31819040	-3.46654820	2.32795561
H	-2.16247100	1.42466261	4.01723555	H	0.21168766	-2.72159765	3.83881254
C	2.05638425	-1.68966513	3.07161958	C	-0.09780274	2.60011467	3.05972555
C	1.59893580	-0.99747383	4.18796246	C	-0.51483576	1.76069860	4.08582640
C	0.61638514	-0.01096078	4.04689204	C	-0.53570493	0.37119075	3.89494945
C	0.10891875	0.24390293	2.78863457	C	-0.14357568	-0.13337112	2.66419689
C	0.57300779	-0.43558416	1.64475925	C	0.31555247	0.70839568	1.61817222
C	1.55568500	-1.41031389	1.79424531	C	0.32525051	2.08071145	1.82248563
H	2.81296221	-2.44723966	3.18618274	H	-0.08602631	3.66560477	3.21380323
H	1.99862371	-1.21725117	5.16201296	H	-0.82458996	2.17391059	5.02963915
H	0.25709345	0.52776066	4.90594835	H	-0.86143917	-0.28372419	4.68382087
H	1.94283973	-1.94610020	0.94261300	H	0.66932803	2.75724631	1.05689393
C	1.26727291	0.95443738	-2.28552428	C	-1.63985566	0.05858880	-1.65297781
C	-0.04341446	-0.48816919	-4.40405814	C	-0.43487777	0.49135840	-4.22916830
C	1.64645122	1.08600417	-3.62311427	C	-2.39603204	0.29137769	-2.79283011
H	2.45254520	1.75299407	-3.86877981	H	-3.46734482	0.28878639	-2.72466184

(2) Two different S_1 /S_0 CIs for DDPYM

Two S_1/S_0 conical intersections for molecular motor DDPYM were obtained from CASSCF(10,9)/6-31G(d) method implemented in MOLPRO[S3,S4] program. According to the characteristic dihedral angles C5-C2-C1-C3, the two CIs are named ECI and ZCI, respectively.

*E*CI-DDPYM				*Z*CI-DDPYM			
C	0.27359461	-0.52111587	-1.01392826	C	-0.55143699	-0.22304712	-1.02189681
C	0.36119727	-0.17462600	0.39066156	C	-0.40484027	0.11383732	0.38023459
C	1.45176384	0.58563363	0.96226813	C	-0.88941688	1.35847804	0.93778145
C	0.46441649	-1.73127550	-3.16269503	C	-1.46054095	-1.05976418	-3.16360292
C	0.82091975	-1.80920761	-1.64144756	C	-1.78025787	-0.89980109	-1.64169737
C	2.31794522	-1.99892496	-1.38137456	C	-2.16606305	-2.21334515	-0.96044763
O	2.42241285	1.06532662	0.41609799	O	-1.43374588	2.28732592	0.37979042
H	1.35867723	-1.73979785	-3.77754027	H	-1.36999787	-2.10709996	-3.43609462
H	-0.14615096	-2.57177478	-3.47643395	H	-2.23859243	-0.63361014	-3.78762294
H	0.29227679	-2.64408070	-1.18655925	H	-2.60330602	-0.19974132	-1.51881333
H	2.52057160	-2.05244628	-0.31912758	H	-2.35656213	-2.06075249	0.09481302
H	2.89093923	-1.17246278	-1.78638963	H	-1.37655166	-2.95277562	-1.05876482
H	2.66392529	-2.92060745	-1.84006573	H	-3.06569742	-2.62213227	-1.41053618
C	-1.31500696	1.51667387	-3.46398411	C	1.77814253	0.72090433	-3.54387282
C	-0.26680233	-0.42733508	-3.28487314	C	-0.15159194	-0.34449032	-3.32048817
C	-0.32330038	0.19886669	-2.02824612	C	0.30132474	0.08584044	-2.06176656
H	-1.04568029	0.24887208	-5.24268694	H	0.76763713	-0.09985259	-5.31845736

C	-1.19673787	2.39134775	-1.12592322	C	2.26954631	1.41083529	-1.19343191
H	-1.73287381	3.22574432	-1.55454549	H	2.52143125	0.71053698	-0.41135924
H	-1.77777195	1.96007821	-0.32443511	H	3.17471177	1.79925363	-1.63748532
H	-0.24668906	2.72912845	-0.73844618	H	1.69047542	2.22163176	-0.77594613
H	-1.83147226	2.38725285	-3.81308754	H	2.66866772	1.18515659	-3.91529931
N	1.17807798	0.70803113	2.31743439	N	-0.59385490	1.32442471	2.29311436
C	2.03276663	1.39869133	3.24475874	C	-0.92144925	2.38398477	3.20816104
H	2.38347308	0.72964411	4.02455458	H	-0.02707732	2.79668271	3.66563052
H	2.88060180	1.77580744	2.69458600	H	-1.42298339	3.15902674	2.65001119
H	1.51269618	2.23016075	3.71126302	H	-1.57972660	2.02952835	3.99535709
C	-2.43112744	-1.27022163	2.73232575	C	1.31980210	-2.31399531	2.75088804
C	-1.88243030	-0.71429422	3.88419683	C	1.17251316	-1.53253616	3.89297023
C	-0.65521305	-0.02506657	3.83537780	C	0.53095713	-0.28058954	3.82853999
C	-0.01790310	0.08324155	2.63277555	C	0.05612152	0.14555961	2.62136704
C	-0.55503098	-0.47815239	1.43992381	C	0.18842798	-0.63555990	1.43818200
C	-1.77552398	-1.15802489	1.50069863	C	0.83216163	-1.87479629	1.51460095
H	-3.36914266	-1.79403972	2.78817954	H	1.81312270	-3.26769981	2.81772044
H	-2.39635209	-0.80965360	4.82366283	H	1.55081062	-1.88319082	4.83622420
H	-0.23801067	0.40217413	4.72966105	H	0.42271431	0.31879907	4.71473330
H	-2.20495706	-1.59264925	0.61473581	H	0.95004597	-2.48533730	0.63653634
N	-0.97612909	1.39991662	-2.16810051	N	1.49843813	0.73935286	-2.22901834
C	-0.89289313	0.39150736	-4.19248026	C	0.77190809	0.04829527	-4.25797441

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