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Electronic Supplementary Information

for

A Comprehensive Study of Isomerization and Protonation Reactions in the Photocycle of Photoactive Yellow Protein

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Contents

1. Computational Details

1.1 Model Setup: The NMR structure of PYP (PDB code: 3PHY) [S1] containing the native chromophore of the p-coumaric acid (pCA) was used to construct the initial QM/MM model. Six Na^+ counterions were added using the xleap module of the AMBER9 package[S2] to neutralize the system in accordance with experimental conditions. The 1046 crystal water molecules in the protein were kept in the model.

1.2 Equilibrium Molecular Dynamics (MD): The initially constructed system was equilibrated for 1 ns using classical canonical MD simulations (at 298 K). The general Amber force field (GAFF), the Amber99 force field,[S2] and the TIP3P water model were used for the chromophore, the amino acid residues of the PYP, and the water molecules, respectively. A cutoff radius of 9.0 Å was used for truncating the electrostatic and van der Waals interactions. All MD simulations were performed with the TINKER4.2 package.[S3] Starting from a MD snapshot, the initial QM/MM structure was manually generated with an appropriate intermolecular hydrogen-bonding network.

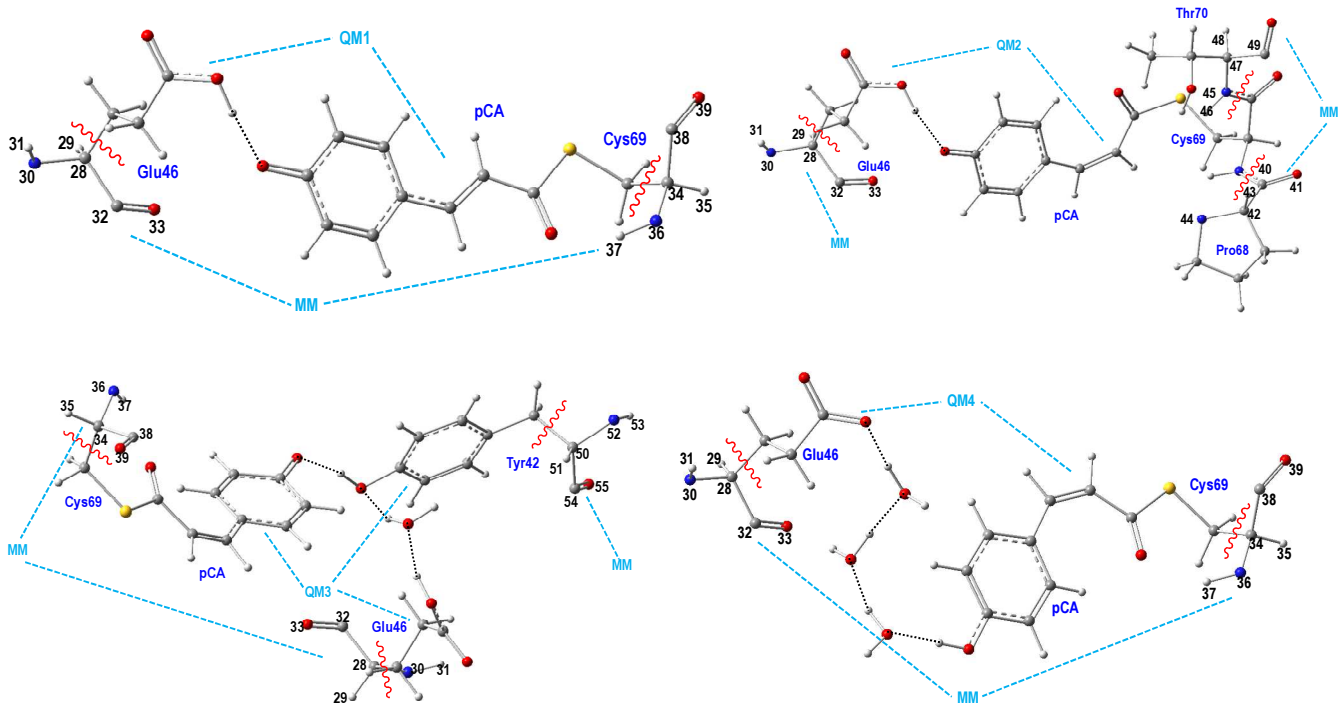
1.3 QM/MM Computational Protocol:

The four QM/MM partitionings are shown in Scheme S1. To explicitly describe the first step of photo-isomerization, the QM1 subsystem (33 atoms) including the pCA chromophore and a portion of the Glu46 and Cys69 residues was used. To comprehensively account for the later isomerization steps of $I_{CP} \rightarrow pR_2$ and $pR_1 \rightarrow pR_2$, as well as subsequent processes involving two typical structural deformations via a simultaneous torsion along the non-adjacent or adjacent two bonds (d/f and d/e), the QM2 subsystem includes the whole Cys69 residue with 40 atoms. To compute the MEPs of the protonation/deprotonation steps, another one and three crystal water molecules have been added to the QM3 and QM4 subsystems, respectively. Moreover, a portion of Tyr42 was also cast into the

QM3 subsystem to account for its role of proton transfer relay. Consequently, the numbers of atoms of QM3 and QM4 increase to 52 and 42. The MM subsystem includes the remaining residues, water molecules, and counterions. The boundary separating the QM and MM regions was treated by the hydrogen link-atom scheme (the wavy lines in Scheme S1). To reduce the strong electrostatic interactions between a link atom and its nearest MM atoms, some point charges were set to zero, and the neighboring MM point charges were re-parameterized (Table S1). For the remaining MM atoms, standard force-field point charges were used.

1.3.1 QM Method: The calculations of the QM parts were conducted at the complete active space self-consistent field (CASSCF) level of theory with appropriate basis sets and active spaces. The constrained minimum energy profiles (MEPs) for the isomerization and proton transfer reactions were computed by stepwise optimizations at the CASSCF level of theory with a 14e/11o active space using the 6-31G* basis set. To describe proton transfer at the ground state, the corresponding donor σ/σ* orbital and the acceptor n orbital were included in the active space. The rest of 10e/9o came from the high-lying occupied π and the low-lying π* orbitals that are mainly distributed in the phenoxy ring of pCA.

Geometry optimizations were performed using a 2-root state-averaged CASSCF approach (S_0 and S_1, equal weights) for the S_1 state and a state-specific approach for the S_0 state. Single-point energies at all optimized structures were determined from the 4-root state-averaged CASPT2//CASSCF calculations to include more dynamical electron correlation. These calculations were performed without an ionization potential-electron affinity (IPEA) shift but included an energy-level shift of 0.2 a.u. to avoid intruder state problems.



Scheme S1. *The chosen QM/MM partitioning: QM1: pCA + a portion of the Glu46 and Cys69 residues; QM2: pCA + a portion of the Glu46 residue + the Cys69 residue; QM3: pCA + a portion of the Glu46, Cys69, Tyr42 residue + one crystal water molecule; QM4: pCA + a portion of the residue Glu46, Cys69 + three crystal water molecules; the MM subsystem includes the other amino acid residues, counterions, and water molecules. See texts for details.*

Table S1. *Re-parameterized point charges (a.u.) for the MM atoms near the QM/MM boundary.*

C28	0.0000	C40	0.0000	C50	0.0000
H29	0.1144	O41	-0.3748	H51	0.1144
N30	-0.4157	C42	0.0130	N52	-0.4157
H31	0.2719	H43	0.2641	H53	0.2719
C32	0.5973	N44	-0.1048	C54	0.5973
O33	-0.5679	N45	0.0000	O55	-0.5679
C34	0.0000	H46	0.0719		
H35	0.1144	C47	-0.0546		
N36	-0.4157	H48	0.0007		

H37	0.2719	C49	0.4973
C38	0.5973		
O39	-0.5679		

1.3.2 Vertical Excitation Energies: Vertical excitation energies, oscillator strengths and transition dipole moments to the three lowest excited singlet states of QM1 at the Franck-Condon (FC) point were computed using the CASPT2//CASSCF and CASSI//CASSCF methods at the CASSCF-optimized S_0 minimum.

1.3.3 Optimizations of Minima, Intermediates and Minimum Energy Paths: The local minima and intermediates for the S_0 and S_1 states were fully optimized at the QM (CASSCF)/AMBER level. At the same computational level, the minimum-energy paths for the isomerization and the proton transfer reaction were also computed using reaction-coordinate-constrained optimizations, in which the chosen reaction coordinate was fixed at a given value and all remaining degrees of freedom were fully relaxed.

1.3.4 Program Packages: The CASSCF calculations were performed using GAUSSIAN03.[S4] The CASPT2 and CASSI calculations were performed using MOLCAS7.6,[S5] whereas the MM calculations were conducted under the AMBER99[S2] force field using TINKER4.2.[S3] The interface between the QM and MM parts was coded by Ferré et al. and included in the Molcas program.[S6]

2. References

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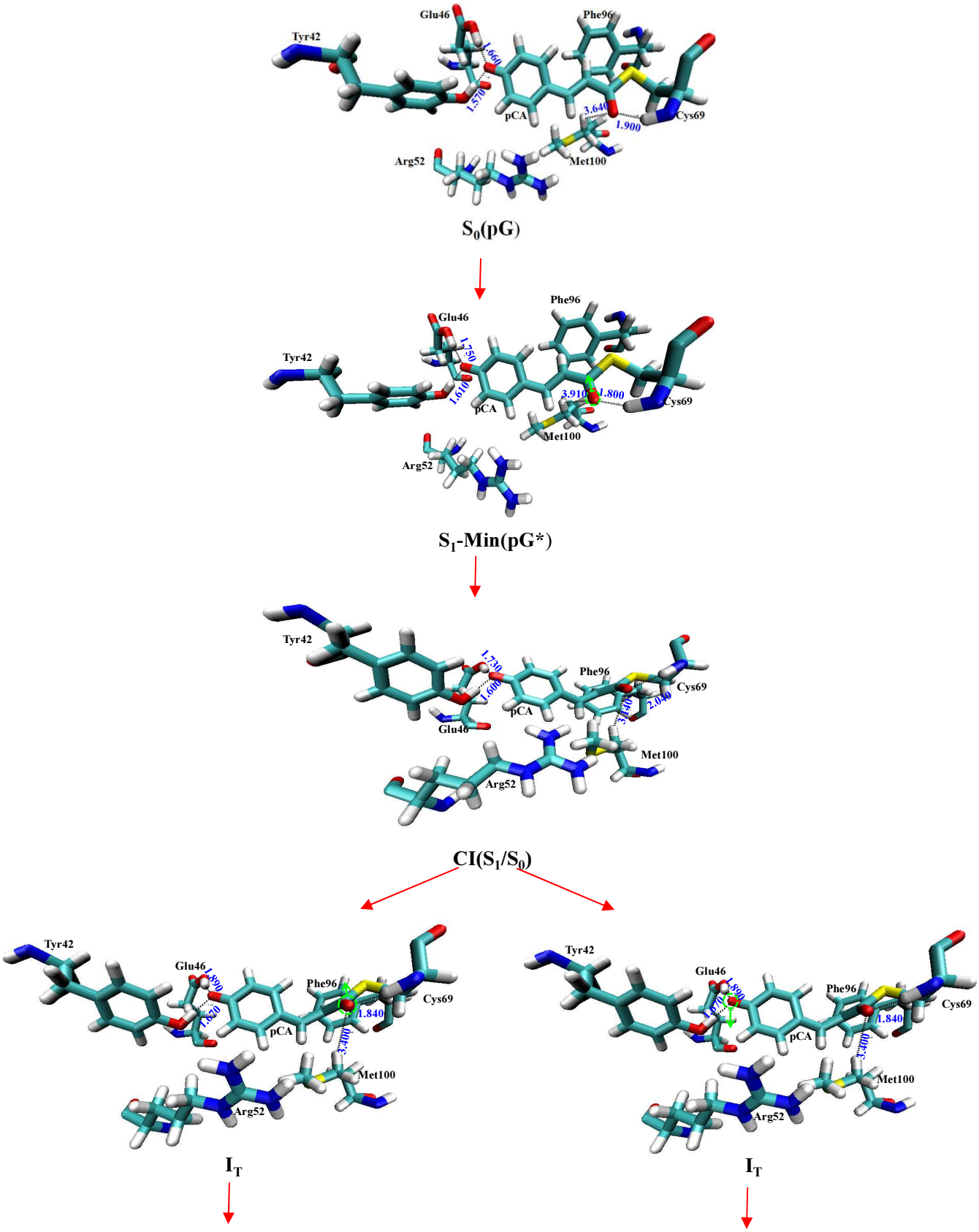
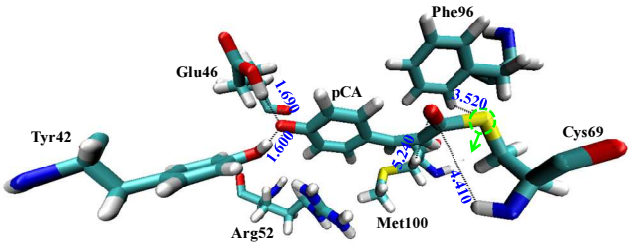
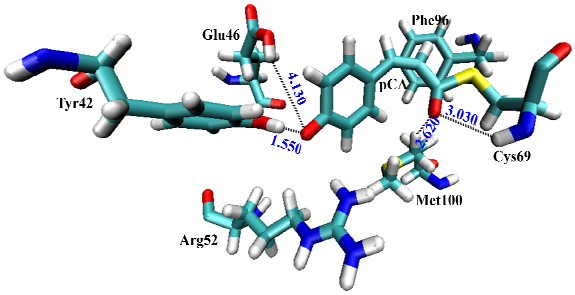
3. Figures

Figure S3-1. The structural evolvement of the binding pocket in photocycle of PYP.

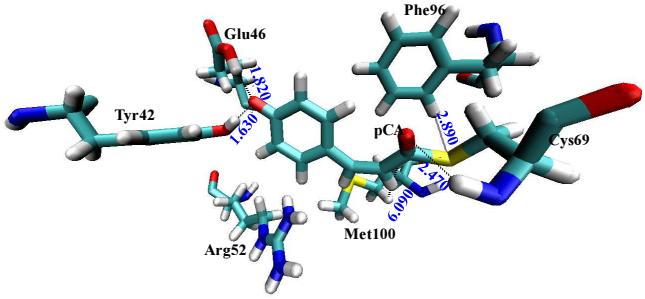




I_{CP}



pR_1



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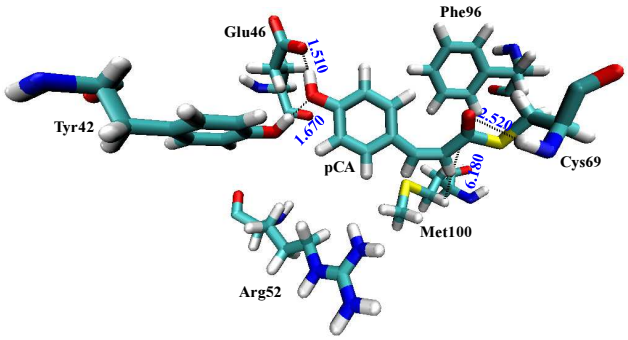
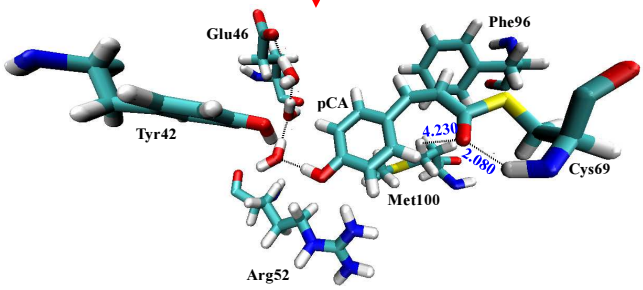
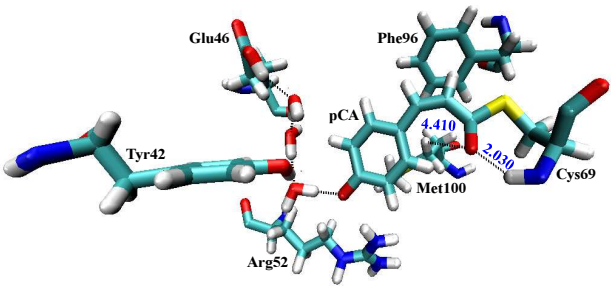


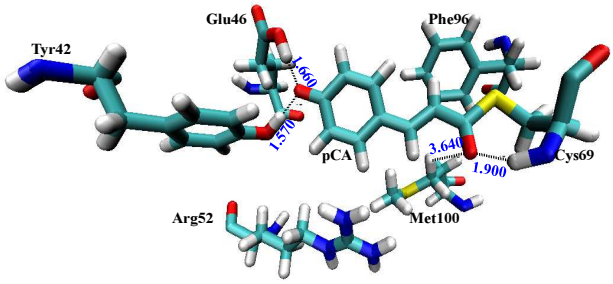
pB'



pB


Glu46
Phe96
pCA
4.410
2.030
Tyr42
Cys69
Met100
Arg52

pG'


Glu46
Phe96
Tyr42
1.660
1.570
pCA
3.640
1.900
Cys69
Arg52
Met100

S_0(pG)

4. Tables

Table S4-1. *Vertical excitation energies ($E_{\perp}$, eV), oscillator strengths (f), transition dipole moments (D.M., Debye), and the characters of singly occupied orbitals of different transitions at the Franck-Condon (FC) geometrie for PYP. The values were computed with the 4-root state-average CASPT2//CASSCF(14e,11o)/AMBER method.*

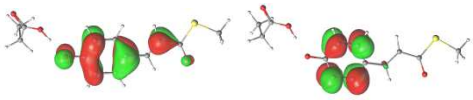
state	$E_{\perp}$	*f*	*D.M.*	*singly occupied orbitals*
S_0			33.21	
S_1	2.88(431nm)	1.059	40.05	
S_2	3.93	0.050	32.56	
S_3	4.57	0.050	39.95	

Table S4-2*. Absolute energies (A.E., hartree), relative energies (ΔE, kcal/mol), and MM energies (hartree) of optimized structures for initial excited state relaxation along the reaction coordinate of C9-C10-C11-C12 dihedral angle(°) in PYP. The corresponding energy profiles are plotted in Figure 2 of the main article.*

C9C10C11C12	**CASPT2 A.E.**	**MM part**	**ΔE**
S_0-min(170.3°)			
Root1 (S_0)	-1200.527041	-28.167790	0
Root2 ($S_1(^1\pi\pi^*)$)	-1200.421290		66.4
Root3	-1200.382426		90.7
Root4	-1200.358930		105.5
S_1-min(155.5°)			
Root1 (S_0)	-1200.515266	-28.168868	6.7
Root2 ($S_1(^1\pi\pi^*)$)	-1200.426049		62.7
Root3	-1200.373523		95.7
Root4	-1200.357454		105.7
S_1-(150°)			
Root1 (S_0)	-1200.510706	-28.169752	9.0
Root2 ($S_1(^1\pi\pi^*)$)	-1200.424819		62.9
Root3	-1200.372740		95.6

Root4	-1200.353770		107.5
S_1-(145°)			
Root1 (S_0)	-1200.507475	-28.170155	10.8
Root2 ($S_1(^1\pi\pi^*)$)	-1200.424510		62.8
Root3	-1200.372819		95.3
Root4	-1200.351532		108.6
S_1-(135°)			
Root1 (S_0)	-1200.499501	-28.176536	11.8
Root2 ($S_1(^1\pi\pi^*)$)	-1200.423685		59.3
Root3	-1200.371533		92.1
Root4	-1200.346698		107.7
S_1-(130°)			
Root1 (S_0)	-1200.494666	-28.176180	15.1
Root2 ($S_1(^1\pi\pi^*)$)	-1200.423168		59.9
Root3	-1200.370217		93.1
Root4	-1200.343212		110.1
S_1-(125°)			
Root1 (S_0)	-1200.489192	-28.176395	18.4
Root2 ($S_1(^1\pi\pi^*)$)	-1200.422975		59.9
Root3	-1200.367891		94.4
Root4	-1200.339099		112.5
S_1-(120°)			
Root1 (S_0)	-1200.480195	-28.174463	25.2
Root2 ($S_1(^1\pi\pi^*)$)	-1200.423912		60.5
Root3	-1200.362428		99.1
Root4	-1200.331988		118.2
S_1-(115°)			
Root1 (S_0)	-1200.460898	-28.171869	38.9
Root2 ($S_1(^1\pi\pi^*)$)	-1200.429356		58.7
Root3	-1200.351798		107.4
Root4	-1200.317181		129.1
S_1-(110°)			
Root1 (S_0)	-1200.442327	-28.174583	48.9
Root2 ($S_1(^1\pi\pi^*)$)	-1200.430277		56.5
Root3	-1200.344080		110.5
Root4	-1200.317325		127.3
S_1-(105°)			
Root1 (S_0)	-1200.443464	-28.180674	44.4
Root2 ($S_1(^1\pi\pi^*)$)	-1200.430953		52.24
Root3	-1200.342955		107.44
Root4	-1200.324869		118.74
S_1-(100°)			
Root1 (S_0)	-1200.442202	-28.180215	45.4
Root2 ($S_1(^1\pi\pi^*)$)	-1200.431152		52.4
Root3	-1200.342284		108.1
Root4	-1200.327690		117.3
S_1-(95°)			
Root1 (S_0)	-1200.441184	-28.180118	46.1
Root2 ($S_1(^1\pi\pi^*)$)	-1200.430484		52.8

Root3	-1200.341169		108.9
Root4	-1200.328492		116.8
S_1-(90°)			
Root1 (S_0)	-1200.439983	-28.180847	46.4
Root2 ($S_1(^1\pi\pi^*)$)	-1200.429247		53.2
Root3	-1200.339840		109.3
Root4	-1200.329574		115.7
CI(S_1/S_0)-(85°)			
Root1 (S_0)	-1200.430265	-28.180023	53.0
Root2 ($S_1(^1\pi\pi^*)$)	-1200.435536		49.7
Root3	-1200.338231		110.8
Root4	-1200.324136		119.6
S_1-(80°)			
Root1 (S_0)	-1200.436677	-28.179502	49.3
Root2 ($S_1(^1\pi\pi^*)$)	-1200.426471		55.7
Root3	-1200.338193		111.1
Root4	-1200.318237		123.7
S_1-(75°)			
Root1 (S_0)	-1200.433430	-28.179968	51.1
Root2 ($S_1(^1\pi\pi^*)$)	-1200.424271		56.8
Root3	-1200.336145		112.1
Root4	-1200.317167		124.0
S_1-(70°)			
Root1 (S_0)	-1200.432017	-28.180116	51.9
Root2 ($S_1(^1\pi\pi^*)$)	-1200.422398		57.9
Root3	-1200.334494		113.1
Root4	-1200.316406		124.4
S_1-(65°)			
Root1 (S_0)	-1200.428825	-28.179916	54.0
Root2 ($S_1(^1\pi\pi^*)$)	-1200.419005		60.2
Root3	-1200.331083		115.3
Root4	-1200.316691		124.4
S_1-(60°)			
Root1 (S_0)	-1200.425952	-28.179413	56.1
Root2 ($S_1(^1\pi\pi^*)$)	-1200.415751		62.5
Root3	-1200.328065		117.5
Root4	-1200.315511		125.4
S_1-(55°)			
Root1 (S_0)	-1200.423297	-28.179399	57.8
Root2 ($S_1(^1\pi\pi^*)$)	-1200.412379		64.6
Root3	-1200.324887		119.5
Root4	-1200.315526		125.4
S_1-(50°)			
Root1 (S_0)	-1200.421286	-28.179691	58.9
Root2 ($S_1(^1\pi\pi^*)$)	-1200.408700		66.8
Root3	-1200.322046		121.2
Root4	-1200.313963		126.2
S_1-(45°)			
Root1 (S_0)	-1200.419595	-28.179217	60.3

Root2 ($S_1(^1\pi\pi^*)$)	-1200.404733		69.6
Root3	-1200.319526		123.0
Root4	-1200.312765		127.3
S_1-(40°)			
Root1 (S_0)	-1200.416833	-28.179634	61.7
Root2 ($S_1(^1\pi\pi^*)$)	-1200.399758		72.4
Root3	-1200.316883		124.4
Root4	-1200.303701		132.7

***Table S4-2-(I)**. Absolute energies (A.E., hartree), relative energies (ΔE, kcal/mol), and MM energies (hartree) of optimized structures for ground state relaxation of photoisomerization along the reaction coordinate of C8-C9-C10-C11 and C9-C10-C11-C12 dihedral angle(°) in PYP. The corresponding energy profiles are plotted in Figure 2-(I) of the main article.*

C8C9C10C11 C9C10C11C12	**CASPT2 A.E.**	**MM part**	**ΔE**
S_0- (80°)			
Root1 (S_0)	-1200.450041	-28.174844	43.9
Root2 ($S_1(^1\pi\pi^*)$)	-1200.408313		70.1
Root3	-1200.282033		149.3
Root4	-1200.295490		140.9
S_0-(75°)			
Root1 (S_0)	-1200.448316	-28.174266	45.3
Root2 ($S_1(^1\pi\pi^*)$)	-1200.402582		74.0
Root3	-1200.285581		147.5
Root4	-1200.295308		141.4
S_0-(70°)			
Root1 (S_0)	-1200.445425	-28.174453	47.0
Root2 ($S_1(^1\pi\pi^*)$)	-1200.394241		79.2
Root3	-1200.288554		145.5
Root4	-1200.290304		144.4
S_0-(65°)			
Root1 (S_0)	-1200.443738	-28.17442	48.1
Root2 ($S_1(^1\pi\pi^*)$)	-1200.387965		83.1
Root3	-1200.293245		142.5
Root4	-1200.289827		144.7
S_0-(60°)			
Root1 (S_0)	-1200.440302	-28.173357	50.9
Root2 ($S_1(^1\pi\pi^*)$)	-1200.378246		89.9
Root3	-1200.294707		142.3
Root4	-1200.285754		147.9
S_0-(55°)			
Root1 (S_0)	-1200.443454	-28.174294	48.4
Root2 ($S_1(^1\pi\pi^*)$)	-1200.374927		91.4

Root3	-1200.304710		135.4
Root4	-1200.288390		145.7
S_0-(50°)			
Root1 (S_0)	-1200.441307	-28.176702	48.2
Root2 ($S_1(^1\pi\pi^*)$)	-1200.368555		93.9
Root3	-1200.301570		135.9
Root4	-1200.289140		143.7
S_0-(45°)			
Root1 (S_0)	-1200.442971	-28.177059	46.9
Root2 ($S_1(^1\pi\pi^*)$)	-1200.367418		94.3
Root3	-1200.293262		140.9
Root4	-1200.301601		135.6
S_0-(40°)			
Root1 (S_0)	-1200.448134	-28.174781	45.1
Root2 ($S_1(^1\pi\pi^*)$)	-1200.365705		96.9
Root3	-1200.289586		144.6
Root4	-1200.299060		138.7
S_0-(35°)			
Root1 (S_0)	-1200.452489	-28.178131	40.3
Root2 ($S_1(^1\pi\pi^*)$)	-1200.369559		92.3
Root3	-1200.291359		141.4
Root4	-1200.308654		130.6
S_0-(30°)			
Root1 (S_0)	-1200.444410	-28.190357	37.7
Root2 ($S_1(^1\pi\pi^*)$)	-1200.372144		83.0
Root3	-1200.291482		133.7
Root4	-1200.303131		126.3
S_0-(25°)			
Root1 (S_0)	-1200.446394	-28.188511	37.6
Root2 ($S_1(^1\pi\pi^*)$)	-1200.372117		84.2
Root3	-1200.290961		135.1
Root4	-1200.306315		125.5
S_0-(20°)			
Root1 (S_0)	-1200.447345	-28.188119	37.3
Root2 ($S_1(^1\pi\pi^*)$)	-1200.374729		82.8
Root3	-1200.293151		134.0
Root4	-1200.309209		123.9
S_0-(15°)			
Root1 (S_0)	-1200.447149	-28.190418	35.9
Root2 ($S_1(^1\pi\pi^*)$)	-1200.374784		81.3
Root3	-1200.293045		132.6
Root4	-1200.309226		122.5
S_0-(10°)			
Root1 (S_0)	-1200.446808	-28.192861	34.6
Root2 ($S_1(^1\pi\pi^*)$)	-1200.375905		79.1
Root3	-1200.293798		130.6
Root4	-1200.309269		120.9
S_0-(5°)			
Root1 (S_0)	-1200.451621	-28.192601	31.8

Root2 ($S_1(^1\pi\pi^*)$)	-1200.376926		78.6
Root3	-1200.295910		129.5
Root4	-1200.312454		119.1
S_0-(0°)			
Root1 (S_0)	-1200.453110	-28.194486	29.6
Root2 ($S_1(^1\pi\pi^*)$)	-1200.378095		76.7
Root3	-1200.297324		127.4
Root4	-1200.313610		117.2
S_0-(-9.6°)			
Root1 (S_0)	-1200.472898	-28.184370	23.6
Root2 ($S_1(^1\pi\pi^*)$)	-1200.379944		81.9
Root3	-1200.323978		117.0
Root4	-1200.327529		114.8

***Table S4-2-(II)**. Absolute energies (A.E., hartree), relative energies (⊿E, kcal/mol), and MM energies (hartree) of optimized structures for ground state relaxation of photoisomerization along the reaction coordinate of C9-C10-C11-C12 and C11-C12-S13-C14 dihedral angle(°) in PYP. The corresponding energy profiles are plotted in Figure 2-(II) of the main article.*

C9C10C11C12 C11C12S13C14	**CASPT2 A.E.**	**MM part**	**ΔE**
S_0-(80°)			
Root1 (S_0)	-1200.449224	-28.179779	41.3
Root2 ($S_1(^1\pi\pi^*)$)	-1200.408851		66.6
Root3	-1200.278605		148.4
Root4	-1200.295739		137.6
S_0-(75°)			
Root1 (S_0)	-1200.452839	-28.174501	42.3
Root2 ($S_1(^1\pi\pi^*)$)	-1200.405437		72.1
Root3	-1200.323079		123.7
Root4	-1200.288707		145.3
S_0-(70°)			
Root1 (S_0)	-1200.451882	-28.170052	45.7
Root2 ($S_1(^1\pi\pi^*)$)	-1200.403422		76.1
Root3	-1200.292962		145.4
Root4	-1200.301682		140.0
S_0-(65°)			
Root1 (S_0)	-1200.457913	-28.164088	45.7
Root2 ($S_1(^1\pi\pi^*)$)	-1200.400716		81.6
Root3	-1200.324133		129.6
Root4	-1200.292575		149.4
S_0-(60°)			
Root1 (S_0)	-1200.469460	-28.169439	35.1
Root2 ($S_1(^1\pi\pi^*)$)	-1200.398379		79.7

Root3	-1200.336241		118.7
Root4	-1200.305861		137.8
S_0-(55°)			
Root1 (S_0)	-1200.477653	-28.179914	23.4
Root2 ($S_1(^1\pi\pi^*)$)	-1200.398559		73.0
Root3	-1200.343801		107.4
Root4	-1200.316092		124.8
S_0-(50°)			
Root1 (S_0)	-1200.478490	-28.185060	19.6
Root2 ($S_1(^1\pi\pi^*)$)	-1200.390142		75.1
Root3	-1200.321332		118.2
Root4	-1200.327883		114.1
S_0-(45°)			
Root1 (S_0)	-1200.484505	-28.184874	16.0
Root2 ($S_1(^1\pi\pi^*)$)	-1200.388657		76.1
Root3	-1200.336421		108.9
Root4	-1200.330302		112.7
S_0-(40°)			
Root1 (S_0)	-1200.485767	-28.185681	14.7
Root2 ($S_1(^1\pi\pi^*)$)	-1200.390796		74.3
Root3	-1200.337147		107.9
Root4	-1200.331985		111.2
S_0-(35°)			
Root1 (S_0)	-1200.486302	-28.184922	14.8
Root2 ($S_1(^1\pi\pi^*)$)	-1200.391212		74.5
Root3	-1200.338175		107.8
Root4	-1200.332359		111.4
S_0-(30°)			
Root1 (S_0)	-1200.488202	-28.184863	13.7
Root2 ($S_1(^1\pi\pi^*)$)	-1200.394032		72.8
Root3	-1200.338767		107.4
Root4	-1200.333967		110.4
S_0-(25°)			
Root1 (S_0)	-1200.489531	-28.185203	12.6
Root2 ($S_1(^1\pi\pi^*)$)	-1200.395554		71.6
Root3	-1200.339705		106.6
Root4	-1200.334720		109.8
S_0-(20°)			
Root1 (S_0)	-1200.490305	-28.185228	12.1
Root2 ($S_1(^1\pi\pi^*)$)	-1200.396986		70.7
Root3	-1200.340040		106.4
Root4	-1200.335003		109.6
S_0-(15°)			
Root1 (S_0)	-1200.490858	-28.186945	10.7
Root2 ($S_1(^1\pi\pi^*)$)	-1200.398527		68.6
Root3	-1200.340053		105.3
Root4	-1200.334837		108.6
S_0-(10°)			
Root1 (S_0)	-1200.491899	-28.188541	9.0

Root2 ($S_1(^1\pi\pi^*)$)	-1200.398918		67.4
Root3	-1200.340432		104.1
Root4	-1200.334716		107.7
S_0-(5°)			
Root1 (S_0)	-1200.497236	-28.190311	4.6
Root2 ($S_1(^1\pi\pi^*)$)	-1200.399281		66.0
Root3	-1200.343916		100.8
Root4	-1200.338045		104.5
S_0-(0°)			
Root1 (S_0)	-1200.498805	-28.192148	2.4
Root2 ($S_1(^1\pi\pi^*)$)	-1200.399290		64.9
Root3	-1200.345445		98.7
Root4	-1200.339375		102.5

***Table S4-2-(III)**. Absolute energies (A.E., hartree), relative energies (⊿E, kcal/mol), and MM energies (hartree) of optimized structures for ground state relaxation of photoisomerization along the reaction coordinate of C9-C10-C11-C12 and C11-C12-S13-C14 dihedral angle(°) in PYP. The corresponding energy profiles are plotted in Figure 2-(III) of the main article.*

(OBF)C9C10C11C12	**CASPT2 A.E.**	**MM part**	**ΔE**
S_0- (80°)			
Root1 (S_0)	-1200.449486	-28.172972	45.4
Root2 ($S_1(^1\pi\pi^*)$)	-1200.409095		70.8
Root3	-1200.279174		152.3
Root4	-1200.295082		142.3
S_0-(75°)			
Root1 (S_0)	-1200.449183	-28.171141	46.8
Root2 ($S_1(^1\pi\pi^*)$)	-1200.406571		73.5
Root3	-1200.281776		151.8
Root4	-1200.299512		140.7
S_0-(70°)			
Root1 (S_0)	-1200.449429	-28.167898	48.6
Root2 ($S_1(^1\pi\pi^*)$)	-1200.402676		78.0
Root3	-1200.293876		146.2
Root4	-1200.294896		145.6
S_0-(65°)			
Root1 (S_0)	-1200.462417	-28.171206	38.4
Root2 ($S_1(^1\pi\pi^*)$)	-1200.401285		76.8
Root3	-1200.328172		122.6
Root4	-1200.297847		141.7
S_0-(60°)			
Root1 (S_0)	-1200.469888	-28.172478	32.9
Root2 ($S_1(^1\pi\pi^*)$)	-1200.397924		78.1

Root3	-1200.336208		116.8
Root4	-1200.306266		135.6
S_0-(55°)			
Root1 (S_0)	-1200.475573	-28.17342	28.8
Root2 ($S_1(^1\pi\pi^*)$)	-1200.396904		78.1
Root3	-1200.340864		113.3
Root4	-1200.312657		131.0
S_0-(50°)			
Root1 (S_0)	-1200.479343	-28.181937	21.1
Root2 ($S_1(^1\pi\pi^*)$)	-1200.378376		84.4
Root3	-1200.335972		111.0
Root4	-1200.320779		120.6
S_0-(45°)			
Root1 (S_0)	-1200.479670	-28.183323	20.0
Root2 ($S_1(^1\pi\pi^*)$)	-1200.375171		85.6
Root3	-1200.336321		109.9
Root4	-1200.317581		121.7
S_0-(40°)			
Root1 (S_0)	-1200.481302	-28.182044	19.8
Root2 ($S_1(^1\pi\pi^*)$)	-1200.376688		85.4
Root3	-1200.337968		109.7
Root4	-1200.318382		122.0
S_0-(35°)			
Root1 (S_0)	-1200.481052	-28.182378	19.7
Root2 ($S_1(^1\pi\pi^*)$)	-1200.373940		86.9
Root3	-1200.337462		109.8
Root4	-1200.314767		124.1
S_0-(30°)			
Root1 (S_0)	-1200.480636	-28.183310	19.4
Root2 ($S_1(^1\pi\pi^*)$)	-1200.371832		87.7
Root3	-1200.336541		109.8
Root4	-1200.311650		125.4
S_0-(25°)			
Root1 (S_0)	-1200.481196	-28.182282	19.7
Root2 ($S_1(^1\pi\pi^*)$)	-1200.372042		88.2
Root3	-1200.336865		110.2
Root4	-1200.311773		126.0
S_0-(20°)			
Root1 (S_0)	-1200.481617	-28.180622	20.5
Root2 ($S_1(^1\pi\pi^*)$)	-1200.370621		90.1
Root3	-1200.336966		111.2
Root4	-1200.309176		128.7
S_0-(15°)			
Root1 (S_0)	-1200.479920	-28.181571	20.9
Root2 ($S_1(^1\pi\pi^*)$)	-1200.366034		92.4
Root3	-1200.334340		112.3
Root4	-1200.302085		132.5
S_0-(10°)			
Root1 (S_0)	-1200.479846	-28.18118	21.2

Root2 ($S_1(^1\pi\pi^*)$)	-1200.365881		92.7
Root3	-1200.334181		112.6
Root4	-1200.302192		132.7
S_0-(8.8°)			
Root1 (S_0)	-1200.478848	-28.182332	21.1
Root2 ($S_1(^1\pi\pi^*)$)	-1200.364891		92.6
Root3	-1200.332778		112.8
Root4	-1200.299056		133.9
(OBF)C11C12S13C14	**CASPT2 A.E.**	**MM part**	**ΔE**
S_0-(-130°)			
Root1 (S_0)	-1200.479940	-28.183422	19.7
Root2 ($S_1(^1\pi\pi^*)$)	-1200.364500		92.2
Root3	-1200.334035		111.3
Root4	-1200.299418		133.0
S_0-(-125°)			
Root1 (S_0)	-1200.480798	-28.182491	19.8
Root2 ($S_1(^1\pi\pi^*)$)	-1200.364485		92.8
Root3	-1200.335216		111.1
Root4	-1200.299850		133.3
S_0-(-120°)			
Root1 (S_0)	-1200.479657	-28.182508	20.5
Root2 ($S_1(^1\pi\pi^*)$)	-1200.360139		95.5
Root3	-1200.333694		112.1
Root4	-1200.295203		136.2
S_0-(-115°)			
Root1 (S_0)	-1200.479044	-28.180962	21.9
Root2 ($S_1(^1\pi\pi^*)$)	-1200.356877		98.5
Root3	-1200.334116		112.8
Root4	-1200.292564		138.9
S_0-(-110°)			
Root1 (S_0)	-1200.478629	-28.179392	23.1
Root2 ($S_1(^1\pi\pi^*)$)	-1200.354889		100.7
Root3	-1200.334711		113.4
Root4	-1200.290565		141.1
S_0-(-105°)			
Root1 (S_0)	-1200.478084	-28.177195	24.8
Root2 ($S_1(^1\pi\pi^*)$)	-1200.352859		103.4
Root3	-1200.338221		112.6
Root4	-1200.289491		143.2
S_0-(-100°)			
Root1 (S_0)	-1200.477145	-28.175576	26.4
Root2 ($S_1(^1\pi\pi^*)$)	-1200.349888		106.3
Root3	-1200.340286		112.3
Root4	-1200.286558		146.0
S_0-(-95°)			
Root1 (S_0)	-1200.476780	-28.173367	28.0
Root2 ($S_1(^1\pi\pi^*)$)	-1200.350925		107.0
Root3	-1200.341634		112.8

Root4	-1200.288111		146.4
S_0-(-90°)			
Root1 (S_0)	-1200.475430	-28.169649	31.2
Root2 ($S_1(^1\pi\pi^*)$)	-1200.344553		113.3
Root3	-1200.352853		108.1
Root4	-1200.282036		152.6
S_0-(-85°)			
Root1 (S_0)	-1200.473122	-28.16797	33.7
Root2 ($S_1(^1\pi\pi^*)$)	-1200.337449		118.9
Root3	-1200.389264		86.3
Root4	-1200.275070		158.0
S_0-(-80°)			
Root1 (S_0)	-1200.473567	-28.163913	36.0
Root2 ($S_1(^1\pi\pi^*)$)	-1200.341290		119.0
Root3	-1200.360508		106.9
Root4	-1200.279017		158.1
S_0-(-75°)			
Root1 (S_0)	-1200.472643	-28.162043	37.7
Root2 ($S_1(^1\pi\pi^*)$)	-1200.341230		120.2
Root3	-1200.340989		120.4
S_0-(-70°)			
Root1 (S_0)	-1200.472228	-28.157918	40.6
Root2 ($S_1(^1\pi\pi^*)$)	-1200.340408		123.3
Root3	-1200.359331		111.4
Root4	-1200.277410		162.8
S_0-(-65°)			
Root1 (S_0)	-1200.473324	-28.158179	39.7
Root2 ($S_1(^1\pi\pi^*)$)	-1200.348529		118.0
Root3	-1200.340202		123.3
Root4	-1200.285317		157.7
S_0-(-60°)			
Root1 (S_0)	-1200.495406	-28.185342	8.8
Root2 ($S_1(^1\pi\pi^*)$)	-1200.394851		71.9
Root3	-1200.342663		104.7
Root4	-1200.334764		109.6
S_0-(-55°)			
Root1 (S_0)	-1200.499311	-28.187677	4.9
Root2 ($S_1(^1\pi\pi^*)$)	-1200.398634		68.1
Root3	-1200.346041		101.1
Root4	-1200.338971		105.5

***Table S4-3-(I)**. Absolute energies (A.E., hartree), relative energies (∆E, kcal/mol), and MM energies (hartree) of optimized structures for ground state relaxation of BP isomerization along the reaction coordinate of C11-C12-S13-C14 and S13-C14-C15-C16 dihedral angle(°) in PYP. The corresponding energy profiles are plotted in Figure 3 of the main article.*

(BP) C11C12S13C14 S13C14C15C16	CASPT2 A.E.	MM part	ΔE
S_0- (-55°)			
Root1 (S_0)	-1407.852591	-28.191908	0.0
Root2 ($S_1(^1\pi\pi^*)$)	-1407.757244		59.8
Root3	-1407.696373		98.0
Root4	-1407.690397		101.8
S_0-(-60°)			
Root1 (S_0)	-1407.858980	-28.180427	3.2
Root2 ($S_1(^1\pi\pi^*)$)	-1407.766104		61.5
Root3	-1407.704596		100.1
Root4	-1407.697510		104.5
S_0-(-70°)			
Root1 (S_0)	-1407.858221	-28.175947	6.5
Root2 ($S_1(^1\pi\pi^*)$)	-1407.766736		63.9
Root3	-1407.706558		101.7
Root4	-1407.700792		105.3
S_0-(-80°)			
Root1 (S_0)	-1407.858081	-28.170274	10.1
Root2 ($S_1(^1\pi\pi^*)$)	-1407.773261		63.4
Root3	-1407.707981		104.3
Root4	-1407.703967		106.8
S_0-(-90°)			
Root1 (S_0)	-1407.853267	-28.173559	11.1
Root2 ($S_1(^1\pi\pi^*)$)	-1407.767552		64.9
Root3	-1407.702117		105.9
Root4	-1407.699913		107.3
S_0-(-100°)			
Root1 (S_0)	-1407.851199	-28.173837	12.2
Root2 ($S_1(^1\pi\pi^*)$)	-1407.764266		66.8
Root3	-1407.700247		106.9
Root4	-1407.697348		108.8
S_0-(-110°)			
Root1 (S_0)	-1407.844847	-28.17378	16.2
Root2 ($S_1(^1\pi\pi^*)$)	-1407.754837		72.7
Root3	-1407.693932		110.9
Root4	-1407.692441		111.9
S_0-(-120°)			
Root1 (S_0)	-1407.845545	-28.178365	12.9
Root2 ($S_1(^1\pi\pi^*)$)	-1407.754976		69.8
Root3	-1407.689227		111.0
Root4	-1407.689925		110.6
S_0-(-130°)			
Root1 (S_0)	-1407.847671	-28.179951	10.6
Root2 ($S_1(^1\pi\pi^*)$)	-1407.754693		68.9
Root3	-1407.690880		109.0
Root4	-1407.690537		109.2

S_0-(-140°)			
Root1 (S_0)	-1407.850729	-28.18523	5.4
Root2 ($S_1(^1\pi\pi^*)$)	-1407.755955		64.8
Root3	-1407.694418		103.4
Root4	-1407.692907		104.4
S_0-(-150°)			
Root1 (S_0)	-1407.853960	-28.188307	1.4
Root2 ($S_1(^1\pi\pi^*)$)	-1407.757885		61.7
Root3	-1407.698245		99.1
Root4	-1407.696503		100.2
S_0-(-160°)			
Root1 (S_0)	-1407.859380	-28.196450	-7.1
Root2 ($S_1(^1\pi\pi^*)$)	-1407.761785		54.1
Root3	-1407.702682		91.2
Root4	-1407.700811		92.4
S_0-(-170°)			
Root1 (S_0)	-1407.863975	-28.195800	-9.6
Root2 ($S_1(^1\pi\pi^*)$)	-1407.766911		51.3
Root3	-1407.708036		88.3
Root4	-1407.706895		89.0
S_0-(-175°)			
Root1 (S_0)	-1407.865855	-28.195814	-10.8
Root2 ($S_1(^1\pi\pi^*)$)	-1407.768479		50.3
Root3	-1407.712209		85.6
Root4	-1407.709500		87.3

***Table S4-3-(II)**. Absolute energies (A.E., hartree), relative energies (∆E, kcal/mol), and MM energies (hartree) of optimized structures for proton transfer (reaction coordinate: O3-H4 distance) in PYP. The corresponding energy profiles are plotted in Figure 3 of the main article.*

O3-H4	**CASPT2 A.E.**	**MM part**	**ΔE**
S_0- (1.1Å)			
Root1 (S_0)	-1407.864193	-28.196036	-9.9
Root2 ($S_1(^1\pi\pi^*)$)	-1407.764400		52.8
Root3	-1407.712638		85.2
Root4	-1407.705088		90.0
S_0-(1.2Å)			
Root1 (S_0)	-1407.861722	-28.192794	-6.3
Root2 ($S_1(^1\pi\pi^*)$)	-1407.752380		62.3
Root3	-1407.710925		88.3
Root4	-1407.689959		101.5
S_0-(1.3Å)			
Root1 (S_0)	-1407.859203	-28.192788	-4.7
Root2 ($S_1(^1\pi\pi^*)$)	-1407.743913		67.6

Root3	-1407.710112		88.9
Root4	-1407.678396		108.8
S_0-(1.4Å)			
Root1 (S_0)	-1407.858432	-28.195615	-6.0
Root2 ($S_1(^1\pi\pi^*)$)	-1407.738750		69.1
Root3	-1407.708511		88.1
Root4	-1407.672878		110.4
S_0-(1.51Å)			
Root1 (S_0)	-1407.858392	-28.196505	-6.5
Root2 ($S_1(^1\pi\pi^*)$)	-1407.730334		73.8
Root3	-1407.712505		85.0
Root4	-1407.669672		111.9

***Table S4-4-(I)**. Absolute energies (A.E., hartree), relative energies (∆E, kcal/mol), and MM energies (hartree) of optimized structures for ground state relaxation of BP isomerization along the reaction coordinate of C10-C11-C12-S13 and C12-S13-C14-C15 dihedral angle(°) in PYP. The corresponding energy profiles are plotted in Figure 4-(I) of the main article.*

(BP) C10C11C12S13 C12S13C14C15	**CASPT2 A.E.**	**MM part**	**ΔE**
S_0- (-173°)			
Root1 (S_0)	-1407.858392	-28.196505	-6.5
Root2 ($S_1(^1\pi\pi^*)$)	-1407.730334		73.8
S_0-(-170°)			
Root1 (S_0)	-1407.853091	-28.198484	-4.4
Root2 ($S_1(^1\pi\pi^*)$)	-1407.713886		82.9
S_0-(-160°)			
Root1 (S_0)	-1407.846626	-28.204338	-4.1
Root2 ($S_1(^1\pi\pi^*)$)	-1407.700777		87.5
S_0-(-150°)			
Root1 (S_0)	-1407.843708	-28.204449	-2.3
Root2 ($S_1(^1\pi\pi^*)$)	-1407.697265		89.6
S_0-(-140°)			
Root1 (S_0)	-1407.837971	-28.202006	2.8
Root2 ($S_1(^1\pi\pi^*)$)	-1407.689201		96.2
S_0-(-130°)			
Root1 (S_0)	-1407.833545	-28.201168	6.1
Root2 ($S_1(^1\pi\pi^*)$)	-1407.683763		100.1
S_0-(-120°)			
Root1 (S_0)	-1407.828987	-28.197640	11.2
Root2 ($S_1(^1\pi\pi^*)$)	-1407.677724		106.1
S_0-(-110°)			
Root1 (S_0)	-1407.835579	-28.189391	12.3
Root2 ($S_1(^1\pi\pi^*)$)	-1407.683518		107.7

S_0-(-100°)			
Root1 (S_0)	-1407.824374	-28.198585	13.5
Root2 ($S_1(^1\pi\pi^*)$)	-1407.665681		113.1
S_0-(-90°)			
Root1 (S_0)	-1407.817266	-28.197965	18.4
Root2 ($S_1(^1\pi\pi^*)$)	-1407.656686		119.1
S_0-(-80°)			
Root1 (S_0)	-1407.814057	-28.198372	20.1
Root2 ($S_1(^1\pi\pi^*)$)	-1407.653673		120.8
S_0-(-70°)			
Root1 (S_0)	-1407.816430	-28.198382	18.6
Root2 ($S_1(^1\pi\pi^*)$)	-1407.657948		118.1
S_0-(-60°)			
Root1 (S_0)	-1407.823360	-28.199101	13.8
Root2 ($S_1(^1\pi\pi^*)$)	-1407.668614		110.9
S_0-(-50°)			
Root1 (S_0)	-1407.827991	-28.197605	11.9
Root2 ($S_1(^1\pi\pi^*)$)	-1407.679359		105.1
S_0-(-40°)			
Root1 (S_0)	-1407.832506	-28.201818	6.4
Root2 ($S_1(^1\pi\pi^*)$)	-1407.680527		101.8
S_0-(-30°)			
Root1 (S_0)	-1407.842490	-28.192355	6.1
Root2 ($S_1(^1\pi\pi^*)$)	-1407.690953		101.1
S_0-(-29.6°)			
Root1 (S_0)	-1407.853031	-28.184416	4.4
Root2 ($S_1(^1\pi\pi^*)$)	-1407.701430		99.6
(OBF)C10C11C12S13	**CASPT2 A.E.**	**MM part**	**ΔE**
S_0-(-40°)			
Root1 (S_0)	-1407.846606	-28.189029	5.6
Root2 ($S_1(^1\pi\pi^*)$)	-1407.701585		96.6
S_0-(-50°)			
Root1 (S_0)	-1407.841211	-28.191688	7.3
Root2 ($S_1(^1\pi\pi^*)$)	-1407.690221		102.0
S_0-(-60°)			
Root1 (S_0)	-1407.836238	-28.194516	8.6
Root2 ($S_1(^1\pi\pi^*)$)	-1407.679199		107.2
S_0-(-70°)			
Root1 (S_0)	-1407.831041	-28.194779	11.7
Root2 ($S_1(^1\pi\pi^*)$)	-1407.670266		112.6
S_0-(-80°)			
Root1 (S_0)	-1407.826353	-28.190634	17.3
Root2 ($S_1(^1\pi\pi^*)$)	-1407.664704		118.7
S_0-(-90°)			
Root1 (S_0)	-1407.824260	-28.187205	20.7
Root2 ($S_1(^1\pi\pi^*)$)	-1407.662886		122.0
S_0-(-100°)			
Root1 (S_0)	-1407.811710	-28.190492	26.5

Root2 ($S_1(^1\pi\pi^*)$)	-1407.652387		126.5
S_0-(-110°)			
Root1 (S_0)	-1407.808661	-28.188558	29.7
Root2 ($S_1(^1\pi\pi^*)$)	-1407.653500		127.0
S_0-(-120°)			
Root1 (S_0)	-1407.801403	-28.190969	32.7
Root2 ($S_1(^1\pi\pi^*)$)	-1407.641771		132.9
S_0-(-130°)			
Root1 (S_0)	-1407.802364	-28.189786	32.8
Root2 ($S_1(^1\pi\pi^*)$)	-1407.645232		131.5
S_0-(-140°)			
Root1 (S_0)	-1407.800257	-28.192894	32.2
Root2 ($S_1(^1\pi\pi^*)$)	-1407.646038		129.0
S_0-(-150°)			
Root1 (S_0)	-1407.796611	-28.198845	30.8
Root2 ($S_1(^1\pi\pi^*)$)	-1407.629890		135.4
S_0-(-160°)			
Root1 (S_0)	-1407.800046	-28.198401	28.9
Root2 ($S_1(^1\pi\pi^*)$)	-1407.633559		133.4
S_0-(-170°)			
Root1 (S_0)	-1407.800262	-28.201338	26.9
Root2 ($S_1(^1\pi\pi^*)$)	-1407.630508		133.4
S_0-(-173°)			
Root1 (S_0)	-1407.802607	-28.204903	23.2
Root2 ($S_1(^1\pi\pi^*)$)	-1407.633755		129.2

Table S4-4-(II). *Absolute energies (A.E., hartree), relative energies (∆E, kcal/mol), and MM energies (hartree) of optimized structures for proton transfer (reaction coordinate: O26-H27 distance and O22-H4 distance) in PYP. The corresponding energy profiles are plotted in Figure 4-(II) of the main article.*

O26-H27	**CASPT2 A.E.**	**MM part**	**ΔE**
S_0- (0.95Å)			
Root1 (S_0)	-1429.094380	-28.129141	27.9
Root2 ($S_1(^1\pi\pi^*)$)	-1428.941783		123.6
S_0- (1.0Å)			
Root1 (S_0)	-1429.145977	-28.12203	0.0
Root2 ($S_1(^1\pi\pi^*)$)	-1428.999122		92.2
S_0-(1.1Å)			
Root1 (S_0)	-1429.138770	-28.12098	5.2
Root2 ($S_1(^1\pi\pi^*)$)	-1428.993132		96.6
S_0-(1.2Å)			
Root1 (S_0)	-1429.131481	-28.127662	5.6
Root2 ($S_1(^1\pi\pi^*)$)	-1428.993684		92.0

S_0-(1.3Å)			
Root1 (S_0)	-1429.134638	-28.12606	4.6
Root2 ($S_1(^1\pi\pi^*)$)	-1428.998196		90.2
S_0-(1.4Å)			
Root1 (S_0)	-1429.140037	-28.1276	0.2
Root2 ($S_1(^1\pi\pi^*)$)	-1429.003999		85.6
S_0-(1.5Å)			
Root1 (S_0)	-1429.141797	-28.128503	-1.4
Root2 ($S_1(^1\pi\pi^*)$)	-1429.006104		83.7
S_0-(1.6Å)			
Root1 (S_0)	-1429.141862	-28.12806	-1.2
Root2 ($S_1(^1\pi\pi^*)$)	-1429.006471		83.8
O22-H4	**CASPT2 A.E.**	**MM part**	**ΔE**
S_0- (1.6Å)			
Root1 (S_0)	-1429.140150	-28.127634	0.1
Root2 ($S_1(^1\pi\pi^*)$)	-1429.005193		84.8
S_0-(1.5Å)			
Root1 (S_0)	-1429.136676	-28.125504	3.7
Root2 ($S_1(^1\pi\pi^*)$)	-1429.016322		79.2
S_0-(1.4Å)			
Root1 (S_0)	-1429.139328	-28.125723	1.9
Root2 ($S_1(^1\pi\pi^*)$)	-1429.021996		75.5
S_0-(1.3Å)			
Root1 (S_0)	-1429.141779	-28.126207	0.0
Root2 ($S_1(^1\pi\pi^*)$)	-1429.027915		71.5
S_0-(1.2Å)			
Root1 (S_0)	-1429.145266	-28.125239	-1.6
Root2 ($S_1(^1\pi\pi^*)$)	-1429.035548		67.3
S_0-(1.1Å)			
Root1 (S_0)	-1429.148267	-28.128278	-5.4
Root2 ($S_1(^1\pi\pi^*)$)	-1429.043766		60.2
S_0-(1.0Å)			
Root1 (S_0)	-1429.152419	-28.127685	-7.6
Root2 ($S_1(^1\pi\pi^*)$)	-1429.049230		57.2

***Table S4-4-(III)**. Absolute energies (A.E., hartree), relative energies (ΔE, kcal/mol), and MM energies (hartree) of optimized structures for ground state relaxation of OBF isomerization along the reaction coordinate of C9-C10-C11-C12 dihedral angle(°) in PYP. The corresponding energy profiles are plotted in Figure 4-(III) of the main article.*

(OBF) C9C10C11C12	**CASPT2 A.E.**	**MM part**	**ΔE**
S_0- (-1.9°)			
Root1 (S_0)	-1429.152419	-28.127685	-7.6
Root2 ($S_1(^1\pi\pi^*)$)	-1429.049230		57.2
S_0-(10°)			

Root1 (S_0)	-1429.148840	-28.129242	-6.3
Root2 ($S_1(^1\pi\pi^*)$)	-1429.046106		58.1
S_0-(20°)			
Root1 (S_0)	-1429.147491	-28.120952	-0.3
Root2 ($S_1(^1\pi\pi^*)$)	-1429.044620		64.3
S_0-(30)			
Root1 (S_0)	-1429.145830	-28.120612	1.0
Root2 ($S_1(^1\pi\pi^*)$)	-1429.043662		65.1
S_0-(40°)			
Root1 (S_0)	-1429.141363	-28.123477	2.0
Root2 ($S_1(^1\pi\pi^*)$)	-1429.040262		65.4
S_0-(50°)			
Root1 (S_0)	-1429.139136	-28.119786	5.7
Root2 ($S_1(^1\pi\pi^*)$)	-1429.040293		67.7
S_0-(60°)			
Root1 (S_0)	-1429.134390	-28.12056	8.2
Root2 ($S_1(^1\pi\pi^*)$)	-1429.038494		68.4
S_0-(70°)			
Root1 (S_0)	-1429.126561	-28.120008	13.5
Root2 ($S_1(^1\pi\pi^*)$)	-1429.033136		72.1
S_0-(80°)			
Root1 (S0)	-1429.118857	-28.120711	17.8
Root2 (S1(1ππ*))	-1429.029995		73.6
S_0-(90°)			
Root1 (S_0)	-1429.110130	-28.118323	24.8
Root2 ($S_1(^1\pi\pi^*)$)	-1429.028956		75.8
S_0-(100°)			
Root1 (S_0)	-1429.091646	-28.131821	27.9
Root2 ($S_1(^1\pi\pi^*)$)	-1429.046048		56.6
S_0-(110°)			
Root1 (S_0)	-1429.088301	-28.133401	29.1
Root2 ($S_1(^1\pi\pi^*)$)	-1429.046868		55.1
S_0-(120°)			
Root1 (S_0)	-1429.116483	-28.108818	26.8
Root2 ($S_1(^1\pi\pi^*)$)	-1429.026556		83.2
S_0-(130°)			
Root1 (S_0)	-1429.124051	-28.109189	21.8
Root2 ($S_1(^1\pi\pi^*)$)	-1429.029681		81.0
S_0-(140°)			
Root1 (S_0)	-1429.113174	-28.128019	16.8
Root2 ($S_1(^1\pi\pi^*)$)	-1429.018126		76.5
S_0-(150°)			
Root1 (S_0)	-1429.117815	-28.129631	12.9
Root2 ($S_1(^1\pi\pi^*)$)	-1429.019958		74.3
S_0-(160°)			
Root1 (S_0)	-1429.126318	-28.127978	8.6
Root2 ($S_1(^1\pi\pi^*)$)	-1429.023337		73.2
S_0-(170°)			
Root1 (S_0)	-1429.137535	-28.126533	2.5

Root2 ($S_1(^1\pi\pi^*)$)	-1429.030875		69.4

Table S4-5-(I). *Absolute energies (A.E., hartree), relative energies (∆E, kcal/mol), and MM energies (hartree) of optimized structures for proton transfer (reaction coordinate: O19-H18 distance) in PYP. The corresponding energy profiles are plotted in Figure 5 of the main article.*

O19-H18	**CASPT2 A.E.**	**MM part**	**ΔE**
S_0- (1.0Å)			
Root1 (S_0)	-1622.390069	-28.150408	0.0
Root2 ($S_1(^1\pi\pi^*)$)	-1622.288786		63.6
S_0-(1.1Å)			
Root1 (S_0)	-1622.382590	-28.144181	8.6
Root2 ($S_1(^1\pi\pi^*)$)	-1622.277228		74.7
S_0-(1.2Å)			
Root1 (S_0)	-1622.368338	-28.150368	13.7
Root2 ($S_1(^1\pi\pi^*)$)	-1622.249882		88.0
S_0-(1.3Å)			
Root1 (S_0)	-1622.374107	-28.150524	9.9
Root2 ($S_1(^1\pi\pi^*)$)	-1622.249083		88.4
S_0-(1.4Å)			
Root1 (S_0)	-1622.376705	-28.150866	8.1
Root2 ($S_1(^1\pi\pi^*)$)	-1622.226122		102.6
S_0-(1.5Å)			
Root1 (S_0)	-1622.377729	-28.148989	8.6
Root2 ($S_1(^1\pi\pi^*)$)	-1622.225296		104.3
S_0-(1.6Å)			
Root1 (S_0)	-1622.381129	-28.147348	7.5
Root2 ($S_1(^1\pi\pi^*)$)	-1622.228480		103.3
S_0- (1.7Å)			
Root1 (S_0)	-1622.381678	-28.148069	6.7
Root2 ($S_1(^1\pi\pi^*)$)	-1622.228747		102.7
S_0-(1.8Å)			
Root1 (S_0)	-1622.382690	-28.147659	6.4
Root2 ($S_1(^1\pi\pi^*)$)	-1622.229627		102.4
S_0-(1.9Å)			
Root1 (S_0)	-1622.381934	-28.149699	5.5
Root2 ($S_1(^1\pi\pi^*)$)	-1622.228996		101.5

Table S4-5-(II)*. Absolute energies (A.E., hartree), relative energies (∆E, kcal/mol), and MM energies (hartree) of optimized structures for ground state relaxation of isomerization along the reaction coordinate of C11-C12-S13-C14 and C12-S13-C14-C15 dihedral angle(°) in PYP. The corresponding energy profiles are plotted in Figure 5 of the main article.*

(BP) C11C12S13C14 C12S13C14C15	CASPT2 A.E.	MM part	ΔE
S_0- (-178°)			
Root1 (S_0)	-1407.828497	-28.185387	19.2
Root2 ($S_1(^1\pi\pi^*)$)	-1407.739447		75.1
S_0-(-170°)			
Root1 (S_0)	-1407.834572	-28.177697	20.2
Root2 ($S_1(^1\pi\pi^*)$)	-1407.746022		75.8
S_0-(-160°)			
Root1 (S_0)	-1407.834458	-28.17572	21.5
Root2 ($S_1(^1\pi\pi^*)$)	-1407.747936		75.8
S_0-(-150°)			
Root1 (S_0)	-1407.828697	-28.172857	26.9
Root2 ($S_1(^1\pi\pi^*)$)	-1407.746235		78.7
S_0-(-140°)			
Root1 (S_0)	-1407.824083	-28.163773	35.5
Root2 ($S_1(^1\pi\pi^*)$)	-1407.748059		83.2
S_0-(-130°)			
Root1 (S_0)	-1407.813018	-28.177383	33.9
Root2 ($S_1(^1\pi\pi^*)$)	-1407.751630		72.5
S_0-(-120°)			
Root1 (S_0)	-1407.824884	-28.174243	28.5
Root2 ($S_1(^1\pi\pi^*)$)	-1407.748978		76.1
S_0-(-110°)			
Root1 (S_0)	-1407.826823	-28.173908	27.5
Root2 ($S_1(^1\pi\pi^*)$)	-1407.751180		74.9
S_0-(-100°)			
Root1 (S_0)	-1407.834927	-28.171685	23.8
Root2 ($S_1(^1\pi\pi^*)$)	-1407.755624		73.5
S_0-(-90°)			
Root1 (S_0)	-1407.842914	-28.163586	23.8
Root2 ($S_1(^1\pi\pi^*)$)	-1407.758626		76.7
S_0-(-80°)			
Root1 (S_0)	-1407.828167	-28.178211	23.9
Root2 ($S_1(^1\pi\pi^*)$)	-1407.737781		80.6
S_0-(-70°)			
Root1 (S_0)	-1407.833284	-28.177476	21.2
Root2 ($S_1(^1\pi\pi^*)$)	-1407.736295		82.0
S_0-(-60°)			
Root1 (S_0)	-1407.833816	-28.180282	19.1
Root2 ($S_1(^1\pi\pi^*)$)	-1407.731823		83.1
S_0-(-50°)			
Root1 (S_0)	-1407.838324	-28.180865	15.9
Root2 ($S_1(^1\pi\pi^*)$)	-1407.741040		76.9
S_0-(-40°)			
Root1 (S_0)	-1407.848813	-28.181721	8.8
Root2 ($S_1(^1\pi\pi^*)$)	-1407.750598		70.4

S_0-(-30°)			
Root1 (S_0)	-1407.846854	-28.18904	5.4
Root2 ($S_1(^1\pi\pi^*)$)	-1407.751567		65.2
S_0-(-20°)			
Root1 (S_0)	-1407.849627	-28.194665	0.1
Root2 ($S_1(^1\pi\pi^*)$)	-1407.753705		60.3
S_0-(-9°)			
Root1 (S_0)	-1407.860629	-28.190691	-4.3
Root2 ($S_1(^1\pi\pi^*)$)	-1407.759688		59.1
(OBF)C11C12S13C14	**CASPT2 A.E.**	**MM part**	**ΔE**
S_0-(-20°)			
Root1 (S_0)	-1407.858891	-28.191437	-3.7
Root2 ($S_1(^1\pi\pi^*)$)	-1407.759053		59.0
S_0-(-30°)			
Root1 (S_0)	-1407.857331	-28.19054	-2.1
Root2 ($S_1(^1\pi\pi^*)$)	-1407.758284		60.0
S_0-(-40°)			
Root1 (S_0)	-1407.855971	-28.188858	-0.2
Root2 ($S_1(^1\pi\pi^*)$)	-1407.757891		61.3
S_0-(-50°)			
Root1 (S_0)	-1407.851324	-28.184759	5.3
Root2 ($S_1(^1\pi\pi^*)$)	-1407.749466		69.2
S_0-(-60°)			
Root1 (S_0)	-1407.851660	-28.174417	11.6
Root2 ($S_1(^1\pi\pi^*)$)	-1407.751582		74.4
S_0-(-70°)			
Root1 (S_0)	-1407.852442	-28.175967	10.1
Root2 ($S_1(^1\pi\pi^*)$)	-1407.753745		72.0
S_0-(-80°)			
Root1 (S_0)	-1407.854706	-28.17735	7.8
Root2 ($S_1(^1\pi\pi^*)$)	-1407.759028		67.8
S_0-(-90°)			
Root1 (S_0)	-1407.855267	-28.178708	6.6
Root2 ($S_1(^1\pi\pi^*)$)	-1407.760880		65.8
S_0-(-100°)			
Root1 (S_0)	-1407.857762	-28.182797	2.5
Root2 ($S_1(^1\pi\pi^*)$)	-1407.765042		60.7
S_0-(-110°)			
Root1 (S_0)	-1407.860312	-28.183763	0.3
Root2 ($S_1(^1\pi\pi^*)$)	-1407.767124		58.7
S_0-(-120°)			
Root1 (S_0)	-1407.862059	-28.189662	-4.5
Root2 ($S_1(^1\pi\pi^*)$)	-1407.770036		53.2
S_0-(-130°)			
Root1 (S_0)	-1407.864438	-28.191354	-7.1
Root2 ($S_1(^1\pi\pi^*)$)	-1407.771102		51.5
S_0-(-140°)			
Root1 (S_0)	-1407.866411	-28.193475	-9.7

Root2 ($S_1(^1\pi\pi^*)$)	-1407.771965		49.6
S_0-(-150°)			
Root1 (S_0)	-1407.867528	-28.195235	-11.5
Root2 ($S_1(^1\pi\pi^*)$)	-1407.772239		48.3
S_0-(-160°)			
Root1 (S_0)	-1407.867770	-28.195373	-11.7
Root2 ($S_1(^1\pi\pi^*)$)	-1407.771272		48.9
S_0-(-173°)			
Root1 (S_0)	-1407.865855	-28.195814	-10.8
Root2 ($S_1(^1\pi\pi^*)$)	-1407.768479		50.3

5. Cartesian Coordinates

S_0 minimum (QM1)

C	2.946818609	-0.692207356	-3.715090544
H	2.513265748	-1.190780030	-4.573908123
H	3.096297736	-1.432443400	-2.940652430
C	1.982450076	0.399143176	-3.209287175
H	2.368920995	0.851282382	-2.305669063
H	1.827671409	1.182959018	-3.936191869
C	0.670908453	-0.271372789	-2.864859748
O	0.614770230	-1.145170836	-2.041885529
O	-0.414737139	0.062608634	-3.519048338
H	-0.292487708	0.739224331	-4.239327600
C	-6.118193680	0.941509336	-14.293665358
H	-6.418369051	0.109141998	-14.913287995
H	-5.371587924	1.516079308	-14.826995538
S	-5.394531039	0.178378820	-12.818638441
O	-4.525369970	2.625345844	-12.595149320
C	-4.473507610	1.518599923	-12.113989138
C	-3.729889144	1.171747546	-10.919560521
H	-3.915252351	0.209339402	-10.485084991
C	-2.885002446	2.078409554	-10.369429017
H	-2.717621005	2.980490428	-10.931428167
C	-2.212932296	2.000620451	-9.096880502
C	-1.380356542	3.053348832	-8.675335366
H	-1.238905764	3.908107871	-9.313532812
C	-0.747600493	3.030838367	-7.449204480
H	-0.087217993	3.828735671	-7.160329954
C	-0.910128680	1.942196283	-6.568158175
O	-0.232399874	1.838898433	-5.482051029
C	-1.812775964	0.923624695	-6.961962464
H	-1.983330796	0.105483626	-6.286190629
C	-2.423188472	0.942806815	-8.193539854
H	-3.078396040	0.131266319	-8.455849365
H	3.931488705	-0.281476728	-3.926147169
H	-6.911157744	1.644911754	-14.052567283

S_1 minimum

C	2.909529547	-0.729029922	-3.732552250
H	2.482377317	-1.211379948	-4.603207292
H	3.056989138	-1.486519584	-2.973585564
C	1.943321716	0.353214317	-3.209292822
H	2.338442910	0.806593246	-2.310232825
H	1.776066075	1.137073096	-3.934201257
C	0.640832003	-0.327160852	-2.853493323
O	0.586161421	-1.191857557	-2.026202901
O	-0.456214564	-0.002438404	-3.507797284
H	-0.349210265	0.698448774	-4.190507517
C	-6.194459605	0.836082659	-14.162677532
H	-6.465791588	-0.009586077	-14.777565567
H	-5.448672010	1.421044800	-14.685101368
S	-5.478284451	0.116946041	-12.657355746
O	-4.669777885	2.605558774	-12.499912232
C	-4.493879267	1.479110848	-12.032736088
C	-3.595774483	1.154435687	-11.014694049
H	-3.572994636	0.146374496	-10.655257493
C	-2.682216666	2.153886788	-10.515970845
H	-2.552333729	3.046584433	-11.087380354
C	-2.118816915	2.089221551	-9.200649727
C	-1.327166296	3.166319348	-8.692619512
H	-1.163762701	4.031324571	-9.306265409
C	-0.781437859	3.120123275	-7.431112280
H	-0.158568390	3.918168811	-7.065116996
C	-0.979700597	1.974295365	-6.575848126
O	-0.351158806	1.879048577	-5.484769095
C	-1.842575242	0.948800636	-7.044182797
H	-2.026627423	0.109730751	-6.397996679
C	-2.381877541	0.985831312	-8.313446550
H	-3.010417899	0.182015682	-8.636667167
H	3.896487700	-0.313203654	-3.923990232
H	-7.009197831	1.525102834	-13.953485987

CI(S_0/S_1)

C	2.837643517	-0.656490172	-4.650233480
H	2.230000162	-0.993222706	-5.481745270
H	3.130307862	-1.524085750	-4.075485539
C	2.015560363	0.305981584	-3.769887086
H	2.597013689	0.635308673	-2.919203717
H	1.687200488	1.178329813	-4.317991931
C	0.826365928	-0.469189820	-3.251604152
O	0.967862172	-1.451253942	-2.577409725
O	-0.385531634	-0.116240438	-3.617393988
H	-0.460496768	0.748379865	-4.096845843
C	-7.507066731	1.472079548	-12.811257212
H	-7.932208739	0.702069717	-13.439737324
H	-6.831061370	2.063823540	-13.415263987
S	-6.609637998	0.560671270	-11.522998271

O	-5.465135984	2.917441604	-11.215960318
C	-5.319491906	1.729659511	-11.060051842
C	-4.095889048	1.044035523	-10.655836043
H	-4.190881439	-0.041388319	-10.670878276
C	-2.887174528	1.635455213	-10.122046432
H	-2.184506873	2.005218139	-10.838478131
C	-2.594660379	1.975091824	-8.765798375
C	-1.501899390	2.834968944	-8.489626537
H	-1.082677844	3.416134063	-9.286549111
C	-0.938816416	2.933459170	-7.238226961
H	-0.117128684	3.600099782	-7.070727545
C	-1.390517761	2.141832924	-6.143288535
O	-0.805316368	2.169542428	-5.018319549
C	-2.494195771	1.299001175	-6.415297706
H	-2.852806382	0.679753820	-5.615918744
C	-3.081087229	1.230238423	-7.665673006
H	-3.877771732	0.530875442	-7.807104199
H	3.769978824	-0.187860198	-4.969159876
H	-8.225205820	2.182586161	-12.397689634

I_T

C	2.883645218	-0.740823939	-4.579524440
H	2.273411265	-1.085626468	-5.406344815
H	3.181359608	-1.604430086	-4.002082024
C	2.068302015	0.222706722	-3.691066383
H	2.650320084	0.529457041	-2.832850843
H	1.761666178	1.110956092	-4.226389703
C	0.870033883	-0.552136149	-3.195911898
O	0.982825606	-1.529038515	-2.518001307
O	-0.342663465	-0.194390584	-3.592117847
H	-0.394251729	0.654805425	-4.068799470
C	-7.458929329	1.285663199	-12.700938943
H	-7.857252739	0.492859369	-13.319845391
H	-6.760498124	1.861641217	-13.294634117
S	-6.597546880	0.467685971	-11.322403845
O	-5.633374608	2.902821178	-10.951411011
C	-5.297754680	1.698613455	-10.928390055
C	-4.086367927	1.121026648	-10.747605009
H	-4.034464555	0.059832842	-10.838523957
C	-2.908861694	1.814329120	-10.188009646
H	-2.229308628	2.279283111	-10.882995167
C	-2.612844460	2.074131231	-8.885995431
C	-1.485666391	2.941161488	-8.559635470
H	-1.077799158	3.553542202	-9.342358155
C	-0.969174754	3.018081730	-7.314633277
H	-0.160042606	3.682155483	-7.076029795
C	-1.468401354	2.150641196	-6.247192276
O	-0.909530694	2.111413001	-5.159139737
C	-2.627233588	1.309926929	-6.552403774
H	-2.994146471	0.681334176	-5.761853658
C	-3.188618544	1.312116294	-7.783924171

H	-4.029223986	0.682229565	-8.005094967
H	3.816094626	-0.269423268	-4.898824939
H	-8.206390923	2.006140098	-12.361363733

I_{CT}

C	2.880650662	-0.678935876	-4.760801584
H	2.219076716	-1.106666137	-5.503713640
H	3.271222996	-1.485974923	-4.154689784
C	2.085074373	0.301659200	-3.874737419
H	2.705512334	0.665614548	-3.065761674
H	1.718244698	1.152116748	-4.430882578
C	0.929096346	-0.480039336	-3.287144394
O	1.117424088	-1.462310000	-2.621809072
O	-0.301620994	-0.127686355	-3.577541242
H	-0.418453602	0.733772938	-4.061081430
C	-8.113389874	1.152820860	-11.876294836
H	-8.561622266	0.331034603	-12.413361113
H	-7.590485598	1.778939153	-12.588666952
S	-6.915289401	0.353411086	-10.746473787
O	-6.045896479	2.801822715	-10.526117077
C	-5.700215621	1.655704101	-10.558288726
C	-4.296648027	1.216400591	-10.728777253
H	-4.201477250	0.791988939	-11.714244464
C	-3.143140268	1.462128725	-10.077684074
H	-2.280042062	1.233465864	-10.677194166
C	-2.783869588	1.782595747	-8.686476875
C	-1.661746189	2.597414625	-8.463406227
H	-1.216486477	3.124155023	-9.290840633
C	-1.088064969	2.728295325	-7.212243618
H	-0.233907478	3.367731009	-7.083077272
C	-1.569432292	2.008981679	-6.086836647
O	-0.990070217	2.070802975	-4.950409290
C	-2.695991885	1.182151462	-6.329326353
H	-3.077141588	0.602181002	-5.506944426
C	-3.283253984	1.076261713	-7.582728441
H	-4.105765035	0.393521263	-7.716758455
H	3.755209333	-0.197913791	-5.191717291
H	-8.803981689	1.810392047	-11.356734220

I_{CP}(QM2)

C	2.961604758	-0.534074403	-4.485769752
H	2.436647497	-0.975067127	-5.323274782
H	3.346536037	-1.337510044	-3.871671647
C	1.967098903	0.311594700	-3.663093444
H	2.441337389	0.695067929	-2.769138871
H	1.572621077	1.145255451	-4.225615035
C	0.850926642	-0.627127476	-3.257357642
O	1.072757692	-1.627820466	-2.631365140
O	-0.368158571	-0.390057754	-3.683442881
H	-0.501605379	0.468278373	-4.167448814

N	-8.377237544	2.748002055	-11.823941849
H	-7.591451822	2.869967277	-11.235149344
C	-8.473857319	1.458770788	-12.454053044
H	-9.065479389	1.553494595	-13.356737301
C	-7.061993580	0.964376254	-12.871271892
H	-7.112665742	0.606872942	-13.889858402
H	-6.394424151	1.814797791	-12.883422436
S	-6.308828038	-0.431694935	-11.967322107
C	-9.237498508	0.432639066	-11.607409292
O	-10.036450901	-0.300126053	-12.107586041
O	-5.285816616	-0.316484734	-9.616306179
C	-5.198828661	0.220304556	-10.670741220
C	-4.138018378	1.151552248	-11.071746288
H	-4.159976159	1.414862703	-12.112973965
C	-3.093008058	1.637653701	-10.341797233
H	-2.453672177	2.266089653	-10.937316270
C	-2.588307167	1.564410697	-8.977120071
C	-1.586313777	2.496590415	-8.640316638
H	-1.241153466	3.191652476	-9.387531212
C	-1.016701427	2.565837989	-7.381620925
H	-0.267286807	3.307171102	-7.167626990
C	-1.418351489	1.697226116	-6.336296888
O	-0.924223173	1.766952363	-5.168356862
C	-2.389302040	0.716348194	-6.698502733
H	-2.688295849	0.010212034	-5.943077286
C	-2.958769675	0.657886592	-7.953791656
H	-3.691591777	-0.093977451	-8.151713261
H	-9.272077754	3.210632418	-11.685092460
H	-9.040880849	0.387596962	-10.546683551
H	3.830425799	0.041567834	-4.774686513

pR_1

C	2.975992702	0.247208872	-5.098713331
H	2.350540246	-0.057611689	-5.927230756
H	3.247797251	-0.639258013	-4.539900494
C	2.204463555	1.220999422	-4.186105080
H	2.736798134	1.375056577	-3.260168028
H	2.059039921	2.192993061	-4.639868332
C	0.875478382	0.590498790	-3.864442752
O	0.764452110	-0.458637353	-3.305008005
O	-0.220927639	1.207371886	-4.288078234
H	-0.018081187	2.034202585	-4.752620070
N	-8.278793325	4.400048256	-12.712698690
H	-7.361647500	4.616927895	-12.397893050
C	-8.518081509	3.094191806	-13.251372978
H	-9.090681826	3.166966320	-14.172834031
C	-7.187325349	2.385998191	-13.609011706
H	-7.333074839	1.795138174	-14.501254820
H	-6.427204882	3.122116876	-13.828338054
S	-6.545503673	1.197839895	-12.390733335
C	-9.375422790	2.192411056	-12.338576090

O	-10.110030880	1.359991377	-12.796186085
O	-4.810213796	3.097747152	-11.751808852
C	-5.153687793	1.971375809	-11.541109945
C	-4.626795045	0.978953203	-10.588119770
H	-5.078624535	0.013801316	-10.715739119
C	-3.778704856	1.081044661	-9.531950298
H	-3.741926609	0.171926916	-8.951635423
C	-2.954338668	2.141431564	-8.973550611
C	-2.293311034	3.136106333	-9.722101094
H	-2.321820146	3.095135679	-10.794484768
C	-1.580315881	4.139156728	-9.102069614
H	-1.048032520	4.872080125	-9.680617936
C	-1.551526739	4.287593995	-7.679252488
O	-1.026372073	5.289983818	-7.123874774
C	-2.135855624	3.223287925	-6.944252225
H	-2.147992796	3.311782268	-5.869716545
C	-2.802490838	2.187310920	-7.577405500
H	-3.254809553	1.414853628	-6.976282106
H	-9.090446342	4.985609468	-12.582232685
H	-9.290758558	2.327792033	-11.266710268
H	3.916426659	0.684463212	-5.410891612

pR_1- pR_2 intermediate

C	4.219833790	-1.384346316	-6.159641700
H	3.426071615	-1.913636967	-6.672481712
H	4.735660151	-2.091085546	-5.522263261
C	3.621651558	-0.245046393	-5.316265036
H	4.401376263	0.284361654	-4.783265185
H	3.091617258	0.473044726	-5.925579829
C	2.681906398	-0.822333174	-4.282435506
O	3.017838678	-1.698508868	-3.533413813
O	1.452030499	-0.365143281	-4.225234874
H	1.204567759	0.284419967	-4.934115029
N	-9.065640417	2.617383483	-9.098794166
H	-8.225258950	2.610898469	-8.560962805
C	-9.585390638	1.295078432	-9.389642947
H	-10.397651786	1.399426915	-10.094231500
C	-8.575130944	0.258428428	-9.962093507
H	-8.155913817	-0.369660765	-9.188110607
H	-9.150192200	-0.408807639	-10.586885411
S	-7.223949706	0.844276075	-11.018834808
C	-10.172579949	0.599573238	-8.159841423
O	-11.225112862	0.044967882	-8.155365907
O	-4.735664617	1.232805769	-10.617447197
C	-5.725070442	0.993435578	-10.006651977
C	-5.839540159	0.820291793	-8.556834217
H	-6.837608721	0.704222765	-8.196122503
C	-4.889492639	0.688919165	-7.594708908
H	-5.342354956	0.483585358	-6.642341999
C	-3.451036695	0.789173943	-7.417632125
C	-3.001679939	0.476038521	-6.124869780

H	-3.715634802	0.128587393	-5.399898854
C	-1.679193385	0.583884281	-5.744652646
H	-1.370313435	0.304832533	-4.752206592
C	-0.707367215	1.024081667	-6.648254549
O	0.545594317	1.049786330	-6.336605504
C	-1.161122577	1.384348681	-7.948948308
H	-0.427996756	1.746030070	-8.646554315
C	-2.479670909	1.248353044	-8.335683107
H	-2.767226927	1.491900337	-9.338397157
H	-9.826664242	3.259302707	-8.888028318
H	-9.558332006	0.614904874	-7.248902477
H	4.978787542	-1.004917634	-6.843452320

pR_2

C	3.815979054	-1.293832638	-5.046478192
H	3.074346088	-1.793142535	-5.657308025
H	4.323207343	-2.044778419	-4.454750049
C	3.116343155	-0.275626752	-4.124001748
H	3.832591399	0.183564313	-3.454306333
H	2.629089344	0.504708774	-4.686893335
C	2.103003464	-1.019437972	-3.283201362
O	2.435864087	-1.898690091	-2.537350832
O	0.822428891	-0.741580244	-3.407407042
H	0.583970299	-0.023241591	-4.036618920
N	-9.247840272	2.213313330	-8.983111733
H	-8.472181733	2.224504915	-8.359259224
C	-9.654308725	0.876552093	-9.351349776
H	-10.502507834	0.942269356	-10.017291297
C	-8.547901917	0.012880299	-10.029284200
H	-8.072291164	-0.651066153	-9.319962262
H	-9.014746055	-0.608918064	-10.779570543
S	-7.220056232	0.882096934	-10.877415204
C	-10.106219375	0.052705185	-8.148004998
O	-11.120864415	-0.572013147	-8.122418802
O	-6.402615656	0.880060718	-8.384907651
C	-6.130394655	1.239948503	-9.494655685
C	-4.998618729	2.074243712	-9.900057211
H	-5.144402691	2.560936575	-10.845497455
C	-3.865844310	2.427419736	-9.238716515
H	-3.365272478	3.224945049	-9.744675689
C	-3.103728692	2.047549096	-8.058866678
C	-2.027545344	2.899623328	-7.751045542
H	-1.880987207	3.787307971	-8.341425209
C	-1.133743862	2.635146905	-6.737991898
H	-0.316472382	3.309536963	-6.559429502
C	-1.211348663	1.448111465	-5.984865620
O	-0.293500662	1.136274864	-5.135231424
C	-2.317303877	0.601601188	-6.268585484
H	-2.406889648	-0.310321058	-5.702920617
C	-3.231079726	0.886614118	-7.271075374
H	-4.036915847	0.200545841	-7.458196154

H	-10.043628714	2.834495214	-8.876577134
H	-9.427343651	0.027384494	-7.289042106
H	4.594403248	-0.816928962	-5.637722487

pB'

C	3.525264028	-1.326585963	-5.239401088
H	2.763862407	-1.771839478	-5.867727579
H	3.979291498	-2.125486036	-4.662954388
C	2.858549828	-0.307496959	-4.294028033
H	3.583539048	0.065580588	-3.580870592
H	2.455990307	0.532498138	-4.843718235
C	1.728594119	-1.021197709	-3.551964857
O	2.053882295	-1.911783805	-2.773812585
O	0.539632982	-0.689787185	-3.818515781
H	0.005154583	0.564513462	-4.469663544
N	-9.135609980	2.305632381	-8.940396704
H	-8.386583132	2.265091424	-8.282227262
C	-9.593198437	0.983903556	-9.333709917
H	-10.400372022	1.094467490	-10.042478441
C	-8.493930335	0.075140564	-9.957289265
H	-8.034820758	-0.566993155	-9.218420451
H	-8.966609340	-0.566315961	-10.686272625
S	-7.131785445	0.889786466	-10.814322512
C	-10.127781814	0.188550003	-8.147161437
O	-11.174296976	-0.381629314	-8.156915338
O	-6.283861455	0.876807072	-8.324227743
C	-6.004900906	1.179691269	-9.445364306
C	-4.811776710	1.924366878	-9.879200166
H	-4.924623785	2.378231287	-10.846150724
C	-3.669378805	2.253715039	-9.230081613
H	-3.125431976	2.990609815	-9.779919582
C	-2.916779397	1.931172986	-8.009767655
C	-1.922114154	2.888053614	-7.688116101
H	-1.828225352	3.769404423	-8.295000172
C	-1.069612257	2.723214493	-6.632261966
H	-0.329148167	3.466744507	-6.407420215
C	-1.121013291	1.547771348	-5.845090964
O	-0.239310109	1.478367767	-4.863356669
C	-2.073392436	0.590221665	-6.162107348
H	-2.132378072	-0.315672434	-5.586561525
C	-2.972566189	0.798612137	-7.224936251
H	-3.706763294	0.039736757	-7.428126239
H	-9.922851045	2.947361376	-8.818063836
H	-9.492037263	0.149517193	-7.266706170
H	4.339893688	-0.887740307	-5.806337515

pB'- pB intermediate

C	4.001077027	-0.623902480	-8.244288587
H	3.023943325	-1.016468362	-8.504401695
H	4.430419807	-1.297620044	-7.513176876

C	3.858051460	0.791044193	-7.647403797
H	4.761510073	1.059324871	-7.117298477
H	3.684947284	1.531759418	-8.414777802
C	2.663944514	0.783686804	-6.696280189
O	2.772348865	0.145324578	-5.653605425
O	1.617315636	1.356511116	-7.110423247
H	-0.267113820	1.285795599	-6.621731180
N	-9.311730275	3.805858391	-11.111491521
H	-8.536437186	3.692377388	-11.717357931
C	-9.931889286	2.566095254	-10.726452259
H	-10.879500745	2.380390484	-11.227258094
C	-9.058829324	1.326591133	-11.032288716
H	-9.523694815	0.455067383	-10.589769639
H	-9.008509860	1.175377088	-12.099134286
S	-7.324670552	1.272237057	-10.414166667
C	-10.242507600	2.531041304	-9.237111203
O	-11.291716645	2.151811937	-8.809802056
O	-7.185555992	2.613883552	-12.583518374
C	-6.501763258	2.025792513	-11.781149084
C	-5.058711712	1.936828002	-12.098710362
H	-4.983197806	2.140168080	-13.150063210
C	-3.860741274	1.790221519	-11.484248209
H	-3.069264933	1.897309928	-12.201671798
C	-3.285063643	1.602067944	-10.146245813
C	-1.913915034	1.888125438	-10.057680486
H	-1.385445957	2.221336297	-10.932444928
C	-1.204552016	1.750291291	-8.875599267
H	-0.152581803	1.949801756	-8.842960303
C	-1.863419025	1.290543007	-7.736296790
O	-1.231038073	1.075360122	-6.569759253
C	-3.227529201	0.987799899	-7.810442725
H	-3.724496484	0.620776148	-6.930411382
C	-3.922854819	1.141288977	-8.990528522
H	-4.961315872	0.872189079	-9.014024945
H	-9.992450236	4.549861124	-11.247682483
H	-9.454054666	2.857238442	-8.556103423
H	4.690651483	-0.634973614	-9.088747101

pB

C	4.391339131	0.857503717	-9.963197370
H	3.399383820	0.440794021	-9.819079757
H	5.014183806	0.496396483	-9.152343040
C	4.314484078	2.394031430	-9.919885430
H	5.307756712	2.818372638	-9.876747112
H	3.814357163	2.809111571	-10.786600186
C	3.527019161	2.763620986	-8.666141070
O	4.151014685	2.715421146	-7.598128346
O	2.320101082	3.018346726	-8.805687015
H	-0.383245658	4.291602983	-15.616511906
N	-9.362682742	4.703227295	-13.114579918
H	-8.368468336	4.709283702	-13.145887155

C	-9.953670222	3.706443888	-12.269711556
H	-10.978717669	3.544088582	-12.581510306
C	-9.226491992	2.353588111	-12.421363013
H	-9.927327725	1.549759250	-12.240470968
H	-8.855451267	2.250446057	-13.430530274
S	-7.902635721	1.967434693	-11.237198106
C	-10.052131163	4.097504494	-10.787523759
O	-10.984402355	3.777288577	-10.116249930
O	-6.240437276	3.100132403	-12.955318627
C	-6.355707056	2.516774791	-11.916872783
C	-5.270027501	2.102218514	-10.990877157
H	-5.616881370	1.602732824	-10.105044443
C	-3.938123889	2.188097737	-11.154957347
H	-3.367608621	1.765057532	-10.344193401
C	-3.101059474	2.831867383	-12.200298424
C	-2.693039415	2.176045445	-13.351478972
H	-3.049932543	1.187034514	-13.564519118
C	-1.776615409	2.773907493	-14.221525852
H	-1.453059161	2.252571413	-15.102476165
C	-1.263267820	4.025854101	-13.927853329
O	-0.345446404	4.649470195	-14.716504228
C	-1.656532719	4.682501507	-12.764748459
H	-1.266175554	5.661029834	-12.556618072
C	-2.547348414	4.083858002	-11.912780549
H	-2.824712933	4.580293277	-11.001669779
H	-9.902034958	5.551530573	-13.190185429
H	-9.257091401	4.711442851	-10.370693010
H	4.848148348	0.497115326	-10.880994771

pR_1(QM3)

C	1.007950815	6.949987395	-0.266679461
H	0.079915057	7.479494162	-0.081681764
H	1.808089776	7.660671223	-0.102674393
C	1.016134890	6.470787868	-1.705736228
C	-0.167863213	6.370950748	-2.424146685
H	-1.096814037	6.609975349	-1.940732038
C	-0.190498223	5.968100226	-3.751610478
H	-1.118956416	5.895461864	-4.290414435
C	0.998641418	5.631400195	-4.386405733
O	1.045461655	5.072553935	-5.610884787
H	0.240677817	5.206255478	-6.173992140
C	2.196830691	5.766311500	-3.697905888
H	3.114164400	5.508203286	-4.190961122
C	2.197825471	6.188720201	-2.383679421
H	3.141603410	6.288550547	-1.876859408
C	3.097614721	0.023354132	-5.058038349
H	2.508567913	-0.365567423	-5.879368526
H	3.479071532	-0.814067812	-4.488457624
C	2.214240385	0.905077763	-4.157244758
H	2.783329092	1.302188738	-3.327634323
H	1.795791459	1.736836012	-4.703217056

C	1.117643554	0.034596155	-3.587548269
O	1.361366587	-0.951617298	-2.955842590
O	-0.133643288	0.334150233	-3.856153053
H	-0.233825335	1.225313127	-4.214783460
C	-7.347060676	2.127475991	-13.803907634
H	-7.705375217	1.511641342	-14.616131898
H	-6.630678773	2.832001567	-14.207831645
S	-6.568964588	0.936763383	-12.693542580
O	-5.258030270	3.054036731	-11.830951649
C	-5.406271630	1.868720471	-11.705263268
C	-4.771587682	0.934132891	-10.775775548
H	-5.143878869	-0.067119453	-10.884578465
C	-3.863422784	1.100474657	-9.778613096
H	-3.720882553	0.190017018	-9.218278896
C	-3.059812954	2.188362675	-9.265579457
C	-2.688240317	3.359329595	-9.967681460
H	-2.986479936	3.470075180	-10.990624845
C	-1.936409200	4.343993965	-9.371123172
H	-1.638730932	5.211338167	-9.928960079
C	-1.536156627	4.278224938	-7.995549403
O	-0.921588924	5.234754372	-7.435074918
C	-1.873269173	3.080016550	-7.325486702
H	-1.608203204	2.977013395	-6.291394611
C	-2.597503913	2.076409238	-7.948933280
H	-2.832674706	1.188474151	-7.384554208
O	-0.422412382	2.927359497	-4.320711939
H	-0.464518818	3.393224906	-3.494960682
H	0.124009983	3.466263543	-4.889802435
H	1.082093559	6.182314458	0.503127644
H	3.971335747	0.578298148	-5.393126179
H	-8.120462275	2.728663839	-13.331062997

pB

C	1.150310952	6.997118937	-0.131713353
H	0.284010432	7.608465506	0.097367162
H	2.019955836	7.628552863	-0.009705933
C	1.040267923	6.503272048	-1.557336713
C	-0.213106547	6.275159558	-2.111460558
H	-1.090174254	6.460989198	-1.519758424
C	-0.350202371	5.779462825	-3.392971605
H	-1.323415371	5.595633739	-3.812228817
C	0.778569723	5.468057201	-4.133637949
O	0.648708838	4.830542499	-5.337869596
H	-0.091726204	5.049118040	-7.060074096
C	2.032349506	5.745000739	-3.627878815
H	2.903286505	5.493716530	-4.201007251
C	2.154284153	6.271318843	-2.351041551
H	3.139168946	6.456389960	-1.960611079
C	3.135191264	0.121971534	-5.085388404
H	2.533894453	-0.258108610	-5.905044471
H	3.500629742	-0.723677336	-4.519449032

C	2.270041533	1.013664601	-4.179434324
H	2.858618997	1.400972022	-3.357846391
H	1.859473263	1.852584116	-4.731339974
C	1.136288342	0.150361465	-3.622054410
O	1.456966807	-0.732677557	-2.830623404
O	-0.021617218	0.366137131	-4.043070787
H	-0.533056827	1.870644787	-4.363768636
C	-7.407794349	2.099208909	-13.728197134
H	-7.795866538	1.472752868	-14.518685389
H	-6.679098862	2.772799867	-14.159572637
S	-6.645973054	0.918034186	-12.596699016
O	-5.259857016	3.016177961	-11.812957982
C	-5.459365147	1.843547504	-11.654529616
C	-4.826840830	0.916989484	-10.696651854
H	-5.242917994	-0.071380500	-10.743705184
C	-3.855080892	1.081306408	-9.771410041
H	-3.688374332	0.191365819	-9.188450868
C	-2.982680036	2.181941083	-9.357076956
C	-2.608282719	3.278877772	-10.155865779
H	-2.993809824	3.372318700	-11.148777985
C	-1.739996576	4.232402908	-9.671501006
H	-1.421629943	5.057368448	-10.277352334
C	-1.246809937	4.148522467	-8.359506931
O	-0.421704331	5.133279094	-7.981822175
C	-1.619542446	3.092355619	-7.556621852
H	-1.338104844	2.996724257	-6.534264848
C	-2.457670693	2.109181079	-8.082748765
H	-2.700004504	1.273276970	-7.450775766
O	-0.876907853	2.781582262	-4.489415180
H	-1.267853818	3.017813495	-3.659603605
H	0.195882985	4.002770219	-5.127321669
H	1.180604068	6.227889319	0.642305068
H	4.019799207	0.653597563	-5.446065124
H	-8.159501162	2.729291432	-13.256414343

pB(QM4)

C	3.447304328	0.107052173	-5.032742841
H	2.774759088	-0.465295879	-5.664783818
H	3.958050276	-0.592661442	-4.386289743
C	2.639932313	1.099838724	-4.175873760
H	3.299701691	1.652069934	-3.520526219
H	2.119120748	1.823667680	-4.787117167
C	1.649619256	0.321598190	-3.295279955
O	2.136363745	-0.501675122	-2.522204038
O	0.424433033	0.543478275	-3.423617963
H	-1.351175004	5.374649691	-8.125972862
C	-9.182185515	-0.030991589	-11.652970977
H	-9.686437934	-0.778928267	-12.244427785
H	-8.692216014	0.661546768	-12.326040358
S	-7.963144282	-0.969774613	-10.703838981
O	-7.132108560	1.462413930	-10.298665107

C	-6.876724604	0.298826516	-10.122664352
C	-5.723904717	-0.278620593	-9.419882992
H	-5.796529214	-1.343194201	-9.296896379
C	-4.588835018	0.288527181	-8.942187281
H	-3.946299874	-0.433025350	-8.467567730
C	-4.008878560	1.633287936	-8.914435586
C	-2.820889130	1.785933966	-8.191234493
H	-2.377060599	0.941668279	-7.695287882
C	-2.183342873	3.016958170	-8.082595621
H	-1.266567092	3.088947543	-7.536489357
C	-2.727900109	4.126531411	-8.688952260
O	-2.174869555	5.344051498	-8.615696931
C	-3.896894462	4.000433320	-9.440549534
H	-4.272312123	4.860763426	-9.956407232
C	-4.521320198	2.773922263	-9.560213814
H	-5.398885056	2.702331836	-10.161597722
O	-0.585326744	1.981442761	-5.234342603
H	-1.180393932	2.620923171	-4.860781370
H	-0.144732131	1.474348983	-4.479600572
O	1.107013600	3.177953474	-6.842589496
H	1.652843142	2.540596525	-7.301501585
H	0.517995946	2.695659413	-6.245186747
O	0.105122397	5.558445226	-7.171410661
H	0.637607096	4.747790587	-7.145017522
H	0.663143555	6.293473536	-6.960037159
H	4.219632348	0.613446292	-5.619819891
H	-9.834058912	0.591532173	-11.044385179

pB-pG' Intermediate

C	3.365177517	0.175084990	-5.137748308
H	2.679447772	-0.373557062	-5.775915273
H	3.863867880	-0.537192633	-4.496294977
C	2.585339964	1.189175226	-4.278953467
H	3.264260172	1.787711139	-3.686699152
H	2.008460477	1.870347459	-4.886196923
C	1.720381711	0.433268877	-3.286331943
O	2.194127739	-0.387448643	-2.545653523
O	0.437282749	0.666612169	-3.242641715
H	-1.179528087	5.289970583	-8.128600598
C	-9.160483692	-0.008572735	-11.672362889
H	-9.678003589	-0.775497299	-12.232328835
H	-8.677107421	0.656609396	-12.373615615
S	-7.942443132	-0.930439942	-10.706350139
O	-7.107848747	1.505838506	-10.303899146
C	-6.858641770	0.342600986	-10.119319952
C	-5.719926627	-0.243965009	-9.405575733
H	-5.802414406	-1.308829452	-9.290440205
C	-4.574089144	0.305365697	-8.929698116
H	-3.938966101	-0.432356135	-8.469454353
C	-3.968969007	1.634439352	-8.895469556
C	-2.737657439	1.746239577	-8.236289597

H	-2.286813859	0.877005497	-7.791226130
C	-2.059681374	2.954311124	-8.140888093
H	-1.103743195	2.994926547	-7.659027969
C	-2.611788894	4.096198347	-8.690542861
O	-2.016604822	5.284189264	-8.636541329
C	-3.833079348	4.011502522	-9.365530139
H	-4.222112485	4.895586675	-9.828783703
C	-4.491733368	2.802184535	-9.480922212
H	-5.406046518	2.760897962	-10.029895082
O	-0.604497619	2.035875055	-5.164647239
H	-1.227825486	2.730520589	-4.973016774
H	0.108200026	1.304882726	-3.932682720
O	1.023110632	3.162821322	-6.696923457
H	1.494656102	2.664006152	-7.354479794
H	0.056164884	2.460690078	-5.796507042
O	0.140063018	5.296128413	-7.212114604
H	0.664994384	4.314787366	-7.028628426
H	0.711469657	6.034087783	-7.060752818
H	4.134797636	0.677956136	-5.721855743
H	-9.818452893	0.610889593	-11.069336256

pG'

C	3.467113915	0.187523006	-5.153391512
H	2.789103051	-0.391107005	-5.769530909
H	3.999721857	-0.501845127	-4.512492780
C	2.665418616	1.177920409	-4.291402324
H	3.321770605	1.859926768	-3.764117800
H	2.010479320	1.791394298	-4.890229539
C	1.883133153	0.451339421	-3.213689311
O	2.333224762	-0.480713115	-2.609498276
O	0.672948670	0.868695620	-2.934165018
H	-0.662146426	5.416406327	-7.814433145
C	-9.270272148	0.047837857	-11.740211615
H	-9.807407112	-0.682512956	-12.327537506
H	-8.799922476	0.749717413	-12.416608620
S	-8.031992729	-0.931895074	-10.862584112
O	-7.197799619	1.486075922	-10.355421589
C	-6.944184384	0.313645751	-10.201386030
C	-5.830091435	-0.299043109	-9.511400123
H	-5.920126393	-1.365676138	-9.420679933
C	-4.675779856	0.237338975	-9.014378594
H	-4.064508048	-0.518561404	-8.548483747
C	-4.051275119	1.528564494	-8.969874576
C	-2.823928105	1.626021343	-8.278333523
H	-2.406706331	0.743208734	-7.822331168
C	-2.129220725	2.807781934	-8.168715831
H	-1.186768639	2.832763582	-7.658629551
C	-2.612636435	4.011282014	-8.745664504
O	-1.985368076	5.100451583	-8.663489786
C	-3.845169995	3.909482795	-9.454378840
H	-4.211220075	4.797558950	-9.932449632

C	-4.521222850	2.719708165	-9.574683213
H	-5.424735418	2.697793575	-10.144544085
O	-0.660334322	2.007811240	-4.994191400
H	-1.375818598	2.624888550	-4.872613980
H	0.302965035	1.477938393	-3.581447374
O	1.148329394	3.159749284	-6.647833218
H	1.607038538	2.668736018	-7.325470933
H	-0.068248199	2.448758777	-5.612839250
O	0.118827583	5.590054994	-7.221715679
H	0.968722921	4.044694033	-6.970290973
H	0.251407689	6.527260764	-7.209872480
H	4.219697278	0.706603983	-5.735798399
H	-9.901776508	0.644449675	-11.093520556

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C	3.536549024	-0.479241101	-5.490588563
H	2.886889074	-1.112966521	-6.078985509
H	4.005646737	-1.095146118	-4.736897251
C	2.708635856	0.626208952	-4.803025722
H	3.351197146	1.266504998	-4.208838550
H	2.172963633	1.238362035	-5.516099299
C	1.744058520	-0.048965864	-3.841171876
O	2.145584283	-0.785968939	-2.981402666
O	0.455963918	0.134549640	-3.980581585
H	0.183998519	0.684286536	-4.760539599
C	-8.949897235	-0.025729806	-12.252320728
H	-9.493342108	-0.831810125	-12.721546534
H	-8.432931862	0.538683056	-13.015093537
S	-7.745257560	-0.845666255	-11.169862312
O	-6.927531599	1.617734983	-11.162073088
C	-6.671215709	0.497918980	-10.781025727
C	-5.538530117	0.174523546	-9.942105847
H	-5.472254265	-0.809940742	-9.521701352
C	-4.646911194	1.163750064	-9.694422107
H	-4.781741609	2.066405671	-10.262210245
C	-3.558318365	1.189931013	-8.759169478
C	-2.718503323	2.313700609	-8.730784463
H	-2.918355287	3.142225172	-9.389654642
C	-1.636247810	2.391189393	-7.883060819
H	-0.984982226	3.241637051	-7.946836362
C	-1.358024060	1.361123706	-6.961572937
O	-0.319297023	1.386119573	-6.204099732
C	-2.271699847	0.273730449	-6.924899419
H	-2.102442880	-0.503122987	-6.200551969
C	-3.315699148	0.175552952	-7.814947770
H	-3.959182424	-0.685869617	-7.772027156
O	5.204985971	5.285878620	-5.718261095
H	5.139520723	4.628899461	-5.022780174
H	5.933258667	5.013345081	-6.269878528
O	3.030727727	6.673212612	-6.990671124
H	3.768922999	6.208850474	-6.599502772

H	2.705720338	7.256000332	-6.317847493
O	0.611457607	5.623394378	-8.190109303
H	1.514072801	5.860708096	-7.987620476
H	0.376453872	5.057349874	-7.456197610
H	4.352664989	-0.046207242	-6.076968179
H	-9.559221342	0.708092410	-11.723481147