Energy Landscape of Perylenediimide Chromophoric Aggregates

Pallavi Panthakkal Das,†[a] Aniruddha Mazumder,†[a] Megha Rajeevan,[a] Rotti Srinivasamurthy Swathi*[a] and Mahesh Hariharan*[a]

[a]School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram (IISER TVM), Maruthamala P. O., Vithura, Thiruvananthapuram 695551, Kerala, India.

*E-mail:swathi@iisertvm.ac.in

[a]School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram (IISER TVM), Maruthamala P. O., Vithura, Thiruvananthapuram 695551, Kerala, India.

*E-mail:mahesh@iisertvm.ac.in

Electronic Supplementary Information (ESI)

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Section 1: Tables

Table S1: Reported crystal structures of perylenediimide and perylene derivatives showing the interplanar distances.

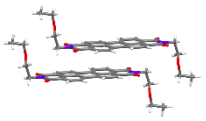
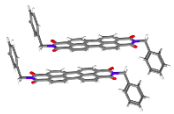
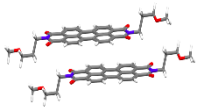
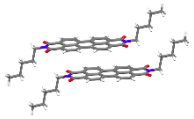
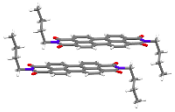
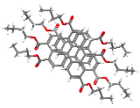
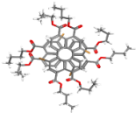
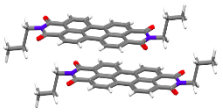
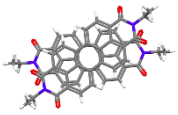
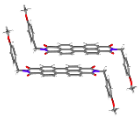
Literature	CCDC references	Molecular formula	Structure	Interplanar distance, d (Å)
Graser and co-workers, *Acta Crystallogr. Sect. C*, 1986, **42**, 189-195.	1140271	$C_{32}H_{26}N_2O_6$		3.426
	1140281	$C_{38}H_{22}N_2O_4$		3.416
	1140272	$C_{32}H_{26}N_2O_6$		3.467
	1140273	$C_{34}H_{30}N_2O_4$		3.359
	1140278	$C_{32}H_{26}N_2O_4$		3.400
Hariharan and co-workers, *Angew. Chem. Int. Ed.* 2018, **57**, 15696 –15701.	1865424	$C_{40}H_{44}O_8$		3.46–3.6
	1865425	$C_{40}H_{42}Br_2O_8$		3.390
Graser and co-workers, *Acta Crystallogr. Sect. C*, 1986, **42**, 195-198.	1140265	$C_{30}H_{22}N_2O_4$		3.415
	1140266	$C_{28}H_{18}N_2O_4$		3.453
Xie and co-workers, *J. Phys. Chem. Lett.* 2018, 9, **3**, 596–600.	1581050	$C_{40}H_{26}N_2O_6$		3.440

Table S2: List of stationary points obtained from the potential energy scan of PDI dimer and their corresponding interaction energies.

Stationary point	X (Å)	Y (Å)	Slip angle, θ (°)	Interaction Energy (kcal mol^{-1})
M_1	1.0	1.4	74.8	-26.99
M_2	0.3	1.4	85.4	-25.86
M_3	3.3	1.0	47.2	-25.52
M_4	1.4	0.0	67.7	-25.17
M_5	3.0	0.2	48.5	-24.35
M_6	2.4	1.4	58.0	-23.19
M_7	5.6	0.0	31.4	-21.39
M_8	4.5	0.0	36.9	-19.09
M_9	0.0	0.0	90.0	-15.43

Table S3: Total interaction energies (E_{int}) and their various contributing components; electrostatics (E_{ele}), exchange (E_{ex}), induction (E_{ind}) and dispersion (E_{dis}) calculated through SAPT at stationary points of PDI dimer in kcal mol^{-1}.

Stationary point	Coordinate (Å)	Rotation angle, ϕ (°)	Slip angle, θ (°)	E_{ele}	E_{ex}	E_{ind}	E_{dis}	E_{int}
R_1, M_9	(0,0)	0	90.0	-5.78	45.19	-1.78	-61.37	-23.74
R_2	(0,0)	30	90.0	-12.33	32.32	-4.06	-56.43	-40.49
R_3	(0,0)	60	90.0	-8.76	33.03	-2.27	-49.73	-27.74
R_4	(0,0)	90	90.0	-9.59	27.47	-3.15	-46.83	-30.10
M_1	(1,1.4)	0	74.8	-8.93	29.71	-3.78	-53.93	-36.93
M_2	(0.3,1.4)	0	85.4	-8.13	31.36	-3.68	-55.02	-35.48
M_3	(3.3,1.0)	0	47.2	-9.41	25.96	-3.43	-47.52	-34.40
M_4	(1.4,0.0)	0	67.7	-8.03	34.99	-3.66	-58.23	-34.93
M_5	(3.0,0.2)	0	48.5	-9.96	31.96	-3.30	-52.02	-33.32
M_6	(2.4,1.4)	0	58.0	-10.35	30.91	-3.05	-49.38	-31.87
M_7	(5.6,0.0)	0	31.4	-8.68	19.63	-2.24	-36.69	-27.98
M_8	(4.5,0.0)	0	36.9	-10.69	31.81	-2.10	-44.97	-25.94

Table S4: Geometrical parameters of the different dimer structures before and after optimisation. θ = slip angle in degrees, ϕ = rotation angle in degrees and d = interplanar distance (Å).

Dimer	Geometric Parameters	Before Optimisation	After Optimisation	Imaginary Frequencies after Optimisation
H	θ	74.8	74.32	0
	ϕ	0	0.67	
	d	3.4	3.3	
M	θ	54.7	46.06	0
	ϕ	0	1.09	
	d	3.4	3.33	
J	θ	48.5	46.08	0
	ϕ	0	1.24	
	d	3.4	3.28	
X	θ	90	87.05	0
	ϕ	30	31.27	
	d	3.4	3.405	
(+)	θ	90	87.74	0
	ϕ	90	90	
	d	3.4	3.40	

Table S5: Interaction energies obtained through DFT at the ωB97XD/6-311+G(d,p) level of theory in vacuum for different PDI dimers in kcal mol^{-1}.

Dimer System	Coordinate (Å)	Rotation angle, ϕ (°)	Slip angle, θ (°)	Interaction Energy (kcal mol^{-1})
X-dimer	(0,0,3.4)	30	90	-29.85
H-dimer	(1.0,1.4,3.4)	0	74.8	-26.99
J-dimer	(3,0.2,3.4)	0	48.5	-24.35
M-dimer	(2.5,0.9,3.4)	0	54.7	-23.63
(+)-dimer	(0,0,3.4)	90	90	-23.59
H*-dimer	(0,0,3.4)	0	90	-15.43

Table S6: Topological properties of the electron density obtained from the QTAIM analysis performed on different PDI dimer geometries.

Dimer	BCPs (3, -1)	Interactions	ρ(r) (e Å^{-3})	∇^{2}ρ(r) (e Å^{-5})
H*	91	O2●●●O42	0.00359	0.01355
	102	C5●●●C45	0.00356	0.01479
	139	N4●●●N44	0.00539	0.01443
	196	O3●●●O43	0.00377	0.01353
X	109	N37●●●078	0.00345	0.01163
	135	C35●●●C76	0.00352	0.01446
(+)	128	C7●●●C53	0.00546	0.01454
H	133	O2●●●C45	0.00340	0.01284
	145	C6●●●C56	0.00577	0.01612
	187	N4●●●C55	0.00452	0.01403
M	107	C35●●●C69	0.00476	0.01569
	132	N38●●●C71	0.00570	0.01573
	182	O39●●●C72	0.00474	0.01464
J	178	O39●●●C72	0.00402	0.01303
	126	N38●●●C71	0.00486	0.01386
	158	C32●●●C41	0.00535	0.01521

Table S7: List of stationary points obtained from the potential energy scan of perylene dimer and their corresponding interaction energies.

Stationary point	X (Å)	Y (Å)	Slip angle, θ (°)	Energy (kcal mol^{-1})
M'$_1$	1.0	1.3	74.6	-19.22
M'$_2$	1.3	0.5	71.1	-18.22
M'$_3$	2.8	0.2	50.6	-16.11
M'$_4$	3.1	1.2	49.9	-16.17
M'$_5$	2.5	1.4	55.8	-15.57
M'$_6$	0.0	0.0	90.0	-10.57
M'$_7$	5.3	0.0	32.7	-9.49

Table S8: Total interaction energies (E_{int}) and their various contributing components; electrostatics (E_{ele}), exchange (E_{ex}), induction (E_{ind}) and dispersion (E_{dis}) calculated through SAPT at stationary points of perylene dimer in kcal mol^{-1}.

Stationary point	Coordinate (Å)	Rotation angle, ϕ (°)	Slip angle, θ (°)	E_{ele}	E_{ex}	E_{ind}	E_{dis}	E_{int}
R'$_1$, M'$_6$	(0,0)	0	90.0	-12.05	43.09	-1.00	-49.84	-19.81
R'$_2$	(0,0)	32	90.0	-10.38	30.63	-3.24	-47.38	-30.37
R'$_3$	(0,0)	60	90.0	-11.08	34.33	-1.90	-46.01	-24.65
R'$_4$	(0,0)	90	90.0	-10.20	29.58	-2.96	-45.68	-29.27
M'$_1$	(1.0,1.3)	0	74.6	-9.87	27.53	-2.81	-43.61	-28.76
M'$_2$	(1.3,0.5)	0	71.1	-9.44	24.82	-2.39	-40.26	-27.26
M'$_2$	(1.3,0.5)	0	71.1	-9.44	24.82	-2.39	-40.26	-27.26
M'$_3$	(2.8,0.2)	0	50.6	-8.80	24.99	-2.07	-38.15	-24.03
M'$_4$	(3.1,1.2)	0	49.9	-8.11	20.05	-1.99	-33.42	-23.47
M'$_5$	(2.5,1.4)	0	55.8	-9.26	24.45	-2.08	-36.56	-23.45
M'$_7$	(5.3,0)	0	32.7	-5.85	17.23	-1.36	-24.30	-14.28

Table S9: Total interaction energies (E_{int}) and their components; electrostatics (E_{ele}), exchange (E_{ex}), induction (E_{ind}), and dispersion (E_{dis}) obtained through SAPT for different perylene dimers in kcal mol^{-1}.

Dimer System	E_{ele}	E_{ex}	E_{ind}	E_{dis}	E_{int}
X-dimer	-10.38	30.63	-3.24	-47.38	-30.37
(+)-dimer	-10.20	29.58	-2.96	-45.68	-29.27
H-dimer	-9.87	27.53	-2.81	-43.61	-28.76
M-dimer	-9.25	27.16	-1.96	-40.38	-24.42
J-dimer	-8.80	24.99	-2.07	-38.15	-24.03
H*-dimer	-12.05	43.09	-1.00	-49.84	-19.81

Section 2: Figures

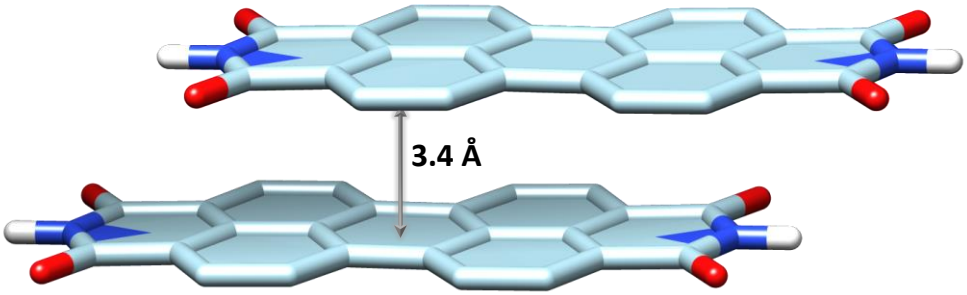


Figure S1: PDI dimer model showing the interplanar distance of 3.4 Å between the monomers.

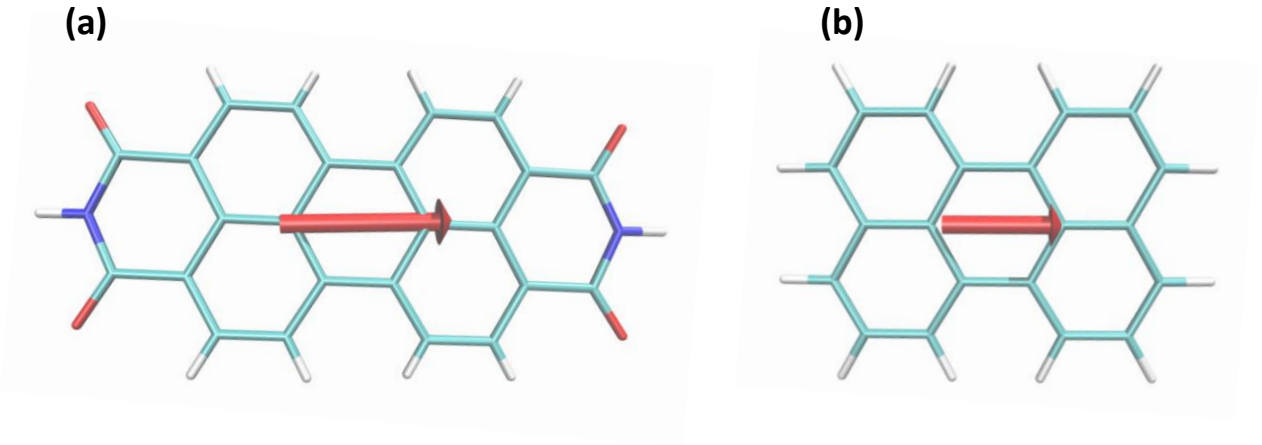


Figure S2: Transition dipole moment vectors (μ) of (a) PDI and (b) perylene for the S_0 to S_1 transition.

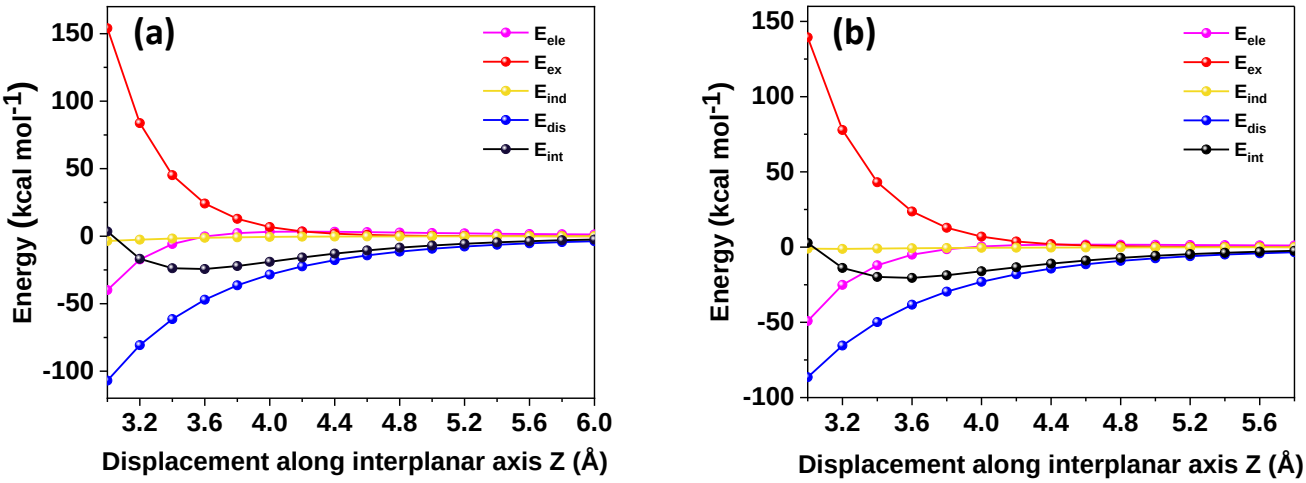


Figure S3: Variation of the total interaction energy (E_{int}) and the components; electrostatics (E_{ele}), exchange (E_{ex}), induction (E_{ind}), and dispersion (E_{dis}) computed through SAPT as a function of

displacement along interplanar axis Z in (a) PDI dimer and (b) perylene dimer.

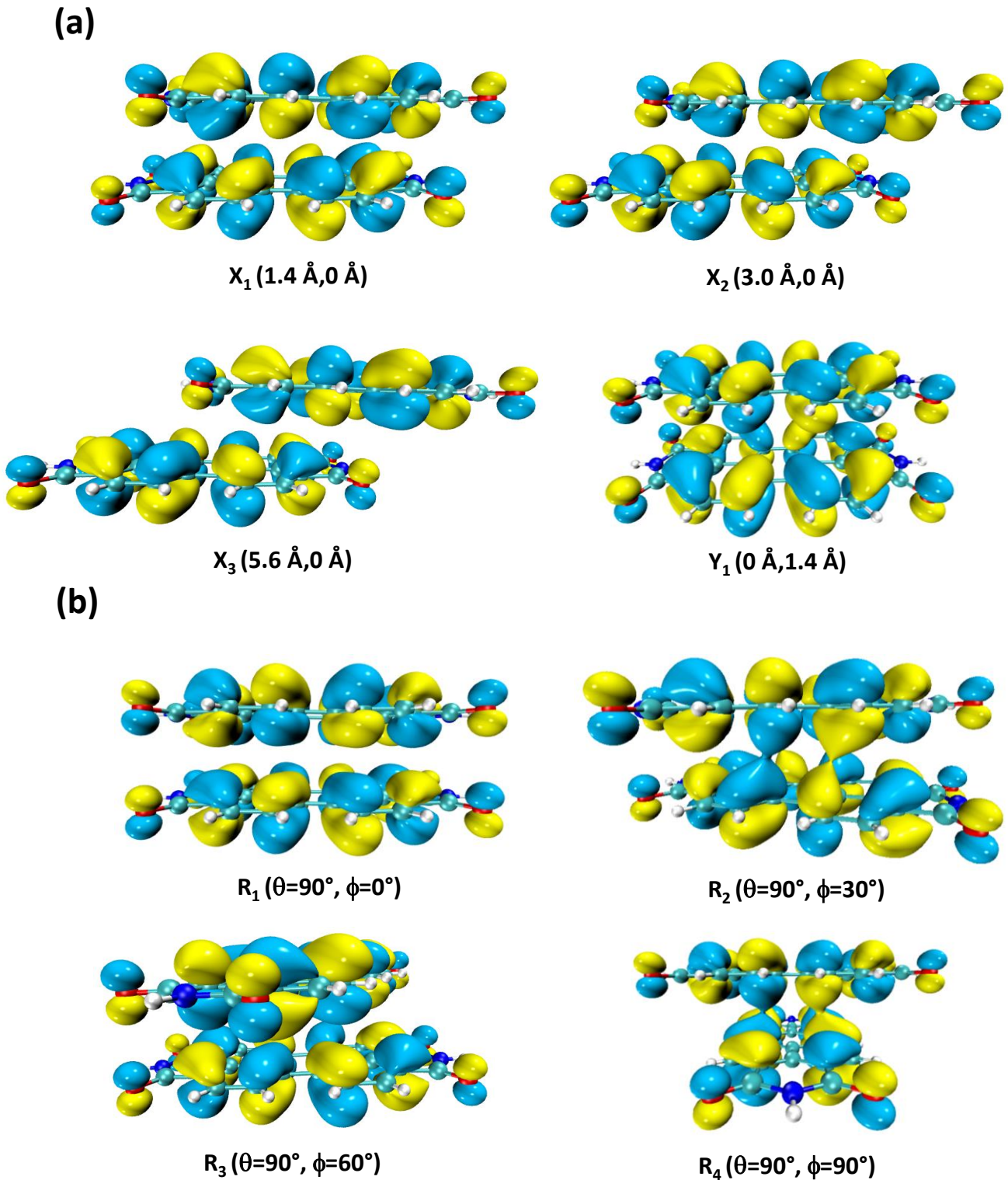


Figure S4: HOMO isosurfaces (isovalue=0.017 a.u.) of stationary points obtained from 1D SAPT scan by (a) displacing one of the monomers along long axis X or short axis Y and (b) rotating along the interplanar axis Z.

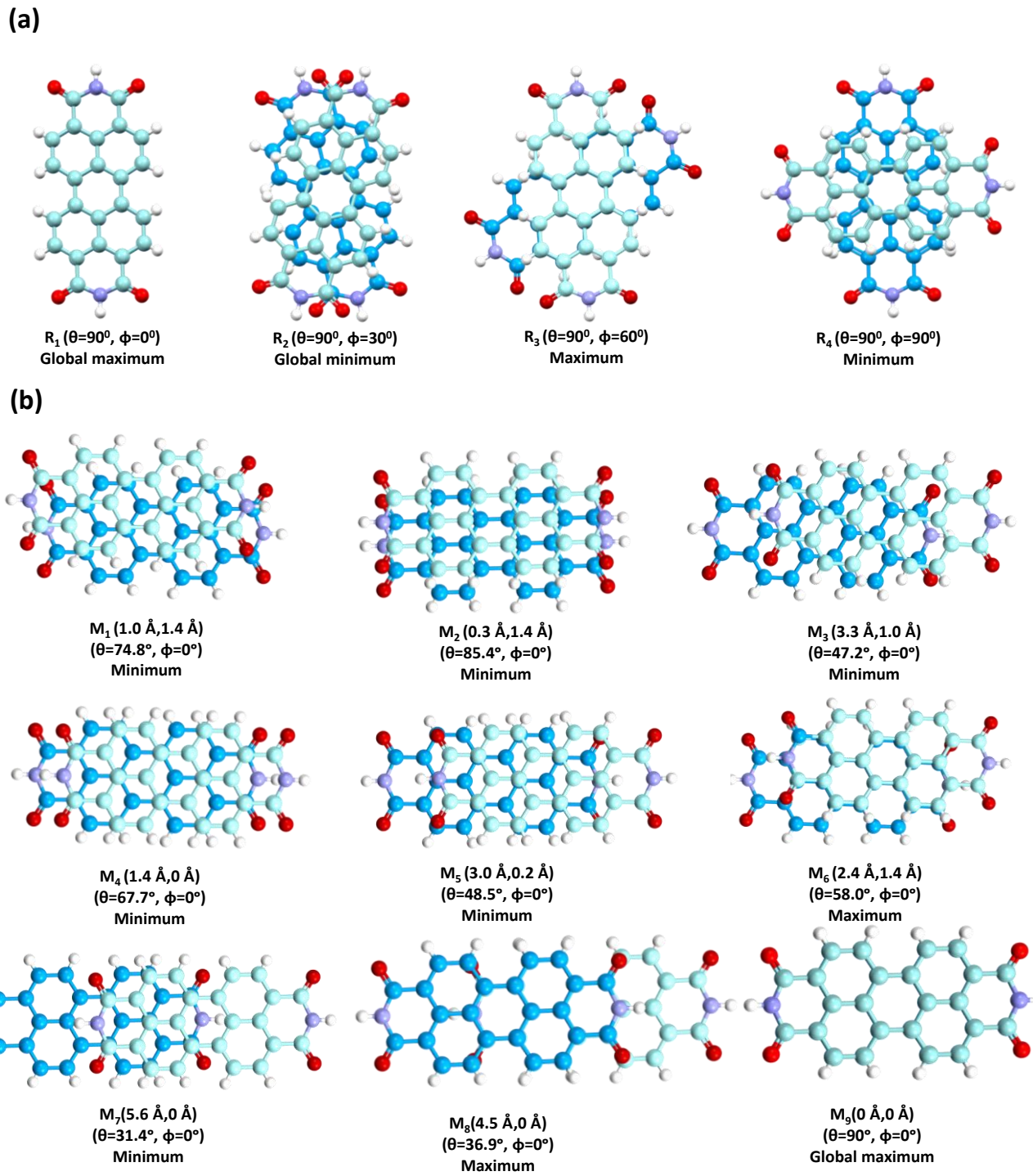


Figure S5: Stationary point geometries obtained from (a) the 1D SAPT scan after rotation about interplanar axis and (b) the PES scan after displacing along long and short axes of one monomer in the PDI dimer.

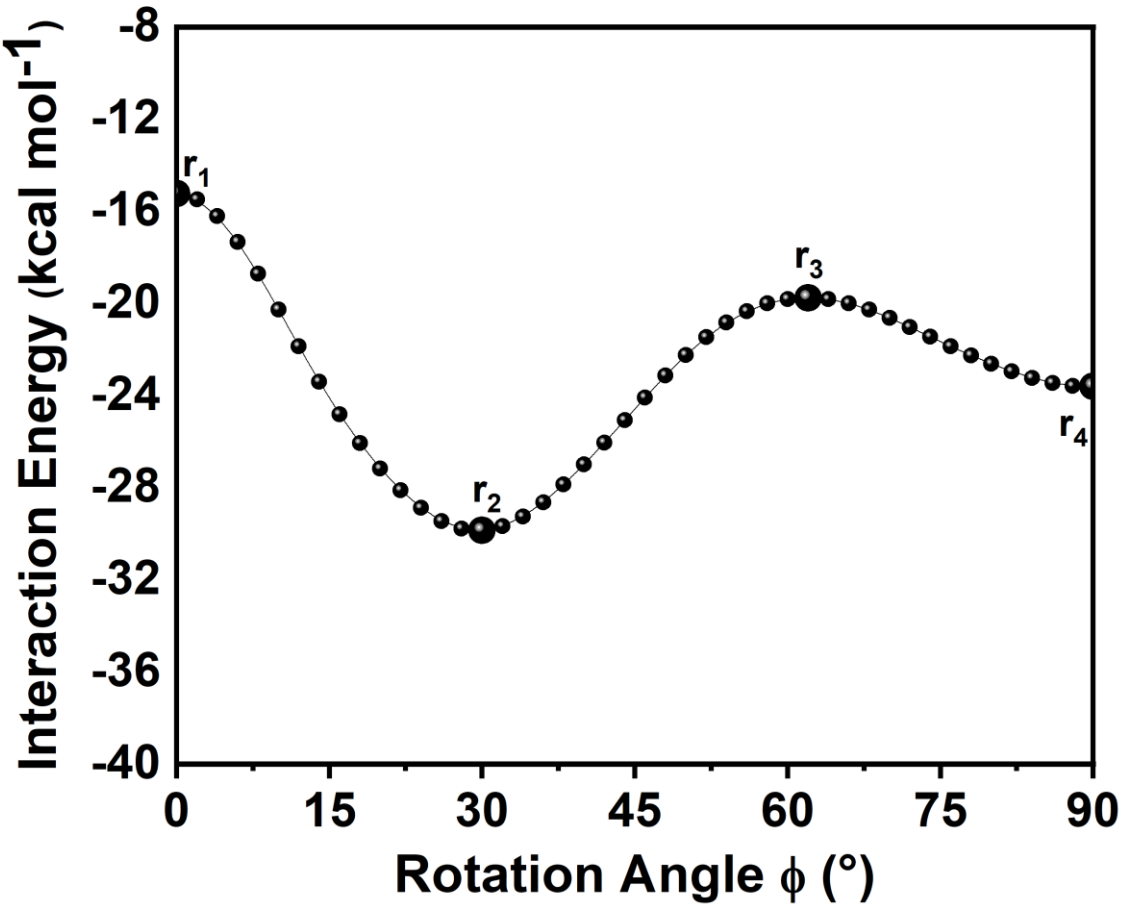


Figure S6: Rigid PES scan of PDI dimer showing interaction energy as a function of the rotation of one monomer about the interplanar axis Z. Step size for rotation=2°.

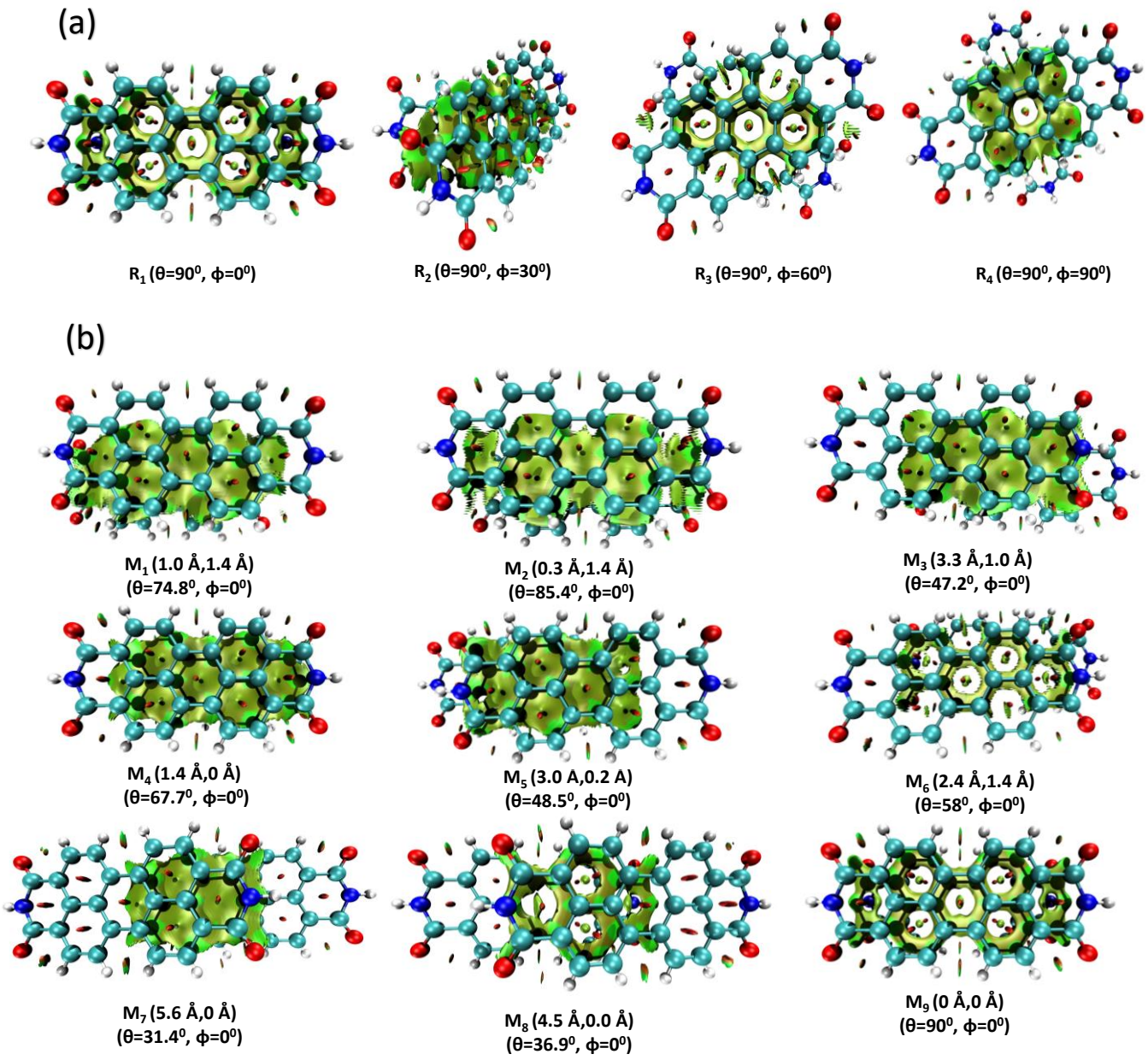


Figure S7: NCI isosurfaces of stationary points obtained from the PES scan of PDI dimer after (a) rotation about interplanar axis and (b) displacement along long and short axes showing the non-covalent interactions. Green surfaces and red surfaces represent stabilizing and destabilizing interactions, respectively.

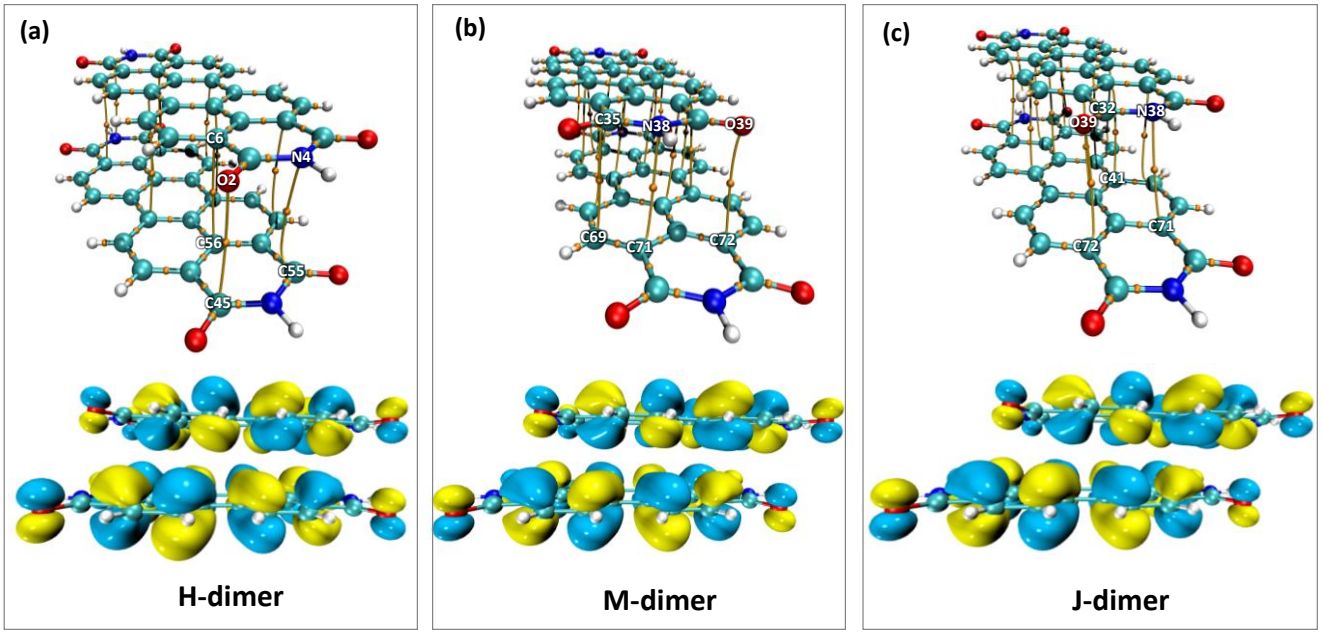


Figure S8: QTAIM plots (top) showing the BCPs between the monomers and HOMO isosurfaces (isovalue=0.017 a.u.) (bottom) showing the interactions between the orbital lobes of the two monomers in (a) H-, (b) M- and (c) J-dimers of PDI.

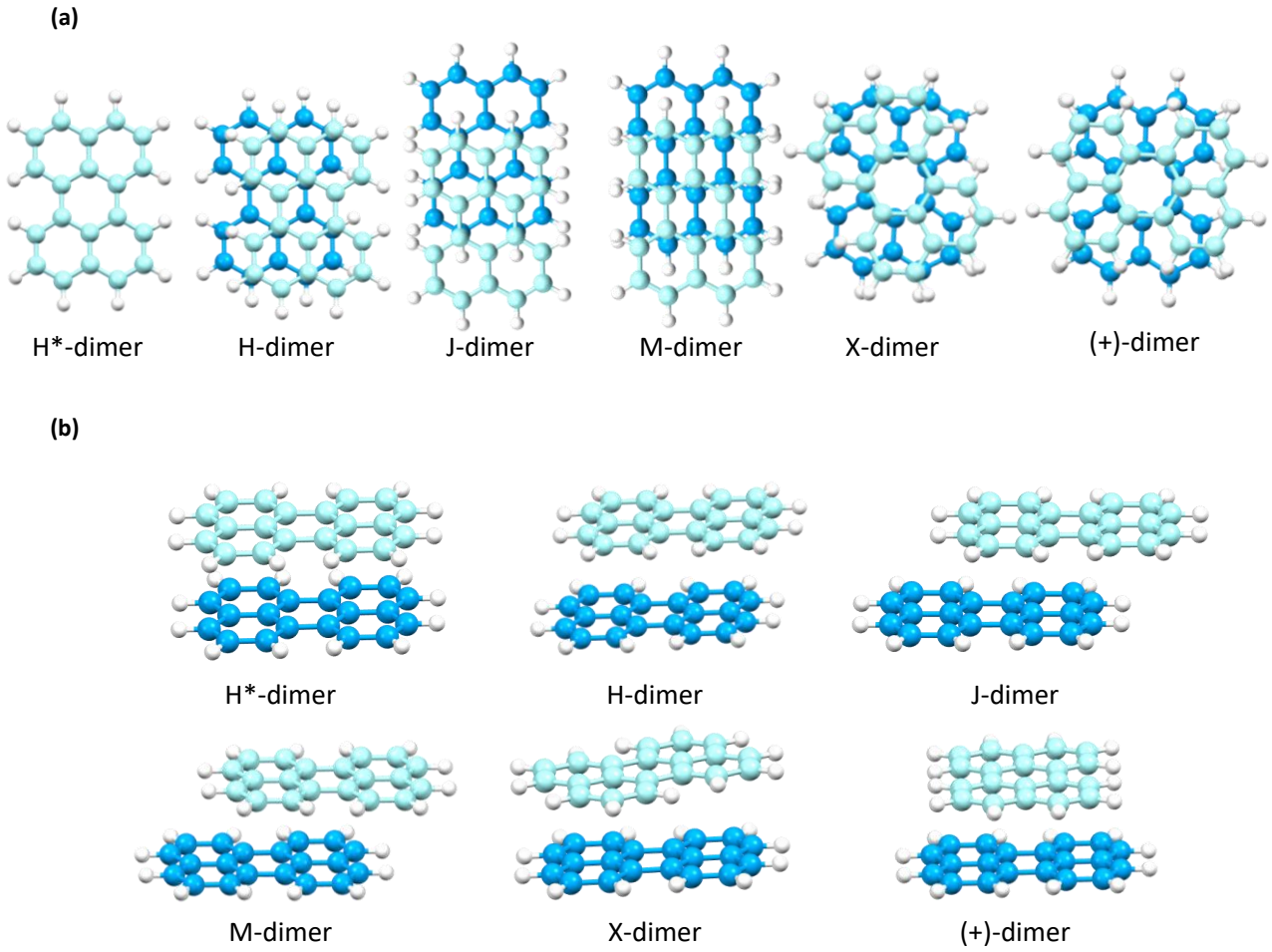


Figure S9: Geometries of different perylene dimers shown in (a) top view and (b) side view.

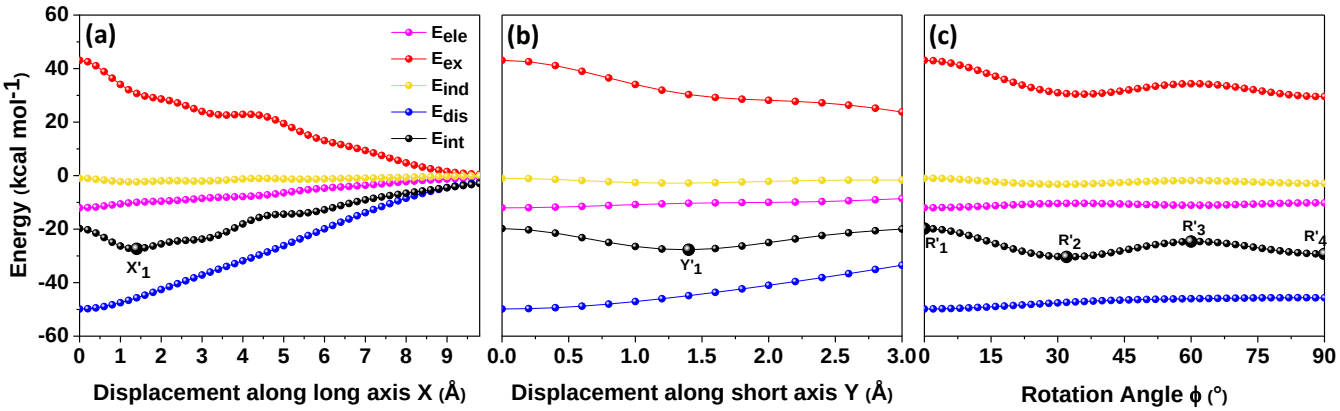


Figure S10: Variation of the total interaction energy (E_{int}) and the components; electrostatics (E_{ele}), exchange (E_{ex}), induction (E_{ind}), and dispersion (E_{dis})) computed through SAPT as a function of (a) displacement along long axis X, (b) displacement along short axis Y and (c) rotation about the interplanar axis Z in perylene dimer.

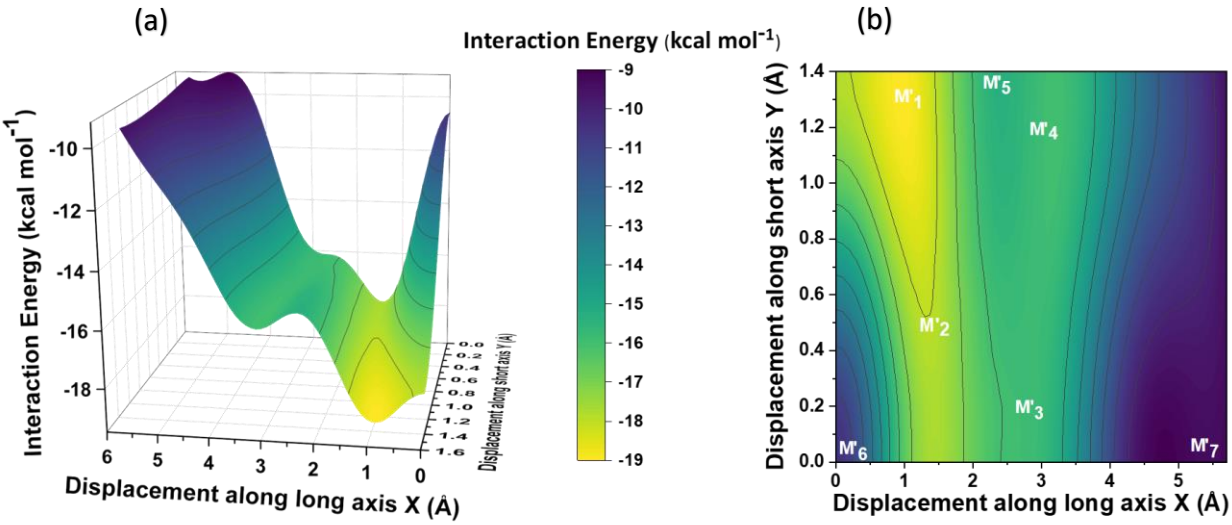


Figure S11: (a) Potential energy surface (PES) of perylene dimer showing interaction energy as a function of displacement along long axis X and short axis Y. (b) 2-D contour plot showing the stationary points on the PES. Step size for displacement=0.1 Å.

Section 4: Cartesian Coordinates of PDI Dimer Systems Studied:

4.1. H*-dimer:

C	1.43370000	0.00000000	-0.03610000
O	-5.71290000	-2.21470000	-0.00640000
O	-5.67220000	2.29930000	-0.00650000
N	-5.62360000	0.05170000	0.00000000
C	-5.05620000	-1.15910000	-0.00870000
C	-3.57890000	-1.19680000	0.03460000
C	-2.90160000	-2.37310000	0.00830000
C	-1.49180000	-2.40130000	0.02440000
C	-0.74610000	-1.23400000	0.01590000
C	-1.43380000	0.00000000	0.03610000
C	-0.71300000	1.25730000	0.01850000
C	-1.44110000	2.42950000	0.01010000
C	-2.83910000	2.44780000	0.01440000
C	-3.54650000	1.25930000	0.00450000
C	-5.03590000	1.29560000	-0.02640000
C	-2.87960000	0.02500000	0.02800000
H	-1.04140000	3.14480000	-0.00200000
H	-3.23720000	3.16850000	0.02000000
H	-6.57510000	0.04350000	0.01310000
H	-3.39160000	-3.19280000	-0.02420000
H	-1.04820000	-3.24480000	0.03380000
C	0.71300000	-1.25730000	-0.01850000
C	0.74610000	1.23400000	-0.01580000
C	1.44110000	-2.42950000	-0.01010000
C	1.49170000	2.40130000	-0.02440000
C	2.87960000	-0.02500000	-0.02800000
C	2.83910000	-2.44780000	-0.01440000
H	1.04140000	-3.14480000	0.00200000
C	2.90160000	2.37300000	-0.00830000
H	1.04820000	3.24480000	-0.03370000
C	3.57890000	1.19680000	-0.03460000
C	3.54650000	-1.25930000	-0.00450000
H	3.23720000	-3.16850000	-0.02000000
H	3.39160000	3.19280000	0.02420000
C	5.05620000	1.15910000	0.00870000
C	5.03590000	-1.29560000	0.02640000
O	5.71290000	2.21470000	0.00640000
N	5.62360000	-0.05170000	0.00000000
O	5.67230000	-2.29930000	0.00640000
H	6.57510000	-0.04350000	-0.01310000

C	1.43370000	0.00000000	3.36390000
O	-5.71290000	-2.21470000	3.39360000
O	-5.67220000	2.29930000	3.39350000
N	-5.62360000	0.05170000	3.40000000
C	-5.05620000	-1.15910000	3.39130000
C	-3.57890000	-1.19680000	3.43460000
C	-2.90160000	-2.37310000	3.40830000
C	-1.49180000	-2.40130000	3.42440000
C	-0.74610000	-1.23400000	3.41590000
C	-1.43380000	0.00000000	3.43610000
C	-0.71300000	1.25730000	3.41850000
C	-1.44110000	2.42950000	3.41010000
C	-2.83910000	2.44780000	3.41440000
C	-3.54650000	1.25930000	3.40450000
C	-5.03590000	1.29560000	3.37360000
C	-2.87960000	0.02500000	3.42800000
H	-1.04140000	3.14480000	3.39800000
H	-3.23720000	3.16850000	3.42000000
H	-6.57510000	0.04350000	3.41310000
H	-3.39160000	-3.19280000	3.37580000
H	-1.04820000	-3.24480000	3.43380000
C	0.71300000	-1.25730000	3.38150000
C	0.74610000	1.23400000	3.38420000
C	1.44110000	-2.42950000	3.38990000
C	1.49170000	2.40130000	3.37560000
C	2.87960000	-0.02500000	3.37200000
C	2.83910000	-2.44780000	3.38560000
H	1.04140000	-3.14480000	3.40200000
C	2.90160000	2.37300000	3.39170000
H	1.04820000	3.24480000	3.36630000
C	3.57890000	1.19680000	3.36540000
C	3.54650000	-1.25930000	3.39550000
H	3.23720000	-3.16850000	3.38000000
H	3.39160000	3.19280000	3.42420000
C	5.05620000	1.15910000	3.40870000
C	5.03590000	-1.29560000	3.42640000
O	5.71290000	2.21470000	3.40640000
N	5.62360000	-0.05170000	3.40000000
O	5.67230000	-2.29930000	3.40640000
H	6.57510000	-0.04350000	3.38690000

4.2. H-dimer:

C	2.43370000	1.40000000	-0.03610000
O	-4.71290000	-0.81470000	-0.00640000

O	-4.67220000	3.69930000	-0.00650000
N	-4.62360000	1.45170000	0.00000000
C	-4.05620000	0.24090000	-0.00870000
C	-2.57890000	0.20320000	0.03460000
C	-1.90160000	-0.97310000	0.00830000
C	-0.49180000	-1.00130000	0.02440000
C	0.25390000	0.16600000	0.01590000
C	-0.43380000	1.40000000	0.03610000
C	0.28700000	2.65730000	0.01850000
C	-0.44110000	3.82950000	0.01010000
C	-1.83910000	3.84780000	0.01440000
C	-2.54650000	2.65930000	0.00450000
C	-4.03590000	2.69560000	-0.02640000
C	-1.87960000	1.42500000	0.02800000
H	-0.04140000	4.54480000	-0.00200000
H	-2.23720000	4.56850000	0.02000000
H	-5.57510000	1.44350000	0.01310000
H	-2.39160000	-1.79280000	-0.02420000
H	-0.04820000	-1.84480000	0.03380000
C	1.71300000	0.14270000	-0.01850000
C	1.74610000	2.63400000	-0.01580000
C	2.44110000	-1.02950000	-0.01010000
C	2.49170000	3.80130000	-0.02440000
C	3.87960000	1.37500000	-0.02800000
C	3.83910000	-1.04780000	-0.01440000
H	2.04140000	-1.74480000	0.00200000
C	3.90160000	3.77300000	-0.00830000
H	2.04820000	4.64480000	-0.03370000
C	4.57890000	2.59680000	-0.03460000
C	4.54650000	0.14070000	-0.00450000
H	4.23720000	-1.76850000	-0.02000000
H	4.39160000	4.59280000	0.02420000
C	6.05620000	2.55910000	0.00870000
C	6.03590000	0.10440000	0.02640000
O	6.71290000	3.61470000	0.00640000
N	6.62360000	1.34830000	0.00000000
O	6.67230000	-0.89930000	0.00640000
H	7.57510000	1.35650000	-0.01310000
C	1.43370000	0.00000000	3.36390000
O	-5.71290000	-2.21470000	3.39360000
O	-5.67220000	2.29930000	3.39350000
N	-5.62360000	0.05170000	3.40000000
C	-5.05620000	-1.15910000	3.39130000
C	-3.57890000	-1.19680000	3.43460000
C	-2.90160000	-2.37310000	3.40830000

C	-1.49180000	-2.40130000	3.42440000
C	-0.74610000	-1.23400000	3.41590000
C	-1.43380000	0.00000000	3.43610000
C	-0.71300000	1.25730000	3.41850000
C	-1.44110000	2.42950000	3.41010000
C	-2.83910000	2.44780000	3.41440000
C	-3.54650000	1.25930000	3.40450000
C	-5.03590000	1.29560000	3.37360000
C	-2.87960000	0.02500000	3.42800000
H	-1.04140000	3.14480000	3.39800000
H	-3.23720000	3.16850000	3.42000000
H	-6.57510000	0.04350000	3.41310000
H	-3.39160000	-3.19280000	3.37580000
H	-1.04820000	-3.24480000	3.43380000
C	0.71300000	-1.25730000	3.38150000
C	0.74610000	1.23400000	3.38420000
C	1.44110000	-2.42950000	3.38990000
C	1.49170000	2.40130000	3.37560000
C	2.87960000	-0.02500000	3.37200000
C	2.83910000	-2.44780000	3.38560000
H	1.04140000	-3.14480000	3.40200000
C	2.90160000	2.37300000	3.39170000
H	1.04820000	3.24480000	3.36630000
C	3.57890000	1.19680000	3.36540000
C	3.54650000	-1.25930000	3.39550000
H	3.23720000	-3.16850000	3.38000000
H	3.39160000	3.19280000	3.42420000
C	5.05620000	1.15910000	3.40870000
C	5.03590000	-1.29560000	3.42640000
O	5.71290000	2.21470000	3.40640000
N	5.62360000	-0.05170000	3.40000000
O	5.67230000	-2.29930000	3.40640000
H	6.57510000	-0.04350000	3.38690000

4.3. J-dimer:

C	4.43370000	0.20000000	-0.03610000
O	-2.71290000	-2.01470000	-0.00640000
O	-2.67220000	2.49930000	-0.00650000
N	-2.62360000	0.25170000	0.00000000
C	-2.05620000	-0.95910000	-0.00870000
C	-0.57890000	-0.99680000	0.03460000
C	0.09840000	-2.17310000	0.00830000
C	1.50820000	-2.20130000	0.02440000
C	2.25390000	-1.03400000	0.01590000

C	1.56620000	0.20000000	0.03610000
C	2.28700000	1.45730000	0.01850000
C	1.55890000	2.62950000	0.01010000
C	0.16090000	2.64780000	0.01440000
C	-0.54650000	1.45930000	0.00450000
C	-2.03590000	1.49560000	-0.02640000
C	0.12040000	0.22500000	0.02800000
H	1.95860000	3.34480000	-0.00200000
H	-0.23720000	3.36850000	0.02000000
H	-3.57510000	0.24350000	0.01310000
H	-0.39160000	-2.99280000	-0.02420000
H	1.95180000	-3.04480000	0.03380000
C	3.71300000	-1.05730000	-0.01850000
C	3.74610000	1.43400000	-0.01580000
C	4.44110000	-2.22950000	-0.01010000
C	4.49170000	2.60130000	-0.02440000
C	5.87960000	0.17500000	-0.02800000
C	5.83910000	-2.24780000	-0.01440000
H	4.04140000	-2.94480000	0.00200000
C	5.90160000	2.57300000	-0.00830000
H	4.04820000	3.44480000	-0.03370000
C	6.57890000	1.39680000	-0.03460000
C	6.54650000	-1.05930000	-0.00450000
H	6.23720000	-2.96850000	-0.02000000
H	6.39160000	3.39280000	0.02420000
C	8.05620000	1.35910000	0.00870000
C	8.03590000	-1.09560000	0.02640000
O	8.71290000	2.41470000	0.00640000
N	8.62360000	0.14830000	0.00000000
O	8.67230000	-2.09930000	0.00640000
H	9.57510000	0.15650000	-0.01310000
C	1.43370000	0.00000000	3.36390000
O	-5.71290000	-2.21470000	3.39360000
O	-5.67220000	2.29930000	3.39350000
N	-5.62360000	0.05170000	3.40000000
C	-5.05620000	-1.15910000	3.39130000
C	-3.57890000	-1.19680000	3.43460000
C	-2.90160000	-2.37310000	3.40830000
C	-1.49180000	-2.40130000	3.42440000
C	-0.74610000	-1.23400000	3.41590000
C	-1.43380000	0.00000000	3.43610000
C	-0.71300000	1.25730000	3.41850000
C	-1.44110000	2.42950000	3.41010000
C	-2.83910000	2.44780000	3.41440000
C	-3.54650000	1.25930000	3.40450000

C	-5.03590000	1.29560000	3.37360000
C	-2.87960000	0.02500000	3.42800000
H	-1.04140000	3.14480000	3.39800000
H	-3.23720000	3.16850000	3.42000000
H	-6.57510000	0.04350000	3.41310000
H	-3.39160000	-3.19280000	3.37580000
H	-1.04820000	-3.24480000	3.43380000
C	0.71300000	-1.25730000	3.38150000
C	0.74610000	1.23400000	3.38420000
C	1.44110000	-2.42950000	3.38990000
C	1.49170000	2.40130000	3.37560000
C	2.87960000	-0.02500000	3.37200000
C	2.83910000	-2.44780000	3.38560000
H	1.04140000	-3.14480000	3.40200000
C	2.90160000	2.37300000	3.39170000
H	1.04820000	3.24480000	3.36630000
C	3.57890000	1.19680000	3.36540000
C	3.54650000	-1.25930000	3.39550000
H	3.23720000	-3.16850000	3.38000000
H	3.39160000	3.19280000	3.42420000
C	5.05620000	1.15910000	3.40870000
C	5.03590000	-1.29560000	3.42640000
O	5.71290000	2.21470000	3.40640000
N	5.62360000	-0.05170000	3.40000000
O	5.67230000	-2.29930000	3.40640000
H	6.57510000	-0.04350000	3.38690000

4.4. M-dimer:

C	3.82870000	0.00000000	-0.03610000
O	-3.31790000	-2.21470000	-0.00640000
O	-3.27720000	2.29930000	-0.00650000
N	-3.22860000	0.05170000	0.00000000
C	-2.66120000	-1.15910000	-0.00870000
C	-1.18390000	-1.19680000	0.03460000
C	-0.50660000	-2.37310000	0.00830000
C	0.90320000	-2.40130000	0.02440000
C	1.64890000	-1.23400000	0.01590000
C	0.96120000	0.00000000	0.03610000
C	1.68200000	1.25730000	0.01850000
C	0.95390000	2.42950000	0.01010000
C	-0.44410000	2.44780000	0.01440000
C	-1.15150000	1.25930000	0.00450000
C	-2.64090000	1.29560000	-0.02640000
C	-0.48460000	0.02500000	0.02800000

H	1.35360000	3.14480000	-0.00200000
H	-0.84220000	3.16850000	0.02000000
H	-4.18010000	0.04350000	0.01310000
H	-0.99660000	-3.19280000	-0.02420000
H	1.34680000	-3.24480000	0.03380000
C	3.10800000	-1.25730000	-0.01850000
C	3.14110000	1.23400000	-0.01580000
C	3.83610000	-2.42950000	-0.01010000
C	3.88670000	2.40130000	-0.02440000
C	5.27460000	-0.02500000	-0.02800000
C	5.23410000	-2.44780000	-0.01440000
H	3.43640000	-3.14480000	0.00200000
C	5.29660000	2.37300000	-0.00830000
H	3.44320000	3.24480000	-0.03370000
C	5.97390000	1.19680000	-0.03460000
C	5.94150000	-1.25930000	-0.00450000
H	5.63220000	-3.16850000	-0.02000000
H	5.78660000	3.19280000	0.02420000
C	7.45120000	1.15910000	0.00870000
C	7.43090000	-1.29560000	0.02640000
O	8.10790000	2.21470000	0.00640000
N	8.01860000	-0.05170000	0.00000000
O	8.06730000	-2.29930000	0.00640000
H	8.97010000	-0.04350000	-0.01310000
C	1.43370000	0.00000000	3.36390000
O	-5.71290000	-2.21470000	3.39360000
O	-5.67220000	2.29930000	3.39350000
N	-5.62360000	0.05170000	3.40000000
C	-5.05620000	-1.15910000	3.39130000
C	-3.57890000	-1.19680000	3.43460000
C	-2.90160000	-2.37310000	3.40830000
C	-1.49180000	-2.40130000	3.42440000
C	-0.74610000	-1.23400000	3.41590000
C	-1.43380000	0.00000000	3.43610000
C	-0.71300000	1.25730000	3.41850000
C	-1.44110000	2.42950000	3.41010000
C	-2.83910000	2.44780000	3.41440000
C	-3.54650000	1.25930000	3.40450000
C	-5.03590000	1.29560000	3.37360000
C	-2.87960000	0.02500000	3.42800000
H	-1.04140000	3.14480000	3.39800000
H	-3.23720000	3.16850000	3.42000000
H	-6.57510000	0.04350000	3.41310000
H	-3.39160000	-3.19280000	3.37580000
H	-1.04820000	-3.24480000	3.43380000

C	0.71300000	-1.25730000	3.38150000
C	0.74610000	1.23400000	3.38420000
C	1.44110000	-2.42950000	3.38990000
C	1.49170000	2.40130000	3.37560000
C	2.87960000	-0.02500000	3.37200000
C	2.83910000	-2.44780000	3.38560000
H	1.04140000	-3.14480000	3.40200000
C	2.90160000	2.37300000	3.39170000
H	1.04820000	3.24480000	3.36630000
C	3.57890000	1.19680000	3.36540000
C	3.54650000	-1.25930000	3.39550000
H	3.23720000	-3.16850000	3.38000000
H	3.39160000	3.19280000	3.42420000
C	5.05620000	1.15910000	3.40870000
C	5.03590000	-1.29560000	3.42640000
O	5.71290000	2.21470000	3.40640000
N	5.62360000	-0.05170000	3.40000000
O	5.67230000	-2.29930000	3.40640000
H	6.57510000	-0.04350000	3.38690000

4.5. X-dimer:

C	1.43370000	0.00000000	-0.03610000
O	-5.71290000	-2.21470000	-0.00640000
O	-5.67220000	2.29930000	-0.00650000
N	-5.62360000	0.05170000	0.00000000
C	-5.05620000	-1.15910000	-0.00870000
C	-3.57890000	-1.19680000	0.03460000
C	-2.90160000	-2.37310000	0.00830000
C	-1.49180000	-2.40130000	0.02440000
C	-0.74610000	-1.23400000	0.01590000
C	-1.43380000	0.00000000	0.03610000
C	-0.71300000	1.25730000	0.01850000
C	-1.44110000	2.42950000	0.01010000
C	-2.83910000	2.44780000	0.01440000
C	-3.54650000	1.25930000	0.00450000
C	-5.03590000	1.29560000	-0.02640000
C	-2.87960000	0.02500000	0.02800000
H	-1.04140000	3.14480000	-0.00200000
H	-3.23720000	3.16850000	0.02000000
H	-6.57510000	0.04350000	0.01310000
H	-3.39160000	-3.19280000	-0.02420000
H	-1.04820000	-3.24480000	0.03380000
C	0.71300000	-1.25730000	-0.01850000

C	0.74610000	1.23400000	-0.01580000
C	1.44110000	-2.42950000	-0.01010000
C	1.49170000	2.40130000	-0.02440000
C	2.87960000	-0.02500000	-0.02800000
C	2.83910000	-2.44780000	-0.01440000
H	1.04140000	-3.14480000	0.00200000
C	2.90160000	2.37300000	-0.00830000
H	1.04820000	3.24480000	-0.03370000
C	3.57890000	1.19680000	-0.03460000
C	3.54650000	-1.25930000	-0.00450000
H	3.23720000	-3.16850000	-0.02000000
H	3.39160000	3.19280000	0.02420000
C	5.05620000	1.15910000	0.00870000
C	5.03590000	-1.29560000	0.02640000
O	5.71290000	2.21470000	0.00640000
N	5.62360000	-0.05170000	0.00000000
O	5.67230000	-2.29930000	0.00640000
H	6.57510000	-0.04350000	-0.01310000
C	1.24170000	0.71690000	3.36390000
O	-3.84010000	-4.77440000	3.39360000
O	-6.06190000	-0.84480000	3.39350000
N	-4.89610000	-2.76710000	3.40000000
C	-3.79930000	-3.53190000	3.39130000
C	-2.50100000	-2.82590000	3.43460000
C	-1.32640000	-3.50590000	3.40830000
C	-0.09130000	-2.82540000	3.42440000
C	-0.02910000	-1.44170000	3.41590000
C	-1.24170000	-0.71690000	3.43610000
C	-1.24610000	0.73240000	3.41850000
C	-2.46280000	1.38350000	3.41010000
C	-3.68260000	0.70030000	3.41440000
C	-3.70100000	-0.68260000	3.40450000
C	-5.00910000	-1.39590000	3.37360000
C	-2.50630000	-1.41810000	3.42800000
H	-2.47430000	2.20270000	3.39800000
H	-4.38780000	1.12540000	3.42000000
H	-5.71590000	-3.24990000	3.41310000
H	-1.34080000	-4.46080000	3.37580000
H	0.71470000	-3.33420000	3.43380000
C	1.24610000	-0.73240000	3.38150000
C	0.02910000	1.44170000	3.38420000
C	2.46280000	-1.38350000	3.38990000
C	0.09130000	2.82540000	3.37560000
C	2.50630000	1.41810000	3.37200000
C	3.68260000	-0.70030000	3.38560000

H	2.47430000	-2.20270000	3.40200000
C	1.32640000	3.50590000	3.39170000
H	-0.71470000	3.33410000	3.36630000
C	2.50100000	2.82590000	3.36540000
C	3.70100000	0.68260000	3.39550000
H	4.38780000	-1.12540000	3.38000000
H	1.34080000	4.46080000	3.42420000
C	3.79930000	3.53190000	3.40870000
C	5.00910000	1.39590000	3.42640000
O	3.84010000	4.77440000	3.40640000
N	4.89600000	2.76700000	3.40000000
O	6.06200000	0.84490000	3.40640000
H	5.71590000	3.24990000	3.38690000

4.6. (+)-dimer:

C	1.43370000	0.00000000	-0.03610000
O	-5.71290000	-2.21470000	-0.00640000
O	-5.67220000	2.29930000	-0.00650000
N	-5.62360000	0.05170000	0.00000000
C	-5.05620000	-1.15910000	-0.00870000
C	-3.57890000	-1.19680000	0.03460000
C	-2.90160000	-2.37310000	0.00830000
C	-1.49180000	-2.40130000	0.02440000
C	-0.74610000	-1.23400000	0.01590000
C	-1.43380000	0.00000000	0.03610000
C	-0.71300000	1.25730000	0.01850000
C	-1.44110000	2.42950000	0.01010000
C	-2.83910000	2.44780000	0.01440000
C	-3.54650000	1.25930000	0.00450000
C	-5.03590000	1.29560000	-0.02640000
C	-2.87960000	0.02500000	0.02800000
H	-1.04140000	3.14480000	-0.00200000
H	-3.23720000	3.16850000	0.02000000
H	-6.57510000	0.04350000	0.01310000
H	-3.39160000	-3.19280000	-0.02420000
H	-1.04820000	-3.24480000	0.03380000
C	0.71300000	-1.25730000	-0.01850000
C	0.74610000	1.23400000	-0.01580000
C	1.44110000	-2.42950000	-0.01010000
C	1.49170000	2.40130000	-0.02440000
C	2.87960000	-0.02500000	-0.02800000
C	2.83910000	-2.44780000	-0.01440000
H	1.04140000	-3.14480000	0.00200000
C	2.90160000	2.37300000	-0.00830000

H	1.04820000	3.24480000	-0.03370000
C	3.57890000	1.19680000	-0.03460000
C	3.54650000	-1.25930000	-0.00450000
H	3.23720000	-3.16850000	-0.02000000
H	3.39160000	3.19280000	0.02420000
C	5.05620000	1.15910000	0.00870000
C	5.03590000	-1.29560000	0.02640000
O	5.71290000	2.21470000	0.00640000
N	5.62360000	-0.05170000	0.00000000
O	5.67230000	-2.29930000	0.00640000
H	6.57510000	-0.04350000	-0.01310000
C	0.00000000	1.43370000	3.36390000
O	2.21470000	-5.71290000	3.39360000
O	-2.29930000	-5.67220000	3.39350000
N	-0.05170000	-5.62360000	3.40000000
C	1.15910000	-5.05620000	3.39130000
C	1.19680000	-3.57890000	3.43460000
C	2.37310000	-2.90160000	3.40830000
C	2.40130000	-1.49180000	3.42440000
C	1.23400000	-0.74610000	3.41590000
C	0.00000000	-1.43380000	3.43610000
C	-1.25730000	-0.71300000	3.41850000
C	-2.42950000	-1.44110000	3.41010000
C	-2.44780000	-2.83910000	3.41440000
C	-1.25930000	-3.54650000	3.40450000
C	-1.29560000	-5.03590000	3.37360000
C	-0.02500000	-2.87960000	3.42800000
H	-3.14480000	-1.04140000	3.39800000
H	-3.16850000	-3.23720000	3.42000000
H	-0.04350000	-6.57510000	3.41310000
H	3.19280000	-3.39160000	3.37580000
H	3.24480000	-1.04820000	3.43380000
C	1.25730000	0.71300000	3.38150000
C	-1.23400000	0.74610000	3.38420000
C	2.42950000	1.44110000	3.38990000
C	-2.40130000	1.49170000	3.37560000
C	0.02500000	2.87960000	3.37200000
C	2.44780000	2.83910000	3.38560000
H	3.14480000	1.04140000	3.40200000
C	-2.37300000	2.90160000	3.39170000
H	-3.24480000	1.04820000	3.36630000
C	-1.19680000	3.57890000	3.36540000
C	1.25930000	3.54650000	3.39550000
H	3.16850000	3.23720000	3.38000000
H	-3.19280000	3.39160000	3.42420000

C	-1.15910000	5.05620000	3.40870000
C	1.29560000	5.03590000	3.42640000
O	-2.21470000	5.71290000	3.40640000
N	0.05170000	5.62360000	3.40000000
O	2.29930000	5.67230000	3.40640000
H	0.04350000	6.57510000	3.38690000