Supporting Information for:

The role of CT excitations in PDI aggregates

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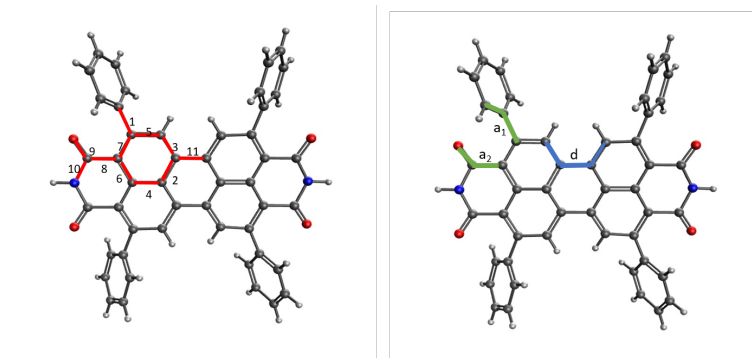## Contents

1 PDI molecule

Figure S1: Analysed bond distances, angles and dihedrals in the optimized and crystal structures.

Table S1: Optimized and crystal structure bond lengths (Å), angles (°) and dihedral (°) of the PDI molecule. See Figure S1 for labelling. Crystal bond lengths are given by the mean value of analogue bonds.

	Optimized	Crystal
C···C(1)	1.49	1.50
C···C(2)	1.42	1.42
C···C(3)	1.38	1.38
C···C(4)	1.42	1.41
C···C(5)	1.41	1.43
C···C(6)	1.43	1.42
C···C(7)	1.39	1.38
C···C(8)	1.49	1.51
C···O(9)	1.21	1.21
C···N(10)	1.38	1.40
C···C(11)	1.48	1.48
a_1	121.0	123.5
a_2	125.4	119.7
d_1	6.3	5.5

Table S2: MO energies (in eV) for PDI **2** and the optimized PDI **3** computed at CAM-B3LYP/6-31G(d) level.

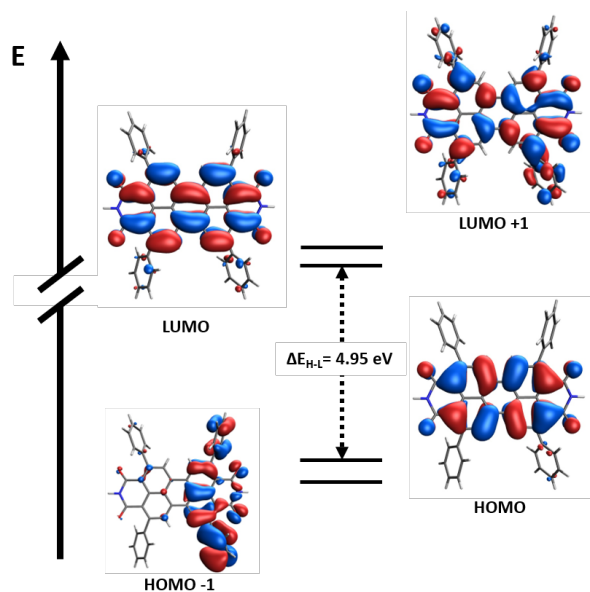|	HOMO-1	HOMO	LUMO	LUMO+1
PDI **2**	-0.281	-0.262	-0.08	-0.023
PDI **3**	-0.329	-0.266	-0.093	-0.026

Figure S2: Frontier molecular orbitals of the PDI **2** derivative computed at CAM-B3LYP/6-31G(d).

Table S3: Vertical excitation energies (in eV) and oscillator strengths (in parenthesis) to the lowest singlet and triplet excited states computed at CAM-B3LYP/6-31G(d) level for the PDI **2**. Orbital-to-orbtial composition correspond to TDA transitions. H=HOMO; L=LUMO.

State	TDDFT	TDA	Composition
S_1	3.01(0.720)	3.19(0.986)	95 % H→L
S_2	3.42(0.047)	3.47(0.057)	75 % H-1→L
S_3	3.58(0.234)	3.61(0.232)	72 % H-2→L
S_4	3.88(0.010)	3.91(0.015)	57 % H-3→L
S_5	3.94(0.006)	3.97(0.010)	41 % H-9→L
T_1	1.46	1.93	88% H→L
T_2	2.67	2.95	31% H-2→L,24% H→L+1
T_3	2.92	3.05	32% H-1→L,10% H→L+1
T_4	3.05	3.14	55% H-2→L
T_5	3.11	3.34	40% H→L+3

3

Table S4: Vertical excitation energies (in eV) and oscillator strengths (in parenthesis) to the lowest singlet and triplet excited states computed at B3LYP/6-31G(d) level for the PDI **2**. Orbital-to-orbtial composition correspond to TDA transitions. H=HOMO; L=LUMO.

State	TDDFT	TDA	Composition
S_1	2.60(0.275)	2.63(0.440)	93% H-1→L
S_2	2.63(0.314)	2.72(0.083)	94% H-2→L
S_3	2.71(0.079)	2.79(0.733)	90% H→L
S_4	2.92(0.032)	2.93(0.088)	90% H-3→L
S_5	3.02(0.041)	3.02(0.075)	92% H→4-L
T_1	1.57	1.75	95% H→L
T_2	2.40	2.42	92% H→1-L
T_3	2.51	2.53	91% H→2-L
T_4	2.63	2.69	67% H→3-L
T_5	2.86	2.88	60% H→4-L

Table S5: Vertical excitation energies (in eV) and oscillator strengths (in parenthesis) to the lowest singlet and triplet excited states computed at ωB97X/6-31G(d) level for the PDI **2**. Orbital-to-orbtial composition correspond to TDA transitions. H=HOMO; L=LUMO.

State	TDDFT	TDA	Composition
S_1	3.21(0.785)	3.40(1.035)	92% H→L
S_2	3.74(0.042)	3.82(0.050)	57% H→1-L
S_3	3.90(0.289)	3.97(0.296)	54% H→2-L
S_4	4.20(0.003)	4.23(0.005)	39% H→9-L
S_5	4.26(0.011)	4.31(0.028)	45% H→10-L
T_1	1.42	2.06	83% H→L
T_2	2.68	3.08	33% H→L+2
T_3	3.06	3.26	43% H→1-L
T_4	3.17	3.35	37% H→2-L
T_5	3.23	3.46	30% H→L+4

Table S6: Vertical excitation energies (in eV) and oscillator strengths (in parenthesis) to the lowest singlet and triplet excited states computed at CAM-B3LYP/6-311+G(d) level for the PDI **2**. Orbital-to-orbtial composition correspond to TDA transitions. H=HOMO; L=LUMO.

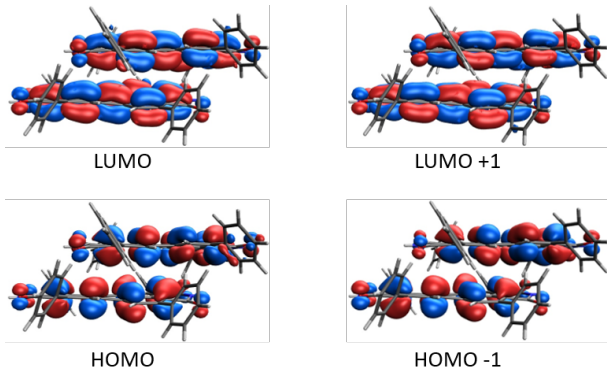| State	TDDFT	TDA	Composition
S_1	2.94(0.699)	3.11(0.945)	94 % H→L
S_2	3.37(0.043)	3.42(0.054)	75 % H-1→L
S_3	3.54(0.279)	3.57(0.285)	72 % H-2→L
S_4	3.85(0.012)	3.88(0.016)	69 % H-3→L
S_5	3.94(0.004)	3.96(0.006)	44 % H-9→L
T_1	1.47	1.92	88% H→L
T_2	2.66	2.92	41% H-1→L,18% H→L+1
T_3	2.88	3.01	21% H-1→L,16% H→L+1
T_4	3.00	3.09	53% H-2→L
T_5	3.08	3.30	75% H-1→L

2 *Intra-* and *inter-*column PDI dimers

Figure S3: Molecular orbital diagram of **D2** computed at the TDA, CAM-B3LYP/6-31G(d) level.

Table S7 shows low-lying singlet and triplet excited state energies and oscillator strengths for the *intra* and *inter* column dimers of PDI from the crystal structure of **1**. Excitated state distribution in the *inter-*dimer, near degeneracy between pairs of states, indicates weak coupling. Energy splitting between low-lying states is much larger for the *intra-*dimer.

Table S7: Excitation energies (in eV) and oscillator strengths (f) to the lowest singlet and triplet excited states of *inter-*column and *intra-* (**D2**) dimers computed at the TDA, CAM-B3LYP/6-31G(d) level.

state	*inter* ΔE	f	*intra* ΔE	f
S_1	3.17	2.042	3.04	0.0000
S_2	3.19	0.021	3.12	1.1228
S_3	3.38	0.116	3.29	0.0000
S_4	3.47	0.056	3.38	0.5012
S_5	3.60	0.421	3.42	0.0000
S_6	3.61	0.035	3.43	0.2152
T_1	1.93	-	1.92	-
T_2	1.94	-	1.94	-
T_3	2.89	-	2.94	-
T_4	2.94	-	2.94	-
T_5	3.04	-	2.96	-
T_6	3.04	-	2.97	-

Table S8: Excitation energies (in eV) and oscillator strengths (f) to the lowest singlet and triplet excited states of *inter*-column and *intra*- (**D2**) dimers computed at the TDA, ωB97X-D/6-31G(d) level.

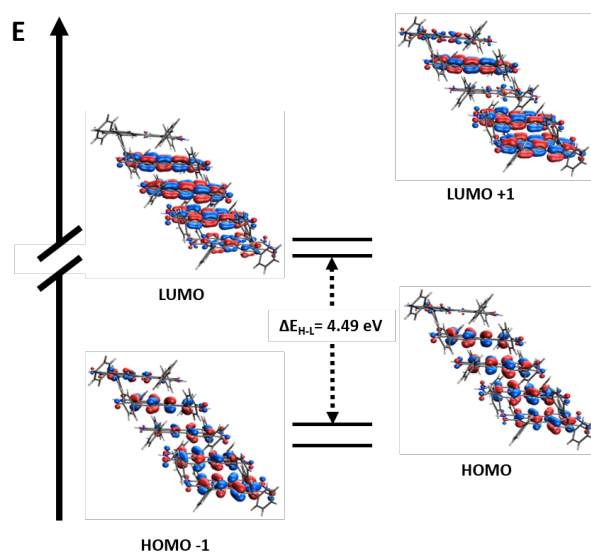|	inter		intra	
state	ΔE	f	ΔE	f
S_1	3.21	2.049	3.08	0.000
S_2	3.23	0.017	3.19	1.442
S_3	3.48	0.119	3.47	0.000
S_4	3.55	0.057	3.49	0.218
S_5	3.68	0.487	3.53	0.000
S_6	3.69	0.002	3.57	0.188
T_1	1.99	-	1.98	-
T_2	1.99	-	1.99	-
T_3	2.96	-	2.99	-
T_4	3.00	-	3.00	-
T_5	3.09	-	3.03	-
T_6	3.10	-	3.04	-

3 PDI pentamer

Figure S4: Frontier molecular orbitals of the PDI pentamer aggregate computed at CAM-B3LYP/6-31G(d).

4 Diabatic states of PDI dimers

Table S9: Transition energies (in eV), oscillator strengths (in parenthesis), and diabatic contributions ω (in %) obtained through the ER diabatization for four excited singlet and triplet states of **D1** and **D2** dimers computed at the (TDA) CAM-B3LYP/6-31G(d) level. Diabatic states correspond to the ones mainly obtained as H,H-1→L,L+1 electronic promotions. LE_A = A*B, LE_B = AB*, CT_{AB} = A^+B^-, CT_{BA} = A^-B^+.

state	ΔE (f)	$\omega(LE_A)$	$\omega(LE_B)$	$\omega(CT_{AB})$	$\omega(CT_{BA})$
D1 dimer					
$S_{1,+}$	2.96 (1.009)	25	25	25	25
$S_{2,-}$	3.04 (0.000)	48	48	2	2
$S_{3,-}$	3.27 (0.000)	2	2	48	48
$S_{8,+}$	3.58 (0.645)	25	25	25	25
$T_{1,+}$	1.87	47	47	3	3
$T_{2,-}$	1.95	50	50	0	0
$T_{9,-}$	3.26	0	0	50	50
$T_{11,+}$	3.33	3	3	47	47
D2 dimer					
$S_{1,-}$	3.04 (0.000)	48	48	2	2
$S_{2,+}$	3.12 (1.123)	26	26	24	24
$S_{3,-}$	3.29 (0.000)	2	2	48	48
$S_{4,+}$	3.38 (0.502)	24	24	26	26
$T_{1,-}$	1.92	49	49	1	1
$T_{2,+}$	1.94	50	50	0	0
$T_{9,-}$	3.29	0	0	50	50
$T_{12,+}$	3.35	1	1	49	49

Table S10: Diabatic electronic energies (in eV) and electronic couplings obtained through the Boys diabatization of the four lowest excited singlets and triplet states of the PDI *intra*-dimers **D1** (unit cell) computed at the (TDA) CAM-B3LYP/6-31G(d) level.

dimer	$E(^1LE)$	$E(^1CT)$	V_{DC}	V_e	V_h	V_{CT}
D1	3.16	3.27	105	-176	-134	-3

dimer	$E(^3LE)$	$E(^3CT)$	V_{DC}	V_e	V_h	V_{CT}
D1	1.95	3.25	0	-183	-145	-3

Table S11: Transition energies (in eV), oscillator strengths (in parenthesis), and diabatic contributions ω (in %) obtained through the Boys diabatization for four excited singlet and triplet states of **D1** dimer computed at the (TDA) CAM-B3LYP/6-31G(d) level. Diabatic states correspond to the ones mainly obtained as H,H-1→L,L+1 electronic promotions. LE_A = A*B, LE_B = AB*, CT_{AB} = A$^+$B$^-$, CT_{BA} = A$^-$B$^+$.

state	ΔE (f)	$\omega(LE_A)$	$\omega(LE_B)$	$\omega(CT_{AB})$	$\omega(CT_{BA})$
$S_{1,+}$	2.96 (1.009)	25	25	25	25
$S_{2,-}$	3.04 (0.000)	48	48	2	2
$S_{3,-}$	3.27 (0.000)	2	2	48	48
$S_{8,+}$	3.58 (0.645)	25	25	25	25
$T_{1,+}$	1.87	47	47	3	3
$T_{2,-}$	1.95	50	50	0	0
$T_{9,-}$	3.26	0	0	50	50
$T_{11,+}$	3.33	3	3	47	47

5 Triplet excitons along intermolecular distortions
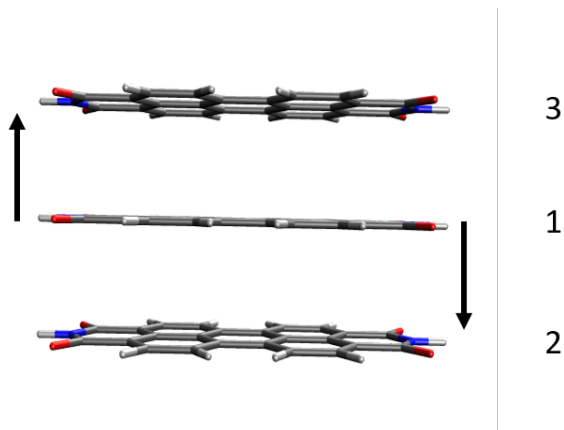

Figure S5: Molecular trimer of PDI **3**. Numbers indicate molecular labelling in Tables S12-S17.

Table S12: Diabatic electronic energies (in eV) and electronic couplings (in meV) obtained through the ER diabatization of the seven lowest excited triplet states of the eclipsed trimer along the vertical distortion (3.7 Å) computed at the (TDA) CAM-B3LYP/6-31G(d) level. $LE_1 = 1^*23$, $LE_2 = 12^*3$, $LE_3 = 123^*$, $CT_{12} = 1^+2^-3$, $CT_{13} = 1^+23^-$, $CT_{21} = 1^-2^+3$, $CT_{31} = 1^-23^+$.

H_{diab}	$^3LE_1$	$^3LE_3$	$^3LE_2$	$^3CT_{31}$	$^3CT_{21}$	$^3CT_{12}$	$^3CT_{13}$
$^3LE_1$	1.69	6	6	-219	219	230	-230
$^3LE_3$	6	1.70	-3	239	7	10	231
$^3LE_2$	6	-3	1.70	-7	-239	-231	-10
$^3CT_{31}$	-219	239	-7	2.87	10	84	-7
$^3CT_{21}$	219	7	-239	10	2.87	-7	84
$^3CT_{12}$	230	10	-231	84	-7	2.95	0
$^3CT_{13}$	-230	231	-10	-7	84	0	2.95

Table S13: Diabatic electronic energies (in eV) and electronic couplings (in meV) obtained through the ER diabatization of the seven lowest excited triplet states of the eclipsed trimer along the vertical distortion (4.0 Å) computed at the (TDA) CAM-B3LYP/6-31G(d) level. $LE_1 = 1^*23$, $LE_2 = 12^*3$, $LE_3 = 123^*$, $CT_{12} = 1^+2^-3$, $CT_{13} = 1^+23^-$, $CT_{21} = 1^-2^+3$, $CT_{31} = 1^-23^+$.

H_{diab}	$^3LE_1$	$^3LE_3$	$^3LE_2$	$^3CT_{31}$	$^3CT_{21}$	$^3CT_{12}$	$^3CT_{13}$
$^3LE_1$	1.70	1	1	139	139	-148	-148
$^3LE_3$	1	1.70	0	-151	2	-3	142
$^3LE_2$	1	0	1.70	2	-151	142	-3
$^3CT_{31}$	139	-151	2	3.00	-3	35	2
$^3CT_{21}$	139	2	-151	-3	3.00	2	35
$^3CT_{12}$	-148	-3	142	35	2	3.08	0
$^3CT_{13}$	-148	142	-3	2	35	0	3.08

Table S14: Diabatic electronic energies (in eV) and electronic couplings (in meV) obtained through the ER diabatization of the seven lowest excited triplet states of the eclipsed trimer along the vertical distortion (4.2 Å) computed at the (TDA) CAM-B3LYP/6-31G(d) level. $LE_1 = 1^*23$, $LE_2 = 12^*3$, $LE_3 = 123^*$, $CT_{12} = 1^+2^-3$, $CT_{13} = 1^+23^-$, $CT_{21} = 1^-2^+3$, $CT_{31} = 1^-23^+$.

H_{diab}	$^3LE_1$	$^3LE_3$	$^3LE_2$	$^3CT_{31}$	$^3CT_{21}$	$^3CT_{12}$	$^3CT_{13}$
$^3LE_1$	1.70	0	0	101	101	109	109
$^3LE_3$	0	1.70	0	1	-110	-102	1
$^3LE_2$	0	0	1.70	-110	1	1	-102
$^3CT_{31}$	101	1	-110	3.06	-1	-19	-1
$^3CT_{21}$	101	-110	1	-1	3.06	-1	-19
$^3CT_{12}$	109	-102	1	-19	-1	3.15	0
$^3CT_{13}$	109	1	-102	-1	-19	0	3.15

Table S15: Diabatic electronic energies (in eV) and electronic couplings (in meV) obtained through the ER diabatization of the seven lowest excited triplet states of the eclipsed trimer along the vertical distortion (4.8 Å) computed at the (TDA) CAM-B3LYP/6-31G(d) level. $LE_1 = 1^*23$, $LE_2 = 12^*3$, $LE_3 = 123^*$, $CT_{12} = 1^+2^-3$, $CT_{13} = 1^+23^-$, $CT_{21} = 1^-2^+3$, $CT_{31} = 1^-23^+$.

H_{diab}	$^3LE_2$	$^3LE_3$	$^3LE_1$	$^3CT_{31}$	$^3CT_{21}$	$^3CT_{12}$	$^3CT_{13}$
$^3LE_2$	1.70	0	0	0	-38	34	0
$^3LE_3$	0	1.70	0	-38	0	0	34
$^3LE_1$	0	0	1.70	34	34	-38	-38
$^3CT_{31}$	0	-38	34	3.21	0	2	0
$^3CT_{21}$	-38	0	34	0	3.21	0	2
$^3CT_{12}$	34	0	-38	2	0	3.30	0
$^3CT_{13}$	0	34	-38	0	2	0	3.30

Table S16: Diabatic electronic energies (in eV) and electronic couplings (in meV) obtained through the ER diabatization of the seven lowest excited triplet states of the eclipsed trimer along the vertical distortion (5.3 Å) computed at the (TDA) CAM-B3LYP/6-31G(d) level. $LE_1 = 1^*23$, $LE_2 = 12^*3$, $LE_3 = 123^*$, $CT_{12} = 1^+2^-3$, $CT_{13} = 1^+23^-$, $CT_{21} = 1^-2^+3$, $CT_{31} = 1^-23^+$.

H_{diab}	$^3LE_3$	$^3LE_2$	$^3LE_1$	$^3CT_{31}$	$^3CT_{21}$	$^3CT_{12}$	$^3CT_{13}$
$^3LE_3$	1.70	0	0	-13	0	0	-12
$^3LE_2$	0	1.70	0	0	-13	12	0
$^3LE_1$	0	0	1.70	12	12	-13	13
$^3CT_{31}$	-13	0	12	3.30	0	0	0
$^3CT_{21}$	0	-13	12	0	3.30	0	0
$^3CT_{12}$	0	12	-13	0	0	3.39	0
$^3CT_{13}$	-12	0	13	0	0	0	3.39

Table S17: Transition energies (in eV), oscillator strengths (in parenthesis), and diabatic contributions ω (in %) obtained through the ER diabatization for the lowest seven excited triplet states of the eclipsed trimer along the vertical distortion computed at the (TDA) CAM-B3LYP/6-31G(d) level.

state	ΔE (f)	$\omega(\mathrm{LE_1})$	$\omega(\mathrm{LE_3})$	$\omega(\mathrm{LE_2})$	$\omega(\mathrm{CT_{31}})$	$\omega(\mathrm{CT_{21}})$	$\omega(\mathrm{CT_{12}})$	$\omega(\mathrm{CT_{13}})$
displacement = 3.7 Å								
$T_{1,+}$	1.46 (-)	57	14	14	5	4	3	3
$T_{2,-}$	1.61 (-)	0	47	47	2	2	1	1
$T_{3,+}$	1.70 (-)	33	33	34	0	0	0	0
$T_{4,+}$	2.83 (-)	0	0	0	31	31	19	19
$T_{5,+}$	2.97 (-)	3	1	1	45	45	3	2
$T_{6,-}$	3.07 (-)	6	2	2	2	2	43	43
$T_{7,-}$	3.09 (-)	0	3	3	17	17	30	30
displacement = 4.0 Å								
$T_{1,-}$	1.61 (-)	63	15	15	3	2	1	1
$T_{2,-}$	1.67 (-)	0	49	49	1	1	0	0
$T_{3,+}$	1.70 (-)	32	34	34	0	0	0	0
$T_{4,-}$	3.00 (-)	0	0	0	40	40	10	10
$T_{5,+}$	3.04 (-)	2	0	0	49	49	0	0
$T_{6,+}$	3.12 (-)	0	1	1	9	9	40	40
$T_{7,+}$	3.13 (-)	2	1	1	0	0	48	48
displacement = 4.2 Å								
$T_{1,-}$	1.65 (-)	65	16	16	1	1	1	1
$T_{2,+}$	1.69 (-)	0	49	49	1	1	0	0
$T_{3,+}$	1.70 (-)	32	34	34	0	0	0	0
$T_{4,-}$	3.06 (-)	0	0	0	46	46	4	4
$T_{5,+}$	3.08 (-)	2	0	0	49	49	0	0
$T_{6,+}$	3.16 (-)	0	0	0	4	4	46	46
$T_{7,+}$	3.17 (-)	2	0	0	0	0	49	49
displacement = 4.8 Å								
$T_{1,-}$	1.70 (-)	17	17	66	0	0	0	0
$T_{2,+}$	1.70 (-)	50	50	0	0	0	0	0
$T_{3,+}$	1.70 (-)	33	33	34	0	0	0	0
$T_{4,-}$	3.21 (-)	0	0	0	50	50	0	0
$T_{5,+}$	3.21 (-)	0	0	0	50	50	0	0
$T_{6,-}$	3.30 (-)	0	0	0	0	0	50	50
$T_{7,-}$	3.30 (-)	0	0	0	0	0	50	50
displacement = 5.3 Å								
$T_{1,+}$	1.70 (-)	28	28	44	0	0	0	0
$T_{2,-}$	1.70 (-)	0	50	50	0	0	0	0
$T_{3,-}$	1.70 (-)	22	22	56	0	0	0	0
$T_{4,+}$	3.30 (-)	0	0	0	51	49	0	0
$T_{5,-}$	3.30 (-)	0	0	0	49	51	0	0
$T_{6,-}$	3.39 (-)	0	0	0	0	0	53	47
$T_{7,+}$	3.30 (-)	0	0	0	0	0	47	53

6 Optimized geometries

All structures have been optimized at the CAM-B3LYP/6-31G(d) level. Cartesian coordinates given in Angstroms.

PDI molecule **2**

C	2.2500844120	3.0073935957	-0.1366396492
C	0.8864001229	2.6633382184	-0.1099147550
C	5.1939167598	-0.1076703044	-0.0410415235
N	5.4990643451	1.2411997885	0.0065804308
C	4.6429204154	2.3274730734	0.0507210176
O	-5.1096572692	-3.4538506983	0.1571358448
O	-6.0995782626	0.9151471645	-0.1063267845
C	-4.2244926070	2.9277317980	0.3414931134
C	-4.2212051168	3.9374953329	-0.6193743245
C	-4.9727619546	5.0927543208	-0.4326913414
C	-5.7177825592	5.2582177763	0.7269801057
C	-5.7122670751	4.2607367101	1.6979714176
C	-4.9730379033	3.1036647006	1.5062432015
C	2.5448846586	4.4613667385	-0.2894306151
C	3.1651719371	4.9525536879	-1.4391787079
C	3.3381974676	6.3166227256	-1.6156853269
C	2.8975327245	7.2108712122	-0.6440122766
C	2.2758313845	6.7308740984	0.5006884294
C	2.0909747913	5.3630118731	0.6717983501
O	6.0892576786	-0.9201276595	-0.1517748830
O	5.1012441178	3.4456344031	0.1676629897
C	4.2172654242	-2.9369258427	0.2856641168
C	4.9697264742	-3.1247854420	1.4460248643
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PDI molecule **3**

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