SUPPLEMENTARY INFORMATION

Synthesis and properties of pyrrolo[3,2-*b*]pyrrole-1,4-diones (isoDPP) derivatives

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Kohn-Sham molecular orbital energies

Compound **2**

Molecular Orbital	Symmetry	Energy (eV)
HOMO-3	A_u	-6.906
HOMO-2	A_g	-6.870
HOMO-1	A_g	-6.198
HOMO	A_u	-6.100
LUMO	A_u	-2.650
LUMO+1	A_u	-0.752
LUMO+2	A_g	-0.736
LUMO+3	A_g	-0.653

Compound **3**

Molecular Orbital	Symmetry	Energy (eV)
HOMO-3	A_g	-6.725
HOMO-2	A_u	-6.707
HOMO-1	A_u	-5.933
HOMO	A_g	-5.875
LUMO	A_u	-2.708
LUMO+1	A_u	-0.763
LUMO+2	A_g	-0.713
LUMO+3	A_g	-0.663

Compound **7**

Molecular Orbital	Symmetry	Energy (eV)
HOMO-3	A_u	-6.072
HOMO-2	A_g	-6.065
HOMO-1	A_g	-5.947
HOMO	A_u	-5.710
LUMO	A_u	-2.579
LUMO+1	A_g	-0.561
LUMO+2	A_u	-0.538
LUMO+3	A_u	-0.265

Excitation energies form TDDFT

Compound **2**

	Symmetry	Energy (eV)	f (a.u.)	Largest molecular orbital contributions
S_1	A_g	2.71766	0	HOMO → LUMO (98 %), HOMO-5 → LUMO (0.4 %), HOMO → LUMO+6 (0.3 %)
S_2	A_u	3.24079	0.37940	HOMO-1 → LUMO (86 %), HOMO-2 → LUMO (6 %), HOMO-4 → LUMO (5 %)
S_3	A_u	3.57964	0.077534	HOMO-2 → LUMO (77%), HOMO-8→LUMO (12%), HOMO-1 → LUMO (6%)
S_4	A_g	3.65915	0	HOMO-3 → LUMO (98%), HOMO-11 → LUMO (0.3%), HOMO-1→ LUMO+8 (0.2%)
S_5	A_u	3.84565	0.0065232	HOMO-8 → LUMO (39%), HOMO-4 → LUMO (32%), HOMO-7 → LUMO (13%)
S_6	A_u	3.99465	0.052762	HOMO-4 → LUMO (58%), HOMO-7 → LUMO (21%), HOMO-8 → LUMO (14%)
S_7	A_g	4.00528	0	HOMO-5 → LUMO (86%), HOMO-6 → LUMO (8%), HOMO-9 → LUMO (2%)
S_8	A_g	4.06003	0	HOMO-6 → LUMO (69%), HOMO-5 → LUMO (12%), HOMO-9 → LUMO (9%)
S_9	A_u	4.20508	0.019059	HOMO-7 → LUMO (63%), HOMO-8 → LUMO (33%), HOMO-4 → LUMO (2%)
S_{10}	A_g	4.30224	0	HOMO-9 → LUMO (56%), HOMO-6 → LUMO (21%), HOMO-11 → LUMO (20%)

	Symmetry	Energy (eV)	f (a.u.)	Largest molecular orbital contributions
T_1	A_u	2.1681	0	HOMO-1 → LUMO (92 %), HOMO-10 → LUMO (4 %), HOMO-4 → LUMO (1 %)
T_2	A_g	2.203	0	HOMO →LUMO (96 %), HOMO-9 → LUMO (1%), HOMO-1 → LUMO+5 (0.6 %)
T_3	A_u	3.3085	0	HOMO-2 → LUMO (56%), HOMO-8→LUMO (23%), HOMO-4 → LUMO (11%)
T_4	A_g	3.5096	0	HOMO-3 → LUMO (90%), HOMO-6 → LUMO (2%), HOMO-9→ LUMO (2%)
T_5	A_u	3.6345	0	HOMO-2 → LUMO (37%), HOMO-4 → LUMO (34%), HOMO-7 → LUMO (13%)
T_6	A_u	3.6718	0	HOMO-8 → LUMO (35%), HOMO-4 → LUMO (30%), HOMO-10 → LUMO (12%)
T_7	A_g	3.7234	0	HOMO-5 → LUMO (68%), HOMO-1 → LUMO+5 (9%), HOMO → LUMO+5 (3%)
T_8	A_g	3.85	0	HOMO-9 → LUMO (32%), HOMO-6 → LUMO (31%), HOMO-11 → LUMO (28%)
T_9	A_u	4.0009	0	HOMO-4 → LUMO (17%), HOMO→ LUMO+5 (13%), HOMO-10 → LUMO (13%)
T_{10}	A_g	4.0283	0	HOMO → LUMO+1 (24%), HOMO-4 → LUMO+2 (14%), HOMO-6 → LUMO+4 (9%)

Compound **3**

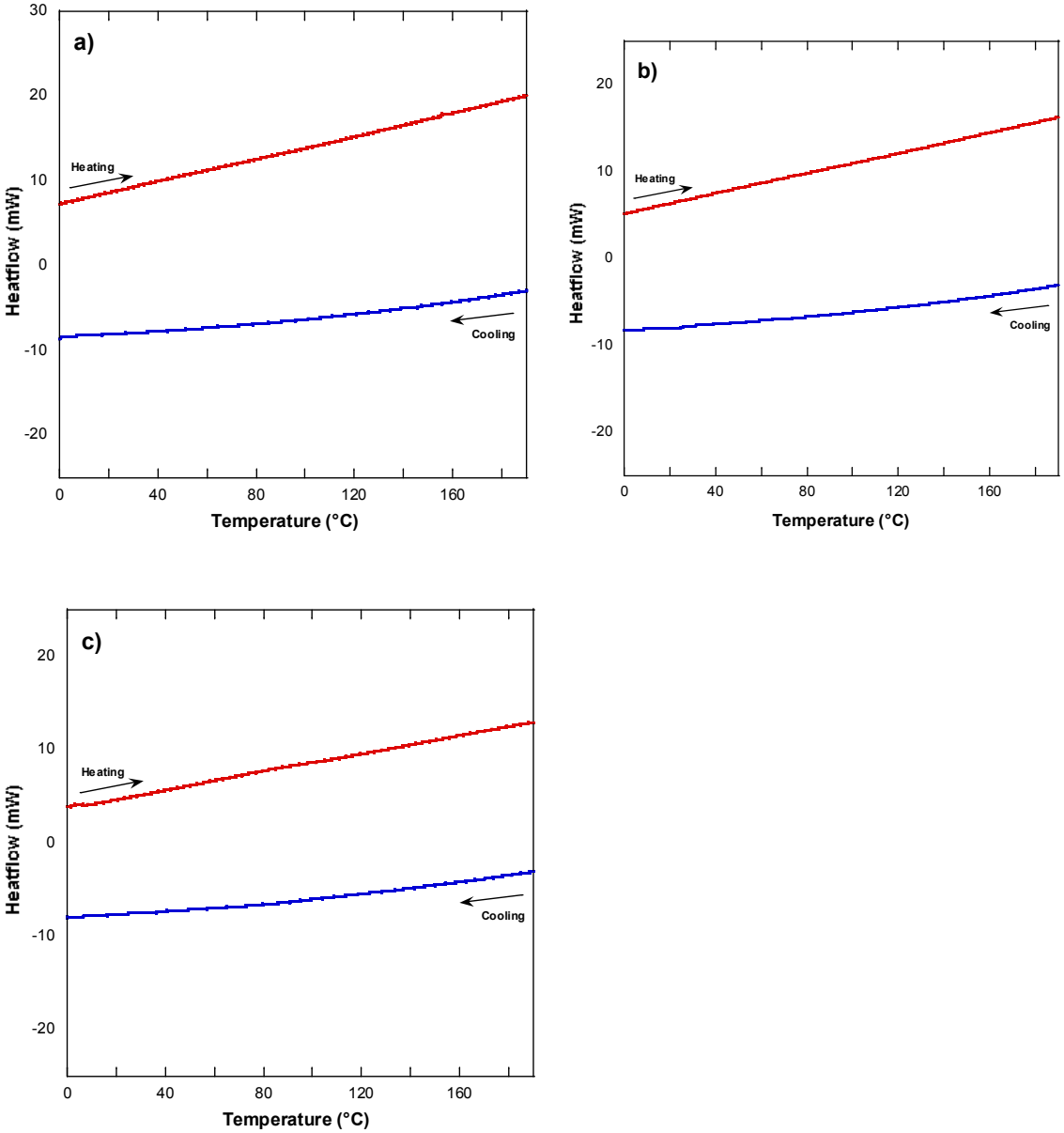
	Symmetry	Energy (eV)	f (a.u.)	Largest molecular orbital contributions
S_1	A_g	2.5881	0	HOMO-1 → LUMO (97 %), HOMO-5 → LUMO (0.6 %), HOMO-9 → LUMO (0.4 %)
S_2	A_u	2.9067	4.41E-01	HOMO→ LUMO (93 %), HOMO-3 → LUMO (2 %), HOMO-4 → LUMO (2 %)
S_3	A_g	3.4161	0	HOMO-2 → LUMO (99%), HOMO-1→LUMO (0.2%), HOMO-11 → LUMO (0.1%)
S_4	A_u	3.4411	6.49E-02	HOMO-3 → LUMO (93%), HOMO-8 → LUMO (3%), HOMO→ LUMO (2%)
S_5	A_u	3.7464	5.19E-03	HOMO-8 → LUMO (39%), HOMO-4 → LUMO (33%), HOMO-7 → LUMO (23%)
S_6	A_u	3.9112	2.75E-02	HOMO-4 → LUMO (61%), HOMO-7 → LUMO (22%), HOMO-8 → LUMO (14%)
S_7	A_g	3.9172	0	HOMO-5 → LUMO (97%), HOMO-6 → LUMO (0.7%), HOMO-1 → LUMO (0.5%)
S_8	A_g	3.9949	0	HOMO-6 → LUMO (87%), HOMO-11 → LUMO (8%), HOMO-9 → LUMO (4%)
S_9	A_u	4.1229	8.84E-03	HOMO-7 → LUMO (55%), HOMO-8 → LUMO (43%), HOMO-4 → LUMO (1%)
S_{10}	A_g	4.2528	0	HOMO-9 → LUMO (51%), HOMO-11 → LUMO (35%), HOMO-6 → LUMO (11%)

	Symmetry	Energy (eV)	f (a.u.)	Largest molecular orbital contributions
T_1	A_u	1.90655	0	HOMO → LUMO (93 %), HOMO-10 → LUMO (2 %), HOMO-3 → LUMO (0.8 %)
T_2	A_g	2.02993	0	HOMO-1 → LUMO (96 %), HOMO-9 → LUMO (1%), HOMO → LUMO+3 (0.6 %)
T_3	A_u	3.1779	0	HOMO-3 → LUMO (89 %), HOMO-8 → LUMO (5 %), HOMO-4 → LUMO (1 %)
T_4	A_g	3.20334	0	HOMO-2 → LUMO (95%), HOMO-3 → LUMO+5 (0.9%), HOMO-3→ LUMO+3 (0.8%)
T_5	A_u	3.43211	0	HOMO-4 → LUMO (39%), HOMO-8 → LUMO (22%), HOMO-7 → LUMO (17%)
T_6	A_g	3.50326	0	HOMO-5 → LUMO (47%), HOMO → LUMO+3 (9%), HOMO → LUMO+5 (9%)
T_7	A_u	3.58024	0	HOMO-8 → LUMO (34%), HOMO-10 → LUMO (19%), HOMO-4 → LUMO (10%)
T_8	A_u	3.81089	0	HOMO-4 → LUMO (36%), HOMO → LUMO+6 (15%), HOMO-1 → LUMO+3 (9%)
T_9	A_g	3.83866	0	HOMO-6 → LUMO (37%), HOMO-11 → LUMO (36%), HOMO-9 → LUMO (20%)
T_{10}	A_g	3.88209	0	HOMO-5 → LUMO (40%), HOMO → LUMO+3 (12%), HOMO → LUMO+2 (10%)

Compound **7**

	Symmetry	Energy (eV)	f (a.u.)	Largest molecular orbital contributions
S_1	A_g	2.45272	0	HOMO → LUMO (98 %), HOMO-13 → LUMO (0.5 %), HOMO-5 → LUMO (0.3 %)
S_2	A_u	2.86395	4.50E-02	HOMO-2 → LUMO (60%), HOMO-1 → LUMO (39 %), HOMO-4 → LUMO (0.9 %)
S_3	A_g	2.90833	0	HOMO-3 → LUMO (99%), HOMO→LUMO (0.3%), HOMO-5 → LUMO (0.1%)
S_4	A_u	3.06083	1.28E-02	HOMO-4 → LUMO (82%), HOMO-2 → LUMO (10%), HOMO-1→ LUMO (6%)
S_5	A_u	3.25786	5.01E-01	HOMO-1 → LUMO (52%), HOMO-2 → LUMO (29%), HOMO-4 → LUMO (15%)
S_6	A_g	3.40255	0	HOMO-5 → LUMO (98%), HOMO→ LUMO (0.4%), HOMO-9 → LUMO (0.4%)
S_7	A_u	3.48479	6.91E-04	HOMO-6 → LUMO (94%), HOMO-8 → LUMO (2%), HOMO-4 → LUMO (2%)
S_8	A_g	3.77644	0	HOMO-7 → LUMO (61%), HOMO-9 → LUMO (36%), HOMO-15 → LUMO (1%)
S_9	A_u	4.09238	9.85E-03	HOMO-8 → LUMO (97%), HOMO-6 → LUMO (2%), HOMO-12 → LUMO (0.2%)
S_{10}	A_g	4.11606	0	HOMO-9 → LUMO (62%), HOMO-7 → LUMO (38%), HOMO-15 → LUMO (0.2%)

	Symmetry	Energy (eV)	f (a.u.)	Largest molecular orbital contributions
T_1	A_g	2.01668	0	HOMO → LUMO (89%), HOMO-5 → LUMO (7%) HOMO-3 → LUMO (1%)
T_2	A_u	2.02813	0	HOMO-1 → LUMO (69%), HOMO-2 → LUMO (21%), HOMO-4 → LUMO (5%)
T_3	A_u	2.66682	0	HOMO-2 → LUMO (69%), HOMO-1→LUMO (26%), HOMO-4 → LUMO (3%)
T_4	A_g	2.6892	0	HOMO-3 → LUMO (92%), HOMO → LUMO (3%), HOMO-5→ LUMO (3%)
T_5	A_u	3.00231	0	HOMO-4 → LUMO (82%), HOMO-6 → LUMO (8%), HOMO-2 → LUMO (7%)
T_6	A_g	3.24481	0	HOMO-5 → LUMO (87%), HOMO→ LUMO (6%), HOMO-3 → LUMO (4%)
T_7	A_u	3.2673	0	HOMO-6 → LUMO (84%), HOMO-4 → LUMO (9%), HOMO-8 → LUMO (2%)
T_8	A_g	3.56249	0	HOMO-7 → LUMO (47%), HOMO-9 → LUMO (46%), HOMO-15 → LUMO (3%)
T_9	A_u	3.82754	0	HOMO-4 → LUMO+4 (22%), HOMO → LUMO+3 (22%), HOMO-5 → LUMO+3 (8%)
T_{10}	A_g	3.83267	0	HOMO → LUMO+4 (24%), HOMO-4 → LUMO+4 (22%), HOMO-5 → LUMO+4 (9%)



S1. DSC thermograms of a) **2**, b) **3** and c) **7**.