Supporting information

Role of Intermolecular Interactions in Molecular Packing of Alkoxy-Substituted Bis-1,3,4-oxadiazole Derivatives

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Figure S1 a) Molecular structure with displacement ellipsoids at the 50% probability level; b) the top view of the nearest dimer along the π-stacking direction; c) pitch and d) roll angle of π-stacking; e) layer structure of BOXD-4 [1]

Figure S2 a) Molecular structure with displacement ellipsoids at the 50% probability level; b) the top view of the nearest dimer along the π-stacking direction; c) pitch and d) roll angle of π-stacking; e) layer structure of BOXD-6 [2]

Figure S3 Crystal packing of BOXD [3]

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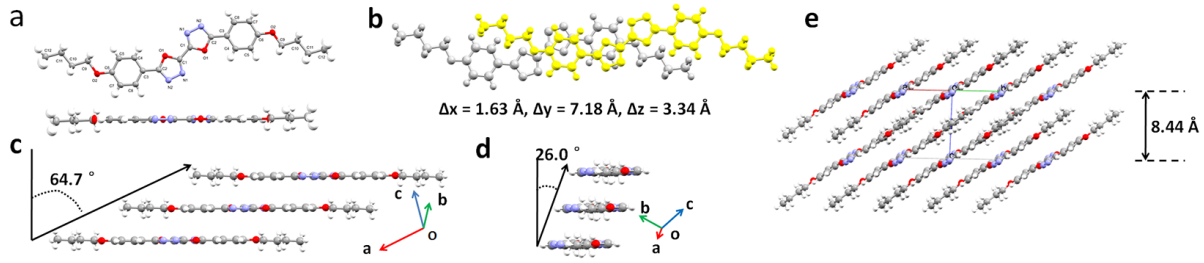

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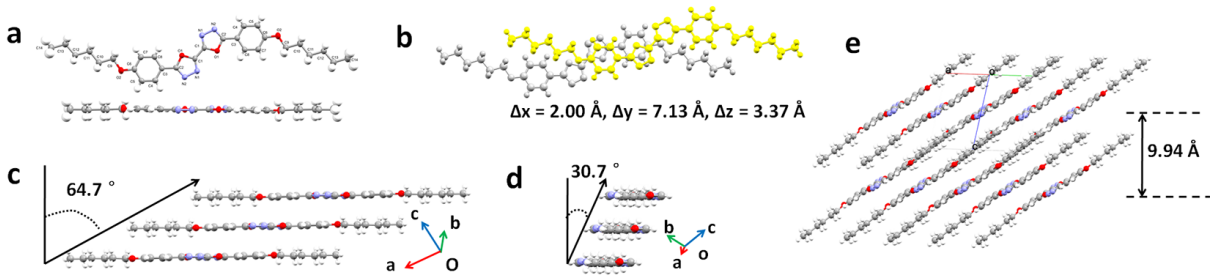

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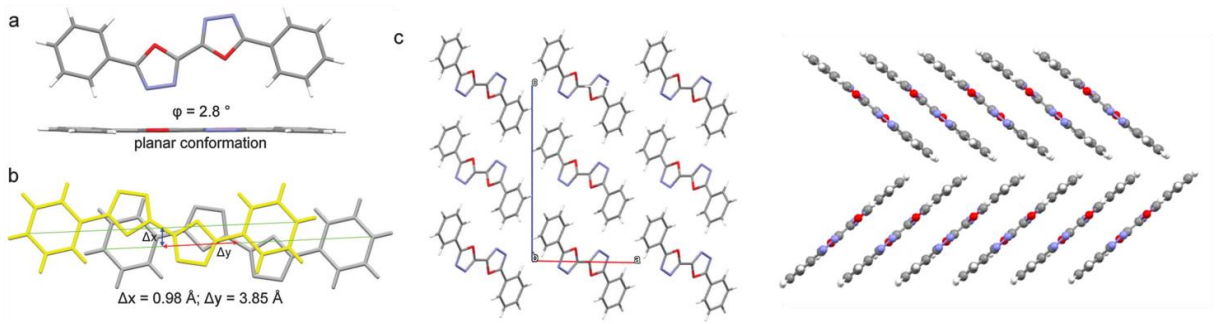

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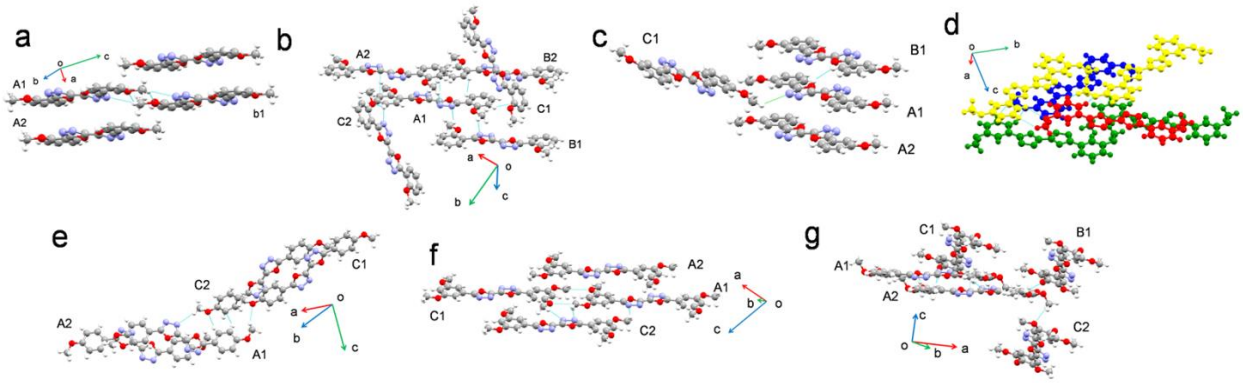

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(AnAm stands molecules in the same π-stacking; AnBm stands molecules in adjacent π-stacking within same molecular layer; AnCm stands molecules in adjacent molecular layers)

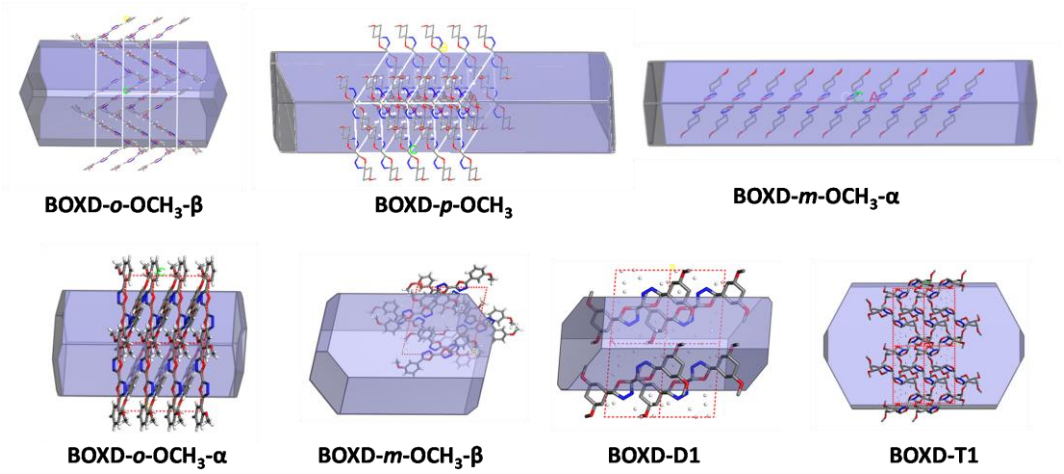

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Table S1 Summary of the crystallographic data for the bis-1,3-4-oxadiazole derivatives investigated

	BOXD-*o*-OCH_3-α [a]	BOXD-*o*-OCH_3-β	BOXD-*m*-OCH_3-α	BOXD-*m*-OCH_3-β	BOXD-*p*-OCH_3 [a]	BOXD-4 [a]	BOXD-6 [a]	BOXD-D1	BOXD-T1
empirical formula	$C_{18}H_{14}N_4O_4$	$C_{18}H_{14}N_4O_4$	$C_{18}H_{14}N_4O_4$	$C_{18}H_{14}N_4O_4$	$C_{18}H_{14}N_4O_4$	$C_{24}H_{26}N_4O_4$	$C_{28}H_{34}N_4O_4$	$C_{20}H_{18}N_4O_6$	$C_{22}H_{22}N_4O_8$
mol wt	350.33	350.33	350.33	350.33	350.33	434.49	490.59	410.38	470.43
crystal system	monoclinic	monoclinic	monoclinic	Triclinic	monoclinic	Triclinic	Triclinic	triclinic	monoclinic
space group	p21/n	P 21/n	P 21/n	P-1	P2(1)/n	P-1	P -1	P -1	P 21/c
Z	2	4	2	6	2	1	1	1	2
a,Å	3.9373(8)	6.7141(13)	3.8988(1)	13.390(3)	6.4194(13)	8.0873(16)	8.134(6)	6.4074(2)	16.537(3)
b, Å	11.632(2)	17.328(3)	24.1759	13.630(3)	8.2680(17)	8.1278(16)	8.142(7)	7.9906(3)	8.4623(17)
c, Å	16.943(3)	14.207(3)	8.4422	14.290(3)	15.213(3)	9.3175(19)	10.657(12)	10.0891(3)	7.6313(15)
α, °	90	90	90	76.08(3)	90	107.15(3)	110.13(4)	69.7350(10)	90
β, °	96.33(3)	97.88(3)	91.735	77.50(3)	92.69(3)	105.03(3)	93.00(4)	75.0100(10)	95.88(3)
γ, °	90	90	90	75.03(3)	90	97.99(3)	98.55(3)	83.8380(10)	90
ρ	1.509	1.421	1.463	1.447	1.443	1.313	1.251	1.456	1.471
V, $Å^3$	771.2(3)	1637.3(6)	759.37	2412.2(9)	806.5(3)	549.59(19)	651.2(10)	468.00(3)	1062.3(4)
Total number of reflections	7218	14908	10119	17731	7435	5423	6429	10362	10040
Number of unique reflections	1744	3615	1964	8186	1814	2492	2936	2304	2420
Rint	0.0412	0.0432	0.0212	0.0441	0.0285	0.0204	0.0282	0.0219	0.0152
GOF	1.013	0.984	1.035	0.947	1.087	1.079	1.006	1.039	1.069
Final R indices R1, wR2	0.0399, 0.1239	0.0445, 0.1014	0.0414, 0.0932	0.0592, 0.1226	0.0368,0.0916	0.0386, 0.1226	0.0507, 0.1281	0.0388, 0.1017	0.0439, 0.1214
R indices (all data) R1,wR2	0.0464, 0.1298	0.0726, 0.1091	0.0581, 0.1041	0.1294, 0.1388	0.0580,0.0983	0.0478, 0.1270	0.0883, 0.1432	0.0456, 0.1072	0.0498, 0.1244

[a] These structures have been reported before and their CCDC codes are 1448062, 293679, 857686 and 1018246, respectively.

Table S2 Intermolecular interactions for different dimers of all these compound investgated.

		type	distance	Total SAPT0	Electrostatics	Exchange	Induction	Dispersion
BOXD-*o*-OCH_3-α	A1A2	π-π	3.52	-16.73	-5.76	18.95	-2.40	-27.52
	A1B1	C(methoxy)-H…N(oxadiazole)	3.45	-9.33	-8.06	4.20	-1.62	-3.84
		C(methoxy)-H…O(methoxy)	3.46					
BOXD-*o*-OCH_3-β	A1A2	π-π	3.72	-18.34	-10.30	16.22	-1.80	-22.46
	A1C1	Ar -H...π (benzene)	3.55	-5.09	-2.32	4.36	-0.68	-6.46
	A1B1	C (methoxy)-H…N (oxadiazole)	3.38	-8.65	-7.45	4.06	-1.54	-3.73
	A1B2	Ar -H…C(benzene)	3.71	-6.69	-2.83	2.33	-0.99	-5.21
	A1C2	Ar -H…N(oxadiazole)	3.39	-4.13	-2.66	3.05	-1.04	-3.47
		Ar -H…O(methoxy)	3.54					
BOXD-*m*-OCH_3-α	A1A2	π-π	3.49	-19.29	-8.82	19.29	-2.06	-27.70
	A1B1	Ar -H…C(benzene)	3.79	-6.79	-3.33	2.82	-1.00	-5.27
	A1C1	C(methoxy)-H…N(oxadiazole)	3.60	-3.78	-2.46	1.75	-0.49	-10.79
BOXD-*m*-OCH_3-β	4-4	π-π	3.43	-17.43	-9.67	16.99	-1.95	-22.80
	3-3	π-π	3.47	-18.06	-7.17	18.97	-1.95	-27.90
	1-3	π-π	3.09	-17.14	-10.13	16.48	-1.86	-21.63
	2-4	π-π	3.09	-17.08	-9.73	15.22	-1.66	-20.90
	1-2-1	Ar -H…O (mothoxy)	3.46	-5.35	-3.18	2.82	-0.77	-4.23
	1-2-2	Ar -H…O (mothoxy)	3.46	-5.43	-3.23	2.83	-0.78	-4.26
	3-4-1	Ar -H…O (mothoxy)	3.43	-5.39	-3.23	3.00	-0.78	-4.38
	3-4-2	Ar -H…O (mothoxy)	3.47	-5.38	-3.18	2.80	-0.78	-4.21
BOXD-*p*-OCH_3	A1A2	π-π	3.34	-16.92	-8.46	17.84	-1.48	-24.81
	A1C2	C (methoxy)-H…N (oxadiazole)	3.57	-7.01	-4.75	4.81	-1.06	-6.01
		Ar -H…O (methoxy)	3.45					
		Ar -H...π (benzene)	3.54					
	A1C1	C (methoxy)-H…O (methoxy)	3.58	-1.74	-1.13	1.06	-0.24	-1.43
BOXD-4	A1A2	π-π	3.34	-21.78	-11.28	20.23	-2.24	-28.49
BOXD-6	A1A2	π-π	3.37	-22.43	-10.59	19.27	-2.18	-28.93
BOXD-D1	A1A2	π-π	3.32	-21.04	-11.30	20.06	-2.48	-27.33
	A1C1	C(methoxy)-H…N(oxadiazole)	3.39	-6.01	-4.74	4.80	-1.14	-4.92
	A1C2	C(methoxy)-H…O(methoxy)	3.17	-3.82	-2.55	3.02	-0.62	-3.67
BOXD-T1		C-H…O	3.42					
	A1C1	C-H...π	3.45	-15.04	-7.89	9.67	-1.80	-15.01
		π-π	/					
	A1A2	C(methoxy)-H…O(oxadiazole)	3.24	-7.29	-2.83	7.60	-1.44	-10.62
	A1C2	C(methoxy)-H…O(methoxy)	3.53	-4.53	-2.30	3.29	-0.59	-4.94
	A1B1	C(methoxy)-H…O(methoxy)	3.48	-3.06	-2.12	1.20	-0.37	-1.77

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3. F. Chen, T. Tian, B. Bai, J. Wang, H. Wang and M. Li, *J. Mater. Chem. C*, 2016, **4**, 4451-4458.