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Theoretical insight into the disordered structure of (Z)-2-((E)-(4-methoxybenzylidene)hydrazono)-1,2-diphenylethanone : the role of non-covalent interactions

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Supporting Information

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Table S1 Comparison of bond lengths between three conformers in the crystal structures of o-**MHDE** and d-**MHDE** (Å)

bonds [i]	bond lengths [i]	bonds [ii]	bond lengths [ii]	bonds [iii]	bond lengths [iii]	ΔB [iv]	ΔB [v]	ΔB [vi]
C1A—C2A	1.367(12)	C1B—C2B	1.375(11)	C1—C2	1.360(2)	0.008	0.007	0.015
C1A—C6A	1.368(6)	C1B—C6B	1.354(11)	C1—C6	1.398(2)	0.014	0.030	0.044
C2A—C3A	1.418(10)	C2B—C3B	1.412(7)	C2—C3	1.391(2)	0.006	0.027	0.021
C3A—O1A	1.385(6)	C3B—O1B	1.349(6)	C3—O1	1.3589(18)	0.036	0.0261	0.0099
C3A—C4A	1.357(5)	C3B—C4B	1.395(5)	C3—C4	1.372(2)	0.038	0.015	0.023
C4A—C5A	1.384(5)	C4B—C5B	1.378(5)	C4—C5	1.385(2)	0.006	0.001	0.007

C5A—C6A	1.379(7)	C5B—C6B	1.370(5)	C5—C6	1.388(2)	0.009	0.009	0.018
C6A—C7A	1.580(7)	C6B—C7B	1.592(7)	C6—C7	1.453(2)	0.012	0.127	0.139
C7A—N1A	1.272(9)	C7B—N1B	1.219(7)	C7—N1	1.2635(19)	0.053	0.0085	0.0445
C8A—N2A	1.306(5)	C8B—N2B	1.219(6)	C8—N2	1.2865(17)	0.087	0.0195	0.0675
C8A—C9A	1.445(6)	C8B—C9B	1.563(7)	C8—C9	1.4751(19)	0.118	0.0301	0.0879
C8A—C15A	1.534(5)	C8B—C15B	1.500(3)	C8—C15	1.5245(18)	0.034	0.0095	0.0245
C9A—C14A	1.375(4)	C9B—C14B	1.387(6)	C9—C14	1.386(2)	0.012	0.011	0.001
C9A—C10A	1.374(12)	C9B—C10B	1.399(7)	C9—C10	1.393(2)	0.025	0.019	0.006
C10A—C11A	1.386(12)	C10B—C11B	1.394(13)	C10—C11	1.385(2)	0.008	0.001	0.009
C11A—C12A	1.394(5)	C11B—C12B	1.378(13)	C11—C12	1.375(2)	0.016	0.019	0.003
C12A—C13A	1.364(4)	C12B—C13B	1.383(5)	C12—C13	1.365(3)	0.019	0.001	0.018
C13A—C14A	1.381(5)	C13B—C14B	1.376(5)	C13—C14	1.381(2)	0.005	0.000	0.005
C15A—O2A	1.213(2)	C15B—O2B	1.208(3)	C15—O2	1.2156(15)	0.005	0.0026	0.0076
C15A—C16A	1.482(3)	C15B—C16B	1.478(3)	C15—C16	1.4794(19)	0.004	0.0026	0.0014
C16A—C17A	1.390(3)	C16B—C17B	1.398(3)	C16—C17	1.3850(18)	0.008	0.005	0.013
C16A—C21A	1.406(3)	C16B—C21B	1.357(3)	C16—C21	1.3911(19)	0.049	0.0149	0.0341
C17A—C18A	1.376(4)	C17B—C18B	1.314(4)	C17—C18	1.381(2)	0.062	0.005	0.067

C18A—C19A	1.368(4)	C18B—C19B	1.410(5)	C18—C19	1.368(3)	0.042	0.000	0.042
C19A—C20A	1.339(4)	C19B—C20B	1.409(4)	C19—C20	1.371(3)	0.070	0.032	0.038
C20A—C21A	1.407(4)	C20B—C21B	1.407(3)	C20—C21	1.380(3)	0.000	0.027	0.027
C22A—O1A	1.462(7)	C22B—O1B	1.400(4)	C22—O1	1.419(3)	0.062	0.043	0.019
N1A—N2A	1.363(8)	N1B—N2B	1.411(4)	N1—N2	1.4092(16)	0.048	0.0462	0.0018

[i]: bonds in part A of d-**MHDE**.

[ii]: bonds in part B of d-**MHDE**.

[iii]: bonds in o-**MHDE**.

[iv]: absolute values of bond length differences between parts A and B of d-**MHDE**.

[v]: absolute values of bond length differences between part A of d-**MHDE** and o-**MHDE**.

[vi]: absolute values of bond length differences between part B of d-**MHDE** and o-**MHDE**.

Table S2 Comparison of bond angles between three conformers in the crystal structures of o-**MHDE** and d-**MHDE** (°)

bonds [i]	bond angles [i]	bonds [ii]	bond angles [ii]	bonds [iii]	bond angles [iii]	ΔA [iv]	ΔA [v]	ΔA [vi]
C2A—C1A—C6A	112.2(6)	C6B—C1B—C2B	122.0(6)	C2—C1—C6	120.35(15)	9.80	8.15	1.65
C1A—C2A—C3A	121.6(9)	C1B—C2B—C3B	117.7(5)	C1—C2—C3	120.69(16)	3.90	0.91	2.99
C4A—C3A—O1A	127.6(4)	O1B—C3B—C4B	124.2(5)	O1—C3—C4	124.98(15)	3.40	2.62	0.78
O1A—C3A—C2A	108.4(6)	O1B—C3B—C2B	115.9(4)	O1—C3—C2	114.92(15)	7.50	6.52	0.98
C4A—C3A—C2A	123.9(6)	C4B—C3B—C2B	119.9(4)	C4—C3—C2	120.10(15)	4.00	3.80	0.20
C3A—C4A—C5A	113.8(5)	C5B—C4B—C3B	118.7(4)	C3—C4—C5	119.14(15)	4.90	5.34	0.44

C6A—C5A—C4A	120.8(4)	C6B—C5B—C4B	121.5(4)	C4—C5—C6	121.40(15)	0.70	0.60	0.10
C1A—C6A—C5A	126.6(5)	C1B—C6B—C5B	119.2(5)	C5—C6—C1	118.31(14)	7.40	8.29	0.89
C1A—C6A—C7A	120.5(5)	C1B—C6B—C7B	123.3(5)	C1—C6—C7	121.03(13)	2.80	0.53	2.27
C5A—C6A—C7A	112.9(4)	C5B—C6B—C7B	117.3(4)	C5—C6—C7	120.64(13)	4.40	7.74	3.34
N1A—C7A—C6A	118.1(5)	N1B—C7B—C6B	112.9(4)	N1—C7—C6	121.58(13)	5.20	3.48	8.68
N2A—C8A—C9A	121.9(4)	N2B—C8B—C9B	121.5(3)	N2—C8—C9	120.94(12)	0.40	0.96	0.56
N2A—C8A—C15A	120.8(4)	N2B—C8B—C15B	118.9(3)	N2—C8—C15	120.14(12)	1.90	0.66	1.24
C9A—C8A—C15A	116.8(3)	C15B—C8B—C9B	118.3(3)	C9—C8—C15	118.84(11)	1.50	2.04	0.54

C10A—C9A—C14A	113.1(6)	C14B—C9B—C10B	123.4(6)	C14—C9—C10	118.35(15)	10.30	5.25	5.05
C14A—C9A—C8A	124.1(3)	C14B—C9B—C8B	117.0(4)	C14—C9—C8	120.82(13)	7.10	3.28	3.82
C10A—C9A—C8A	122.3(6)	C10B—C9B—C8B	118.3(4)	C10—C9—C8	120.84(14)	4.00	1.46	2.54
C9A—C10A—C11A	127.1(10)	C11B—C10B—C9B	116.9(6)	C11—C10—C9	120.08(18)	10.20	7.02	3.18
C10A—C11A—C12A	113.2(6)	C12B—C11B—C10B	120.7(9)	C12—C11—C10	120.37(19)	7.50	7.17	0.33
C13A—C12A—C11A	122.4(3)	C11B—C12B—C13B	120.0(6)	C13—C12—C11	120.11(18)	2.40	2.29	0.11
C12A—C13A—C14A	117.9(3)	C14B—C13B—C12B	121.4(5)	C12—C13—C14	120.02(19)	3.50	2.12	1.38
C9A—C14A—C13A	124.1(3)	C13B—C14B—C9B	117.0(5)	C13—C14—C9	121.07(18)	7.10	3.03	4.07

O2A—C15A—C16A	122.41(19)	O2B—C15B—C16B	123.76(19)	O2—C15—C16	122.56(12)	1.35	0.15	1.20
O2A—C15A—C8A	119.7(2)	O2B—C15B—C8B	119.22(19)	O2—C15—C8	118.01(12)	0.48	1.69	1.21
C16A—C15A—C8A	117.79(19)	C16B—C15B—C8B	117.02(17)	C16—C15—C8	119.39(11)	0.77	1.60	2.37
C17A—C16A—C21A	119.68(19)	C21B—C16B—C17B	118.71(19)	C17—C16—C21	118.94(14)	0.97	0.74	0.23
C17A—C16A—C15A	120.08(17)	C17B—C16B—C15B	118.88(18)	C17—C16—C15	121.70(12)	1.20	1.62	2.82
C21A—C16A—C15A	120.24(16)	C21B—C16B—C15B	122.35(18)	C21—C16—C15	119.36(13)	2.11	0.88	2.99
C18A—C17A—C16A	121.6(2)	C18B—C17B—C16B	120.9(2)	C18—C17—C16	120.45(15)	0.70	1.15	0.45
C19A—C18A—C17A	116.8(3)	C17B—C18B—C19B	122.3(3)	C19—C18—C17	120.02(18)	5.50	3.22	2.28

C20A—C19A—C18A	124.6(3)	C20B—C19B—C18B	118.1(3)	C18—C19—C20	120.24(18)	6.50	4.36	2.14
C19A—C20A—C21A	119.3(3)	C21B—C20B—C19B	117.6(2)	C19—C20—C21	120.40(18)	1.70	1.10	2.80
C16A—C21A—C20A	117.9(2)	C16B—C21B—C20B	122.3(2)	C20—C21—C16	119.91(16)	4.40	2.01	2.39
C7A—N1A—N2A	113.0(6)	C7B—N1B—N2B	111.8(4)	C7—N1—N2	114.00(12)	1.20	1.00	2.20
C8A—N2A—N1A	109.2(5)	C8B—N2B—N1B	116.3(3)	C8—N2—N1	110.54(11)	7.10	1.34	5.76
C3A—O1A—C22A	116.6(4)	C3B—O1B—C22B	119.9(4)	C3—O1—C22	118.98(17)	3.30	2.38	0.92

[i]: bonds in part A of d-**MHDE**.

[ii]: bonds in part B of d-**MHDE**.

[iii]: bonds in o-**MHDE**.

[iv]: absolute values of bond angle differences between parts A and B of d-**MHDE**.

[v]: absolute values of bond angle differences between part A of d-**MHDE** and o-**MHDE**.

[vi]**:** absolute values of bond angle differences between part B of d-**MHDE** and o-**MHDE**.

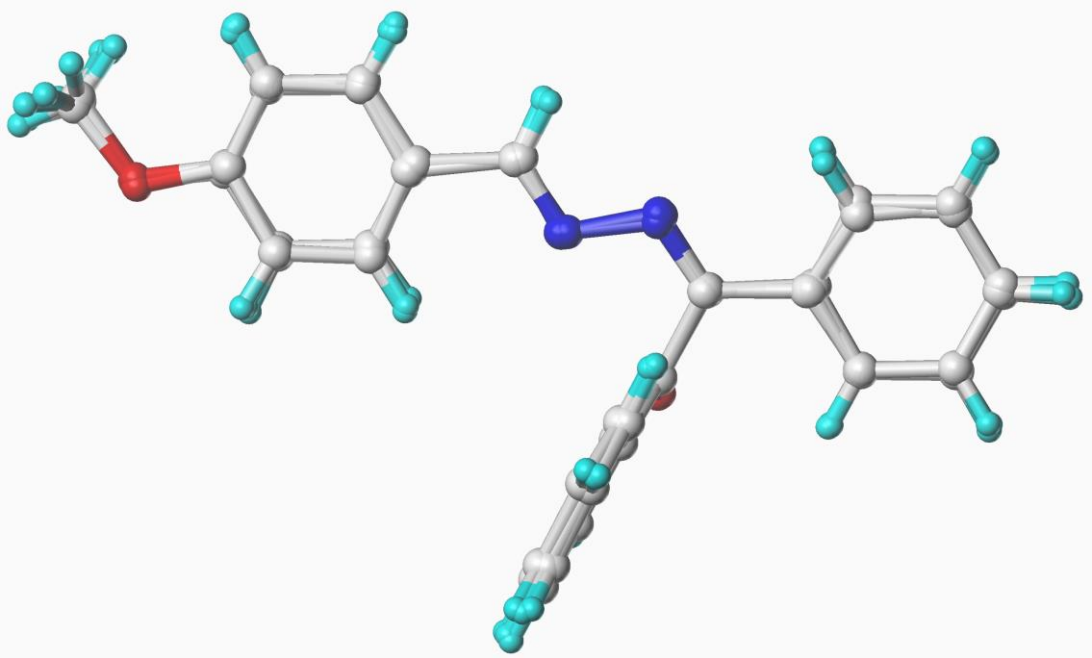

Fig. S1 The overlapping of three conformers in the crystal structures of o-**MHDE** and d-**MHDE**.

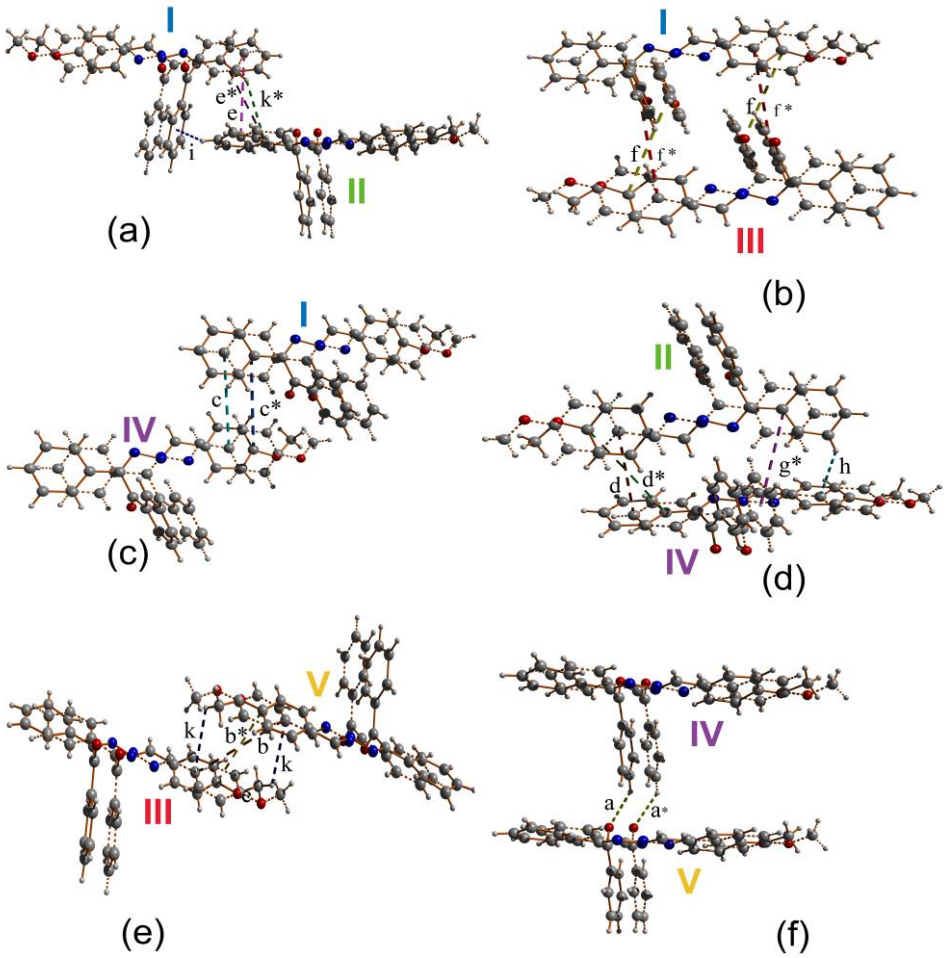

Fig. S2 The intermolecular interactions in various molecule pairings of d-**MHDE**. The indices I, II, III, IV and V for five molecules are the same as that in **Fig. 3**. Some molecule pairs such as I-V, II-III and III-IV are not shown because there are no valuable NCIs between them. Another molecule pair II-V is not shown because all NCIs are the same as that in II-IV.