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Structural and Computational Analysis of H-bond mediated anion···anion interactions in new salts of Fumaric and Maleic Acids

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Materials and Methods

N-Benzylphenethylamine (95% purity), 6-Methylquinoline (98% purity), 1,4-Dioxa-8-azaspiro(4.5)decane (98% purity) and m-Xylylenediamine (99% purity) were purchased from Sigma-Aldrich. Ethanol (96% Technical grade) was purchased from PanReac.

Synthesis and crystallization

Employing the same synthesis conditions, the series of the six salts was produced by introducing the following materials on separate crystallizers: 40 mg MA / 75 mg NBPEA (I); 40 mg FA / 75 mg NBPEA (II); 40 mg MA / 50 mg 1,4-DAD (III); 40 mg FA / 50 mg 1,4-DAD (IV); 40 mg MA / 50 mg 6-MQ (V); 40 mg FA / 45 mg MXDA (VI). We dissolve each pair of coformers in 10 ml of ethanol and leave them under magnetic stirring for 20 min at room temperature. A few days later, a series of colorless single crystals suitable for SCXRD have been formed.

Geometric parameters of hydrogen bonds in compounds I-VI

Table S1. Hydrogen-bond geometry in Compound I

D—H…A	D—H (Å)	H…A (Å)	D…A (Å)	D—H…A (°)
O1A—H1A···O8A	1.01 (3)	1.45 (3)	2.4551 (16)	177 (3)
N8—H8A···O7Ai	0.89 (2)	1.98 (2)	2.834 (2)	160 (2)
N8—H8B···O8A	0.94 (2)	1.93 (2)	2.8712 (19)	174 (2)
N8—H8B···O7A	0.94 (2)	2.58 (2)	3.153 (2)	120 (2)
C5A—H5A···O8Aii	0.95	2.59	3.443 (2)	150
C7—H7A···O1Aiii	0.99	2.49	3.440 (2)	161
C9—H9A···O2Aiii	0.99	2.54	3.246 (2)	128
C9—H9B···O2Aiv	0.99	2.43	3.368 (2)	158

Symmetry codes: (i) x+1, y, z; (ii) x−1, y, z; (iii) −x, y−1/2, −z+1/2; (iv) −x−1, y−1/2, −z+1/2.

Table S2. Hydrogen-bond geometry in Compound II (Å, °)

D—H…A	D—H (Å)	H…A (Å)	D…A (Å)	D—H…A (°)
N8—H8A···O3A	0.91 (3)	1.93 (4)	2.778 (4)	155 (4)
N8—H8B···O7A	0.94 (4)	1.83 (4)	2.762 (5)	174 (6)
O5A—H5A···O5Ai	1.23 (1)	1.23 (1)	2.459 (5)	180 (1)
O1A—H1A···O1Aii	1.22 (1)	1.22 (1)	2.442 (5)	180 (1)

Symmetry codes: (i) −x+1, −y+1, −z+1; (ii) −x+1, −y, −z+2.

Table S3. Hydrogen-bond geometry in Compound III (Å, °)

D—H…A	D—H (Å)	H…A (Å)	D…A (Å)	D—H…A (°)
N8—H8B···O7A	0.92 (2)	2.12 (2)	2.865 (2)	138 (2)
N8—H8A···O8Ai	0.94 (2)	1.93 (2)	2.8498 (18)	168 (2)
O1A—H1A···O8A	0.97 (2)	1.49 (2)	2.4484 (18)	175 (3)
N8—H8A···O7Ai	0.94 (2)	2.53 (2)	3.163 (2)	125 (2)
C2—H2A···O2Aii	0.97	2.52	3.444 (3)	160
C4A—H4A···O1Ai	0.93	2.56	3.322 (2)	140
C5A—H5A···O8Ai	0.93	2.58	3.4371 (19)	154

Symmetry codes: (i) x, y−1, z; (ii) x−1, −y+1/2, z−1/2.

Table S4. Hydrogen-bond geometry in Compound IV (Å, °)

D—H…A	D—H (Å)	H…A (Å)	D…A (Å)	D—H…A (°)
C2—H2A···O13ii	0.99	2.56	3.3824 (18)	140
C6—H6B···O12iii	0.99	2.50	3.3363 (16)	142
N8—H8A···O12	0.939 (17)	1.728 (17)	2.6590 (15)	170.6 (15)
N8—H8B···O13iii	0.922 (17)	1.782 (17)	2.6855 (14)	166.1 (14)
C14—H14···O13iii	0.95	2.791 (3)	3.711 (3)	163.33

Symmetry codes: (ii) x+1, y−1, z; (iii) x+1, y, z.

Table S5. Hydrogen-bond geometry in Compound V (Å, °)

D—H…A	D—H (Å)	H…A (Å)	D…A (Å)	D—H…A (°)
N1—H1···O5A	0.97 (2)	1.70 (2)	2.6729 (15)	173.3 (19)
O1A—H1A···O6A	1.05 (2)	1.40 (2)	2.4544 (13)	178 (2)
C2—H2···O6A	0.95	2.58	3.2268 (17)	126
C3—H3···O2Ai	0.95	2.34	3.2874 (17)	174
C3A—H3A···O1Aii	0.95	2.58	3.4601 (16)	154
C4—H4···O2Aiii	0.95	2.46	3.3260 (17)	152
C4A—H4A···O6Aii	0.95	2.58	3.3918 (16)	143

Symmetry codes: (i) −x+1, −y, −z; (ii) x−1, y, z; (iii) x+1, y, z+1.

Table S6. Hydrogen-bond geometry in Compound VI (Å, °)

D—H…A	D—H (Å)	H…A (Å)	D…A (Å)	D—H…A (°)
N1—H1A···O1B	1.02 (2)	1.80 (2)	2.7851 (19)	161 (2)
N1—H1B···O7Bi	1.00 (2)	2.27 (3)	2.9193 (18)	122 (2)
N1—H1C···O2Wii	1.01 (2)	1.83 (2)	2.8117 (19)	165 (2)
N1—H1B···O1Wi	1.00 (2)	1.90 (2)	2.770 (2)	145 (2)
N10—H10C···O3Biii	0.97 (2)	1.89 (2)	2.8451 (18)	171 (2)
N10—H10A···O2W	0.98 (2)	1.89 (2)	2.8440 (19)	165 (2)
O3W—H3WB···O1A	1.02 (2)	1.70 (2)	2.7165 (17)	171 (3)
O3W—H3WA···O3Biii	1.02 (2)	1.70 (2)	2.7245 (17)	178 (3)
O8A—H8A···O3Ai	1.03 (2)	1.51 (2)	2.5386 (16)	176 (3)
O8B—H8B···O1Biv	1.03 (2)	1.53 (2)	2.5520 (15)	171 (3)
O2W—H2WB···O3Wiv	0.93 (3)	1.77 (3)	2.6897 (17)	172 (2)
O2W—H2WA···O3Av	1.02 (2)	1.76 (2)	2.7719 (17)	178 (2)

O1W—H1WA···O1Avi	1.04 (2)	2.13 (3)	2.898 (2)	129 (3)
O1W—H1WB···O7Avii	1.03 (2)	1.78 (2)	2.706 (2)	148 (2)
N10—H10B···O1A	1.00 (2)	2.05 (2)	3.0048 (18)	161 (2)
C5A—H5A···O3W	0.95	2.50	3.314 (2)	144
C5B—H5B···O3Wiii	0.95	2.49	3.286 (2)	142
C8—H8···O3Biii	0.95	2.51	3.411 (2)	159
C9—H9A···O7B	0.99	2.47	3.293 (2)	140

Symmetry codes: (i) x+1, y, z; (ii) x+1/2, −y+3/2, z−1/2; (iii) −x, −y+2, −z+1; (iv) x−1, y, z; (v) −x−1/2, y+1/2, −z+3/2; (vi) x−1/2, −y+3/2, z−1/2; (vii) −x, −y+1, −z+1.