

## Pseudopolymorphs - a variety of self-organization of *para*-sulphonato-calix[8]arene and phenanthroline in the solid state

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**Table S1. Interactions present in the structure of complex 1.**

Hydrogen bonding (Å and °)				
<i>D</i> —H⋯ <i>A</i>	<i>d</i> ( <i>D</i> —H)	<i>d</i> (H⋯ <i>A</i> )	<i>d</i> ( <i>D</i> ⋯ <i>A</i> )	<(D—H⋯ <i>A</i> )
O4A—H4A1⋯O1A1 <sup>1</sup>	0.84	2.39	2.82(3)	113
O4A—H4A1⋯O1A2 <sup>1</sup>	0.84	1.89	2.37(4)	115
O4B—H4B1⋯O4C	0.84	2.02	2.86(2)	174
O4C—H4C1⋯O1W	0.84	1.90	2.61(2)	142
O4D—H4D1⋯O1W	0.84	2.55	3.23(2)	138
O4D—H4D1⋯O4E	0.84	2.65	2.89(2)	99
O4E—H4E1⋯O1W	0.84	2.34	3.11(2)	153
O4F—H4F1⋯O2H	0.84	1.94	2.71(2)	152
O4G—H4G1⋯O2G <sup>2</sup>	0.84	1.91	2.74(2)	167
O4H—H4H1⋯O1B1 <sup>1</sup>	0.84	1.84	2.59(3)	149
O4H—H4H1⋯O1B2 <sup>1</sup>	0.84	2.02	2.61(4)	127
N2X—H2X1⋯O5W	0.88	1.84	2.69(3)	163
N2Y—H2Y1⋯O22W	0.88	1.85	2.71(3)	163
N2O—H2O1⋯O32W	0.88	1.95	2.80(4)	163
N1Z—H1ZN⋯O3B1 <sup>1</sup>	0.88	2.21	3.01(4)	151
N2W—H2W1⋯O2C1 <sup>1</sup>	0.88	2.38	3.10(3)	140
N2V—H2V1⋯O18W	0.88	1.79	2.51(5)	137
N2M—H2M1⋯O18W	0.88	2.09	2.91(5)	156
C7A—H7A1⋯O1A1 <sup>1</sup>	0.99	2.58	3.23(3)	124
C1Q—H1Q⋯O8W	0.95	2.17	3.03(3)	150
C1R—H1R⋯O3C <sup>3</sup>	0.95	2.55	3.37(6)	145
C1Y—H1Y⋯O3A1 <sup>4</sup>	0.95	2.59	3.50(4)	160
C1Y—H1Y⋯O3A2 <sup>4</sup>	0.95	2.38	3.28(6)	158
C2L—H2L⋯O3G <sup>5</sup>	0.95	2.44	3.09(4)	126
C2T—H2T⋯O3G <sup>5</sup>	0.95	2.57	3.21(3)	124
C2W—H2W⋯O3F2 <sup>2</sup>	0.95	1.93	2.87(4)	169
C3X—H3X⋯O2G <sup>2</sup>	0.95	2.49	3.41(2)	163
C3Z—H3Z⋯O1G <sup>2</sup>	0.95	2.34	3.09(2)	136
C6W—H6W⋯O1C2 <sup>1</sup>	0.95	2.51	3.26(6)	136
C7O—H7O⋯O4B <sup>1</sup>	0.95	2.55	3.37(3)	144
C7Q—H7Q⋯O1F1 <sup>4</sup>	0.95	2.40	3.12(4)	132
C7Z—H7Z⋯O2E1 <sup>6</sup>	0.95	2.48	3.21(3)	134

C8L—H8L···O1A1 <sup>7</sup>	0.95	2.55	3.39(4)	147
C8L—H8L···O1A2 <sup>7</sup>	0.95	2.54	3.36(6)	144
C8X—H8X···O4C <sup>6</sup>	0.95	2.50	3.28(3)	139
C8Z—H8Z···O1D <sup>6</sup>	0.95	2.60	3.46(3)	151
C8Z—H8Z···O3D <sup>6</sup>	0.95	2.41	3.27(3)	151
C7E—H7E2···O22W <sup>1</sup>	0.99	2.52	3.34(4)	140
C7E—H7E2···O23W <sup>1</sup>	0.99	2.47	3.40(6)	156
C11T—H11T···O4A <sup>5</sup>	0.95	2.49	3.24(4)	136
C11Y—H11Y···O4F <sup>4</sup>	0.95	2.44	3.37(4)	166
C12M—H12M···O4B <sup>5</sup>	0.95	2.44	3.18(4)	135
C7H—H7H1···O1B2 <sup>1</sup>	0.99	2.32	3.09(5)	134
C3V—H3V···O3H	0.95	2.17	3.06(2)	156

Symmetry operations: (1) 1-x,-y,1-z; (2) -x,1-y,1-z; (3) x,1+y,-1+z; (4) 1+x,y,z; (5) 1-x,1-y,1-z; (6) -x,-y,1-z; (7) x,1+y,z.

### Interactions X—H··· $\pi$ (Å and °)

C—H···CgJ	$d(\text{H}\cdots\text{Cg})$	$\perp d(\text{H}\cdots\pi)$	$\gamma$	$\langle \text{C—H}\cdots\text{Cg}$	$d(\text{C}\cdots\text{Cg})$	$\langle \text{C—H}, \pi$
C3T—H3T···CgH <sup>1</sup>	2.82	2.71	15.71	160	3.72(2)	56
C7C—H7C1···CgV3 <sup>1</sup>	3.00	2.76	22.98	121	3.61(2)	53
C7C—H7C2···CgJ3 <sup>1</sup>	2.85	2.82	8.59	148	3.73(2)	66
C6X—H6X···CgE <sup>2</sup>	2.69	-2.62	12.39	160	3.60(2)	77
C7X—H7X···CgD <sup>2</sup>	2.74	-2.69	10.55	158	3.64(2)	59
C1O—H1O···CgH	2.99	-2.78	21.67	135	3.72(2)	60
C2M—H2M···CgL1	2.79	2.69	15.78	112	3.27(2)	19
C7C—H7C1···CgM3 <sup>1</sup>	2.85	2.60	24.14	113	3.36(2)	46
C11L—H11L···CgH <sup>1</sup>	3.00	2.84	18.71	162	3.91(2)	62

### Interactions $\pi\cdots\pi$ (Å and °)

CgI···CgJ	$d(\text{CgI}\cdots\text{CgJ})$	$\alpha$	$\beta$	$\gamma$	CgI perp.	CgJ perp.
CgA···CgA <sup>3</sup>	3.98(2)	0	23.72	23.72	3.65(2)	3.65(2)
CgC···CgV2 <sup>1</sup>	4.62(2)	6.8	32.75	38.18	3.63(2)	3.89(2)
CgC···CgV3 <sup>1</sup>	4.48(2)	11.1	37.86	30.60	3.86(2)	3.54(2)
CgD···CgJ1 <sup>4</sup>	3.77(2)	3.7	20.14	23.78	-3.45(2)	3.54(2)
CgD···CgJ1 <sup>1</sup>	4.81(2)	3.7	44.57	42.46	3.55(2)	3.42(2)
CgD···CgJ2 <sup>4</sup>	4.54(2)	7.4	45.08	41.37	-3.41(2)	3.21(2)
CgD···CgJ2 <sup>1</sup>	4.20(2)	7.4	26.66	33.93	3.49(2)	3.76(2)
CgD···CgJ3 <sup>4</sup>	3.52(2)	6.6	18.56	11.94	-3.44(2)	3.34(2)
CgD···CgJ3 <sup>1</sup>	4.62(2)	6.6	38.34	39.03	3.59(2)	3.63(2)
CgG···CgG <sup>5</sup>	3.69(2)	0	25.53	25.53	-3.33(2)	-3.33(2)
CgH···CgY1 <sup>6</sup>	4.92(2)	5.0	13.44	64.69	-2.11(2)	-4.79(2)
CgK1···CgK2 <sup>1</sup>	4.13(2)	6.1	30.35	26.67	3.70(2)	3.57(2)
CgK1···CgK3 <sup>1</sup>	4.71(2)	7.0	39.35	33.28	-3.93(2)	3.64(2)
CgK1···CgT1 <sup>1</sup>	3.58(2)	1.2	22.92	23.30	-3.29(2)	-3.30(2)
CgK1···CgT3 <sup>1</sup>	4.83(2)	1.5	46.48	46.24	-3.34(2)	-3.33(2)
CgK2···CgK3 <sup>1</sup>	4.00(2)	7.9	16.81	24.56	-3.64(2)	3.83(2)
CgK2···CgT1 <sup>1</sup>	4.25(2)	7.3	43.55	40.57	-3.23(2)	-3.08(2)
CgK2···CgT3 <sup>1</sup>	4.00(2)	5.2	32.88	34.17	-3.31(2)	-3.36(2)
CgK3···CgK3 <sup>1</sup>	3.91(2)	0	13.39	13.39	-3.80(2)	-3.80(2)
CgK3···CgT1 <sup>1</sup>	3.47(2)	7.7	18.48	25.86	-3.12(2)	3.29(2)
CgK3···CgT3 <sup>1</sup>	4.55(2)	5.6	42.89	44.59	-3.24(2)	3.34(2)
CgR1···CgW1	3.73(2)	6.9	26.50	19.73	-3.51(2)	3.34(2)
CgR1···CgW2 <sup>7</sup>	3.41(2)	6.9	10.34	16.53	-3.26(2)	-3.35(2)
CgR1···CgW3	4.22(2)	6.9	34.59	33.71	-3.51(2)	3.48(2)
CgR1···CgW3 <sup>7</sup>	4.28(2)	6.9	35.07	40.24	-3.26(2)	-3.50(2)

CgR2...CgW1	4.77(2)	2.2	46.75	44.54	-3.40(2)	3.27(2)
CgR2...CgW1 <sup>7</sup>	3.71(2)	2.2	24.13	24.51	-3.38(2)	-3.39(2)
CgR2...CgW2	3.74(2)	2.2	23.99	24.37	-3.40(2)	3.41(2)
CgR2...CgW3	4.28(2)	2.2	39.07	37.27	-3.40(2)	3.32(2)
CgR2...CgW3 <sup>7</sup>	3.76(2)	2.2	24.08	26.17	-3.38(2)	-3.43(2)
CgR3...CgW1	3.56(2)	2.0	19.40	19.76	-3.35(2)	3.35(2)
CgR3...CgW1 <sup>7</sup>	4.63(2)	2.0	43.91	42.13	-3.43(2)	-3.33(2)
CgR3...CgW2	4.87(2)	2.0	44.98	46.60	-3.35(2)	3.45(2)
CgR3...CgW2 <sup>7</sup>	3.88(2)	2.0	28.18	27.94	-3.43(2)	-3.42(2)
CgR3...CgW3	4.19(2)	2.0	35.04	37.04	-3.35(2)	3.43(2)
CgR3...CgW3 <sup>7</sup>	3.52(2)	2.0	13.97	12.52	-3.43(2)	-3.41(2)
CgT1...CgV1	4.33(2)	7.9	38.34	32.53	-3.65(2)	3.40(2)
CgT2...CgV1	3.72(2)	8.9	22.48	31.22	-3.18(2)	3.44(2)
CgT2...CgV2	4.10(2)	5.9	42.17	44.51	-2.92(2)	3.04(2)
CgT2...CgV3	3.58(2)	6.4	26.72	27.73	-3.16(2)	3.20(2)
CgT3...CgV1	3.74(2)	6.6	22.94	27.14	-3.34(2)	3.45(2)
CgT3...CgV3	3.79(2)	2.8	31.10	28.57	-3.33(2)	3.24(2)
CgW1...CgZ1	3.90(2)	2.3	29.27	28.17	-3.44(2)	3.40(2)
Cg W1...CgZ2	4.07(2)	3.0	34.33	31.51	-3.47(2)	3.36(2)
Cg W1...CgZ3	3.58(2)	1.9	15.91	17.04	3.42(2)	3.44(2)
Cg W2...CgZ2	3.85(2)	3.0	29.18	32.17	-3.25(2)	3.36(2)
Cg W3...CgZ2	3.63(2)	3.0	22.39	23.02	-3.34(2)	3.36(2)
Cg W3...CgZ3	3.94(2)	1.9	29.24	30.45	-3.40(2)	3.44(2)
CgX1...CgY1 <sup>6</sup>	3.59(2)	4.0	19.10	19.14	-3.39(2)	3.39(2)
CgX1...CgY2 <sup>6</sup>	4.57(2)	5.8	41.44	44.69	-3.24(2)	3.42(2)
CgX1...CgY3 <sup>6</sup>	3.73(2)	5.6	21.22	25.46	-3.37(2)	3.48(2)
CgX1...CgZ1	3.59(2)	3.0	18.29	20.51	3.36(2)	-3.41(2)
CgX1...CgZ2	4.59(2)	4.1	43.95	44.48	3.28(2)	-3.31(2)
CgX1...CgZ3	3.60(2)	1.9	21.00	21.60	3.35(2)	-3.36(2)
CgX2...CgY2 <sup>6</sup>	4.64(2)	7.9	40.64	47.53	-3.13(2)	3.52(2)
CgX2...CgZ2	4.11(2)	3.0	35.26	32.67	3.46(2)	-3.36(2)
CgX2...CgZ3	4.39(2)	0.5	40.47	40.03	3.36(2)	-3.34(2)
CgX3...CgY1 <sup>6</sup>	4.85(2)	4.6	47.17	46.10	-3.37(2)	3.30(2)
CgX3...CgY2 <sup>6</sup>	3.64(2)	7.5	15.23	22.73	-3.36(2)	3.51(2)
CgX3...CgY3 <sup>6</sup>	4.20(2)	6.1	34.13	37.59	-3.33(2)	3.48(2)
CgX3...CgZ1	4.76(2)	3.4	43.19	46.35	3.28(2)	-3.47(2)
CgX3...CgZ2	4.54(2)	1.7	42.49	41.73	3.39(2)	-3.35(2)
CgX3...CgZ3	3.56(2)	1.1	19.31	20.00	3.35(2)	-3.36(2)
CgY1...CgY1 <sup>8</sup>	3.98(2)	0	31.29	31.29	3.40(2)	3.40(2)
CgY1...CgY2 <sup>8</sup>	4.03(2)	3.8	34.06	30.23	3.48(2)	3.34(2)
CgY1...CgY3 <sup>8</sup>	3.83(2)	1.6	27.82	26.22	3.43(2)	3.38(2)
CgC...CgM2 <sup>1</sup>	4.04(2)	1.7	32.94	33.32	3.38(2)	3.39(2)
CgC...CgM3 <sup>1</sup>	4.04(2)	4.3	36.09	35.79	3.27(2)	3.26(2)
CgL1...CgM1	4.27(2)	19.9	35.93	53.43	-2.54(2)	3.45(2)
CgL1...CgQ2 <sup>1</sup>	4.61(2)	12.3	48.31	36.93	-3.69(2)	-3.07(2)
CgL2...CgM1	3.72(2)	12.2	21.42	12.25	-3.63(2)	3.46(2)
CgL2...CgM2	4.98(2)	12.8	34.02	43.70	-3.60(2)	4.13(2)
CgL2...CgM3	3.88(2)	10.0	18.19	19.95	-3.65(2)	3.69(2)
CgL2...CgQ2 <sup>1</sup>	3.80(2)	9.5	27.14	35.68	-3.09(2)	-3.38(2)
CgO1...CgO1 <sup>5</sup>	4.26(2)	0	38.05	38.05	3.35(2)	3.35(2)
CgO1...CgO2 <sup>5</sup>	3.76(2)	3.5	24.73	23.61	3.44(2)	3.41(2)
CgO1...CgO3 <sup>5</sup>	3.60(2)	3.7	17.67	17.84	3.42(2)	3.43(2)
CgO1...CgX1	3.45(2)	9.0	11.95	20.96	3.22(2)	-3.38(2)
CgO1...CgX3	4.74(2)	11.4	38.59	48.70	3.13(2)	-3.71(2)
CgO2...CgX1	4.81(2)	11.4	47.13	38.46	3.77(2)	-3.27(2)

CgO2...CgX2	4.68(2)	13.5	44.82	34.62	3.86(2)	-3.32(2)
CgO2...CgX3	3.91(2)	13.6	23.42	9.86	3.85(2)	-3.58(2)
CgO3...CgO3 <sup>2</sup>	4.40(2)	0	40.53	40.53	3.34(2)	3.34(2)
CgO3...CgX1	3.85(2)	7.1	27.53	28.69	3.38(2)	-3.42(2)
CgO3...CgX2	4.11(2)	9.2	34.64	34.54	3.38(2)	-3.38(2)
CgO3...CgX3	3.77(2)	9.1	17.59	26.62	3.37(2)	-3.60(2)
CgQ1...CgQ1 <sup>1</sup>	4.45(2)	0	43.01	43.01	3.25(2)	3.25(2)
CgQ1...CgQ2 <sup>1</sup>	3.47(2)	1.2	19.09	20.20	3.26(2)	3.28(2)
CgQ1...CgQ3 <sup>1</sup>	3.62(2)	0.5	25.69	25.67	3.26(2)	3.26(2)
CgQ2...CgQ3 <sup>1</sup>	4.77(2)	0.7	47.62	46.90	3.26(2)	3.22(2)
CgQ3...CgQ3 <sup>1</sup>	4.24(2)	0	40.01	40.01	3.25(2)	3.25(2)

Symmetry operations: (1) 1-x,1-y,1-z; (2) -x,-y,1-z; (3) 1-x,-y,1-z; (4) -1+x,-1+y,1+z; (5) -x,1-y,1-z; (6) -1+x,y,z; (7) 1-x,1-y,-z; (8) 2-x,-y,1-z.

CgI – center of gravity of ring number I;  $\alpha$  – dihedral angle between planes I and J ( $^\circ$ );  $\beta$  – angle between Cg I...Cg J vector and normal to plane I ( $^\circ$ );  $\gamma$  – angle between Cg I...Cg J vector and normal to plane J ( $^\circ$ ); Cg...Cg – distance between ring centroids ( $\text{\AA}$ ); CgI perp. – perpendicular distance of CgI on ring J ( $\text{\AA}$ ); CgJ perp. – perpendicular distance of CgJ on ring J ( $\text{\AA}$ );  $\perp d(\text{H}\cdots\pi)$  – distance between H atom and plane of the ring

**Table S2. Interactions present in the structure of complex 2.**

Hydrogen bonding ( $\text{\AA}$ and $^\circ$ )				
$D\text{---}H\cdots A$	$d(D\text{---}H)$	$d(H\cdots A)$	$d(D\cdots A)$	$\angle(D\text{---}H\cdots A)$
O1S—H1S...O2A1 <sup>1</sup>	0.84	1.96	2.69(1)	145
O4A—H4A1...O4D <sup>2</sup>	0.84	1.81	2.628(8)	164
O4B—H4B1...O4C	0.84	1.87	2.685(7)	164
O4C—H4C1...O4D	0.84	1.68	2.477(8)	159
N2X—H2X1...O3C <sup>3</sup>	0.88	1.97	2.772(9)	151
N2Z—H2Z1...O1W	0.88	1.91	2.705(9)	150
N1V—H1V1...O3W	0.88	1.91	2.73(1)	155
N1U—H1U1...O4W	0.88	1.97	2.80(1)	157
N2Y—H2YN...O13W	0.88	1.85	2.676(1)	155
N2W—H2W1...O14W	0.88	1.88	2.747(1)	167
C7A—H7A1...O1S	0.99	2.38	3.37(1)	174
C1U—H1U...O9W <sup>4</sup>	0.95	2.59	3.16(2)	119
C1U—H1U...O3B1	0.95	2.63	3.43(2)	142
C2U—H2U...O4A	0.95	2.69	3.27(2)	120
C3V—H3V...O6W <sup>4</sup>	0.95	2.50	3.33(1)	146
C3X—H3X...O3A1 <sup>2</sup>	0.95	2.34	3.25(1)	162
C6X—H6X...O5W <sup>5</sup>	0.95	2.53	3.39(1)	151
C6Y—H6Y...O2C	0.95	2.30	3.15(1)	150
C6Z—H6Z...O1C <sup>3</sup>	0.95	2.45	3.24(1)	141
C7Z—H7Z...O5W <sup>3</sup>	0.95	2.57	3.21(1)	125
C8U—H8U...O1B1	0.95	2.38	3.31(1)	167
C8Y—H8Y...O2W	0.95	2.37	3.218(1)	148
C11U—H11U...O3A1 <sup>6</sup>	0.95	2.56	3.43(1)	152
C11V—H11V...O6W <sup>4</sup>	0.95	2.43	3.28(1)	149
C11X—H11X...O2A1 <sup>2</sup>	0.95	2.47	3.39(2)	164

Symmetry operations: (1)  $\frac{1}{2}\text{-x}, -1/2\text{-y}, -z$ ; (2)  $\frac{1}{2}\text{-x}, 1/2\text{-y}, -z$ ; (3)  $\frac{1}{2}\text{-x}, 1/2\text{+y}, 1/2\text{-z}$ ; (4)  $-1/2\text{+x}, 1/2\text{+y}, z$ ; (5)  $x, 1\text{+y}, z$ ; (6)  $-x, -y, -z$ .

Interactions $X\text{---}H\cdots\pi$ ( $\text{\AA}$ and $^\circ$ )						
$C\text{---}H\cdots CgJ$	$d(H\cdots Cg)$	$\perp d(H\cdots\pi)$	$\gamma$	$\angle C\text{---}H\cdots Cg$	$d(C\cdots Cg)$	$\angle C\text{---}H, \pi$
C7B—H7B1...CgZ3	2.87	-2.78	14.16	136	3.643(9)	48
C3Y—H3Y...CgD <sup>1</sup>	2.94	-2.78	19.40	161	3.85(1)	84

C7C–H7C1…CgX3 <sup>2</sup>	2.84	2.82	7.66	140	3.656(8)	43
C8X–H8X…CgB <sup>3</sup>	2.89	-2.69	21.24	165	3.816(9)	59
C8Z–H8Z…CgD	2.66	2.65	6.45	151	3.526(8)	58
C12Z–H12Z…CgA <sup>4</sup>	2.58	2.56	6.41	154	3.453(8)	58
C1W–H1W…CgD <sup>1</sup>	2.93	-2.77	19.25	167	3.86(3)	84
C2W–H2W…CgX1 <sup>5</sup>	2.84	2.63	21.85	153	3.71(3)	42

**Interactions  $\pi \cdots \pi$  (Å and °)**

<b>CgI…CgJ</b>	<b>d(CgI…CgJ)</b>	<b><math>\alpha</math></b>	<b><math>\beta</math></b>	<b><math>\gamma</math></b>	<b>CgI perp.</b>	<b>CgJ perp.</b>
CgC…CgX2 <sup>2</sup>	3.497(4)	4.0(4)	18.27	21.30	3.259(3)	-3.321(3)
CgC…CgX3 <sup>2</sup>	4.763(5)	6.0(4)	42.30	48.30	3.168(3)	-3.523(4)
CgC…CgZ2	3.665(4)	8.7(4)	19.54	24.71	-3.330(3)	3.454(3)
CgU1…CgU2 <sup>6</sup>	3.818(5)	0.6(4)	25.68	26.15	-3.427(3)	-3.441(4)
CgU1…CgU3 <sup>6</sup>	3.687(5)	1.5(4)	22.30	22.56	-3.405(3)	-3.411(3)
CgU1…CgV3	4.901(5)	8.6(4)	45.61	44.81	-3.477(3)	3.428(3)
CgU2…CgU3 <sup>6</sup>	4.411(5)	1.0(4)	39.04	39.33	-3.412(4)	-3.426(3)
CgU2…CgV1	4.719(5)	8.2(4)	48.71	40.64	-3.581(4)	3.114(3)
CgU2…CgV2	3.839(5)	8.2(4)	15.09	21.31	-3.576(4)	3.707(3)
CgU2…CgV3	3.730(5)	8.0(4)	23.37	16.28	-3.580(4)	3.424(3)
CgU3…CgU3 <sup>6</sup>	3.597(5)	0	18.14	18.14	-3.418(3)	-3.418(3)
CgU3…CgV1	4.269(5)	7.2(4)	42.05	37.95	-3.366(3)	3.170(3)
CgU3…CgV3	3.644(5)	7.0(4)	19.24	22.28	-3.372(3)	3.440(3)
CgV1…CgY1	3.618(6)	8.0(5)	21.39	29.28	-3.156(3)	3.369(5)
CgV1…CgY3	4.585(6)	8.3(5)	40.48	46.57	-3.152(3)	3.487(5)
CgV1…CgW1	3.56(1)	5.2	21.18	24.14	-3.248(3)	3.32(1)
CgV1…CgW2	4.98(2)	9	47.30	49.36	-3.242(3)	3.38(3)
CgV1…CgW3	3.54(2)	6.7	23.54	23.62	-3.242(3)	3.24(2)
CgV2…CgY2	3.660(7)	9.1(6)	28.46	19.42	-3.451(3)	3.217(6)
CgV2…CgY3	3.764(6)	8.7(5)	21.94	23.36	-3.456(3)	3.492(5)
CgV2…CgW2	3.76(3)	9	26.52	17.43	-3.582(3)	3.36(2)
CgV2…CgW3	4.63(2)	7	45.67	40.23	-3.535(3)	3.24(2)
CgV3…CgY1	3.698(6)	8.0(5)	24.55	20.83	-3.456(3)	3.363(5)
CgV3…CgY2	4.566(7)	8.6(6)	44.75	40.25	-3.485(3)	3.242(6)
CgV3…CgY3	3.621(6)	8.3(5)	15.58	17.36	-3.456(3)	3.488(5)
CgV3…CgW1	3.81(1)	5.3	29.65	24.70	-3.463(3)	3.31(1)
CgV3…CgW2	4.50(3)	9	41.20	37.45	-3.568(3)	3.38(3)
CgV3…CgW3	4.08(2)	6.7	37.39	30.96	-3.501(3)	3.24(2)
CgX1…CgZ2	3.594(5)	2.1(4)	5.28	3.22	3.588(3)	-3.580(3)
CgX1…CgZ3	4.413(5)	3.5(4)	38.02	35.04	3.614(3)	-3.477(3)
CgX2…CgZ1	4.580(5)	8.4(4)	44.37	45.26	3.224(4)	-3.274(3)
CgX3…CgZ1	3.964(5)	6.2(4)	33.66	29.51	3.450(4)	-3.299(3)
CgX3…CgZ2	4.133(5)	2.8(4)	29.81	32.35	3.491(4)	-3.586(3)
CgX3…CgZ3	3.908(5)	4.1(4)	25.77	27.83	3.456(4)	-3.519(3)
CgY1…CgY1 <sup>7</sup>	3.955(7)	7	30.92	30.92	3.393(5)	3.393(5)
CgY1…CgY2 <sup>7</sup>	4.078(7)	6.6(7)	31.13	33.83	3.388(5)	3.491(6)
CgY1…CgY3 <sup>7</sup>	3.785(7)	6.5(6)	19.49	25.96	3.403(5)	3.568(5)
CgY1…CgW1 <sup>7</sup>	4.12(1)	10.3	34.59	38.00	3.252(5)	3.40(1)
CgY1…CgW2 <sup>7</sup>	3.82(2)	6	28.62	30.27	3.296(5)	3.35(3)
CgY1…CgW3 <sup>7</sup>	3.41(2)	7.9	21.68	13.92	3.313(5)	3.17(2)
CgY2…CgW1 <sup>7</sup>	3.99(1)	10.6	31.63	23.55	3.660(6)	3.40(1)
CgY3…CgY3 <sup>7</sup>	3.999(7)	6	27.15	27.15	3.558(5)	3.558(5)
CgY3…CgW1 <sup>7</sup>	3.91(1)	10.3	29.36	21.97	3.629(5)	3.41(1)
CgY3…CgW3 <sup>7</sup>	4.58(1)	7.8	46.16	39.20	3.546(5)	3.17(2)
CgW1…CgW1 <sup>7</sup>	4.29(1)	12	41.37	41.37	3.23(1)	3.22(1)

CgW1...CgW2 <sup>7</sup>	3.74(2)	10	20.79	28.00	3.31(1)	3.50(3)
CgW1...CgW3 <sup>7</sup>	3.38(2)	11	22.78	11.98	3.31(1)	3.12(2)
CgW3...CgW3 <sup>7</sup>	3.63(2)	9	31.27	31.27	3.10(2)	3.10(2)

Symmetry operations: (1)  $-1/2+x, 1/2+y, z$ ; (2)  $x, -1+y, z$ ; (3)  $x, 1+y, z$ ; (4)  $1/2-x, 1/2-y, -z$ ; (5)  $-1/2+x, -1/2+y, z$ ; (6)  $-x, 1-y, -z$ ; (7)  $-x, y, 1/2-z$ .

CgI – center of gravity of ring number I;  $\alpha$  – dihedral angle between planes I and J ( $^\circ$ );  $\beta$  – angle between Cg I...Cg J vector and normal to plane I ( $^\circ$ );  $\gamma$  – angle between Cg I...Cg J vector and normal to plane J ( $^\circ$ ); Cg...Cg – distance between ring centroids ( $\text{\AA}$ ); CgI perp. – perpendicular distance of CgI on ring J ( $\text{\AA}$ ); CgJ perp. – perpendicular distance of CgJ on ring I ( $\text{\AA}$ );  $\perp d(\text{H}\cdots\pi)$  – distance between H atom and plane of the ring

**Table S3. Interactions present in the structure of complex 3.**

Hydrogen bonding ( $\text{\AA}$ and $^\circ$ )				
$D-H\cdots A$	$d(D-H)$	$d(H\cdots A)$	$d(D\cdots A)$	$\angle(D-H\cdots A)$
O4B—H4B1...O4C	0.84	1.86	2.558(4)	139
O4D—H4D1...O4E	0.84	1.89	2.725(4)	177
O4F—H4F1...O4G	0.84	1.86	2.547(4)	138
O4H—H4H1...O4A	0.84	1.87	2.706(4)	171
N1X—H1XN...O6W	0.88	2.07	2.901(4)	156
N2Q—H2QN...O12W	0.88	1.99	2.806(6)	153
N2Z—H2ZN...O7W	0.88	2.02	2.869(7)	161
N1L—H1LN...O7W	0.88	2.27	2.893(8)	127
N1W—H1WN...O13W	0.88	1.87	2.732(5)	166
N2U—H2UN...O6W	0.88	2.12	2.866(5)	142
N1T—H1TN...O11W	0.88	2.00	2.858(5)	166
N2R—H2RN...O1D <sup>1</sup>	0.88	1.98	2.766(4)	149
N2Y—H2YN...O7W	0.88	1.94	2.760(5)	154
N1P—H1PN...O1W <sup>2</sup>	0.88	1.85	2.659(4)	151
N2O—H2ON...O9W <sup>3</sup>	0.88	1.91	2.696(6)	148
N1V—H1VN...O32W	0.88	2.16	3.02(2)	166
N2M—H2MN...O28W	0.88	2.27	3.12(3)	160
N1K—H1KN...O34W	0.88	2.38	3.22(3)	160
N1N—H1NN...O2H1	0.88	2.24	3.110(1)	168
N1N—H1NN...O2H2	0.88	2.11	2.956(1)	162
O1W—H1W1...O2F <sup>4</sup>	0.85(6)	1.95(6)	2.764(4)	162
O1W—H1W2...O3W	0.84(6)	1.89(6)	2.718(4)	171
O2W—H2W1...O3E <sup>4</sup>	0.90(6)	1.90(6)	2.791(4)	169
O2W—H2W2...O2E <sup>5</sup>	0.78(6)	2.12(6)	2.900(4)	174
O3W—H3W1...O1D <sup>1</sup>	0.91(6)	2.00(6)	2.888(4)	162
O3W—H3W2...O3C1 <sup>1</sup>	0.84(6)	2.06(6)	2.85(2)	155
O4W—H4W1...O3A <sup>6</sup>	0.93(6)	1.82(6)	2.744(5)	175
O4W—H4W2...O1A <sup>3</sup>	0.81(6)	2.07(6)	2.866(5)	170
O5W—H5W1...O2E <sup>5</sup>	0.97(6)	1.81(6)	2.766(5)	168
O5W—H5W2...O1F <sup>4</sup>	0.89(6)	1.88(6)	2.764(4)	177
O6W—H6W1...O2W	0.95(6)	2.04(6)	2.886(4)	147
O6W—H6W2...O1F <sup>4</sup>	0.93(6)	1.85(6)	2.778(4)	172
O8W—H8W1...O5W <sup>3</sup>	0.95(6)	1.80(6)	2.736(5)	167
O8W—H8W2...O3D	0.95(6)	1.86(6)	2.805(5)	175
O10W—H1WW...O1E	0.85(4)	2.04(4)	2.882(5)	171
O10W—H2WW...O8W	0.83(5)	1.94(5)	2.768(6)	177
O13W—H6WW...O14W	0.84(5)	1.84(6)	2.670(7)	168
O14W—H7WW...O3E <sup>4</sup>	0.94(5)	2.47(9)	2.801(6)	101
O14W—H8WW...O3G	0.83(7)	2.04(8)	2.732(7)	140
O15W—H5W3...O2C1	0.92(6)	1.95(6)	2.87(2)	175
O15W—H5W4...O3A <sup>6</sup>	0.80(3)	2.05(3)	2.849(5)	175

O16W—H6W4···O11W	0.85(8)	2.06(8)	2.797(8)	145
C1L—H1L···N1Y	0.95	2.47	3.390(8)	164
C1N—H1N···O2A <sup>7</sup>	0.95	2.43	3.178(6)	136
C1O—H1O···O3G <sup>3</sup>	0.95	2.59	3.283(8)	130
C1P—H1P···O2F <sup>5</sup>	0.95	2.56	3.153(5)	121
C1U—H1U···O5W	0.95	2.59	3.436(6)	149
C1W—H1W···O2W	0.95	2.34	3.268(5)	166
C1X—H1X···O3F <sup>4</sup>	0.95	2.25	3.180(5)	167
C2P—H2P···O1E <sup>4</sup>	0.95	2.38	3.197(6)	144
C2R—H2R···O1C1 <sup>1</sup>	0.95	2.58	3.120(18)	116
C2U—H2U···O3D <sup>5</sup>	0.95	2.50	3.242(5)	135
C2X—H2X···O1G <sup>4</sup>	0.95	2.60	3.205(8)	122
C2Z—H3L···O4G	1.00	2.48	3.387(9)	150
C3P—H3P···O1G	0.95	2.39	3.259(8)	152
C3R—H3R···O17W <sup>4</sup>	0.95	2.48	3.361(8)	154
C3X—H3X···O1G <sup>4</sup>	0.95	2.55	3.180(7)	124
C3Z—H3Z···O4F	0.95	2.56	3.487(9)	166
C3Z—H3Z···O4G	0.95	2.31	2.984(9)	128
C4A—H4A···O3A <sup>8</sup>	0.95	2.65	3.454(1)	143
C4E—H4E···O3E <sup>8</sup>	0.95	2.56	3.375(2)	144
C6O—H6O···O2B1 <sup>9</sup>	0.95	2.43	3.03(2)	121
C6O—H6O···O21W <sup>3</sup>	0.95	2.53	3.298(8)	138
C6P—H6P···O3C1 <sup>10</sup>	0.95	2.46	3.04(3)	119
C6Q—H6Q···O4W	0.95	2.57	3.342(7)	139
C6R—H6R···O2D <sup>1</sup>	0.95	2.38	3.171(5)	140
C6U—H6U···N2X	0.95	2.34	3.240(5)	158
C6Y—H6Y···O1B1 <sup>6</sup>	0.95	2.51	3.45(1)	169
C7D—H7D1···O16W	0.99	2.39	3.321(7)	156
C7O—H7O···O2A <sup>7</sup>	0.95	2.30	3.165(7)	151
C7R—H7R···O2D	0.95	2.54	3.335(6)	142
C7W—H7W···O4A	0.95	2.56	3.439(5)	154
C8R—H8R···O10W	0.95	2.43	3.273(6)	149
C8U—H8U···O4C	0.95	2.36	3.203(5)	147
C8W—H8W···O15W <sup>5</sup>	0.95	2.43	3.329(6)	159
C8Y—H8Y···O2C1 <sup>6</sup>	0.95	2.43	3.34(1)	160
C11L—H11L···O4F	0.95	2.43	3.364(9)	168
C11P—H11P···O2G	0.95	2.45	3.322(7)	153
C11Q—H11Q···O3G <sup>3</sup>	0.95	2.50	3.445(6)	175
C11R—H11R···O1G <sup>4</sup>	0.95	2.57	3.269(8)	131
C12O—H12O···O1C1 <sup>11</sup>	0.95	2.57	3.34(2)	138
C12U—H12U···O4B	0.95	2.52	3.451(5)	168
C7H—H7H2···O4H	0.95	2.56	2.939(5)	102

Symmetry operations: (1) 1-x,-y,1-z; (2) -x,1-y,1-z; (3) 1+x,y,z; (4) 1-x,1-y,1-z; (5) -1+x,y,z; (6) 1-x,-y,-z; (7) 1-x,1-y,-z; (8) 2-x,1-y,1-z; (9) 1+x,1+y,z; (10) -1+x,1+y,z; (11) x,1+y,z.

#### Interactions X—H··· $\pi$ (Å and °)

C—H···CgJ	$d(\text{H}\cdots\text{Cg})$	$\perp d(\text{H}\cdots\pi)$	$\gamma$	$\angle \text{C—H}\cdots\text{Cg}$	$d(\text{C}\cdots\text{Cg})$	$\angle \text{C—H}, \pi$
C2Y—H2Y···CgC	2.68	-2.63	10.31	142	3.475(2)	62
C3O—H3O···CgF	2.54	2.51	8.77	144	3.360(2)	59
C3W—H3W···CgD <sup>1</sup>	2.74	2.59	19.34	144	3.554(2)	72
C7Q—H7Q···CgA <sup>2</sup>	2.93	-2.92	6.56	139	3.709(2)	56
C7X—H7X···CgG	2.42	2.41	4.86	164	3.342(2)	75
C8P—H8P···CgB <sup>3</sup>	2.45	-2.43	6.76	146	3.284(3)	61
C8Q—H8Q···CgH <sup>2</sup>	2.86	-2.72	17.98	145	3.681(3)	72
C8X—H8X···CgF	2.77	-2.73	9.68	164	3.689(3)	71

C1V–H1V···CgH	2.98	2.79	20.36	156	3.864(2)	57
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**Interactions  $\pi\cdots\pi$  (Å and °)**

<b>CgI···CgJ</b>	<b><i>d</i>(CgI···CgJ)</b>	<b><math>\alpha</math></b>	<b><math>\beta</math></b>	<b><math>\gamma</math></b>	<b>CgI perp.</b>	<b>CgJ perp.</b>
CgA···CgY1	4.198(5)	12.69	32.07	43.09	3.066(1)	3.557(1)
CgA···CgY3	4.131(6)	12.76	31.27	41.99	3.071(4)	3.531(4)
CgC···CgR1 <sup>4</sup>	4.872(5)	2.24	51.81	30.23	-4.209(4)	3.012(4)
CgD···CgU2	4.963(4)	7.27	18.83	53.16	-2.976(3)	-4.698(3)
CgE···CgW1 <sup>2</sup>	4.983(5)	54.53	5.69	58.64	2.593(4)	4.958(4)
CgE···CgX2	4.423(5)	9.06	35.26	43.49	-3.209(2)	-3.611(2)
CgE···CgX3	3.815(5)	9.47	25.52	32.88	-3.204(4)	-3.443(4)
CgN1···CgO2	4.587(5)	57.88	34.07	24.80	-4.164(4)	3.800(4)
CgN1···CgY2 <sup>5</sup>	4.416(5)	58.72	32.61	28.91	3.866(4)	-3.720(4)
CgN1···CgV3	4.711(4)	2.21	44.60	43.06	-3.442(4)	3.354(4)
CgN2···CgV1	3.655(5)	1.56	22.12	22.95	-3.365(4)	3.386(4)
CgN2···CgV1 <sup>5</sup>	3.830(4)	1.56	29.20	28.92	-3.352(3)	-3.343(3)
CgN2···CgV2	4.303(4)	3.43	40.79	37.47	-3.415(4)	3.258(4)
CgN2···CgV2 <sup>5</sup>	4.308(4)	3.43	41.71	39.11	-3.342(3)	-3.216(4)
CgN2···CgV3	3.605(4)	1.85	20.96	21.75	-3.349(4)	3.367(4)
CgN2···CgV3 <sup>5</sup>	4.088(4)	1.85	35.60	36.89	-3.270(1)	-3.324(1)
CgN3···CgV1	3.933(4)	2.88	30.21	33.04	-3.297(4)	3.399(4)
CgN3···CgV2 <sup>5</sup>	4.571(4)	2.11	45.51	44.48	-3.262(4)	-3.203(4)
CgN3···CgV3	4.076(4)	0.27	33.62	33.77	-3.389(4)	3.394(4)
CgO1···CgP1 <sup>2</sup>	3.747(5)	2.69	24.16	21.64	-3.483(3)	3.419(4)
CgO1···CgP3 <sup>2</sup>	4.011(4)	1.36	29.62	29.92	-3.477(4)	3.487(4)
CgO2···CgP2 <sup>2</sup>	3.709(5)	3.39	24.95	22.60	-3.424(3)	3.363(3)
CgO2···CgP3 <sup>2</sup>	4.059(5)	2.35	31.24	32.10	-3.439(4)	3.471(4)
CgO3···CgP1 <sup>2</sup>	4.032(4)	3.45	31.85	31.69	-3.431(4)	3.425(4)
CgO3···CgP2 <sup>2</sup>	3.959(4)	3.37	31.81	29.42	-3.448(2)	3.364(2)
CgO3···CgP3 <sup>2</sup>	3.578(6)	2.42	14.38	16.67	-3.428(3)	3.466(3)
CgQ1···CgW1 <sup>2</sup>	3.848(4)	4.67	29.42	27.94	3.400(3)	-3.352(3)
CgQ1···CgW2 <sup>2</sup>	4.078(4)	3.76	34.91	34.45	3.363(2)	-3.344(2)
CgQ1···CgW3 <sup>2</sup>	3.635(5)	3.98	25.81	21.84	3.374(4)	-3.272(3)
CgQ1···CgZ1	3.764(5)	5.31	33.01	28.15	3.319(3)	3.156(4)
CgQ1···CgZ3	3.690(5)	6.44	23.89	24.81	3.349(1)	3.374(1)
CgQ2···CgW2 <sup>2</sup>	3.709(8)	6.26	25.59	29.78	3.219(4)	-3.345(4)
CgQ2···CgZ2	3.439(4)	5.80	11.36	15.78	3.309(4)	3.371(4)
CgQ2···CgZ3	4.402(4)	6.61	41.62	39.21	3.411(4)	3.291(4)
CgQ3···CgW2 <sup>2</sup>	3.628(4)	4.64	24.04	19.44	3.421(4)	-3.313(4)
CgQ3···CgW3 <sup>2</sup>	4.618(4)	4.92	44.98	42.15	3.424(4)	-3.266(4)
CgQ3···CgZ1	4.779(5)	5.00	48.47	43.49	3.467(4)	3.168(4)
CgQ3···CgZ2	3.848(4)	6.49	29.77	25.11	3.484(4)	3.340(4)
CgQ3···CgZ3	3.582(5)	5.76	19.26	14.56	3.467(3)	3.382(3)
CgR2···CgT1	4.913(5)	9.70	57.31	49.54	3.188(4)	2.653(4)
CgR2···CgT2 <sup>4</sup>	3.733(4)	10.09	18.48	28.56	3.279(4)	-3.541(4)
CgR2···CgT3 <sup>4</sup>	4.397(4)	9.72	37.14	41.18	3.309(4)	-3.505(4)
CgT1···CgU1	3.586(4)	4.93	15.55	13.25	-3.490(2)	-3.454(2)
CgT1···CgU3	4.745(5)	3.49	45.02	44.37	-3.392(3)	-3.354(3)
CgT2···CgU1	4.768(5)	3.59	44.12	45.90	-3.318(4)	-3.423(4)
CgT2···CgU2	4.006(5)	3.96	34.34	31.45	-3.417(4)	-3.308(3)
CgT2···CgU3	3.520(6)	3.28	15.04	14.06	-3.415(4)	-3.400(4)
CgT3···CgU1	3.810(5)	4.07	24.91	24.82	-3.458(4)	-3.456(4)
CgT3···CgU3	3.827(4)	3.10	27.46	25.50	-3.454(3)	-3.396(3)
CgU1···CgW1	3.573(4)	4.28	21.03	17.54	-3.407(4)	3.335(4)



CgU1...CgW2	4.817(4)	4.02	43.30	44.83	-3.416(3)	3.506(3)
CgU1...CgW3	3.681(4)	4.36	18.71	22.46	-3.402(4)	3.487(4)
CgU2...CgW2	4.299(4)	4.97	37.75	41.72	-3.209(4)	3.399(4)
CgU3...CgW1	4.574(4)	5.26	41.63	43.19	-3.335(3)	3.419(3)
CgU3...CgW2	3.591(4)	4.31	18.37	18.89	-3.398(3)	3.408(3)
CgU3...CgW3	3.846(5)	4.51	24.43	28.10	-3.392(4)	3.501(4)
CgX1...CgX2 <sup>6</sup>	3.489(5)	4.01	16.90	18.50	3.308(3)	3.338(3)
CgX1...CgX3 <sup>6</sup>	4.245(4)	3.18	41.04	39.57	3.272(4)	3.202(4)
CgX2...CgX2 <sup>6</sup>	4.966(4)	0	48.58	48.58	3.285(4)	3.285(4)
CgX2...CgX3 <sup>6</sup>	3.643(5)	1.08	25.18	24.30	3.320(3)	3.297(3)
CgX3...CgX3 <sup>6</sup>	3.673(4)	0	26.54	26.54	3.286(4)	3.286(4)
CgY1...CgY2 <sup>7</sup>	3.582(4)	3.25	22.22	19.46	-3.377(4)	-3.316(4)
CgY1...CgY3 <sup>7</sup>	3.776(4)	1.23	28.37	27.29	-3.356(4)	-3.322(4)
CgY2...CgY3 <sup>7</sup>	4.083(6)	2.48	36.23	36.28	-3.292(4)	-3.294(4)
CgY3...CgY3 <sup>7</sup>	3.550(4)	0	20.63	20.63	-3.323(4)	3.323(4)
CgZ1...CgV1	4.039(4)	6.61	27.89	33.32	3.375(3)	-3.570(3)
CgZ2...CgV2	3.629(4)	3.71	11.74	14.16	3.519(3)	-3.554(3)
CgZ2...CgV3	4.356(5)	1.37	37.17	36.46	3.504(4)	-3.471(4)
CgZ3...CgV1	3.789(4)	4.74	20.92	23.72	3.469(4)	-3.539(4)
CgZ3...CgV2	4.476(5)	1.89	39.22	39.87	3.435(4)	-3.467(4)
CgZ3...CgV3	3.840(4)	2.16	23.60	23.96	3.509(4)	-3.518(4)
CgL1...CgQ1	4.060(4)	4.34	30.75	34.96	3.327(3)	3.489(3)
CgL1...CgQ3	4.821(4)	3.59	42.51	45.96	3.351(4)	3.554(4)
CgL1...CgM1	3.697(5)	5.97	26.32	32.24	3.127(2)	-3.314(2)
CgL1...CgM3	4.032(4)	8.37	37.28	41.90	3.001(3)	-3.209(3)
CgL2...CgQ1	4.949(5)	4.22	45.28	44.07	3.556(3)	3.483(4)
CgL2...CgQ2	4.119(4)	4.74	30.76	29.87	3.572(4)	3.539(4)
CgL2...CgQ3	3.719(5)	3.51	17.35	15.58	3.582(3)	3.550(4)
CgL2...CgM1	4.626(4)	6.11	44.15	42.83	3.392(4)	-3.319(4)
CgL2...CgM2	3.613(5)	3.74	20.02	18.58	3.424(3)	-3.394(4)
CgL2...CgM3	3.880(4)	8.48	34.22	25.92	3.490(4)	-3.208(4)
CgL3...CgQ1	3.661(5)	4.41	17.41	16.75	3.506(3)	3.493(3)
CgL3...CgQ2	4.807(4)	4.62	42.81	45.19	3.387(4)	3.526(4)
CgL3...CgQ3	3.786(5)	3.61	20.29	22.29	3.503(4)	3.551(4)
CgL3...CgM1	3.440(4)	5.87	15.67	12.60	3.357(4)	-3.312(4)
CgL3...CgM2	4.846(5)	3.52	45.37	45.63	3.389(3)	-3.405(3)
CgL3...CgM3	3.890(4)	8.32	34.25	30.59	3.348(4)	-3.215(4)
CgM1...CgN2	3.629(5)	1.65	20.69	19.07	3.430(4)	-3.395(4)
CgM1...CgN2 <sup>5</sup>	3.645(4)	1.65	22.30	21.68	-3.387(4)	-3.373(4)
CgM1...CgN3	4.236(5)	2.49	37.66	35.21	3.461(5)	-3.353(4)
CgM2...CgN2	4.488(4)	2.20	41.40	43.14	3.275(4)	-3.367(4)
CgM2...CgN2 <sup>5</sup>	4.569(5)	2.20	43.89	44.97	-3.232(4)	-3.292(4)
CgM2...CgN3 <sup>5</sup>	4.861(5)	0.63	48.18	48.55	-3.218(3)	-3.242(3)
CgM3...CgN2	3.874(4)	4.74	29.68	28.93	3.390(4)	-3.365(4)
CgM3...CgN2 <sup>5</sup>	3.522(4)	4.74	15.82	18.08	-3.348(3)	-3.388(3)
CgM3...CgN3 <sup>5</sup>	3.824(4)	5.24	25.42	29.37	-3.333(4)	-3.454(4)

Symmetry operations: (1)  $-1+x,y,z$ ; (2)  $1+x,y,z$ ; (3)  $x,1+y,z$ ; (4)  $1-x,-y,1-z$ ; (5)  $1-x,1-y,-z$ ; (6)  $1-x,1-y,1-z$ ; (7)  $1-x,-y,-z$ .

CgI – center of gravity of ring I;  $\alpha$  – dihedral angle between planes I and J ( $^\circ$ );  $\beta$  – angle between Cg I...Cg J vector and normal to plane I ( $^\circ$ );  $\gamma$  – angle between Cg I...Cg J vector and normal to plane J ( $^\circ$ ); Cg...Cg – distance between ring centroids ( $\text{\AA}$ ); CgI perp. – perpendicular distance of CgI on ring J ( $\text{\AA}$ ); CgJ perp. – perpendicular distance of CgJ on ring I ( $\text{\AA}$ );  $\perp d(\text{H}\cdots\pi)$  – distance between H atom and plane of the ring

