Supporting Information

Supramolecular Interactions and Aromaticity in Phenazine –Hydroxybenzoic Acid Co-crystals

*Kinga Wzgarda-Raj**

Department of Physical Chemistry, Faculty of Chemistry, University of Lodz, Pomorska 163/165, 90-236 Lodz, Poland

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Table S1. Bond Lengths for (**I**).

Atom	Atom	Length [Å]	Atom	Atom	Length [Å]
O(29C)	C(27C)	1.2375(15)	C(21C)	C(26C)	1.4068(17)
O(29B)	C(27B)	1.2339(15)	C(23A)	C(22A)	1.3838(18)
O(30A)	C(24A)	1.3472(15)	C(7A)	C(6A)	1.4295(18)
O(29A)	C(27A)	1.2340(15)	C(27B)	C(21B)	1.4721(17)
O(30C)	C(24C)	1.3499(15)	C(14D)	C(13D)	1.4296(18)
O(30B)	C(24B)	1.3494(15)	C(2D)	C(3D)	1.4238(18)
O(28C)	C(27C)	1.3120(15)	C(21B)	C(22B)	1.3966(17)
O(28B)	C(27B)	1.3139(15)	C(21B)	C(26B)	1.4046(17)
O(28A)	C(27A)	1.3095(15)	C(2B)	C(3B)	1.4235(18)
N(1A)	C(14A)	1.3421(16)	C(14B)	C(13B)	1.4295(18)
N(1A)	C(2A)	1.3396(16)	C(26A)	C(25A)	1.3803(18)
N(8B)	C(7B)	1.3428(16)	C(25C)	C(26C)	1.3799(18)
N(8B)	C(9B)	1.3453(17)	C(25B)	C(26B)	1.3783(18)
N(8D)	C(9D)	1.3450(17)	C(3D)	C(4D)	1.363(2)
N(8D)	C(7D)	1.3434(16)	C(6D)	C(5D)	1.3642(19)
N(1D)	C(14D)	1.3413(17)	C(13A)	C(12A)	1.364(2)
N(1D)	C(2D)	1.3422(17)	C(10D)	C(11D)	1.368(2)
N(1B)	C(2B)	1.3426(17)	C(6B)	C(5B)	1.363(2)
N(1B)	C(14B)	1.3407(18)	C(3A)	C(4A)	1.364(2)
N(8A)	C(9A)	1.3425(17)	C(10A)	C(11A)	1.360(2)
N(8A)	C(7A)	1.3385(18)	C(10B)	C(11B)	1.367(2)
C(24C)	C(23C)	1.4021(17)	C(3B)	C(4B)	1.363(2)
C(24C)	C(25C)	1.3966(18)	C(4D)	C(5D)	1.421(2)
C(9D)	C(14D)	1.4341(18)	C(13D)	C(12D)	1.358(2)
C(9D)	C(10D)	1.4242(18)	C(11A)	C(12A)	1.417(2)
C(14A)	C(9A)	1.4341(17)	C(5B)	C(4B)	1.417(2)
C(14A)	C(13A)	1.4262(18)	C(6A)	C(5A)	1.359(2)
C(22C)	C(23C)	1.3811(17)	N(8C)	C(9C)	1.342(2)
C(22C)	C(21C)	1.3994(17)	N(8C)	C(7C)	1.334(2)
C(7D)	C(2D)	1.4348(17)	C(13B)	C(12B)	1.359(2)
C(7D)	C(6D)	1.4289(18)	C(11D)	C(12D)	1.422(2)
C(7B)	C(2B)	1.4336(17)	C(4A)	C(5A)	1.423(2)
C(7B)	C(6B)	1.4256(18)	N(1C)	C(14C)	1.347(2)
C(9B)	C(14B)	1.4359(19)	N(1C)	C(2C)	1.334(2)
C(9B)	C(10B)	1.4237(19)	C(11B)	C(12B)	1.424(2)
C(27C)	C(21C)	1.4707(17)	C(9C)	C(14C)	1.433(3)
C(21A)	C(27A)	1.4727(17)	C(9C)	C(10C)	1.419(3)
C(21A)	C(22A)	1.3986(17)	C(7C)	C(2C)	1.434(2)
C(21A)	C(26A)	1.4049(17)	C(7C)	C(6C)	1.428(3)
C(2A)	C(7A)	1.4390(19)	C(14C)	C(13C)	1.416(3)
C(2A)	C(3A)	1.4258(18)	C(2C)	C(3C)	1.419(3)
C(24B)	C(23B)	1.4022(17)	C(13C)	C(12C)	1.358(3)
C(24B)	C(25B)	1.3973(18)	C(3C)	C(4C)	1.366(3)
C(23B)	C(22B)	1.3806(17)	C(12C)	C(11C)	1.435(3)
C(9A)	C(10A)	1.4255(18)	C(5C)	C(6C)	1.353(3)
C(24A)	C(23A)	1.4020(17)	C(5C)	C(4C)	1.423(3)
C(24A)	C(25A)	1.3981(18)	C(11C)	C(10C)	1.358(3)

Table S2. Bond Angles for (**I**).

Atom	Atom	Atom	Angle [°]	Atom	Atom	Atom	Angle [°]
C(2A)	N(1A)	C(14A)	117.86(11)	C(22B)	C(21B)	C(27B)	119.86(11)
C(7B)	N(8B)	C(9B)	117.59(11)	C(22B)	C(21B)	C(26B)	119.12(12)
C(7D)	N(8D)	C(9D)	117.65(11)	C(26B)	C(21B)	C(27B)	120.96(11)
C(14D)	N(1D)	C(2D)	116.95(11)	C(23B)	C(22B)	C(21B)	120.68(11)
C(14B)	N(1B)	C(2B)	117.08(11)	C(23A)	C(22A)	C(21A)	120.56(11)
C(7A)	N(8A)	C(9A)	116.99(11)	N(1B)	C(2B)	C(7B)	121.59(12)
O(30C)	C(24C)	C(23C)	122.91(11)	N(1B)	C(2B)	C(3B)	119.49(12)
O(30C)	C(24C)	C(25C)	117.03(11)	C(3B)	C(2B)	C(7B)	118.92(12)
C(25C)	C(24C)	C(23C)	120.06(12)	N(1B)	C(14B)	C(9B)	121.74(12)
N(8D)	C(9D)	C(14D)	120.85(12)	N(1B)	C(14B)	C(13B)	119.38(12)
N(8D)	C(9D)	C(10D)	119.80(12)	C(13B)	C(14B)	C(9B)	118.88(13)
C(10D)	C(9D)	C(14D)	119.33(12)	C(25A)	C(26A)	C(21A)	120.55(12)
N(1A)	C(14A)	C(9A)	120.94(11)	C(26C)	C(25C)	C(24C)	119.87(11)
N(1A)	C(14A)	C(13A)	119.89(11)	C(26A)	C(25A)	C(24A)	119.86(11)
C(13A)	C(14A)	C(9A)	119.16(12)	C(25C)	C(26C)	C(21C)	120.54(11)
C(23C)	C(22C)	C(21C)	120.54(11)	C(26B)	C(25B)	C(24B)	119.82(12)
N(8D)	C(7D)	C(2D)	120.98(11)	C(4D)	C(3D)	C(2D)	120.37(13)
N(8D)	C(7D)	C(6D)	119.78(11)	C(25B)	C(26B)	C(21B)	120.61(12)
C(6D)	C(7D)	C(2D)	119.22(12)	C(5D)	C(6D)	C(7D)	119.57(12)
N(8B)	C(7B)	C(2B)	121.14(11)	C(12A)	C(13A)	C(14A)	119.83(13)
N(8B)	C(7B)	C(6B)	119.74(11)	C(11D)	C(10D)	C(9D)	119.68(14)
C(6B)	C(7B)	C(2B)	119.11(12)	C(5B)	C(6B)	C(7B)	119.88(13)
N(8B)	C(9B)	C(14B)	120.86(12)	C(4A)	C(3A)	C(2A)	119.64(14)
N(8B)	C(9B)	C(10B)	119.62(12)	C(11A)	C(10A)	C(9A)	120.35(13)
C(10B)	C(9B)	C(14B)	119.51(12)	C(11B)	C(10B)	C(9B)	119.53(14)
C(22C)	C(23C)	C(24C)	119.86(11)	C(4B)	C(3B)	C(2B)	120.35(13)
O(29C)	C(27C)	O(28C)	122.41(12)	C(3D)	C(4D)	C(5D)	120.49(13)
O(29C)	C(27C)	C(21C)	122.79(11)	C(6D)	C(5D)	C(4D)	121.37(13)
O(28C)	C(27C)	C(21C)	114.80(10)	C(12D)	C(13D)	C(14D)	119.97(14)
C(22A)	C(21A)	C(27A)	120.08(11)	C(10A)	C(11A)	C(12A)	120.72(13)
C(22A)	C(21A)	C(26A)	119.21(12)	C(13A)	C(12A)	C(11A)	121.11(13)
C(26A)	C(21A)	C(27A)	120.71(11)	C(6B)	C(5B)	C(4B)	121.15(13)
N(1A)	C(2A)	C(7A)	120.75(12)	C(5A)	C(6A)	C(7A)	120.12(14)
N(1A)	C(2A)	C(3A)	119.76(12)	C(7C)	N(8C)	C(9C)	116.91(15)
C(3A)	C(2A)	C(7A)	119.48(12)	C(12B)	C(13B)	C(14B)	120.07(14)
O(30B)	C(24B)	C(23B)	122.90(11)	C(10D)	C(11D)	C(12D)	121.00(13)
O(30B)	C(24B)	C(25B)	117.06(11)	C(13D)	C(12D)	C(11D)	120.98(13)
C(25B)	C(24B)	C(23B)	120.04(12)	C(3B)	C(4B)	C(5B)	120.58(13)
C(22B)	C(23B)	C(24B)	119.72(11)	C(3A)	C(4A)	C(5A)	121.08(13)
N(8A)	C(9A)	C(14A)	121.67(12)	C(2C)	N(1C)	C(14C)	116.82(15)
N(8A)	C(9A)	C(10A)	119.50(12)	C(10B)	C(11B)	C(12B)	121.12(13)
C(10A)	C(9A)	C(14A)	118.82(12)	C(13B)	C(12B)	C(11B)	120.88(13)
O(30A)	C(24A)	C(23A)	122.96(11)	C(6A)	C(5A)	C(4A)	121.01(13)
O(30A)	C(24A)	C(25A)	116.97(11)	N(8C)	C(9C)	C(14C)	121.39(17)
C(25A)	C(24A)	C(23A)	120.06(12)	N(8C)	C(9C)	C(10C)	119.61(17)
O(29A)	C(27A)	O(28A)	122.40(12)	C(10C)	C(9C)	C(14C)	118.98(17)
O(29A)	C(27A)	C(21A)	122.81(11)	N(8C)	C(7C)	C(2C)	121.80(17)
O(28A)	C(27A)	C(21A)	114.79(11)	N(8C)	C(7C)	C(6C)	119.63(17)
C(22C)	C(21C)	C(27C)	120.18(11)	C(6C)	C(7C)	C(2C)	118.56(18)

Atom	Atom	Atom	Angle [°]	Atom	Atom	Atom	Angle [°]
C(22C)	C(21C)	C(26C)	119.13(12)	N(1C)	C(14C)	C(9C)	121.49(16)
C(26C)	C(21C)	C(27C)	120.69(11)	N(1C)	C(14C)	C(13C)	119.91(17)
C(22A)	C(23A)	C(24A)	119.75(12)	C(13C)	C(14C)	C(9C)	118.59(17)
N(8A)	C(7A)	C(2A)	121.78(12)	N(1C)	C(2C)	C(7C)	121.57(17)
N(8A)	C(7A)	C(6A)	119.54(12)	N(1C)	C(2C)	C(3C)	119.47(16)
C(6A)	C(7A)	C(2A)	118.67(12)	C(3C)	C(2C)	C(7C)	118.96(17)
O(29B)	C(27B)	O(28B)	122.39(12)	C(12C)	C(13C)	C(14C)	121.2(2)
O(29B)	C(27B)	C(21B)	122.59(11)	C(4C)	C(3C)	C(2C)	120.85(19)
O(28B)	C(27B)	C(21B)	115.02(11)	C(13C)	C(12C)	C(11C)	120.2(2)
N(1D)	C(14D)	C(9D)	121.84(11)	C(6C)	C(5C)	C(4C)	121.18(19)
N(1D)	C(14D)	C(13D)	119.12(12)	C(5C)	C(6C)	C(7C)	120.55(19)
C(13D)	C(14D)	C(9D)	119.04(12)	C(3C)	C(4C)	C(5C)	119.9(2)
N(1D)	C(2D)	C(7D)	121.70(12)	C(10C)	C(11C)	C(12C)	120.1(2)
N(1D)	C(2D)	C(3D)	119.31(12)	C(11C)	C(10C)	C(9C)	120.94(19)
C(3D)	C(2D)	C(7D)	118.98(12)				

Table S3. Torsion Angles for (**I**).

Atom	Atom	Atom	Atom	Angle [°]	Atom	Atom	Atom	Atom	Angle [°]
O(29C)	C(27C)	C(21C)	C(22C)	-0.6(2)	C(7A)	N(8A)	C(9A)	C(14A)	-0.63(18)
O(29C)	C(27C)	C(21C)	C(26C)	-179.31(12)	C(7A)	N(8A)	C(9A)	C(10A)	178.70(11)
O(29B)	C(27B)	C(21B)	C(22B)	-2.5(2)	C(7A)	C(2A)	C(3A)	C(4A)	-0.05(19)
O(29B)	C(27B)	C(21B)	C(26B)	174.78(12)	C(7A)	C(6A)	C(5A)	C(4A)	0.0(2)
O(30A)	C(24A)	C(23A)	C(22A)	178.99(11)	C(27B)	C(21B)	C(22B)	C(23B)	177.45(11)
O(30A)	C(24A)	C(25A)	C(26A)	-179.98(12)	C(27B)	C(21B)	C(26B)	C(25B)	-176.93(12)
O(30C)	C(24C)	C(23C)	C(22C)	179.79(11)	C(14D)	N(1D)	C(2D)	C(7D)	0.86(17)
O(30C)	C(24C)	C(25C)	C(26C)	-179.46(11)	C(14D)	N(1D)	C(2D)	C(3D)	-178.36(11)
O(30B)	C(24B)	C(23B)	C(22B)	-179.67(12)	C(14D)	C(9D)	C(10D)	C(11D)	-0.09(18)
O(30B)	C(24B)	C(25B)	C(26B)	-179.87(12)	C(14D)	C(13D)	C(12D)	C(11D)	-0.2(2)
O(28C)	C(27C)	C(21C)	C(22C)	178.78(11)	C(2D)	N(1D)	C(14D)	C(9D)	-1.47(18)
O(28C)	C(27C)	C(21C)	C(26C)	0.08(18)	C(2D)	N(1D)	C(14D)	C(13D)	178.24(11)
O(28B)	C(27B)	C(21B)	C(22B)	177.33(12)	C(2D)	C(7D)	C(6D)	C(5D)	-0.48(18)
O(28B)	C(27B)	C(21B)	C(26B)	-5.44(19)	C(2D)	C(3D)	C(4D)	C(5D)	0.8(2)
N(1A)	C(14A)	C(9A)	N(8A)	0.02(18)	C(22B)	C(21B)	C(26B)	C(25B)	0.3(2)
N(1A)	C(14A)	C(9A)	C(10A)	-179.31(10)	C(22A)	C(21A)	C(27A)	O(29A)	11.2(2)
N(1A)	C(14A)	C(13A)	C(12A)	178.98(11)	C(22A)	C(21A)	C(27A)	O(28A)	-168.17(12)
N(1A)	C(2A)	C(7A)	N(8A)	-0.76(18)	C(22A)	C(21A)	C(26A)	C(25A)	-0.5(2)
N(1A)	C(2A)	C(7A)	C(6A)	179.09(11)	C(2B)	N(1B)	C(14B)	C(9B)	-1.20(18)
N(1A)	C(2A)	C(3A)	C(4A)	-179.09(11)	C(2B)	N(1B)	C(14B)	C(13B)	179.16(11)
N(8B)	C(7B)	C(2B)	N(1B)	-0.05(18)	C(2B)	C(7B)	C(6B)	C(5B)	-0.18(18)
N(8B)	C(7B)	C(2B)	C(3B)	179.59(11)	C(2B)	C(3B)	C(4B)	C(5B)	1.2(2)
N(8B)	C(7B)	C(6B)	C(5B)	-178.88(11)	C(14B)	N(1B)	C(2B)	C(7B)	0.86(18)
N(8B)	C(9B)	C(14B)	N(1B)	0.77(18)	C(14B)	N(1B)	C(2B)	C(3B)	-178.77(11)
N(8B)	C(9B)	C(14B)	C(13B)	-179.59(11)	C(14B)	C(9B)	C(10B)	C(11B)	0.48(19)
N(8B)	C(9B)	C(10B)	C(11B)	179.59(11)	C(14B)	C(13B)	C(12B)	C(11B)	0.2(2)
N(8D)	C(9D)	C(14D)	N(1D)	1.21(18)	C(26A)	C(21A)	C(27A)	O(29A)	-168.75(13)
N(8D)	C(9D)	C(14D)	C(13D)	-178.49(11)	C(26A)	C(21A)	C(27A)	O(28A)	11.86(18)
N(8D)	C(9D)	C(10D)	C(11D)	178.58(11)	C(26A)	C(21A)	C(22A)	C(23A)	-0.4(2)
N(8D)	C(7D)	C(2D)	N(1D)	0.05(18)	C(25C)	C(24C)	C(23C)	C(22C)	-0.36(19)
N(8D)	C(7D)	C(2D)	C(3D)	179.27(10)	C(25A)	C(24A)	C(23A)	C(22A)	-0.1(2)
N(8D)	C(7D)	C(6D)	C(5D)	-178.88(11)	C(25B)	C(24B)	C(23B)	C(22B)	0.7(2)

N(1D)	C(14D)	C(13D)	C(12D)	-179.75(12)	C(3D)	C(4D)	C(5D)	C(6D)	-0.4(2)
N(1D)	C(2D)	C(3D)	C(4D)	178.18(11)	C(26B)	C(21B)	C(22B)	C(23B)	0.2(2)
N(1B)	C(2B)	C(3B)	C(4B)	178.24(11)	C(6D)	C(7D)	C(2D)	N(1D)	-178.33(10)
N(1B)	C(14B)	C(13B)	C(12B)	179.77(12)	C(6D)	C(7D)	C(2D)	C(3D)	0.89(17)
N(8A)	C(9A)	C(10A)	C(11A)	-178.49(11)	C(13A)	C(14A)	C(9A)	N(8A)	178.76(10)
N(8A)	C(7A)	C(6A)	C(5A)	179.84(12)	C(13A)	C(14A)	C(9A)	C(10A)	-0.57(17)
C(24C)	C(25C)	C(26C)	C(21C)	-0.6(2)	C(10D)	C(9D)	C(14D)	N(1D)	179.87(11)
C(9D)	N(8D)	C(7D)	C(2D)	-0.35(17)	C(10D)	C(9D)	C(14D)	C(13D)	0.17(18)
C(9D)	N(8D)	C(7D)	C(6D)	178.02(10)	C(10D)	C(11D)	C(12D)	C(13D)	0.3(2)
C(9D)	C(14D)	C(13D)	C(12D)	-0.04(19)	C(6B)	C(7B)	C(2B)	N(1B)	-178.73(11)
C(9D)	C(10D)	C(11D)	C(12D)	-0.1(2)	C(6B)	C(7B)	C(2B)	C(3B)	0.90(17)
C(14A)	N(1A)	C(2A)	C(7A)	0.12(17)	C(6B)	C(5B)	C(4B)	C(3B)	-0.4(2)
C(14A)	N(1A)	C(2A)	C(3A)	179.14(10)	C(3A)	C(2A)	C(7A)	N(8A)	-179.79(11)
C(14A)	C(9A)	C(10A)	C(11A)	0.86(19)	C(3A)	C(2A)	C(7A)	C(6A)	0.07(18)
C(14A)	C(13A)	C(12A)	C(11A)	-0.1(2)	C(3A)	C(4A)	C(5A)	C(6A)	0.1(2)
C(22C)	C(21C)	C(26C)	C(25C)	0.2(2)	C(10A)	C(11A)	C(12A)	C(13A)	0.4(2)
C(7D)	N(8D)	C(9D)	C(14D)	-0.25(17)	C(10B)	C(9B)	C(14B)	N(1B)	179.87(11)
C(7D)	N(8D)	C(9D)	C(10D)	-178.90(10)	C(10B)	C(9B)	C(14B)	C(13B)	-0.49(18)
C(7D)	C(2D)	C(3D)	C(4D)	-1.06(19)	C(10B)	C(11B)	C(12B)	C(13B)	-0.3(2)
C(7D)	C(6D)	C(5D)	C(4D)	0.2(2)	N(8C)	C(9C)	C(14C)	N(1C)	-0.1(2)
C(7B)	N(8B)	C(9B)	C(14B)	0.08(17)	N(8C)	C(9C)	C(14C)	C(13C)	178.28(15)
C(7B)	N(8B)	C(9B)	C(10B)	-179.02(10)	N(8C)	C(9C)	C(10C)	C(11C)	-177.81(16)
C(7B)	C(2B)	C(3B)	C(4B)	-1.40(19)	N(8C)	C(7C)	C(2C)	N(1C)	-0.3(2)
C(7B)	C(6B)	C(5B)	C(4B)	-0.1(2)	N(8C)	C(7C)	C(2C)	C(3C)	-179.72(15)
C(9B)	N(8B)	C(7B)	C(2B)	-0.42(17)	N(8C)	C(7C)	C(6C)	C(5C)	178.65(16)
C(9B)	N(8B)	C(7B)	C(6B)	178.26(10)	N(1C)	C(14C)	C(13C)	C(12C)	177.59(17)
C(9B)	C(14B)	C(13B)	C(12B)	0.12(19)	N(1C)	C(2C)	C(3C)	C(4C)	-177.54(16)
C(9B)	C(10B)	C(11B)	C(12B)	-0.1(2)	C(9C)	N(8C)	C(7C)	C(2C)	1.5(2)
C(23C)	C(24C)	C(25C)	C(26C)	0.7(2)	C(9C)	N(8C)	C(7C)	C(6C)	-177.19(14)
C(23C)	C(22C)	C(21C)	C(27C)	-178.58(11)	C(9C)	C(14C)	C(13C)	C(12C)	-0.8(3)
C(23C)	C(22C)	C(21C)	C(26C)	0.15(19)	C(7C)	N(8C)	C(9C)	C(14C)	-1.3(2)
C(27C)	C(21C)	C(26C)	C(25C)	178.90(12)	C(7C)	N(8C)	C(9C)	C(10C)	177.23(15)
C(21A)	C(26A)	C(25A)	C(24A)	1.1(2)	C(7C)	C(2C)	C(3C)	C(4C)	1.9(3)
C(2A)	N(1A)	C(14A)	C(9A)	0.23(17)	C(14C)	N(1C)	C(2C)	C(7C)	-1.1(2)
C(2A)	N(1A)	C(14A)	C(13A)	-178.50(10)	C(14C)	N(1C)	C(2C)	C(3C)	178.34(15)
C(2A)	C(7A)	C(6A)	C(5A)	-0.02(19)	C(14C)	C(9C)	C(10C)	C(11C)	0.7(3)
C(2A)	C(3A)	C(4A)	C(5A)	0.0(2)	C(14C)	C(13C)	C(12C)	C(11C)	1.4(3)
C(24B)	C(23B)	C(22B)	C(21B)	-0.7(2)	C(2C)	N(1C)	C(14C)	C(9C)	1.3(2)
C(24B)	C(25B)	C(26B)	C(21B)	-0.3(2)	C(2C)	N(1C)	C(14C)	C(13C)	-177.10(14)
C(23B)	C(24B)	C(25B)	C(26B)	-0.2(2)	C(2C)	C(7C)	C(6C)	C(5C)	-0.1(2)
C(9A)	N(8A)	C(7A)	C(2A)	0.99(18)	C(2C)	C(3C)	C(4C)	C(5C)	-1.6(3)
C(9A)	N(8A)	C(7A)	C(6A)	-178.87(11)	C(13C)	C(12C)	C(11C)	C(10C)	-0.9(3)
C(9A)	C(14A)	C(13A)	C(12A)	0.22(19)	C(12C)	C(11C)	C(10C)	C(9C)	-0.2(3)
C(9A)	C(10A)	C(11A)	C(12A)	-0.8(2)	C(6C)	C(7C)	C(2C)	N(1C)	178.36(15)
C(24A)	C(23A)	C(22A)	C(21A)	0.7(2)	C(6C)	C(7C)	C(2C)	C(3C)	-1.1(2)
C(27A)	C(21A)	C(22A)	C(23A)	179.61(11)	C(6C)	C(5C)	C(4C)	C(3C)	0.4(3)
C(27A)	C(21A)	C(26A)	C(25A)	179.44(12)	C(4C)	C(5C)	C(6C)	C(7C)	0.4(3)
C(21C)	C(22C)	C(23C)	C(24C)	-0.06(19)	C(10C)	C(9C)	C(14C)	N(1C)	-178.60(15)
C(23A)	C(24A)	C(25A)	C(26A)	-0.8(2)	C(10C)	C(9C)	C(14C)	C(13C)	-0.2(2)

Table S4. Bond Lengths for (**II**).

Atom	Atom	Length [Å]	Atom	Atom	Length [Å]
O(31A)	C(24A)	1.356(3)	C(2A)	C(3A)	1.428(3)
O(32A)	C(25A)	1.358(3)	C(2B)	C(7B)	1.434(3)
O(30A)	C(23A)	1.359(3)	C(2B)	C(3B)	1.420(4)
N(1C)	C(7C)	1.342(3)	C(6C)	C(5C)	1.350(4)
N(1C)	C(2C)	1.350(3)	C(14A)	C(9A)	1.437(3)
O(28A)	C(27A)	1.273(3)	C(14A)	C(13A)	1.418(4)
N(1A)	C(2A)	1.340(3)	C(2D)	C(3D)	1.431(3)
N(1A)	C(14A)	1.347(3)	C(14B)	C(9B)	1.439(3)
N(1B)	C(2B)	1.348(3)	C(14B)	C(13B)	1.427(4)
N(1B)	C(14B)	1.341(3)	C(7B)	C(6B)	1.430(4)
O(29A)	C(27A)	1.267(3)	C(7A)	C(6A)	1.426(4)
N(8B)	C(7B)	1.336(3)	C(9A)	C(10A)	1.427(3)
N(8B)	C(9B)	1.347(3)	C(3C)	C(4C)	1.364(4)
N(1D)	C(7D)	1.347(3)	C(3A)	C(4A)	1.358(4)
N(1D)	C(2D)	1.342(3)	C(9B)	C(10B)	1.424(4)
N(8A)	C(7A)	1.341(3)	C(5C)	C(4C)	1.430(4)
N(8A)	C(9A)	1.342(3)	C(3D)	C(4D)	1.354(4)
C(25A)	C(24A)	1.401(3)	C(6D)	C(5D)	1.360(4)
C(25A)	C(26A)	1.384(3)	C(13B)	C(12B)	1.359(4)
C(21A)	C(27A)	1.490(3)	C(4A)	C(5A)	1.427(4)
C(21A)	C(26A)	1.396(3)	C(3B)	C(4B)	1.361(4)
C(21A)	C(22A)	1.401(3)	C(13A)	C(12A)	1.361(4)
C(24A)	C(23A)	1.402(3)	C(6A)	C(5A)	1.361(4)
C(7C)	C(2C)1	1.439(3)	C(4D)	C(5D)	1.424(4)
C(7C)	C(6C)	1.432(3)	C(6B)	C(5B)	1.350(4)
C(2C)	C(3C)	1.422(3)	C(10A)	C(11A)	1.356(4)
C(23A)	C(22A)	1.381(3)	C(10B)	C(11B)	1.351(4)
C(7D)	C(2D)2	1.437(3)	C(12B)	C(11B)	1.427(4)
C(7D)	C(6D)	1.421(4)	C(12A)	C(11A)	1.415(5)
C(2A)	C(7A)	1.440(3)	C(4B)	C(5B)	1.428(4)

Symmetry: [1]*2-x,1-y,1-z*; [2]*-x,1-y,2-z*

Table S5. Bond Angles for (**II**).

Atom	Atom	Atom	Angle [˚]	Atom	Atom	Atom	Angle [˚]
C(7C)	N(1C)	C(2C)	117.5(2)	N(1D)	C(2D)	C(7D)	121.6(2)
C(2A)	N(1A)	C(14A)	117.9(2)	N(1D)	C(2D)	C(3D)	119.5(2)
C(14B)	N(1B)	C(2B)	117.8(2)	C(3D)	C(2D)	C(7D)	118.9(2)
C(7B)	N(8B)	C(9B)	117.0(2)	N(1B)	C(14B)	C(9B)	121.0(2)
C(2D)	N(1D)	C(7D)	117.3(2)	N(1B)	C(14B)	C(13B)	120.1(2)
C(7A)	N(8A)	C(9A)	116.9(2)	C(13B)	C(14B)	C(9B)	118.9(2)
O(32A)	C(25A)	C(24A)	114.6(2)	N(8B)	C(7B)	C(2B)	122.2(2)
O(32A)	C(25A)	C(26A)	125.3(2)	N(8B)	C(7B)	C(6B)	119.3(2)

Atom	Atom	Atom	Angle [°]	Atom	Atom	Atom	Angle [°]
C(26A)	C(25A)	C(24A)	120.1(2)	C(6B)	C(7B)	C(2B)	118.5(2)
C(26A)	C(21A)	C(27A)	119.7(2)	N(8A)	C(7A)	C(2A)	121.8(2)
C(26A)	C(21A)	C(22A)	120.7(2)	N(8A)	C(7A)	C(6A)	119.3(2)
C(22A)	C(21A)	C(27A)	119.6(2)	C(6A)	C(7A)	C(2A)	119.0(2)
O(31A)	C(24A)	C(25A)	120.8(2)	N(8A)	C(9A)	C(14A)	122.0(2)
O(31A)	C(24A)	C(23A)	119.4(2)	N(8A)	C(9A)	C(10A)	119.3(2)
C(25A)	C(24A)	C(23A)	119.8(2)	C(10A)	C(9A)	C(14A)	118.8(2)
N(1C)	C(7C)	C(2C)	121.5(2)	C(4C)	C(3C)	C(2C)	120.0(2)
N(1C)	C(7C)	C(6C)	120.0(2)	C(4A)	C(3A)	C(2A)	119.8(2)
C(6C)	C(7C)	C(2C)	118.5(2)	N(8B)	C(9B)	C(14B)	121.4(2)
O(28A)	C(27A)	C(21A)	117.7(2)	N(8B)	C(9B)	C(10B)	119.2(2)
O(29A)	C(27A)	O(28A)	124.5(2)	C(10B)	C(9B)	C(14B)	119.4(2)
O(29A)	C(27A)	C(21A)	117.8(2)	C(6C)	C(5C)	C(4C)	121.1(2)
N(1C)	C(2C)	C(7C)	121.0(2)	C(4D)	C(3D)	C(2D)	120.0(2)
N(1C)	C(2C)	C(3C)	119.5(2)	C(3C)	C(4C)	C(5C)	120.6(2)
C(3C)	C(2C)	C(7C)	119.4(2)	C(5D)	C(6D)	C(7D)	120.1(2)
O(30A)	C(23A)	C(24A)	114.2(2)	C(12B)	C(13B)	C(14B)	119.6(3)
O(30A)	C(23A)	C(22A)	125.5(2)	C(3A)	C(4A)	C(5A)	121.2(2)
C(22A)	C(23A)	C(24A)	120.4(2)	C(4B)	C(3B)	C(2B)	119.9(3)
N(1D)	C(7D)	C(2D)	121.0(2)	C(12A)	C(13A)	C(14A)	120.0(3)
N(1D)	C(7D)	C(6D)	119.9(2)	C(5A)	C(6A)	C(7A)	120.1(2)
C(6D)	C(7D)	C(2D)2	119.1(2)	C(3D)	C(4D)	C(5D)	121.0(2)
C(25A)	C(26A)	C(21A)	119.6(2)	C(5B)	C(6B)	C(7B)	120.3(2)
C(23A)	C(22A)	C(21A)	119.4(2)	C(11A)	C(10A)	C(9A)	120.1(3)
N(1A)	C(2A)	C(7A)	120.8(2)	C(6A)	C(5A)	C(4A)	120.7(2)
N(1A)	C(2A)	C(3A)	120.0(2)	C(6D)	C(5D)	C(4D)	120.9(3)
C(3A)	C(2A)	C(7A)	119.1(2)	C(11B)	C(10B)	C(9B)	119.8(3)
N(1B)	C(2B)	C(7B)	120.6(2)	C(13B)	C(12B)	C(11B)	121.2(3)
N(1B)	C(2B)	C(3B)	119.9(2)	C(13A)	C(12A)	C(11A)	121.0(3)
C(3B)	C(2B)	C(7B)	119.6(2)	C(10A)	C(11A)	C(12A)	120.9(2)
C(5C)	C(6C)	C(7C)	120.3(2)	C(3B)	C(4B)	C(5B)	120.6(3)
N(1A)	C(14A)	C(9A)	120.6(2)	C(10B)	C(11B)	C(12B)	121.1(3)
N(1A)	C(14A)	C(13A)	120.3(2)	C(6B)	C(5B)	C(4B)	121.1(3)
C(13A)	C(14A)	C(9A)	119.2(2)				

Symmetry: [1]*2-x,1-y,1-z*; [2]*-x,1-y,2-z*

Table S6. Torsion Angles for (**II**).

Atom	Atom	Atom	Atom	Angle [°]	Atom	Atom	Atom	Atom	Angle [°]
O(31A)	C(24A)	C(23A)	O(30A)	1.2(3)	C(22A)	C(21A)	C(27A)	O(29A)	170.5(2)
O(31A)	C(24A)	C(23A)	C(22A)	-178.9(2)	C(22A)	C(21A)	C(26A)	C(25A)	0.8(3)
O(32A)	C(25A)	C(24A)	O(31A)	-0.6(3)	C(2A)	N(1A)	C(14A)	C(9A)	-0.3(3)
O(32A)	C(25A)	C(24A)	C(23A)	-179.7(2)	C(2A)	N(1A)	C(14A)	C(13A)	179.8(2)
O(32A)	C(25A)	C(26A)	C(21A)	179.2(2)	C(2A)	C(7A)	C(6A)	C(5A)	0.8(4)
O(30A)	C(23A)	C(22A)	C(21A)	179.4(2)	C(2A)	C(3A)	C(4A)	C(5A)	1.0(4)
N(1C)	C(7C)	C(6C)	C(5C)	-180.0(2)	C(2B)	N(1B)	C(14B)	C(9B)	0.0(3)
N(1C)	C(2C)	C(3C)	C(4C)	179.2(2)	C(2B)	N(1B)	C(14B)	C(13B)	179.2(2)
N(1A)	C(2A)	C(7A)	N(8A)	-1.7(3)	C(2B)	C(7B)	C(6B)	C(5B)	0.4(4)
N(1A)	C(2A)	C(7A)	C(6A)	178.5(2)	C(2B)	C(3B)	C(4B)	C(5B)	0.3(4)

Atom	Atom	Atom	Atom	Angle [°]	Atom	Atom	Atom	Atom	Angle [°]
N(1A)	C(2A)	C(3A)	C(4A)	-179.4(2)	C(14A)	N(1A)	C(2A)	C(7A)	1.1(3)
N(1A)	C(14A)	C(9A)	N(8A)	0.0(3)	C(14A)	N(1A)	C(2A)	C(3A)	-179.3(2)
N(1A)	C(14A)	C(9A)	C(10A)	179.8(2)	C(14A)	C(9A)	C(10A)	C(11A)	0.4(4)
N(1A)	C(14A)	C(13A)	C(12A)	-179.9(2)	C(14A)	C(13A)	C(12A)	C(11A)	-0.2(4)
N(1B)	C(2B)	C(7B)	N(8B)	0.1(3)	C(2D)	N(1D)	C(7D)	C(2D)	-0.8(4)
N(1B)	C(2B)	C(7B)	C(6B)	-179.2(2)	C(2D)	N(1D)	C(7D)	C(6D)	179.3(2)
N(1B)	C(2B)	C(3B)	C(4B)	178.9(2)	C(2D)2	C(7D)	C(6D)	C(5D)	-1.1(4)
N(1B)	C(14B)	C(9B)	N(8B)	-0.6(3)	C(2D)	C(3D)	C(4D)	C(5D)	0.9(4)
N(1B)	C(14B)	C(9B)	C(10B)	179.6(2)	C(14B)	N(1B)	C(2B)	C(7B)	0.3(3)
N(1B)	C(14B)	C(13B)	C(12B)	-179.7(2)	C(14B)	N(1B)	C(2B)	C(3B)	-179.1(2)
N(8B)	C(7B)	C(6B)	C(5B)	-178.9(2)	C(14B)	C(9B)	C(10B)	C(11B)	0.1(4)
N(8B)	C(9B)	C(10B)	C(11B)	-179.6(2)	C(14B)	C(13B)	C(12B)	C(11B)	0.0(4)
N(1D)	C(7D)	C(6D)	C(5D)	178.8(2)	C(7B)	N(8B)	C(9B)	C(14B)	1.0(3)
N(1D)	C(2D)	C(3D)	C(4D)	179.7(2)	C(7B)	N(8B)	C(9B)	C(10B)	-179.2(2)
N(8A)	C(7A)	C(6A)	C(5A)	-179.1(2)	C(7B)	C(2B)	C(3B)	C(4B)	-0.6(4)
N(8A)	C(9A)	C(10A)	C(11A)	-179.8(2)	C(7B)	C(6B)	C(5B)	C(4B)	-0.7(4)
C(25A)	C(24A)	C(23A)	O(30A)	-179.7(2)	C(7A)	N(8A)	C(9A)	C(14A)	-0.4(3)
C(25A)	C(24A)	C(23A)	C(22A)	0.2(3)	C(7A)	N(8A)	C(9A)	C(10A)	179.7(2)
C(24A)	C(25A)	C(26A)	C(21A)	-1.0(3)	C(7A)	C(2A)	C(3A)	C(4A)	0.2(3)
C(24A)	C(23A)	C(22A)	C(21A)	-0.5(3)	C(7A)	C(6A)	C(5A)	C(4A)	0.4(4)
C(7C)	N(1C)	C(2C)	C(7C)	-0.8(3)	C(9A)	N(8A)	C(7A)	C(2A)	1.2(3)
C(7C)	N(1C)	C(2C)	C(3C)	178.82(19)	C(9A)	N(8A)	C(7A)	C(6A)	-179.0(2)
C(7C)1	C(2C)	C(3C)	C(4C)	-1.2(3)	C(9A)	C(14A)	C(13A)	C(12A)	0.2(4)
C(7C)	C(6C)	C(5C)	C(4C)	1.2(4)	C(9A)	C(10A)	C(11A)	C(12A)	-0.4(4)
C(27A)	C(21A)	C(26A)	C(25A)	179.8(2)	C(3A)	C(2A)	C(7A)	N(8A)	178.8(2)
C(27A)	C(21A)	C(22A)	C(23A)	-179.1(2)	C(3A)	C(2A)	C(7A)	C(6A)	-1.0(3)
C(2C)	N(1C)	C(7C)	C(2C)	0.8(3)	C(3A)	C(4A)	C(5A)	C(6A)	-1.3(4)
C(2C)	N(1C)	C(7C)	C(6C)	-178.9(2)	C(9B)	N(8B)	C(7B)	C(2B)	-0.8(3)
C(2C)1	C(7C)	C(6C)	C(5C)	0.3(3)	C(9B)	N(8B)	C(7B)	C(6B)	178.6(2)
C(2C)	C(3C)	C(4C)	C(5C)	-0.2(4)	C(9B)	C(14B)	C(13B)	C(12B)	-0.5(3)
C(7D)	N(1D)	C(2D)	C(7D)	0.8(4)	C(9B)	C(10B)	C(11B)	C(12B)	-0.5(4)
C(7D)	N(1D)	C(2D)	C(3D)	-178.8(2)	C(13B)	C(14B)	C(9B)	N(8B)	-179.9(2)
C(7D)2	C(2D)	C(3D)	C(4D)	0.1(4)	C(13B)	C(14B)	C(9B)	C(10B)	0.4(3)
C(7D)	C(6D)	C(5D)	C(4D)	0.2(4)	C(13B)	C(12B)	C(11B)	C(10B)	0.5(4)
C(26A)	C(25A)	C(24A)	O(31A)	179.7(2)	C(3B)	C(2B)	C(7B)	N(8B)	179.5(2)
C(26A)	C(25A)	C(24A)	C(23A)	0.5(3)	C(3B)	C(2B)	C(7B)	C(6B)	0.2(3)
C(26A)	C(21A)	C(27A)	O(28A)	172.0(2)	C(3B)	C(4B)	C(5B)	C(6B)	0.3(4)
C(26A)	C(21A)	C(27A)	O(29A)	-8.6(3)	C(13A)	C(14A)	C(9A)	N(8A)	179.9(2)
C(26A)	C(21A)	C(22A)	C(23A)	0.0(3)	C(13A)	C(14A)	C(9A)	C(10A)	-0.3(3)
C(22A)	C(21A)	C(27A)	O(28A)	-8.9(3)	C(13A)	C(12A)	C(11A)	C(10A)	0.3(4)

Symmetry: [1]*2-x,1-y,1-z*; [2]*-x,1-y,2-z*

Table S7. Short ring interactions (π–π) for structure (**I**).

Cg(I) → Cg(J)	Cg…Cg [Å]	Slippage [Å]	*symmetry*
Cg1 → Cg8	3.7211(8)	1.332	*1-x,1-y,1-z*
Cg1 → Cg9	4.8618(8)	3.436	*1-x,1-y,1-z*
Cg1 → Cg10	3.4691(6)	0.289	*1-x,1-y,1-z*
Cg1 → Cg11	4.1169(6)	2.265	*1-x,1-y,1-z*
Cg1 → Cg12	3.6212(6)	1.090	*1-x,1-y,1-z*
Cg1 → Cg19	4.2221(7)	2.604	*x,y,z*

Cg1 → Cg20	5.7877(8)	4.769	*x,y,z*
Cg1 → Cg21	3.6007(7)	1.431	*x,y,z*
Cg1 → Cg22	4.9285(6)	3.662	*x,y,z*
Cg1 → Cg23	3.7373(6)	1.733	*x,y,z*
Cg1 → Cg24	4.2026(6)	2.606	*x,y,z*
Cg2 → Cg7	4.8715(8)	3.482	*1-x,1-y,1-z*
Cg2 → Cg8	3.6601(8)	1.138	*1-x,1-y,1-z*
Cg2 → Cg10	4.1411(7)	2.297	*1-x,1-y,1-z*
Cg2 → Cg11	5.7732(7)	4.670	*1-x,1-y,1-z*
Cg2 → Cg12	4.8848(7)	3.482	*1-x,1-y,1-z*
Cg2 → Cg19	3.5620(7)	1.312	*x,y,z*
Cg2 → Cg20	4.1437(8)	2.588	*x,y,z*
Cg2 → Cg21	4.3608(8)	2.822	*x,y,z*
Cg2 → Cg22	3.6773(7)	1.681	*x,y,z*
Cg2 → Cg23	3.8025(7)	1.861	*x,y,z*
Cg2 → Cg24	3.5389(7)	1.315	*x,y,z*
Cg3 → Cg7	3.7093(8)	1.410	*1-x,1-y,1-z*
Cg3 → Cg8	5.5623(8)	4.791	*-x,1-y,1-z*
Cg3 → Cg8	5.0819(8)	3.763	*1-x,1-y,1-z*
Cg3 → Cg9	3.6344(8)	1.008	*1-x,1-y,1-z*
Cg3 → Cg10	4.2949(7)	2.591	*1-x,1-y,1-z*
Cg3 → Cg11	3.4767(7)	0.315	*1-x,1-y,1-z*
Cg3 → Cg12	3.7267(7)	1.410	*1-x,1-y,1-z*
Cg3 → Cg19	5.8183(8)	4.724	*x,y,z*
Cg3 → Cg21	4.2190(8)	2.602	*x,y,z*
Cg3 → Cg23	4.9360(7)	3.619	*x,y,z*
Cg3 → Cg24	5.8044(7)	4.726	*x,y,z*
Cg4 → Cg7	4.1234(6)	2.291	*1-x,1-y,1-z*
Cg4 → Cg8	3.4973(7)	0.279	*1-x,1-y,1-z*
Cg4 → Cg9	5.7698(7)	4.650	*1-x,1-y,1-z*
Cg4 → Cg10	3.6358(6)	1.116	*1-x,1-y,1-z*
Cg4 → Cg11	4.8787(6)	3.476	*1-x,1-y,1-z*
Cg4 → Cg12	4.1390(6)	2.291	*1-x,1-y,1-z*
Cg4 → Cg19	3.7191(6)	1.701	*x,y,z*
Cg4 → Cg20	4.8861(7)	3.652	*x,y,z*
Cg4 → Cg21	3.8212(7)	1.917	*x,y,z*
Cg4 → Cg22	4.1789(6)	2.598	*x,y,z*
Cg4 → Cg23	3.5786(6)	1.374	*x,y,z*
Cg4 → Cg24	3.6970(5)	1.704	*x,y,z*
Cg5 → Cg7	3.4628(6)	0.306	*1-x,1-y,1-z*
Cg5 → Cg8	4.3001(7)	2.553	*1-x,1-y,1-z*
Cg5 → Cg9	4.1240(7)	2.207	*1-x,1-y,1-z*
Cg5 → Cg10	3.7253(6)	1.387	*1-x,1-y,1-z*
Cg5 → Cg11	3.6221(6)	1.047	*1-x,1-y,1-z*
Cg5 → Cg12	3.4814(6)	0.305	*1-x,1-y,1-z*
Cg5 → Cg19	4.9470(6)	3.644	*x,y,z*
Cg5 → Cg21	3.7392(7)	1.764	*x,y,z*
Cg5 → Cg22	5.8113(6)	4.759	*x,y,z*
Cg5 → Cg23	4.2169(6)	2.602	*x,y,z*
Cg5 → Cg24	4.9306(6)	3.646	*x,y,z*
Cg6 → Cg7	3.6221(6)	1.081	*1-x,1-y,1-z*
Cg6 → Cg8	3.7396(7)	1.342	*1-x,1-y,1-z*
Cg6 → Cg9	4.8756(7)	3.426	*1-x,1-y,1-z*
Cg6 → Cg10	3.4888(6)	0.294	*1-x,1-y,1-z*

Cg6 → Cg11	4.1332(6)	2.255	*1-x,1-y,1-z*
Cg6 → Cg12	3.6399(5)	1.081	*1-x,1-y,1-z*
Cg6 → Cg19	4.2067(6)	2.597	*x,y,z*
Cg6 → Cg20	5.7767(7)	4.761	*x,y,z*
Cg6 → Cg21	3.5826(7)	1.433	*x,y,z*
Cg6 → Cg22	4.9154(6)	3.654	*x,y,z*
Cg6 → Cg23	3.7199(5)	1.728	*x,y,z*
Cg6 → Cg24	4.1873(5)	2.599	*x,y,z*
Cg7 → Cg1	3.6035(7)	1.073	*1-x,1-y,1-z*
Cg7 → Cg2	4.8716(8)	3.423	*1-x,1-y,1-z*
Cg7 → Cg3	3.7093(8)	1.336	*1-x,1-y,1-z*
Cg7 → Cg4	4.1235(6)	2.251	*1-x,1-y,1-z*
Cg7 → Cg5	3.4628(6)	0.263	*1-x,1-y,1-z*
Cg7 → Cg6	3.6222(6)	1.072	*1-x,1-y,1-z*
Cg7 → Cg7	4.1946(7)	2.529	*-x,1-y,1-z*
Cg7 → Cg8	5.7240(8)	4.666	*-x,1-y,1-z*
Cg7 → Cg9	3.6524(7)	1.495	*-x,1-y,1-z*
Cg7 → Cg10	4.8795(6)	3.568	*-x,1-y,1-z*
Cg7 → Cg11	3.7483(6)	1.704	*-x,1-y,1-z*
Cg7 → Cg12	4.1803(6)	2.530	*-x,1-y,1-z*
Cg8 → Cg1	3.7211(8)	1.431	*1-x,1-y,1-z*
Cg8 → Cg2	3.6601(8)	0.995	*1-x,1-y,1-z*
Cg8 → Cg3	5.5623(8)	4.805	*-x,1-y,1-z*
Cg8 → Cg3	5.0819(8)	3.782	*1-x,1-y,1-z*
Cg8 → Cg4	3.4973(7)	0.344	*1-x,1-y,1-z*
Cg8 → Cg5	4.3000(7)	2.610	*1-x,1-y,1-z*
Cg8 → Cg6	3.7397(7)	1.432	*1-x,1-y,1-z*
Cg8 → Cg7	5.7240(8)	4.591	*-x,1-y,1-z*
Cg8 → Cg9	4.1600(8)	2.474	*-x,1-y,1-z*
Cg8 → Cg11	4.8562(7)	3.486	*-x,1-y,1-z*
Cg8 → Cg12	5.7137(7)	4.592	*-x,1-y,1-z*
Cg9 → Cg1	4.8619(8)	3.452	*1-x,1-y,1-z*
Cg9 → Cg3	3.6345(8)	1.097	*1-x,1-y,1-z*
Cg9 → Cg4	5.7698(7)	4.641	*1-x,1-y,1-z*
Cg9 → Cg5	4.1240(7)	2.265	*1-x,1-y,1-z*
Cg9 → Cg6	4.8756(7)	3.452	*1-x,1-y,1-z*
Cg9 → Cg7	3.6524(7)	1.485	*-x,1-y,1-z*
Cg9 → Cg8	4.1600(8)	2.554	*-x,1-y,1-z*
Cg9 → Cg9	4.5043(9)	3.017	*-x,1-y,1-z*
Cg9 → Cg10	3.7307(7)	1.726	*-x,1-y,1-z*
Cg9 → Cg11	3.9282(7)	2.068	*-x,1-y,1-z*
Cg9 → Cg12	3.6360(7)	1.487	*-x,1-y,1-z*
Cg10 → Cg1	3.4692(6)	0.309	*1-x,1-y,1-z*
Cg10 → Cg2	4.1412(7)	2.192	*1-x,1-y,1-z*
Cg10 → Cg3	4.2950(7)	2.566	*1-x,1-y,1-z*
Cg10 → Cg4	3.6358(6)	1.033	*1-x,1-y,1-z*
Cg10 → Cg5	3.7253(6)	1.400	*1-x,1-y,1-z*
Cg10 → Cg6	3.4889(6)	0.309	*1-x,1-y,1-z*
Cg10 → Cg7	4.8795(6)	3.532	*-x,1-y,1-z*
Cg10 → Cg9	3.7307(7)	1.699	*-x,1-y,1-z*
Cg10 → Cg10	5.7324(6)	4.642	*-x,1-y,1-z*
Cg10 → Cg11	4.1747(6)	2.501	*-x,1-y,1-z*
Cg10 → Cg12	4.8673(6)	3.533	*-x,1-y,1-z*
Cg11 → Cg1	4.1169(6)	2.268	*1-x,1-y,1-z*

Cg11 → Cg2	5.7732(7)	4.629	*1-x,1-y,1-z*
Cg11 → Cg3	3.4768(7)	0.234	*1-x,1-y,1-z*
Cg11 → Cg4	4.8787(6)	3.455	*1-x,1-y,1-z*
Cg11 → Cg5	3.6221(6)	1.088	*1-x,1-y,1-z*
Cg11 → Cg6	4.1332(6)	2.268	*1-x,1-y,1-z*
Cg11 → Cg7	3.7483(6)	1.713	*-x,1-y,1-z*
Cg11 → Cg8	4.8562(7)	3.572	*-x,1-y,1-z*
Cg11 → Cg9	3.9282(7)	2.079	*-x,1-y,1-z*
Cg11 → Cg10	4.1748(6)	2.545	*-x,1-y,1-z*
Cg11 → Cg11	3.6523(6)	1.494	*-x,1-y,1-z*
Cg11 → Cg12	3.7323(5)	1.714	*-x,1-y,1-z*
Cg12 → Cg1	3.6212(6)	1.059	*1-x,1-y,1-z*
Cg12 → Cg2	4.8848(7)	3.408	*1-x,1-y,1-z*
Cg12 → Cg3	3.7268(7)	1.352	*1-x,1-y,1-z*
Cg12 → Cg4	4.1391(6)	2.236	*1-x,1-y,1-z*
Cg12 → Cg5	3.4814(6)	0.276	*1-x,1-y,1-z*
Cg12 → Cg6	3.6400(5)	1.059	*1-x,1-y,1-z*
Cg12 → Cg7	4.1803(6)	2.522	*-x,1-y,1-z*
Cg12 → Cg8	5.7136(7)	4.655	*-x,1-y,1-z*
Cg12 → Cg9	3.6360(7)	1.506	*-x,1-y,1-z*
Cg12 → Cg10	4.8673(6)	3.559	*-x,1-y,1-z*
Cg12 → Cg11	3.7322(5)	1.704	*-x,1-y,1-z*
Cg12 → Cg12	4.1661(5)	2.523	*-x,1-y,1-z*
Cg13 → Cg25	5.2352(9)	3.974	*x,y,z*
Cg13 → Cg26	5.1727(9)	3.969	*x,y,z*
Cg13 → Cg27	3.5722(9)	0.980	*x,y,z*
Cg14 → Cg26	3.8497(10)	1.764	*x,y,z*
Cg14 → Cg27	4.1061(10)	2.192	*x,y,z*
Cg15 → Cg25	3.8664(10)	1.583	*x,y,z*
Cg15 → Cg27	4.3729(10)	2.636	*x,y,z*
Cg16 → Cg26	4.4019(8)	2.799	*x,y,z*
Cg16 → Cg27	3.6616(8)	1.281	*x,y,z*
Cg17 → Cg25	4.4469(8)	2.739	*x,y,z*
Cg17 → Cg27	3.8126(8)	1.657	*x,y,z*
Cg18 → Cg25	5.2629(8)	3.964	*x,y,z*
Cg18 → Cg26	5.1997(8)	3.975	*x,y,z*
Cg18 → Cg27	3.5317(8)	0.973	*x,y,z*
Cg19 → Cg1	4.2221(7)	2.580	*x,y,z*
Cg19 → Cg2	3.5621(7)	1.301	*x,y,z*
Cg19 → Cg3	5.8182(8)	4.777	*x,y,z*
Cg19 → Cg4	3.7192(6)	1.661	*x,y,z*
Cg19 → Cg5	4.9471(6)	3.659	*x,y,z*
Cg19 → Cg6	4.2067(6)	2.580	*x,y,z*
Cg19 → Cg19	3.5831(7)	1.013	*1-x,2-y,-z*
Cg19 → Cg20	3.7552(7)	1.428	*1-x,2-y,-z*
Cg19 → Cg21	4.8175(8)	3.348	*1-x,2-y,-z*
Cg19 → Cg22	3.4777(6)	0.367	*1-x,2-y,-z*
Cg19 → Cg23	4.0828(6)	2.179	*1-x,2-y,-z*
Cg19 → Cg24	3.6080(6)	1.011	*1-x,2-y,-z*
Cg20 → Cg1	5.7877(8)	4.665	*x,y,z*
Cg20 → Cg2	4.1437(8)	2.463	*x,y,z*
Cg20 → Cg4	4.8861(7)	3.531	*x,y,z*
Cg20 → Cg6	5.7768(7)	4.666	*x,y,z*
Cg20 → Cg19	3.7553(7)	1.530	*1-x,2-y,-z*

Cg20 → Cg20	5.1550(8)	3.877	*1-x,2-y,-z*
Cg20 → Cg21	3.6427(8)	0.921	*1-x,2-y,-z*
Cg20 → Cg22	4.3586(7)	2.707	*1-x,2-y,-z*
Cg20 → Cg23	3.5067(7)	0.438	*1-x,2-y,-z*
Cg20 → Cg24	3.7794(7)	1.530	*1-x,2-y,-z*
Cg21 → Cg1	3.6006(7)	1.367	*x,y,z*
Cg21 → Cg2	4.3607(8)	2.790	*x,y,z*
Cg21 → Cg3	4.2188(8)	2.674	*x,y,z*
Cg21 → Cg4	3.8211(7)	1.857	*x,y,z*
Cg21 → Cg5	3.7391(7)	1.769	*x,y,z*
Cg21 → Cg6	3.5825(7)	1.368	*x,y,z*
Cg21 → Cg19	4.8176(8)	3.415	*1-x,2-y,-z*
Cg21 → Cg20	3.6427(8)	1.070	*1-x,2-y,-z*
Cg21 → Cg22	4.1023(7)	2.230	*1-x,2-y,-z*
Cg21 → Cg23	5.7164(7)	4.603	*1-x,2-y,-z*
Cg21 → Cg24	4.8361(7)	3.415	*1-x,2-y,-z*
Cg22 → Cg1	4.9285(6)	3.599	*x,y,z*
Cg22 → Cg2	3.6774(7)	1.612	*x,y,z*
Cg22 → Cg4	4.1790(6)	2.519	*x,y,z*
Cg22 → Cg5	5.8114(6)	4.733	*x,y,z*
Cg22 → Cg6	4.9155(6)	3.600	*x,y,z*
Cg22 → Cg19	3.4777(6)	0.410	*1-x,2-y,-z*
Cg22 → Cg20	4.3586(7)	2.659	*1-x,2-y,-z*
Cg22 → Cg21	4.1022(7)	2.113	*1-x,2-y,-z*
Cg22 → Cg22	3.7666(6)	1.496	*1-x,2-y,-z*
Cg22 → Cg23	3.6180(6)	0.964	*1-x,2-y,-z*
Cg22 → Cg24	3.5036(5)	0.408	*1-x,2-y,-z*
Cg23 → Cg1	3.7373(6)	1.713	*x,y,z*
Cg23 → Cg2	3.8025(7)	1.853	*x,y,z*
Cg23 → Cg3	4.9359(7)	3.693	*x,y,z*
Cg23 → Cg4	3.5786(6)	1.337	*x,y,z*
Cg23 → Cg5	4.2169(6)	2.631	*x,y,z*
Cg23 → Cg6	3.7199(5)	1.714	*x,y,z*
Cg23 → Cg19	4.0829(6)	2.215	*1-x,2-y,-z*
Cg23 → Cg20	3.5068(7)	0.322	*1-x,2-y,-z*
Cg23 → Cg21	5.7163(7)	4.573	*1-x,2-y,-z*
Cg23 → Cg22	3.6181(6)	1.044	*1-x,2-y,-z*
Cg23 → Cg23	4.8308(6)	3.399	*1-x,2-y,-z*
Cg23 → Cg24	4.1048(6)	2.215	*1-x,2-y,-z*
Cg24 → Cg1	4.2025(6)	2.574	*x,y,z*
Cg24 → Cg2	3.5388(7)	1.304	*x,y,z*
Cg24 → Cg3	5.8042(7)	4.770	*x,y,z*
Cg24 → Cg4	3.6970(5)	1.658	*x,y,z*
Cg24 → Cg5	4.9305(6)	3.653	*x,y,z*
Cg24 → Cg6	4.1872(5)	2.575	*x,y,z*
Cg24 → Cg19	3.6081(6)	1.003	*1-x,2-y,-z*
Cg24 → Cg20	3.7794(7)	1.435	*1-x,2-y,-z*
Cg24 → Cg21	4.8362(7)	3.340	*1-x,2-y,-z*
Cg24 → Cg22	3.5037(5)	0.368	*1-x,2-y,-z*
Cg24 → Cg23	4.1049(6)	2.170	*1-x,2-y,-z*
Cg24 → Cg24	3.6330(5)	1.002	*1-x,2-y,-z*
Cg25 → Cg13	5.2352(9)	4.111	*x,y,z*
Cg25 → Cg15	3.8664(10)	1.890	*x,y,z*
Cg25 → Cg17	4.4469(8)	2.967	*x,y,z*

Cg25 → Cg18	5.2629(8)	4.112	*x,y,z*
Cg26 → Cg13	5.1727(9)	3.831	*x,y,z*
Cg26 → Cg14	3.8498(10)	1.751	*x,y,z*
Cg26 → Cg16	4.4019(8)	2.727	*x,y,z*
Cg26 → Cg18	5.1997(8)	3.828	*x,y,z*
Cg27 → Cg13	3.5723(9)	1.124	*x,y,z*
Cg27 → Cg14	4.1060(10)	2.258	*x,y,z*
Cg27 → Cg15	4.3729(10)	2.926	*x,y,z*
Cg27 → Cg16	3.6616(8)	1.342	*x,y,z*
Cg27 → Cg17	3.8126(8)	1.883	*x,y,z*
Cg27 → Cg18	3.5317(8)	1.124	*x,y,z*

Cg-Cg - Distance between ring Centroids (Ang.); Slippage - Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang).

Table S8. Contacts X–Y…Cg for structure (**I**).

X-Y…Cg	**Y…Cg [Å]**	**X…Cg [Å]**	**X-Y…Cg [°]**	***symmetry***
C27B-O29B…Cg13	3.4572(12)	3.9740(15)	105.76(8)	*x,y,z*
C27B-O29B…Cg16	3.4480(11)	3.5819(15)	86.08(8)	*x,y,z*
C27B-O29B…Cg18	3.4983(11)	4.0103(14)	105.61(8)	*x,y,z*
C27C-O29C…Cg14	3.6866(13)	3.5882(16)	75.74(8)	*x,y,z*
C4A-H4A…Cg27	2.96	3.5942(17)	125	*1+x,1+y,z*
C11B-H11B…Cg25	2.90	3.5746(17)	129	*1-x,1-y,1-z*
C11D-H11D…Cg26	2.86	3.5507(17)	131	*x,y,z*

Table S9. Definitions of ring centroids (Cg) for structure (**I**).

Cg	**Ring size**	**Atoms defining the ring**
Cg1	6	N1A, N8A, C2A, C7A, C9A, C14A
Cg2	6	C2A, C3A, C4A, C5A, C6A, C7A
Cg3	6	C9A, C10A, C11A, C12A, C13A, C14A
Cg4	10	N1A, N8A, C2A, C3A, C4A, C5A, C6A, C7A, C9A, C14A
Cg5	10	N1A, N8A, C2A, C7A, C9A, C10A, C11A, C12A, C13A, C14A
Cg6	14	N1A, N8A, C2A, C3A, C4A, C5A, C6A, C7A, C9A, C10A, C11A, C12A, C13A, C14A
Cg7	6	N1B, N8B, C2B, C7B, C9B, C14B
Cg8	6	C2B, C3B, C4B, C5B, C6B, C7B
Cg9	6	C9B, C10B, C11B, C12B, C13B, C14B
Cg10	10	N1B, N8B, C2B, C3B, C4B, C5B, C6B, C7B, C9B, C14B
Cg11	10	N1B, N8B, C2B, C7B, C9B, C10B, C11B, C12B, C13B, C14B
Cg12	14	N1B, N8B, C2B, C3B, C4B, C5B, C6B, C7B, C9B, C10B, C11B, C12B, C13B, C14B
Cg13	6	N1C, N8C, C2C, C7C, C9C, C14C
Cg14	6	C2C, C3C, C4C, C5C, C6C, C7C
Cg15	6	C9C, C10C, C11C, C12C, C13C, C14C
Cg16	10	N1C, N8C, C2C, C3C, C4C, C5C, C6C, C7C, C9C, C14C
Cg17	10	N1C, N8C, C2C, C7C, C9C, C10C, C11C, C12C, C13C, C14C
Cg18	14	N1C, N8C, C2C, C3C, C4C, C5C, C6C, C7C, C9C, C10C, C11C, C12C, C13C, C14C
Cg19	6	N1D, N8D, C2D, C7D, C9D, C14D
Cg20	6	C2D, C3D, C4D, C5D, C6D, C7D
Cg21	6	C9D, C10D, C11D, C12D, C13D, C14D
Cg22	10	N1D, N8D, C2D, C3D, C4D, C5D, C6D, C7D, C9D, C14D
Cg23	10	N1D, N8D, C2D, C7D, C9D, C10D, C11D, C12D, C13D, C14D
Cg24	14	N1D, N8D, C2D, C3D, C4D, C5D, C6D, C7D, C9D, C10D, C11D, C12D, C13D, C14D

Cg25	6	C21A, C22A, C23A, C24A, C25A, C26A
Cg26	6	C21B, C22B, C23B, C24B, C25B, C26B
Cg27	6	C21C, C22C, C23C, C24C, C25C, C26C

Table S10. Short ring interactions (π–π) for structure (**II**).

Cg(I) → Cg(J)	**Cg···Cg [Å]**	**Slippage [Å]**	***symmetry***
Cg1 → Cg1	3.5710(12)	1.309	*2-x,-y,-z*
Cg1 → Cg2	4.8747(14)	3.566	*2-x,-y,-z*
Cg1 → Cg3	3.5974(15)	1.378	*2-x,-y,-z*
Cg1 → Cg4	4.1099(12)	2.418	*2-x,-y,-z*
Cg1 → Cg5	3.3834(12)	0.638	*2-x,-y,-z*
Cg1 → Cg6	3.5711(11)	1.308	*2-x,-y,-z*
Cg1 → Cg19	3.6495(13)	1.474	*1+x,y,z*
Cg1 → Cg19	3.6495(13)	1.474	*1-x,1-y,-z*
Cg1 → Cg20	3.9680(15)	2.081	*1+x,y,z*
Cg1 → Cg20	4.7018(13)	3.351	*1-x,1-y,-z*
Cg1 → Cg21	4.7018(13)	3.351	*1+x,y,z*
Cg1 → Cg21	3.9680(15)	2.081	*1-x,1-y,-z*
Cg1 → Cg22	3.6252(12)	1.362	*1+x,y,z*
Cg1 → Cg22	4.0414(11)	2.308	*1-x,1-y,-z*
Cg1 → Cg23	4.0414(11)	2.308	*1+x,y,z*
Cg1 → Cg23	3.6252(12)	1.362	*1-x,1-y,-z*
Cg1 → Cg24	3.6495(11)	1.474	*1+x,y,z*
Cg1 → Cg24	3.6495(11)	1.474	*1-x,1-y,-z*
Cg2 → Cg1	4.8747(14)	3.555	*2-x,-y,-z*
Cg2 → Cg3	3.5715(15)	1.278	*2-x,-y,-z*
Cg2 → Cg4	5.7912(13)	4.734	*2-x,-y,-z*
Cg2 → Cg5	4.1021(13)	2.388	*2-x,-y,-z*
Cg2 → Cg6	4.8752(13)	3.555	*2-x,-y,-z*
Cg2 → Cg19	3.9762(15)	2.126	*1+x,y,z*
Cg2 → Cg19	3.9762(15)	2.126	*1-x,1-y,-z*
Cg2 → Cg20	5.4245(16)	4.229	*1+x,y,z*
Cg2 → Cg20	3.6620(15)	1.539	*1-x,1-y,-z*
Cg2 → Cg21	3.6620(15)	1.539	*1+x,y,z*
Cg2 → Cg21	5.4245(16)	4.229	*1-x,1-y,-z*
Cg2 → Cg22	4.6110(14)	3.137	*1+x,y,z*
Cg2 → Cg22	3.6327(13)	1.428	*1-x,1-y,-z*
Cg2 → Cg23	3.6327(13)	1.428	*1+x,y,z*
Cg2 → Cg23	4.6110(14)	3.137	*1-x,1-y,-z*
Cg2 → Cg24	3.9762(13)	2.126	*1+x,y,z*
Cg2 → Cg24	3.9762(13)	2.126	*1-x,1-y,-z*
Cg3 → Cg1	3.5975(15)	1.386	*2-x,-y,-z*
Cg3 → Cg2	3.5715(15)	1.310	*2-x,-y,-z*
Cg3 → Cg3	4.9318(17)	3.648	*2-x,-y,-z*
Cg3 → Cg4	3.3835(14)	0.646	*2-x,-y,-z*
Cg3 → Cg5	4.1552(15)	2.499	*2-x,-y,-z*
Cg3 → Cg6	3.5971(14)	1.383	*2-x,-y,-z*
Cg3 → Cg19	4.6938(14)	3.303	*1+x,y,z*
Cg3 → Cg19	4.6938(14)	3.303	*1-x,1-y,-z*
Cg3 → Cg20	3.6431(15)	1.374	*1+x,y,z*
Cg3 → Cg21	3.6431(15)	1.374	*1-x,1-y,-z*
Cg3 → Cg22	4.0285(13)	2.229	*1+x,y,z*

Cg3 → Cg22	5.5382(14)	4.437	*1-x,1-y,-z*
Cg3 → Cg23	5.5382(14)	4.437	*1+x,y,z*
Cg3 → Cg23	4.0285(13)	2.229	*1-x,1-y,-z*
Cg3 → Cg24	4.6938(13)	3.303	*1+x,y,z*
Cg3 → Cg24	4.6938(13)	3.303	*1-x,1-y,-z*
Cg4 → Cg1	4.1099(12)	2.411	*2-x,-y,-z*
Cg4 → Cg2	5.7912(13)	4.739	*2-x,-y,-z*
Cg4 → Cg3	3.3834(14)	0.604	*2-x,-y,-z*
Cg4 → Cg4	4.8853(11)	3.576	*2-x,-y,-z*
Cg4 → Cg5	3.5712(11)	1.294	*2-x,-y,-z*
Cg4 → Cg6	4.1102(10)	2.411	*2-x,-y,-z*
Cg4 → Cg19	3.6295(12)	1.398	*1+x,y,z*
Cg4 → Cg19	3.6295(12)	1.398	*1-x,1-y,-z*
Cg4 → Cg20	4.6074(14)	3.121	*1+x,y,z*
Cg4 → Cg20	4.0413(12)	2.319	*1-x,1-y,-z*
Cg4 → Cg21	4.0413(12)	2.319	*1+x,y,z*
Cg4 → Cg21	4.6074(14)	3.121	*1-x,1-y,-z*
Cg4 → Cg22	3.9784(12)	2.114	*1+x,y,z*
Cg4 → Cg22	3.6546(11)	1.509	*1-x,1-y,-z*
Cg4 → Cg23	3.6546(11)	1.509	*1+x,y,z*
Cg4 → Cg23	3.9784(12)	2.114	*1-x,1-y,-z*
Cg4 → Cg24	3.6295(10)	1.398	*1+x,y,z*
Cg4 → Cg24	3.6295(10)	1.398	*1-x,1-y,-z*
Cg5 → Cg1	3.3834(12)	0.644	*2-x,-y,-z*
Cg5 → Cg2	4.1021(13)	2.405	*2-x,-y,-z*
Cg5 → Cg3	4.1552(15)	2.497	*2-x,-y,-z*
Cg5 → Cg4	3.5713(11)	1.309	*2-x,-y,-z*
Cg5 → Cg5	3.6020(12)	1.393	*2-x,-y,-z*
Cg5 → Cg6	3.3833(11)	0.640	*2-x,-y,-z*
Cg5 → Cg19	4.0378(12)	2.274	*1+x,y,z*
Cg5 → Cg19	4.0378(12)	2.274	*1-x,1-y,-z*
Cg5 → Cg20	3.6199(13)	1.306	*1+x,y,z*
Cg5 → Cg20	5.5423(13)	4.455	*1-x,1-y,-z*
Cg5 → Cg21	5.5423(13)	4.455	*1+x,y,z*
Cg5 → Cg21	3.6199(13)	1.306	*1-x,1-y,-z*
Cg5 → Cg22	3.6465(11)	1.424	*1+x,y,z*
Cg5 → Cg22	4.7061(11)	3.340	*1-x,1-y,-z*
Cg5 → Cg23	4.7061(11)	3.340	*1+x,y,z*
Cg5 → Cg23	3.6465(11)	1.424	*1-x,1-y,-z*
Cg5 → Cg24	4.0378(10)	2.274	*1+x,y,z*
Cg5 → Cg24	4.0378(10)	2.274	*1-x,1-y,-z*
Cg6 → Cg1	3.5712(11)	1.300	*2-x,-y,-z*
Cg6 → Cg2	4.8752(13)	3.563	*2-x,-y,-z*
Cg6 → Cg3	3.5971(14)	1.368	*2-x,-y,-z*
Cg6 → Cg4	4.1103(10)	2.414	*2-x,-y,-z*
Cg6 → Cg5	3.3834(11)	0.618	*2-x,-y,-z*
Cg6 → Cg6	3.5713(10)	1.299	*2-x,-y,-z*
Cg6 → Cg19	3.6501(11)	1.463	*1+x,y,z*
Cg6 → Cg19	3.6501(11)	1.463	*1-x,1-y,-z*
Cg6 → Cg20	3.9688(13)	2.074	*1+x,y,z*
Cg6 → Cg20	4.7020(12)	3.345	*1-x,1-y,-z*
Cg6 → Cg21	4.7020(12)	3.345	*1+x,y,z*
Cg6 → Cg21	3.9688(13)	2.074	*1-x,1-y,-z*
Cg6 → Cg22	3.6259(11)	1.351	*1+x,y,z*

Cg6 → Cg22	4.0417(10)	2.300	*1-x,1-y,-z*
Cg6 → Cg23	4.0417(10)	2.300	*1+x,y,z*
Cg6 → Cg23	3.6259(11)	1.351	*1-x,1-y,-z*
Cg6 → Cg24	3.6501(9)	1.463	*1+x,y,z*
Cg6 → Cg24	3.6501(9)	1.463	*1-x,1-y,-z*
Cg7 → Cg7	3.5163(12)	0.965	*-x,2-y,1-z*
Cg7 → Cg8	4.0849(15)	2.256	*-x,2-y,1-z*
Cg7 → Cg9	4.4107(15)	2.818	*-x,2-y,1-z*
Cg7 → Cg10	3.6267(12)	1.274	*-x,2-y,1-z*
Cg7 → Cg11	3.8125(12)	1.749	*-x,2-y,1-z*
Cg7 → Cg12	3.5294(11)	0.961	*-x,2-y,1-z*
Cg7 → Cg13	3.6749(12)	1.654	*x,y,z*
Cg7 → Cg13	3.6753(12)	1.655	*-x,1-y,1-z*
Cg7 → Cg14	3.7698(13)	1.820	*x,y,z*
Cg7 → Cg14	4.9039(14)	3.662	*-x,1-y,1-z*
Cg7 → Cg15	4.9037(14)	3.662	*x,y,z*
Cg7 → Cg15	3.7699(13)	1.820	*-x,1-y,1-z*
Cg7 → Cg16	3.5295(11)	1.274	*x,y,z*
Cg7 → Cg16	4.1713(12)	2.588	*-x,1-y,1-z*
Cg7 → Cg17	4.1711(12)	2.588	*x,y,z*
Cg7 → Cg17	3.5297(11)	1.274	*-x,1-y,1-z*
Cg7 → Cg18	3.6750(11)	1.654	*x,y,z*
Cg7 → Cg18	3.6752(11)	1.655	*-x,1-y,1-z*
Cg8 → Cg7	4.0850(15)	2.315	*-x,2-y,1-z*
Cg8 → Cg8	5.6745(17)	4.585	*-x,2-y,1-z*
Cg8 → Cg9	3.5484(16)	0.933	*-x,2-y,1-z*
Cg8 → Cg10	4.8067(14)	3.441	*-x,2-y,1-z*
Cg8 → Cg11	3.6377(14)	1.305	*-x,2-y,1-z*
Cg8 → Cg12	4.0966(14)	2.314	*-x,2-y,1-z*
Cg8 → Cg13	4.8798(15)	3.571	*x,y,z*
Cg8 → Cg13	4.8802(15)	3.571	*-x,1-y,1-z*
Cg8 → Cg14	3.6476(15)	1.557	*x,y,z*
Cg8 → Cg15	3.6478(15)	1.558	*-x,1-y,1-z*
Cg8 → Cg16	4.1383(14)	2.481	*x,y,z*
Cg8 → Cg16	5.7748(14)	4.711	*-x,1-y,1-z*
Cg8 → Cg17	5.7746(14)	4.711	*x,y,z*
Cg8 → Cg17	4.1385(14)	2.481	*-x,1-y,1-z*
Cg8 → Cg18	4.8799(14)	3.571	*x,y,z*
Cg8 → Cg18	4.8801(14)	3.571	*-x,1-y,1-z*
Cg9 → Cg7	4.4106(15)	2.840	*-x,2-y,1-z*
Cg9 → Cg8	3.5483(16)	0.962	*-x,2-y,1-z*
Cg9 → Cg10	3.8230(14)	1.754	*-x,2-y,1-z*
Cg9 → Cg11	5.2200(14)	3.984	*-x,2-y,1-z*
Cg9 → Cg12	4.4209(14)	2.839	*-x,2-y,1-z*
Cg9 → Cg13	3.7647(14)	1.847	*x,y,z*
Cg9 → Cg13	3.7650(14)	1.847	*-x,1-y,1-z*
Cg9 → Cg14	5.1076(15)	3.884	*x,y,z*
Cg9 → Cg14	3.6752(14)	1.727	*-x,1-y,1-z*
Cg9 → Cg15	3.6750(14)	1.727	*x,y,z*
Cg9 → Cg15	5.1077(15)	3.884	*-x,1-y,1-z*
Cg9 → Cg16	4.3315(14)	2.807	*x,y,z*
Cg9 → Cg16	3.5257(13)	1.338	*-x,1-y,1-z*
Cg9 → Cg17	3.5255(13)	1.337	*x,y,z*
Cg9 → Cg17	4.3316(14)	2.807	*-x,1-y,1-z*

Cg9 → Cg18	3.7647(13)	1.847	*x,y,z*
Cg9 → Cg18	3.7649(13)	1.847	*-x,1-y,1-z*
Cg10 → Cg7	3.6266(12)	1.297	*-x,2-y,1-z*
Cg10 → Cg8	4.8066(14)	3.411	*-x,2-y,1-z*
Cg10 → Cg9	3.8231(14)	1.703	*-x,2-y,1-z*
Cg10 → Cg10	4.0954(12)	2.300	*-x,2-y,1-z*
Cg10 → Cg11	3.5347(12)	0.947	*-x,2-y,1-z*
Cg10 → Cg12	3.6395(11)	1.294	*-x,2-y,1-z*
Cg10 → Cg13	4.1568(12)	2.540	*x,y,z*
Cg10 → Cg13	4.1572(12)	2.540	*-x,1-y,1-z*
Cg10 → Cg14	3.5135(12)	1.243	*x,y,z*
Cg10 → Cg14	5.7848(13)	4.754	*-x,1-y,1-z*
Cg10 → Cg15	5.7846(13)	4.754	*x,y,z*
Cg10 → Cg15	3.5137(12)	1.243	*-x,1-y,1-z*
Cg10 → Cg16	3.6599(11)	1.606	*x,y,z*
Cg10 → Cg16	4.9002(11)	3.628	*-x,1-y,1-z*
Cg10 → Cg17	4.9000(11)	3.628	*x,y,z*
Cg10 → Cg17	3.6601(11)	1.606	*-x,1-y,1-z*
Cg10 → Cg18	4.1569(10)	2.540	*x,y,z*
Cg10 → Cg18	4.1571(10)	2.540	*-x,1-y,1-z*
Cg11 → Cg7	3.8124(12)	1.761	*-x,2-y,1-z*
Cg11 → Cg8	3.6376(14)	1.251	*-x,2-y,1-z*
Cg11 → Cg9	5.2200(14)	3.976	*-x,2-y,1-z*
Cg11 → Cg10	3.5347(12)	0.964	*-x,2-y,1-z*
Cg11 → Cg11	4.4197(12)	2.845	*-x,2-y,1-z*
Cg11 → Cg12	3.8245(11)	1.759	*-x,2-y,1-z*
Cg11 → Cg13	3.5271(12)	1.308	*x,y,z*
Cg11 → Cg13	3.5275(12)	1.308	*-x,1-y,1-z*
Cg11 → Cg14	4.3339(13)	2.802	*x,y,z*
Cg11 → Cg14	4.1650(13)	2.610	*-x,1-y,1-z*
Cg11 → Cg15	4.1648(13)	2.610	*x,y,z*
Cg11 → Cg15	4.3341(13)	2.802	*-x,1-y,1-z*
Cg11 → Cg16	3.7719(11)	1.843	*x,y,z*
Cg11 → Cg16	3.6744(11)	1.694	*-x,1-y,1-z*
Cg11 → Cg17	3.6741(11)	1.693	*x,y,z*
Cg11 → Cg17	3.7721(11)	1.843	*-x,1-y,1-z*
Cg11 → Cg18	3.5272(10)	1.308	*x,y,z*
Cg11 → Cg18	3.5274(10)	1.308	*-x,1-y,1-z*
Cg12 → Cg7	3.5294(11)	0.956	*-x,2-y,1-z*
Cg12 → Cg8	4.0966(14)	2.264	*-x,2-y,1-z*
Cg12 → Cg9	4.4210(14)	2.806	*-x,2-y,1-z*
Cg12 → Cg10	3.6396(11)	1.278	*-x,2-y,1-z*
Cg12 → Cg11	3.8246(11)	1.736	*-x,2-y,1-z*
Cg12 → Cg12	3.5426(10)	0.952	*-x,2-y,1-z*
Cg12 → Cg13	3.6632(11)	1.649	*x,y,z*
Cg12 → Cg13	3.6636(11)	1.650	*-x,1-y,1-z*
Cg12 → Cg14	3.7580(12)	1.829	*x,y,z*
Cg12 → Cg14	4.8954(12)	3.653	*-x,1-y,1-z*
Cg12 → Cg15	4.8952(12)	3.653	*x,y,z*
Cg12 → Cg15	3.7581(12)	1.829	*-x,1-y,1-z*
Cg12 → Cg16	3.5171(10)	1.277	*x,y,z*
Cg12 → Cg16	4.1612(10)	2.580	*-x,1-y,1-z*
Cg12 → Cg17	4.1610(10)	2.580	*x,y,z*
Cg12 → Cg17	3.5173(10)	1.277	*-x,1-y,1-z*

Cg12 → Cg18	3.6633(9)	1.650	*x,y,z*
Cg12 → Cg18	3.6635(9)	1.650	*-x,1-y,1-z*
Cg13 → Cg7	3.6750(12)	1.562	*x,y,z*
Cg13 → Cg7	3.6753(12)	1.562	*-x,1-y,1-z*
Cg13 → Cg8	4.8800(15)	3.579	*x,y,z*
Cg13 → Cg8	4.8802(15)	3.579	*-x,1-y,1-z*
Cg13 → Cg9	3.7647(14)	1.811	*x,y,z*
Cg13 → Cg9	3.7649(14)	1.811	*-x,1-y,1-z*
Cg13 → Cg10	4.1570(12)	2.502	*x,y,z*
Cg13 → Cg10	4.1572(12)	2.502	*-x,1-y,1-z*
Cg13 → Cg11	3.5272(12)	1.211	*x,y,z*
Cg13 → Cg11	3.5274(12)	1.211	*-x,1-y,1-z*
Cg13 → Cg12	3.6633(11)	1.566	*x,y,z*
Cg13 → Cg12	3.6636(11)	1.566	*-x,1-y,1-z*
Cg14 → Cg7	3.7698(13)	1.744	*x,y,z*
Cg14 → Cg7	4.9039(14)	3.578	*-x,1-y,1-z*
Cg14 → Cg8	3.6477(15)	1.466	*x,y,z*
Cg14 → Cg9	5.1075(15)	3.891	*x,y,z*
Cg14 → Cg9	3.6752(14)	1.575	*-x,1-y,1-z*
Cg14 → Cg10	3.5135(12)	1.093	*x,y,z*
Cg14 → Cg10	5.7848(13)	4.716	*-x,1-y,1-z*
Cg14 → Cg11	4.3339(13)	2.780	*x,y,z*
Cg14 → Cg11	4.1649(13)	2.493	*-x,1-y,1-z*
Cg14 → Cg12	3.7580(12)	1.746	*x,y,z*
Cg14 → Cg12	4.8955(12)	3.580	*-x,1-y,1-z*
Cg15 → Cg7	4.9038(14)	3.579	*x,y,z*
Cg15 → Cg7	3.7699(13)	1.744	*-x,1-y,1-z*
Cg15 → Cg8	3.6478(15)	1.466	*-x,1-y,1-z*
Cg15 → Cg9	3.6750(14)	1.576	*x,y,z*
Cg15 → Cg9	5.1076(15)	3.890	*-x,1-y,1-z*
Cg15 → Cg10	5.7847(13)	4.716	*x,y,z*
Cg15 → Cg10	3.5136(12)	1.093	*-x,1-y,1-z*
Cg15 → Cg11	4.1648(13)	2.494	*x,y,z*
Cg15 → Cg11	4.3341(13)	2.780	*-x,1-y,1-z*
Cg15 → Cg12	4.8954(12)	3.581	*x,y,z*
Cg15 → Cg12	3.7581(12)	1.746	*-x,1-y,1-z*
Cg16 → Cg7	3.5295(11)	1.149	*x,y,z*
Cg16 → Cg7	4.1714(12)	2.502	*-x,1-y,1-z*
Cg16 → Cg8	4.1384(14)	2.456	*x,y,z*
Cg16 → Cg8	5.7748(14)	4.717	*-x,1-y,1-z*
Cg16 → Cg9	4.3315(14)	2.796	*x,y,z*
Cg16 → Cg9	3.5257(13)	1.218	*-x,1-y,1-z*
Cg16 → Cg10	3.6599(11)	1.514	*x,y,z*
Cg16 → Cg10	4.9002(11)	3.593	*-x,1-y,1-z*
Cg16 → Cg11	3.7720(11)	1.787	*x,y,z*
Cg16 → Cg11	3.6743(11)	1.569	*-x,1-y,1-z*
Cg16 → Cg12	3.5172(10)	1.153	*x,y,z*
Cg16 → Cg12	4.1613(10)	2.505	*-x,1-y,1-z*
Cg17 → Cg7	4.1712(12)	2.502	*x,y,z*
Cg17 → Cg7	3.5297(11)	1.149	*-x,1-y,1-z*
Cg17 → Cg8	5.7747(14)	4.717	*x,y,z*
Cg17 → Cg8	4.1385(14)	2.456	*-x,1-y,1-z*
Cg17 → Cg9	3.5255(13)	1.218	*x,y,z*
Cg17 → Cg9	4.3316(14)	2.796	*-x,1-y,1-z*

Cg17 → Cg10	4.9001(11)	3.593	*x,y,z*
Cg17 → Cg10	3.6601(11)	1.514	*-x,1-y,1-z*
Cg17 → Cg11	3.6742(11)	1.569	*x,y,z*
Cg17 → Cg11	3.7721(11)	1.786	*-x,1-y,1-z*
Cg17 → Cg12	4.1611(10)	2.505	*x,y,z*
Cg17 → Cg12	3.5173(10)	1.153	*-x,1-y,1-z*
Cg18 → Cg7	3.6751(11)	1.531	*x,y,z*
Cg18 → Cg7	3.6752(11)	1.531	*-x,1-y,1-z*
Cg18 → Cg8	4.8800(14)	3.563	*x,y,z*
Cg18 → Cg8	4.8801(14)	3.563	*-x,1-y,1-z*
Cg18 → Cg9	3.7648(13)	1.790	*x,y,z*
Cg18 → Cg9	3.7648(13)	1.790	*-x,1-y,1-z*
Cg18 → Cg10	4.1570(10)	2.481	*x,y,z*
Cg18 → Cg10	4.1571(10)	2.481	*-x,1-y,1-z*
Cg18 → Cg11	3.5273(10)	1.175	*x,y,z*
Cg18 → Cg11	3.5273(10)	1.175	*-x,1-y,1-z*
Cg18 → Cg12	3.6634(9)	1.535	*x,y,z*
Cg18 → Cg12	3.6635(9)	1.535	*-x,1-y,1-z*
Cg19 → Cg1	3.6495(13)	1.512	*-1+x,y,z*
Cg19 → Cg1	3.6494(13)	1.512	*1-x,1-y,-z*
Cg19 → Cg2	3.9762(15)	2.238	*-1+x,y,z*
Cg19 → Cg2	3.9762(15)	2.238	*1-x,1-y,-z*
Cg19 → Cg3	4.6937(14)	3.283	*-1+x,y,z*
Cg19 → Cg3	4.6937(14)	3.283	*1-x,1-y,-z*
Cg19 → Cg4	3.6294(12)	1.503	*-1+x,y,z*
Cg19 → Cg4	3.6294(12)	1.503	*1-x,1-y,-z*
Cg19 → Cg5	4.0377(12)	2.271	*-1+x,y,z*
Cg19 → Cg5	4.0377(12)	2.271	*1-x,1-y,-z*
Cg19 → Cg6	3.6501(11)	1.515	*-1+x,y,z*
Cg19 → Cg6	3.6501(11)	1.515	*1-x,1-y,-z*
Cg20 → Cg1	3.9679(15)	2.155	*-1+x,y,z*
Cg20 → Cg1	4.7017(13)	3.294	*1-x,1-y,-z*
Cg20 → Cg2	5.4245(16)	4.322	*-1+x,y,z*
Cg20 → Cg2	3.6619(15)	1.585	*1-x,1-y,-z*
Cg20 → Cg3	3.6431(15)	1.349	*-1+x,y,z*
Cg20 → Cg4	4.6073(14)	3.211	*-1+x,y,z*
Cg20 → Cg4	4.0412(12)	2.293	*1-x,1-y,-z*
Cg20 → Cg5	3.6199(13)	1.352	*-1+x,y,z*
Cg20 → Cg5	5.5423(13)	4.391	*1-x,1-y,-z*
Cg20 → Cg6	3.9689(13)	2.158	*-1+x,y,z*
Cg20 → Cg6	4.7020(12)	3.295	*1-x,1-y,-z*
Cg21 → Cg1	4.7018(13)	3.294	*-1+x,y,z*
Cg21 → Cg1	3.9679(15)	2.155	*1-x,1-y,-z*
Cg21 → Cg2	3.6619(15)	1.585	*-1+x,y,z*
Cg21 → Cg2	5.4245(16)	4.322	*1-x,1-y,-z*
Cg21 → Cg3	3.6431(15)	1.349	*1-x,1-y,-z*
Cg21 → Cg4	4.0412(12)	2.293	*-1+x,y,z*
Cg21 → Cg4	4.6073(14)	3.211	*1-x,1-y,-z*
Cg21 → Cg5	5.5423(13)	4.391	*-1+x,y,z*
Cg21 → Cg5	3.6199(13)	1.352	*1-x,1-y,-z*
Cg21 → Cg6	4.7020(12)	3.295	*-1+x,y,z*
Cg21 → Cg6	3.9689(13)	2.158	*1-x,1-y,-z*
Cg22 → Cg1	3.6251(12)	1.425	*-1+x,y,z*
Cg22 → Cg1	4.0414(11)	2.287	*1-x,1-y,-z*

Cg22 → Cg2	4.6110(14)	3.231	*-1+x,y,z*
Cg22 → Cg2	3.6327(13)	1.544	*1-x,1-y,-z*
Cg22 → Cg3	4.0284(13)	2.199	*-1+x,y,z*
Cg22 → Cg3	5.5381(14)	4.391	*1-x,1-y,-z*
Cg22 → Cg4	3.9783(12)	2.206	*-1+x,y,z*
Cg22 → Cg4	3.6545(11)	1.549	*1-x,1-y,-z*
Cg22 → Cg5	3.6465(11)	1.430	*-1+x,y,z*
Cg22 → Cg5	4.7061(11)	3.302	*1-x,1-y,-z*
Cg22 → Cg6	3.6260(11)	1.429	*-1+x,y,z*
Cg22 → Cg6	4.0418(10)	2.288	*1-x,1-y,-z*
Cg23 → Cg1	4.0414(11)	2.287	*-1+x,y,z*
Cg23 → Cg1	3.6251(12)	1.425	*1-x,1-y,-z*
Cg23 → Cg2	3.6327(13)	1.544	*-1+x,y,z*
Cg23 → Cg2	4.6110(14)	3.231	*1-x,1-y,-z*
Cg23 → Cg3	5.5382(14)	4.391	*-1+x,y,z*
Cg23 → Cg3	4.0284(13)	2.199	*1-x,1-y,-z*
Cg23 → Cg4	3.6545(11)	1.549	*-1+x,y,z*
Cg23 → Cg4	3.9783(12)	2.206	*1-x,1-y,-z*
Cg23 → Cg5	4.7061(11)	3.302	*-1+x,y,z*
Cg23 → Cg5	3.6465(11)	1.430	*1-x,1-y,-z*
Cg23 → Cg6	4.0418(10)	2.288	*-1+x,y,z*
Cg23 → Cg6	3.6260(11)	1.429	*1-x,1-y,-z*
Cg24 → Cg1	3.6495(11)	1.480	*-1+x,y,z*
Cg24 → Cg1	3.6494(11)	1.480	*1-x,1-y,-z*
Cg24 → Cg2	3.9762(13)	2.231	*-1+x,y,z*
Cg24 → Cg2	3.9762(13)	2.231	*1-x,1-y,-z*
Cg24 → Cg3	4.6937(13)	3.258	*-1+x,y,z*
Cg24 → Cg3	4.6937(13)	3.258	*1-x,1-y,-z*
Cg24 → Cg4	3.6294(10)	1.481	*-1+x,y,z*
Cg24 → Cg4	3.6294(10)	1.481	*1-x,1-y,-z*
Cg24 → Cg5	4.0377(10)	2.243	*-1+x,y,z*
Cg24 → Cg5	4.0377(10)	2.243	*1-x,1-y,-z*
Cg24 → Cg6	3.6501(9)	1.483	*-1+x,y,z*
Cg24 → Cg6	3.6501(9)	1.483	*1-x,1-y,-z*

Cg-Cg - Distance between ring Centroids (Ang.); Slippage - Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang).

Table S11. Definitions of ring centroids (Cg) for structure (**II**).

Cg	Ring size	Atoms defining the ring
Cg1	6	N1A, N8A, C2A, C7A, C9A, C14A
Cg2	6	C2A, C3A, C4A, C5A, C6A, C7A
Cg3	6	C9A, C10A, C11A, C12A, C13A, C14A
Cg4	10	N1A, N8A, C2A, C3A, C4A, C5A, C6A, C7A, C9A, C14A
Cg5	10	N1A, N8A, C2A, C7A, C9A, C10A, C11A, C12A, C13A, C14A
Cg6	14	N1A, N8A, C2A, C3A, C4A, C5A, C6A, C7A, C9A, C10A, C11A, C12A, C13A, C14A
Cg7	6	N1B, N8B, C2B, C7B, C9B, C14B
Cg8	6	C2B, C3B, C4B, C5B, C6B, C7B
Cg9	6	C9B, C10B, C11B, C12B, C13B, C14B
Cg10	10	N1B, N8B, C2B, C3B, C4B, C5B, C6B, C7B, C9B, C14B
Cg11	10	N1B, N8B, C2B, C7B, C9B, C10B, C11B, C12B, C13B, C14B
Cg12	14	N1B, N8B, C2B, C3B, C4B, C5B, C6B, C7B, C9B, C10B, C11B, C12B, C13B, C14B
Cg13	6	N1C, C2C, C7C
Cg14	6	C2C, C3C, C4C, C5C, C6C, C7C

Cg15	6	C7C, C2C, C3C, C4C, C5C, C6C
Cg16	10	N1C, C2C, C3C, C4C, C5C, C6C, C7C
Cg17	10	N1C, C2C, C7C, C3C, C4C, C5C, C6C
Cg18	14	N1C, C2C, C3C, C4C, C5C, C6C, C7C
Cg19	6	N1D, C2D, C7D
Cg20	6	C2D, C3D, C4D, C5D, C6D, C7D
Cg21	6	C7D, C2D, C3D, C4D, C5D, C6D
Cg22	10	N1D, C2D, C3D, C4D, C5D, C6D, C7D
Cg23	10	N1D, C2D, C7D, C3D, C4D, C5D, C6D
Cg24	14	N1D, C2D, C3D, C4D, C5D, C6D, C7D
Cg25	6	C21A, C22A, C23A, C24A, C25A, C26A

Table S12. HOMA (with GEO and EN components) for 2-hydroxybenzoic acid, 4-hydroxybenzoic acid, 2,4,6-trihydroxybenzoic acid and 3,4,5-trihydroxybenzoic acid.

Refcode	HOMA	GEO	EN	Type of acid
SALIAC[1]	0.740	0.014	0.246	2-hydroxybenzoic acid
JOZZIH01[2]	0.671	0.002	0.327	4-hydroxybenzoic acid
XIPVEY[3]	0.587	0.024	0.389	2,4,6-trihydroxybenzoic acid
IJUMEG[4]	0.639	0.003	0.000	3,4,5-trihydroxybenzoic acid

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Note: Baseline HOMA values for the corresponding pure hydroxybenzoic acids were calculated from their reported crystal structures. These values serve as an experimental reference for gauging the magnitude of geometry-based aromaticity changes upon co-crystallisation. For consistency, HOMA (together with the GEO and EN terms) was evaluated using the same aromatic ring atom sets as in the co-crystals.