STRUCTURAL CHEMISTRY

Volume 74 (2018)

Supporting information for article:

The new heteropolyoxometalate compound (C6H8N)5[HAs2Mo6O26(H2O)]·3H2O: crystal structure and Hirshfeld surface analysis

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Supplementary material

Table S1. Bond lengths for **1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Mo(1)	O(1)	1.889(2)	As(2)	O(10)	1.687(2)
Mo(1)	O(1W)	2.395(2)	As(2)	O(11)	1.6819(19)
Mo(1)	O(6)	1.910(2)	As(2)	O(12)	1.661(2)
Mo(1)	O(9)	2.3140(19)	As(2)	O(13)	1.735(2)
Mo(1)	O(15)	1.696(2)	C(1A)	N(1A)	1.472(4)
Mo(1)	O(16)	1.727(2)	C(1A)	C(2A)	1.369(5)
Mo(2)	O(1)	1.889(2)	C(1A)	C(6A)	1.383(4)
Mo(2)	O(2)	1.957(2)	C(2A)	C(3A)	1.388(5)
Mo(2)	O(7)	2.2358(19)	C(3A)	C(4A)	1.377(5)
Mo(2)	O(10)	2.319(2)	C(4A)	C(5A)	1.389(6)
Mo(2)	O(17)	1.701(2)	C(5A)	C(6A)	1.392(5)
Mo(2)	O(18)	1.724(2)	C(1B)	N(1B)	1.459(4)
Mo(3)	O(2)	1.909(2)	C(1B)	C(2B)	1.392(5)
Mo(3)	O(3)	1.890(2)	C(1B)	C(6B)	1.383(5)
Mo(3)	O(7)	2.3099(19)	C(2B)	C(3B)	1.373(5)
Mo(3)	O(11)	2.331(2)	C(3B)	C(4B)	1.386(5)
Mo(3)	O(19)	1.704(2)	C(4B)	C(5B)	1.390(5)
Mo(3)	O(20)	1.735(2)	C(5B)	C(6B)	1.370(5)
Mo(4)	O(3)	1.946(2)	C(1C)	N(1C)	1.474(4)
Mo(4)	O(4)	1.870(2)	C(1C)	C(2C)	1.381(4)
Mo(4)	O(8)	2.249(2)	C(1C)	C(6C)	1.380(4)
Mo(4)	O(11)	2.375(2)	C(2C)	C(3C)	1.389(4)
Mo(4)	O(21)	1.727(2)	C(3C)	C(4C)	1.381(4)
Mo(4)	O(22)	1.709(2)	C(4C)	C(5C)	1.387(4)
Mo(5)	O(4)	1.950(2)	C(5C)	C(6C)	1.388(4)
Mo(5)	O(5)	1.914(2)	C(1D)	N(1D)	1.468(4)
Mo(5)	O(8)	2.274(2)	C(1D)	C(2D)	1.387(4)
Mo(5)	O(12)	2.266(2)	C(1D)	C(6D)	1.387(4)
Mo(5)	O(23)	1.711(2)	C(2D)	C(3D)	1.390(5)
Mo(5)	O(24)	1.703(2)	C(3D)	C(4D)	1.382(5)
Mo(6)	O(1W)	2.436(2)	C(4D)	C(5D)	1.383(5)
Mo(6)	O(5)	1.864(2)	C(5D)	C(6D)	1.387(4)
Mo(6)	O(6)	1.986(2)	C(1E)	N(1E)	1.466(4)
Mo(6)	O(9)	2.289(2)	C(1E)	C(2E)	1.388(4)
Mo(6)	O(25)	1.702(2)	C(1E)	C(6E)	1.382(4)
Mo(6)	O(26)	1.703(2)	C(2E)	C(3E)	1.386(5)
As(1)	O(7)	1.6880(19)	C(3E)	C(4E)	1.387(5)
As(1)	O(8)	1.6943(19)	C(4E)	C(5E)	1.384(5)
As(1)	O(9)	1.698(2)	C(5E)	C(6E)	1.392(4)
As(1)	O(14)	1.6734(19)			

Table S2. Values of valence angles for **1**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O(1)	Mo(1)	O(1W)	77.18(8)	O(25)	Mo(6)	O(5)	101.10(10)
O(1)	Mo(1)	O(6)	145.91(9)	O(25)	Mo(6)	O(6)	93.51(9)
O(1)	Mo(1)	O(9)	83.40(8)	O(25)	Mo(6)	O(9)	154.37(9)
O(6)	Mo(1)	O(1W)	72.92(8)	O(25)	Mo(6)	O(26)	104.75(11)
O(6)	Mo(1)	O(9)	70.71(8)	O(26)	Mo(6)	O(1W)	165.27(9)
O(9)	Mo(1)	O(1W)	68.37(7)	O(26)	Mo(6)	O(5)	102.22(10)
O(15)	Mo(1)	O(1)	99.15(10)	O(26)	Mo(6)	O(6)	101.07(9)
O(15)	Mo(1)	O(1W)	93.46(9)	O(26)	Mo(6)	O(9)	97.82(9)

O(15)	Mo(1)	O(6)	98.63(10)	O(7)	As(1)	O(8)	109.01(10)
O(15)	Mo(1)	O(9)	160.76(9)	O(7)	As(1)	O(9)	109.54(10)
O(15)	Mo(1)	O(16)	104.31(10)	O(8)	As(1)	O(9)	108.57(10)
O(16)	Mo(1)	O(1)	100.25(9)	O(14)	As(1)	O(7)	111.05(10)
O(16)	Mo(1)	O(1W)	162.21(9)	O(14)	As(1)	O(8)	109.17(10)
O(16)	Mo(1)	O(6)	103.19(9)	O(14)	As(1)	O(9)	109.47(10)
O(16)	Mo(1)	O(9)	93.89(8)	O(10)	As(2)	O(13)	102.07(10)
O(1)	Mo(2)	O(2)	152.78(9)	O(11)	As(2)	O(10)	114.30(10)
O(1)	Mo(2)	O(7)	85.90(8)	O(11)	As(2)	O(13)	107.76(10)
O(1)	Mo(2)	O(10)	77.66(8)	O(12)	As(2)	O(10)	110.14(10)
O(2)	Mo(2)	O(7)	73.44(8)	O(12)	As(2)	O(11)	113.56(10)
O(2)	Mo(2)	O(10)	80.72(8)	O(12)	As(2)	O(13)	108.16(10)
O(7)	Mo(2)	O(10)	77.77(7)	Mo(1)	O(1)	Mo(2)	162.11(12)
O(17)	Mo(2)	O(1)	101.57(10)	Mo(1)	O(1W)	Mo(6)	84.60(6)
O(17)	Mo(2)	O(2)	94.48(9)	Mo(3)	O(2)	Mo(2)	118.28(10)
O(17)	Mo(2)	O(7)	163.48(9)	Mo(3)	O(3)	Mo(4)	121.24(10)
O(17)	Mo(2)	O(10)	89.35(9)	Mo(4)	O(4)	Mo(5)	119.53(10)
O(17)	Mo(2)	O(18)	104.96(11)	Mo(6)	O(5)	Mo(5)	154.86(12)
O(18)	Mo(2)	O(1)	97.73(10)	Mo(1)	O(6)	Mo(6)	113.13(10)
O(18)	Mo(2)	O(2)	99.18(10)	Mo(2)	O(7)	Mo(3)	93.77(7)
O(18)	Mo(2)	O(7)	88.38(9)	As(1)	O(7)	Mo(2)	135.81(11)
O(18)	Mo(2)	O(10)	165.62(9)	As(1)	O(7)	Mo(3)	123.56(10)
O(2)	Mo(3)	O(7)	72.54(8)	Mo(4)	O(8)	Mo(5)	93.74(7)
O(2)	Mo(3)	O(11)	80.93(8)	As(1)	O(8)	Mo(4)	125.38(11)
O(3)	Mo(3)	O(2)	145.09(9)	As(1)	O(8)	Mo(5)	140.51(11)
O(3)	Mo(3)	O(7)	79.37(8)	Mo(6)	O(9)	Mo(1)	89.88(7)
O(3)	Mo(3)	O(11)	74.05(8)	As(1)	O(9)	Mo(1)	133.94(11)
O(7)	Mo(3)	O(11)	79.99(7)	As(1)	O(9)	Mo(6)	132.95(10)
O(19)	Mo(3)	O(2)	98.80(9)	As(2)	O(10)	Mo(2)	128.90(11)
O(19)	Mo(3)	O(3)	103.14(10)	Mo(3)	O(11)	Mo(4)	90.53(7)
O(19)	Mo(3)	O(7)	164.32(8)	As(2)	O(11)	Mo(3)	127.27(11)
O(19)	Mo(3)	O(11)	85.80(9)	As(2)	O(11)	Mo(4)	126.61(11)
O(19)	Mo(3)	O(20)	105.37(10)	As(2)	O(12)	Mo(5)	125.86(11)
O(20)	Mo(3)	O(2)	100.71(9)	C(2A)	C(1A)	N(1A)	119.3(3)
O(20)	Mo(3)	O(3)	99.23(9)	C(2A)	C(1A)	C(6A)	121.7(3)
O(20)	Mo(3)	O(7)	89.31(9)	C(6A)	C(1A)	N(1A)	118.9(3)
O(20)	Mo(3)	O(11)	168.20(9)	C(1A)	C(2A)	C(3A)	119.1(3)
O(3)	Mo(4)	O(8)	80.33(8)	C(4A)	C(3A)	C(2A)	120.6(4)
O(3)	Mo(4)	O(11)	72.08(7)	C(3A)	C(4A)	C(5A)	119.6(4)
O(4)	Mo(4)	O(3)	148.87(9)	C(4A)	C(5A)	C(6A)	120.3(4)
O(4)	Mo(4)	O(8)	73.68(8)	C(1A)	C(6A)	C(5A)	118.6(4)
O(4)	Mo(4)	O(11)	84.13(8)	C(2B)	C(1B)	N(1B)	119.6(3)
O(8)	Mo(4)	O(11)	73.37(7)	C(6B)	C(1B)	N(1B)	118.5(3)
O(21)	Mo(4)	O(3)	98.08(9)	C(6B)	C(1B)	C(2B)	121.8(3)
O(21)	Mo(4)	O(4)	101.20(9)	C(3B)	C(2B)	C(1B)	118.5(3)
O(21)	Mo(4)	O(8)	161.63(9)	C(2B)	C(3B)	C(4B)	120.3(3)
O(21)	Mo(4)	O(11)	88.67(9)	C(3B)	C(4B)	C(5B)	120.3(3)
O(22)	Mo(4)	O(3)	97.63(9)	C(6B)	C(5B)	C(4B)	120.0(3)
O(22)	Mo(4)	O(4)	100.70(10)	C(5B)	C(6B)	C(1B)	119.0(3)
O(22)	Mo(4)	O(8)	93.43(9)	C(2C)	C(1C)	N(1C)	118.8(3)
O(22)	Mo(4)	O(11)	164.23(9)	C(6C)	C(1C)	N(1C)	119.6(3)
O(22)	Mo(4)	O(21)	104.91(10)	C(6C)	C(1C)	C(2C)	121.6(3)
O(4)	Mo(5)	O(8)	71.73(8)	C(1C)	C(2C)	C(3C)	118.3(3)
O(4)	Mo(5)	O(12)	79.53(8)	C(4C)	C(3C)	C(2C)	121.4(3)
O(5)	Mo(5)	O(4)	148.63(9)	C(3C)	C(4C)	C(5C)	119.1(3)
O(5)	Mo(5)	O(8)	82.66(8)	C(4C)	C(5C)	C(6C)	120.5(3)

O(5)	Mo(5)	O(12)	79.74(8)	C(1C)	C(6C)	C(5C)	119.1(3)
O(12)	Mo(5)	O(8)	83.23(7)	C(2D)	C(1D)	N(1D)	119.0(3)
O(23)	Mo(5)	O(4)	98.91(9)	C(6D)	C(1D)	N(1D)	119.3(3)
O(23)	Mo(5)	O(5)	102.92(10)	C(6D)	C(1D)	C(2D)	121.7(3)
O(23)	Mo(5)	O(8)	166.95(9)	C(1D)	C(2D)	C(3D)	118.7(3)
O(23)	Mo(5)	O(12)	86.16(9)	C(4D)	C(3D)	C(2D)	120.2(3)
O(24)	Mo(5)	O(4)	97.86(10)	C(3D)	C(4D)	C(5D)	120.2(3)
O(24)	Mo(5)	O(5)	98.53(10)	C(4D)	C(5D)	C(6D)	120.6(3)
O(24)	Mo(5)	O(8)	86.90(9)	C(1D)	C(6D)	C(5D)	118.5(3)
O(24)	Mo(5)	O(12)	170.11(9)	C(2E)	C(1E)	N(1E)	117.6(3)
O(24)	Mo(5)	O(23)	103.70(11)	C(6E)	C(1E)	N(1E)	120.2(3)
O(5)	Mo(6)	O(1W)	81.47(8)	C(6E)	C(1E)	C(2E)	122.1(3)
O(5)	Mo(6)	O(6)	148.22(9)	C(3E)	C(2E)	C(1E)	118.5(3)
O(5)	Mo(6)	O(9)	85.56(8)	C(2E)	C(3E)	C(4E)	120.6(3)
O(6)	Mo(6)	O(1W)	70.82(8)	C(5E)	C(4E)	C(3E)	119.9(3)
O(6)	Mo(6)	O(9)	70.06(8)	C(4E)	C(5E)	C(6E)	120.6(3)
O(9)	Mo(6)	O(1W)	68.05(7)	C(1E)	C(6E)	C(5E)	118.4(3)
O(25)	Mo(6)	O(1W)	88.31(9)				

Table S3. Values of torsion angles for **1**.

A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
O(1W)	Mo(1)	O(1)	Mo(2)	102.0(4)	O(18)	Mo(2)	O(1)	Mo(1)	72.7(4)
O(1W)	Mo(6)	O(5)	Mo(5)	-132.6(3)	O(19)	Mo(3)	O(3)	Mo(4)	68.20(13)
O(2)	Mo(2)	O(1)	Mo(1)	-55.3(5)	O(20)	Mo(3)	O(3)	Mo(4)	176.48(12)
O(2)	Mo(3)	O(3)	Mo(4)	-59.3(2)	O(21)	Mo(4)	O(4)	Mo(5)	172.21(12)
O(3)	Mo(4)	O(4)	Mo(5)	45.0(2)	O(22)	Mo(4)	O(4)	Mo(5)	-80.07(13)
O(6)	Mo(1)	O(1)	Mo(2)	72.9(4)	O(25)	Mo(6)	O(5)	Mo(5)	140.9(3)
O(6)	Mo(6)	O(5)	Mo(5)	-103.3(3)	O(26)	Mo(6)	O(5)	Mo(5)	32.9(3)
O(7)	Mo(2)	O(1)	Mo(1)	-15.1(4)	N(1A)	C(1A)	C(2A)	C(3A)	179.3(3)
O(7)	Mo(3)	O(3)	Mo(4)	-95.98(12)	N(1A)	C(1A)	C(6A)	C(5A)	-179.5(4)
O(7)	As(1)	O(8)	Mo(4)	-51.37(14)	C(1A)	C(2A)	C(3A)	C(4A)	-0.4(7)
O(7)	As(1)	O(8)	Mo(5)	119.56(16)	C(2A)	C(1A)	C(6A)	C(5A)	-2.5(6)
O(7)	As(1)	O(9)	Mo(1)	18.54(17)	C(2A)	C(3A)	C(4A)	C(5A)	-1.2(7)
O(7)	As(1)	O(9)	Mo(6)	-134.73(13)	C(3A)	C(4A)	C(5A)	C(6A)	1.0(7)
O(8)	Mo(4)	O(4)	Mo(5)	10.39(11)	C(4A)	C(5A)	C(6A)	C(1A)	0.8(7)
O(8)	As(1)	O(7)	Mo(2)	-103.20(15)	C(6A)	C(1A)	C(2A)	C(3A)	2.3(6)
O(8)	As(1)	O(7)	Mo(3)	39.52(14)	N(1B)	C(1B)	C(2B)	C(3B)	174.0(3)
O(8)	As(1)	O(9)	Mo(1)	137.47(13)	N(1B)	C(1B)	C(6B)	C(5B)	-173.4(3)
O(8)	As(1)	O(9)	Mo(6)	-15.80(17)	C(1B)	C(2B)	C(3B)	C(4B)	-0.8(5)
O(9)	Mo(1)	O(1)	Mo(2)	32.7(4)	C(2B)	C(1B)	C(6B)	C(5B)	2.6(5)
O(9)	Mo(6)	O(5)	Mo(5)	-64.1(3)	C(2B)	C(3B)	C(4B)	C(5B)	2.8(5)
O(9)	As(1)	O(7)	Mo(2)	15.46(17)	C(3B)	C(4B)	C(5B)	C(6B)	-2.1(5)
O(9)	As(1)	O(7)	Mo(3)	158.18(10)	C(4B)	C(5B)	C(6B)	C(1B)	-0.6(5)
O(9)	As(1)	O(8)	Mo(4)	-170.63(11)	C(6B)	C(1B)	C(2B)	C(3B)	-1.9(5)
O(9)	As(1)	O(8)	Mo(5)	0.30(19)	N(1C)	C(1C)	C(2C)	C(3C)	-179.4(3)
O(10)	Mo(2)	O(1)	Mo(1)	-93.4(4)	N(1C)	C(1C)	C(6C)	C(5C)	179.4(3)
O(10)	As(2)	O(11)	Mo(3)	13.04(16)	C(1C)	C(2C)	C(3C)	C(4C)	0.7(5)
O(10)	As(2)	O(11)	Mo(4)	-112.40(13)	C(2C)	C(1C)	C(6C)	C(5C)	-0.9(5)
O(10)	As(2)	O(12)	Mo(5)	96.18(14)	C(2C)	C(3C)	C(4C)	C(5C)	-2.2(5)
O(11)	Mo(3)	O(3)	Mo(4)	-13.46(10)	C(3C)	C(4C)	C(5C)	C(6C)	2.1(5)
O(11)	Mo(4)	O(4)	Mo(5)	84.75(12)	C(4C)	C(5C)	C(6C)	C(1C)	-0.6(5)
O(11)	As(2)	O(10)	Mo(2)	-15.89(17)	C(6C)	C(1C)	C(2C)	C(3C)	0.9(5)
O(11)	As(2)	O(12)	Mo(5)	-33.48(16)	N(1D)	C(1D)	C(2D)	C(3D)	177.1(3)
O(12)	As(2)	O(10)	Mo(2)	-145.15(13)	N(1D)	C(1D)	C(6D)	C(5D)	-177.1(3)
O(12)	As(2)	O(11)	Mo(3)	140.57(12)	C(1D)	C(2D)	C(3D)	C(4D)	0.1(5)
O(12)	As(2)	O(11)	Mo(4)	15.13(16)	C(2D)	C(1D)	C(6D)	C(5D)	2.2(5)

O(13)	As(2)	O(10)	Mo(2)	100.14(14)	C(2D)	C(3D)	C(4D)	C(5D)	1.9(5)
O(13)	As(2)	O(11)	Mo(3)	-99.64(13)	C(3D)	C(4D)	C(5D)	C(6D)	-1.9(5)
O(13)	As(2)	O(11)	Mo(4)	134.92(12)	C(4D)	C(5D)	C(6D)	C(1D)	-0.2(5)
O(13)	As(2)	O(12)	Mo(5)	-153.04(13)	C(6D)	C(1D)	C(2D)	C(3D)	-2.2(5)
O(14)	As(1)	O(7)	Mo(2)	136.49(14)	N(1E)	C(1E)	C(2E)	C(3E)	-179.9(3)
O(14)	As(1)	O(7)	Mo(3)	-80.79(13)	N(1E)	C(1E)	C(6E)	C(5E)	179.6(3)
O(14)	As(1)	O(8)	Mo(4)	70.10(14)	C(1E)	C(2E)	C(3E)	C(4E)	0.6(5)
O(14)	As(1)	O(8)	Mo(5)	-118.98(17)	C(2E)	C(1E)	C(6E)	C(5E)	-0.3(4)
O(14)	As(1)	O(9)	Mo(1)	-103.44(15)	C(2E)	C(3E)	C(4E)	C(5E)	-0.9(5)
O(14)	As(1)	O(9)	Mo(6)	103.29(15)	C(3E)	C(4E)	C(5E)	C(6E)	0.6(5)
O(15)	Mo(1)	O(1)	Mo(2)	-166.5(4)	C(4E)	C(5E)	C(6E)	C(1E)	0.0(5)
O(16)	Mo(1)	O(1)	Mo(2)	-60.1(4)	C(6E)	C(1E)	C(2E)	C(3E)	0.0(4)
O(17)	Mo(2)	O(1)	Mo(1)	179.8(4)					

Table S4. The geometry of hydrogen bonds in the crystal of **1**.

D–H	**A**	**d(D···A) (Å)**	**< D–H···A (°)**
O1W–H1WA	O2W	2.578(3)	177(6)
O1W–H1WB	O10*	2.835(3)	164(4)
O2W–H2WA	O19^{i}	2.833(3)	156(4)
O2W–H2WB	O21^{i}	2.873(3)	164(4)
O3W–H3WA	O26	2.777(3)	162(5)
O3W–H3WB	O23^{ii}	2.799(3)	146(5)
O4W–H4WA	O3Wiii	2.811(4)	165(4)
O4W–H4WB	O18	3.057(4)	113(3)
N1A–H1AA	O16^{iv}	2.873(3)	175(5)
N1A–H1AB	O6^{v}	2.721(3)	169(4)
N1A–H1AC	O21	2.806(3)	163(4)
N1B–H1BA	O18^{iv}	2.888(4)	102
C1B–H1BA	O20^{iv}	2.992(4)	157
C13–H13	O18^{iv}	2.852(3)	166(5)
N1B–H1BB	O12	2.808(4)	166
N1B–H1BC	O4W^{iv}	2.764(4)	159
N1C–H1CA	O14^{iv}	2.851(3)	165(4)
N1C–H1CB	O20^{iv}	2.875(3)	171(5)
N1C–H1CC	O10	2.922(3)	175(4)
N1D–H1DA	O22	2.884(3)	148
N1D–H1DB	O3W	2.861(4)	172
N1D–H1DC	O14	2.747(3)	171
N1E–H1EA	O14	2.763(3)	167(5)
N1E–H1EB	O16	2.868(3)	162(4)
N1E–H1EC	O2^{vi}	2.708(3)	172(4)
C2A–H2A	O21	3.243(4)	130
C2B–H2B	O4W^{iv}	3.249(5)	128
C2C–H2C	O1	3.371(4)	162
C2C–H2C	O17	3.122(4)	129
C2D–H2D	O22	3.226(4)	127
C3E–H3E	O24^{ii}	3.179(4)	151
C6D–H6D	O23^{ii}	3.288(4)	156
C6E–H6E	O6	3.267(3)	138

Symmetry codes: (i) x, –*y* + 1/2, *z* + 1/2; (ii) –*x*, *y* + 1/2, –*z* + 3/2; (iii) *x* + 1, *y*, *z*; (iv) –*x* + 1, *y* – 1/2, –*z* + 3/2; (v) *x*, –*y* + 1/2, *z* – 1/2; (vi) –*x* + 1, *y* + 1/2, –*z* +3/2; (*) intramolecular interaction.

Table S5. The geometry of C−H···π contacts is the crystal of **1**.

D–H	***Cg*I**	**d(D··· *Cg*I) (Å)**	**< D–H··· *Cg*I (°)**
C5C–H5C	16[vii]	3.407(3)	129

Symmetry code: (vii) *–x* + 1, *–y*, *–z* + 2.
*Cg*16 represents the centre of gravity of the C1B–C6B aromatic ring (Fig. 1).

Table S6. The geometry of π–π interactions in the crystal of **MWC12k2k**.

***Cg*I**	***Cg*J**	***Cg*I···*Cg*J (Å)**	**Dihedral angle (°)**	**Interplanar distance (Å)**	**Offset (Å)**
16	18[viii]	3.776(2)	7.50(16)	3.464(2)	1.503(2)
18	16[ii]	3.776(2)	7.50(16)	3.147(2)	2.087(2)

Symmetry codes: (viii) *–x*, *y* – 1/2, *–z* + 2; (ii) *–x*, *y* + 1/2, *–z* + 3/2.
*Cg*16 and *Cg*18 represent the centres of gravity of the C1B–C6B and C1D−C6D aromatic rings, respectively (Fig. 1).
*Cg*I···*Cg*J is the distance between ring centroids.
The dihedral angle is the angle between the mean planes of *Cg*I and *Cg*J.
The interplanar distance is the perpendicular distance from *Cg*I to ring J.
The offset is the perpendicular distance from ring I to ring J.