Crystal structure of aquamagnesiumphthalocyanine pyridine (2/3), $2(C_{32}H_{16}N_8)Mg(H_2O) \cdot 3C_5H_5N$

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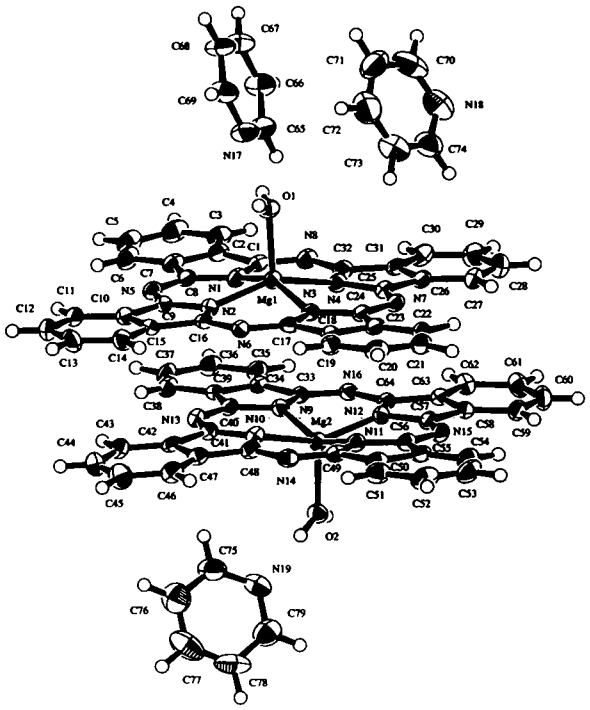

Abstract

$C_{79}H_{51}Mg_2N_{19}O_2$, triclinic, $P\bar{1}$ (No. 2), $a = 13.586(8)$ Å, $b = 15.640(9)$ Å, $c = 17.67(1)$ Å, $\alpha = 102.96(5)°$, $\beta = 112.59(4)°$, $\gamma = 104.01(5)°$, $V = 3145.0$ Å^3, $Z = 2$, $R_{gt}(F) = 0.053$, $wR_{ref}(F^2) = 0.157$, $T = 223$ K.

Source of material

Magnesiumphthalocyanine was purchased from Aldrich Chemical Industry Inc. The product was purified once by sublimation. using a two-zone furnace [1]. The single crystals were then grown from solution in pyridine by solvent evaporation at room temperature.

Discussion

Magnesiumphthalocyanine (MgPc) is a blue pigment and used also as a photocoonductor for laser printers [2,3]. MgPc is known to accommodate water and/or solvent molecules upon crystallization [4-6]. Thus, the electronic spectra vary significantly due to intermolecular interactions in the molecular arrangement [7]. The present structure analysis has been carried out in order to study the correlation between crystal and electronic structures in MgPc complexes. When MgPc was recrystallized from solution in pyridine, two kinds of complexes were obtained: $MgPc(H_2O) \cdot 2$(pyridine) and $2(MgPc)(H_2O) \cdot 3$(pyridine). The former coincides with the structure reported by Fischer and others [3] while the latter is reported here. The complex is composed of two MgPc molecules arranged in convex pairs together with two water and three pyridine molecules. The O atom of water is coordinated to the central Mg atom of MgPc. The Mg atom is shifted by about 0.45 Å out of the plane of the four nitrogen atoms, forming a pyramidal structure. The electron-rich nitrogen of pyridine is hydrogen-bonded to the water molecule in the N···HO form. This H-bond formation occurs in both MgPc molecules. In addition, the third pyridine molecule exists alongside the hydrogen-bonded pyridine molecule as shown in the figure. However, this pyridine molecule is rather free because no hydrogen bond is recognized between the pyridine and water molecules. The complex molecules are then stacked alternately nearly along the (a,b)-diagonal direction. The essential difference between $MgPc(H_2O) \cdot 2$(pyridine) and $2(MgPc)(H_2O) \cdot 3$(pyridine) is that two pyridine molecules are hydrogen-bonded to one water molelcule in the former case while there is only one pyridine molecule in the latter case.

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Table 1. Data collection and handling.

Crystal:	blue platelet, size 0.07 × 0.12 × 0.28 mm
Wavelength:	Mo K_α radiation (0.7107 Å)
μ:	0.93 cm^{-1}
Diffractometer, scan mode:	Rigaku AFC7R, $\omega/2\theta$
$2\theta_{max}$:	50°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	14969, 11075
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 11068
$N(param)_{refined}$:	919
Programs:	teXsan [8], SHELX-86 [9], ORTEPII [10]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1)	2*i*	0.5485	0.0599	–0.0299	0.043
H(2)	2*i*	0.6370	–0.0066	–0.1041	0.051
H(3)	2*i*	0.8315	0.0660	–0.0592	0.051
H(4)	2*i*	0.9456	0.2031	0.0657	0.045
H(5)	2*i*	1.2109	0.4357	0.2766	0.037
H(6)	2*i*	1.3908	0.5505	0.3772	0.045
H(7)	2*i*	1.4123	0.6660	0.4966	0.046
H(8)	2*i*	1.2539	0.6732	0.5178	0.041
H(9)	2*i*	1.0096	0.7328	0.6146	0.028
H(10)	2*i*	0.9141	0.7916	0.6866	0.040
H(11)	2*i*	0.7169	0.7369	0.6257	0.071
H(12)	2*i*	0.5965	0.5923	0.4918	0.076
H(13)	2*i*	0.3399	0.3714	0.2818	0.038
H(14)	2*i*	0.1630	0.2559	0.1802	0.048
H(15)	2*i*	0.1440	0.1411	0.0595	0.050
H(16)	2*i*	0.3074	0.1365	0.0430	0.044
H(17)	2*i*	0.4827	0.2585	–0.1066	0.031

Table 2. Continued.

Atom	Site	x	y	z	U_{iso}
H(18)	2*i*	0.5813	0.1952	–0.1763	0.030
H(19)	2*i*	0.7792	0.2639	–0.1166	0.046
H(20)	2*i*	0.8849	0.4040	0.0175	0.029
H(21)	2*i*	1.1425	0.6386	0.2183	0.039
H(22)	2*i*	1.3177	0.7593	0.3179	0.049
H(23)	2*i*	1.3329	0.8772	0.4324	0.050
H(24)	2*i*	1.1727	0.8750	0.4555	0.040
H(25)	2*i*	0.9267	0.9248	0.5469	0.045
H(26)	2*i*	0.8277	0.9853	0.6160	0.051
H(27)	2*i*	0.6310	0.9182	0.5568	0.054
H(28)	2*i*	0.5242	0.7880	0.4276	0.044
H(29)	2*i*	0.2672	0.5682	0.2111	0.034
H(30)	2*i*	0.0867	0.4522	0.1060	0.047
H(31)	2*i*	0.0699	0.3325	–0.0086	0.046
H(32)	2*i*	0.2325	0.3239	–0.0239	0.038
H(33)	2*i*	0.8911	0.3525	0.4500	0.050
H(34)	2*i*	0.7957	0.2532	0.3446	0.050

Table 2. Continued.

Atom	Site	x	y	z	U_{iso}
H(35)	2*i*	0.7402	0.7528	0.1458	0.050
H(36)	2*i*	0.6079	0.6507	0.0547	0.050
H(37)	2*i*	0.6357	0.0819	0.1976	0.053
H(38)	2*i*	0.5771	–0.0790	0.1626	0.056
H(39)	2*i*	0.6852	–0.1413	0.2576	0.061
H(40)	2*i*	0.8528	–0.0387	0.3843	0.057
H(41)	2*i*	0.9020	0.1234	0.4162	0.055
H(42)	2*i*	0.3600	–0.0918	0.2808	0.098
H(43)	2*i*	0.5601	–0.0184	0.3845	0.092
H(44)	2*i*	0.6515	0.1429	0.4169	0.088
H(45)	2*i*	0.5391	0.2233	0.3494	0.099
H(46)	2*i*	0.3466	0.1448	0.2562	0.066
H(47)	2*i*	0.9585	0.7837	0.1793	0.063
H(48)	2*i*	1.1213	0.8960	0.2025	0.078
H(49)	2*i*	1.1179	1.0392	0.1907	0.084
H(50)	2*i*	0.9458	1.0648	0.1506	0.082
H(51)	2*i*	0.7834	0.9461	0.1269	0.065

Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mg(1)	2*i*	0.78493(8)	0.38513(7)	0.30082(6)	0.0259(5)	0.0221(5)	0.0258(5)	0.0106(4)	0.0142(3)	0.0067(4)
Mg(2)	2*i*	0.70044(8)	0.61540(7)	0.20140(6)	0.0253(4)	0.0235(5)	0.0259(5)	0.0109(4)	0.0147(3)	0.0074(4)
O(1)	2*i*	0.8156(2)	0.3053(1)	0.3754(1)	0.036(1)	0.023(1)	0.029(1)	0.0113(8)	0.0144(8)	0.0073(9)
O(2)	2*i*	0.6818(2)	0.6989(1)	0.1289(1)	0.027(1)	0.027(1)	0.028(1)	0.0077(8)	0.0113(8)	0.0101(9)
N(1)	2*i*	0.7662(2)	0.3020(2)	0.1858(2)	0.032(1)	0.029(1)	0.027(1)	0.018(1)	0.0152(9)	0.010(1)
N(2)	2*i*	0.9467(2)	0.4604(2)	0.3284(2)	0.027(1)	0.025(1)	0.028(1)	0.0119(9)	0.0161(9)	0.011(1)
N(3)	2*i*	0.7921(2)	0.5027(2)	0.3843(2)	0.030(1)	0.020(1)	0.029(1)	0.0124(9)	0.0178(9)	0.009(1)
N(4)	2*i*	0.6112(2)	0.3448(2)	0.2405(2)	0.029(1)	0.030(1)	0.024(1)	0.016(1)	0.0139(9)	0.010(1)
N(5)	2*i*	0.9651(2)	0.3529(2)	0.2162(2)	0.036(1)	0.028(1)	0.029(1)	0.018(1)	0.0199(9)	0.012(1)
N(6)	2*i*	0.9966(2)	0.5901(2)	0.4589(2)	0.027(1)	0.022(1)	0.030(1)	0.0109(9)	0.0167(9)	0.010(1)
N(7)	2*i*	0.5909(2)	0.4554(2)	0.3489(2)	0.030(1)	0.024(1)	0.028(1)	0.0149(9)	0.0152(9)	0.010(1)
N(8)	2*i*	0.5615(2)	0.2119(2)	0.1129(2)	0.035(1)	0.028(1)	0.029(1)	0.015(1)	0.015(1)	0.010(1)
N(9)	2*i*	0.6955(2)	0.4971(2)	0.1201(1)	0.025(1)	0.024(1)	0.026(1)	0.0095(9)	0.0149(9)	0.009(1)
N(10)	2*i*	0.8734(2)	0.6544(2)	0.2670(2)	0.026(1)	0.027(1)	0.026(1)	0.0129(9)	0.0117(9)	0.009(1)
N(11)	2*i*	0.7142(2)	0.6959(2)	0.3162(2)	0.030(1)	0.026(1)	0.025(1)	0.0135(9)	0.0148(9)	0.010(1)
N(12)	2*i*	0.5362(2)	0.5391(2)	0.1688(2)	0.025(1)	0.024(1)	0.026(1)	0.0106(9)	0.0150(9)	0.009(1)
N(13)	2*i*	0.8969(2)	0.5473(2)	0.1575(2)	0.025(1)	0.028(1)	0.032(1)	0.0139(9)	0.0146(9)	0.012(1)
N(14)	2*i*	0.9187(2)	0.7846(2)	0.3950(2)	0.032(1)	0.022(1)	0.025(1)	0.009(1)	0.012(1)	0.008(1)
N(15)	2*i*	0.5123(2)	0.6457(2)	0.2782(2)	0.033(1)	0.031(1)	0.030(1)	0.019(1)	0.0201(9)	0.013(1)
N(16)	2*i*	0.4911(2)	0.4082(2)	0.0417(2)	0.029(1)	0.022(1)	0.028(1)	0.0113(9)	0.0168(9)	0.010(1)
N(17)	2*i*	0.7734(2)	0.1180(2)	0.3102(2)	0.050(2)	0.027(1)	0.050(2)	0.014(1)	0.019(1)	0.016(1)
N(18)	2*i*	0.3377(3)	0.0222(3)	0.2630(2)	0.065(2)	0.060(2)	0.045(2)	0.005(2)	0.028(1)	0.011(2)
N(19)	2*i*	0.8548(2)	0.8528(2)	0.1503(2)	0.044(2)	0.041(2)	0.040(2)	0.004(1)	0.016(1)	0.017(1)
C(1)	2*i*	0.6686(2)	0.2299(2)	0.1226(2)	0.030(1)	0.021(1)	0.024(1)	0.012(1)	0.011(1)	0.008(1)
C(2)	2*i*	0.6952(3)	0.1697(2)	0.0627(2)	0.038(2)	0.030(2)	0.028(1)	0.019(1)	0.018(1)	0.014(1)
C(3)	2*i*	0.6285(3)	0.0882(2)	–0.0102(2)	0.045(2)	0.030(2)	0.030(2)	0.018(1)	0.016(1)	0.009(1)
C(4)	2*i*	0.6810(3)	0.0500(2)	–0.0545(2)	0.059(2)	0.031(2)	0.037(2)	0.024(1)	0.021(2)	0.007(1)
C(5)	2*i*	0.7982(3)	0.0936(2)	–0.0267(2)	0.058(2)	0.043(2)	0.034(2)	0.031(1)	0.026(1)	0.008(1)
C(6)	2*i*	0.8660(3)	0.1745(2)	0.0466(2)	0.048(2)	0.041(2)	0.034(2)	0.028(1)	0.024(1)	0.011(1)
C(7)	2*i*	0.8132(3)	0.2127(2)	0.0917(2)	0.039(2)	0.029(2)	0.028(1)	0.019(1)	0.016(1)	0.011(1)
C(8)	2*i*	0.8556(2)	0.2952(2)	0.1700(2)	0.034(1)	0.029(1)	0.028(1)	0.019(1)	0.019(1)	0.015(1)
C(9)	2*i*	1.0062(2)	0.4285(2)	0.2888(2)	0.029(1)	0.024(1)	0.032(1)	0.013(1)	0.019(1)	0.014(1)
C(10)	2*i*	1.1263(2)	0.4882(2)	0.3382(2)	0.030(1)	0.028(2)	0.029(1)	0.013(1)	0.017(1)	0.013(1)
C(11)	2*i*	1.2195(2)	0.4836(2)	0.3252(2)	0.032(1)	0.035(2)	0.035(1)	0.019(1)	0.021(1)	0.017(1)
C(12)	2*i*	1.3255(3)	0.5517(2)	0.3850(2)	0.037(2)	0.045(2)	0.048(2)	0.023(1)	0.029(1)	0.024(1)
C(13)	2*i*	1.3382(3)	0.6211(3)	0.4564(2)	0.027(2)	0.042(2)	0.044(2)	0.008(1)	0.018(1)	0.018(1)
C(14)	2*i*	1.2452(3)	0.6255(2)	0.4696(2)	0.036(2)	0.031(2)	0.035(2)	0.012(1)	0.021(1)	0.011(1)
C(15)	2*i*	1.1381(2)	0.5580(2)	0.4099(2)	0.027(1)	0.025(1)	0.030(1)	0.010(1)	0.017(1)	0.015(1)
C(16)	2*i*	1.0214(2)	0.5379(2)	0.4012(2)	0.031(1)	0.024(1)	0.029(1)	0.014(1)	0.019(1)	0.016(1)
C(17)	2*i*	0.8899(2)	0.5732(2)	0.4491(2)	0.034(1)	0.023(1)	0.027(1)	0.013(1)	0.018(1)	0.013(1)
C(18)	2*i*	0.8617(2)	0.6302(2)	0.5107(2)	0.032(1)	0.023(1)	0.029(1)	0.015(1)	0.019(1)	0.014(1)
C(19)	2*i*	0.9266(3)	0.7068(2)	0.5891(2)	0.033(1)	0.024(2)	0.035(2)	0.011(1)	0.018(1)	0.009(1)
C(20)	2*i*	0.8696(3)	0.7433(2)	0.6303(2)	0.048(2)	0.027(2)	0.032(2)	0.016(1)	0.021(1)	0.007(1)
C(21)	2*i*	0.7510(3)	0.7044(2)	0.5954(2)	0.048(2)	0.033(2)	0.036(2)	0.022(1)	0.029(1)	0.014(1)
C(22)	2*i*	0.6857(2)	0.6278(2)	0.5188(2)	0.034(1)	0.029(2)	0.034(1)	0.017(1)	0.022(1)	0.012(1)
C(23)	2*i*	0.7428(2)	0.5906(2)	0.4770(2)	0.031(1)	0.025(1)	0.028(1)	0.015(1)	0.015(1)	0.013(1)
C(24)	2*i*	0.7004(2)	0.5102(2)	0.3970(2)	0.029(1)	0.024(1)	0.027(1)	0.015(1)	0.015(1)	0.012(1)

Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(25)	2*i*	0.5504(2)	0.3802(2)	0.2764(2)	0.028(1)	0.025(1)	0.033(1)	0.014(1)	0.017(1)	0.013(1)
C(26)	2*i*	0.4292(2)	0.3214(2)	0.2238(2)	0.027(1)	0.024(1)	0.029(1)	0.013(1)	0.013(1)	0.011(1)
C(27)	2*i*	0.3334(3)	0.3241(2)	0.2342(2)	0.029(1)	0.034(2)	0.037(2)	0.017(1)	0.017(1)	0.014(1)
C(28)	2*i*	0.2289(3)	0.2562(3)	0.1733(2)	0.030(2)	0.047(2)	0.048(2)	0.018(1)	0.020(1)	0.019(2)
C(29)	2*i*	0.2183(3)	0.1871(3)	0.1014(2)	0.026(2)	0.042(2)	0.043(2)	0.011(1)	0.008(1)	0.014(2)
C(30)	2*i*	0.3144(3)	0.1834(2)	0.0917(2)	0.036(2)	0.038(2)	0.032(2)	0.019(1)	0.010(1)	0.012(1)
C(31)	2*i*	0.4198(2)	0.2505(2)	0.1538(2)	0.029(1)	0.027(1)	0.029(1)	0.014(1)	0.011(1)	0.015(1)
C(32)	2*i*	0.5366(3)	0.2677(2)	0.1663(2)	0.032(1)	0.031(2)	0.027(1)	0.016(1)	0.014(1)	0.013(1)
C(33)	2*i*	0.5997(2)	0.4258(2)	0.0546(2)	0.027(1)	0.020(1)	0.027(1)	0.010(1)	0.016(1)	0.008(1)
C(34)	2*i*	0.6300(2)	0.3672(2)	–0.0040(2)	0.028(1)	0.021(1)	0.032(1)	0.013(1)	0.016(1)	0.011(1)
C(35)	2*i*	0.5676(3)	0.2881(2)	–0.0798(2)	0.035(2)	0.026(2)	0.031(2)	0.014(1)	0.017(1)	0.008(1)
C(36)	2*i*	0.6263(3)	0.2526(2)	–0.1208(2)	0.044(2)	0.026(2)	0.034(2)	0.016(1)	0.019(1)	0.007(1)
C(37)	2*i*	0.7448(3)	0.2954(2)	–0.0861(2)	0.041(2)	0.037(2)	0.035(2)	0.026(1)	0.024(1)	0.012(1)
C(38)	2*i*	0.8078(3)	0.3729(2)	–0.0102(2)	0.032(1)	0.033(2)	0.030(1)	0.017(1)	0.016(1)	0.011(1)
C(39)	2*i*	0.7487(2)	0.4087(2)	0.0304(2)	0.027(1)	0.024(1)	0.031(1)	0.013(1)	0.017(1)	0.016(1)
C(40)	2*i*	0.7878(2)	0.4901(2)	0.1085(2)	0.027(1)	0.023(1)	0.025(1)	0.014(1)	0.014(1)	0.010(1)
C(41)	2*i*	0.9350(2)	0.6222(2)	0.2298(2)	0.025(1)	0.027(1)	0.027(1)	0.012(1)	0.012(1)	0.012(1)
C(42)	2*i*	1.0543(2)	0.6844(2)	0.2798(2)	0.029(1)	0.027(1)	0.030(1)	0.017(1)	0.012(1)	0.016(1)
C(43)	2*i*	1.1490(3)	0.6854(2)	0.2659(2)	0.027(1)	0.037(2)	0.036(2)	0.017(1)	0.014(1)	0.017(1)
C(44)	2*i*	1.2516(3)	0.7579(3)	0.3248(2)	0.030(2)	0.044(2)	0.051(2)	0.013(1)	0.022(1)	0.020(2)
C(45)	2*i*	1.2609(3)	0.8278(3)	0.3942(2)	0.030(2)	0.044(2)	0.040(2)	0.006(1)	0.010(1)	0.009(2)
C(46)	2*i*	1.1664(3)	0.8272(2)	0.4080(2)	0.031(2)	0.029(2)	0.033(2)	0.010(1)	0.010(1)	0.007(1)
C(47)	2*i*	1.0626(2)	0.7547(2)	0.3499(2)	0.030(1)	0.028(2)	0.026(1)	0.013(1)	0.010(1)	0.012(1)
C(48)	2*i*	0.9460(2)	0.7324(2)	0.3400(2)	0.024(1)	0.024(1)	0.027(1)	0.010(1)	0.009(1)	0.009(1)
C(49)	2*i*	0.8110(2)	0.7647(2)	0.3834(2)	0.032(1)	0.023(1)	0.024(1)	0.012(1)	0.012(1)	0.009(1)
C(50)	2*i*	0.7815(3)	0.8199(2)	0.4447(2)	0.042(2)	0.025(1)	0.024(1)	0.016(1)	0.017(1)	0.010(1)
C(51)	2*i*	0.8458(3)	0.8971(2)	0.5222(2)	0.050(2)	0.030(2)	0.035(2)	0.018(1)	0.022(1)	0.010(1)
C(52)	2*i*	0.7866(3)	0.9323(2)	0.5627(2)	0.063(2)	0.033(2)	0.032(2)	0.026(2)	0.021(1)	0.007(1)
C(53)	2*i*	0.6682(3)	0.8920(2)	0.5275(2)	0.062(2)	0.046(2)	0.041(2)	0.037(1)	0.030(1)	0.018(1)
C(54)	2*i*	0.6050(3)	0.8154(2)	0.4515(2)	0.050(2)	0.037(2)	0.036(2)	0.026(1)	0.027(1)	0.014(1)
C(55)	2*i*	0.6629(3)	0.7789(2)	0.4096(2)	0.035(1)	0.025(1)	0.030(1)	0.016(1)	0.017(1)	0.014(1)
C(56)	2*i*	0.6228(2)	0.7009(2)	0.3288(2)	0.033(1)	0.024(1)	0.022(1)	0.015(1)	0.016(1)	0.008(1)
C(57)	2*i*	0.4743(2)	0.5725(2)	0.2058(2)	0.028(1)	0.030(2)	0.027(1)	0.017(1)	0.016(1)	0.014(1)
C(58)	2*i*	0.3541(2)	0.5132(2)	0.1526(2)	0.027(1)	0.032(2)	0.031(1)	0.015(1)	0.017(1)	0.019(1)
C(59)	2*i*	0.2583(3)	0.5177(2)	0.1622(2)	0.034(1)	0.043(2)	0.034(2)	0.023(1)	0.020(1)	0.021(1)
C(60)	2*i*	0.1538(3)	0.4501(3)	0.1014(2)	0.029(1)	0.055(2)	0.044(2)	0.019(1)	0.022(1)	0.022(2)
C(61)	2*i*	0.1432(3)	0.3789(3)	0.0324(2)	0.025(1)	0.044(2)	0.041(2)	0.006(1)	0.015(1)	0.014(2)
C(62)	2*i*	0.2396(3)	0.3734(2)	0.0229(2)	0.028(1)	0.035(2)	0.035(2)	0.010(1)	0.017(1)	0.013(1)
C(63)	2*i*	0.3448(2)	0.4418(2)	0.0836(2)	0.031(1)	0.026(1)	0.033(1)	0.015(1)	0.020(1)	0.015(1)
C(64)	2*i*	0.4629(2)	0.4616(2)	0.0962(2)	0.028(1)	0.021(1)	0.028(1)	0.012(1)	0.017(1)	0.011(1)
C(65)	2*i*	0.6802(3)	0.0575(3)	0.2371(2)	0.046(2)	0.038(2)	0.048(2)	0.015(2)	0.013(2)	0.018(2)
C(66)	2*i*	0.6447(3)	–0.0384(3)	0.2152(2)	0.053(2)	0.036(2)	0.039(2)	0.009(2)	0.011(2)	0.011(2)
C(67)	2*i*	0.7089(3)	–0.0752(2)	0.2712(3)	0.067(2)	0.028(2)	0.054(2)	0.015(2)	0.025(2)	0.017(2)
C(68)	2*i*	0.8064(3)	–0.0144(3)	0.3460(2)	0.054(2)	0.035(2)	0.050(2)	0.016(2)	0.014(2)	0.025(2)
C(69)	2*i*	0.8354(3)	0.0814(3)	0.3635(2)	0.047(2)	0.041(2)	0.041(2)	0.008(2)	0.012(2)	0.019(2)
C(70)	2*i*	0.4016(4)	–0.0251(3)	0.2994(3)	0.130(3)	0.037(2)	0.078(2)	0.019(2)	0.081(2)	0.016(2)
C(71)	2*i*	0.5185(4)	0.0179(4)	0.3581(3)	0.111(3)	0.107(3)	0.091(3)	0.085(2)	0.074(2)	0.067(2)
C(72)	2*i*	0.5688(4)	0.1115(4)	0.3759(3)	0.057(2)	0.101(4)	0.064(3)	0.028(2)	0.028(2)	0.041(2)
C(73)	2*i*	0.5054(4)	0.1577(3)	0.3376(3)	0.059(2)	0.051(2)	0.038(2)	0.006(2)	0.017(2)	0.012(2)
C(74)	2*i*	0.3935(3)	0.1115(3)	0.2838(3)	0.057(2)	0.061(2)	0.053(2)	0.020(2)	0.027(2)	0.030(2)
C(75)	2*i*	0.9550(3)	0.8422(3)	0.1730(3)	0.050(2)	0.049(2)	0.054(2)	0.014(2)	0.017(2)	0.028(2)
C(76)	2*i*	1.0521(3)	0.9079(3)	0.1867(3)	0.047(2)	0.069(3)	0.060(3)	0.014(2)	0.015(2)	0.020(2)
C(77)	2*i*	1.0495(4)	0.9913(3)	0.1796(3)	0.066(3)	0.056(3)	0.065(3)	–0.012(2)	0.026(2)	0.016(2)
C(78)	2*i*	0.9497(4)	1.0067(3)	0.1570(3)	0.103(3)	0.040(2)	0.070(3)	0.024(2)	0.042(2)	0.033(2)
C(79)	2*i*	0.8537(3)	0.9360(3)	0.1428(3)	0.063(2)	0.062(2)	0.045(2)	0.031(2)	0.023(2)	0.022(2)

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