Crystal structure of 2,6-diaminopyridinium bis(2,6-pyridinedicarboxylato)chromium(III) 2,6-pyridinedicarboxylic acid hemihydrate, $C_{26}H_{18}CrN_6O_{12} \cdot 0.5H_2O$

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Abstract

$C_{26}H_{18}CrN_6O_{12.50}$, monoclinic, $P12_1/c1$ (No. 14), $a = 15.233(4)$ Å, $b = 25.208(6)$ Å, $c = 14.685(3)$ Å, $\beta = 103.893(5)^\circ$, $V = 5474.0$ Å³, $Z = 8$, $R_{\text{gt}}(F) = 0.057$, $wR_{\text{all}}(F^2) = 0.151$, $T = 110$ K.

Source of material

The title compound was synthesized by the reaction between ligand LH_2 , $[H_2pyda]^{2+}[pydc]^{2-}$, ($pyda = 2,6\text{-pyridinediamine}$ and $H_2pydc = 2,6\text{-pyridinedicarboxylic acid}$) that is a new self-assembling system [1], and chromium(III) chloride hexahydrate in water. The resulting violet solution was left to slow concentration at room temperature. After five days, dark red block shaped crystals were isolated.

Discussion

Our goal was to generate a self-assembling coordination compound [2] using a self-assembling system ligand. We found out that the counter ion $[H_2pyda]^{2+}$ has an important role in the complexation process and results in the formation of a novel Cr(III) complex. The molecular structure consists of monomeric units $[Hpyda][Cr(pydc)_2] \cdot H_2pydc, 0.5H_2O$ in which the two $[pydc]^{2-}$ units act as a tridentate ligands through two oxygen and one nitrogen atoms and $[Hpyda]^+$ as counter ion. The ionic crystal contains $[Hpyda]^+$ and $[Cr(pydc)_2]^-$. It has a rather complicated crystal structure with two crystallographic independent pairs of ions in the unit cell along with solvating molecules of water and $[H_2pydc]$, which are bonded to the complex via hydrogen bondings. The two kinds of molecule arrangements are shown in the figure.

The structural data found in this work for the unit $[Hpyda]^+$ are comparable well with those of the LH_2 [1]. The length of the C—N (ring) bonds (1.360 Å – 1.357 Å, mean 1.358 Å) agree with 1.37 Å found in $[H_2pyda]^{2+}$. The structure is strongly stabilized by a complicated network of hydrogen bonds between the crystallization water, $[Hpyda]^+$, $[H_2pydc]$ and $[Cr(pydc)_2]^-$. This complex self-assemble into layers by hydrogen bonding and ion pairing. The Cr(III) atom is in the center of a distorted octahedron consisting of six donor atoms of two tridentate ligands of $[pydc]^{2-}$. The angles O3—Cr1—O1 and O7—Cr1—O5 are 157.86° and 157.32° , respectively. This indicate that four carboxylate groups of the two dianions are oriented in a flattened tetrahedral arrangement around the Cr(III) atom. The two dianionic $[pydc]^{2-}$ units are almost perpendicular to each other (i.e., O1—Cr1—N2—C12 torsion angle is 83.20° , N2—Cr1—O1 and N2—Cr1—O3 angles are 97.35° and 104.75° , respectively). This data are well in agreement with the previous reports [3–6]. An important feature of this structure is the presence of the counter ion $[Hpyda]^+$ that has been formed from LH_2 (the protonation sites in LH_2 are the two $-NH_2$ nitrogens while the protonation site of the counter ion is its pyridine nitrogen).

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Table 1. Data collection and handling.

Crystal:	dark read prism, size 0.1 × 0.2 × 0.3 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	4.99 cm ⁻¹
Diffractometer, scan mode:	Bruker SMART CCD, ϕ/ω
2 $\theta_{\max}$:	65.1°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	71342, 18860
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 10976
$N(\text{param})_{\text{refined}}$:	980
Program:	SHELXTL- 97 [7]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(2)	4e	-0.137(2)	0.2623(9)	0.075(2)	0.021(6)
H(3)	4e	-0.034(2)	0.330(1)	0.129(2)	0.042(8)
H(4)	4e	0.113(2)	0.309(1)	0.207(2)	0.027(6)
H(9)	4e	0.147(1)	-0.0678(9)	0.268(2)	0.017(5)
H(10)	4e	0.172(2)	-0.096(1)	0.121(2)	0.028(6)
H(11)	4e	0.157(2)	-0.033(1)	0.001(2)	0.031(7)
H(16)	4e	0.333(2)	1.0848(9)	0.228(2)	0.022(6)
H(17)	4e	0.297(2)	1.110(1)	0.370(2)	0.027(6)
H(18)	4e	0.309(2)	1.0546(9)	0.493(2)	0.026(6)
H(23)	4e	0.591(2)	0.740(1)	0.429(2)	0.039(7)
H(24)	4e	0.466(2)	0.6846(9)	0.401(2)	0.022(6)
H(25)	4e	0.322(2)	0.718(1)	0.345(2)	0.036(7)

Table 2. Continued.

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(18O)	4e	0.414(2)	0.961(1)	0.026(2)	0.031(7)
H(20O)	4e	0.346(2)	1.067(1)	0.064(2)	0.049(9)
H(30)	4e	0.385(2)	0.9861(9)	-0.259(2)	0.018(6)
H(31)	4e	0.317(2)	1.066(1)	-0.321(2)	0.033(7)
H(32)	4e	0.279(2)	1.1285(9)	-0.212(2)	0.024(6)
H(22O)	4e	0.140(2)	-0.057(1)	0.442(2)	0.025(7)
H(24O)	4e	0.075(2)	0.052(1)	0.505(2)	0.040(9)
H(37)	4e	0.211(2)	-0.1279(9)	0.703(2)	0.021(6)
H(38)	4e	0.192(2)	-0.073(1)	0.832(2)	0.030(6)
H(39)	4e	0.124(2)	0.011(1)	0.788(2)	0.047(8)
H(7N)	4e	0.410(2)	0.795(1)	0.633(2)	0.041(8)
H(8A)	4e	0.543(2)	0.828(1)	0.680(2)	0.047(9)
H(8B)	4e	0.623(2)	0.798(1)	0.692(2)	0.030(7)
H(9A)	4e	0.237(2)	0.715(1)	0.552(2)	0.031(7)
H(9B)	4e	0.264(2)	0.771(1)	0.573(2)	0.038(8)
H(44)	4e	0.612(2)	0.702(1)	0.658(2)	0.040(7)
H(45)	4e	0.511(2)	0.636(1)	0.613(2)	0.028(6)
H(46)	4e	0.355(2)	0.6479(9)	0.573(2)	0.022(6)
H(10N)	4e	0.112(2)	0.189(1)	-0.047(2)	0.030(7)
H(11A)	4e	-0.087(2)	0.171(1)	-0.183(2)	0.048(9)
H(11B)	4e	-0.005(2)	0.143(1)	-0.136(2)	0.034(8)
H(12A)	4e	0.240(2)	0.229(1)	0.023(2)	0.027(7)
H(12B)	4e	0.250(2)	0.281(1)	0.047(2)	0.045(8)
H(49)	4e	-0.097(2)	0.264(1)	-0.177(2)	0.042(8)
H(50)	4e	-0.022(2)	0.3433(9)	-0.124(2)	0.023(6)
H(51)	4e	0.125(2)	0.339(1)	-0.035(2)	0.035(7)
H(25A)	4e	0.417(2)	0.876(1)	0.736(2)	0.042(9)
H(25B)	4e	0.391(2)	0.891(1)	0.651(2)	0.06(1)

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Cr(1)	4e	0.07538(2)	0.11798(1)	0.16532(2)	0.0238(2)	0.0154(2)	0.0167(2)	0.0018(1)	0.0036(1)	0.0009(1)
Cr(2)	4e	0.41199(2)	0.90255(1)	0.34322(2)	0.0245(2)	0.0173(2)	0.0163(2)	0.0028(1)	0.0034(1)	0.0016(1)
O(1)	4e	-0.0558(1)	0.11016(6)	0.1072(1)	0.0256(7)	0.0182(7)	0.0225(7)	-0.0001(6)	0.0037(5)	0.0003(5)
O(2)	4e	-0.1819(1)	0.15459(6)	0.0400(1)	0.0250(8)	0.0260(8)	0.0386(9)	-0.0032(6)	-0.0027(6)	0.0011(7)
O(3)	4e	0.19089(9)	0.15454(6)	0.2242(1)	0.0254(7)	0.0213(7)	0.0246(7)	0.0031(6)	0.0030(6)	0.0005(6)
O(4)	4e	0.2512(1)	0.23342(7)	0.2753(1)	0.0246(8)	0.0315(9)	0.044(1)	-0.0011(7)	-0.0016(7)	-0.0055(7)
O(5)	4e	0.0677(1)	0.08744(6)	0.2895(1)	0.0305(8)	0.0183(7)	0.0198(7)	0.0032(6)	0.0064(6)	0.0008(5)
O(6)	4e	0.0945(1)	0.01528(6)	0.38104(9)	0.0326(8)	0.0235(8)	0.0186(7)	0.0038(6)	0.0063(6)	0.0036(6)
O(7)	4e	0.0987(1)	0.11902(6)	0.0379(1)	0.0333(8)	0.0191(7)	0.0190(7)	0.0026(6)	0.0073(6)	0.0025(5)
O(8)	4e	0.1138(1)	0.06668(6)	-0.0802(1)	0.056(1)	0.0290(9)	0.0184(7)	0.0016(8)	0.0113(7)	-0.0003(6)
O(9)	4e	0.4175(1)	0.93198(6)	0.21678(9)	0.0332(8)	0.0208(7)	0.0179(6)	0.0051(6)	0.0064(6)	0.0011(5)
O(10)	4e	0.3941(1)	1.00393(6)	0.1255(1)	0.048(1)	0.0255(8)	0.0182(7)	0.0092(7)	0.0109(6)	0.0039(6)
O(11)	4e	0.3976(1)	0.90462(6)	0.47369(9)	0.0304(8)	0.0221(7)	0.0186(7)	0.0045(6)	0.0064(6)	0.0019(5)
O(12)	4e	0.3550(1)	0.95572(6)	0.5803(1)	0.0452(9)	0.0279(8)	0.0171(7)	0.0038(7)	0.0099(6)	0.0013(6)
O(13)	4e	0.5455(1)	0.89964(6)	0.3861(1)	0.0256(7)	0.0194(7)	0.0238(7)	0.0014(6)	0.0039(6)	0.0018(6)
O(14)	4e	0.6653(1)	0.84625(6)	0.4286(1)	0.0240(7)	0.0250(8)	0.0392(9)	0.0002(6)	0.0039(6)	0.0020(7)
O(15)	4e	0.2879(1)	0.87538(6)	0.2942(1)	0.0251(7)	0.0284(8)	0.0237(7)	0.0023(6)	0.0038(6)	0.0030(6)
O(16)	4e	0.2015(1)	0.80222(7)	0.2756(1)	0.0251(8)	0.0384(9)	0.0336(9)	-0.0043(7)	0.0003(6)	-0.0001(7)
O(17)	4e	0.4338(2)	0.91092(7)	-0.1398(1)	0.083(1)	0.0288(9)	0.0268(8)	0.0165(9)	0.0116(9)	-0.0031(7)
O(18)	4e	0.4288(1)	0.93846(7)	-0.0003(1)	0.053(1)	0.0226(8)	0.0211(7)	0.0100(7)	0.0089(7)	0.0002(6)
O(19)	4e	0.2714(1)	1.15994(6)	-0.0485(1)	0.051(1)	0.0238(8)	0.0383(9)	0.0112(7)	0.0173(8)	0.0077(7)
O(20)	4e	0.3215(1)	1.09872(7)	0.0589(1)	0.056(1)	0.0265(9)	0.0252(8)	0.0142(8)	0.0152(7)	0.0019(7)
O(21)	4e	0.2046(1)	-0.15286(6)	0.5327(1)	0.0442(9)	0.0226(8)	0.0323(8)	0.0075(7)	0.0059(7)	-0.0009(6)
O(22)	4e	0.1581(1)	-0.08533(7)	0.4385(1)	0.044(1)	0.0243(9)	0.0225(7)	0.0076(7)	0.0081(7)	-0.0012(6)
O(23)	4e	0.0649(1)	0.08958(7)	0.6809(1)	0.061(1)	0.0281(9)	0.0337(9)	0.0130(8)	0.0049(8)	-0.0073(7)
O(24)	4e	0.0631(1)	0.07217(7)	0.5332(1)	0.046(1)	0.0197(8)	0.0291(8)	0.0061(7)	0.0060(7)	0.0003(7)
O(25)	4e	0.4137(1)	0.86823(7)	0.6866(1)	0.061(1)	0.0240(9)	0.0198(8)	0.0116(8)	0.0047(8)	-0.0005(7)
N(1)	4e	0.0351(1)	0.19250(6)	0.1608(1)	0.0208(8)	0.0183(8)	0.0177(7)	-0.0001(6)	0.0043(6)	-0.0004(6)
N(2)	4e	0.1100(1)	0.04326(6)	0.1523(1)	0.0218(8)	0.0174(8)	0.0182(7)	0.0007(6)	0.0033(6)	-0.0001(6)
N(3)	4e	0.3789(1)	0.97801(7)	0.3538(1)	0.0242(8)	0.0186(8)	0.0168(7)	-0.0001(6)	0.0029(6)	0.0003(6)
N(4)	4e	0.4334(1)	0.82498(7)	0.3497(1)	0.0250(8)	0.0203(8)	0.0168(7)	0.0008(7)	0.0047(6)	0.0011(6)
N(5)	4e	0.3561(1)	1.03202(7)	-0.0688(1)	0.0276(9)	0.0221(9)	0.0189(8)	0.0016(7)	0.0059(6)	0.0022(6)
N(6)	4e	0.1311(1)	-0.02573(7)	0.5804(1)	0.0222(8)	0.0193(8)	0.0215(8)	-0.0003(6)	0.0045(6)	0.0000(6)
N(7)	4e	0.4259(1)	0.76704(8)	0.6284(1)	0.0257(9)	0.0183(9)	0.0286(9)	0.0012(7)	0.0045(7)	-0.0030(7)
N(8)	4e	0.5690(2)	0.80249(9)	0.6768(2)	0.023(1)	0.022(1)	0.067(2)	0.0006(8)	0.002(1)	-0.009(1)
N(9)	4e	0.2773(1)	0.74017(8)	0.5807(2)	0.026(1)	0.021(1)	0.042(1)	0.0008(8)	0.0001(8)	-0.0016(8)

Table 3. Continued.

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
N(10)	4e	0.0871(1)	0.21657(7)	-0.0609(1)	0.0241(9)	0.0173(9)	0.0254(9)	0.0018(7)	0.0015(7)	0.0018(7)
N(11)	4e	-0.0353(2)	0.16929(9)	-0.1453(2)	0.031(1)	0.025(1)	0.038(1)	-0.0075(9)	-0.0071(9)	0.0073(8)
N(12)	4e	0.2160(1)	0.25425(9)	0.0306(1)	0.026(1)	0.022(1)	0.036(1)	-0.0009(8)	0.0003(8)	-0.0061(8)
C(1)	4e	-0.0500(1)	0.20338(8)	0.1163(1)	0.0216(9)	0.0198(9)	0.0182(9)	0.0013(7)	0.0037(7)	0.0009(7)
C(2)	4e	-0.0785(1)	0.25557(8)	0.1045(1)	0.025(1)	0.021(1)	0.024(1)	0.0043(8)	0.0029(8)	0.0004(8)
C(3)	4e	-0.0163(2)	0.29546(9)	0.1384(2)	0.032(1)	0.017(1)	0.027(1)	0.0027(8)	0.0049(8)	-0.0007(8)
C(4)	4e	0.0723(2)	0.28296(9)	0.1835(2)	0.028(1)	0.019(1)	0.026(1)	-0.0019(8)	0.0049(8)	-0.0021(8)
C(5)	4e	0.0965(1)	0.23008(8)	0.1935(1)	0.0212(9)	0.021(1)	0.0201(9)	-0.0010(7)	0.0042(7)	-0.0013(7)
C(6)	4e	-0.1025(1)	0.15313(8)	0.0841(1)	0.026(1)	0.020(1)	0.0221(9)	-0.0009(8)	0.0056(8)	0.0022(7)
C(7)	4e	0.1879(1)	0.20564(9)	0.2356(1)	0.023(1)	0.026(1)	0.023(1)	0.0018(8)	0.0030(8)	-0.0012(8)
C(8)	4e	0.1143(1)	0.01007(8)	0.2247(1)	0.0218(9)	0.0190(9)	0.0173(9)	-0.0003(7)	0.0031(7)	0.0003(7)
C(9)	4e	0.1386(1)	-0.04227(8)	0.2171(1)	0.027(1)	0.020(1)	0.023(1)	-0.0012(8)	0.0049(8)	0.0021(8)
C(10)	4e	0.1563(2)	-0.05887(8)	0.1327(2)	0.032(1)	0.018(1)	0.026(1)	0.0006(8)	0.0058(8)	-0.0013(8)
C(11)	4e	0.1482(2)	-0.02390(8)	0.0576(2)	0.033(1)	0.022(1)	0.0206(9)	0.0002(8)	0.0070(8)	-0.0037(8)
C(12)	4e	0.1250(1)	0.02799(8)	0.0707(1)	0.025(1)	0.021(1)	0.0170(9)	-0.0012(8)	0.0041(7)	-0.0005(7)
C(13)	4e	0.0907(1)	0.03873(8)	0.3064(1)	0.0195(9)	0.0187(9)	0.0197(9)	0.0005(7)	0.0034(7)	-0.0016(7)
C(14)	4e	0.1119(1)	0.07351(8)	0.0013(1)	0.028(1)	0.021(1)	0.0211(9)	0.0004(8)	0.0054(8)	0.0025(8)
C(15)	4e	0.3708(1)	1.00993(8)	0.2795(1)	0.0234(9)	0.0199(9)	0.0183(9)	0.0013(8)	0.0039(7)	0.0011(7)
C(16)	4e	0.3396(1)	1.06149(8)	0.2828(1)	0.028(1)	0.018(1)	0.023(1)	-0.0012(8)	0.0039(8)	0.0001(8)
C(17)	4e	0.3175(2)	1.07824(9)	0.3651(2)	0.029(1)	0.019(1)	0.024(1)	0.0024(8)	0.0042(8)	-0.0002(8)
C(18)	4e	0.3254(1)	1.04417(8)	0.4412(1)	0.026(1)	0.026(1)	0.0180(9)	0.0002(8)	0.0060(8)	-0.0038(8)
C(19)	4e	0.3571(1)	0.99348(8)	0.4327(1)	0.0229(9)	0.021(1)	0.0166(8)	0.0007(8)	0.0016(7)	0.0007(7)
C(20)	4e	0.3959(1)	0.98040(8)	0.2001(1)	0.025(1)	0.022(1)	0.0184(9)	0.0034(8)	0.0039(7)	0.0020(7)
C(21)	4e	0.3707(1)	0.94875(8)	0.5034(1)	0.026(1)	0.024(1)	0.0186(9)	0.0005(8)	0.0033(7)	0.0011(8)
C(22)	4e	0.5175(1)	0.80781(8)	0.3855(1)	0.025(1)	0.019(1)	0.0185(9)	0.0037(8)	0.0034(7)	0.0012(7)
C(23)	4e	0.5325(2)	0.75424(9)	0.4053(2)	0.027(1)	0.022(1)	0.031(1)	0.0028(8)	0.0046(9)	0.0039(8)
C(24)	4e	0.4584(2)	0.72030(9)	0.3872(2)	0.037(1)	0.019(1)	0.030(1)	-0.0002(9)	0.0040(9)	0.0019(9)
C(25)	4e	0.3716(2)	0.73966(9)	0.3521(2)	0.031(1)	0.024(1)	0.025(1)	-0.0059(9)	0.0029(8)	0.0011(8)
C(26)	4e	0.3609(1)	0.79338(8)	0.3337(1)	0.026(1)	0.024(1)	0.0187(9)	-0.0009(8)	0.0036(7)	-0.0003(8)
C(27)	4e	0.5839(1)	0.85360(8)	0.4024(1)	0.026(1)	0.022(1)	0.0199(9)	0.0007(8)	0.0052(7)	0.0015(7)
C(28)	4e	0.2749(1)	0.82474(9)	0.2980(1)	0.028(1)	0.030(1)	0.0175(9)	0.0012(9)	0.0023(8)	0.0022(8)
C(29)	4e	0.3785(1)	0.99835(8)	-0.1298(1)	0.029(1)	0.022(1)	0.0197(9)	-0.0010(8)	0.0056(8)	-0.0018(8)
C(30)	4e	0.3671(2)	1.01029(9)	-0.2243(2)	0.033(1)	0.028(1)	0.020(1)	-0.0027(9)	0.0077(8)	-0.0015(8)
C(31)	4e	0.3292(2)	1.05866(9)	-0.2571(1)	0.029(1)	0.033(1)	0.0173(9)	-0.0060(9)	0.0034(8)	0.0047(8)
C(32)	4e	0.3042(1)	1.09358(9)	-0.1952(2)	0.024(1)	0.026(1)	0.024(1)	-0.0023(8)	0.0048(8)	0.0050(8)
C(33)	4e	0.3209(1)	1.07858(8)	-0.1012(1)	0.024(1)	0.022(1)	0.025(1)	0.0007(8)	0.0080(8)	0.0025(8)
C(34)	4e	0.4161(2)	0.94608(9)	-0.0909(2)	0.040(1)	0.027(1)	0.023(1)	0.0031(9)	0.0065(9)	-0.0033(8)
C(35)	4e	0.3018(2)	1.11589(9)	-0.0287(2)	0.033(1)	0.024(1)	0.027(1)	0.0043(9)	0.0118(9)	0.0027(8)
C(36)	4e	0.1649(1)	-0.07407(8)	0.6027(1)	0.0229(9)	0.0185(9)	0.025(1)	-0.0009(8)	0.0069(8)	0.0009(8)
C(37)	4e	0.1872(1)	-0.09380(8)	0.6939(2)	0.028(1)	0.019(1)	0.026(1)	0.0004(8)	0.0062(8)	0.0025(8)
C(38)	4e	0.1729(1)	-0.06137(9)	0.7652(2)	0.026(1)	0.027(1)	0.022(1)	-0.0043(8)	0.0060(8)	0.0033(8)
C(39)	4e	0.1363(1)	-0.01137(9)	0.7433(2)	0.025(1)	0.028(1)	0.024(1)	-0.0021(8)	0.0080(8)	-0.0041(8)
C(40)	4e	0.1174(1)	0.00464(8)	0.6500(2)	0.023(1)	0.022(1)	0.026(1)	-0.0011(8)	0.0045(8)	-0.0006(8)
C(41)	4e	0.1782(1)	-0.10756(8)	0.5222(2)	0.028(1)	0.023(1)	0.025(1)	0.0018(8)	0.0058(8)	0.0011(8)
C(42)	4e	0.0795(2)	0.05913(9)	0.6233(2)	0.033(1)	0.021(1)	0.028(1)	0.0028(9)	0.0034(9)	-0.0016(8)
C(43)	4e	0.5176(1)	0.75993(9)	0.6502(2)	0.024(1)	0.023(1)	0.029(1)	0.0004(8)	0.0037(8)	-0.0013(8)
C(44)	4e	0.5509(2)	0.70885(9)	0.6444(2)	0.025(1)	0.025(1)	0.032(1)	0.0019(9)	0.0029(9)	-0.0038(9)
C(45)	4e	0.4897(2)	0.66827(9)	0.6162(2)	0.033(1)	0.017(1)	0.028(1)	0.0032(9)	0.0040(9)	-0.0028(8)
C(46)	4e	0.3976(2)	0.67629(9)	0.5928(2)	0.029(1)	0.020(1)	0.028(1)	0.0000(8)	0.0012(8)	0.0011(8)
C(47)	4e	0.3654(1)	0.72765(8)	0.5991(1)	0.027(1)	0.020(1)	0.0217(9)	-0.0008(8)	0.0035(8)	0.0001(8)
C(48)	4e	0.0024(1)	0.21675(9)	-0.1172(1)	0.025(1)	0.025(1)	0.0224(9)	-0.0028(8)	0.0042(8)	0.0040(8)
C(49)	4e	-0.0403(2)	0.26521(9)	-0.1406(2)	0.025(1)	0.026(1)	0.025(1)	0.0010(8)	0.0031(8)	0.0055(8)
C(50)	4e	0.0069(2)	0.31115(9)	-0.1086(2)	0.034(1)	0.021(1)	0.028(1)	0.0068(9)	0.0118(9)	0.0072(8)
C(51)	4e	0.0938(2)	0.31007(9)	-0.0534(2)	0.033(1)	0.019(1)	0.030(1)	-0.0022(9)	0.0109(9)	-0.0004(8)

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