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Crystal structure of 2-(2,6-diisopropyl-phenylamino)-6-(2,4,6-triisopropyl-phenyl)-pyridinium [2-(2,6-diisopropyl-phenylamido)-6-(2,4,6-triisopropyl-phenyl)-pyridinium]-(μ-chloro)-di(μ-oxo)-tetrachloro-tetrahydrofuran-dichromate(IV) pentane solvate, $(C_{32}H_{45}N_2)[(C_{32}H_{44}N_2)Cl_5Cr_2O_2(C_4H_8O)]\cdot C_5H_{12}$

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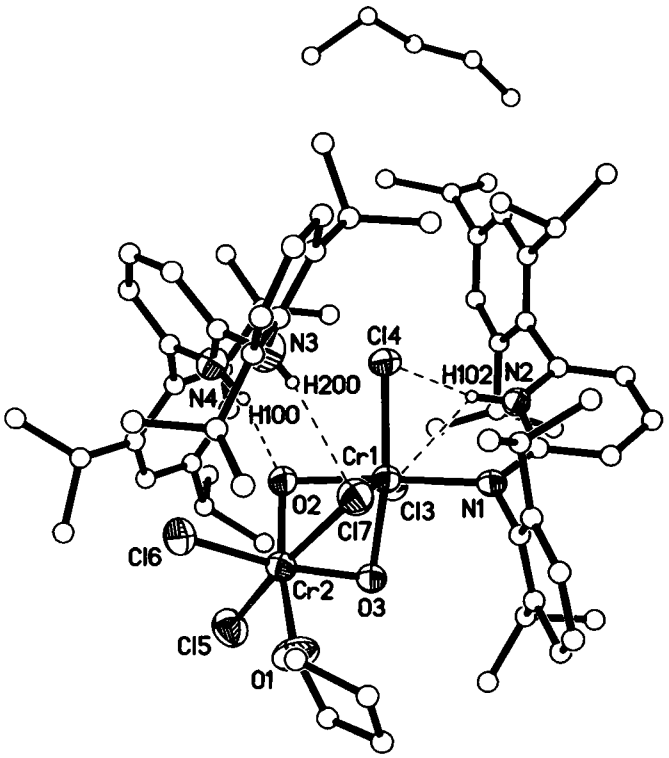

Abstract

$C_{73}H_{109}Cl_5Cr_2N_4O_3$, monoclinic, $P12_1/c1$ (no. 14), a = 14.499(5) Å, b = 17.826(5) Å, c = 30.234(5) Å, β = 90.095(5)°, V = 7814.2 Å^3, Z = 4, $R_{gt}(F)$ = 0.063, $wR_{ref}(F^2)$ = 0.176, T = 193 K.

Source of material

$CrCl_3(thf)_3$ (0.43 g, 1.15 mmol), KAp* (0.57 g, 1.15 mmol) (Ap* = deprotonated (2,6-diisopropyl-phenyl)-[6-(2,4,6-triisopropyl-phenyl)-pyridin-2-yl]-amine) [1] and THF (30 mL) were stirred for 16 h in a Schlenk flask. The solvent was removed under vacuum and a mixture of *n*-pentane/ether (60 mL; 1:1, *v*/*v*) was added. The suspension was filtered and upon standing at –80 °C for five days, green crystals of the title complex were formed.

Experimental details

The H atoms attached to N atoms were included in the refinement process due to their importance with regard to the H-bond pattern.

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Discussion

The title compound is a dinuclear chromium(IV) complex. Each of the chromium atoms adopts an octahedral coordination. They are coordinated by two chloro ligands and connected via a μ-chloro and two μ-oxygen bridges with bond angles of ∠Cr1–O2–Cr2 = 89.21°, ∠Cr1–O3–Cr2 = 90.55° and ∠Cr1–Cl7–Cr2 = 71.23°. The coordination spheres are completed by the amido atom of the aminopyridinato ligand for Cr1 and by one THF for Cr2. The Cr1 atom is deviated by 0.1759 Å from the plane through Cl3, Cl4, Cl7, O3; and the Cr2 atom lies in the appropriate plane (Cl5, Cl6, Cl7, O3; deviation of only 0.0661 Å). The angle between the Cl_3O planes is 73.2°. In both aminopyridinato ligands, the $N_{pyridine}$ atoms are protonated and inter- and intramolecular hydrogen bonds are formed. The H102—$N_{pyridine}$ moiety of the aminopyridinato ligand coordinated to the Cr1 forms intermolecular hydrogen bonds to the adjacent chloro ligands of the Cr1 (d(H102···Cl3) = 2.601 Å, d(H102···Cl4) = 2.401 Å). The protonated aminopyridinato molecule is coordinated over intermolecular hydrogen bonds N4–H100···O2 (d(H100···O2) = 1.887 Å) and N3–H200···Cl7 (d(H200···Cl7) = 2.482 Å). The Cr1—Cr2 distance of 2.817 Å indicates a proximity close enough to observe metal-metal interactions. One uncoordinated *n*-pentane molecule was also found in the crystal structure.

Table 1. Data collection and handling.

Crystal:	green prism, size 0.21 × 0.33 × 0.34 mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ:	4.93 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS II, ω
$2\theta_{max}$:	52.54°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	99835, 15537
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 8968
$N(param)_{refined}$:	771
Programs:	SIR97 [2], SHELXL-97 [3]

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

Atom	Site	x	y	z	U_{iso}
H(3)	4*e*	1.2514	0.1273	0.3133	0.063
H(4)	4*e*	1.2685	0.2321	0.3573	0.071
H(5)	4*e*	1.1477	0.3151	0.3670	0.068
H(7)	4*e*	0.9156	0.2893	0.3301	0.068
H(8A)	4*e*	0.9333	0.4148	0.3060	0.135
H(8B)	4*e*	0.9805	0.3582	0.2718	0.135

Table 2. Continued.

Atom	Site	x	y	z	U_{iso}
H(8C)	4e	1.0429	0.4048	0.3058	0.135
H(9A)	4e	0.9214	0.3855	0.3838	0.121
H(9B)	4e	1.0307	0.3751	0.3882	0.121
H(9C)	4e	0.9628	0.3094	0.4037	0.121
H(10)	4e	1.0429	0.0680	0.2601	0.061
H(11A)	4e	1.1410	−0.0376	0.2673	0.096
H(11B)	4e	1.1140	−0.0067	0.3153	0.096
H(11C)	4e	1.2135	0.0113	0.2950	0.096
H(12A)	4e	1.1540	0.0456	0.2042	0.112
H(12B)	4e	1.2256	0.0995	0.2290	0.112
H(12C)	4e	1.1331	0.1335	0.2081	0.112
H(14)	4e	1.0674	0.2576	0.2318	0.061
H(15)	4e	1.0400	0.2929	0.1598	0.071
H(16)	4e	0.9002	0.2618	0.1249	0.059
H(20)	4e	0.6329	0.0588	0.1139	0.074
H(22)	4e	0.5560	0.2718	0.1366	0.067
H(24)	4e	0.7701	0.3317	0.1839	0.061
H(25A)	4e	0.6628	0.3921	0.2289	0.152
H(25B)	4e	0.6675	0.3044	0.2400	0.152
H(25C)	4e	0.5835	0.3369	0.2115	0.152
H(26A)	4e	0.7183	0.3812	0.1160	0.138
H(26B)	4e	0.7000	0.4385	0.1558	0.138
H(26C)	4e	0.6168	0.3900	0.1361	0.138
H(27)	4e	0.4668	0.1998	0.1010	0.129
H(28A)	4e	0.5416	0.1661	0.0438	0.303
H(28B)	4e	0.4312	0.1689	0.0447	0.303
H(28C)	4e	0.4835	0.0899	0.0466	0.303
H(29A)	4e	0.4404	0.1343	0.1627	0.169
H(29B)	4e	0.4102	0.0674	0.1304	0.169
H(29C)	4e	0.3602	0.1473	0.1270	0.169
H(30)	4e	0.8463	0.0703	0.1712	0.070
H(31A)	4e	0.9040	0.0115	0.1068	0.147
H(31B)	4e	0.8912	0.0997	0.0990	0.147
H(31C)	4e	0.8176	0.0418	0.0791	0.147
H(32A)	4e	0.8066	−0.0574	0.1595	0.119
H(32B)	4e	0.7137	−0.0324	0.1349	0.119
H(32C)	4e	0.7269	−0.0156	0.1865	0.119
H(34)	4e	0.5198	0.2533	0.4431	0.068
H(35)	4e	0.3950	0.1772	0.4320	0.074
H(36)	4e	0.4099	0.0624	0.3947	0.064
H(40)	4e	0.5959	−0.0641	0.2605	0.054
H(42)	4e	0.6421	−0.1697	0.3761	0.058
H(44)	4e	0.6078	−0.0125	0.4451	0.061
H(45A)	4e	0.4946	−0.0830	0.4838	0.099
H(45B)	4e	0.4769	−0.1330	0.4406	0.099
H(45C)	4e	0.4512	−0.0457	0.4403	0.099
H(46A)	4e	0.6566	−0.1153	0.4880	0.095
H(46B)	4e	0.7246	−0.1036	0.4470	0.095
H(46C)	4e	0.6494	−0.1692	0.4458	0.095
H(47)	4e	0.6679	−0.2371	0.3113	0.078
H(48A)	4e	0.6339	−0.2639	0.2390	0.200
H(48B)	4e	0.6001	−0.1796	0.2310	0.200
H(48C)	4e	0.5440	−0.2332	0.2637	0.200
H(49A)	4e	0.7978	−0.1623	0.2970	0.188

Table 2. Continued.

Atom	Site	x	y	z	U_{iso}
H(49B)	4e	0.7546	−0.1385	0.2503	0.188
H(49C)	4e	0.7836	−0.2238	0.2591	0.188
H(50)	4e	0.5449	0.1144	0.3058	0.053
H(51A)	4e	0.5566	0.1239	0.2286	0.076
H(51B)	4e	0.5713	0.0352	0.2246	0.076
H(51C)	4e	0.6481	0.0860	0.2481	0.076
H(52A)	4e	0.4070	0.1045	0.2633	0.100
H(52B)	4e	0.3979	0.0589	0.3087	0.100
H(52C)	4e	0.4165	0.0151	0.2634	0.100
H(53A)	4e	1.0906	−0.0179	0.3920	0.089
H(53B)	4e	1.1049	−0.0466	0.4421	0.089
H(54A)	4e	1.2235	0.0315	0.4463	0.110
H(54B)	4e	1.1954	0.0714	0.4004	0.110
H(55A)	4e	1.1695	0.1322	0.4802	0.114
H(55B)	4e	1.1229	0.1629	0.4354	0.114
H(56A)	4e	1.0423	0.0672	0.4997	0.077
H(56B)	4e	0.9927	0.1332	0.4720	0.077
H(59)	4e	0.7561	0.3821	0.5255	0.109
H(60)	4e	0.6816	0.4818	0.4931	0.124
H(61)	4e	0.6251	0.4722	0.4215	0.100
H(63)	4e	0.6210	0.3053	0.3559	0.108
H(64A)	4e	0.6637	0.3985	0.3052	0.192
H(64B)	4e	0.7469	0.3783	0.3379	0.192
H(64C)	4e	0.6887	0.4536	0.3452	0.192
H(65A)	4e	0.4811	0.3560	0.3802	0.252
H(65B)	4e	0.5007	0.3797	0.3300	0.252
H(65C)	4e	0.5171	0.4388	0.3691	0.252
H(66)	4e	0.7907	0.2015	0.4751	0.081
H(67A)	4e	0.7428	0.1600	0.5449	0.204
H(67B)	4e	0.6571	0.1865	0.5153	0.204
H(67C)	4e	0.6954	0.2396	0.5538	0.204
H(68A)	4e	0.8964	0.2131	0.5336	0.187
H(68B)	4e	0.8613	0.2968	0.5426	0.187
H(68C)	4e	0.9127	0.2771	0.4973	0.187
C(102)	4e	0.177(2)	0.159(2)	0.013(1)	0.36(1)
H(10A)	4e	0.2002	0.1091	0.0223	0.430
H(10B)	4e	0.1222	0.1474	−0.0053	0.430
C(100)	4e	0.309(1)	0.1509(9)	−0.0501(6)	0.220(6)
H(10C)	4e	0.3234	0.1912	−0.0711	0.330
H(10D)	4e	0.2872	0.1067	−0.0663	0.330
H(10E)	4e	0.3647	0.1379	−0.0333	0.330
C(101)	4e	0.242(2)	0.175(1)	−0.0215(9)	0.32(1)
H(10F)	4e	0.1995	0.1987	−0.0430	0.386
H(10G)	4e	0.2746	0.2174	−0.0077	0.386
C(103)	4e	0.128(2)	0.183(2)	0.056(1)	0.46(2)
H(10H)	4e	0.0641	0.1983	0.0496	0.549
H(10I)	4e	0.1606	0.2267	0.0692	0.549
C(104)	4e	0.126(2)	0.118(2)	0.091(1)	0.40(2)
H(10J)	4e	0.0829	0.1307	0.1148	0.597
H(10K)	4e	0.1882	0.1117	0.1039	0.597
H(10L)	4e	0.1072	0.0715	0.0768	0.597
H(100)	4e	0.678(3)	0.104(3)	0.379(2)	0.06(1)
H(200)	4e	0.737(4)	0.213(4)	0.403(2)	0.09(2)
H(102)	4e	0.821(3)	0.168(3)	0.238(2)	0.05(1)

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}
Cr(1)	4e	0.86463(4)	0.11275(4)	0.32048(2)	0.0281(3)	0.0406(3)	0.0323(3)	0.0007(3)	−0.0016(2)	0.0053(3)
Cr(2)	4e	0.89206(4)	0.03704(4)	0.40122(2)	0.0341(3)	0.0395(3)	0.0345(3)	−0.0003(3)	−0.0030(3)	0.0044(3)
Cl(3)	4e	0.83810(7)	0.02962(6)	0.26447(3)	0.0443(5)	0.0461(6)	0.0384(5)	−0.0016(4)	−0.0030(4)	0.0010(4)
Cl(4)	4e	0.74219(6)	0.19365(6)	0.30653(3)	0.0336(5)	0.0494(6)	0.0416(6)	0.0080(4)	0.0006(4)	0.0066(4)
Cl(5)	4e	0.89298(9)	−0.09078(6)	0.39672(4)	0.0684(7)	0.0392(6)	0.0564(7)	0.0032(5)	0.0081(6)	0.0031(5)
Cl(6)	4e	0.80481(7)	0.04663(6)	0.46453(3)	0.0506(6)	0.0495(6)	0.0377(6)	−0.0022(5)	0.0037(4)	0.0026(4)
Cl(7)	4e	0.89829(8)	0.17066(6)	0.39168(4)	0.0489(6)	0.0524(6)	0.0486(7)	−0.0022(5)	−0.0015(5)	0.0054(5)
N(1)	4e	0.9547(2)	0.1779(2)	0.2836(1)	0.027(2)	0.043(2)	0.038(2)	0.000(1)	−0.007(1)	0.010(2)
N(4)	4e	0.6209(2)	0.1178(2)	0.3912(1)	0.037(2)	0.038(2)	0.038(2)	−0.003(2)	0.003(1)	−0.007(2)
N(2)	4e	0.8627(2)	0.1899(2)	0.2208(1)	0.029(2)	0.049(2)	0.030(2)	−0.000(2)	−0.003(1)	0.009(2)
O(2)	4e	0.7845(2)	0.0507(2)	0.36175(9)	0.032(1)	0.045(2)	0.035(2)	−0.000(1)	0.000(1)	0.007(1)

Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(3)	4e	0.6905(3)	0.2275(2)	0.4142(1)	0.054(2)	0.046(2)	0.050(2)	−0.010(2)	0.005(2)	−0.017(2)
O(3)	4e	0.9602(2)	0.0445(2)	0.34452(9)	0.031(1)	0.049(2)	0.040(2)	−0.001(1)	−0.004(1)	0.012(1)
O(1)	4e	1.0115(2)	0.0378(2)	0.4366(1)	0.043(2)	0.085(2)	0.047(2)	0.012(2)	−0.013(1)	−0.015(2)
C(1)	4e	1.0432(3)	0.1939(2)	0.3037(1)	0.030(2)	0.047(2)	0.038(2)	−0.006(2)	−0.005(2)	0.011(2)
C(2)	4e	1.1169(3)	0.1439(3)	0.2969(1)	0.031(2)	0.057(3)	0.042(2)	−0.001(2)	−0.004(2)	0.012(2)
C(3)	4e	1.2005(3)	0.1602(3)	0.3174(2)	0.027(2)	0.077(3)	0.054(3)	0.000(2)	−0.005(2)	0.013(3)
C(4)	4e	1.2109(3)	0.2226(3)	0.3433(2)	0.040(2)	0.078(3)	0.060(3)	−0.014(2)	−0.017(2)	0.015(3)
C(5)	4e	1.1390(3)	0.2716(3)	0.3493(2)	0.055(3)	0.062(3)	0.053(3)	−0.015(2)	−0.015(2)	0.005(2)
C(6)	4e	1.0528(3)	0.2584(3)	0.3297(2)	0.044(2)	0.051(3)	0.046(3)	−0.006(2)	−0.012(2)	0.008(2)
C(7)	4e	0.9755(3)	0.3155(3)	0.3355(2)	0.056(3)	0.048(3)	0.066(3)	−0.002(2)	−0.012(2)	−0.001(2)
C(8)	4e	0.9838(5)	0.3790(3)	0.3017(2)	0.107(5)	0.059(4)	0.105(5)	0.005(3)	−0.028(4)	0.013(3)
C(9)	4e	0.9723(5)	0.3494(3)	0.3820(2)	0.090(4)	0.063(3)	0.090(5)	0.005(3)	−0.011(3)	−0.021(3)
C(10)	4e	1.1096(3)	0.0764(3)	0.2669(2)	0.036(2)	0.064(3)	0.053(3)	0.008(2)	−0.003(2)	0.004(2)
C(11)	4e	1.1480(4)	0.0043(3)	0.2881(2)	0.053(3)	0.072(3)	0.067(4)	0.011(3)	0.001(2)	0.008(3)
C(12)	4e	1.1601(4)	0.0899(4)	0.2231(2)	0.081(4)	0.088(4)	0.055(3)	0.008(3)	0.012(3)	0.004(3)
C(13)	4e	0.9440(2)	0.2041(2)	0.2427(1)	0.029(2)	0.040(2)	0.040(2)	0.000(2)	−0.004(2)	0.012(2)
C(14)	4e	1.0104(3)	0.2448(3)	0.2182(2)	0.032(2)	0.070(3)	0.050(3)	−0.013(2)	−0.007(2)	0.020(2)
C(15)	4e	0.9942(3)	0.2658(3)	0.1756(2)	0.040(2)	0.082(4)	0.056(3)	−0.011(2)	0.001(2)	0.031(3)
C(16)	4e	0.9107(3)	0.2479(3)	0.1548(2)	0.034(2)	0.071(3)	0.041(3)	0.002(2)	−0.001(2)	0.020(2)
C(17)	4e	0.8453(3)	0.2107(2)	0.1778(1)	0.035(2)	0.045(2)	0.035(2)	0.005(2)	−0.004(2)	0.006(2)
C(18)	4e	0.7519(3)	0.1925(2)	0.1599(1)	0.039(2)	0.053(2)	0.029(2)	0.004(2)	−0.005(2)	0.005(2)
C(19)	4e	0.7330(3)	0.1203(2)	0.1440(1)	0.059(3)	0.046(2)	0.037(2)	0.001(2)	−0.010(2)	0.007(2)
C(20)	4e	0.6470(4)	0.1074(3)	0.1249(2)	0.071(3)	0.061(3)	0.053(3)	−0.017(3)	−0.022(2)	0.009(2)
C(21)	4e	0.5809(3)	0.1642(3)	0.1214(2)	0.053(3)	0.079(4)	0.060(3)	−0.017(3)	−0.023(2)	0.017(3)
C(22)	4e	0.6014(3)	0.2334(3)	0.1382(2)	0.046(3)	0.070(3)	0.053(3)	0.002(2)	−0.013(2)	0.007(2)
C(23)	4e	0.6863(3)	0.2500(2)	0.1576(1)	0.039(2)	0.052(2)	0.038(2)	0.005(2)	−0.007(2)	0.007(2)
C(24)	4e	0.7032(3)	0.3282(3)	0.1761(2)	0.046(2)	0.060(3)	0.046(3)	0.011(2)	−0.009(2)	−0.006(2)
C(25)	4e	0.6496(6)	0.3416(4)	0.2177(2)	0.150(7)	0.092(5)	0.063(4)	0.026(5)	0.020(4)	−0.010(4)
C(26)	4e	0.6828(6)	0.3899(3)	0.1431(2)	0.160(7)	0.056(3)	0.061(4)	−0.009(4)	−0.026(4)	0.006(3)
C(27)	4e	0.4878(5)	0.1463(5)	0.1003(3)	0.079(4)	0.134(6)	0.109(6)	−0.047(4)	−0.061(4)	0.041(5)
C(28)	4e	0.4859(6)	0.1425(9)	0.0558(3)	0.084(6)	0.42(2)	0.102(7)	−0.011(9)	−0.052(5)	−0.07(1)
C(29)	4e	0.4189(4)	0.1218(5)	0.1328(3)	0.045(3)	0.136(7)	0.156(7)	−0.016(4)	−0.005(4)	−0.057(6)
C(30)	4e	0.8025(4)	0.0577(3)	0.1467(2)	0.080(3)	0.052(3)	0.044(3)	0.011(2)	−0.008(2)	0.006(2)
C(31)	4e	0.8589(5)	0.0522(4)	0.1041(2)	0.128(6)	0.091(5)	0.075(4)	0.060(4)	0.026(4)	0.020(4)
C(32)	4e	0.7584(5)	−0.0190(3)	0.1579(2)	0.122(5)	0.044(3)	0.072(4)	0.004(3)	−0.017(4)	0.000(3)
C(33)	4e	0.6147(3)	0.1857(2)	0.4115(1)	0.045(2)	0.044(2)	0.040(2)	−0.002(2)	0.000(2)	−0.006(2)
C(34)	4e	0.5269(3)	0.2072(3)	0.4278(2)	0.055(3)	0.052(3)	0.063(3)	0.001(2)	0.011(2)	−0.013(2)
C(35)	4e	0.4537(3)	0.1621(3)	0.4214(2)	0.048(3)	0.063(3)	0.073(4)	0.005(2)	0.015(2)	−0.016(3)
C(36)	4e	0.4624(3)	0.0933(3)	0.3993(2)	0.036(2)	0.054(3)	0.071(3)	−0.004(2)	0.009(2)	−0.009(2)
C(37)	4e	0.5470(3)	0.0713(2)	0.3845(1)	0.034(2)	0.042(2)	0.047(3)	−0.004(2)	0.002(2)	−0.005(2)
C(38)	4e	0.5683(2)	0.0008(2)	0.3604(1)	0.026(2)	0.042(2)	0.049(3)	−0.004(2)	−0.001(2)	0.000(2)
C(39)	4e	0.5679(3)	0.0010(2)	0.3139(1)	0.029(2)	0.041(2)	0.045(2)	−0.004(2)	−0.001(2)	−0.000(2)
C(40)	4e	0.5961(3)	−0.0635(2)	0.2919(2)	0.044(2)	0.038(2)	0.052(3)	0.001(2)	0.004(2)	−0.003(2)
C(41)	4e	0.6248(3)	−0.1271(2)	0.3148(2)	0.044(2)	0.037(2)	0.066(3)	0.002(2)	0.004(2)	−0.003(2)
C(42)	4e	0.6234(3)	−0.1260(2)	0.3605(2)	0.042(2)	0.041(2)	0.062(3)	−0.003(2)	0.000(2)	0.005(2)
C(43)	4e	0.5957(3)	−0.0635(2)	0.3845(2)	0.031(2)	0.045(2)	0.050(3)	−0.006(2)	−0.001(2)	0.002(2)
C(44)	4e	0.5926(3)	−0.0643(3)	0.4346(2)	0.050(3)	0.056(3)	0.045(3)	−0.012(2)	−0.006(2)	0.003(2)
C(45)	4e	0.4949(3)	−0.0832(3)	0.4514(2)	0.056(3)	0.088(4)	0.054(3)	−0.016(3)	0.006(2)	0.004(3)
C(46)	4e	0.6620(4)	−0.1179(3)	0.4558(2)	0.058(3)	0.072(3)	0.060(3)	−0.010(3)	−0.010(2)	0.018(3)
C(47)	4e	0.6628(4)	−0.1946(3)	0.2898(2)	0.079(4)	0.040(3)	0.077(4)	0.010(2)	0.007(3)	−0.004(2)
C(48)	4e	0.6055(5)	−0.2199(4)	0.2528(3)	0.079(5)	0.109(6)	0.21(1)	0.020(4)	−0.022(5)	−0.107(7)
C(49)	4e	0.7580(4)	−0.1784(5)	0.2725(3)	0.050(3)	0.128(6)	0.197(9)	0.021(4)	−0.003(4)	−0.095(6)
C(50)	4e	0.5339(3)	0.0684(2)	0.2876(2)	0.036(2)	0.040(2)	0.055(3)	−0.004(2)	0.003(2)	0.002(2)
C(51)	4e	0.5818(3)	0.0794(3)	0.2433(2)	0.045(2)	0.059(3)	0.048(3)	0.002(2)	−0.003(2)	0.006(2)
C(52)	4e	0.4294(3)	0.0611(3)	0.2801(2)	0.037(2)	0.063(3)	0.099(4)	0.009(2)	0.000(3)	0.023(3)
C(53)	4e	1.0948(3)	−0.0018(4)	0.4233(2)	0.042(3)	0.113(5)	0.068(4)	0.025(3)	−0.009(2)	−0.005(3)
C(54)	4e	1.1719(4)	0.0541(4)	0.4294(2)	0.063(4)	0.123(6)	0.088(5)	−0.005(4)	0.010(3)	0.043(4)
C(55)	4e	1.1300(4)	0.1185(4)	0.4548(3)	0.074(4)	0.101(5)	0.110(6)	−0.038(4)	−0.025(4)	0.026(4)
C(56)	4e	1.0376(4)	0.0914(3)	0.4703(2)	0.071(3)	0.070(3)	0.049(3)	−0.011(3)	−0.021(3)	−0.002(2)
C(57)	4e	0.6919(3)	0.3005(3)	0.4348(2)	0.069(3)	0.043(3)	0.048(3)	−0.010(2)	0.004(2)	−0.012(2)
C(58)	4e	0.7327(4)	0.3062(3)	0.4763(2)	0.085(4)	0.049(3)	0.044(3)	−0.013(3)	0.002(2)	−0.009(2)
C(59)	4e	0.7288(6)	0.3761(3)	0.4972(2)	0.160(7)	0.052(3)	0.061(4)	−0.003(4)	−0.028(4)	−0.019(3)
C(60)	4e	0.6867(6)	0.4356(4)	0.4776(2)	0.180(8)	0.053(4)	0.078(5)	0.001(4)	−0.017(5)	−0.023(3)
C(61)	4e	0.6514(5)	0.4294(3)	0.4354(2)	0.132(6)	0.044(3)	0.074(4)	0.008(3)	−0.014(4)	−0.006(3)
C(62)	4e	0.6536(4)	0.3619(3)	0.4131(2)	0.090(4)	0.052(3)	0.064(4)	0.002(3)	−0.009(3)	−0.011(3)
C(63)	4e	0.6196(5)	0.3591(4)	0.3653(2)	0.127(6)	0.067(4)	0.075(4)	0.021(4)	−0.037(4)	−0.017(3)
C(64)	4e	0.6855(8)	0.4010(5)	0.3358(2)	0.22(1)	0.107(6)	0.063(5)	0.025(6)	−0.011(6)	0.013(4)
C(65)	4e	0.5209(8)	0.3858(6)	0.3607(4)	0.18(1)	0.141(8)	0.18(1)	0.052(8)	−0.110(9)	−0.043(7)
C(66)	4e	0.7781(4)	0.2394(3)	0.4987(2)	0.100(4)	0.060(3)	0.041(3)	−0.003(3)	−0.002(3)	−0.008(2)
C(67)	4e	0.7126(7)	0.2032(5)	0.5310(3)	0.169(8)	0.124(7)	0.116(7)	0.032(6)	0.069(6)	0.057(6)
C(68)	4e	0.8703(6)	0.2583(5)	0.5199(3)	0.150(7)	0.093(5)	0.130(7)	0.004(5)	−0.061(6)	−0.022(5)

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