Crystal structure of chloro{2,2'-[(*R,R*)-cyclohexane-1,2-diylbis(nitrilomethylidyne)]-bis[6-tert-butyl-4-(triphenylphosphoniomethyl)phenolato]-*O,N,N',O'*}-iron(III) bis(hexafluorophosphate) tris(ethanol) solvate, $[\text{Fe}(\text{C}_{66}\text{H}_{68}\text{N}_2\text{O}_2\text{P}_2)\text{Cl}](\text{PF}_6)_2 \cdot 3\text{C}_2\text{H}_6\text{O}$

A. Pajunen^{*†}, I. Mutikainen[†], A. Haikarainen[‡] and J. Sipilä[‡][†] University of Helsinki, Department of Chemistry, Laboratory of Inorganic Chemistry, Box 55, FIN-00014, Helsinki, Finland[‡] University of Helsinki, Department of Chemistry, Laboratory of Organic Chemistry, Box 55, FIN-00014, Helsinki, Finland

Received August 21, 2000. CCDC-No. 1267/521

Table 1. Data collection and handling.

Crystal:	red plate, size 0.20 × 0.25 × 0.40 mm
Wavelength:	Mo K_{α} radiation (0.71069 Å)
μ :	3.89 cm ⁻¹
Diffractometer, scan mode:	Rigaku AFC7S, 2 θ / ω
2 θ_{max} :	48°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	12071, 12071
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3625
$N(\text{param})_{\text{refined}}$:	973
Programs:	SHELXTL/P [3], SHELXL-97 [4]

Abstract

$\text{C}_{72}\text{H}_{86}\text{ClF}_{12}\text{FeN}_2\text{O}_5\text{P}_4$, triclinic, $P1$ (No. 1), $a = 14.094(9)$ Å, $b = 21.59(1)$ Å, $c = 13.660(7)$ Å, $\alpha = 107.52(4)^\circ$, $\beta = 101.97(5)^\circ$, $\gamma = 80.80(5)^\circ$, $V = 3856.8$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.118$, $wR_{\text{ref}}(F^2) = 0.32$, $T = 193$ K.

Source of material

The complex cation as a chloride salt [1,2] was dissolved in methylenechloride and an excess of NH_4PF_6 in ethanol was added. The solution was filtered and allowed to evaporate slowly at room temperature yielding crystals of $[\text{Fe}(\text{C}_{66}\text{H}_{68}\text{N}_2\text{O}_2\text{P}_2)\text{Cl}](\text{PF}_6)_2 \cdot 3\text{C}_2\text{H}_6\text{O}$ suitable for X-ray structure determination.

Experimental details

The poor quality and the weak diffraction power of the crystals resulted in a rather high R -value and low $N(hkl)_{\text{gt}}/\text{parameter}$ ratio. Attempts to refine all non-hydrogen atoms anisotropically failed, most of the carbon atoms become non-positive definitive. Therefore, the O, N and C positions were refined isotropically. The positions of the hydrogen atoms in the ethanol solvate molecules were not determined.

Discussion

The two independent molecules have very similar structures. The cations and anions are approximately related by a center of symmetry, except for the cyclohexyl ring atoms. The Fe^{III} atom is pentacoordinated in a distorted square-pyramidal environment with four N and O atoms in the basal coordination plane and the Cl atom at the apex of the pyramid. The structure contains ill-defined and disordered ethanol solvate molecules.

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

Atom	Site	Occ.	x	y	z	U_{iso}
O(1A)	1a		1.038(1)	0.3003(9)	0.634(1)	0.066(5)
O(2A)	1a		1.048(1)	0.166(1)	0.534(2)	0.076(6)
N(1A)	1a		0.894(1)	0.277(1)	0.730(1)	0.062(5)
N(2A)	1a		0.949(2)	0.154(1)	0.681(2)	0.066(6)
C(1A)	1a		0.872(2)	0.335(1)	0.741(2)	0.056(6)
H(1A)	1a		0.8195	0.3544	0.7750	0.068
C(2A)	1a		0.921(2)	0.377(2)	0.705(2)	0.078(9)
C(3A)	1a		0.887(2)	0.448(1)	0.747(2)	0.059(7)
H(3A)	1a		0.8437	0.4588	0.7938	0.070
C(4A)	1a		0.912(2)	0.494(1)	0.726(2)	0.060(7)
C(5A)	1a		1.004(2)	0.474(2)	0.670(2)	0.078(9)
H(5A)	1a		1.0328	0.5060	0.6580	0.093
C(6A)	1a		1.046(2)	0.404(1)	0.635(2)	0.059(7)
C(7A)	1a		1.002(2)	0.355(2)	0.655(2)	0.067(8)
C(8A)	1a		0.954(3)	0.088(2)	0.628(3)	0.10(1)
H(8A)	1a		0.9203	0.0600	0.6446	0.122
C(9A)	1a		1.016(2)	0.064(1)	0.543(2)	0.055(7)
C(10A)	1a		1.012(2)	0.001(1)	0.512(2)	0.046(6)
H(10A)	1a		0.9806	-0.0191	0.5459	0.055
C(11A)	1a		1.056(2)	-0.035(1)	0.425(2)	0.044(5)
C(12A)	1a		1.101(2)	0.005(1)	0.387(2)	0.071(8)
H(12A)	1a		1.1379	-0.0161	0.3352	0.085
C(13A)	1a		1.093(2)	0.077(1)	0.423(2)	0.045(6)
C(14A)	1a		1.048(2)	0.101(1)	0.500(2)	0.061(7)
C(15A)	1a		1.149(3)	0.385(2)	0.598(3)	0.11(1)
C(16A)	1a		1.216(2)	0.356(1)	0.666(2)	0.066(8)
H(16A)	1a		1.2300	0.3869	0.7328	0.099
H(16B)	1a		1.2755	0.3397	0.6383	0.099

* Correspondence author (e-mail: Aarne.Pajunen@Helsinki.fi)

Table 2. Continued

Atom	Site	Occ.	x	y	z	U _{iso}
H(16C)	1a		1.1892	0.3196	0.6742	0.099
C(17A)	1a		1.111(2)	0.342(2)	0.480(3)	0.10(1)
H(17A)	1a		1.0608	0.3679	0.4458	0.150
H(17B)	1a		1.0865	0.3038	0.4815	0.150
H(17C)	1a		1.1649	0.3296	0.4415	0.150
C(18A)	1a		1.183(2)	0.444(2)	0.571(3)	0.09(1)
H(18A)	1a		1.1979	0.4783	0.6345	0.130
H(18B)	1a		1.1310	0.4607	0.5250	0.130
H(18C)	1a		1.2395	0.4294	0.5388	0.130
C(19A)	1a		0.890(2)	0.562(1)	0.737(2)	0.071(8)
H(19A)	1a		0.8194	0.5708	0.7202	0.085
H(19B)	1a		0.9179	0.5729	0.6864	0.085
C(20A)	1a		0.877(1)	0.693(1)	0.863(1)	0.039(6)
C(21A)	1a		0.884(2)	0.724(1)	0.790(2)	0.052(7)
H(21A)	1a		0.9271	0.7031	0.7435	0.062
C(22A)	1a		0.836(2)	0.782(1)	0.779(2)	0.079(9)
H(22A)	1a		0.8454	0.7997	0.7279	0.094
C(23A)	1a		0.769(2)	0.815(1)	0.848(2)	0.073(8)
H(23A)	1a		0.7324	0.8536	0.8413	0.087
C(24A)	1a		0.759(1)	0.789(1)	0.919(2)	0.044(5)
H(24A)	1a		0.7157	0.8121	0.9639	0.052
C(25A)	1a		0.807(2)	0.732(1)	0.934(2)	0.10(1)
H(25A)	1a		0.7957	0.7169	0.9871	0.115
C(26A)	1a		1.067(2)	0.620(1)	0.885(2)	0.072(8)
C(27A)	1a		1.108(2)	0.675(1)	0.899(1)	0.045(6)
H(27A)	1a		1.0712	0.7148	0.8971	0.053
C(28A)	1a		1.206(2)	0.669(1)	0.918(2)	0.069(8)
H(28A)	1a		1.2394	0.7048	0.9284	0.083
C(29A)	1a		1.260(3)	0.608(1)	0.921(2)	0.10(1)
H(29A)	1a		1.3281	0.6060	0.9340	0.125
C(30A)	1a		1.222(2)	0.551(2)	0.906(2)	0.09(1)
H(30A)	1a		1.2580	0.5117	0.9099	0.111
C(31A)	1a		1.120(2)	0.560(1)	0.885(2)	0.056(7)
H(31A)	1a		1.0862	0.5233	0.8702	0.067
C(32A)	1a		0.913(1)	0.593(1)	0.964(2)	0.043(6)
C(33A)	1a		0.960(2)	0.591(1)	1.058(2)	0.09(1)
H(33A)	1a		1.0231	0.6021	1.0694	0.105
C(34A)	1a		0.940(2)	0.576(1)	1.143(2)	0.053(6)
H(34A)	1a		0.9871	0.5757	1.2016	0.064
C(35A)	1a		0.847(2)	0.560(1)	1.134(2)	0.060(7)
H(35A)	1a		0.8251	0.5521	1.1889	0.072
C(36A)	1a		0.789(2)	0.557(2)	1.041(2)	0.09(1)
H(36A)	1a		0.7282	0.5421	1.0257	0.108
C(37A)	1a		0.823(2)	0.577(1)	0.969(2)	0.080(9)
H(37A)	1a		0.7752	0.5810	0.9116	0.096
C(38A)	1a		1.135(2)	0.104(2)	0.367(3)	0.11(1)
C(39A)	1a		1.064(1)	0.158(1)	0.318(2)	0.043(5)
H(39A)	1a		1.0263	0.1855	0.3691	0.065
H(39B)	1a		1.0206	0.1359	0.2579	0.065
H(39C)	1a		1.1021	0.1835	0.2986	0.065
C(40A)	1a		1.187(2)	0.072(1)	0.280(2)	0.080(8)
H(40A)	1a		1.1452	0.0455	0.2244	0.119
H(40B)	1a		1.2438	0.0454	0.3027	0.119
H(40C)	1a		1.2074	0.1047	0.2561	0.119
C(41A)	1a		1.222(2)	0.150(1)	0.442(2)	0.078(9)
H(41A)	1a		1.1980	0.1793	0.5010	0.118
H(41B)	1a		1.2422	0.1737	0.4021	0.118
H(41C)	1a		1.2773	0.1217	0.4645	0.118
C(42A)	1a		1.078(2)	-0.107(1)	0.379(2)	0.051(7)
H(42A)	1a		1.0914	-0.1143	0.3090	0.061
H(42B)	1a		1.0210	-0.1284	0.3725	0.061
C(43A)	1a		1.200(2)	-0.230(1)	0.370(2)	0.056(7)
C(44A)	1a		1.223(2)	-0.236(2)	0.274(2)	0.09(1)
H(44A)	1a		1.2297	-0.2002	0.2537	0.104
C(45A)	1a		1.235(2)	-0.301(2)	0.209(3)	0.13(1)
H(45A)	1a		1.2496	-0.3081	0.1428	0.151
C(46A)	1a		1.224(2)	-0.353(2)	0.243(2)	0.09(1)
H(46A)	1a		1.2359	-0.3945	0.1996	0.103
C(47A)	1a		1.197(2)	-0.346(1)	0.337(2)	0.072(8)
H(47A)	1a		1.1852	-0.3824	0.3547	0.087
C(48A)	1a		1.189(2)	-0.282(1)	0.407(2)	0.069(8)
H(48A)	1a		1.1767	-0.2743	0.4737	0.083
C(49A)	1a		1.158(1)	-0.154(1)	0.558(2)	0.056(6)

Table 2. Continued.

Atom	Site	Occ.	x	y	z	U _{iso}
C(50A)	1a		1.216(2)	-0.127(1)	0.665(2)	0.09(1)
H(50A)	1a		1.2758	-0.1127	0.6691	0.109
C(51A)	1a		1.182(2)	-0.122(1)	0.758(3)	0.12(1)
H(51A)	1a		1.2224	-0.1084	0.8217	0.141
C(52A)	1a		1.090(2)	-0.138(1)	0.752(3)	0.11(1)
H(52A)	1a		1.0625	-0.1265	0.8126	0.130
C(53A)	1a		1.035(3)	-0.173(2)	0.655(2)	0.11(1)
H(53A)	1a		0.9832	-0.1956	0.6515	0.137
C(54A)	1a		1.068(1)	-0.1703(9)	0.564(2)	0.049(5)
H(54A)	1a		1.0242	-0.1805	0.5019	0.059
C(55A)	1a		1.292(1)	-0.102(1)	0.476(1)	0.034(5)
C(56A)	1a		1.368(2)	-0.137(2)	0.430(2)	0.078(9)
H(56A)	1a		1.3635	-0.1806	0.3912	0.094
C(57A)	1a		1.454(2)	-0.109(2)	0.442(2)	0.12(1)
H(57A)	1a		1.5081	-0.1313	0.4138	0.142
C(58A)	1a		1.450(2)	-0.044(1)	0.499(2)	0.090(9)
H(58A)	1a		1.5036	-0.0214	0.5076	0.108
C(59A)	1a		1.371(2)	-0.013(2)	0.543(2)	0.089(9)
H(59A)	1a		1.3725	0.0314	0.5772	0.107
C(60A)	1a		1.285(3)	-0.042(2)	0.543(3)	0.13(1)
H(60A)	1a		1.2348	-0.0225	0.5806	0.150
C(61A)	1a		0.853(2)	0.239(1)	0.776(2)	0.069(6)
H(61A)	1a		0.7985	0.2244	0.7196	0.082
C(62A)	1a		0.902(2)	0.178(1)	0.778(2)	0.101(9)
H(62A)	1a		0.9585	0.1897	0.8340	0.122
C(63A)	1a		0.858(3)	0.136(2)	0.812(3)	0.13(1)
H(63A)	1a		0.9076	0.1006	0.8243	0.157
H(63B)	1a		0.8087	0.1160	0.7550	0.157
C(64A)	1a		0.813(2)	0.165(2)	0.906(2)	0.11(1)
H(64A)	1a		0.7592	0.1405	0.9019	0.137
H(64B)	1a		0.8607	0.1600	0.9668	0.137
C(65A)	1a		0.778(3)	0.231(2)	0.922(3)	0.12(1)
H(65A)	1a		0.8020	0.2526	0.9942	0.149
H(65B)	1a		0.7078	0.2334	0.9148	0.149
C(66A)	1a		0.797(2)	0.272(2)	0.860(2)	0.09(1)
H(66A)	1a		0.8321	0.3072	0.9071	0.110
H(66B)	1a		0.7351	0.2904	0.8301	0.110
O(1B)	1a		0.650(1)	0.405(1)	0.573(2)	0.080(6)
O(2B)	1a		0.664(1)	0.2835(9)	0.490(1)	0.080(5)
N(1B)	1a		0.752(2)	0.417(1)	0.432(2)	0.086(8)
N(2B)	1a		0.763(1)	0.291(1)	0.350(1)	0.060(5)
C(1B)	1a		0.741(2)	0.477(1)	0.481(2)	0.054(7)
H(1B)	1a		0.7746	0.5049	0.4648	0.064
C(2B)	1a		0.677(2)	0.505(2)	0.563(2)	0.071(8)
C(3B)	1a		0.652(2)	0.583(1)	0.614(2)	0.059(6)
H(3B)	1a		0.6762	0.6126	0.5913	0.071
C(4B)	1a		0.601(2)	0.603(1)	0.687(2)	0.067(7)
C(5B)	1a		0.576(2)	0.563(1)	0.725(2)	0.041(6)
H(5B)	1a		0.5557	0.5820	0.7889	0.049
C(6B)	1a		0.575(2)	0.502(1)	0.691(2)	0.060(7)
C(7B)	1a		0.636(2)	0.468(2)	0.604(2)	0.061(8)
C(8B)	1a		0.788(2)	0.230(2)	0.341(3)	0.12(1)
H(8B)	1a		0.8323	0.2109	0.2966	0.138
C(9B)	1a		0.762(2)	0.188(1)	0.384(2)	0.044(6)
C(10B)	1a		0.794(2)	0.125(2)	0.369(2)	0.082(9)
H(10B)	1a		0.8507	0.1101	0.3404	0.098
C(11B)	1a		0.746(1)	0.078(1)	0.396(2)	0.041(5)
C(12B)	1a		0.680(2)	0.101(1)	0.443(2)	0.058(7)
H(12B)	1a		0.6547	0.0702	0.4645	0.070
C(13B)	1a		0.636(2)	0.159(1)	0.470(2)	0.064(8)
C(14B)	1a		0.685(2)	0.206(1)	0.442(2)	0.064(8)
C(15B)	1a		0.527(1)	0.455(1)	0.736(2)	0.042(5)
C(16B)	1a		0.461(2)	0.504(2)	0.813(2)	0.11(1)
H(16D)	1a		0.5014	0.5322	0.8680	0.161
H(16E)	1a		0.4286	0.4794	0.8425	0.161
H(16F)	1a		0.4133	0.5291	0.7759	0.161
C(17B)	1a		0.467(2)	0.414(2)	0.643(2)	0.10(1)
H(17D)	1a		0.4362	0.3845	0.6644	0.143
H(17E)	1a		0.5082	0.3890	0.5940	0.143
H(17F)	1a		0.4179	0.4413	0.6113	0.143
C(18B)	1a		0.597(3)	0.419(2)	0.783(3)	0.17(2)
H(18D)	1a		0.6379	0.4478	0.8371	0.251
H(18E)	1a		0.6357	0.3916	0.7328	0.251

Table 2. Continued.

Atom	Site	Occ.	x	y	z	U _{iso}
H(18F)	1a		0.5688	0.3929	0.8121	0.251
C(19B)	1a		0.605(2)	0.677(2)	0.726(3)	0.09(1)
H(19C)	1a		0.6668	0.6866	0.7162	0.102
H(19D)	1a		0.6024	0.6912	0.7995	0.102
C(20B)	1a		0.549(2)	0.7112(9)	0.525(2)	0.055(6)
C(21B)	1a		0.640(2)	0.7267(9)	0.535(2)	0.074(8)
H(21B)	1a		0.6848	0.7316	0.5964	0.088
C(22B)	1a		0.661(2)	0.734(1)	0.452(2)	0.072(8)
H(22B)	1a		0.7235	0.7431	0.4535	0.087
C(23B)	1a		0.597(2)	0.730(1)	0.364(2)	0.10(1)
H(23B)	1a		0.6121	0.7387	0.3070	0.121
C(24B)	1a		0.504(2)	0.710(1)	0.360(2)	0.085(9)
H(24B)	1a		0.4615	0.7038	0.2966	0.102
C(25B)	1a		0.472(2)	0.700(1)	0.443(2)	0.065(8)
H(25B)	1a		0.4119	0.6875	0.4428	0.078
C(26B)	1a		0.399(2)	0.679(2)	0.632(2)	0.09(1)
C(27B)	1a		0.312(2)	0.701(2)	0.673(2)	0.084(9)
H(27B)	1a		0.3060	0.7428	0.7197	0.101
C(28B)	1a		0.235(2)	0.664(1)	0.648(2)	0.071(8)
H(28B)	1a		0.1784	0.6797	0.6770	0.086
C(29B)	1a		0.243(2)	0.601(1)	0.577(2)	0.078(8)
H(29B)	1a		0.1901	0.5764	0.5593	0.093
C(30B)	1a		0.324(2)	0.574(2)	0.532(2)	0.10(1)
H(30B)	1a		0.3295	0.5332	0.4850	0.121
C(31B)	1a		0.398(2)	0.617(1)	0.567(2)	0.078(9)
H(31B)	1a		0.4564	0.5991	0.5424	0.094
C(32B)	1a		0.483(1)	0.805(1)	0.741(2)	0.051(7)
C(33B)	1a		0.491(2)	0.851(1)	0.702(2)	0.070(8)
H(33B)	1a		0.5018	0.8427	0.6343	0.084
C(34B)	1a		0.482(2)	0.914(2)	0.767(2)	0.09(1)
H(34B)	1a		0.4876	0.9493	0.7440	0.103
C(35B)	1a		0.467(2)	0.922(2)	0.862(2)	0.078(9)
H(35B)	1a		0.4613	0.9645	0.9061	0.094
C(36B)	1a		0.458(2)	0.874(1)	0.896(2)	0.067(8)
H(36B)	1a		0.4432	0.8825	0.9620	0.081
C(37B)	1a		0.471(2)	0.810(2)	0.835(2)	0.078(9)
H(37B)	1a		0.4713	0.7745	0.8595	0.094
C(38B)	1a		0.552(2)	0.182(1)	0.521(2)	0.045(6)
C(39B)	1a		0.510(2)	0.128(2)	0.539(2)	0.083(9)
H(39D)	1a		0.4533	0.1449	0.5712	0.124
H(39E)	1a		0.5576	0.1070	0.5842	0.124
H(39F)	1a		0.4922	0.0959	0.4738	0.124
C(40B)	1a		0.563(2)	0.235(2)	0.631(2)	0.082(9)
H(40D)	1a		0.5910	0.2713	0.6267	0.123
H(40E)	1a		0.6055	0.2156	0.6818	0.123
H(40F)	1a		0.5005	0.2486	0.6514	0.123
C(41B)	1a		0.462(2)	0.215(1)	0.451(2)	0.080(9)
H(41D)	1a		0.4806	0.2530	0.4415	0.121
H(41E)	1a		0.4065	0.2265	0.4863	0.121
H(41F)	1a		0.4453	0.1838	0.3847	0.121
C(42B)	1a		0.805(2)	0.004(1)	0.357(2)	0.049(6)
H(42C)	1a		0.8101	-0.0180	0.4101	0.059
H(42D)	1a		0.8703	0.0094	0.3513	0.059
C(43B)	1a		0.821(2)	-0.126(1)	0.237(2)	0.067(8)
C(44B)	1a		0.806(2)	-0.152(1)	0.313(2)	0.057(7)
H(44B)	1a		0.7616	-0.1317	0.3584	0.068
C(45B)	1a		0.861(2)	-0.212(1)	0.317(2)	0.066(8)
H(45B)	1a		0.8529	-0.2320	0.3658	0.079
C(46B)	1a		0.927(2)	-0.240(1)	0.251(2)	0.047(6)
H(46B)	1a		0.9640	-0.2793	0.2564	0.056
C(47B)	1a		0.940(2)	-0.212(1)	0.174(2)	0.078(8)
H(47B)	1a		0.9844	-0.2313	0.1298	0.094

Table 2. Continued.

Atom	Site	Occ.	x	y	z	U _{iso}
C(48B)	1a		0.882(1)	-0.1558(9)	0.169(2)	0.034(5)
H(48B)	1a		0.8854	-0.1373	0.1168	0.041
C(49B)	1a		0.787(2)	-0.020(1)	0.132(2)	0.054(7)
C(50B)	1a		0.711(2)	-0.0256(9)	0.046(2)	0.052(6)
H(50B)	1a		0.6509	-0.0386	0.0434	0.062
C(51B)	1a		0.735(3)	-0.010(1)	-0.033(3)	0.12(1)
H(51B)	1a		0.6904	-0.0123	-0.0944	0.139
C(52B)	1a		0.827(2)	0.008(2)	-0.025(3)	0.13(2)
H(52B)	1a		0.8408	0.0186	-0.0817	0.161
C(53B)	1a		0.901(2)	0.012(1)	0.062(2)	0.069(8)
H(53B)	1a		0.9625	0.0237	0.0639	0.083
C(54B)	1a		0.878(2)	-0.001(1)	0.144(2)	0.053(6)
H(54B)	1a		0.9216	0.0024	0.2057	0.063
C(55B)	1a		0.636(2)	-0.042(1)	0.211(2)	0.072(8)
C(56B)	1a		0.565(2)	0.013(2)	0.213(2)	0.11(1)
H(56B)	1a		0.5865	0.0533	0.2197	0.133
C(57B)	1a		0.459(2)	0.010(2)	0.206(2)	0.13(1)
H(57B)	1a		0.4179	0.0479	0.2081	0.151
C(58B)	1a		0.417(2)	-0.047(1)	0.195(2)	0.081(9)
H(58B)	1a		0.3512	-0.0471	0.1922	0.097
C(59B)	1a		0.484(2)	-0.101(2)	0.189(2)	0.10(1)
H(59B)	1a		0.4610	-0.1413	0.1752	0.117
C(60B)	1a		0.586(2)	-0.099(1)	0.202(2)	0.076(8)
H(60B)	1a		0.6250	-0.1370	0.2063	0.091
C(61B)	1a		0.829(2)	0.392(1)	0.366(2)	0.069(6)
H(61B)	1a		0.8893	0.3787	0.4092	0.083
C(62B)	1a		0.788(2)	0.327(2)	0.288(2)	0.11(1)
H(62B)	1a		0.7305	0.3382	0.2395	0.134
C(63B)	1a		0.881(2)	0.295(1)	0.226(2)	0.066(7)
H(63C)	1a		0.9333	0.2793	0.2734	0.080
H(63D)	1a		0.8605	0.2571	0.1693	0.080
C(64B)	1a		0.918(4)	0.338(2)	0.183(4)	0.15(2)
H(64C)	1a		0.8746	0.3396	0.1185	0.175
H(64D)	1a		0.9809	0.3177	0.1658	0.175
C(65B)	1a		0.928(2)	0.403(1)	0.247(2)	0.103(9)
H(65C)	1a		0.9313	0.4292	0.2005	0.124
H(65D)	1a		0.9911	0.4028	0.2918	0.124
C(66B)	1a		0.852(2)	0.441(1)	0.316(2)	0.062(6)
H(66C)	1a		0.8779	0.4778	0.3692	0.074
H(66D)	1a		0.7933	0.4559	0.2746	0.074
O(1)	1a		0.504(1)	1.1062(8)	0.811(1)	0.094(5)
C(1)	1a		0.406(3)	1.124(2)	0.833(3)	0.17(2)
C(2)	1a		0.385(3)	1.093(2)	0.927(4)	0.21(2)
O(2)	1a	0.50	1.546(3)	-0.468(2)	0.300(3)	0.11(1)
C(3)	1a	0.50	1.500(6)	-0.482(4)	0.191(6)	0.18(3)
C(4)	1a	0.50	1.398(4)	-0.512(3)	0.105(4)	0.11(2)
O(3)	1a		1.095(4)	0.044(3)	0.861(5)	0.34(2)
C(5)	1a		1.105(4)	0.073(3)	0.970(4)	0.21(2)
C(6)	1a		1.239(5)	0.059(3)	0.977(5)	0.28(3)
O(4A)	1a	0.50	1.018(2)	0.415(2)	-0.016(2)	0.065(9)
O(4B)	1a	0.50	1.043(4)	0.373(2)	0.002(4)	0.14(2)
C(7)	1a		1.120(3)	0.371(2)	-0.042(3)	0.17(2)
C(8)	1a		1.200(2)	0.434(2)	0.003(2)	0.106(9)
O(5)	1a		0.658(2)	0.170(1)	0.104(2)	0.15(1)
C(9)	1a		0.578(4)	0.169(3)	0.159(4)	0.22(2)
C(10)	1a		0.481(5)	0.173(3)	0.135(5)	0.26(3)
O(6)	1a	0.50	0.622(2)	0.461(1)	0.113(2)	0.066(8)
C(11)	1a	0.50	0.626(3)	0.395(2)	0.052(3)	0.06(1)
C(12)	1a	0.50	0.515(6)	0.352(5)	0.023(8)	0.19(4)
O(7)	1a		1.272(3)	0.247(2)	0.208(3)	0.26(2)
C(13)	1a		1.200(6)	0.252(5)	0.147(7)	0.35(5)
C(14)	1a		1.103(6)	0.216(4)	0.068(6)	0.32(4)

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
Fe(1A)	1a	1.0195(3)	0.2223(2)	0.6626(3)	0.095(3)	0.062(3)	0.063(3)	0.000(3)	0.013(3)	0.021(2)
Cl(1A)	1a	1.1517(7)	0.2084(5)	0.7787(8)	0.100(7)	0.121(8)	0.111(7)	−0.003(6)	−0.037(6)	0.020(7)
P(1A)	1a	0.9320(5)	0.6180(4)	0.8698(6)	0.046(4)	0.070(6)	0.059(5)	−0.010(4)	−0.021(4)	0.030(4)
P(2A)	1a	1.1816(5)	−0.1467(4)	0.4515(6)	0.037(4)	0.060(5)	0.067(5)	−0.026(4)	−0.022(4)	−0.002(4)
Fe(1B)	1a	0.6647(2)	0.3473(2)	0.4392(3)	0.041(2)	0.063(3)	0.077(3)	−0.018(2)	−0.007(2)	−0.009(2)
Cl(1B)	1a	0.5343(6)	0.3624(6)	0.328(1)	0.058(5)	0.19(1)	0.18(1)	−0.051(7)	−0.034(6)	0.09(1)
P(1B)	1a	0.5046(6)	0.7201(4)	0.6558(5)	0.104(6)	0.061(5)	0.029(4)	−0.002(4)	−0.004(4)	0.025(4)
P(2B)	1a	0.7512(6)	−0.0445(4)	0.2394(6)	0.087(6)	0.043(5)	0.054(5)	−0.007(4)	0.000(4)	−0.012(4)
P(5)	1a	0.9374(8)	0.6308(4)	0.4868(6)	0.163(9)	0.065(6)	0.048(5)	−0.037(6)	0.010(5)	0.034(5)
P(6)	1a	0.5392(9)	−0.3043(8)	0.041(1)	0.096(8)	0.21(2)	0.115(9)	−0.023(9)	−0.029(8)	0.09(1)
P(7)	1a	0.1411(7)	−0.1278(4)	0.0628(6)	0.134(8)	0.076(6)	0.034(4)	−0.021(6)	0.001(5)	0.026(4)
P(8)	1a	0.7463(6)	−0.0612(5)	0.6212(7)	0.054(5)	0.106(8)	0.080(6)	−0.002(5)	−0.011(5)	0.002(6)
F(1)	1a	0.881(2)	0.603(2)	0.527(2)	0.25(2)	0.18(2)	0.19(2)	−0.05(2)	0.06(2)	0.08(2)
F(2)	1a	0.886(2)	0.639(1)	0.385(1)	0.20(2)	0.21(2)	0.06(1)	0.12(2)	0.07(1)	0.07(1)
F(3)	1a	0.989(2)	0.565(1)	0.450(3)	0.25(4)	0.08(2)	0.39(5)	−0.04(2)	−0.17(3)	0.00(2)
F(4)	1a	1.002(1)	0.634(1)	0.594(1)	0.06(1)	0.24(2)	0.08(1)	0.07(1)	0.019(9)	0.06(2)
F(5)	1a	0.879(2)	0.695(1)	0.544(2)	0.20(3)	0.15(2)	0.15(2)	0.10(2)	−0.05(2)	−0.10(2)
F(6)	1a	1.020(2)	0.665(2)	0.469(2)	0.12(2)	0.40(5)	0.18(3)	−0.08(2)	0.01(2)	0.15(3)
F(7)	1a	0.645(2)	−0.297(1)	0.126(2)	0.16(2)	0.23(3)	0.10(2)	−0.06(2)	−0.03(2)	0.00(2)
F(8)	1a	0.547(2)	−0.234(1)	0.026(2)	0.26(3)	0.08(1)	0.08(1)	−0.03(2)	−0.00(2)	0.01(1)
F(9)	1a	0.482(2)	−0.257(1)	0.128(2)	0.16(2)	0.14(2)	0.16(2)	0.00(2)	0.07(2)	0.00(2)
F(10)	1a	0.520(3)	−0.372(2)	0.052(2)	0.39(4)	0.24(3)	0.19(3)	−0.12(3)	0.04(3)	0.14(3)
F(11)	1a	0.457(1)	−0.314(1)	−0.058(2)	0.09(1)	0.13(2)	0.13(2)	−0.01(1)	0.02(1)	0.02(1)
F(12)	1a	0.615(1)	−0.342(2)	−0.047(2)	0.06(1)	0.37(4)	0.11(2)	−0.02(2)	−0.02(1)	0.10(2)
F(13)	1a	0.067(2)	−0.089(1)	0.146(1)	0.23(2)	0.14(1)	0.040(8)	−0.02(1)	0.04(1)	−0.026(8)
F(14)	1a	0.234(1)	−0.124(1)	0.149(2)	0.13(2)	0.28(3)	0.20(2)	−0.14(2)	−0.12(2)	0.18(2)
F(15)	1a	0.148(2)	−0.067(1)	0.046(2)	0.20(2)	0.14(2)	0.13(2)	0.04(2)	0.04(2)	0.08(2)
F(16)	1a	0.211(2)	−0.157(1)	−0.019(2)	0.22(3)	0.26(3)	0.10(2)	0.07(2)	0.09(2)	0.11(2)
F(17)	1a	0.124(2)	−0.186(1)	0.089(2)	0.12(1)	0.15(2)	0.13(2)	0.00(1)	0.04(1)	0.07(2)
F(18)	1a	0.057(2)	−0.130(2)	−0.026(1)	0.25(3)	0.30(4)	0.02(1)	0.14(3)	0.00(1)	0.01(2)
F(19)	1a	0.675(1)	−0.064(1)	0.508(2)	0.10(1)	0.13(2)	0.11(1)	−0.06(1)	−0.06(1)	−0.02(1)
F(20)	1a	0.822(2)	−0.056(2)	0.717(2)	0.12(2)	0.29(3)	0.14(2)	0.05(2)	−0.08(2)	−0.09(2)
F(21)	1a	0.690(2)	0.006(1)	0.676(2)	0.15(2)	0.16(2)	0.11(1)	0.06(2)	0.06(1)	−0.06(1)
F(22)	1a	0.792(2)	−0.132(1)	0.566(2)	0.16(2)	0.12(2)	0.17(2)	−0.01(1)	−0.02(1)	0.02(1)
F(23)	1a	0.829(1)	−0.027(1)	0.592(2)	0.12(1)	0.33(3)	0.11(1)	−0.16(2)	−0.05(1)	0.13(2)
F(24)	1a	0.670(3)	−0.098(1)	0.645(2)	0.30(4)	0.12(2)	0.17(2)	−0.11(2)	0.06(2)	−0.02(2)

References

1. Pajunen, A.; Mutikainen, I.; Haikarainen, A.; Sipilä, J.; Pietikäinen, P.: {2,2'-[(*R,R*)-Cyclohexane-1,2-diylbis(nitrilomethylidyne)]bis-[6-*tert*-butyl-4-(triphenylphosphoniomethyl)phenolato]-*O,N,N',O'*copper(II)} dichloride hexakis(deuterochloroform) solvate. *Acta Crystallogr. C* **55** (2000) 321–322.
2. Haikarainen, A.; Sipilä, J.; Pietikäinen, P.: Unpublished results.
3. Sheldrick, G. M.: SHELXTL/PC. Version 4.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA 1990.
4. Sheldrick, G. M.: SHELX-97. Programs for Crystal Structure Analysis. University of Göttingen, Germany 1997.