Redetermination of the crystal structure of *trans*-dichloro-*syn*-bis[*meso*-ethane-1,2-diylbis(methylphenyl-phosphane)]ruthenium(II), $Ru((C_6H_5)(CH_3)P(C_2H_4)P(CH_3)(C_6H_5))_2Cl_2$

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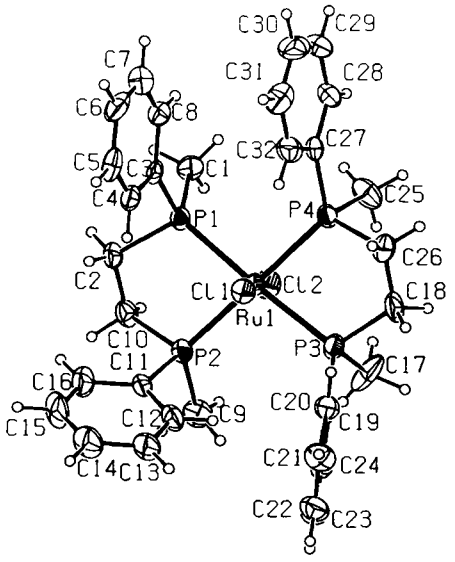

Source of material: preparation described in ref. 1.

The title compound is the first in a series of isomers synthesized by Horner and his coworkers (see ref. 1). An overview on all isomers 1 to 5, crystallographic data, structural data of the isomers 3 and 4, and further references are given in ref. 2. The enumeration of the isomers refers to table 1. in ref. 2. Kawada has already determined the structure of 1 in 1969 (see ref. 3), but he did not publish the coordinates. Therefore a redetermination was undertaken and is presented here. Kawada's description of the structure is confirmed, but it should be noted, that the symmetry *mm*2-C_{2v} of the complex is strongly distorted in the crystal packing. Ru–P distances are 233 pm-234 pm, Ru–Cl are 242 pm and 245 pm.

Table 1. Parameters used for the X-ray data collection

Crystal:	yellow flat needle, size 0.18 x 0.74 x 0.06 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	8.50 cm^{-1}
Diffractometer:	Stoe IPDS
Scan mode:	150 exposures, $\Delta\varphi$ = 1.5°
$T_{measurement}$:	301 K
$2\theta_{max}$:	48.4°
$N(hkl)_{unique}$:	5149
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
$N(param)_{refined}$:	353
Programs:	SHELXS-86, SHELXL-93, PLATON

$C_{32}H_{40}Cl_2P_4Ru$, monoclinic, $P12_1/n1$ (No. 14), a =17.823(3) Å, b =8.742(2) Å, c =21.784(4) Å, β =103.07(2)°, V =3306.2 $Å^3$, Z =4, ρ_m =1.45 $g\cdot cm^{-3}$, $R(F)$ =0.030, $R_w(F^2)$ =0.043.

Table 2. Final atomic coordinates and displacement parameters (in $Å^2$)

Atom	Site	x	y	z	U_{iso}
H(1)	4e	0.1535(2)	–0.0479(4)	0.3269(2)	0.085(2)
H(2)	4e	0.1008(2)	0.0862(4)	0.2944(2)	0.085(2)
H(3)	4e	0.0644(2)	–0.0540(4)	0.3220(2)	0.085(2)
H(4)	4e	0.0789(2)	–0.0099(4)	0.4858(2)	0.085(2)
H(5)	4e	0.0799(2)	–0.1294(4)	0.4321(2)	0.085(2)
H(6)	4e	0.0469(2)	0.2649(4)	0.4889(2)	0.085(2)
H(7)	4e	–0.0646(3)	0.4036(5)	0.4815(2)	0.085(2)
H(8)	4e	–0.1470(3)	0.4380(5)	0.3860(3)	0.085(2)
H(9)	4e	–0.1196(3)	0.3404(5)	0.2961(2)	0.085(2)
H(10)	4e	–0.0091(3)	0.1988(5)	0.3023(2)	0.085(2)
H(11)	4e	0.3640(2)	–0.0791(4)	0.5228(2)	0.085(2)
H(12)	4e	0.3337(2)	–0.1251(4)	0.5824(2)	0.085(2)
H(13)	4e	0.3773(2)	0.0302(4)	0.5814(2)	0.085(2)
H(14)	4e	0.2102(2)	–0.1693(4)	0.4659(2)	0.085(2)
H(15)	4e	0.1798(2)	–0.1695(4)	0.5282(2)	0.085(2)
H(16)	4e	0.3009(2)	0.2815(5)	0.6151(2)	0.085(2)
H(17)	4e	0.2773(3)	0.3617(6)	0.7085(2)	0.085(2)
H(18)	4e	0.1811(3)	0.2462(6)	0.7468(2)	0.085(2)
H(19)	4e	0.1123(3)	0.0532(7)	0.6921(2)	0.085(2)
H(20)	4e	0.1370(3)	–0.0318(5)	0.5989(2)	0.085(2)
H(21)	4e	0.4318(2)	0.1944(5)	0.4099(2)	0.085(2)
H(22)	4e	0.4590(2)	0.1513(5)	0.4814(2)	0.085(2)
H(23)	4e	0.4882(2)	0.3026(5)	0.4560(2)	0.085(2)
H(24)	4e	0.3756(3)	0.5995(5)	0.4510(2)	0.085(2)
H(25)	4e	0.4029(3)	0.5063(5)	0.3988(2)	0.085(2)
H(26)	4e	0.3327(3)	0.5865(5)	0.5443(2)	0.085(2)
H(27)	4e	0.3753(3)	0.6630(5)	0.6488(2)	0.085(2)
H(28)	4e	0.4683(3)	0.5283(6)	0.7163(2)	0.085(2)
H(29)	4e	0.5178(3)	0.3110(6)	0.6823(2)	0.085(2)
H(30)	4e	0.4791(3)	0.2359(5)	0.5790(2)	0.085(2)
H(31)	4e	0.3217(2)	0.2610(4)	0.3058(2)	0.085(2)
H(32)	4e	0.2806(2)	0.3922(4)	0.2616(2)	0.085(2)
H(33)	4e	0.2384(2)	0.2358(4)	0.2644(2)	0.085(2)
H(34)	4e	0.3032(3)	0.6005(5)	0.3412(2)	0.085(2)
H(35)	4e	0.2623(3)	0.6227(5)	0.3972(2)	0.085(2)
H(36)	4e	0.1428(3)	0.4042(5)	0.2217(2)	0.085(2)
H(37)	4e	0.0288(4)	0.5177(7)	0.1733(3)	0.085(2)
H(38)	4e	–0.0427(4)	0.6461(6)	0.2304(3)	0.085(2)
H(39)	4e	0.0007(3)	0.6717(5)	0.3363(3)	0.085(2)
H(40)	4e	0.1148(3)	0.5586(5)	0.3879(2)	0.085(2)

Table 3. Final 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}
Ru(1)	4*e*	0.24201(2)	0.22314(3)	0.43934(2)	0.0441(2)	0.0383(2)	0.0363(2)	–0.0095(2)	0.0146(2)	–0.0044(2)
Cl(1)	4*e*	0.19354(6)	0.4287(1)	0.49355(5)	0.0560(8)	0.0502(6)	0.0480(7)	–0.0015(6)	0.0173(7)	–0.0100(6)
Cl(2)	4*e*	0.29789(6)	0.0125(1)	0.39026(5)	0.0674(9)	0.0586(7)	0.0680(9)	–0.0005(6)	0.0264(8)	–0.0165(7)
P(1)	4*e*	0.12181(6)	0.1094(1)	0.40330(5)	0.0510(9)	0.0411(6)	0.0411(8)	–0.0130(6)	0.0145(7)	–0.0052(6)
P(2)	4*e*	0.25080(7)	0.0543(1)	0.52328(5)	0.0519(9)	0.0431(6)	0.0511(8)	–0.0050(6)	0.0138(7)	0.0048(6)
P(3)	4*e*	0.36341(7)	0.3371(1)	0.46893(5)	0.0521(9)	0.0712(8)	0.0476(9)	–0.0241(7)	0.0179(7)	–0.0115(7)
P(4)	4*e*	0.23260(7)	0.3824(1)	0.35222(5)	0.0571(9)	0.0489(7)	0.0401(8)	–0.0146(6)	0.0156(7)	–0.0000(6)
C(1)	4*e*	0.1086(2)	0.0119(4)	0.3277(2)	0.066(4)	0.060(3)	0.051(3)	–0.010(2)	0.009(3)	–0.014(2)
C(2)	4*e*	0.1085(2)	–0.0467(4)	0.4565(2)	0.063(4)	0.054(3)	0.060(3)	–0.023(3)	0.016(3)	0.008(2)
C(3)	4*e*	0.0313(2)	0.2153(4)	0.3954(2)	0.039(3)	0.039(2)	0.051(3)	–0.018(2)	0.014(3)	–0.004(3)
C(4)	4*e*	0.0135(2)	0.2790(4)	0.4499(2)	0.051(3)	0.060(3)	0.056(3)	–0.021(3)	0.017(3)	–0.003(3)
C(5)	4*e*	–0.0530(3)	0.3619(5)	0.4455(2)	0.056(4)	0.056(3)	0.097(5)	–0.016(3)	0.047(4)	–0.017(3)
C(6)	4*e*	–0.1018(3)	0.3826(5)	0.3885(3)	0.035(4)	0.067(3)	0.134(6)	–0.006(3)	0.005(4)	0.022(4)
C(7)	4*e*	–0.0860(3)	0.3239(5)	0.3350(2)	0.072(5)	0.080(4)	0.072(4)	–0.010(3)	0.020(4)	0.007(3)
C(8)	4*e*	–0.0196(3)	0.2398(5)	0.3388(2)	0.055(3)	0.061(3)	0.054(3)	–0.014(3)	0.010(3)	–0.001(3)
C(9)	4*e*	0.3423(2)	–0.0413(4)	0.5564(2)	0.077(4)	0.065(3)	0.090(4)	0.015(3)	0.011(3)	0.022(3)
C(10)	4*e*	0.1870(2)	–0.1065(4)	0.4933(2)	0.079(4)	0.043(2)	0.056(3)	–0.014(3)	0.021(3)	0.001(2)
C(11)	4*e*	0.2238(3)	0.1128(4)	0.5961(2)	0.056(3)	0.048(3)	0.041(3)	–0.015(2)	0.010(3)	0.008(2)
C(12)	4*e*	0.2628(2)	0.2322(5)	0.6306(2)	0.078(4)	0.079(3)	0.043(3)	–0.022(3)	0.022(3)	0.005(3)
C(13)	4*e*	0.2486(3)	0.2822(6)	0.6864(2)	0.095(5)	0.100(4)	0.041(3)	–0.027(3)	0.019(3)	–0.012(3)
C(14)	4*e*	0.1918(3)	0.2137(6)	0.7091(2)	0.111(5)	0.110(4)	0.054(4)	–0.015(4)	0.038(4)	–0.015(4)
C(15)	4*e*	0.1513(3)	0.0992(7)	0.6766(2)	0.123(6)	0.152(6)	0.061(4)	–0.053(4)	0.062(4)	–0.014(4)
C(16)	4*e*	0.1662(3)	0.0477(5)	0.6205(2)	0.088(4)	0.085(3)	0.077(4)	–0.043(3)	0.022(4)	0.004(3)
C(17)	4*e*	0.4453(2)	0.2342(5)	0.4521(2)	0.044(3)	0.166(5)	0.119(4)	–0.039(4)	0.038(3)	–0.075(4)
C(18)	4*e*	0.3625(3)	0.5144(5)	0.4220(2)	0.125(5)	0.114(4)	0.055(4)	–0.088(4)	0.015(4)	0.009(3)
C(19)	4*e*	0.4013(3)	0.4009(5)	0.5493(2)	0.042(3)	0.051(3)	0.048(3)	–0.022(2)	0.010(3)	0.004(3)
C(20)	4*e*	0.3705(3)	0.5302(5)	0.5714(2)	0.069(4)	0.045(3)	0.056(4)	–0.014(3)	0.002(3)	0.004(3)
C(21)	4*e*	0.3962(3)	0.5762(5)	0.6345(2)	0.105(5)	0.059(3)	0.055(4)	–0.008(3)	0.011(4)	–0.014(3)
C(22)	4*e*	0.4512(3)	0.4959(6)	0.6748(2)	0.094(5)	0.082(4)	0.051(4)	–0.015(3)	0.003(4)	0.007(3)
C(23)	4*e*	0.4811(3)	0.3681(6)	0.6545(2)	0.066(4)	0.085(4)	0.055(4)	–0.001(3)	–0.000(3)	0.007(3)
C(24)	4*e*	0.4570(3)	0.3226(5)	0.5924(2)	0.049(3)	0.067(3)	0.064(4)	–0.010(3)	0.018(3)	–0.007(3)
C(25)	4*e*	0.2731(2)	0.3092(4)	0.2885(2)	0.108(4)	0.097(3)	0.051(3)	0.011(3)	0.040(3)	0.006(3)
C(26)	4*e*	0.2915(3)	0.5510(5)	0.3777(2)	0.068(4)	0.063(3)	0.086(4)	–0.030(3)	0.008(3)	0.012(3)
C(27)	4*e*	0.1422(2)	0.4680(4)	0.3105(2)	0.052(4)	0.039(2)	0.054(4)	–0.016(2)	0.011(3)	0.011(3)
C(28)	4*e*	0.1147(3)	0.4576(5)	0.2458(2)	0.085(5)	0.079(3)	0.044(4)	–0.025(3)	0.005(3)	0.018(3)
C(29)	4*e*	0.0462(4)	0.5253(7)	0.2168(3)	0.095(6)	0.111(5)	0.054(4)	–0.027(4)	–0.009(4)	0.031(4)
C(30)	4*e*	0.0040(4)	0.6024(6)	0.2505(3)	0.081(5)	0.081(4)	0.111(6)	–0.010(4)	–0.029(5)	0.044(5)
C(31)	4*e*	0.0295(3)	0.6164(5)	0.3134(3)	0.063(5)	0.048(3)	0.129(5)	0.004(3)	0.015(4)	0.013(4)
C(32)	4*e*	0.0982(3)	0.5492(5)	0.3444(2)	0.079(4)	0.047(3)	0.065(4)	–0.009(3)	0.008(4)	0.007(3)

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