SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.

Acta Cryst. (1981). B37, 490

The crystal and molecular structure of 2-oxo-2-phenoxy-4H-1,3,2-benzodioxaphosphorin: errata. By Z. GALDECKI and M. L. GŁÓWKA, Institute of General Chemistry, Technical University, 36 Żwirki, 90-924 Łódź, Poland

(Received 22 August 1980; accepted 29 September 1980)

Abstract

E.s.d.'s of bond lengths and angles in Tables 3 and 4 of Gałdecki & Główka [Acta Cryst. (1978). B34, 160–163] are corrected. The mean σ's should be: 0.003 for P-O, 0.004 for O-C, 0.006 for C-C and 0.06 Å for C-H; 0.2 for

O-P-O and P-O-C, 0.3 for O-C-C and 0.3° for C-C-C.

All relevant information is contained in the Abstract.

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Comparison of two independent structure determinations of (1-3-η-2-methylallyl)palladium chloride dimer. By Giuliano Bandoli and Dore A. Clemente, Istituto di Chimica e Tecnologia dei Radioelementi del CNR, Area Ricerca, Corso Stati Uniti, 35100 Padova, Italy

(Received 18 July 1980; accepted 16 October 1980)

Abstract

Two independent structure analyses of $(1-3-\eta-2-methylally)$ palladium chloride dimer are compared by means of half-normal probability plots. No systematic errors are detected in the derived atomic positions, while the thermal parameters differ significantly between the two studies; this can be attributed to absorption effects. [This work: $C_8H_{14}Cl_2Pd_2$, $P\bar{l}$, a=9.266 (9), b=6.332 (6), c=4.985 (4) Å, $\alpha=92.01$ (3), $\beta=90.77$ (3), $\gamma=95.94$ (5)°; R=0.035 for 1155 reflections.]

Introduction

The crystal structure of the title compound was first reported and thoroughly discussed by Mason & Wheeler (1968) (hereinafter MW). The earlier work had been carried out using visual intensity estimates from film; the present study employs diffractometer X-ray data. Comparison of our results with those of MW gives some information on the precision and accuracy available from diffractometer data.

Experimental

Crystals are triclinic, space group $P\bar{1}$, with a=9.266 (9), b=6.332 (6), c=4.985 (4) Å, $\alpha=92.01$ (3), $\beta=90.77$ (3), $\gamma=95.94$ (5)°; crystal size $0.22\times0.16\times0.06$ mm. Intensity data within a Bragg limit of 27° were collected by the use of a Philips PW 1100 diffractometer (Mo $K\alpha$ radiation). The number of independent reflections was 1270; 1155 reflections

Table 1. Coordinates (×10⁴) and $U_{\rm eq}$ (×10²) values of the non-hydrogen atoms

 $U_{\rm eq}=(U_1\,U_2\,U_3)^{1/3},$ where $U_1,\ U_2$ and U_3 are the mean-square displacements along the principal axes of the thermal ellipsoids.

	x	у	z	$U_{\mathrm{eq}}(\mathrm{\AA^2})$
Pd	-1234(1)	912 (1)	2191 (1)	3.5
Cl	1046 (2)	2313 (3)	403 (4)	4.4
C(1)	-1753(10)	3424 (14)	4823 (16)	4.7
C(2)	-3018(8)	2298 (13)	3806 (15)	4.2
C(3)	-3148(9)	127 (14)	4219 (17)	5.1
C(4)	-3999 (10)	3296 (16)	1927 (20)	5.9

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