SHORT COMMUNICATIONS

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Acta Cryst. (1990). C**46**, 1577

Über Tetraphenylphosphoniumbromid-monohydrat.

Von VOLKER KRUG und ULRICH MÜLLER, *Fachbereich Chemie der Universität Marburg, Hans-Meerweinstraße, D-3550 Marburg, Bundesrepublik Deutschland*

(*Eingegangen am* 20. *Mai* 1989; *angenommen am* 27. *Februar* 1990)

Abstract

The crystal structure of $[P(C_6H_5)_4]Br.H_2O$, recently published by Vincent, Knop, Linden, Cameron & Robertson [*Can. J. Chem.* (1988), **66**, 3060–3069], was determined independently. The results are confirmed. Using the same (non-standard) cell setting for $P\bar{1}$, the present lattice parameters are $a = 10{\cdot}035\ (4)$, $b = 10{\cdot}685\ (4)$, $c = 10{\cdot}677\ (3)$ Å, $\alpha = 102{\cdot}45\ (3)$, $\beta = 83{\cdot}30\ (3)$, $\gamma = 108{\cdot}08\ (3)°$; these differ slightly from the earlier determination by 0·020 to 0·030 Å and 0·01 to 0·16°, respectively. Atomic coordinates coincide within 2σ.

Experimentelles

Nachdem wir die Kristallstruktur von $PPh_4Br.H_2O$ bestimmt hatten, erschien die Arbeit von Vincent, Knop, Linden, Cameron & Robertson (1988), in der die gleiche Struktur beschrieben wird. Wir können deren Ergebnisse in vollem Umfang bestätigen. Lediglich bei den Gitterparametern haben wir (bei gleicher Meßtemperature 293 K) geringfügige Abweichungen gefunden (siehe *Abstract*); sie wurden mit 19 Reflexen $16 < \theta < 19°$ bestimmt. Die Atomkoordinaten beider Untersuchungen stimmen innerhalb von 2σ, vielfach auch innerhalb von 1σ überein, so daß wir auf ihre Wiedergabe verzichten. Die Strukturbestimmung erfolgte mit 1398 unabhängigen Reflexen mit $F > 2\sigma(F)$ von 1560 gemessenen Reflexen. Vierkreisdiffraktometer Enraf–Nonius CAD-4, Mo $K\alpha$ Strahlung, $\lambda =$ 0,7107 Å, ω-scan, Absorptionskorrektur des vermessenen Kristalls (0,21 × 0,22 × 0,34 mm), Transmissionsfaktoren 0,62 bis 0,68. Verfeinerung durch Minimieren von $\sum w(|F_o| - |F_c|)^2$, $w = 1{,}4/\sigma^2(F)$, $R = 0{,}034$, $wR = 0{,}027$. Rechenprogramm: *SHELX*76, Sheldrick (1976). In der Struktur sind die Anionen und Wassermoleküle zu zentrosymmetrischen Ringen $(Br^-.H_2O)_2$ assoziiert; die PPh_4^+ Ionen bilden Zickzacklinien wie beim β-$AsPh_4[UCl_6].2CH_2Cl_2$ (Strukturtyp II nach Müller, Klingelhöfer, Eicher & Bohrer, 1984).

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Structure of potassium nitroprusside monohydrate. Corrigendum.

By Y. LE PAGE, *Chemistry Div. NRC, Ottawa, Canada K1A 0R9* and E. E. CASTELLANO, *Instituto de Fisica e Quimica de São Carlos, Universidade de São Paulo, Caixa Postal* 369, 13.560 *São Carlos, Brazil*

(*Received* 5 *February* 1990; *accepted* 2 *March* 1990)

Abstract

Re-examination of the structure of potassium nitroprusside 0·8 hydrate [Castellano, Rivero, Piro & Amalvy (1989). *Acta Cryst.* C**45**, 1207–1210] with the program *MISSYM* [Le Page (1987). *J. Appl. Cryst.* **20**, 264–269; Le Page (1988). *J. Appl. Cryst.* **21**, 983–984] suggested that a center of symmetry could have been overlooked in the original analysis. In fact, refinement in the centric space group *Pnam* (*Pnma*, number 62 with y and z axes relabelled z and $-y$) with the original data, produced the atomic coordinates reported in the present paper and gave residuals $R =$ 0·074 and $wR = 0{\cdot}080$. The structure is essentially that proposed originally except for the fact that the water content of this compound is *one* rather than 0·8 per nitroprusside complex (thus the modified name of the compound in the present communication).

Atomic coordinates from the refinement in space group *Pnam* are given in Table 1.

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Table 1. *Fractional atomic coordinates and isotropic temperature factors* ($Å^2$)

Atom labels are consistent with those used to describe the structure in the subgroup $Pna2_1$.

	x	y	z	B_{iso}
Fe(1)	0·1164 (0)	0·0175 (1)	0·0159 (1)	1·31 (3)
N(1)	0·1402 (2)	0·1181 (5)	−0·0417 (4)	1·7 (2)
O(1)	0·1582 (2)	0·1822 (5)	−0·0843 (3)	3·1 (2)
C(11)	0·0841 (2)	0·1169 (6)	0·0933 (4)	1·4 (2)
N(11)	0·0633 (2)	0·1691 (5)	0·1409 (4)	2·4 (2)
C(12)	0·0638 (2)	0·0086 (6)	−0·0523 (5)	1·7 (2)
N(12)	0·0326 (2)	0·0043 (5)	−0·0957 (5)	3·1 (2)
C(13)	0·1441 (2)	−0·1056 (6)	−0·0503 (4)	1·6 (2)
N(13)	0·1596 (2)	−0·1725 (5)	−0·0943 (4)	2·9 (2)
C(14)	0·1641 (2)	0·0164 (6)	0·0972 (5)	1·8 (2)
N(14)	0·1926 (2)	0·0233 (6)	0·1456 (4)	2·7 (2)
C(15)	0·0891 (2)	−0·1051 (6)	0·0790 (5)	2·0 (2)
N(15)	0·0719 (2)	−0·1760 (5)	0·1175 (5)	3·0 (2)
Fe(2)	0·1181 (0)	0·5113 (1)	−0·0022 (1)	1·29 (3)
N(2)	0·1440 (2)	0·6147 (5)	0·0517 (4)	1·7 (2)
O(2)	0·1623 (2)	0·6838 (4)	0·0887 (3)	2·8 (2)
C(21)	0·0696 (3)	0·4908 (7)	0·0778 (5)	2·5 (3)
N(21)	0·0419 (2)	0·4799 (6)	0·1273 (5)	3·9 (3)
C(22)	0·1499 (2)	0·3869 (6)	0·0525 (4)	1·6 (2)
N(22)	0·1683 (2)	0·3125 (5)	0·0865 (4)	2·6 (2)
C(23)	0·1612 (2)	0·5143 (6)	−0·0922 (4)	1·7 (2)
N(23)	0·1878 (2)	0·5245 (5)	−0·1440 (4)	2·5 (2)
C(24)	0·0807 (2)	0·6153 (6)	−0·0667 (4)	1·7 (2)
N(24)	0·0589 (2)	0·6737 (5)	−0·1045 (5)	2·9 (2)
C(25)	0·0881 (2)	0·3905 (6)	−0·0654 (4)	1·9 (2)
N(25)	0·0696 (2)	0·3230 (5)	−0·1007 (4)	2·7 (2)
Fe(5)	0·2435 (1)	0·0217 (1)	0·75	1·59 (5)
N(5)	0·1868 (3)	0·0233 (8)	0·75	2·5 (3)
O(5)	0·3504 (3)	0·5256 (8)	0·25	4·5 (3)
C(51)	0·2466 (4)	0·1865 (9)	0·75	2·5 (3)
N(51)	0·2495 (3)	0·283 (1)	0·75	4·0 (4)
C(52)	0·2482 (2)	0·0262 (7)	0·8704 (5)	2·1 (3)
N(52)	0·2499 (2)	0·0333 (7)	0·9413 (5)	3·4 (3)
C(53)	0·2481 (3)	−0·148 (1)	0·75	2·0 (3)
N(53)	0·2486 (3)	−0·2462 (8)	0·75	2·4 (3)
C(55)	0·3092 (4)	0·0216 (9)	0·75	2·1 (3)
N(55)	0·1532 (3)	0·5268 (9)	0·25	3·3 (3)
O(*W*1)	0·2506 (2)	0·8290 (8)	0·0562 (5)	7·1 (3)
O(*W*2)	0·0597 (3)	−0·1363 (7)	−0·25	3·5 (3)
O(*W*3)	0·0720 (5)	−0·493 (1)	−0·25	8·1 (4)
O(*W*4)	−0·0199 (3)	−0·2356 (7)	0·25	4·2 (3)
K(1)	0·2535 (1)	0·2071 (2)	0·4288 (1)	3·30 (7)
K(2)	0·0025 (1)	0·3290 (2)	0·25	2·77 (9)
K(4)	0·0230 (1)	0·9780 (2)	0·25	3·21 (9)
K(5)	0·1349 (1)	0·6993 (3)	−0·25	3·8 (1)
K(6)	0·1475 (1)	0·2404 (3)	0·25	3·6 (1)
K(7)	0·0685 (1)	0·6509 (2)	0·25	3·07 (9)
K(8)	0·0015 (1)	0·2262 (2)	0·5013 (1)	3·72 (8)
K(9)	0·2524 (1)	−0·0008 (3)	0·25	5·7 (2)

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Structure de la bétaïne de carboxyméthyl-1 phénylacétylamino-4 triazolium-1,2,4. Errata.

Par L. DUPONT et O. DIDEBERG, *Laboratoire de Cristallographie, Institut de Physique B5, Université de Liège au Sart-Tilman, B-4000 Liège, Belgique* et B. PIROTTE et J. DELARGE, *Laboratoire de Chimie Pharmaceutique, Institut de Pharmacie F1, Université de Liège, rue Fusch 3-5, B-4000 Liège, Belgique*

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Abstract

Some incorrect features in Fig. 1 of Dupont, Dideberg, Pirotte & Delarge [*Acta Cryst.* (1989), C**45**, 1928–1930] are corrected.

Le résumé contient tous les détails pertinents.

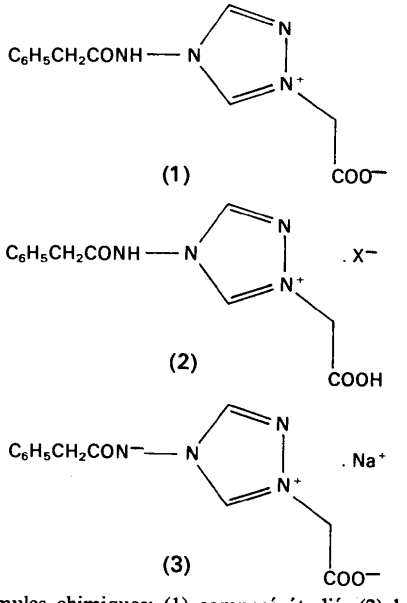

Fig. 1. Formules chimiques: (1) composé étudié, (2) halogénure acide correspondant, (3) amide anionique.

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