Table 1. *Rubidium carnallite*: *final coordinates*, *C*2/*c refinement*; *x*, *y*, *z and* $U_{eq} \times 10^4$.

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	*y*	*z*	U_{eq} (Å^2)
Rb	0	43 (.7)	2500	344 (2)
Mg	5000	0	5000	194 (3)
Cl(1)	2481 (1)	2621 (1)	2532 (1)	306 (2)
Cl(2)	0	0	0	314 (3)
O(1)	4098 (5)	135 (3)	3600 (3)	383 (8)
O(2)	3197 (4)	1008 (4)	512 (3)	374 (9)
O(3)	902 (4)	3125 (3)	4620 (3)	364 (8)

Table 2. *Rubidium carnallite*: *some distances and angles* (Å, °), *C*2/*c refinement*

Rb—Cl(1)	3.369 (1)	O(1)···Cl(1)	3.144 (4)
Rb—Cl(1)	3.288 (1)	O(1)···Cl(1)	3.187 (4)
Rb—Cl(2)	3.321 (1)	O(2)···Cl(1)	3.166 (4)
Mg—O(1)	2.041 (4)	O(2)···Cl(2)	3.187 (4)
Mg—O(2)	2.047 (4)	O(3)···Cl(1)	3.177 (4)
Mg—O(3)	2.041 (3)	O(3)···Cl(2)	3.141 (3)
O(1)—Mg—O(2)	90.02 (14)	Cl(1)···O(1)···Cl(1)	97.98 (10)
O(1)—Mg—O(3)	90.16 (14)	Cl(1)···O(2)···Cl(2)	97.51 (10)
O(2)—Mg—O(3)	90.28 (14)	Cl(1)···O(3)···Cl(2)	96.88 (9)
O(1)—Mg—O(1)	180.0		
O(2)—Mg—O(2)	180.0		
O(3)—Mg—O(3)	180.0		

Table 3. *Ammonium carnallite*: *coordinates*, *space group C*2/*c*;* *x*, *y*, *z* $\times 10^4$

	x	*y*	*z*
NH_4	0	16	2500
Mg	5000	0	5000
Cl(1)	2456	2620	2536
Cl(2)	0	0	0
O(1)	4084	138	3601
O(2)	3185	1004	515
O(3)	898	3114	4622

* These values were obtained by symmetrizing and averaging the *P*1 coordinates in Table 2, Nakaya *et al*. (1983).

13.301 Å, $\alpha = 89.95$, $\beta = 90.06$, $\gamma = 90.00°$. The resulting *C*2/*c* coordinates are given in Table 3. Once again they lead to equal Mg—O distances, at 2.053 (3) Å, in contrast to the rather large variation 1.96 (1) - 2.14 (1) Å reported earlier.

A couple of final comments might be in order. First, the monoclinic unit cells for the Rb and NH_4 carnallites reported by Andress & Saffe (1939) – $a = 13.30$, $b \simeq c \simeq 6.65$ Å, $\beta \simeq 90°$ – correspond to a primitive cell rather than to the *C*-centered cell described here and the axis of symmetry was mislocated. This improper cell probably resulted from the strong pseudosymmetry: reflections with *l* odd are systematically weak, and the Mg, Cl and Rb (or NH_4) atoms alone describe an effectively tetragonal structure. Secondly, in the case of the Rb compound, the rather large deviations of the cell angles α and γ from 90°, plus the appearance of the 203 reflection with seemingly significant intensity, might cast doubt on the assignment of the monoclinic space group and Laue symmetry. However, there is a far larger body of evidence – the satisfactory agreement indexes for averaging in Laue group 2/*m*, and the improved values of the final *R* and (most important) the over-all goodness-of-fit – that argues strongly in favor of the revised description. And the overwhelming disadvantage of attempting refinement in *P*1 is clearly shown in the wide range of apparent Mg—O distances when, in fact, the experimental data seem perfectly consistent with regular coordination.

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Acta Cryst. (1992). C**48**, 219–220

Structures de trois pyrroles substitués dérivés de munchnones. Erratum.

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Abstract

The *Abstract* of the paper by Toupet, Mazari, Texier & Carrié [*Acta Cryst.* (1991), C**47**, 1528–1531] is corrected. Methyl 2-methoxyphenyl-1-methyl-4,5-diphenylpyrrole-3-carboxylate (I), $C_{26}H_{23}NO_3$, $M_r = 397.5$, triclinic, $P\bar{1}$, $a = 10.525$ (2), $b = 10.719$ (1), $c = 10.965$ (1) Å, $\alpha = 71.84$ (1), $\beta = 82.09$ (1), $\gamma = 62.01$ (2)°, $V = 1038$ (1) Å^3, $Z = 2$, $D_x = 1.27$ g cm^{-3}, $\mu = 0.77$ cm^{-1}, $T = 293$ K, $F(000) = 420$, $wR = 0.033$ for 2612 observations. Methyl 5-methoxyphenyl-1-methyl-2,4-diphenylpyrrole-3-carboxylate (II), $C_{26}H_{23}NO_3$, $M_r = 397.5$, monoclinic, $P2_1/n$, $a = 10.940$ (2), $b = 13.649$ (5), $c = 14.418$ (4) Å, $\beta = 98.96$ (2)°, $V = 2126$ (1) Å^3, $Z = 4$, $D_x = 1.24$ g cm^{-3}, $\mu = 0.76$ cm^{-1}, $T =$

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293 K, $F(000) = 840$, $wR = 0.042$ for 1781 observations. Methyl 1-methyl-2-nitrophenyl-4,5-diphenylpyrrole-3-carboxylate (III), $C_{25}H_{20}N_2O_4$, $M_r = 412.5$, monoclinic, $P2_1/n$, $a = 14.675$ (7), $b = 8.278$ (6), $c = 17.397$ (3) Å, $V = 2095$ (2) Å^3, $Z = 4$, $D_x = 1.31$ g cm^{-3}, $\mu = 0.84$ cm^{-1}, $T = 293$ K, $F(000) = 864$, $wR = 0.039$ for 2038 observations. These studies confirm the orientation of the reaction predicted by theoretical calculations.

Le résumé contient tous les détails pertinents.

Acta Cryst. (1992). C**48**, 220

Crystal structure and photochemistry of a methyl phenyl diester derivative of dibenzobarrelene. Erratum.

By James Trotter and Fred C. Wireko, *Department of Chemistry, University of British Columbia, Vancouver, BC, Canada V6T 1Y6*

(*Received* 29 *July* 1991)

Abstract

An error in technical editing is corrected. In the paper by Trotter & Wireko [*Acta Cryst.* (1991), C**47**, 793–797] the title compound is incorrectly named as a 2,3-diester on pages 793, 794 and 796; its correct name is methyl phenyl dibenzobarrelene-11,12-dicarboxylate.

All relevant information is given in the *Abstract.*

Acta Cryst. (1992). C**48**, 220

Structure of the modified nucleoside 2',3'-dideoxy-3'-fluorocytidine. Erratum.

By H. L. De Winter, N. M. Blaton, O. M. Peeters and C. J. De Ranter, *Laboratorium voor Analytische Chemie en Medicinale Fysicochemie, Instituut voor Farmaceutische Wetenschappen, Katholieke Universiteit Leuven, Van Evenstraat* 4, *B*-3000 *Leuven, Belgium*, and A. Van Aerschot and P. Herdewijn, *Laboratorium voor Farmaceutische Chemie, Rega Institute for Medical Research, Katholieke Universiteit Leuven, B*-3000 *Leuven, Belgium*

(*Received* 10 *October* 1991)

Abstract

In the paper by De Winter, Blaton, Peeters, De Ranter, Van Aerschot & Herdewijn [*Acta Cryst.* (1991), C**47**, 832–835] the fractional *y* coordinates of atoms C1'*A*, C3'*A* and F3'*A* should be 0.5916 (3), 0.3130 (3) and 0.3924, respectively.

All relevant information is given in the *Abstract.*

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