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Corrigendum

Volume **48,** Number 3 (1983), in the article "Neutron and X-Ray Diffraction Study on Polymorphism in Lithium Orthotantalate, Li_3TaO_4," by M. Zocchi, M. Gatti, A. Santoro, and R. S. Roth, pages 420–430:

The high-temperature phase of lithium orthotantalate, α-Li_3TaO_4, has been investigated by Zocchi *et al.* (*1*). The structure has been described by these authors in the acentric space group *P*2. From an analysis of the published atomic coordinates, Marsh (*2*) suggested that the correct space group might be *P*2/*n* instead. A refinement in space group *P*2/*n*, based on neutron powder data, shows that Marsh's suggestion is indeed correct.

The corrected Table IV (printed here) shows the atomic coordinates in the centric space group.

TABLE IV

RESULTS OF THE RIETVELD REFINEMENT OF α-Li_3TaO_4 IN SPACE GROUP *P*2/*n*

Atom	*x*	*y*	*z*	*B* (Å²)
Ta(1)	$\frac{1}{4}$	0.580(2)	$\frac{3}{4}$	0.3
Ta(2)	0.403(1)	0.134(1)	0.0821(5)	0.3
O(1)	−0.016(1)	0.142(1)	0.2579(6)	0.5
O(2)	0.487(1)	0.386(1)	0.7432(7)	0.5
O(3)	0.162(2)	0.360(1)	0.0779(5)	0.5
O(4)	0.652(2)	0.357(2)	0.0906(5)	0.5
O(5)	0.681(2)	0.116(2)	0.5876(6)	0.5
O(6)	0.145(2)	0.113(1)	0.5729(5)	0.5
Li(1)	$\frac{3}{4}$	0.124(4)	$\frac{3}{4}$	1.0
Li(2)	0.396(3)	0.416(3)	0.594(2)	1.0
Li(3)	−0.084(4)	0.130(6)	0.096(2)	1.0
Li(4)	$\frac{1}{4}$	0.416(6)	$\frac{1}{4}$	1.0
Li(5)	$\frac{1}{4}$	0.132(7)	$\frac{3}{4}$	1.0
Li(6)	0.608(4)	0.369(4)	−0.081(2)	1.0

$R_N = 6.70$, $R_P = 7.48$, $R_W = 9.67$, $R_E = 5.09$[a]

Note. Numbers in parentheses are standard deviations in the last decimal figure.

[a] For definitions of the *R* factors, see Table II of the original paper (*1*).

In general, the failure to recognize the center of symmetry introduces into the acentric model distortions well without the reported esd's and, as a consequence, significant structural details may be wrong. A detailed discussion of this problem has been given by Schomaker and Marsh (*3*) and by Herbstein and Marsh (*4*).

However, the descriptions of the structure of α-Li_3TaO_4 in space groups *P*2 and *P*2/*n* are quite similar to one another and, for this reason, the conclusions reached in the original paper (*1*) need not be changed. In particular, in the *P*2 model, the oxygen and tantalum coordinates show only a slight distortion from a centrosymmetric structure and this may explain why no difficulties ensued in the refinement based on neutron diffraction data.

In the centric model the two independent Ta–Ta distances are equal within 3σ and the shortest distance equals 3.10 Å, as reported by Zocchi *et al.* (*1*) for the acentric structure. Therefore the important conclusion that the stress introduced by the edge-sharing of the Ta coordination octahedra is smaller in the α phase than in the β phase can be confirmed after refinement of the centric model.

References

1. M. Zocchi, M. Gatti, A. Santoro, and R. S. Roth, *J. Solid State Chem.* **48**, 420 (1983).
2. R. E. Marsh, private communication (1983).
3. V. Schomaker and R. E. Marsh, *Acta Crystallogr. Sect. B* **35**, 1933 (1979).
4. F. H. Herbstein and R. E. Marsh, *Acta Crystallogr. Sect. B* **38**, 1051 (1982).