

Errata

Erratum: Photoelastic constants of calcite from its first-order Raman spectrum
[Phys. Rev. B 28, 2172 (1983)]

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Since our paper was published, we have noticed a few errors.

- (1) In Eq. (A13), the strain for R_x , which should be $-\frac{3}{2}u_{yz}$, was incorrectly given as $\frac{3}{2}u_{yz}$.
(2) The symmetry coordinate S_{5a} in Table I should be

$$S_{5a}^E = (1/\sqrt{2})\{R_x - (2.6445/2R)[(R'_2 - R''_2) - (R'_3 - R''_3)]\} .$$

R was omitted in the original. Now the two parts in the curly brackets are dimensionless. Then the normalization factors are suitably changed.

Consequently, the elements G_{35} and G_{55} of Table II on p. 2176 are altered as $(1.186/r)\mu_0 = 0.035$ and $(2.30)\mu_0 = 0.0862$, respectively, and Eqs. (17c) to (17j) become

$$A_2 = \frac{1}{2/2}\gamma'_{C-O} - (0.7096)\gamma_{Ca-O} , \quad (17c)$$

$$A_3 = \frac{\gamma_{C-O}}{\sqrt{2}} + (0.3029)\gamma_{Ca-O} , \quad (17d)$$

$$A_4 = (0.3015)\gamma_{Ca-O} , \quad (17e)$$

$$A_5 = (-0.3131)\gamma_{Ca-O} , \quad (17f)$$

$$A_6 = (-1.0164)\gamma_{C-O} + (0.9809)\gamma_{Ca-O} , \quad (17g)$$

$$A_7 = (+0.4346)\gamma_{C-O} - (0.4194)\gamma_{Ca-O} , \quad (17h)$$

$$A_8 = (1.6589)\gamma_{C-O} - (1.0289)\gamma_{Ca-O} , \quad (17i)$$

$$A_9 = (-0.7386)\gamma_{C-O} + (0.1378)\gamma_{Ca-O} . \quad (17j)$$

(3) In the equation $\epsilon = 1 + 4\pi bN\alpha$, given on p. 2174, line 1, α (the polarizability tensor) is for one molecule, as N is the number of molecules per unit volume. This should be borne in mind while calculating A and $URle$. A was calculated correctly for one molecule. However, $URle$ was calculated for the entire unit cell by multiplying the value for one molecule by $\sqrt{2}$. Hence, the values given in Table IV should be divided by $\sqrt{2}$.

This changes the value of K^2 of Eq. (19a) to 21.72×10^{-6} if Pockel's value of $P_{11} + P_{12} = 0.297$ is taken, and to 10.75×10^{-6} if Nelson's value of $P_{11} + P_{12} = 0.209$ is taken. Consequently, Eqs. (19a) and (19b) become

$$\sum_i I_{ij}^2 K^2 n_x^2 = 0.0040 = \gamma_{C-O}^2(0.0094) + \gamma_{Ca-O}^2(0.098) + \gamma_{Ca-O}^2(0.021) - \gamma'_{C-O}\gamma_{C-O}(0.029) \\ - \gamma'_{C-O}\gamma_{Ca-O}(0.019) - \gamma_{C-O}\gamma_{Ca-O}(0.0098) , \quad (19a)$$

$$\sum_i I_{ij}^2 K^2 n_x n_z = 0.0032 = \gamma_{C-O}^2(0.036) + \gamma_{Ca-O}^2(0.014) - \gamma_{C-O}\gamma_{Ca-O}(0.013) . \quad (19b)$$

$K^2 = 21.72 \times 10^{-6}$ in these equations. Now the entry against S_{5a}^E of Table IV becomes

	e_{xx}	e_{yy}	e_{yz}	ω_z
S_{5a}^E	1.0179	-1.0179	0.4754	0.5304

The entry against S_{3a}^E should be $-1.0601(e_{xx} - e_{yy})$. This is a consequence of an error in Eqs. (A8). $r \sin\theta$ in the denominator should be replaced by $2r \sin\theta$ and 2, which is multiplying e_{xx} , e_{yy} , and e_{xy} of Eqs. (A10) and (A11), should be dropped.

(4) Then the correct expressions for P'_{14} to P'_{66} on p. 2178 can be obtained and the following equations used to calculate the electro-optical parameters.

$$P'_{14} = -0.0907 = -0.4334\gamma'_{C-O} + 0.2684\gamma_{Ca-O} ,$$

$$P'_{66} = -0.3212 = 0.2223\gamma'_{C-O} + 0.7497\gamma_{C-O} - 1.0218\gamma_{Ca-O} ,$$

$$P'_{44} = -0.4188 = -1.5949\gamma_{C-O} + 1.4074\gamma_{Ca-O} .$$

While Pockel and Nelson reported the same values for P'_{14} and P'_{66} , Nelson's value for $P'_{44} = -0.3520$. Using P'_{14} , P'_{66} , and

TABLE VII. Electro-optical constants calculated with the use of values of Pockel and Nelson. The values given below are accurate up to two digits.

$\gamma_{C-O}(yz)$	0.3460	0.3265
γ'_{C-O}	0.4118	0.4480
γ_{Ca-O}	0.3263	0.4138
$\gamma_{C-O}(yy)$	-0.1063	0.0022

TABLE V. Photoelastic constants.

	Calculated with the use of some values of		Experimental	
	Pockel	Nelson	Pockel	Nelson
P_{13}	0.295	0.346	0.223	0.186
$P_{1[4]}$	-0.0072	-0.0091
P_{31}	0.1076	0.113	0.310	0.241
P_{41}	-0.0232	-0.0018	0.0007	-0.036
P_{33}	0.2139	0.224	0.188	0.139
$P_{4[4]}$	-0.0229	-0.016	...	0.047

(19a), γ'_{C-O} , γ_{C-O} , and γ_{Ca-O} are calculated. γ_{C-O} , thus calculated, is designated $\gamma_{C-O}(yy)$. Substituting for γ_{Ca-O} in p'_{44} , $\gamma_{C-O}(yz)$ is obtained. Table VII is thus altered.

On substituting $\gamma_{C-O}(yz)$ and γ_{Ca-O} in (19b), it is found that the values of the first column satisfy the intensity equation, while the values of the second column do not. It is possible that $P_{11} + P_{12}$ given by Nelson is too small and does not give correct values for K^2 .

Photoelastic constants other than those used in these calculations are calculated from the electro-optical parameters and are given in Table V.

We emphasize that $P_{1[4]}$ is not too small, contrary to what is reported by Nelson and Lax (Refs. 2 and 4 of our paper).

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Erratum: White lines at K edges of light atoms [Phys. Rev. B 31, 5066 (1985)]

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The hydrogenic calculation of the $1s$ excitation spectrum of magnesium discussed in the text and shown in Fig. 8 is incorrect. The correct result is greater by a factor of 2 and so is in better agreement with more realistic calculations than what was shown. This error does not affect any of the paper's conclusions. We thank Professor R. F. Egerton for bringing it to our attention.