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. Publication will be quicker if the contributions are without illustrations.*

Ordering scheme for general positions in *International Tables*. Some corrections and additions. By E. F. Bertaut, *Laboratoire d'Electrostatique et de Physique du Métal, CNRS, Chemin des Martyrs, Grenoble, France* and H. Wondratschek, *Institut für Kristallographie der Universität,* 75 *Karlsruhe* 1, *Kaiserstrasse* 12, *Germany* (*BRD*)

Corrigenda are given for *Acta Cryst.* (1971), A**27**, 298.

The following corrections and additions should be made.

1. To (2) should be added
   $N_0 = I$, the unit subgroup.
2. (3) and the two following lines should read

$$a_0 a_1^{\gamma 1} \ldots a_l^{\gamma l} \ldots a_{k-1}^{\gamma k-1} a_k^{\gamma k} \qquad (3)$$

   ($0 \le \nu_l < n_l$, n_l order of N_l/N_{l-1}, or ν_l any (positive or negative) integer, when n_l infinite) of powers of the generators a_l.
3. The first sentence of the second paragraph, right column of p. 298, should read: In general there are different possible chains N_0, $N_1, \ldots, N_k$ and different possible choices for the coset representatives.
4. The second sentence of the footnote, p. 298, should read: For the systematic generation of all general positions belonging to a given unit cell these fractional translations can be (and in some cases, have to be) introduced as the first generators after the integral translations.

5. In the text of Table 1 the last two formulae should read

$$2_z 32_d = 4_y, \quad 2_x 32_d = 4_y^3.$$

6. On p. 299, right column, eighth line after (6) should read 'block T' instead of 'blocks T'.
7. P. 300, left column, fourth line, $4/mm$ should read $4/mmm$.
8. P. 300, left column, the last three lines should read

$$\{m3m - O_h\} = \{T\} + \{T\}\ (2_d|\tau) + \{T\}\ (\bar{1}|\tau_{\bar{1}}) + \{T\}\ (m|\tau_m)$$

   where

$$(m|\tau_m) = (2_d|\tau)\ (\bar{1}|\tau_{\bar{1}}) .$$

9. P. 300, the end of the first line of the right column should read

$$\{T\} + \{T\}(2_d|\tau) .$$

Traps responsible for 360 and 390°K glow peaks in X-irradiated NaCl:Tl crystals. By R. V. Joshi and T. R. Joshi, *Physics Department, M. S. University of Baroda, Baroda, India*

Correlated measurements on the thermoluminescence and optical absorption of X-irradiated NaCl:Tl indicate that the glow peaks observed at 360 and 390°K may be due respectively to electrons released from F' and some species of higher aggregate centres.

The study of the correlation of the filling and emptying of the thermoluminescence traps with the formation and destruction of some colour centres has been reported by Fischer (1961). The present work is an extension of the earlier study reported from this laboratory, the results of which suggested that the 340°K glow peak in NaCl:Tl could be correlated with the F-band absorption (Joshi & Joshi, 1971). The purpose of the present investigation has been to seek correlation between colour centre absorptions and the glow peaks at 360 and 390°K in NaCl:Tl.

Thallium in the form of TlCl (reagent grade) was thermally diffused in the plates cleaved from a Harshaw NaCl single crystal. The specimens so obtained were examined either in an untreated condition or after thermal pretreatment. The latter involved the annealing of the specimen at 750°C in open air for three hours and rapid quenching to room temperature. The thermal glow curves were recorded by warming the specimen at a uniform rate of $10°.\text{min}^{-1}$. The absorption measurements, which always preceded the

thermoluminescence measurements, were made at room temperature. The concentration of thallium in all the specimens studied was of the order of 10^{-3} mol fraction. It was observed that the experimental results for the specimens with the same history were in general identical. The results obtained for two specimens differing in thermal history are presented for discussion.

Fig. 1 represents the absorption and thermoluminescence data for an untreated specimen. In the Figure curves 1 and 3 indicate the absorption and thermolumiscence of the specimen after 30 minutes X-irradiation at room temperature, whereas curves 2 and 4 exhibit the corresponding data after 30 minutes X-irradiation followed by 30 minutes F-light illumination. It is obvious from the figure that illumination of the specimen with F-light suppresses the F-band absorption and to a certain extent enhances absorption in the F' and R-band regions. In the corresponding thermal glow curve, peaks at 360 and 390°K are discernible. Fig. 2 represents the results on the optical absorption and ther-

moluminescence of a rapidly quenched specimen after 30 minutes X-irradiation. It is significant that the absorption curve in Fig. 2(a) is markedly different from that obtained for the untreated specimen. In this case the absorption in F' and R-band regions appear comparable with that in the F-band. In the corresponding thermal glow curve, Fig. 2(b), there is a dominant glow peak at 390 °K and another at 360 °K.

It is known that if the alkali halides are subjected to prolonged X-irradiation near room temperature, in addition to the F-band, new absorption bands situated on the longer-wavelength side of the F-band are formed. Since the new bands grow at the expense of the F-band by room temperature illumination of X-irradiated crystals with F-band light, these bands have been suggested to be due to electron excess centres such as M,R,N etc. As expected, the illumination of X-irradiated specimens with F-light in the present experiments [Fig. 1(a)] suppresses the F-band, generates the F' band ($\lambda_{F'} = 510m\mu$) and enhances absorption in the R-band region ($\lambda_{R1} = 545m\mu$; $\lambda_{R2} = 596m\mu$). In the corresponding thermoluminescence, the illumination with F-light reduces the strength of the 340 °K glow peak and new glow peaks at 360 and 390 °K appear. The 340 °K glow peak has been previously assigned to F centres (Joshi & Joshi, 1971). It has been reported before that the thermal glow peak at 360 °K in NaCl is due to thermal release of F' electrons (Gudden & Pohl, 1925). It is therefore reason-

Fig. 2. (a) Optical absorption and (b) corresponding thermo-luminescence of an annealed and quenched NaCl:Tl crystal after X-irradiation.

able to assume that the 360 °K glow peak presently observed is associated with F' centres and the 390 °K glow peak with R-type higher aggregate centres. The R-type centres instead of R centres are suggested since the absorption observed in the R-band region coincides neither with the R_1 nor the R_2-band.

The above hypothesis is corroborated by the results give in Fig. 2 for thermally pretreated specimens. In the case of these specimens the F' and R-band region absorptions appear comparable with F-band absorption and the corresponding glow curve exhibits 360 and 390 °K peaks. The suggested thermal stability of F' centres (360 °K) higher than F centres (340 °K) can be inferred from the present understanding of the colouration phenomena in alkali halides (Royce, 1968; Crawford, 1968). It is now generally believed that the mechanism of F centre production at all temperatures involves the creation of Frenkel pairs in the negative ion sub-lattice. The production of Frenkel pairs gives rise to different forms of stable interstitial species at various lattice temperatures. This in turn leads to the generation of F centres, associated with the interstitials, of different thermal stability.
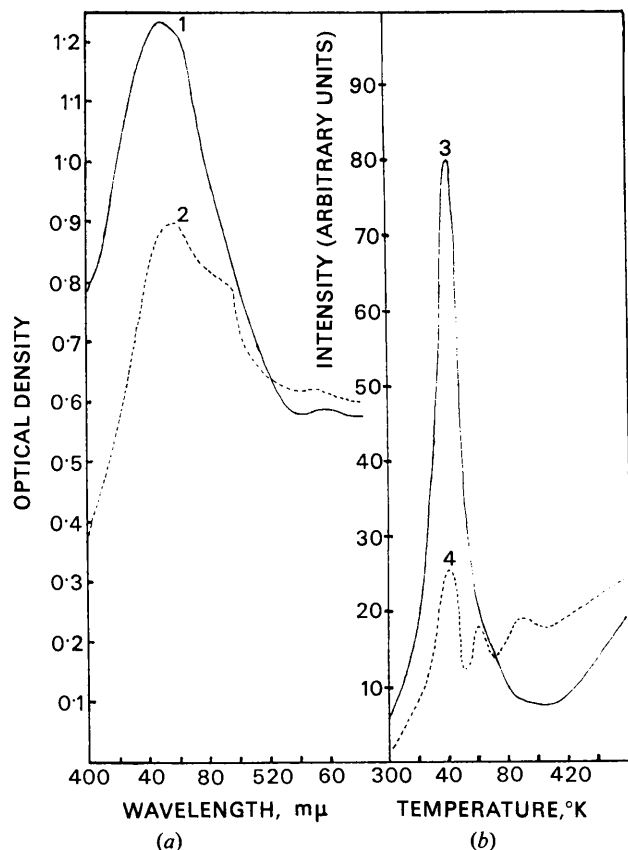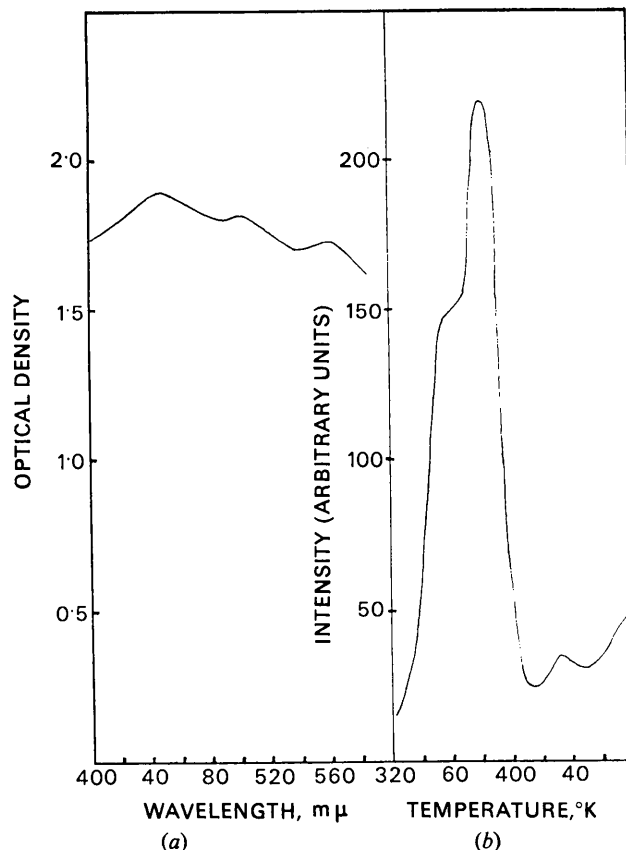

Fig. 1. (a) Optical absorption and (b) corresponding thermo-lumiscence of an untreated NaCl:Tl crystal. Curve 1: after X-irradiation alone; curve 2: after X-irradiation followed by F-light illumination.

References

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