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## 1 Formation Kinetics, Optical and Electro-Optical Properties of $F_2^+$ Centers \*

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$F_2^+$  centers were so far identified in several alkali halides by one absorption band in the 0.6—1.6  $\mu$  region. The formation of these centers was observed empirically after ionizing irradiation followed by different thermal and optical treatments<sup>1</sup>.

We show first, that in additively colored KCl the  $F_2^+$  centers can be formed simply by optical ionization of M centers in their higher absorption transitions in the UV ("L<sub>M</sub>-bands"). A quantitative analysis of these transitions up to 5.5 eV crystals with high M:F ratio and aligned and unaligned M centers shows several excitations. From their polarization properties it appears that most of the structure is due to optical transitions parallel to the M center axis.

Assuming that L<sub>M</sub> excitation (similar to that of L<sub>F</sub> bands) leads to conductive states, UV irradiation of an F + M centers system produces ionized F and M centers ( $\alpha$  and  $F_2^+$ ), while competing capture processes partially destroy them and form F' and M' centers too.

The simple electron kinetics can be quantitatively worked out and shows that the excitation spectrum for UV production of  $F_2^+$  centers should closely follow the absorption ratio of L<sub>M</sub>:L<sub>F</sub>, while the excitation spectrum for the  $F_2^+$  centers bleaching should follow the F' and M' spectrum. Both have been experimentally verified.

Introduction of extra electron traps into the crystal shifts the equilibrium of this reaction to higher  $F_2^+$  center amounts. Different traps are tried out to achieve this objective. For example, if the crystal (containing F + M centers) is X-rayed at He-temperature (as done by Schneider and Rabin<sup>1</sup>) higher amounts of  $F_2^+$  centers are formed, which are not stabilized by F' and M' centers. These extra  $F_2^+$  centers anneal out near 40 °K in complete parallelism with the third stage annealing of the X-ray produced  $\alpha$  centers + interstitial anions. It is thus concluded that these  $\alpha$  centers are the electron traps enhancing the  $F_2^+$  production.

A thorough investigation of the  $F_2^+$  centers formed with these methods reveals (besides the known absorption and emission band at 1.4 and 1.65  $\mu$  resp.) 3 new absorption bands at 492, 390 and 325 m $\mu$ , which all produce under excitation a single emission at 610 m $\mu$  (see Fig.). Temperature dependence, dichroic behavior and polarization properties of these transitions were investigated.

A remarkable analogy exists between the  $F_2^+$  center and the H<sub>2</sub><sup>+</sup> molecule whose quantum states are very accurately calculated<sup>2</sup>. Following

Herman et al.<sup>3</sup> we can surprisingly well fit the observed absorptions of the  $F_2^+$  center to the calculated states of the  $H_2^+$  molecule, corrected with a single dielectric constant  $k_0$  (see Fig.).

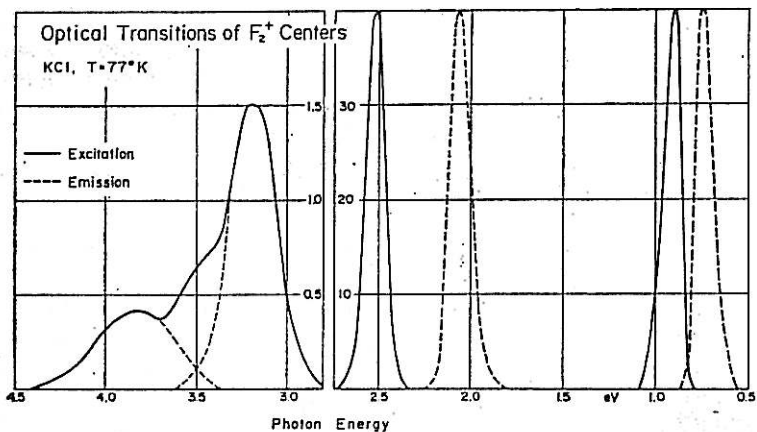
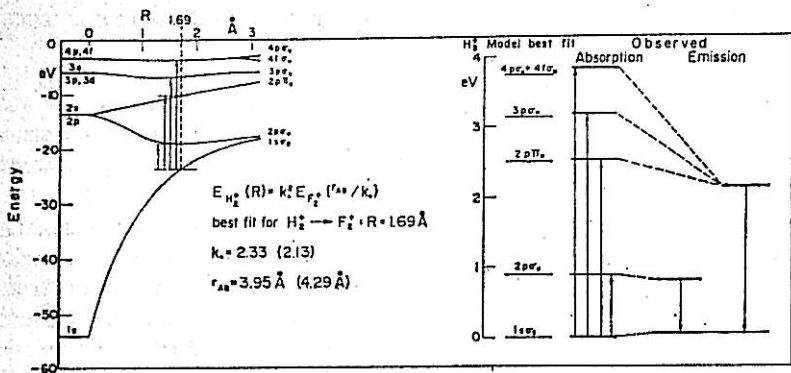


Fig. 1 - The observed optical transitions of the  $F_2^+$  center in KCl and their best fit into the calculated energy level diagram of the  $H_2^+$  molecule.

As most of the  $H_2^+$  transitions are experimentally unobservable, the  $F_2^+$  center can be regarded in part as an experimental model system to check these calculations.

The  $F_2^+$  center is also the realization of a simple double well potential with a charged particle in it. This constitutes the widely used model case from which all consideration about particles in more complicated multi-well potentials, their tunneling, relaxation and localization properties start out.

The two lowest states of the  $F_2^+$  centers can be regarded as the symmetric and asymmetric "tunnelling states" of the double well potential, sepa-

rated by the (large!) tunneling splitting  $2\Delta = 0.89$  eV. The effects of electric fields on this system are accurately predicable. For practical fields ( $\mu E \ll \Delta$ ) only a small amount of electron localization into one of the wells is possible, producing only quadratic Stark effects. Results on electro-optical measurements will be reported. Attempts are under way to create  $F_2^+$  type double vacancy configurations with larger vacancy separation, which have much smaller tunneling splittings (and transitions in the IR) and large dipole moments so that electron localization by fields should be possible.

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<sup>1</sup> I. Schneider and H. Rabin, Phys. Rev. **140**, A 1983 (1965).

<sup>2</sup> D. R. Bates, K. Ledsham and A. L. Stewart, Phil. Trans. Roy. Soc. A, **246**, 215 (1953).

<sup>3</sup> R. Herman, M. C. Wallis and R. F. Wallis, Phys. Rev. **103**, 87 (1956).

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## 2 Role of Thermally Activated Anion Vacancy Processes on the Radiation Intensity Dependence of the F-Colouring in NaCl

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The influence of  $Co^{60}$   $\gamma$ -radiation intensity on the saturation level of the first stage of the room-temperature F-colouring of NaCl, has been investigated in the range 50 to 30.000 R/min. Experimental results have shown that the F-colouring level decreases very slowly with intensity on going from 30.000 to 5.000 R/min, very markedly between 5.000 and 250 R/m and finally for intensities below 25 R/m it stays approximately constant around 70% of the level correspond to 30.000 R/min.

The above dependence might be attributed either to the intensity sensitivity of the radiation induced mechanisms for defect production or the operation of competing secondary reaction among defects which are thermally activated. In fact, recent work on NaCl has revealed the existence of a thermally activated process of trapping of free anion vacancies which saturates in 50-60 minutes at room temperature. This process leads to a decrease in the F-colouring whenever a short dose irradiation is given to an irradiated sample after it has been in the dark for some minutes. Since this behaviour appears to be similar to that observed after a reduction in intensity, a detailed study was undertaken to ascertain the role played by the above process in determining the influence of radiation intensity on F-colouring.

It is known that if, once the saturation of the initial F-colouring has been reached, radiation intensity is shifted to a lower value, the colouring decreases to a new saturation level which is characteristic of the last