ABOUT EXISTING OF THE 'ROTATION' POLARON IN MOLECULAR CRYOCRYSTALS

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The influence of strongly localized carrier (electron or hole) on the nearest environment in a molecular cryocrystal is theoretically investigated. The action of the local electric field on the molecular orientation and relaxation of ideal crystal lattice is considered. A source of carriers is usually injection or radiation with generation of exitons.

The Hamilionian of the system carrier-lattice contains next contributions: (i) carrier,(ii) lattice (iii) carrier-lattice interactions $H_{el} = -\sum Ed$. Here E is electric field of the carrier which is acting on the molecule with an anisotropic dipole moment d, intrinsic for polar molecule or induced for symmetric one, sum is for different neighbor molecules.

In the case of molecular cryocrystal CO (N2) the axes reorientation of the nearest molecules along the electric field is considerable but realized only particularly. Thus for CO (N2) the energetic barrier for the reorientation exceeds 668K (330K) and maximal profit in energy 300K (150K) for each neighbor. For the bigger molecules CO2, N2O the energetic barrier is much higher and the reorientation is much weaker. For H2 crystal under the pressure several types of polarons can exist. The parameters of the crystals and molecules one can find in [1].

[1]CRYOCRYSTALS// Ed. Verkin B.I. et al