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HYDROSTATIC-PRESSURE-TUNING FROM CLASSICAL TO TUNNELING MOTION AND FROM OFF- TO ON-CENTER POTENTIALS FOR Ag^+, Cu^+ AND Li^+ DEFECTS (*)

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Abstract. — The delicate balance among various defect-lattice interaction energies, producing off-center potentials for certain small point-defects, can be drastically upset by increasing the repulsion energy through hydrostatic pressure application. Consequently, the multiwell off-center potential becomes more shallow and transforms eventually into a centro-symmetric single-well potential. This pressure tuning from off- to on-center behaviour has been studied for Ag^+, Cu^+ and Li^+ defects in various hosts through the temperature range 1.5 to 300 K. Dielectric loss measurements show for the classically reorienting Ag^+ and Cu^+ defects a gradual decrease of the reorientation barrier and eventually a change to tunneling behaviour under pressure, and for the quantum-mechanical KCl : Li^+ system a strong increase of the tunneling splitting. The size of the off-center dipole moment $< p >$ was monitored by the real ($\varepsilon \propto < p >^2/T$) and integrated imaginary dielectric response, and — for Cu^+ and Ag^+ ions — by the strength of the parity-forbidden $d \rightarrow s$ transition which becomes partially allowed in off-center potentials. Both optical and dielectric data indicate a rather constant dipole moment, which collapses abruptly at a critical characteristic pressure in a way suggesting a *local phase-transition* picture for the off- to on-center symmetry change.

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