CHIRALITY IN ROTATIONAL ENERGY LEVEL CLUSTERS

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Chirality results when a molecule has two physically distinguishable mirror image forms of its equilibrium structure separated by an essentially insuperable potential energy barrier. The wavefunctions of the optically active rovibrational levels of a molecule having this 'static' chirality only sample one of the two chiral potential minima, and they have mixed parity. Rotation and vibration dynamics can affect optical activity. For example, one can conceive of the possibility that rovibrational levels in highly excited states of an appropriate tunneling vibration will not be optically active since their wavefunctions will observably sample the regions of both potential minima. In this paper we show that rotational motion can produce rovibrational states of significant lifetime that are optically active (having mixed parity) in rotational energy level clusters of molecules such as H_2Se that do not possess static chirality. Such dynamically induced chirality has been mentioned before as being possible in the methane molecule.[a]

[a] P. W. Atkins and J. A. N. F. Gomes, *Chem. Phys. Lett.,* **39**, 519-520 (1976).