CURVILINEAR INTERNAL VALENCE COORDINATE HAMILTONIAN FOR AMMONIA

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A new six-dimensional vibrational Hamiltonian based on curvilinear internal valence coordinates is presented for ammonia. The square of the inversion coordinate adopted is similar to the often used out-of-plane bending coordinate for planar XY_3-type molecules. Conventional symmetrized internal coordinates are employed for the other vibrational degrees of freedom. The exact kinetic energy operator is given in closed form.