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Spontaneous Quantum Electrical Dipole Predicted in Triangular Molecules RYAN REQUIST, PHILIP B. ALLEN, ALEXANDER G. ABANOV, Stony Brook University, TUNNA BARUAH, Naval Research Laboratory — Triangular symmetric molecules are forbidden by symmetry to have a fixed electrical dipole moment. However, with orbital degeneracy and an odd electron count yielding an electronically degenerate ground state (as in Na_3), a quantum dipole moment is shown to exist. Unlike the fixed dipole of a water molecule, the moment does not point in a fixed direction, but lies in the plane of the molecule and takes quantized values μ_0 along any direction of measurement in the plane. An electric field $\vec{F}$ in the plane leads to a linear Stark splitting $\pm\mu_0|\vec{F}|$. Linear Stark splittings are suppressed in low fields by molecular rotation, just as the linear Stark shift of water is suppressed, but will be revealed in moderately large applied fields and low temperatures. With an increasing barrier to the free periodic Jahn-Teller motion of the nuclei, there is a crossover from the quantum dipole to the classical dipole of a rigidly distorted triangular molecule. Density functional theory calculations for Na_3, a simple model system, suggest that its dipole is classical, because there is a large barrier that obstructs free Jahn-Teller motion.

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