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Applications of Curie Symmetry Principle in Molecular Ferroelectrics

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To predict or identify ferroelectricity is essential for extending the family of molecular ferroelectrics and thereby promoting their practical applications in nonvolatile memories, capacitors, piezoelectric sensors and nonlinear optical devices. In this respect, symmetry breaking is of particular importance, since the paraelectric phase adopting any of the 32 crystallographic point groups is always broken into one of the 10 ferroelectric point groups, i.e. C1, C2, C1h, C2v, C4, C4v, C3, C3v, C6 and C6v.1 It is the Curie symmetry principle that determines the group-subgroup relationship between paraelectric and ferroelectric phases, and thus 88 species of potential ferroelectric phase transitions are deduced. However, in some cases such as croconic acid and triglycine sulfate (TGS), the existence of pseudo center of symmetry makes it difficult to accurately recognize the ferroelectric phase. Then inspired by the Neumann's principle, which states that the symmetry of any physical property of a crystal must include the symmetry elements of the point group of the crystal, the temperature-dependent SHG effect and dielectric property become useful for detecting symmetry breaking and ferroelectricity. Consequently, in the light of the Curie symmetry principle and Neumann's principle, ferroelectrics can be effectively distinguished from innumerable compounds with various crystal structures collected in the Cambridge Structural Database. Taking advantage of such strategy and combining with the measurements of ferroelectric hysteresis loops and ferroelectric domains, we have successfully discovered a series of low-temperature and high-temperature molecular ferroelectrics with high performance.2-6 This study does help to avoid blindly searching for molecular ferroelectrics.

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