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Symmetry crossover in layered MPS3 complexes (M= Mn, Fe, Ni) via near-field infrared spectroscopy[1]

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We employ synchrotron-based near-field infrared spectroscopy to reveal the vibrational properties of bulk, few-, and single-sheet members of the $M\mathrm{PS}_3$ (M = Mn, Fe, Ni) family of materials and compare our findings with complementary lattice dynamics calculations. MnPS_3 and the Fe analog are similar in terms of their symmetry crossovers, from $C2/m$ to $P\bar{3}1m$, as the monolayer is approached. These states differ as to the presence of a C_3 rotation around the metal center. On the other hand, NiPS_3 does not show a symmetry crossover, and the lack of a B_u symmetry mode near 450 cm^{-1} suggests that C_3 rotational symmetry is already present - even in the bulk material. We discuss these findings in terms of local symmetry and temperature effects as well as the curious relationship between these symmetry transformations and what takes place under pressure. Time permitting, we will compare the $M\mathrm{PS}_3$ family of materials with complementary work on CrPS_4 - a system in which the P-P dimer is absent.

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