GROUP THEORY OF DIMETHYL METHYL PHOSPHONATE

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The dimethyl methyl phosphonate molecule $(CH_3O\text{-})_2P(=O)\text{-}CH_3$ has five large-amplitude motions, consisting of rather traditional three-fold-barrier internal rotations for each of the three methyl tops, together with less traditional skeletal-flexing internal rotations about each of the two P-O bonds. Experimental evidence (previous talk) indicates that all three methyl tops are inequivalent, with the corresponding splittings in a $(J+1)_{0,J+1}$ - $J_{0,J}$ pattern of the order of 20 MHz, 2 MHz and 0.2 MHz, respectively. A group theoretical treatment which neglects the smallest torsional tunneling motion leads to a permutation-inversion molecular symmetry group G_{18}, which is a subgroup of the group G_{36} used in our earlier study of the methanol dimer. This G_{18} group is chiral, in the sense that two-fold and four-fold separable degeneracies occur, i.e., degeneracies occur which are not intrinsic to the character table of the group, but result instead from an application of time reversal. Results from this G_{18} group nicely explain the qualitative features of the *a*-type spectral patterns, and work is in progress to apply the results also to *b*-type and *c*-type patterns. When rotation of the third methyl top is considered, the appropriate group is G_{54}. Work on splitting patterns from this group is in progress.