

# MOLECULAR SYMMETRY ANALYSIS OF LOW-ENERGY TORSIONAL AND VIBRATIONAL STATES IN THE $S_0$ AND $S_1$ STATES OF *p*-XYLENE TO INTERPRET THE REMPI SPECTRUM

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The electronic transition  $S_1 \leftarrow S_0$  of *p*-xylene (pXyl) has been observed by REMPI spectroscopy.<sup>a</sup> Its analysis required a detailed investigation of the molecular symmetry of pXyl whose methyl groups are almost free internal rotors. The molecular symmetry group of pXyl has 72 operators.<sup>b</sup> This group, called  $[33]D_{2h}$ , is isomorphic to  $G_{36}(\text{EM})$ ,<sup>c</sup> the double group for ethane and dimethyl acetylene even though it is NOT a double group for pXyl. Loosely speaking, the group symbol,  $[33]D_{2h}$ , indicates that is for a molecule with two threefold rotors on a molecular frame with  $D_{2h}$  point group symmetry. The transformation properties of the (i) free internal rotor basis functions for the torsional coordinates, (ii) the asymmetric rotor (Wang) basis functions for the Eulerian angles, (iii) nuclear spin functions, (iv) potential function, and (v) transitions dipole moment functions were determined. The forms of the torsional potential in the  $S_0$  and  $S_1$  states and the dependence of the first order torsional splittings on the potential coefficients have been obtained.

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<sup>a</sup>AM Gardner, WD Tuttle, P. Groner, TG Wright, J. Chem. Phys., submitted Dec 2016

<sup>b</sup>P Groner, JR Durig, J. Chem. Phys., 66 (1977) 1856

<sup>c</sup>PR Bunker, P Jensen, Molecular Symmetry and Spectroscopy (1998, NRC Research Press, Ottawa, 2nd ed.)