TOLUENE INTERNAL ROTATION: REFINED BARRIER HEIGHT IN S_1, SIGN OF V_6, AND MOTION ALONG THE TORSIONAL COORDINATE.[a]

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High resolution electronic spectra of three torsional bands in the $S_1 \leftarrow S_0$ electronic transition of toluene have been recorded in a molecular beam. The analyses of these spectra provide a unique and unambigious determination of the sign of the V_6 hindering potential in both electronic states; $V_6(S_0)$ = -4.874 cm^{-1} and $V_6(S_1)$ = -26.375 cm^{-1}. Furthermore, the data show that both F and the frame rotational constant A_F vary between torsional levels within the S_1 manifold. Information about geometric changes responsible for these differences will be discussed, along with the validity of the one-dimensional, rigid frame-rigid top model.

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