

## PREDISSOCIATION DYNAMICS OF THE T-SHAPED AND LINEAR ISOMERS OF I<sub>2</sub>(B)Ar

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Three-dimensional quantum dynamics models for the predissociation of I<sub>2</sub>(B)Ar were examined by Gray and Roncero.<sup>a</sup> Their calculations predicted highly structured rotational population distributions for the I<sub>2</sub>(B) products. The distributions were characteristic of dynamics controlled by intramolecular vibrational energy redistribution (IVR). To test this model we have examined final state distributions resulting from predissociation of T-shaped I<sub>2</sub>(B)Ar using optical-optical double resonance (OODR) techniques. We observed smooth rotational distributions that are indicative of direct dissociation or IVR occurring with level densities near the statistical limit.

OODR measurements were used to probe the highest vibrational level of I<sub>2</sub>(B) populated by predissociation of T-shaped I<sub>2</sub>(B)Ar. This is a matter of interest as Stevens Miller *et al.*<sup>b</sup> have suggested that previous measurements<sup>c</sup> may be in error, leading to overestimation of the bond strength for the B and X states of I<sub>2</sub>Ar. The previous measurements relied on detection of dispersed fluorescence from I<sub>2</sub>(B), and may have been influenced by non-adiabatic decay channels. OODR is a more sensitive technique, potentially capable of detecting the highest energy products prior to non-radiative decay. However, the OODR experiments yield results that are in agreement with the earlier study.<sup>c</sup> The data do not resolve conflicts associated with the relative bond strengths of the T-shaped and linear isomers.<sup>c</sup>

OODR techniques are being used to characterize the predissociation of linear I<sub>2</sub>(B)Ar. Initial measurements show that I<sub>2</sub>(B) from the linear isomer has less rotational energy than I<sub>2</sub>(B) from the T-shaped complex.

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<sup>a</sup>S. K. Gray and O. Roncero *J. Phys. Chem.* 99, 2512 (1995)

<sup>b</sup>A. E. Stevens Miller, C. Chuang, H. C. Fu, K. Higgins and W. Klemperer *J. Chem. Phys.* 111, 7844 (1999)

<sup>c</sup>J. A. Balzy, B. M. DeKoven, T. D. Russell and D. H. Levy *J. Chem. Phys.* 72, 2439 (1980)