

## MILLIMETER WAVE SPECTROSCOPY OF THE INTERNAL ROTATION BANDS OF He-HCN AND He-DCN.

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Millimeter-wave absorption spectroscopy combined with a pulsed-jet expansion technique was applied to the measurement of the internal-rotation band of the He-HCN complex in the frequency region of 95–125 GHz. In total 13 rovibrational lines, split into nitrogen nuclear hyperfine structure, were observed for the fundamental internal-rotation band,  $j = 1 - 0$ . The observed transition frequencies and the previous MBER data<sup>a</sup> were analyzed to yield an empirical intermolecular potential energy surface, which was obtained by improving the recent *ab initio* potential surface.<sup>b</sup> The surface obtained has a global minimum in the linear configuration (He ···H–C–N) with a well depth of  $30.2 \text{ cm}^{-1}$ , and the saddle point located in the anti-linear configuration (H–C–N ···He) is higher in energy than the global minimum by  $8.92 \text{ cm}^{-1}$ . The distance  $R_m$  from the He atom to the center of mass of HCN along the minimum energy path shows a large angular dependence;  $R_m$  is  $4.169 \text{ \AA}$  and  $4.039 \text{ \AA}$  in the linear and anti-linear forms, respectively, and has a minimum value of  $3.528 \text{ \AA}$  in a T-shaped configuration. The He-DCN was also measured and analyzed. The empirical potential energy surfaces are compared with the *ab initio* potential energy surface<sup>b</sup> for both isotopic species.

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<sup>a</sup>S. Drucker, F. Tao, and W. Klemperer, *J. Phys. Chem.* 99, 2646(1995).

<sup>b</sup>R. R. Toczylowski, F. Doloresco, and S. M. Cybulski, *J. Chem. Phys.* 114, 851(2001).