ROTATIONALLY RESOLVED ELECTRONIC SPECTRUM OF THE PARA-DIFLUOROBENZENE-NITROGEN VAN DER WAALS COMPLEX: STRUCTURE AND INTERNAL MOTION[a]

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The rotationally resolved $S_1 \leftarrow S_0$ fluorescence excitation spectra of p-difluorobenzene and its N_2 complex have been observed. While the spectrum of pDFB is pure b-type, the spectrum of the N_2 complex is a superposition of two pure c-type spectra that result from the internal rotation of the N_2 molecule. The analysis reveals that N_2 molecule lies above the center of the ring plane in the S_0 state; this distance decreases in the S_1 state. The preferred orientation and barrier to internal rotation in the two electronic states are also different. A full discussion of the factors responsible for the differences will be given.

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