THE STRUCTURE, THE INTERNAL ROTATION OF N_2 AND THE ROTATION OF THE ELECTRONIC TRANSITION MOMENT IN THE PARA-DIFLUOROBENZENE-N_2 VAN DER WAALS COMPLEX

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Cold jet $S_1 \leftarrow S_0$ rotational band contours have been obtained at 0.3 cm^{-1} resolution for the p-difluorobenzene-N_2 (pDFB-N_2) van der Waals complex and analyzed with an asymmetric top simulation program. Satisfactory simulation is possible only if it is assumed that the in-plane electronic transition moment of pDFB-N_2 rotates about 37° towards the F-F axis from its position normal to that axis in free pDFB. The vdW bond distances from the ring plane to the N_2 bond parallel to that plane are 3.47Åand 3.42Åin the S_1 and S_0 states, respectively. Several transitions involving the internal rotation of N_2 about an axis perpendicular to the ring plane have been assigned. The band positions are consistent with two-fold rotational barriers of 14.0 cm^{-1} and 19.0 cm^{-1} for the S_0 and S_1 states, respectively. These barriers are in agreement with those recently [a] determined from the assignments of different internal rotor transitions seen in the R2PI spectra.

[a] Y. Hu, W. Lu and S. Yang, J. Photoch. Photobio. A, 106, 91(1997).