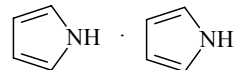


846  
MW $\text{C}_8\text{H}_{10}\text{N}_2$ **1H-Pyrrole dimer**  
(weakly bound complex) $\text{C}_s$   
(effective symmetry class)  
(large-amplitude motion)

$r_0$	$\text{\AA}^a$
$R_{\text{cm}}$	4.116(13)

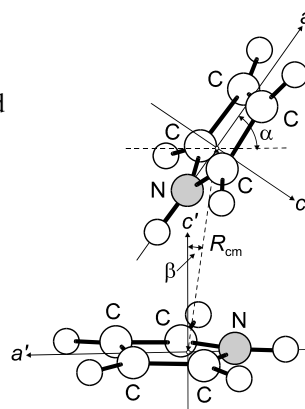
$\theta_0$	$\text{deg}^a$
$\alpha^b$	55.42(42)
$\beta^b$	12.02(29)



The rotational transitions did not show any additional splittings arising from large-amplitude motions. The observed rotational constants are consistent with essentially a T-shaped structure for the dimer. The planes of the two pyrrole monomers form an angle of  $55.4(4)^\circ$  with the nitrogen side of one ring directed to the  $\pi$  electron of the other ring establishing a weak hydrogen bond. Structural parameters were obtained by a least-squares fit to differences in planar moments of inertia between isotopomers, where the effects of the large-amplitude van der Waals vibrations were corrected by the introduction of a scale factor  $s = 0.9979(27)$ , which reduced the moments of inertia of both monomers.

<sup>a</sup>) Estimated standard errors.

<sup>b</sup>) See figure for the definition.



Columberg, G., Bauder, A.: J. Chem. Phys. **106** (1997) 504.