

H₂-HCN

Millimeter-wave spectroscopy of the internal rotation bands of H₂-HCN

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The H₂-HCN complex is a weakly bonded molecular complex including molecular hydrogen. The hydrogen molecule attaches to the nitrogen end of HCN for (ortho)H₂-NCH, while to the hydrogen end for (para)H₂-HCN in the ground state according to the MMW study of the pure rotational transitions of H₂-HCN. In the present study, we have observed the Σ_1 - Σ_0 band of the $j_{\text{HCN}} = 1-0$ internal rotation band of (ortho)H₂-HCN. The assignment of the internal rotation transitions was confirmed by a combination difference of the transition frequencies for the *P* and *R* branch lines. The band origin of the Σ_1 - Σ_0 band has been determined to be 149.8 GHz. This value is larger than that (133GHz) of Ne-HCN, but smaller than that (165 GHz) of Ar-HCN.

H ₂ -HCN		<i>ab initio</i>	
[1]		(ortho)H ₂ -HCN	
$D_e = 173.2 \text{ cm}^{-1}$	(para)H ₂ -HCN	$D_e = 145.3 \text{ cm}^{-1}$	
H ₂	HCN		
		Ar-HCN	
$D_e = 149.2 \text{ cm}^{-1}$	Ne-HCN	$D_e = 62.9 \text{ cm}^{-1}$	
Ar, Ne	1.64 Å, 0.398 Å ³	(ortho)H ₂	
$\alpha_{//}, \alpha$	0.93 Å, 0.788 Å ³	H ₂	
	($Q = 0.66 \cdot 10^{-26} \text{ cgs}$)		
	-HCN		
	H ₂ -HCN		
[2]		[3]	

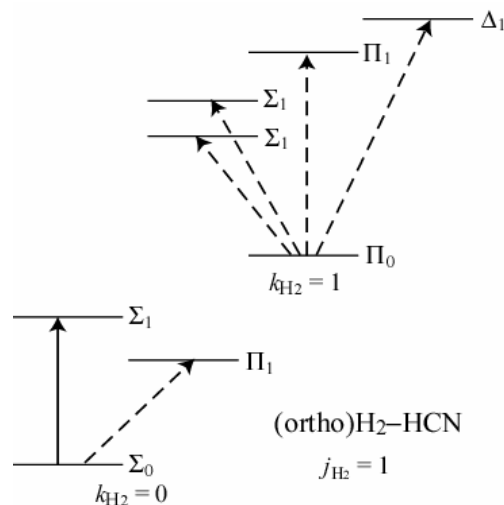


Fig. 1A (ortho)H₂-HCN

(ortho)H ₂	HCN	N	(para)H ₂
HCN	H		
68	210	GHz	71
		8	
(ortho)H ₂ -HCN	(para)H ₂ -HCN	Σ_0	
[2]		Fig. 1	

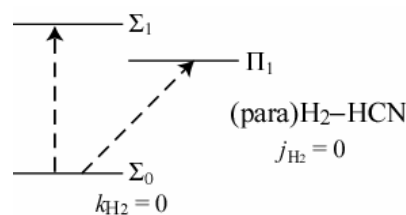
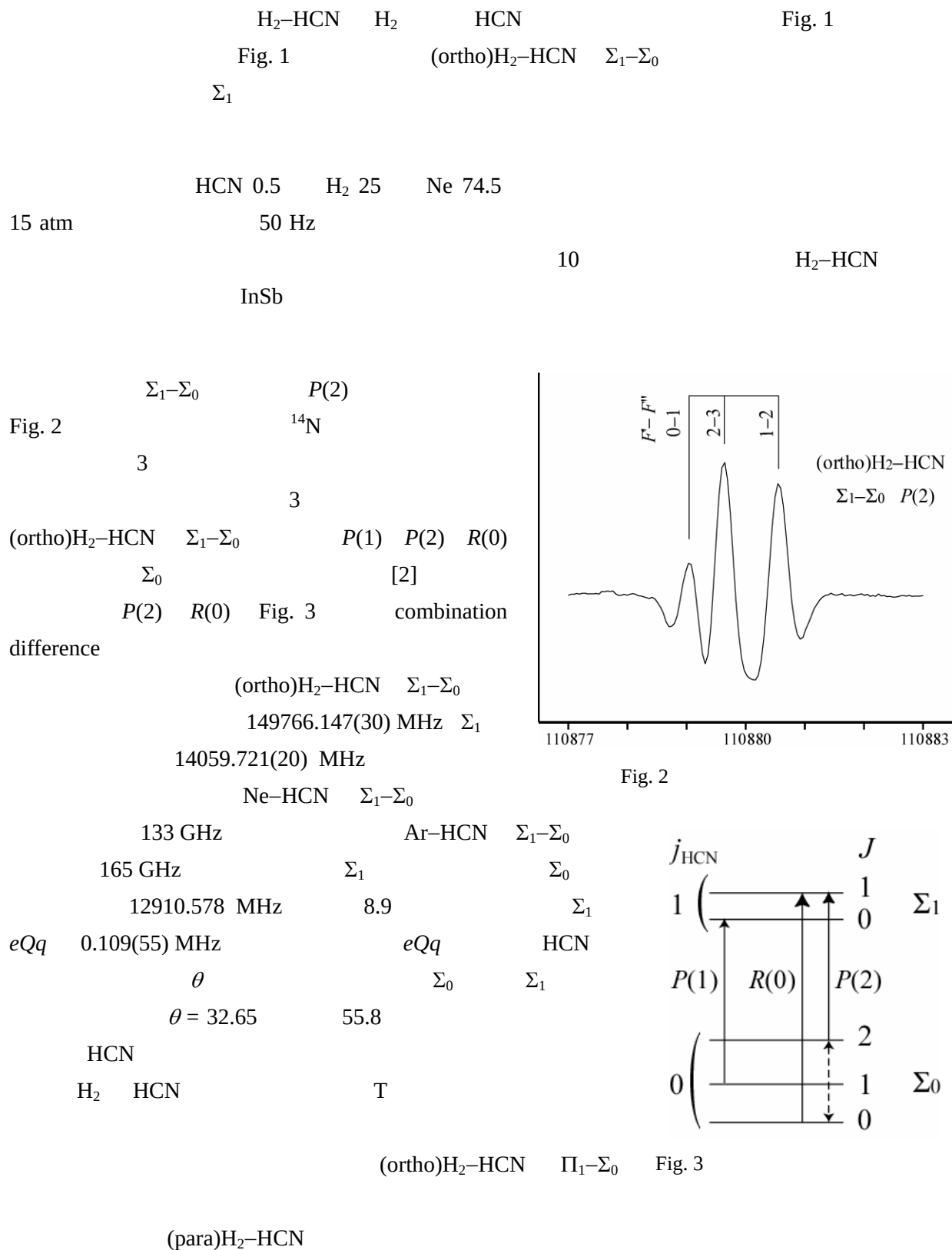


Fig. 1B (para)H₂-HCN



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- [2] M. Ishiguro, T. Tanaka, K. Harada, C. J. Whitham, and K. Tanaka, *J. Chem. Phys.* **115**, 5155 (2001).
- [3] International Symposium on Molecular Spectroscopy, **WF09** (2002), Ohio, USA.