

213  
MW

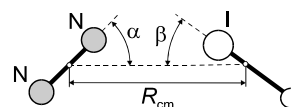
 HIN<sub>2</sub>

 Hydrogen iodide – dinitrogen (1/1)  
(weakly bound complex)

 C<sub>∞v</sub>  
(effective symmetry class)  
(large-amplitude motion)  
HI · N<sub>2</sub>

Isotopic species	$r_0(R_{\text{cm}})$ [Å]	$r_0(\text{N} \dots \text{I})$ [Å]	$\theta_0(\alpha)$ [deg] <sup>a)</sup>	$\theta_0(\beta)$ [deg] <sup>a)</sup>
<sup>14</sup> N <sub>2</sub> · IH	4.197872(67)	3.69748(93)	25.61(22)	23.4546(91)
<sup>14</sup> N <sub>2</sub> · ID	4.174903(72)	3.65476(99)	23.97(25)	19.060(10)
<sup>15</sup> N <sub>2</sub> · IH	4.19797(10)	3.6954(14)	25.14 <sup>b)</sup>	23.343(10)
<sup>14</sup> N <sup>15</sup> N · IH	4.18047(10)	3.6946(14)	25.14(35)	23.353(10)
<sup>15</sup> N <sup>14</sup> N · IH	4.21539(41)	3.6980(34)	25.5(14)	23.444(15)

The rotational transitions of <sup>14</sup>N<sub>2</sub> · IH, <sup>14</sup>N<sub>2</sub> · ID and <sup>15</sup>N<sub>2</sub> · IH show a doubling, which is a consequence of tunneling associated with the interchange of the two nitrogen nuclei. The intermolecular stretching force constant  $k_\sigma$  is 1.46152 N m<sup>-1</sup>.



<sup>a)</sup> The oscillation angles of the N<sub>2</sub> and HI moieties, see figure.

<sup>b)</sup> Assumed.

Jabs, W., McIntosh, A.L., Lucchese, R.R., Bevan, J.W., Brugh, D.J., Suenram, R.D.:  
J. Chem. Phys. **113** (2000) 249.