

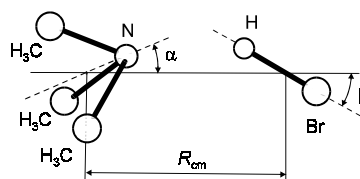
Hydrogen-bonded model ^{a)}:

Isotope	$r_0(R_{\text{cm}})$ [Å] ^{b)}	$r_0(\text{N} \cdots \text{Br})$ [Å] ^{b)}	k_s ^{c)} [N m ⁻¹]	ν_s ^{d)} [cm ⁻¹]
(CH ₃) ₃ ¹⁴ N · H ⁸¹ Br	3.3030(30)	2.9607(30)	82	202
(CH ₃) ₃ ¹⁴ N · H ⁷⁹ Br	3.3026(30)	2.9608(30)	87	208
(CH ₃) ₃ ¹⁴ N · D ⁷⁹ Br	3.2840(30)	2.9596(30)	88	209

Ion-pair model ^{e)}:

Isotope	$r_0(R_{\text{cm}})$ [Å] ^{b)}	$r_0(\text{N} \cdots \text{Br})$ [Å] ^{b)}	k_s ^{c)} [N m ⁻¹]	ν_s ^{d)} [cm ⁻¹]
(CH ₃) ₃ ¹⁴ N · H ⁸¹ Br	3.2959(30)	2.9594(30)	82	202
(CH ₃) ₃ ¹⁴ N · H ⁷⁹ Br	3.2959(30)	2.9594(30)	87	208
(CH ₃) ₃ ¹⁴ N · D ⁷⁹ Br	3.2716(30)	2.9577(30)	88	209

In the heterodimer trimethylamine – hydrogen bromide there is a significant extent of proton transfer from HBr to N(CH₃)₃



^{a)} Hydrogen-bonded model (CH₃)₃N · HBr with $\alpha_{\text{av}} = \beta_{\text{av}} = 10^\circ$. The distance $r(\text{N} \cdots \text{Br}) = \langle R_{\text{cm}}^2 \rangle^{1/2} - r + r'$, where r and r' are the distances of N and Br nuclei from mass centers of (CH₃)₃N and HBr subunits, respectively, then represents the best estimate of the equilibrium value.

^{b)} Uncertainties were not estimated in the original paper.

^{c)} Stretching force constant of the intermolecular vibration.

^{d)} Calculated from k_s by using the expression $\nu_s = (2\pi c)^{-1}(k_s/\mu)^{1/2}$

^{e)} Ion-pair model (CH₃)₃N⁺H...Br⁻ used in analogous version to obtain R_{cm} and $r(\text{N} \cdots \text{Br})$.

The (CH₃)₃N⁺H geometry is assumed unchanged from N(CH₃)₃ but with a hydrogen atom at 1.03 Å from N along the C₃ axis.

Legon, A.C., Wallwork, A.L., Rego, C.A.: J. Chem. Phys. **92** (1990) 6397.