ANHARMONIC AND CORIOLIS INTERACTIONS IN THE $v_3 = 2/v_2 = 1/v_5 = 1/v_3 = v_6 = 1$ LEVEL SYSTEM OF CH_3Br

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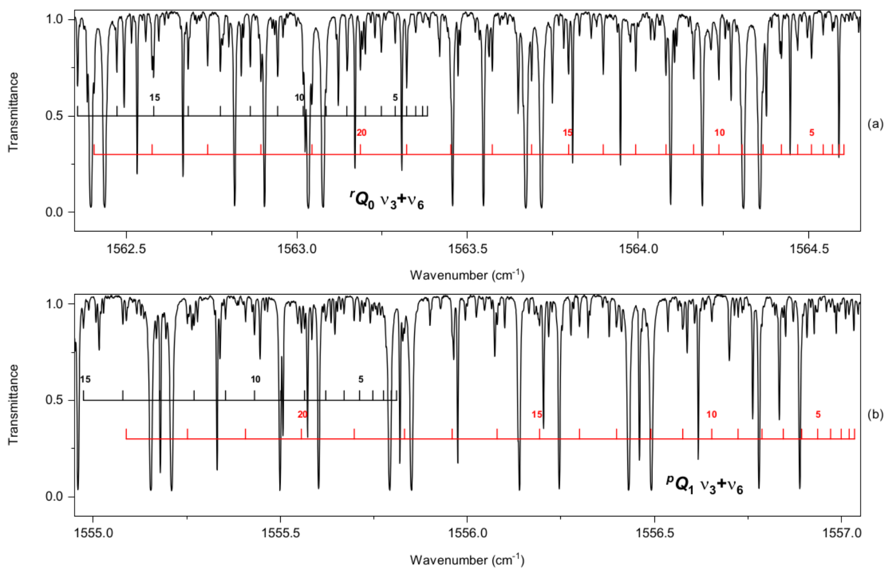
The ν_2/ν_5 band system of CH_3Br, a methyl halide playing an important role in the catalytic destruction of stratospheric ozone, already constituted the subject of several medium and high-resolution studies.
The novelty of the present study consists in considering, besides the strong Coriolis and α-interactions coupling the $v_2 = 1$ and $v_5 = 1$ levels, a large variety of anharmonic and rovibrational interactions involving also the $v_3 = 2$ and $v_3 = v_6 = 1$ levels. Thousands of new data, belonging either to high J and K values in the ν_2 and ν_5 bands or to the, very weak, $\nu_3 + \nu_6$ combination band, were included in the least-squares calculations.



Thanks to the large set of data, including more than 6300 experimental wavenumbers of the ν_2, ν_5, $2\nu_3$ and $\nu_3 + \nu_6$ rovibrational bands, with $J \leq 74$ and $K \leq 18$, combined to the completeness of the theoretical model, the global standard deviation, of 2.34×10^{-4} cm^{-1}, represents a great improvement with respect to the previous high-resolution study of the ν_2/ν_5 band system[1]. Moreover, the present study explores also the reductions' issue, in the spirit of the work of Střiteská *et al*[2] and Sarka *et al*[3]. Two different reductions schemes were thus applied and were proved to be equally successful.

$CH_3{}^{79}Br$:

Parameter	QQ	QC
$(\eta_J^5 + \eta_K^5) \times 10^5$	-20.9766(47)	-20.9704(47)
$\alpha_2^A \times 10^3$	-21.8459(36)	-21.8479(36)
$\alpha_5^A \times 10^3$	46.7461(36)	46.7461(36)
$(\alpha_2^B + 4q_{22}) \times 10^3$	1.02914(10)	1.02865(11)
$(\alpha_5^B - 2q_{22}) \times 10^3$	-0.032513(23)	-0.031836(69)
$(\alpha_2^B + 2\alpha_5^B) \times 10^3$	0.96412(11)	0.964981(95)

$CH_3{}^{81}Br$:

Parameter	QQ	QC
$(\eta_J^5 + \eta_K^5) \times 10^5$	-21.0762(71)	-21.0639(71)
$\alpha_2^A \times 10^3$	-21.8565(43)	-21.8587(44)
$\alpha_5^A \times 10^3$	46.7752(43)	46.7840(43)
$(\alpha_2^B + 4q_{22}) \times 10^3$	1.02346(22)	1.02285(22)
$(\alpha_5^B - 2q_{22}) \times 10^3$	-0.03028(13)	-0.02952(13)
$(\alpha_2^B + 2\alpha_5^B) \times 10^3$	0.96290(34)	0.96382(14)

[1] F. Kwabia Tchana, I. Kleiner, J. Orphal, N. Lacome, O. Bouba, *J. Mol. Spectrosc.* **228** (2004) 441-452.

[2] L. Nová Střiteská, K. Sarka, Š Urban, *J. Mol. Spectrosc.* **256** (2009) 135-140.

[3] K. Sarka, L. Nová Střiteská, A. Ceausu-Velcescu, *J. Mol. Spectrosc.* **311** (2015) 84-99.