

THE ν_1 BAND CONTOUR IN RAMAN SPECTRA
OF METHANE AND ITS GASEOUS
MIXTURES WITH Kr AND Ar

*B.T. Kuyliev, N.D. Orlova¹, L.A. Pozdnyakova¹,
F.H. Tukhvatullin², A. Jumabaev²*

Karshi State University

(Uzbekistan; e-mail: bahromq@rambler.ru),

¹Saint-Petersburg State University (Russia),

²Samarkand State University (Uzbekistan)

S u m m a r y

We have carried out the investigations of the Raman scattering spectra of the ν_1 band of methane (CH₄) and its mixtures with Ar and Kr in the gaseous phase in the temperature interval 140–360 K under a pressure of 4–160 atm. At low pressures, the band represents an asymmetric contour typical of the *Q*-branch with a degraded discrete structure. Starting from ~ 50 Amagat and higher, the real contour is of Lorentzian shape. We have determined the broadening coefficients *k* of the band, which appears to be $k(\text{CH}_4+\text{Kr}) \approx k(\text{CH}_4+\text{Ar}) > k(\text{CH}_4+\text{Ar})$ with increase in pressure. For all studied systems, *k* decreases first of all with increase in temperature, and then it starts to increase. The behavior of the ν_1 band of methane under the above-mentioned conditions is related to the vibrational relaxation process and the dephasing of vibrations. By calculations on the base of Gaussian98W software, the structure of isolated aggregates CH₄–Kr is determined.