Ultra-precise molecular spectroscopy data analysis for the low-pressures range

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There is a need for application of advanced line-shape models for ultra-precise molecular spectra measurements for low and very low pressures. So far the most commonly used profiles for this pressure range [Cygan2012, Kassi2012, DeVizia2012, Casa2009] have been the Voigt profile, the Nelkin-Ghatak profile [Nelkin1964], the Galatry profile [Galatry1961] and the speed-dependent versions of these profiles [Lance1997, Ciurylo2001]. Moreover, the exact speed-dependent Galatry profile has been calculated for the low-pressure range only for the quadratic speed dependence [Ciurylo2001]. The techniques based on the conversion of the transport/relaxation equation into the set of coupled algebraic equations [Lindenfeld1980, Ciurylo2002, Wcislo2012] are very ineffective for the low-pressure range and their accuracy rapidly falls down with the pressure decrease [Lindenfeld1980, Shapiro2000, Wcislo2013].

We extended the perturbation approach [Nienhuis1978, Shapiro2001] to the transport/relaxation equation [Lindenfeld1980, Ciurylo2002, Wcislo2012] such as to allow its application for low pressures including the Doppler limit [Wcislo2013]. We have presented that the relative differences between the profiles generated with our technique and the exact reference profiles are not higher than 10^{-7} and still may be reduced by expanding the set of basis functions. We have applied this technique to the R7 Q8 $^{16}O_2$ B-band rovibronic transition measured at 7 Torr with the signal-to-noise ratio of 220000 [Cygan2012]. We found that the speed-dependent billiard-balls profile (with hypergeometric speed dependence) is best able to reproduce the experimental profile providing the consistency with it corresponding to the signal-to-noise ratio of 92650.

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