

CO₂, H₂ and He Line Broadening Coefficients and Pressure Shifts for the HITRAN Database. J. S. Wilzewski, I. E. Gordon and L. S. Rothman, Harvard-Smithsonian Center for Astrophysics (60 Garden Street, Cambridge, MA, 02138)

Introduction: The goal of this work is to increase the potential of the HITRAN database [1] towards the exploration of the Venusian atmosphere. Line-broadening coefficients, line shifts and temperature dependence exponents of molecules of planetary interest perturbed by CO₂ have been assembled from available peer-reviewed sources, obtained from both experimental and theoretical studies or their extrapolations.

These spectroscopic data are of critical importance for the study of the atmosphere of Venus, since its atmosphere is dominated by CO₂.

Jupiter: H ₂ , He, CH ₄ , C ₂ H ₂ , C ₂ H ₆ , C ₂ H ₆ , H ₂ O, C ₂ H ₂ , C ₂ H ₆ , HD, C ₂ H ₆ , NH ₃ , PH ₃ , CO, GeH ₄ , AsH ₃ , CO ₂ , ...
Saturn: H ₂ , He, CH ₄ , C ₂ H ₂ , C ₂ H ₆ , C ₃ H ₈ , CH ₄ , H ₂ S, H ₂ O, C ₂ H ₆ , NH ₃ , SiH ₄ , PH ₃ , CO, GeH ₄ , AsH ₃ , CO ₂ , ...
Uranus: H ₂ , He, CH ₄ , C ₂ H ₂ , C ₂ H ₆ , C ₂ H ₆ , CO, H ₂ S, ...
Neptune: H ₂ , He, CH ₄ , C ₂ H ₂ , C ₂ H ₆ , C ₂ H ₆ , CH ₄ , C ₂ H ₆ , ...
Venus: CO₂ , N ₂ , SO₂ , H ₂ SO ₄ , CO, O, N ₂ , O ₂ , HCl, HF, Ne, H ₂ S, OCS, H ₂ , H ₂ , He, H ₂ O, O ₂ , Cl, ClO, ClO ₂ , COCl ₂ , NH ₃ , ...
Titan: N ₂ , CH ₄ , Ar, C ₂ H ₆ , C ₃ H ₈ , H ₂ O, CO, CO ₂ , CH ₃ D, CH ₃ , C ₂ H ₆ , NH ₃ , HCN, C ₂ N ₂ , HCN, CH ₃ CN, C ₂ H ₂ , C ₂ H ₂ , ...
HD 189733b: H ₂ , H ₂ O, O, CH ₄ , CO, ...

Figure 1. Overview of constituents of some planetary and lunar atmospheres (list provided by Dr. Linda Brown, JPL). Molecules, for which datasets were already created, are in bold font.

Details: Additionally, the current study investigates pressure effects on molecular spectra in H₂ and He environments, which can be useful in the frame of studying the atmospheres of gas giants. An overview of the molecular systems studied is given in Figure 1.

The data collected here are used to create semi-empirical models for complete molecular data sets spanning the spectral range from microwave to UV wavelengths.

Pressure broadening due to CO₂ is unfortunately only poorly understood and insufficiently studied for the majority of the molecular systems considered in this work, although new HITRAN datasets were created in each case. The data for pressure shifts are especially sparse, while these parameters are not negligible for a detailed study of the Venusian atmosphere, particularly in the near infrared.

For some molecules, like CO, an extensive amount of measurements exist to build a complete database.

However, some of the seven new CO₂-broadening datasets, which are summarized in Table 1, are partly based on very limited amounts of data or default values, highlighting the importance of further work in this field. For example, only a single CO₂ broadening coefficient of SO₂ is available [2] and this is quite old. This datapoint was used to scale all available H₂-broadening coefficients from Refs. [3], [4] and [5] to yield a full CO₂-broadened dataset for SO₂.

Outlook: The fact that some sets are listed as not available in Table 1 is due to the absence of data for these molecular systems. In the near future we will add datasets for CO₂, H₂O, CH₄ and PH₃ perturbed by the three broadeners listed in Table 1 respectively.

	C ₂ H ₂	SO ₂	OCS	HCl	HF	CO	NH ₃
Perturbed by CO₂	Y	Y	Y	Y	Y	Y	Y
Perturbed by H ₂	Y	Y	N	N	N	Y	Y
Perturbed by He	Y	Y	N	Y	Y	Y	Y

Table 1. Prepared datasets: 'N'=Not Yet Available, 'Y'=Available

The present work helps identifying the need for further investigations of broadening, shifting and the temperature dependence of spectral lines in CO₂ environments to enhance future studies of the cytherean atmosphere. A “wishlist” for additional studies in this area will be presented at the meeting.

References:

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Acknowledgements: Support from NASA Planetary Atmospheres grant NNX13AI59G and the German-American Fulbright Commission is greatly acknowledged.