COLLISION-INDUCED INFRARED ABSORPTION BY COLLISIONAL COMPLEXES IN DENSE HYDROGEN-HELIUM GAS MIXTURES AT THOUSANDS OF KELVIN

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The interaction-induced absorption by collisional pairs of H_2 molecules is an important opacity source in the atmospheres of the outer planets and cool stars [a]. The emission spectra of cool white dwarf stars differ significantly in the infrared from the expected blackbody spectra of their cores, which is largely due to absorption by collisional H_2–H_2, H_2–He, and H_2–H complexes in the stellar atmospheres. Using quantum-chemical methods we compute the atmospheric absorption from hundreds to thousands of kelvin [b]. Laboratory measurements of interaction-induced absorption spectra by H_2 pairs exist only at room temperature and below. We show that our results reproduce these measurements closely [c], so that our computational data permit reliable modeling of stellar atmosphere opacities even for the higher temperatures [d].

[a] L. Frommhold, Collision-Induced Absorption in Gases, Cambridge University Press, Cambridge, New York, 1993 and 2006

[b] Xiaoping Li, Katharine L. C. Hunt, Fei Wang, Martin Abel, and Lothar Frommhold, Collision-Induced Infrared Absorption by Molecular Hydrogen Pairs at Thousands of Kelvin, International Journal of Spectroscopy, vol. 2010, Article ID 371201, 11 pages, 2010. doi: 10.1155/2010/371201

[c] M. Abel, L. Frommhold, X. Li, and K. L. C. Hunt, Collision-induced absorption by H_2 pairs: From hundreds to thousands of Kelvin, J. Phys. Chem. A, published online, DOI: 10.1021/jp109441f

[d] L. Frommhold, M. Abel, F. Wang, M. Gustafsson, X. Li, and K. L. C. Hunt, "Infrared atmospheric emission and absorption by simple molecular complexes, from first principles", Mol. Phys. 108, 2265, 2010