COMPUTATION OF COLLISION-INDUCED ABSORPTION BY SIMPLE MOLECULAR COMPLEXES, FOR ASTROPHYSICAL APPLICATIONS

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The interaction-induced absorption by collisional pairs of H_2 molecules is an important opacity source in the atmospheres of various types of planets and cool stars, such as late stars, low-mass stars, brown dwarfs, cool white dwarf stars, the ambers of the smaller, burnt out main sequence stars, exoplanets, etc., and therefore of special astronomical interest [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]. First results for H_2–He complexes [e] have already been applied to astrophysical models [f] and have shown great improvements in these models.

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