

Photoionization of the MgH, AlH, and SiH Molecules

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ABSTRACT: We present photoionization cross sections for the MgH, AlH, and SiH molecules using a distorted-wave approximation. A configuration-average distorted-wave method is used to compute the photoionization cross sections based on earlier molecular structure tabulations.

1. INTRODUCTION

Photoionization cross sections for atoms and molecules are needed to better understand the physics and chemistry of the interstellar medium. In particular AlH lines are found in the spectrum of the small low mass star Proxima Centauri[1].

The rest of this paper is organized as follows: in Section 2 we give a brief review of the configuration-average distorted-wave (CADW) for the photoionization of diatomic molecules, in Section 3 we present CADW photoionization cross sections for AlH, and in Section 4 we give a brief summary. Unless otherwise stated, we will use atomic units.

2. THEORY

The photon ionization of a molecular configuration is given by:

$$(nl\lambda)^w \rightarrow (nl\lambda)^{w-1} \epsilon_e l_e \lambda_e, \quad (1)$$

where again w is the occupation number of the active subshell and $nl\lambda$ and $\epsilon_e l_e \lambda_e$ are quantum numbers of the valence bound electron and the ejected electron.

The configuration-average photon ionization cross section for $\lambda = 0$ is given by[2, 3]:

$$\sigma_{\parallel} = \frac{8\pi\omega}{ck_e} \sum_{l_e} w [D_C(nl\lambda \rightarrow \epsilon_e l_e \lambda_e)]^2 \quad (2)$$

for the electromagnetic field polarization parallel with the internuclear axis and

$$\sigma_{\perp} = \frac{8\pi\omega}{ck_e} \sum_{l_e} w [D_S(nl\lambda \rightarrow \epsilon_e l_e \lambda_e)]^2 \quad (3)$$

for the electromagnetic field polarization perpendicular to the internuclear axis. In both cases $\lambda_e = \lambda$, $k_e = \sqrt{2\epsilon_e}$, ω is the radiation field frequency, and c is the speed of light. The total configuration-average photon ionization cross section is given by:

$$\sigma_{total} = \left(\frac{\sigma_{\parallel} + 2\sigma_{\perp}}{3} \right). \quad (4)$$

We note that configuration-average photon ionization cross sections for $\lambda \neq 0$ are slightly different from those for $\lambda = 0$ [2, 3].

The radial and angular dipole integrals are given by:

$$D_C(nl\lambda \rightarrow \epsilon_e l_e \lambda_e) = \int_0^{\infty} dr \int_0^{\pi} d\theta u_e(r, \theta) r \cos \theta u_{nl\lambda}(r, \theta) \quad (5)$$

and

$$D_S(nl\lambda \rightarrow \epsilon_e l_e \lambda_e) = \int_0^{\infty} dr \int_0^{\pi} d\theta u_e(r, \theta) r \sin \theta u_{nl\lambda}(r, \theta). \quad (5)$$

2.1. Bound and Continuum Orbitals

The bound orbitals, $u_{nl\lambda}(r, \theta)$, for photon ionization are obtained from previous Hartree-Fock-Roothaan calculations for MgH[4], MgH⁺[5], AlH[6], AlH⁺[7], SiH[8], and SiH⁺[9]. The bound orbitals are then transformed[10] onto a two dimensional (r, θ) grid. We note that the conventions of Cade and Huo are used for the transformation. The total scattering potential is given by:

$$V(r, \theta) = -\frac{Z}{\sqrt{r^2 + \frac{R^2}{4} - rR \cos \theta}} - \frac{Z}{\sqrt{r^2 + \frac{R^2}{4} + rR \cos \theta}} + V_{direct}(r, \theta) + V_{exchange}(r, \theta), \quad (7)$$

where Z is the atomic number of each target nucleus and R is the internuclear distance. The bound orbitals for the molecular ion are used to calculate the direct, $V_{direct}(r, \theta)$, and the exchange, $V_{exchange}(r, \theta)$, scattering potentials. The local exchange potential is given by:

$$V_{exchange}(r, \theta) = -\frac{1}{4} \left(\frac{24\rho(r, \theta)}{\pi} \right)^{\frac{1}{3}}, \quad (8)$$

where $\rho(r, \theta)$ is the probability density. The continuum orbitals are calculated by solving a single channel (r, θ) Schrodinger equation.

3. RESULTS

The photoionization cross section for MgH $1\sigma^2 2\sigma^2 1\pi^4 3\sigma^2 4\sigma^2 5\sigma \rightarrow \text{MgH}^+ 1\sigma^2 2\sigma^2 1\pi^4 3\sigma^2 4\sigma^2$ is given in Figure 1. The photoionization cross section for AlH $1\sigma^2 2\sigma^2 1\pi^4 3\sigma^2 4\sigma^2 5\sigma^2 \rightarrow \text{AlH}^+ 1\sigma^2 2\sigma^2 1\pi^4 3\sigma^2 4\sigma^2 5\sigma$ is given in Figure 2. The photoionization cross section for SiH $1\sigma^2 2\sigma^2 1\pi^4 3\sigma^2 4\sigma^2 5\sigma^2 2\pi \rightarrow \text{SiH}^+ 1\sigma^2 2\sigma^2 1\pi^4 3\sigma^2 4\sigma^2 5\sigma^2$ is given in Figure 3.

4. SUMMARY

A configuration-average distorted-wave method has been applied to calculate the photoionization cross sections for the MgH, AlH, and SiH molecules. In the future we plan to calculate photoionization cross sections for other diatomic molecules using the perturbative distorted-wave method.

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References

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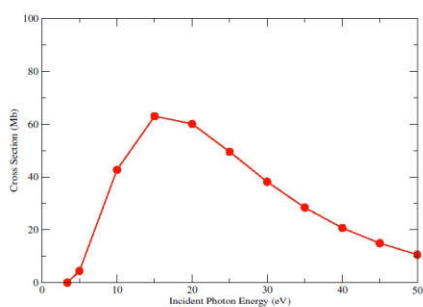


Figure 1. Photoionization of MgH. Solid line (red): 5σ cross section ($1.0 \text{ Mb} = 1.0 \times 10^{-18} \text{ cm}^2$).

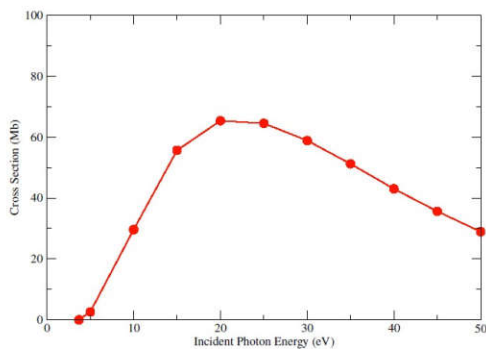


Figure 2. Photoionization of AlH. Solid line (red): $5\sigma^2$ cross section ($1.0 \text{ Mb} = 1.0 \times 10^{-18} \text{ cm}^2$).

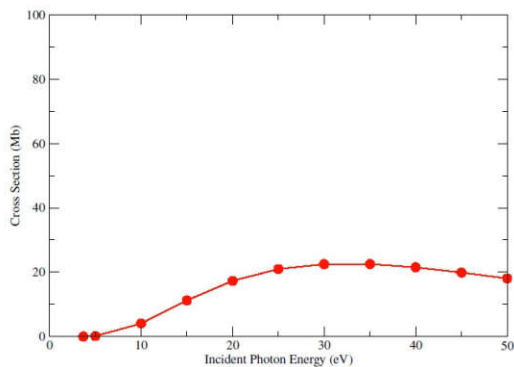


Figure 3. Photoionization of SiH. Solid line (red): 2π cross section ($1.0 \text{ Mb} = 1.0 \times 10^{-18} \text{ cm}^2$).