Positron binding, scattering, and annihilation on atoms and molecules

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The ability of the positron to bind to molecules is key to the strong enhancements of positron annihilation rates in polyatomic molecules [1]. This enhancement is due to positron capture in vibrational Feshbach resonances, observation of which has led to measured values of positron binding energies for over 70 molecules [2]. *Ab initio* calculations of positron binding to nonpolar molecules have proven to be extremely challenging. Here, we use a model-potential approach [3] to calculate elastic *s*-wave scattering cross sections, annihilation rates, and (where applicable) binding energies for positron interactions with atoms and small nonpolar molecules, namely, Be, Mg, He, Ar, H_2, N_2, Cl_2, and CH_4. We write the positron-molecule interaction potential as $V(\mathbf{r}) = V_{\rm st}(\mathbf{r}) + V_{\rm cor}(\mathbf{r})$, where $V_{\rm st}(\mathbf{r})$ is the electrostatic potential of the target, and $V_{\rm cor}(\mathbf{r}) = -\sum_A (\alpha_A/2|\mathbf{r}-\mathbf{r}_A|^4)\{1-\exp[-(|\mathbf{r}-\mathbf{r}_A|/\rho_A)^6]\}$ is a model correlation potential, where the sum is over the target's constituent atoms A, with the nucleus at position $\mathbf{r}_A$ and the hybrid polarizability α_A [4]. The cutoff parameters ρ_A are taken from Ref. [5] for Be, Mg, and He; for Ar we choose it to reproduce the accurate *s*-wave scattering phase shift from many-body-theory calculation [6]; for C and N we use the same value as for H, while for Cl we use the same value as for Ar (due to the similar radii of these atoms). Scattering data are obtained by correctly normalizing Gaussian-based positive-energy positron eigenstates. Our calculations confirm positron binding for Be and Mg, and predict it for Cl_2. Figure 1 shows the annihilation parameter $Z_{\rm eff}$ as a function of positron momentum for all of the species, along with existing calculations. The very large values of $Z_{\rm eff}$ at small momenta for Cl_2, Be and CH_4 are due to the presence of a weakly bound state or low-lying virtual level. The discrepancy with the result of Ref. [5] for Mg is due to the presence of a *p*-wave shape resonance not accounted for here.

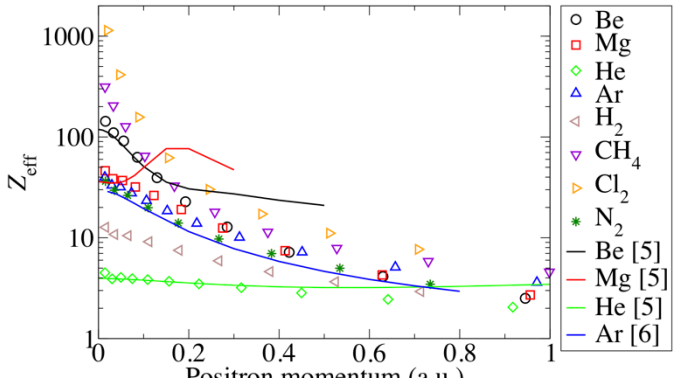

Figure 1 *Annihilation parameter $Z_{\rm eff}$ for Be, Mg, He, Ar, H_2, N_2, Cl_2, and CH_4. Symbols: present results. Lines: previous calculations.*

References

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