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Effective oscillator strength distributions of spherically symmetric atoms for calculating polarizabilities and long-range atom–atom interactions

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ABSTRACT

Effective oscillator strength distributions are systematically generated and tabulated for the alkali atoms, the alkaline-earth atoms, the alkaline-earth ions, the rare gases and some miscellaneous atoms. These effective distributions are used to compute the dipole, quadrupole and octupole static polarizabilities, and are then applied to the calculation of the dynamic polarizabilities at imaginary frequencies. These polarizabilities can be used to determine the long-range C_6, C_8 and C_{10} atom–atom interactions for the dimers formed from any of these atoms and ions, and we present tables covering all of these combinations.

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1. Introduction

The long-range interaction between two spherically symmetric atoms can be written in the general form [1–4]

$$V(R) \approx -\frac{C_6}{R^6} - \frac{C_8}{R^8} - \frac{C_{10}}{R^{10}} + \cdots, \tag{1}$$

where the C_n parameters are the London/van der Waals dispersion coefficients. There are two complementary approaches to the computation of the dispersion coefficients. One approach uses oscillator strength sum-rules [5,6], while the second utilizes Casimir–Polder relations and uses the dynamic polarizabilities computed at imaginary energies [7,8]. These approaches can be regarded as complementary to each other.

The key to the first approach is to generate an oscillator strength distribution that incorporates excitations to bound excited states and to the continuum states. In practice, the oscillator strength distributions are best termed 'effective' oscillator strength distributions [9]. One might find that the lowest few excited states are accurately represented by the distribution, however the higher bound states and continuum states are approximated with a set of discrete effective oscillator strengths and energies. The oscillator strength distributions can be derived from *ab-initio* structure calculations [10–12,4], experimental information such as refractive indices, atomic transition rates and photo-ionization cross sections [5,6], and sometimes both experimental and calculated oscillator strengths are used [12,13].

The Casimir–Polder relation is reliant on being able to calculate the dipole and multipole dynamic polarizabilities at imaginary frequencies. One way to calculate a dynamic polarizability is to use oscillator strength sum-rules in conjunction with a previously-determined oscillator strength distribution. An alternate approach is to directly compute the dynamic polarizability as part of a structure calculation [14–16]. The direct calculation of the dynamic polarizability is the preferred approach for structure calculations.

The present paper reports both effective oscillator strength distributions and dynamic polarizabilities for a number of spherically symmetric atoms and ions. The atoms presented are the noble gases, the alkali atoms and hydrogen, the singly-charged alkaline-earth ions and the alkaline earth atoms. The long-range atom–atom interaction coefficients C_6, C_8 and C_{10} are also presented for any dimer formed from these atoms and ions. A previous tabulation of dynamic polarizabilities for many of these atoms does exist [17]. This previous tabulation only gave the dynamic dipole polarizabilities, while the present tabulation extends this to the quadrupole and octupole polarizabilities that are needed in the evaluation of

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