

ERRATA

Erratum: "On nonadiabatic molecular dynamics simulations of the photofragmentation and geminate recombination dynamics in size-selected $I_2^- \cdot Ar_n$ cluster ions" [J. Chem. Phys. 106, 7102 (1997)]

V. S. Batista^{a)} and D. F. Coker

Department of Chemistry, Boston University, 590 Commonwealth Avenue, Boston, Massachusetts 02215

[S0021-9606(99)00713-8]

After publication of our paper,¹ we have discovered a programming error in the computer code for obtaining minimum energy structures as presented in Sec. II B. Neither the MD simulation scheme nor the qualitative conclusions presented previously are affected by this but there are quantitative differences as described below.

Figure 1 shows the energies of the lowest minimum energy structures, expressed as energy divided by the number of solvent particles (replacing Fig. 1 in the original paper,¹ where the total energy was expressed relative to the I–I energy contribution). The total potential energy is dominated by the negative electrostatic contribution which is the sum of the charge induced dipole, and the induced dipole-induced dipole interactions as observed previously.¹ However, the relative magnitudes of the electrostatic and short range interactions for small clusters are slightly different from the ones reported before.¹

The correct minimum energy structures of the various size argon clusters solvating the I_2^- anion are shown in Fig. 2 (replacing Fig. 2 in the original paper¹). The underlying equilibrium structure of the I_2^- solvation shell is as presented before best understood in terms of forming a cylindrical

stack of staggered hexagonal rings of argon atoms around the I_2^- anion.¹ The first ring packs around the center of the I_2^- bond and subsequent rings pack around the ends of the I_2^- molecule, with individual argon atoms packed onto the ends of the molecule, capping the end rings. The $n=13$ atom cluster is, as presented in the original paper, slightly more stable than its neighboring clusters with a completed central ring and a single completed capped end structure that optimizes the rare gas van der Waals interactions. In larger clusters we also see the second capping structure around the other end of the molecule being established. However, for smaller clusters the competition seen in the original geometries between formation of an incomplete central ring and a partial terminal cap structure is not present. These small minimum energy geometry corrections were found not to produce any significant effect on the percentage photofragment yields, since they mostly changed the optimized geometries of clusters smaller than $n=10$, all of which were so weakly bound that photofragmented completely, whereas the minimum energy geometries presented in the original work for bigger clusters were all global minima or within the energy range of thermal fluctuations.

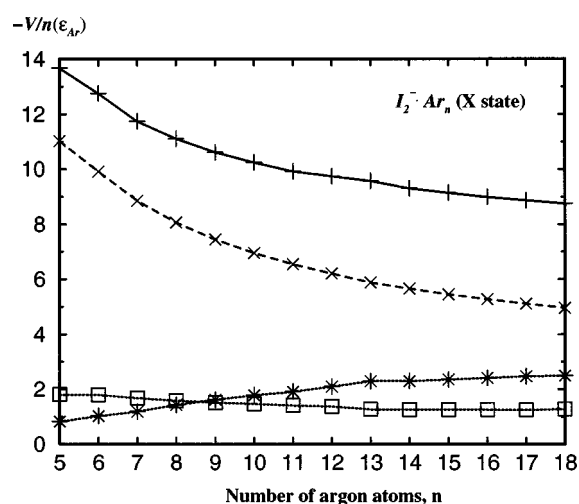


FIG. 1. Contributions to potential energy of minimum energy structures of $I_2^- \cdot Ar_n$ ($5 \leq n \leq 18$) clusters. Energy per Ar atom expressed in units of ϵ_{Ar} (83.26 cm^{-1}): total energy (plus signs), electrostatic polarization energy (crosses), Ar–Ar interaction energy (stars), and Ar–I interaction energy (squares).

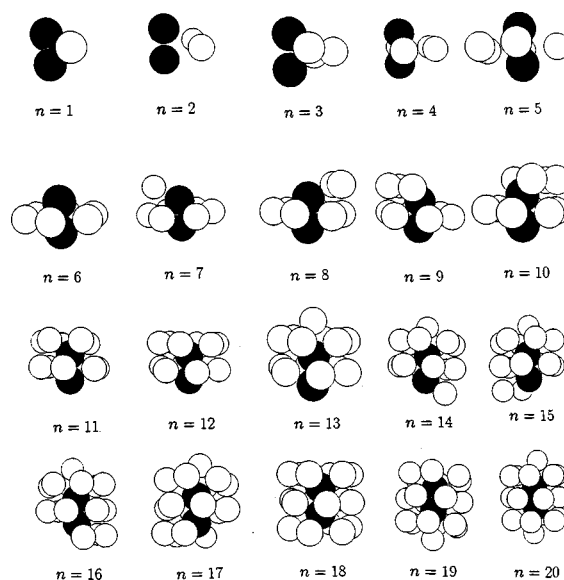


FIG. 2. Minimum energy structures of $I_2^- \cdot Ar_n$ ($1 \leq n \leq 20$), the two black atoms embedded in the cluster are the I_2^- molecule.

We gratefully acknowledge financial support for this work from the National Science Foundation (Grants No. CHE-9058348 and No. CHE-9521793), the Petroleum Research Fund administered by the American Chemical Society (Grant No. 27995-AC6) and a generous allocation of super-

computing time from the Center for Scientific Computing and Visualization at Boston University.

^{a)}Current address: Department of Chemistry, University of California, Berkeley, California 94720.

¹V. S. Batista and D. F. Coker, J. Chem. Phys. **106**, 7102 (1997).