



Data Article

Free energy and enthalpy data of neutral and protonated clusters in the solvent phase

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ABSTRACT

Structures of neutral and protonated acetonitrile in the solvent phase are important to describe proton behavior and to calculate thermodynamic quantities related to the solvation of ions or molecules in acetonitrile. In this work, we provide data related to the calculation of the solvation free energy and enthalpy of the proton in acetonitrile. We have thoroughly explored the potential energy surfaces (PESs) of neutral and protonated acetonitrile clusters from dimer to heptamer in the solvent phase at both MN15/6-31++G(d,p) and MP2/aug-cc-pVDZ levels of theory. We report the structures and relative stability of neutral and protonated acetonitrile clusters in the solvent phase at the MN15/6-31++G(d,p) level of theory. In addition, enthalpies and free energies of neutral and protonated acetonitrile are also reported at the MP2/aug-cc-pVDZ and MP2/CBS levels of theory. Furthermore, Cartesian coordinates of the clusters in the solvent phase as optimized at the MP2/aug-cc-pVDZ level of theory are provided as supplementary file. The data provided in this work will be useful for further investigations that would involve neutral and protonated acetonitrile clusters. The free energies and enthalpies of the investigated clusters in the solvent phase have been used to compute the solvation free energy and enthalpy of the proton in acetonitrile. For more insights on the solvation free energy and enthalpy of the proton in acetonitrile, see the related main research paper [1].

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Specifications Table

Subject	Chemistry
Specific subject area	Physical and Theoretical Chemistry
Type of data	Table Figure
How data were acquired	Data are computed using the quantum computational chemistry program Gaussian 16 suite of programs
Data format	Raw Analyzed
Parameters for data collection	Raw data were collected from the output files of calculations using DFT and the analyzed data were generated using a our home-made programs.
Description of data collection	DFT calculations were performed using the resources of the Center of High Performance Computing (CHPC), South Africa
Data source location	Department of Chemistry University of the Free State Bloemfontein South Africa
Data accessibility	With the article
Related research article	Alhadji Malloum, Jeanet Conradie, Solvation Free Energy of the Proton in Acetonitrile, <i>J. Mol. Liq.</i> 335 (2021) 116,032.

Value of the Data

- The data reported in this work will save computational time to calculate the enthalpies and free energies of the most stable structures of neutral and protonated acetonitrile clusters at high level ab-initio methods.
- The data will be useful for further investigations in the solvent phase involving neutral and protonated acetonitrile clusters.
- The enthalpies and free energies of the global minimum energy clusters in solvent phase as well as the Cartesian coordinates are available for chemistry and physics researchers for further investigation of ions or molecular solvation processes in acetonitrile.
- The present data have been used to compute the proton solvation free energy that could be used to calculate the pKa of molecules in acetonitrile.
- The relative energies of the structures will be useful for the selection of the structures in further investigations.

1. Data Description

The data used to compute the solvation free energy and enthalpy of the proton in acetonitrile is reported in this work. We have reported in [Table 1](#) the free energies and enthalpies of the most stable structures in the solvent phase at the MP2/aug-cc-pVDZ and MP2/CBS levels of theory. The free energies and enthalpies at the MP2/CBS are obtained by replacing the electronic energies calculated at the MP2/aug-cc-pVDZ by those calculated at the MP2/CBS in the free energies and enthalpies calculated at the MP2/aug-cc-pVDZ level of theory. [Fig. 1](#) and [Fig. 2](#) report the structures and relative stabilities of the neutral acetonitrile clusters from dimer to nonamer in the solvent phase. Structures have been optimized in the solvent phase at the MN15/6-31++G(d,p) level of theory. [Figs. 3, 4](#) and [5](#) report the structures and relative stabilities of the protonated acetonitrile clusters from dimer to nonamer as optimized in the solvent phase at the MN15/6-31++G(d,p) level of theory. Besides, we have provided in the supplementary file the Cartesian coordinates of all the structures of neutral and protonated acetonitrile clusters reported in [Figs. 1](#) to [5](#).

Table 1

Free energies and enthalpies of neutral and protonated acetonitrile clusters as computed at the MP2/aug-cc-pVDZ and MP2/CBS levels of theory (in a.u.).

n	MP2/aug-cc-pVDZ			
	Neutral		Protonated	
	ΔH	ΔG	ΔH	ΔG
1	-132.341855	-132.370534	-132.716130	-132.745369
2	-264.686745	-264.734339	-265.081107	-265.126344
3	-397.034415	-397.093913	-397.425713	-397.489322
4	-529.385658	-529.457596	-529.774928	-529.844635
5	-661.732608	-661.820383	-662.126640	-662.213911
6	-794.084172	-794.184548	-794.477710	-794.575247
7	-926.437543	-926.546817	-926.830537	-926.940889
	MP2/CBS			
1	-132.514516	-132.543195	-132.891984	-132.921223
2	-265.031273	-265.078867	-265.427459	-265.472696
3	-397.549412	-397.608910	-397.943813	-398.007422
4	-530.070720	-530.142658	-530.462988	-530.532695
5	-662.586473	-662.674248	-662.984881	-663.072152
6	-795.108702	-795.209078	-795.504891	-795.602428

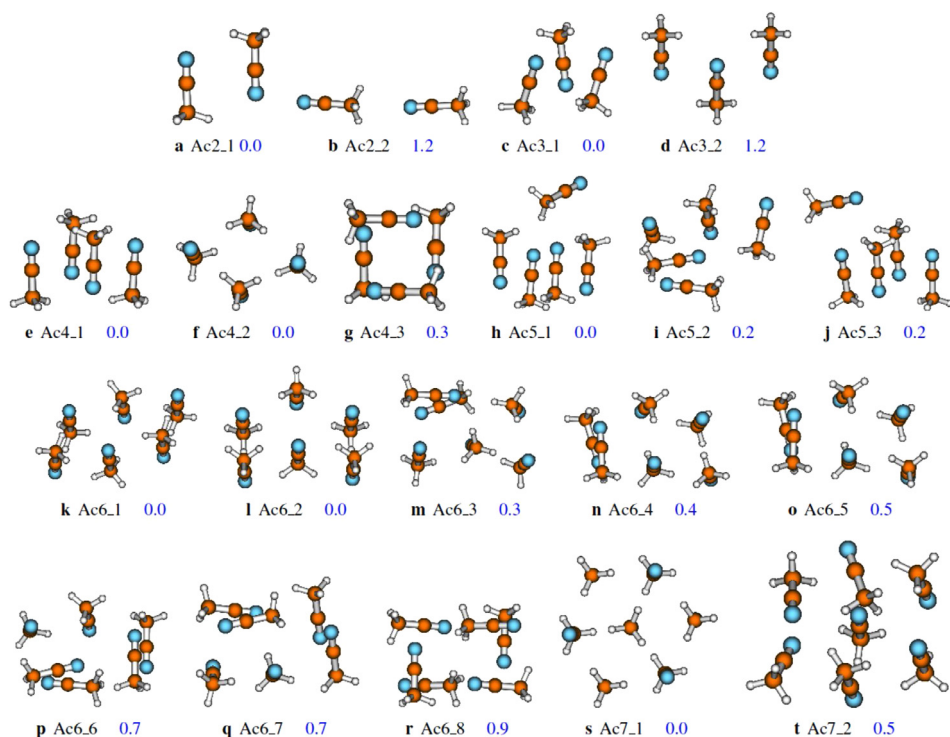


Fig. 1. Structures and relative stabilities of neutral acetonitrile clusters, from dimer to heptamer as optimized in the solvent phase at the MN15/6-31++G(d,p) level of theory. Each sub-caption indicates the name of the structure followed by a number representing the corresponding relative energy (in kcal/mol).

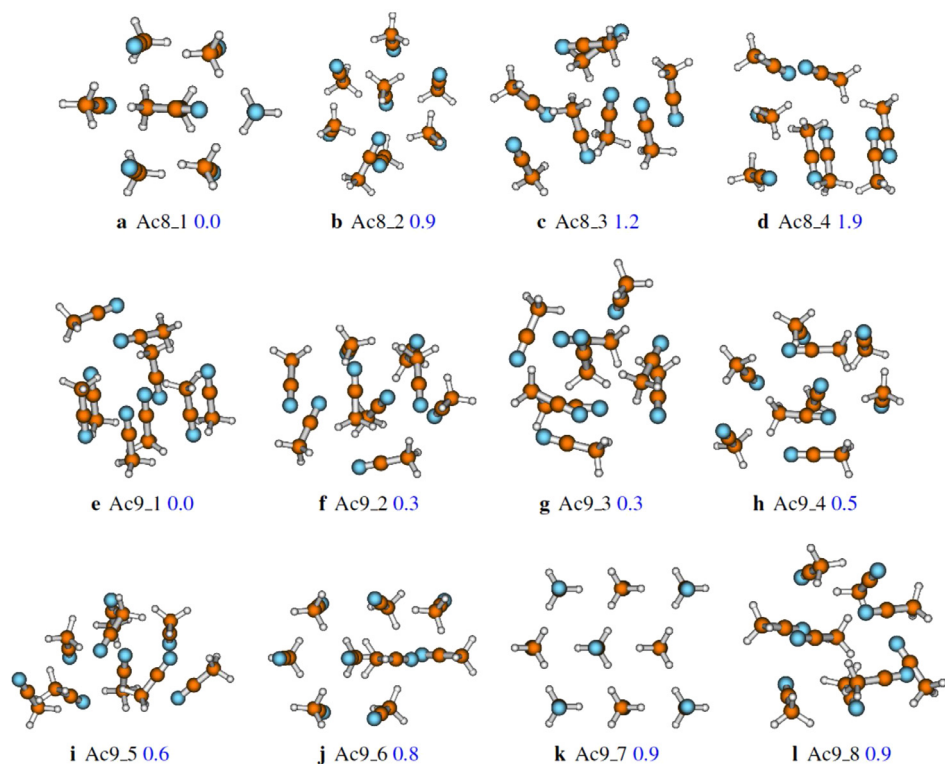


Fig. 2. Structures and relative stabilities of neutral acetonitrile octamer and nonamer as optimized in the solvent phase at the MN15/6–31++G(d,p) level of theory. Each sub-caption indicates the name of the structure followed by a number representing the corresponding relative energy (in kcal/mol).

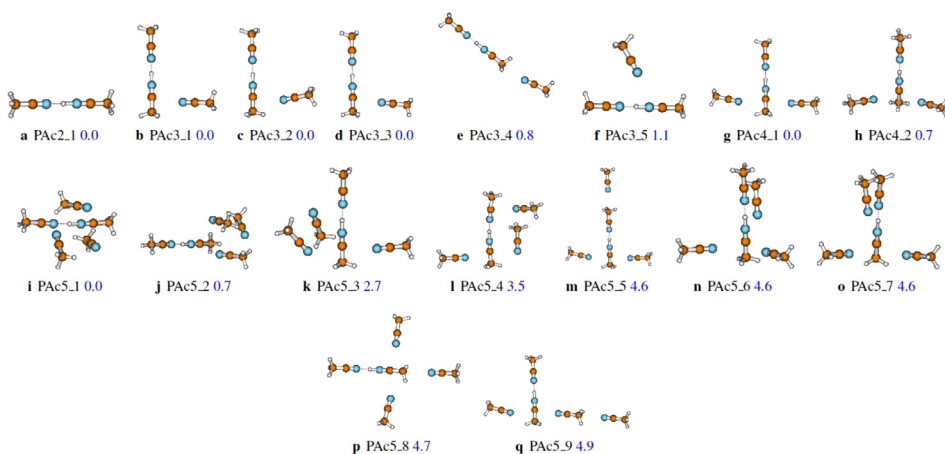


Fig. 3. Structures and relative stabilities of the protonated acetonitrile clusters, from dimer to pentamer, as optimized in the solvent phase at the MN15/6–31++G(d,p) level of theory. Each sub-caption indicates the name of the structure followed by a number representing the corresponding relative energy (in kcal/mol).

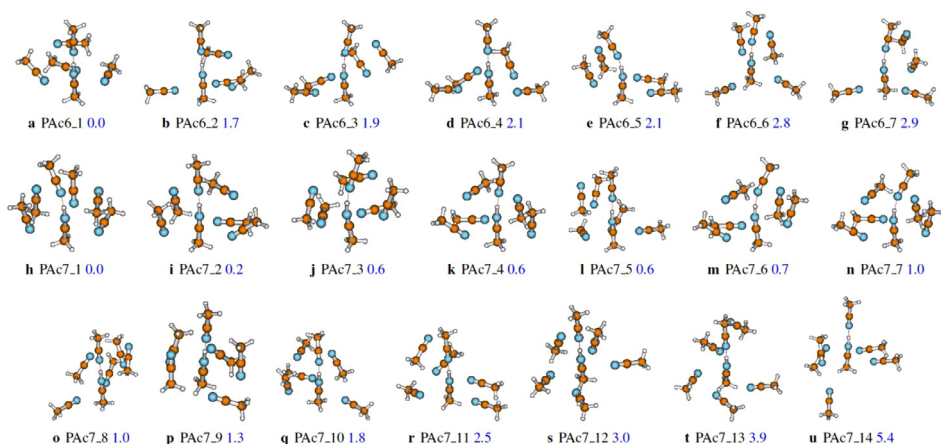


Fig. 4. Structures and relative stabilities of the protonated acetonitrile hexamer and heptamer as optimized in the solvent phase at the MN15/6-31++G(d,p) level of theory. Each sub-caption indicates the name of the structure followed by a number representing the corresponding relative energy (in kcal/mol).

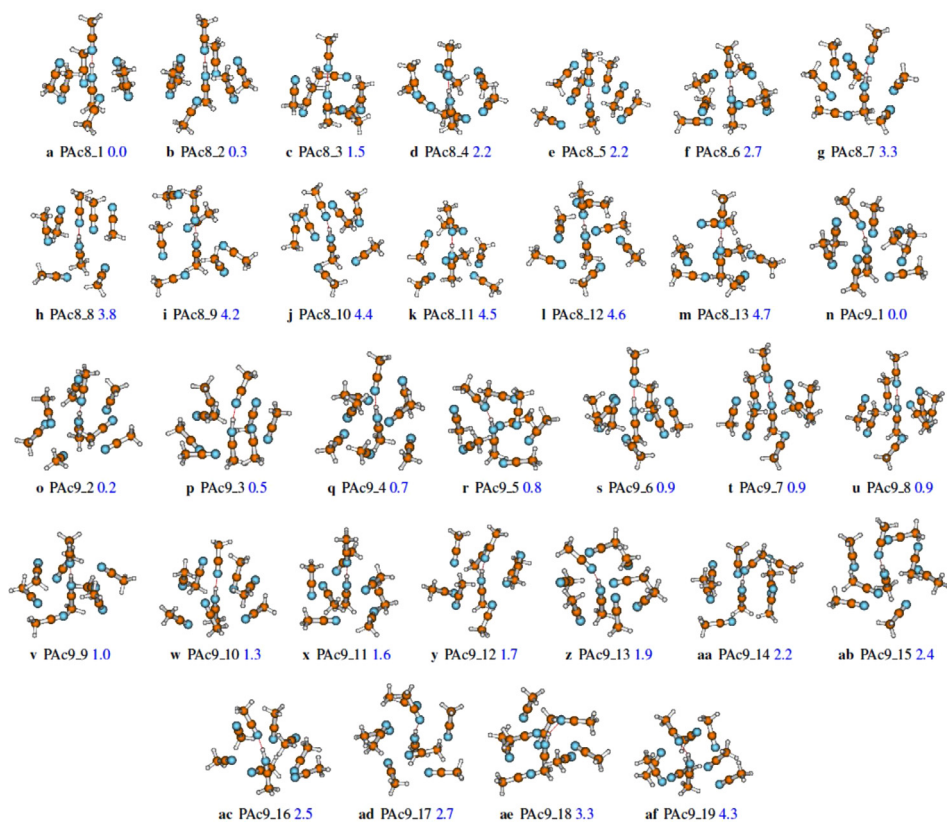


Fig. 5. Structures and relative stabilities of the protonated acetonitrile octamer and nonamer as optimized in the solvent phase at the MN15/6-31++G(d,p) level of theory. Each sub-caption indicates the name of the structure followed by a number representing the corresponding relative energy (in kcal/mol).

2. Experimental Design, Materials and Methods

We generated initial structures using the ABCluster code of Zhan and Dolg [2,3]. The AB-Cluster code is based on the bee colony algorithm to generate global and local minima structures on the PESs of a given molecular cluster. ABCluster uses a classical potential energy based on electrostatic and Lennard-Jones interactions. It is worth noting that the ABCluster has been used successfully in our previous works to generate initial structures on the PESs of molecular clusters [4,5]. The structures generated using ABCluster have been fully optimized at the MN15/aug-cc-pVDZ level of theory. The MN15 structures have been further optimized at the MP2/aug-cc-pVDZ level of theory. For the extrapolation at the complete basis set (CBS) limit, we performed a single point calculations at MP2/aug-cc-pVTZ and MP2/aug-cc-pVQZ levels of theory and we applied extrapolation based on two points. The single point calculation has been performed on the structures optimized at the MP2/aug-cc-pVDZ level of theory. All optimizations, frequency calculations, and single point calculations are performed in the solvent phase using Gaussian 16 suite of programs. For accurate optimizations, we used the *tight* option. For MN15, we used the *ultrafine* grid for the evaluation of integrals. The solvent is modelled as a dielectric continuum medium using the integral equation formalism polarized continuum model (IEF-PCM). We used the dielectric constant of acetonitrile (35.688) to set the solvent to be acetonitrile.

Supporting Information

Cartesian coordinates of neutral and protonated acetonitrile clusters reported in this work as optimized in the solvent phase at the MN15/6-31++G(d,p) level of theory are provided as supplementary file.

CRedit Author Statement

Alhadji Malloum: Conceptualization, Methodology, Validation, Formal analysis, Investigation, Data curation, Writing – original draft, Visualization; **Jeanet Conradie:** Resources, Validation, Writing – review & editing, Supervision, Funding acquisition, Project administration.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships which have, or could be perceived to have, influenced the work reported in this article.

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Supplementary Materials

Supplementary material associated with this article can be found in the online version at doi:[10.1016/j.dib.2021.107144](https://doi.org/10.1016/j.dib.2021.107144).

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