Data for: "A Thermodynamic Landscape of Hydrogen Cyanide-Derived Molecules and Polymers"

SND-ID: 2024-85. **Version**: 1. **DOI**: https://doi.org/10.5878/f7tx-5e29

Download data

sandstroem_et-al_dataset_190324.zip *(154.85 MB)*

Associated documentation

README.txt *(4.69 KB)*

Download all files

2024-85-1.zip *(~154.85 MB)*

Citation

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Description

This study describes a part of the free energy landscape of hydrogen cyanide (HCN)-derived molecules and polymers. The data consists of output from quantum chemical calculations and input files sufficient to reproduce the study.

The program CREST version 2.11 was used to generate polymer conformers. Gaussian16 was used for molecular optimizations. VASP version 5.4.4 was used for calculations of extended system.

SCRIPT
Folder contains scripts used to automate the calculations.

VASP_calc_thermodynamics_project
Folder contains results of VASP calculations on extended HCN-derived polymers.

verification_gasphase

Folder contains CREST and Gaussian16 calculations on HCN-derived molecules and polymers in vacuum. Each subfolder is named after the structure numbering used in the main research article.

verification_water
Folder contains CREST and Gaussian16 calculations on HCN-derived molecules and polymers that include implicit consideration of water solvation. Each subfolder is named following the article's species numbering.

Data contains personal data

No

Language

English

Data format / data structure

Numeric

Text

Responsible department/unit

Department of Chemistry and Chemical Engineering

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Funding 1

- Funding agency: Swedish Research Council
- Funding agency's reference number: 2016-04127
- Project name on the application: Functional Materials Prediction with Implications for the Origin of Life and Planetary Science
- Funding information: This research marks a beginning aimed at identifying entirely new classes of materials, starting with what can be made from one of nature’s simplest building blocks, hydrogen cyanide (HCN). It also intends to further the development of methods for analyzing chemical bonding and predicting material properties. I will combine structure search algorithms with quantum mechanical calculations to explore unknown materials, calculate their properties and seek ways to synthesize those most interesting. HCN is, of course, toxic, and whereas chemists are used to handling dangerous chemicals this is often unpractical, making computational studies ideal for its exploration. The combinatorial possibilities of HCN-based materials are incredibly diverse, varying in mechanical, electronic and chemical properties. Several are expected to be nontoxic; others will be able to teach us structure – function relationships and provide us with design rules for emergent properties such as semiconduction, ferroelectricity and catalytic activity. HCN is ubiquitous in the Universe and molecules and materials made thereof have long been suspected key to the chemistry that gave rise to life. HCN is, for instance, found in ample amounts in the atmosphere of Saturn’s moon Titan, where it has mysteriously vanished at the surface. By collaborating with planetary scientists I will investigate if HCN-based polymers can explain part of the surface chemistry, and, maybe, provide a base for prebiotic chemistry.

Funding 2

- Funding agency: Swedish Research Council
- Funding agency's reference number: 2020-04305
- Project name on the application: Computational Astrobiology: The Rise of Macromolecules
- Funding information: The goal of this project is to enhance our knowledge of chemical structures and processes that may play a role in life’s possible origins. We will apply quantum chemical calculations to study the properties and reactions of in particular hydrogen cyanide, one of the most abundant and widely distributed organic molecules in astrochemical environments.Together with collaborators, we aim to answer the following questions:How can heterocycles, including nucleobase-analogs, form from HCN polymers?What is the catalytic potential of HCN nanocrystals?What role might co-crystals have on worlds such as Saturn’s moon Titan?What are the next steps in the development of computational astrobiology?State-of-the-art computational methods, including steered ab initio molecular dynamics and structure prediction algorithms will be applied to several of these questions for the first time. Outcomes of this research will be concrete predictions of chemical structures and phenomena that will be amenable for verification by low temperature experiments by collaborating groups, by ongoing and future sample-return missions to asteroids and comets, as well as the recently selected Dragonfly mission to Saturn’s moon Titan.

Research area

Theoretical chemistry (Standard för svensk indelning av forskningsämnen 2011)

Physical chemistry (Standard för svensk indelning av forskningsämnen 2011)

Keywords

Hydrogen cyanide, Thermodynamics, Quantum chemistry, Polymerisation

Accessibility level

Access to data through SND
Data are freely accessible

Use of data

Things to consider when using data shared through SND

License

CC0 1.0

Versions

Version 1. 2024-06-05

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Related research data in SND's catalogue

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DataCite

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DCAT-AP-SE 2.0

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Citation (CSL)

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