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Computational Model of Hg (II) Reduction in BrHgOH on Ice Surface

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Question

How much energy is required for the reduction reaction of Hg (II) in BrHgOH on ice surface?

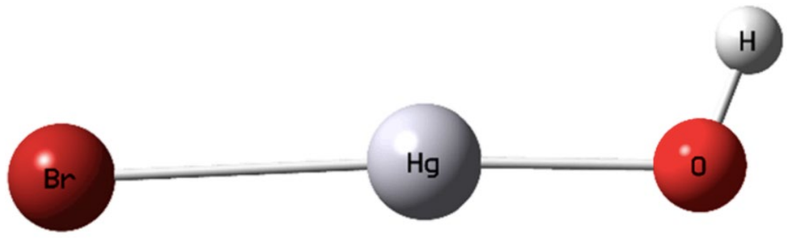


Fig. 1. Ball and Stick Model of BrHgOH Molecule

Background

- According to the World Health Organization (WHO), mercury is among the top ten chemicals or groups of chemicals currently posing major public health concerns due to its' toxicity to humans and other organisms via bioaccumulation.
- Unlike the oxidation of mercury which has been extensively investigated both experimentally and theoretically, the reduction mechanism of mercury is much less studied hence why it is the focus of our investigation.
- While there are many molecules that contribute to the biogeochemical cycle of mercury, we focused on BrHgOH because previous research data indicates that this molecule has the greatest amount of reduced or elemental mercury on ice after deposition.

Methods

- Using VASP code to gradually adjust the thousands place value of the Hg (II) ion as it's gradually reduced on ice.

```
[aqd6030@submit-003 work1$ mkdir job1
[aqd6030@submit-003 work1$ ls
INCAR  job0  job1  job.pbs  KPOINTS  POSCAR  POTCAR
[aqd6030@submit-003 work1$ cp INCAR job1
[aqd6030@submit-003 work1$ cp KPOINTS job1
[aqd6030@submit-003 work1$ cp POSCAR job1
[aqd6030@submit-003 work1$ cp POTCAR job1
[aqd6030@submit-003 work1$ cp job.pbs job1
[aqd6030@submit-003 work1$ cd job1
[aqd6030@submit-003 job11$ ls
INCAR  job.pbs  KPOINTS  POSCAR  POTCAR
[aqd6030@submit-003 job11$ qsub job.pbs
Job will run under the 'open' account, as requested.
37280847.torque01.util.production.int.aci.ics.psu.edu
[aqd6030@submit-003 job11$
```

Fig. 3. Sample VASP code

- Computational modeling of Hg (II) reduction in BrHgOH on ice.

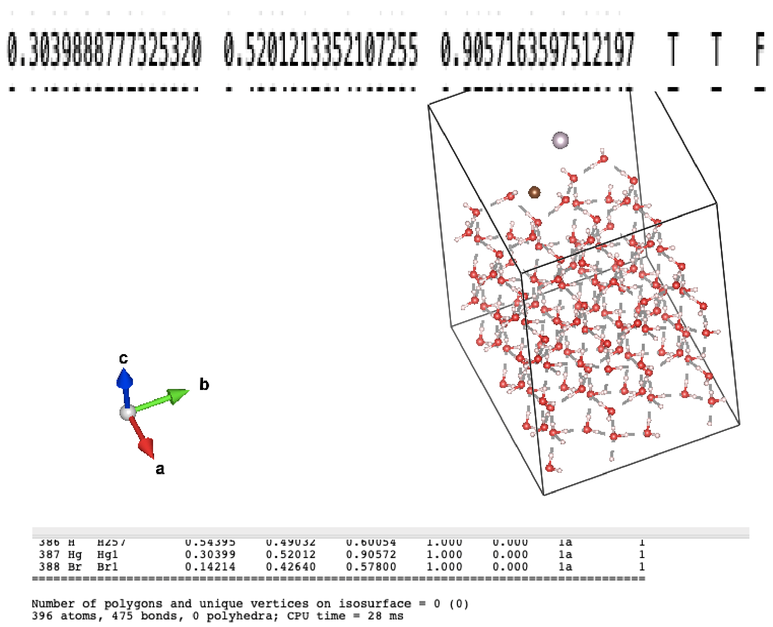
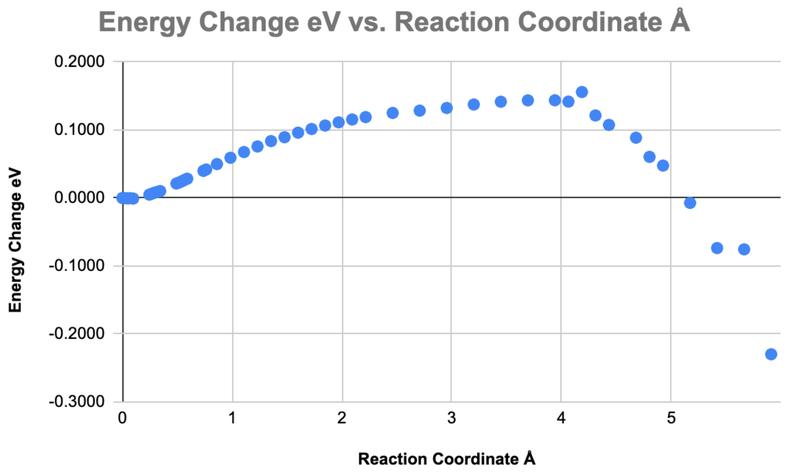


Fig. 2. Visual representation of computational model of HgBrOH on ice containing a total of 129 oxygen atoms, 257 hydrogen atoms, 1 mercury atom and 1 bromine atom.

Data



Conclusion

- Using computational modeling we've demonstrated that the reduction reaction of BrHgOH on ice occurs without an external source of energy.
- Our findings indicate that the activation energy for this particular reaction is low enough to occur spontaneously in Antarctic environmental conditions.
- This reaction is thermodynamically favorable because the products have a lower energy than the reactants.

Bibliography

1. Sibgha Amin, Tabeen Asif, Marwa Khan, Edward Usinowicz, Debashree Mitra, Abu Asaduzzaman, Structural, energetic and vibrational properties of oxidized mercury in the gas and aqueous phases, Computational and Theoretical Chemistry, Volume 1198,(2021),113186, https://doi.org/10.1016/j.comptc.2021.113186.
2. D. Durnford, A. Dastoor, The behavior of mercury in the cryosphere: A review of what we know from observations, J. Geophys. Res. 116 (2011) D06305, https:// doi.org/10.1029/2010JD014809.

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