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PennState Harrisburg

Computational Model of Hg (II) Reduction in BrHgOH & $BrHgO_2H$ on Ice Surface

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Question

How much energy is required for the reduction reaction of Hg (II) in BrHgOH and $BrHgO_2H$ on ice surface?

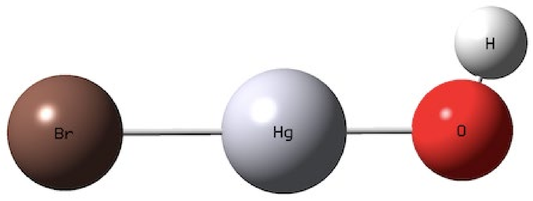

Fig. 1. Ball and Stick Model of BrHgOH Molecule

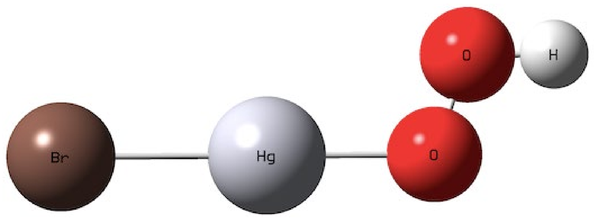

Fig. 2. Ball and Stick Model of $BrHgO_2H$ Molecule

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.
- $BrHgO_2H$ is very similar molecule.
- Based on previous research, there is high probability that these two molecules are forming in the atmosphere.

Methods

- Using VASP code to gradually adjust the thousands place value of the Hg (II) ion as it's gradually reduced on ice.
- Computational modeling of Hg (II) reduction in BrHgOH and $BrHgO_2H$ on ice.

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0.3039888777325320  0.5201213352107255  0.9057163597512197   T   T   F
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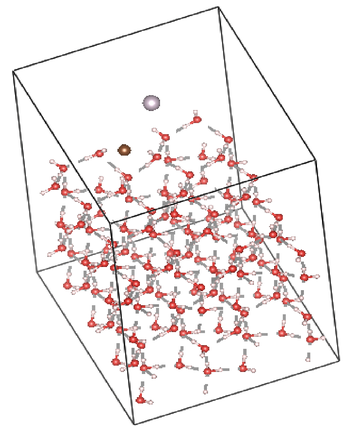
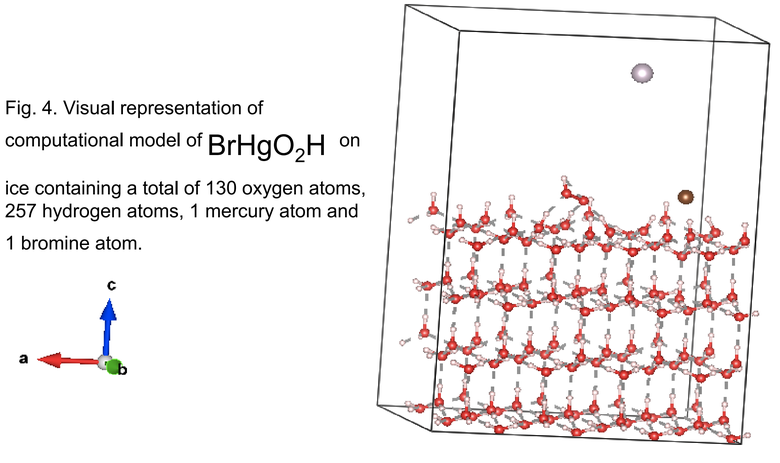
Fig. 3. Visual representation of computational model of BrHgOH on ice containing a total of 129 oxygen atoms, 257 hydrogen atoms, 1 mercury atom and 1 bromine atom.




```
387 Hg   Hg1        0.30399    0.52012    0.90572    1.000    0.000    1a         1
388 Br   Br1        0.14214    0.42640    0.57800    1.000    0.000    1a         1
================================================================================

Number of polygons and unique vertices on isosurface = 0 (0)
396 atoms, 475 bonds, 0 polyhedra; CPU time = 28 ms
```

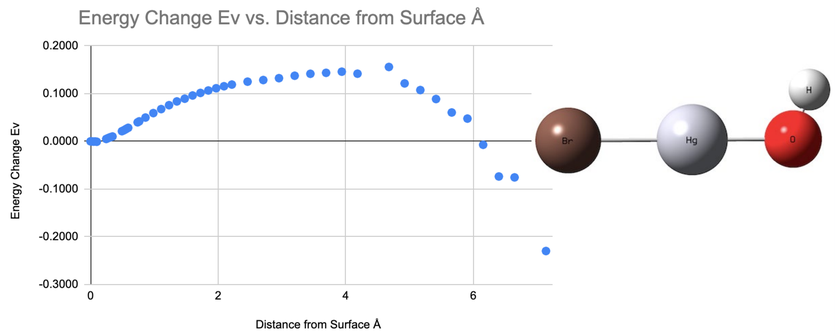
Fig. 4. Visual representation of computational model of $BrHgO_2H$ on ice containing a total of 130 oxygen atoms, 257 hydrogen atoms, 1 mercury atom and 1 bromine atom.

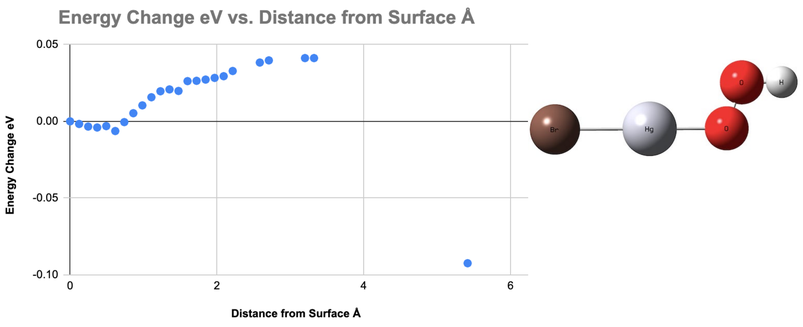



```
388 Hg   Hg1        0.31393    0.50681    0.88426    1.000    0.000    1a         1
389 Br   Br1        0.13094    0.42413    0.57527    1.000    0.000    1a         1
================================================================================

Number of polygons and unique vertices on isosurface = 0 (0)
397 atoms, 478 bonds, 0 polyhedra; CPU time = 44 ms
```

Data





Conclusion

BrHgOH

- The reduction reaction of BrHgOH on ice surface occurs without an external source of energy.
- The reaction's activation energy 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.

$BrHgO_2H$

If indeed this crude data includes from the vertex as well as the lowest point on the energy diagram, then

- the reduction reaction of $BrHgO_2H$ on ice occurs without an external source of energy requiring even less energy than that of BrHgOH.
- the activation energy for this reaction is also low enough to occur spontaneously in Antarctic environmental conditions.
- this reaction is also thermodynamically favorable because the products have a lower energy than the reactants.

Bibliography

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2. Vogelsong, L., Fuentes, J. D., & Asaduzzaman, A. (2023). Deposition and Reduction of Oxidized Mercury on the Ice Surface: Quantum-Chemical Study and Implication of Mercury Activities in the Arctic. *Journal of Physical Chemistry C*, *127*(5), 2657-2665. https://doi.org/10.1021/acs.jpcc.2c07879

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