Properties of size selected sodium doped solvent clusters

Ingo Dauster

Institute of Physical Chemistry, University Göttingen
Tammannstr. 6, 37077 Göttingen, Germany

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Size dependent ionization potential (IP) of sodium doped solvent clusters:

Systems that have already been measured:

- sodium doped ammonia cluster\(^{a,b}\) \(\text{Na(NH}_3\text{)}_n\)
- sodium doped water cluster\(^b\) \(\text{Na(H}_2\text{O)}_n\)


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\textarrow{\textleftarrow} show a strong size dependence of the IP
\textarrow{\textleftarrow} only show a size dependent decrease for clusters up to \( n=4 \), for larger clusters the IP is constant


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What is with other systems?

- methylated water \(\Rightarrow\) methanol
- learn more about the properties and the structures of these clusters
- learn more about solvation of electrons


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\(\text{O} \quad \text{H} \quad \text{CH}_3\)


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Experimental setup
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Na pickup cell

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Experimental setup
Mass spectrum of $\text{Na(MeOH)}_n$

$\lambda_{\text{ion}} = 370 \text{ nm}$
Mass spectrum of Na(MeOH)$_n$}

\[ \lambda_{ion} = 370 \text{ nm} \]
DFT calculations

\[ \text{Na(MeOH)}_1 \]

\[ \Delta E = 434 \text{ kJ/mol} \]
\[ \Delta E = 437 \text{ kJ/mol} \]
\[ \Delta E = 111 \text{ kJ/mol} \]

\[ \Rightarrow \text{no fragmentation} \]

UB3LYP / 6-31+G(d,p)

(Bing Gao and Zhi-feng Liu, Chinese University of Hong Kong)
DFT calculations

Motivation

Experimental setup

First results

Outlook

Acknowledgements

Properties of size selected sodium doped solvent clusters

Na(MeOH)$_2$

$\Rightarrow$ no fragmentation

UB3LYP / 6-31+G(d,p)

$\Delta E=80 \text{ kJ/mol}$

$\Delta E=458 \text{ kJ/mol}$

$\Delta E=381 \text{ kJ/mol}$

$\Delta E=-10 \text{ kJ/mol}$

$\text{Na}^+(\text{MeOH})_2$

$\text{Na}^+_a(\text{MeOH})_2$

$\text{Na}^+_a(\text{MeOH}) + \text{MeOH}$

$\text{Na}^+(\text{MeOH})_2$

$\Rightarrow$ no fragmentation
DFT calculations

\[ \text{Na(MeOH)}_3 \]

\[ \Delta E = 426 \text{ kJ/mol} \]

\[ \Delta E = 339 \text{ kJ/mol} \]

\[ \Delta E = 9 \text{ kJ/mol} \]

\[ \Delta E = 51 \text{ kJ/mol} \]

\( \Rightarrow \) no fragmentation

\( \Rightarrow \) soft ionization

UB3LYP / 6-31+G(d,p)
determination of the size selective IP of Na(MeOH)$_n$ is running
more DFT calculations of bigger clusters
size selectiv IR action spectroscopy of Na(MeOH)$_n$ clusters$^a$
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Thank you for your attention!