universität innsbruck

Vibrational spectroscopy using nuclear wave function

PR Theoretical Chemistry and Computer Chemistry (Advanced)

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Starting Structures

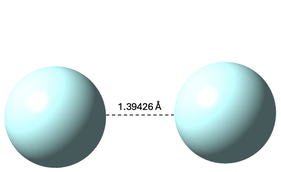

Figure 1: F_2 optimized with B3LYP/6-311++G(3df,3pd)

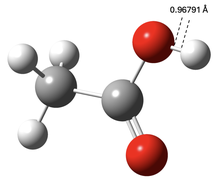

Figure 2: trans-CH_3COOH optimized with B3LYP/6-311++G(3df,3pd)

Calculation of reduced mass and force constant k

The force constant k can be calculated via finite differences from the potential energies of the bond scan.

$$k \approx \frac{E_{min-1} + 2E_{min} + E_{min+1}}{\Delta r^2} \quad \mu = \frac{m_1 \cdot m_2}{m_1 + m_2} \tag{1}$$

Table 1: Reduced mass μ and force constant k

	F_2	trans-CH_3COOH
μ (g/mol)	9.4992016	Col 2
k (kcal/mol)	874.9427	Col 2

With the harmonic oscillator framework the frequency ν and wavenumber can be calculated

$$\nu = \frac{1}{2\pi} \cdot \sqrt{\frac{k}{\mu} \cdot \xi} \Rightarrow \bar{\nu} = \frac{\nu}{c} \tag{2}$$

Table 2: Frequency ν and $\bar{\nu}$ calculated with eq. (2)

	F_2	trans-CH_3COOH
ν / (s^{-1})	3.111e13	Col 2
$\bar{\nu}$ / (cm^{-1})	1037.68	Col 2

Numerov frequency calculation

Numerov method is a numerical method to solve differential equations. This method can be used for the

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{2m}{\hbar}(V - E)\Psi \Rightarrow \frac{\partial^2 \Psi}{\partial x^2} \approx \frac{\Delta g}{\Delta x} \tag{3}$$

Center Column for Landscape Posters

If you ever wondered how the cumulative distribution function of the generalized logistic distribution type I would look like: here it is.

$$F(x;\alpha) = \frac{1}{(1+e^{-x})^{\alpha}} = (1+e^{-1})^{-\alpha}, \quad \alpha > 0 \tag{4}$$

- $F(x;\alpha)$: cumulative distribution function
- α: skewness parameter

Another equation to fill the space here:

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \bigtriangledown \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = - \bigtriangledown \cdot p\mathbf{I} + \bigtriangledown \cdot \tau + \rho g \tag{5}$$

. . . which is the Navier-Stokes equation. If you find an analytic solution you might get a quite nice price!

Content Block With Example Figure

A very simple statistical graph to demonstrate how the figure includes look like in the beamer style and to fill the content such that the demo content looks a little bit nicer.

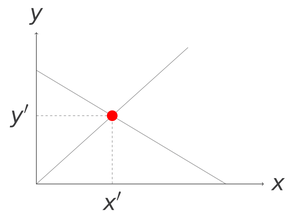

Figure 3: This is just an example figure to demonstrate how figure includes with captions look like.

Center Column for Landscape Posters

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Supported Text Styles and Colors

Both, **bold face** and *italic* styles are supported by the poster theme. Beside text styles a set of default colors and commands which can be used. These colors are based on the colors of the corporate design of our university.

Available colors:

- blue (`uibkblue`)
- light blue (`uibkbluel`)
- orange (`uibkorange`)
- light orange (`uibkorangel`)
- gray (`uibkgray`)
- medium gray (`uibkgraym`)
- light gray (`uibkgrayl`)

Available commands:

command	output example
`\fct{...}`	`example()`
`\class{...}`	“example”
`\pkg{...}`	*example*
`\email{...}`	email
`\doi{...}`	doi:example
`\file{...}`	example
`\dataset{...}`	example

Table 3: Commands provided by the “`beamerstyleuibk`” template.

All commands using verbatim (`\email`, `\doi`, `\file` and `dataset`) use a highlight color which can be adjusted by including e.g., in the preamble if required.

Take Home Message

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References:
Mustermann, M. and Demoman F.C., 2017: A Fake Reference to Demonstrate How This Could Look like. LaTeX poster template demo, **0**(0), 666-999.

Acknowledgements:
Ongoing project funded by the Austrian Science Fund (FWF): TRP 123-456. The computational results presented have been achieved (in part) using the HPC infrastructure LEO of the University of Innsbruck.