Exe 1: Excercises for (Physical and) Theoretical Chemistry
WS 2002/03 $1^{\text {st }}$ IGS semester

Notes: How to tackle the excercises is explained on Friday, you may find them on the web: http://www.tc.chemie.uni-siegen.de/, "Vorlesungsskripte und Übungsblätter ...", "Excercises 2002/3", "Ex1".
You may ask respective questions on Monday morning. Deliver your homework before Wednesday night. It will be returned / discussed on Friday.
$25-30 \%$ of your marks will come from your homework, the rest from a clausur at the end of the lecture.

1) How many dimensions does the vector space have which is spanned by the 4 functions of $\phi: f_{1}=1, f_{2}=\sin ^{2} \phi, f_{3}=\cos ^{2} \phi, f_{4}=\cos 2 \phi$.
2) Determine the scalar products of two vectors. a) $\left\langle v_{1} \mid v_{2}\right\rangle$ with $\left\langle v_{1}\right|=\left|v_{1}\right\rangle^{+}=(1, i)$ and $\left|v_{2}\right\rangle^{+}=(1,-i)$; b) $\left|v_{1}\right\rangle$ and $\left|v_{1}\right\rangle$; c) $\phi \in[0,2 \pi], e^{i \phi}$ and $e^{i \phi}$; d) $e^{i \phi}$ and $e^{-i \phi}$ for $\phi \in[-\pi, \pi]$
3) Determine Eigenvalues and Eigenvectors of $O p_{1}=\left(\begin{array}{ll}0 & 1 \\ 1 & 0\end{array}\right) \cdot$ and of $O p_{2}=d / d x$.
4) a) A bond in a molecule is photodissociated by UV light of wave length $\lambda=350 \mathrm{~nm}$. The bond energy BE is $>$ or $<$ than ...? Give the answer in eV , in $\mathrm{kJ} / \mathrm{mol}$. Which temperature T corresponds to $\mathrm{BE}, \mathrm{BE}=k \cdot T$ ?
b) An ionic molecule $A^{+} B^{-}$with internuclear average separation of 250 pm has a dipole moment of 5D. Determine the atomic 'effective dipole' charges.
