## Exe 1: Excercises for (Physical and) Theoretical Chemistry WS 2002/03 1<sup>st</sup> IGS semester Excercises No. 1 hand out: Fr. 18.10.02, return: We. evening, 23.10. mail-box, AR-K6 left side wall.

**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)  $\langle v_1 | v_2 \rangle$  with  $\langle v_1 | = |v_1\rangle^+ = (1, i)$  and  $|v_2\rangle^+ = (1, -i)$ ; b)  $|v_1\rangle$  and  $|v_1\rangle$ ; 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  $Op_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$  and of  $Op_2 = d/dx$ .

4) a) A bond in a molecule is photodissociated by UV light of wave length  $\lambda = 350$  nm. The bond energy BE is > or < than ...? Give the answer in eV, in kJ/mol. Which temperature T corresponds to BE, 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.