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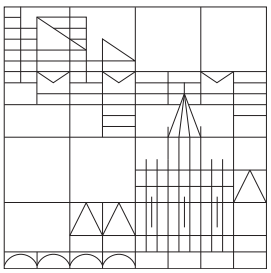

Group theory and symmetries in quantum mechanics
Summer semester 2016 - Exercise sheet 7
Distributed: 10.06.2016, Discussion: 17.06.2016

Problem 23: Vibrations of the CO_2 molecule

The procedure of finding the molecular vibrations of linear molecules, such as CO_2, is somewhat different from what we discussed in the lecture. Assuming that the axis of the molecule is along the $\hat{z}$ direction, only two rotational degrees of freedom has to be removed, because rotations around $\hat{z}$ by an arbitraty angle Φ correspond to the identity operation (we consider the atoms as homogeneous balls). In particular, CO_2 is a molecule with $D_{\infty h}$ symmetry group, whose character table is given below.

			E	$2C_\Phi$	C_2'	i	$2iC_\Phi$	iC_2'
$x^2+y^2,\ z^2$		A_{1g}	1	1	1	1	1	1
		A_{1u}	1	1	1	-1	-1	-1
	R_z	A_{2g}	1	1	-1	1	1	-1
	z	A_{2u}	1	1	-1	-1	-1	1
(xy, yz)	(R_x, R_y)	E_{1g}	2	$2\cos\Phi$	0	2	$2\cos\Phi$	0
	(x, y)	E_{1u}	2	$2\cos\Phi$	0	-2	$-2\cos\Phi$	0
(x^2-y^2, xy)		E_{2g}	2	$2\cos 2\Phi$	0	2	$2\cos 2\Phi$	0
		E_{2u}	2	$2\cos 2\Phi$	0	-2	$-2\cos 2\Phi$	0
		$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

(a) Find the characters of the atomic site representation $\Gamma^{a.s.}$!

(b) Find $\Gamma_{mol.vib.}$, the symmetries of the normal modes of the molecular vibrations! Which are infrared active and which are not?

Problem 24: Vibrations of the ammonia molecule NH_3

The hydrogen atoms in NH_3 are at the corners of an equilateral triangle and the nitrogen atom is either above or below the centre of this triangle.

(a) Which point group corresponds to the symmetries of this molecule? Find $\Gamma^{a.s.}$ and $\Gamma_{mol.vib.}$!

(b) Which modes are infrared active? What is the polarization dependence of the normal mode excitation?