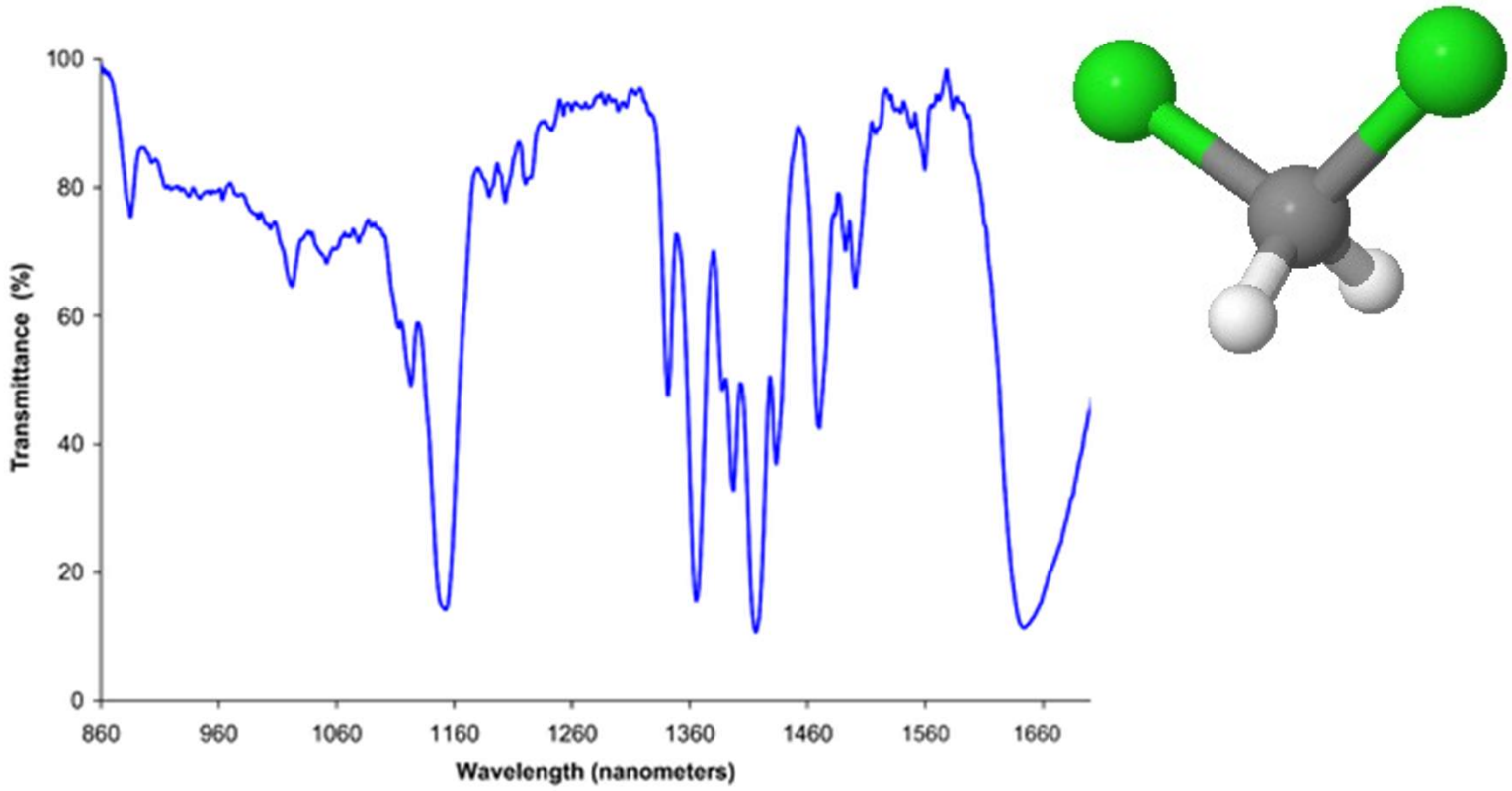
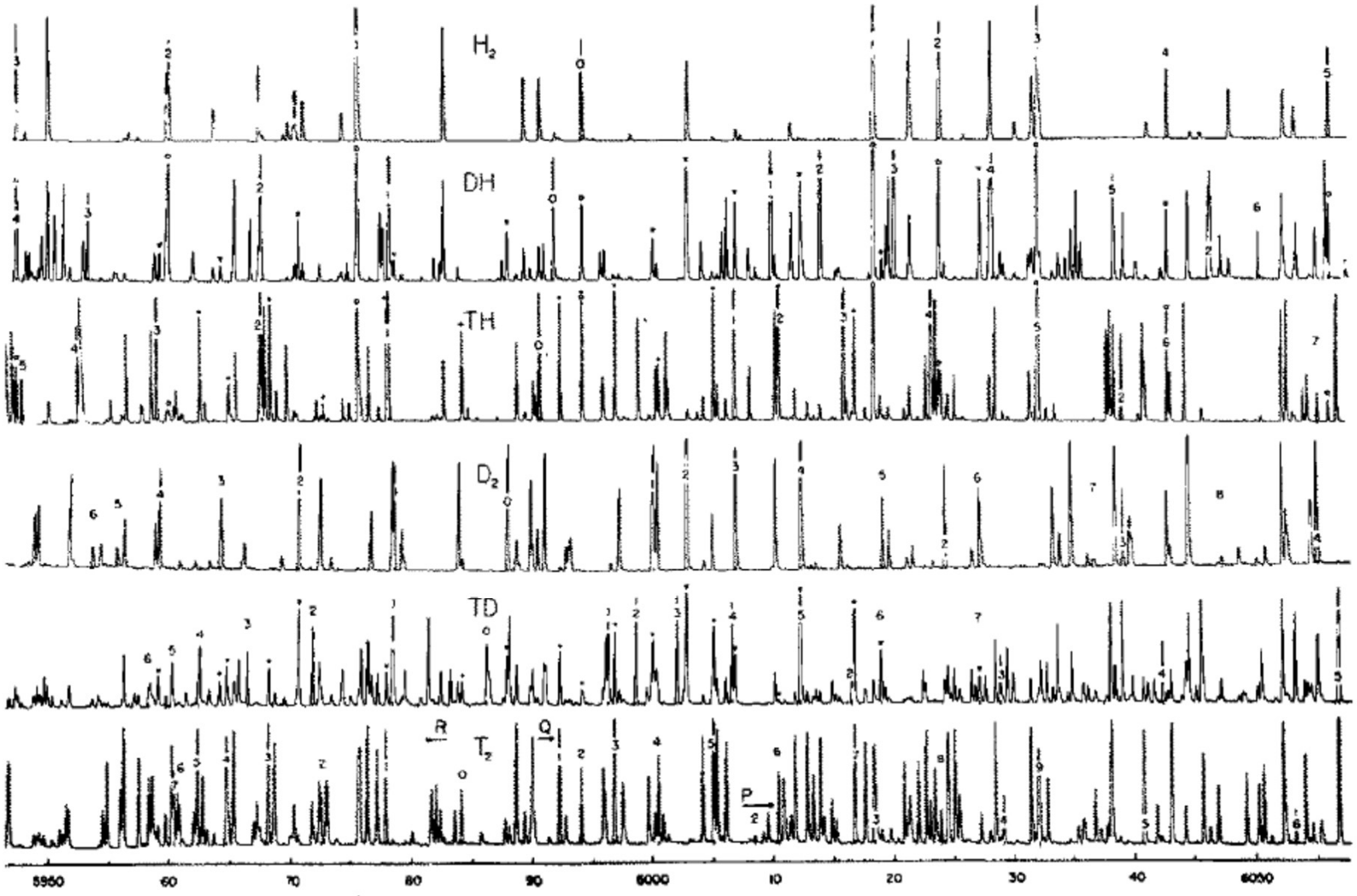
IR absorption spectrum



Near IR absorption spectrum of dichloromethane .

Emission spectra



Dieke, Journal of Molecular Spectroscopy 2, p. 494 (1958)

"Molecular spectroscopy is the study of absorption of light by molecules. In the gas phase at low pressures, molecules exhibit absorption in narrow lines which are very characteristic of the molecule as well as the temperature and pressure of its environment. In the microwave and long-wavelength infrared regions of the spectrum, these lines are due to quantized rotational motion of the molecule. At shorter wavelengths similar lines are due to quantized vibration and electronic motion as well as rotational motion. The precise frequencies of these lines can be fit to quantum mechanical models which can be used both to determine the structure of the molecule and to predict the frequencies and intensities of other lines. Because this absorption is so characteristic, it is very valuable for detecting molecules in the Earth's stratosphere, planetary atmospheres, and even the interstellar medium."

http://spec.jpl.nasa.gov/

Catalog Directory

ID	Name	# lines	Ver.	Catalog	Documentation
1001	H-atom	1	1	c001001.cat	pdf or Tex format
2001	D-atom	1	1	c002001.cat	pdf or Tex format
3001	HD	1	2	c003001.cat	pdf or Tex format
4001	H2D+	32	2*	c004001.cat	pdf or Tex format
7001	Li-6-H	51	2*	c007001.cat	pdf or Tex format
8001	LiH	53	2*	c008001.cat	pdf or Tex format
8002	Li-6-D	80	1	c008002.cat	pdf or Tex format
9001	LiD	90	1	c009001.cat	pdf or Tex format
12001	C-atom	2	2	c012001.cat	pdf or Tex format
13001	C-13-atom	7	2	c013001.cat	pdf or Tex format
13002	CH	508	2*	c013002.cat	pdf or Tex format
13003	CH+	9	2	c013003.cat	pdf or Tex format
14001	N-atom	2	1	c014001.cat	pdf or Tex format
14002	N-atom-D-st	6	3	c014002.cat	pdf or Tex format
14003	13CH	648	1*	c014003.cat	pdf or Tex format
14004	CD	188	1*	c014004.cat	pdf or Tex format
15001	NH	1416	1*	c015001.cat	pdf or Tex format
16001	O-atom	2	2	c016001.cat	pdf or Tex format
17001	OH	3153	5*	c017001.cat	pdf or Tex format
17002	NH3	1716	5*	c017002.cat	pdf or Tex format
17003	CH3D	143	3*	c017003.cat	pdf or Tex format
17004	NH3-v2	4198	5*	c017004.cat	pdf or Tex format
18001	OD	9351	2	c018001.cat	pdf or Tex format
18002	N-15-H3	235	2	c018002.cat	pdf or Tex format
18003	H2O	1376	6*	c018003.cat	pdf or Tex format
18004	NH2D	5036	1	c018004.cat	pdf or Tex format
18005	H2O v2,2v2,v	8608	4*	c018005.cat	pdf or Tex format
18006	13CH3D	143	1*	c018006.cat	pdf or Tex format
18007	17OH	46769	1*	c018007.cat	pdf or Tex format
19001	HO-18	3159	3	c019001.cat	pdf or Tex format
19002	HDO	1401	3	c019002.cat	pdf or Tex format
19003	H2O-17	404	1	c019003.cat	pdf or Tex format
19004	H3O+	304	3*	c019004.cat	pdf or Tex format
19005	H3O+ v1,v3,v	1973	2*	c019005.cat	pdf or Tex format
19006	17OD	113226	1*	c019006.cat	pdf or Tex format
20001	D2O	1137	2	c020001.cat	pdf or Tex format
20002	HF	8	1	c020002.cat	pdf or Tex format
20003	H2O-18	726	1	c020003.cat	pdf or Tex format
20004	18OD	3632	1*	c020004.cat	pdf or Tex format
21001	HDO-18	952	1	c021001.cat	pdf or Tex format
21002	DF	20	1	c021002.cat	pdf or Tex format
25001	CCH	114	1	c025001.cat	pdf or Tex format

Transition rates

$$H = H_0 + H_1$$

We know the eigenstates of H_0 = molecule + EM waves
$|\, i >$ is the initial state, $|\, f >$ is the final state.

H_1 is the perturbation that couples the molecular states to the EM waves.

Fermi's golden rule: $$\Gamma_{i\to f} = \frac{2\pi}{\hbar}|\langle f|H_1|i\rangle|^2\delta(E_f - E_i)$$

Often you can show $|\langle f|H_1|i\rangle| = 0$ by symmetry $\Longrightarrow$ Forbidden transition

Symmetries

Molecules can be classified by their symmetries. The eigenfunctions of the Hamiltonian will also be eigenfunctions of the symmetry operators.

Symmetries belong to a group. for $A, B \in G, AB \in G$

Point symmetries

If one point remains fixed during transformation, symmetries can be represented by 3×3 matrices.

$AB \in G$ for $A, B \in G$

Rotation about the x axis by angle α:

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & \sin\alpha \\ 0 & -\sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Symmetry @ Otterbein

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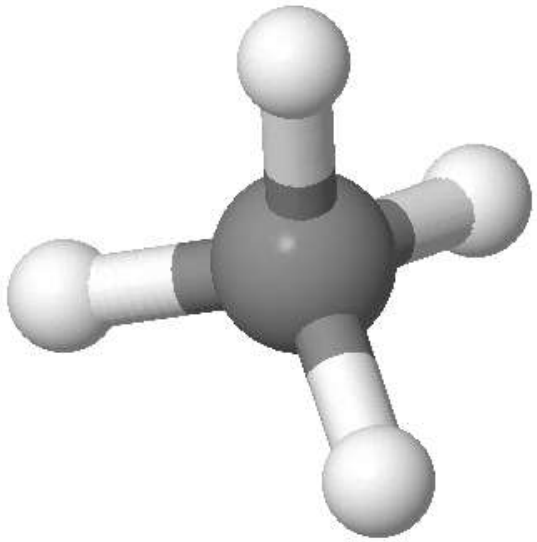


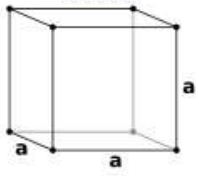
Point Group = T_d

Jmol

Element	Operation	Element	Operation
Show All Proper		*Show All Planes*	
C_3 axis	Rotate	plane (σ_d)	Reflect
C_3 axis	Rotate	plane (σ_d)	Reflect
C_3 axis	Rotate	plane (σ_d)	Reflect
C_3 axis	Rotate	plane (σ_d)	Reflect
C_2 axis	Rotate	plane (σ_d)	Reflect
C_2 axis	Rotate	plane (σ_d)	Reflect
C_2 axis	Rotate		
S_4 axis	Rotate		
S_4 axis	Rotate		
S_4 axis	Rotate		

https://symotter.org/tutorial/intro

The 32 Crystal Classes

Crystal system	Crystal Class	International symbol	Schoenflies symbol	Space groups	2-fold axes	3-fold axes	4-fold axes	6-fold axes	mirror planes	inversion	Examples	Number of symmetry elements
Cubic 	tetrahedral	23	T	195-199	3	4	-	-	-	n		12
	diploidal	$m3$	T_h	200-206	3	4	-	-	3	y		24
	gyroidal	432	O	207-214	6	4	3	-	-	n		24
	hextetrahedral	$\bar{4}3m$	T_d	215-220	3	4	-	-	6	n	216: Zincblende, ZnS, GaAs, GaP, InAs, SiC	24
	hexoctahedral	$m3m$	O_h	221-230	6	4	3	-	9	y	221: CsCl, cubic perovskite 225: fcc, Al, Cu, Ni, Ag, Pt, Au, Pb, γ-Fe, NaCl 227: diamond, C, Si, Ge, α-Sn, spinel 229: bcc, Na, K, Cr, α-Fe, β-Ti, Nb, Mo, Ta	48

http://lamp.tu-graz.ac.at/~hadley/ss2/crystalphysics/crystalclasses/crystalclasses.html