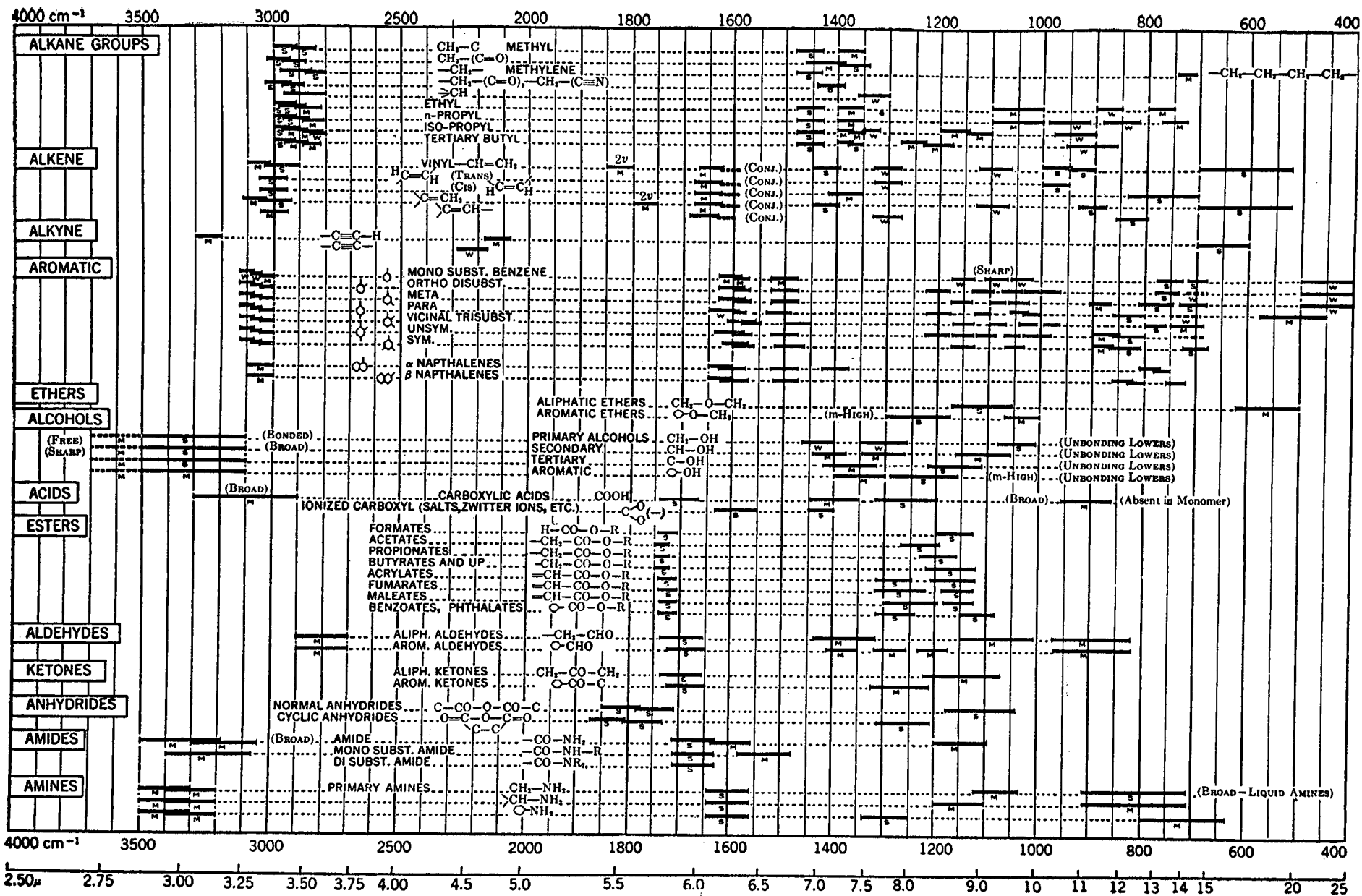


Interpretace spekter

- Oblast otisku prstu – 500 – 1500 cm^{-1}
 - valenční vibrace většiny anorganických molekul
 - deformační vibrace organických molekul – δ HCH, δ CCH, δ COH
 - některé valenční vibrace organických molekul ν C-C, ν C-O
- Charakteristické vibrace – poloha spektrálních pásů funkčních skupin je relativně málo závislá na zbytku molekuly, proto je možné jejich vlnočty tabelovat

Interpretace spekter



Izotopicky substituované molekuly

- Interpretaci IR a RA spekter lze usnadnit izotopickou substitucí ve zkoumané molekule.
- Nedojde ke změně geometrie molekuly, ale změní se hmotnosti atomů.
- Dojde k poklesu frekvencí všech vibrací, jichž se substituovaný atom účastní.

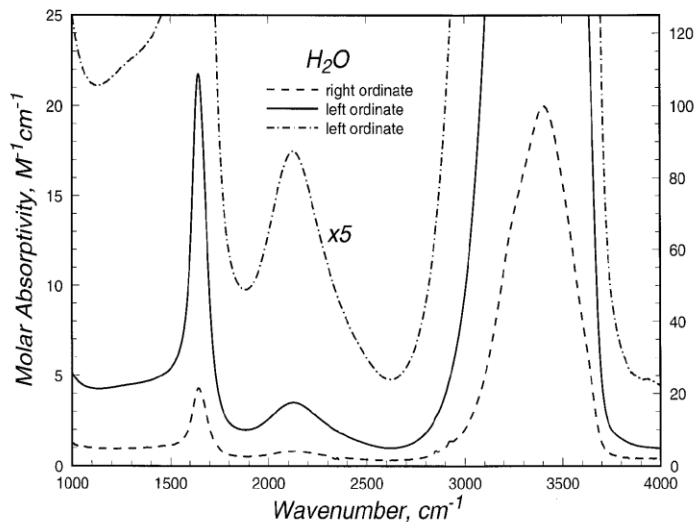


FIG. 1. Molar absorptivity of H_2O in the $1000\text{--}4000\text{ cm}^{-1}$ spectral range at 25°C .

cal studies, are the water absorptions at 1550 and 1650 cm^{-1} , the characteristic wavenumbers of protein amide II (H_2O) and amide I' (D_2O) bands. D_2O never is 100% pure and usually includes HOD molecules from the

traces of H_2O . The absorbance bands at 3404 cm^{-1} (intensity is proportional to content of OH groups) and at 3840 cm^{-1} (intensity is proportional to D_2O content) can be used for quick and precise determination of D_2O

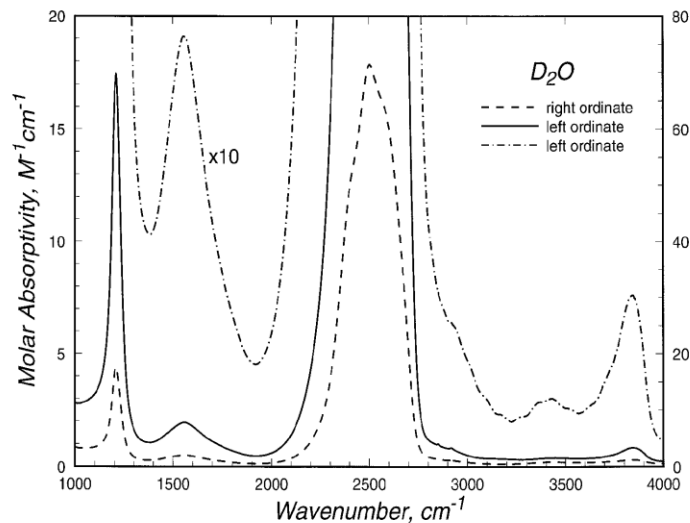



FIG. 2. Molar absorptivity of D_2O in the $1000\text{--}4000\text{ cm}^{-1}$ spectral range at 25°C .

Knihovny spekter

□ http://sdb.s.riodb.aist.go.jp/sdb.s/cgi-bin/cre_index.cgi

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SDBS Compounds and Spectral Search

Compound Name:

Molecular Formula:
C, H, then the other elements are alphabetical order, "%," for the wild card

Molecular Weight: to
Numbers between left and right columns
Up to the first place of a decimal point

CAS Registry No.:
"%," for the wild card.

SDBS No.:
"%," for the wild card.

Atoms:

C(Carbon)	<input type="text"/>	to	<input type="text"/>
H(Hydrogen)	<input type="text"/>	to	<input type="text"/>
N(Nitrogen)	<input type="text"/>	to	<input type="text"/>
O(Oxygen)	<input type="text"/>	to	<input type="text"/>
F(Fluorine)	<input type="text"/>	to	<input type="text"/>
Cl(Chlorine)	<input type="text"/>	to	<input type="text"/>
Br(Bromine)	<input type="text"/>	to	<input type="text"/>
I(Iodine)	<input type="text"/>	to	<input type="text"/>
S(Sulfur)	<input type="text"/>	to	<input type="text"/>
P(Phosphorus)	<input type="text"/>	to	<input type="text"/>
Si(Silicon)	<input type="text"/>	to	<input type="text"/>

Numbers between left and right columns.

Spectrum:
Check the spectra of your interest.
 MS IR
 ¹³C NMR Raman
 ¹H NMR ESR

IR Peaks(cm⁻¹): Allowance
 ±
", " or space is the separator for multiple peaks.
Use "-", to set a range.: eg. 550-750,1650-3000-
Transmittance < %

¹³C NMR Shift(ppm): Allowance
 ±
", " is the separator for multiple shifts, eg. 129.3,18.4,...
No shift regions:
Range defined by two numbers separated by a space, eg. 110 78,...

¹H NMR Shift(ppm): Allowance
 ±
No shift regions:

MS Peaks and intensities:

Mass and its intensity are a set of data separated by a space, eg. 110 22,...

Hit: Sort by: