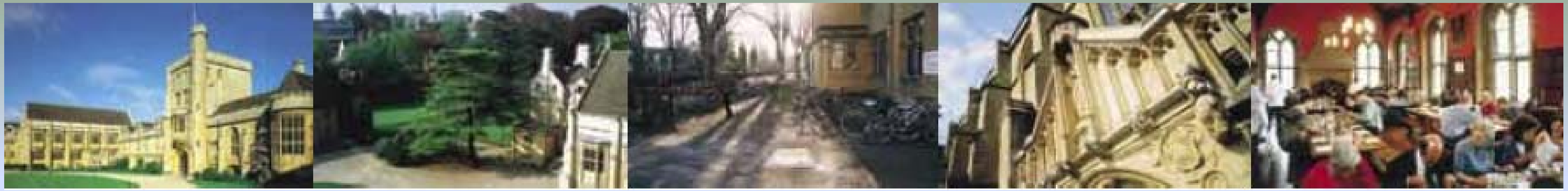


10^{th} Oxford School on Neutron Scattering

University of Oxford, Mansfield College

Chemical Applications of Neutron Scattering

Part 2

Mainly Spectroscopy and Dynamics

Alberto Albinati

University of Milan

Department of Structural Chemistry

Chemical Applications of Neutron Scattering

Part 2

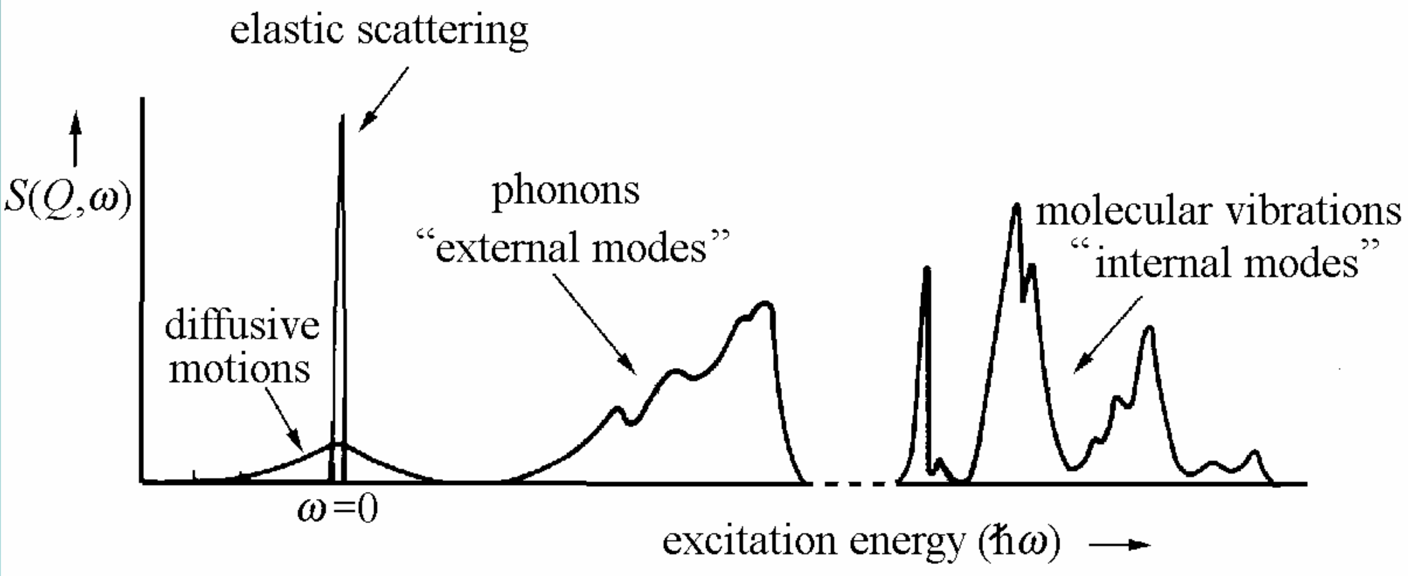
- **INS Spectroscopy**
- **Rotational Tunnelling**
- **QENS**
- **Diffraction, Spectroscopy and ab-initio calculations**

NEUTRON SCATTERING TECHNIQUES

Tipe of Scattering	Range of ω [cm^{-1}] or κ [$Å^{-1}$]	Instrument	*Information*
Coherent Elastic $\frac{d\sigma}{d\Omega}$	$0.5 < \kappa < 15.$	4circle diffract. Laue TOF	***Diffraction*** *Magnetic Diffr.*
	$\kappa < 0.1$	SANS	*Particle size* *Macromolecules*
	$\kappa < 0.1$	Reflectometry	*Absorbed Layers*
Coherent Inelastic $\frac{d^2\sigma}{d\Omega dE} \equiv \frac{d^2\sigma}{d\Omega d\omega}$	$0.5 < \kappa < 15$ $0. < \omega < 1000.$	Triple Axis Constant ***Q*** (TOF)	*Collective Modes* *(Phon)ons etc.*
Incoherent Inelastic	$10 < \omega < 4000.$	Be filter, TOF	***Vibrational Modes***
$\frac{d^2\sigma}{d\Omega dE} \equiv \frac{d^2\sigma}{d\Omega d\omega}$	$10 < \omega < 4000.$	Backscattering	***Rot. Tunnelling***
Incoherent Quasi-Elastic (QENS)	$0.01 < \omega < 5.$ $0.1 < \kappa < 5.$	Backscattering Spin Echo	Diffusion Translations

$\boldsymbol{\kappa} = \mathbf{k_o} - \mathbf{k}$ $\qquad$ $|\mathbf{k_o}| = 2\pi/\lambda$

INS spectrum from a hypothetical molecular crystal



NEUTRON SCATTERING CROSS SECTIONS

INCOHERENT CROSS SECTION

$$\sigma_{inc} = 4\pi \left\langle \left(b - \langle b \rangle\right)^2 \right\rangle$$

σ_{inc} arises from the random distribution of different isotopes with different scattering lengths.

Incoherent Scattering depends on the correlation between **the positions of the same nucleus at different times.**

NO INTERFERENCE EFFECTS $\Rightarrow$

SPECTROSCOPY

Correlation Functions

$$S_{coh}(\mathbf{Q}, \omega) \;\Leftarrow F.T. \Rightarrow\; G(\mathbf{r}, t)$$

$$S_{inc}(\mathbf{Q}, \omega) \;\Leftarrow F.T. \Rightarrow\; G_s(\mathbf{r}, t)$$

- $G(\mathbf{r}, t) \equiv$ **Probability of finding an atom at *r* and at time *t* when there is an atom at r = 0 at *t* = 0.**

- $G_s(\mathbf{r}, t) \equiv$ **Probability of finding an atom at *r* and at time *t* if the *same atom* was at r = 0 at *t* = 0.**

Inelastic Neutron Scattering Measures Atomic Motion

$$\left(\frac{\partial^2\sigma}{\partial\Omega\partial E} = b_{coh}^2 \frac{k'}{k} N\mathbf{S}(\mathbf{Q},\omega)\right)_{coh} \qquad \left(\frac{\partial^2\sigma}{\partial\Omega\partial E} = b_{inc}^2 \frac{k'}{k} N\mathbf{S}_i(\mathbf{Q},\omega)\right)_{incoh}$$

$$\mathbf{S}(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar}\iint \mathbf{G}(\mathbf{r},t)e^{i(\mathbf{Q}.\mathbf{r}-\omega t)}d\mathbf{r}dt \qquad \mathbf{S}_i(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar}\iint \mathbf{G}_s(\mathbf{r},t)e^{i(\mathbf{Q}.\mathbf{r}-\omega t)}d\mathbf{r}dt$$

Inelastic coherent scattering measures *correlated* motions of atoms.
Inelastic incoherent scattering measures *self-correlations* (diffusion, vibrations).

INCOHERENT INELASTIC NEUTRON SCATTERING

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}E} = \frac{1}{4\pi}\frac{k'}{k}\left[b_{coh}S_{coh}\left(\mathbf{Q},\omega\right) + b_{incoh}S_{incoh}\left(\mathbf{Q},\omega\right)\right]$$

$$\frac{\mathrm{d}^2\sigma_{inc}}{\mathrm{d}\Omega\mathrm{d}E} = \sum_{\mathbf{q},j}\frac{k_f}{k_i}\delta\left(\hbar\omega \mp \hbar\omega_j\left(\mathbf{q}\right)\right)\frac{\hbar\left(\overline{n}+\frac{1}{2}\pm\frac{1}{2}\right)}{2\omega_j\left(\mathbf{q}\right)}\ \mathrm{x}\ \sum_r \frac{\left(b_{inc}\right)_r}{4\pi\ m_r}\left|\mathbf{Q}.\mathbf{U}_r^j\left(\mathbf{q}\right)\right|^2 \exp\left(-Q^2\left\langle U^2\right\rangle\right)$$

for a powder sample we can average

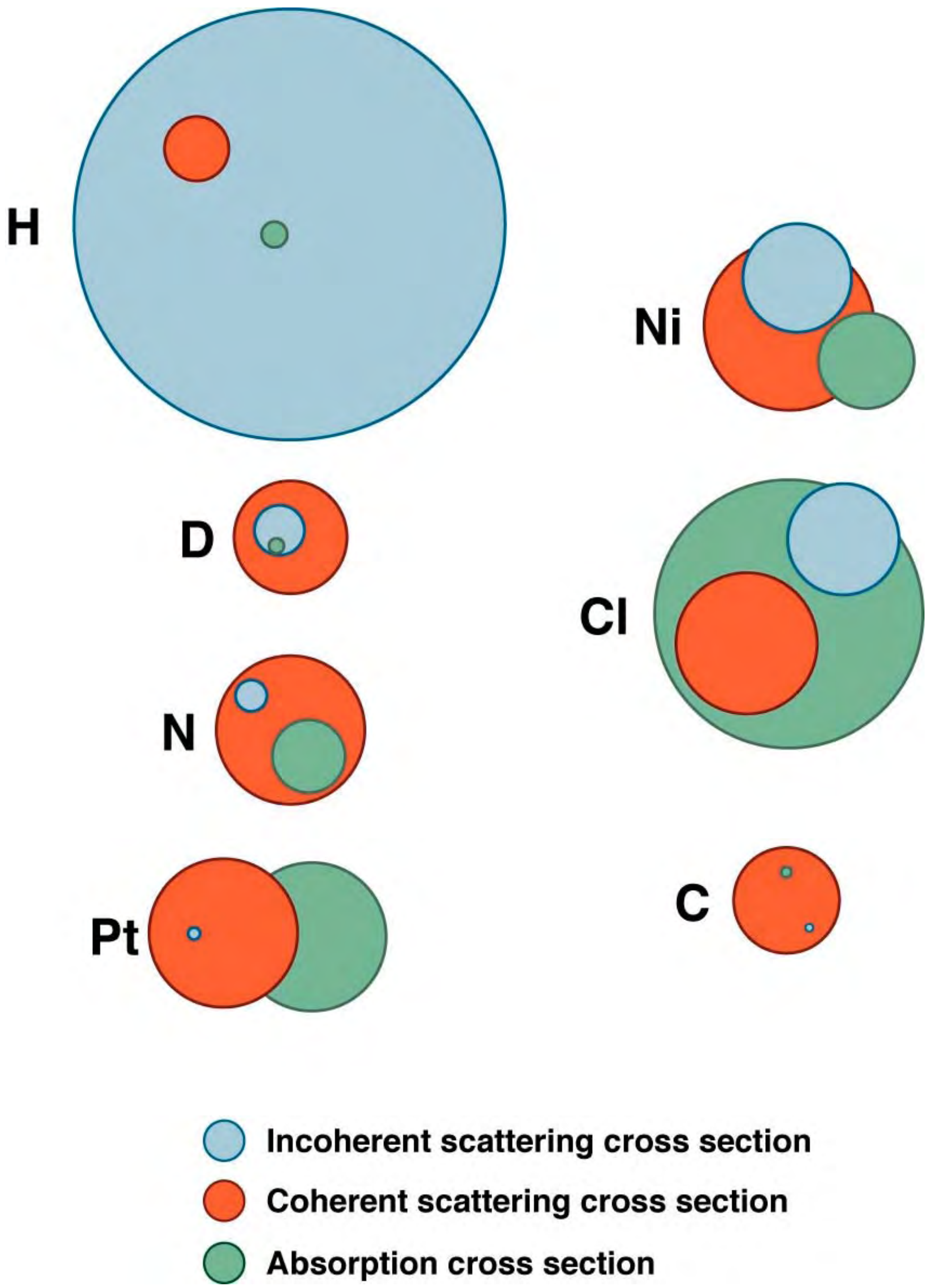
$$\frac{\mathrm{d}^2\sigma_{inc}}{\mathrm{d}\Omega\mathrm{d}E} = \frac{1}{4\pi}\frac{k_f}{k_i}\sigma_{inc}\frac{Q^2\left\langle U^2\right\rangle}{2m}\left(\overline{n}+\frac{1}{2}\pm\frac{1}{2}\right)\exp\left(-2W\right)N\frac{Z\left(\omega\right)}{\omega}$$

at very low T for hydrogenous materials

$$\frac{\mathrm{d}^2\sigma_{inc}}{\mathrm{d}\Omega\mathrm{d}E} = \frac{1}{4\pi}\frac{k_f}{k_i}b_{inc}S_{inc}(\mathbf{Q},\omega)$$

$$S_{inc}\left(\mathbf{Q},\omega\right) = Q^2\left\langle U^2\right\rangle\exp\left(-2W\right)$$

Neutron Incoherent Cross-Sections

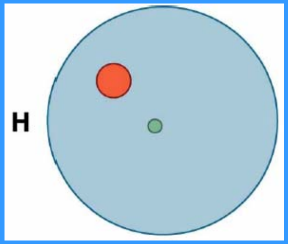


INELASTIC INCOHERENT NEUTRON SCATTERING

•**The energy of the thermal neutrons is comparable to that of the lattice and molecular vibrations:** ***INS is a powerful spectroscopic tool.***

•**The incoherent part of the scattering cross-section describes the single particles dynamics:** ***Vibrational and rotational spectroscopy.***

•**The incoherent scattering cross-section of** ***Hydrogen is very large:***



σ_{inc} (H) = 80.27 (barn)

σ_{inc} (D) = 2.05 (barn)

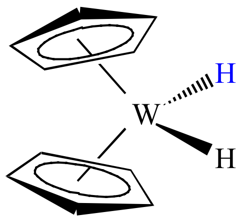
•**The intensity scattered by each mode depends on the** ***value of the incoherent scattering cross-section (σ_{inc}) and the atomic displacements.***

•**Modes involving H atoms** ***will dominate the INS Spectrum.*** **Large amplitude motions** ***will give the strongest peaks.***

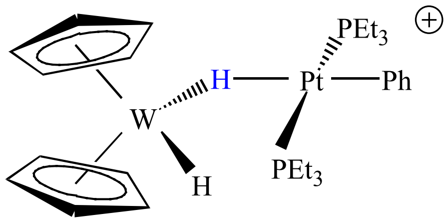
•**The are** ***no selection rules.***

“M-H” Stretching Frequencies and “M-H-M” Formation

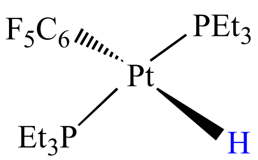
$\nu_{M\text{-}H}$ (cm^{-1})



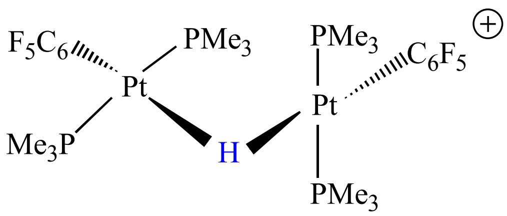
1896



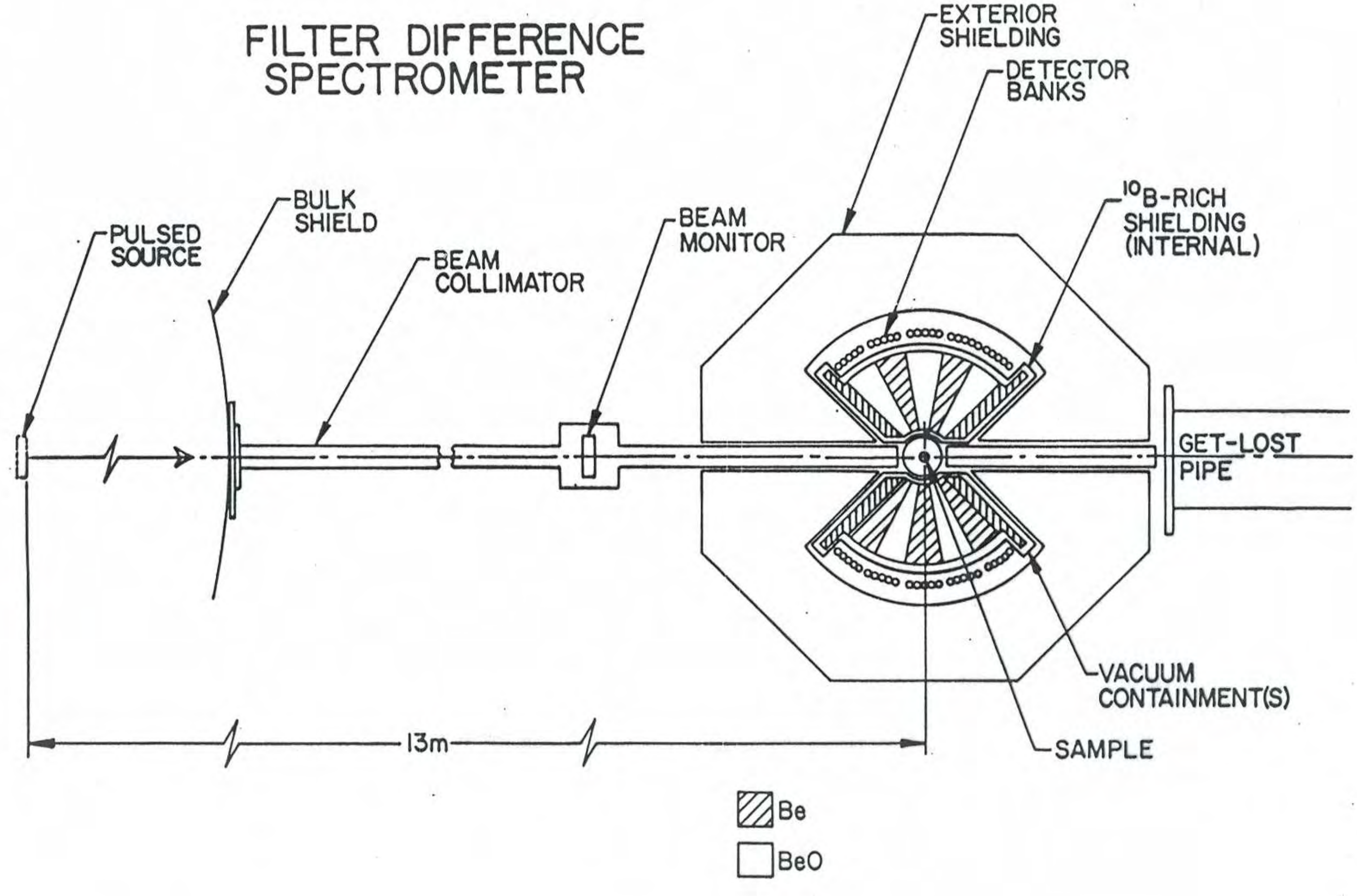
1635



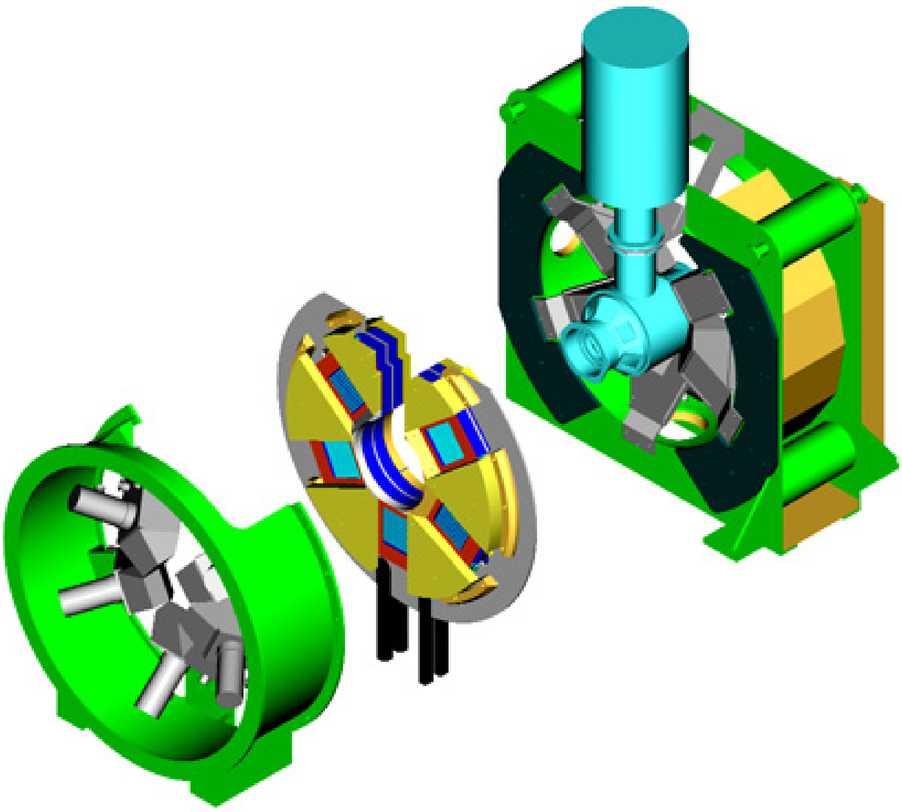
2060

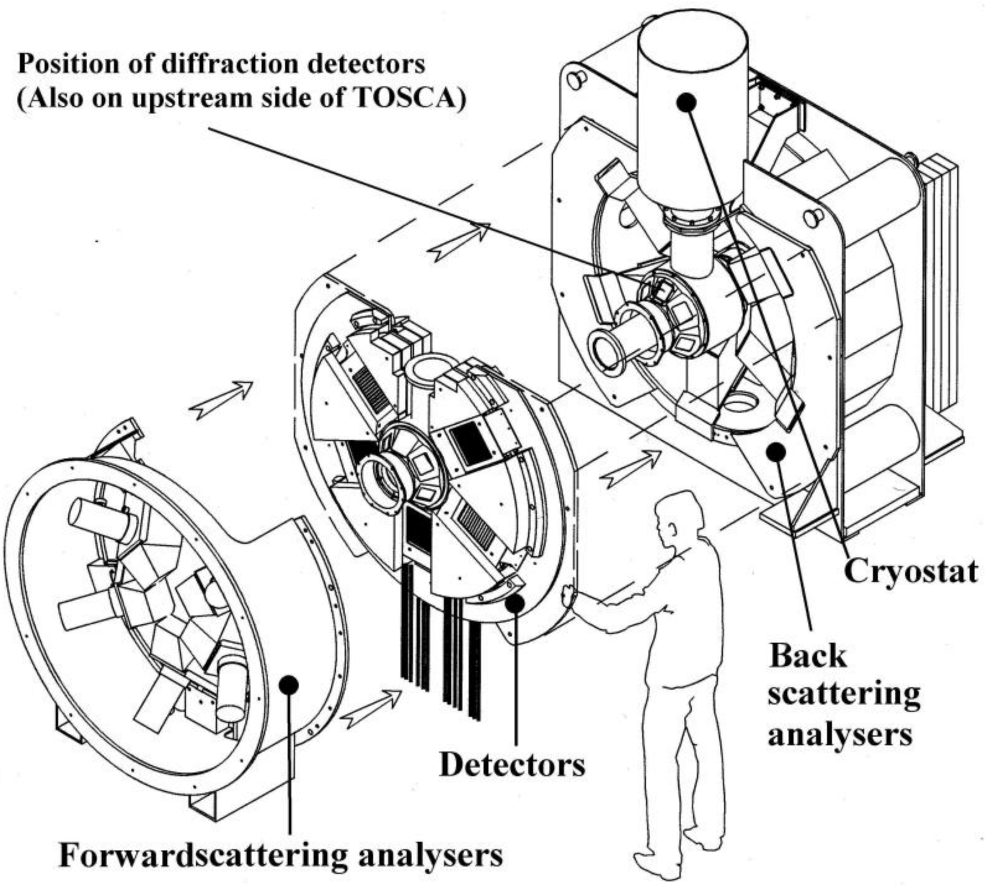


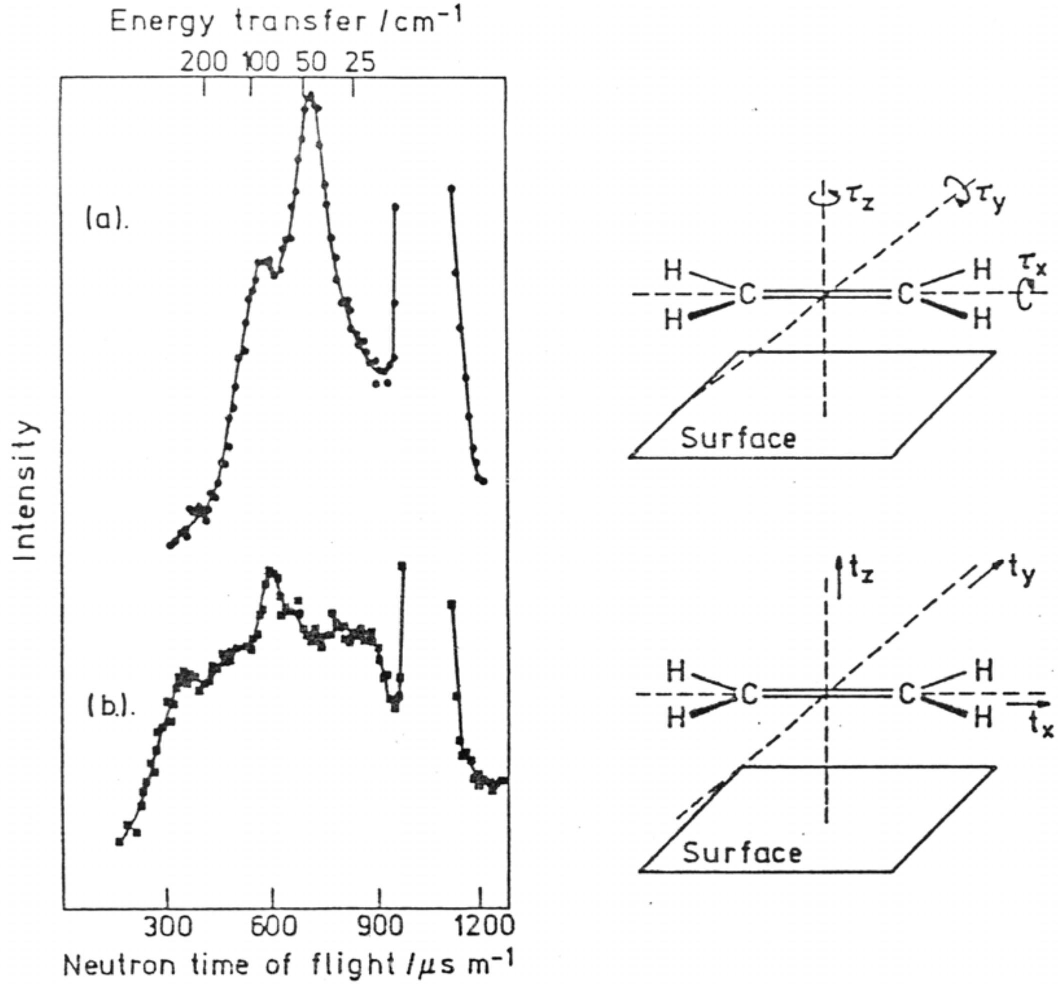
1260 (sym)
1020 (asym)


FILTER DIFFERENCE
SPECTROMETER
EXTERIOR
SHIELDING
DETECTOR
BANKS
BULK
SHIELD
PULSED
SOURCE
BEAM
COLLIMATOR
BEAM
MONITOR
10B-RICH
SHIELDING
(INTERNAL)
GET-LOST
PIPE
VACUUM
CONTAINMENT(S)
13m
SAMPLE
Be
BeO

The TOSCA Spectrometer







The inelastic neutron scattering from (*a*) ethylene adsorbed on an Ag-13X zeolite catalyst and (*b*) the catalyst alone. The spectra were taken on the Harwell DIDO 6H double rotor spectrometer by Howard et al

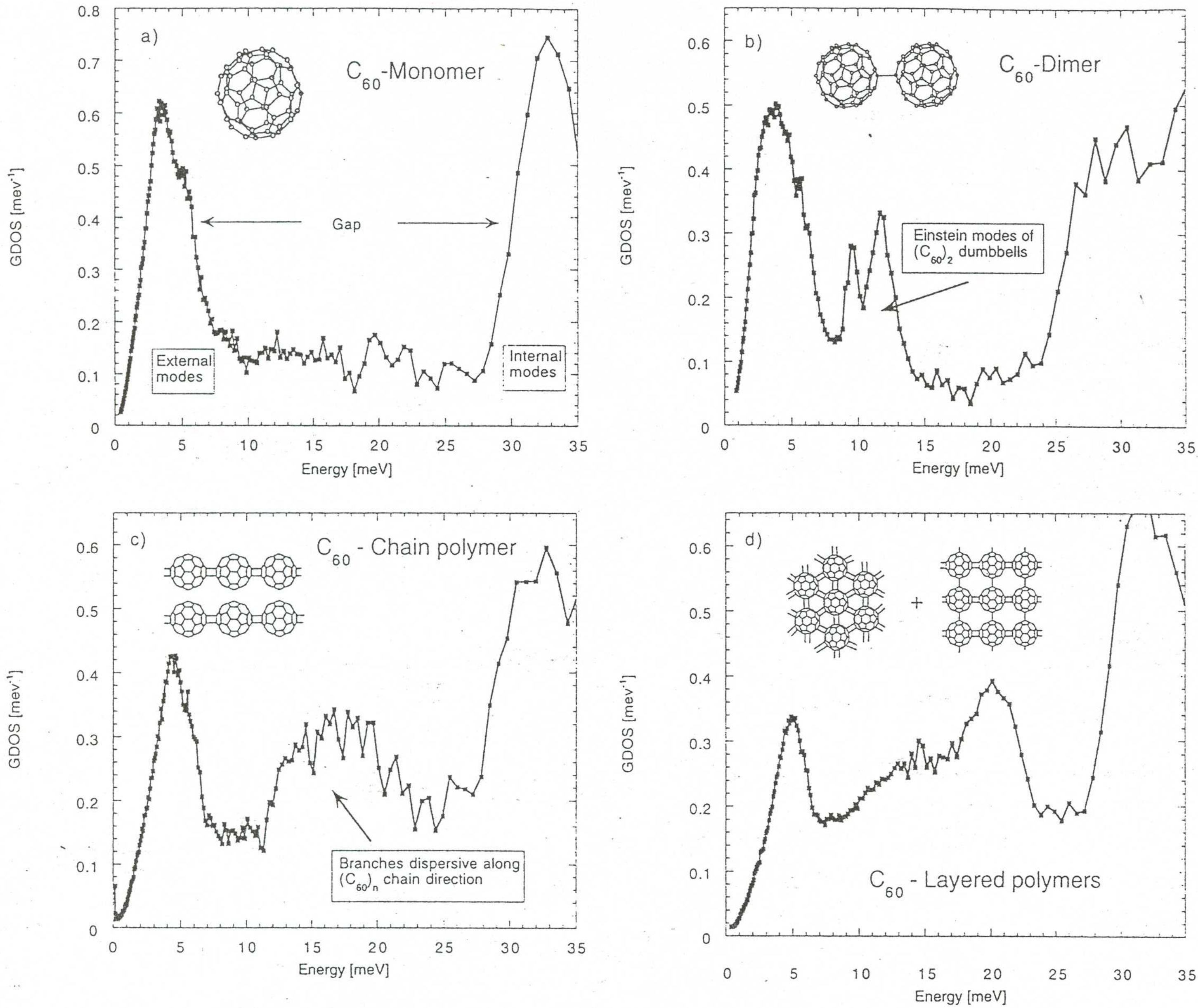
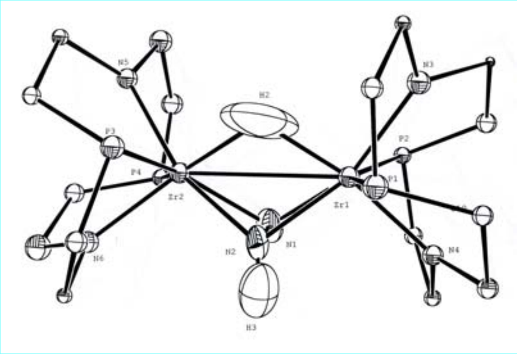
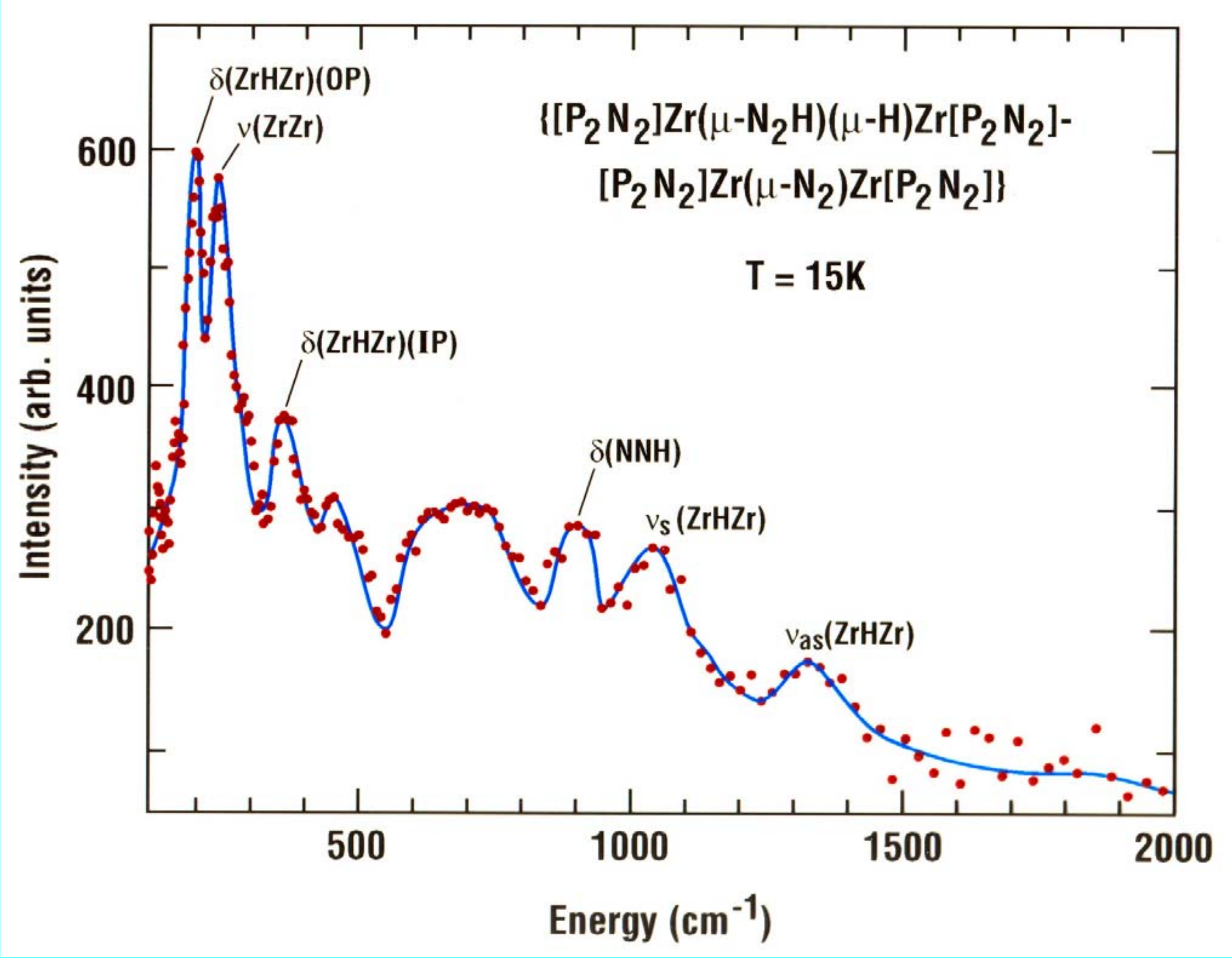


Figure 2. G(ω) as obtained from the INS spectra using the cold time-of-flight instrument IN6 of the ILL. Details about how G(ω) is obtained from the raw data are given in ref. [5]. a. C_{60} at 300 K in the plastic phase; b. $(C_{60})_2$ dimer of Rb_1C_{60}; c. Linear chains in pressure polymerized C_{60} [6]; d. 2-D polymer sheets in pressure polymerized C_{60} (the sample is a mixture of 2D rhomohedral and tetragonal networks) [7].

The INS Difference-Spectrum of $\{[P_2N_2Zr]_2\,(\mu\text{-H})(\mu\text{-}N_2H)\}$



$$\left\langle u_1^2 \right\rangle = \frac{h}{8\pi^2 \mu \nu} \coth\left(\frac{h\nu}{2kT} \right)$$



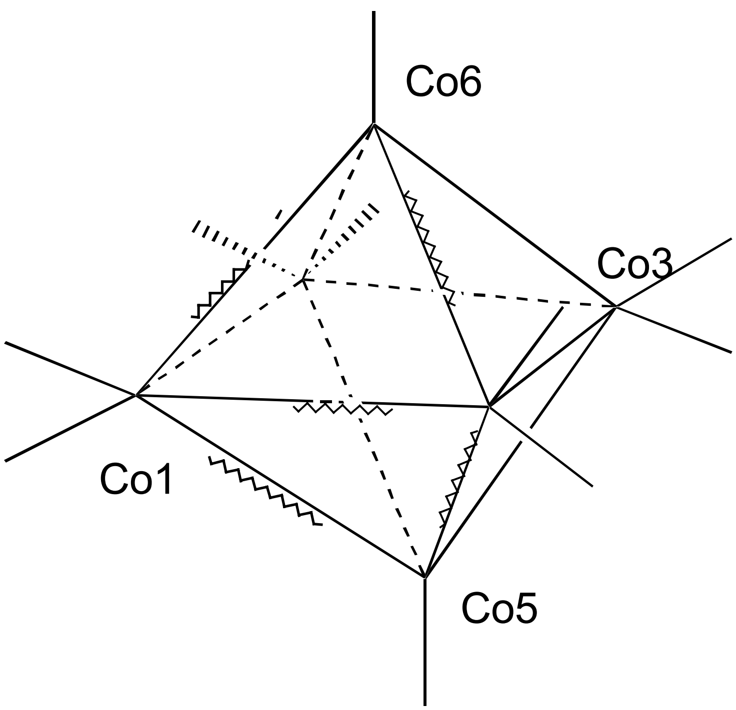
$[(PPh_3)_2N]^+$ $[HCo_6(CO)_{15}]^-$

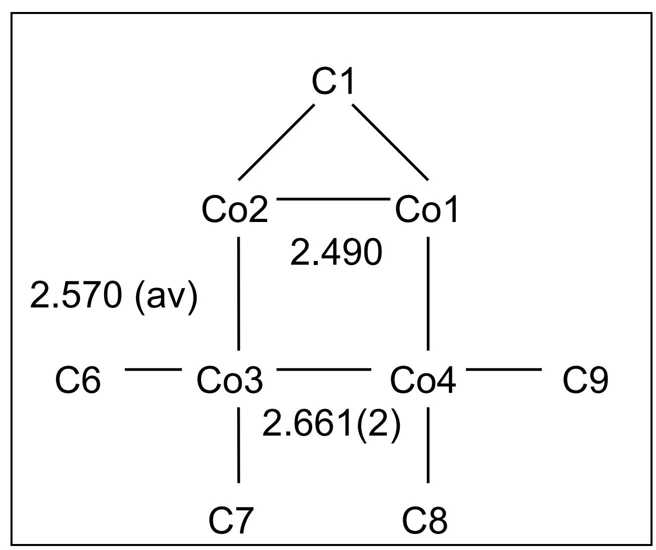
$$[Co_6(CO)_{15}]^{2-} + H^+ \Rightarrow [HCo_6(CO)_{15}]^-$$

NMR τ -13.2

Hydride $\tau \sim$ +10. +50.

Formyl $\tau \sim$ -5. -11.

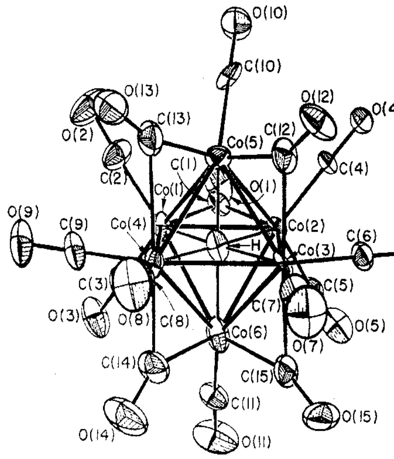


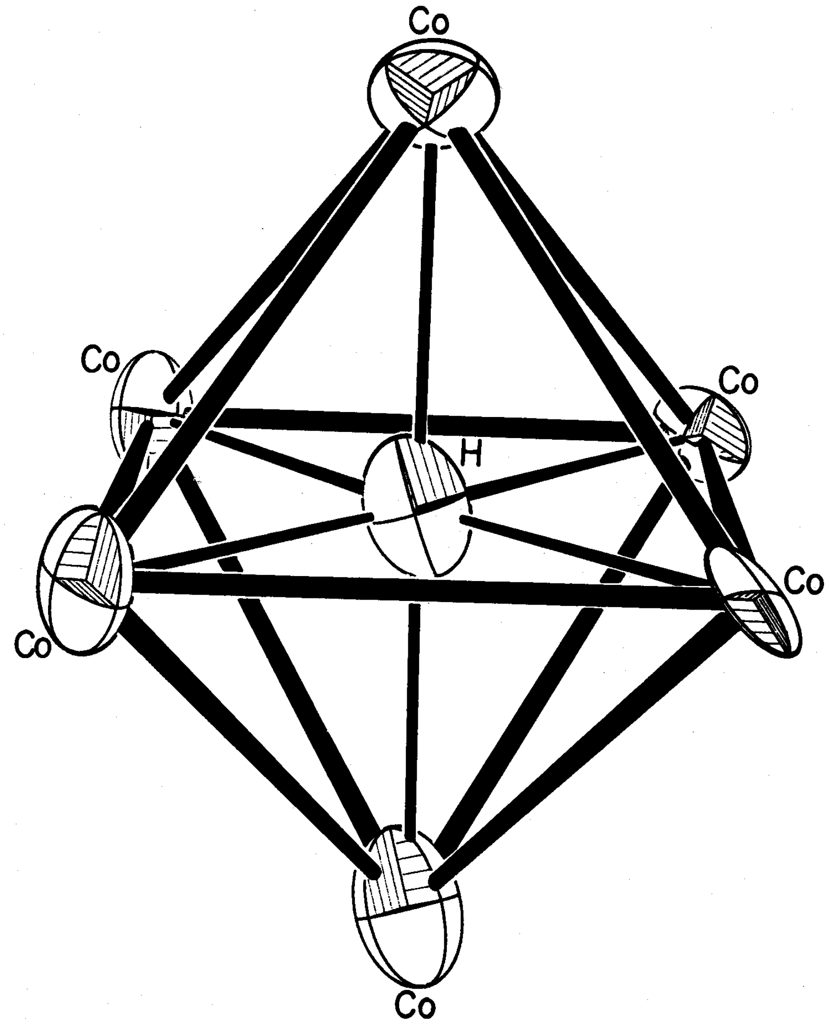


Carbonyl associated H atom ?

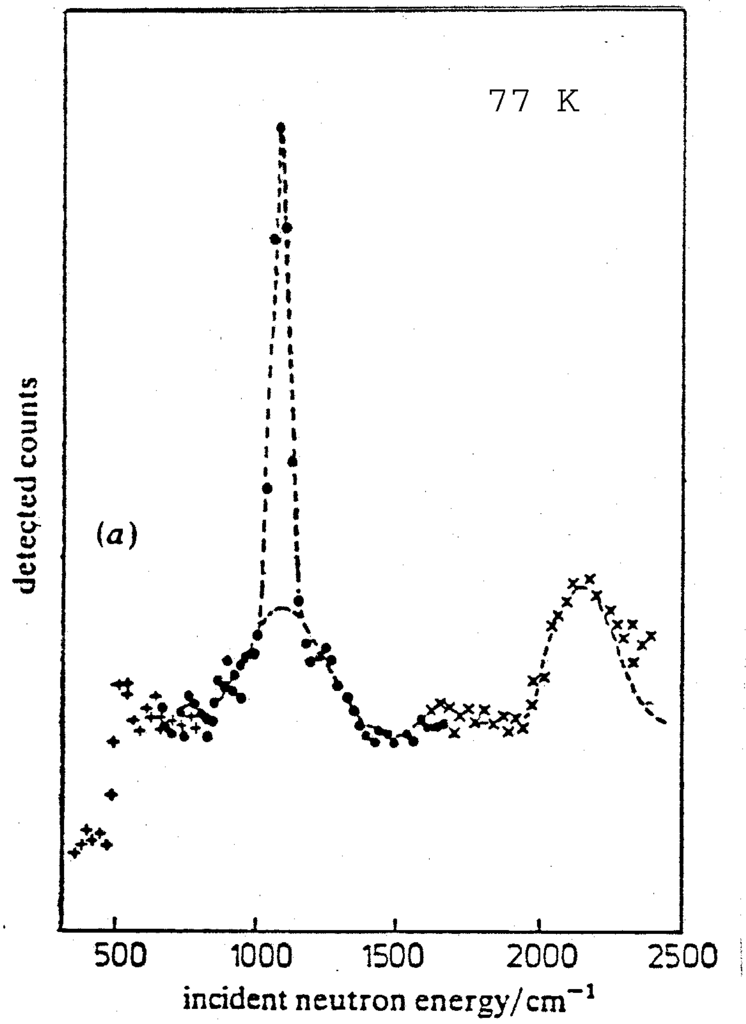
Chini,Longoni & al. JACS (1981) *103,*1458

The Crystal Structure of $[Co(CO)_{15}H]^-$
(Neutron Diffraction)



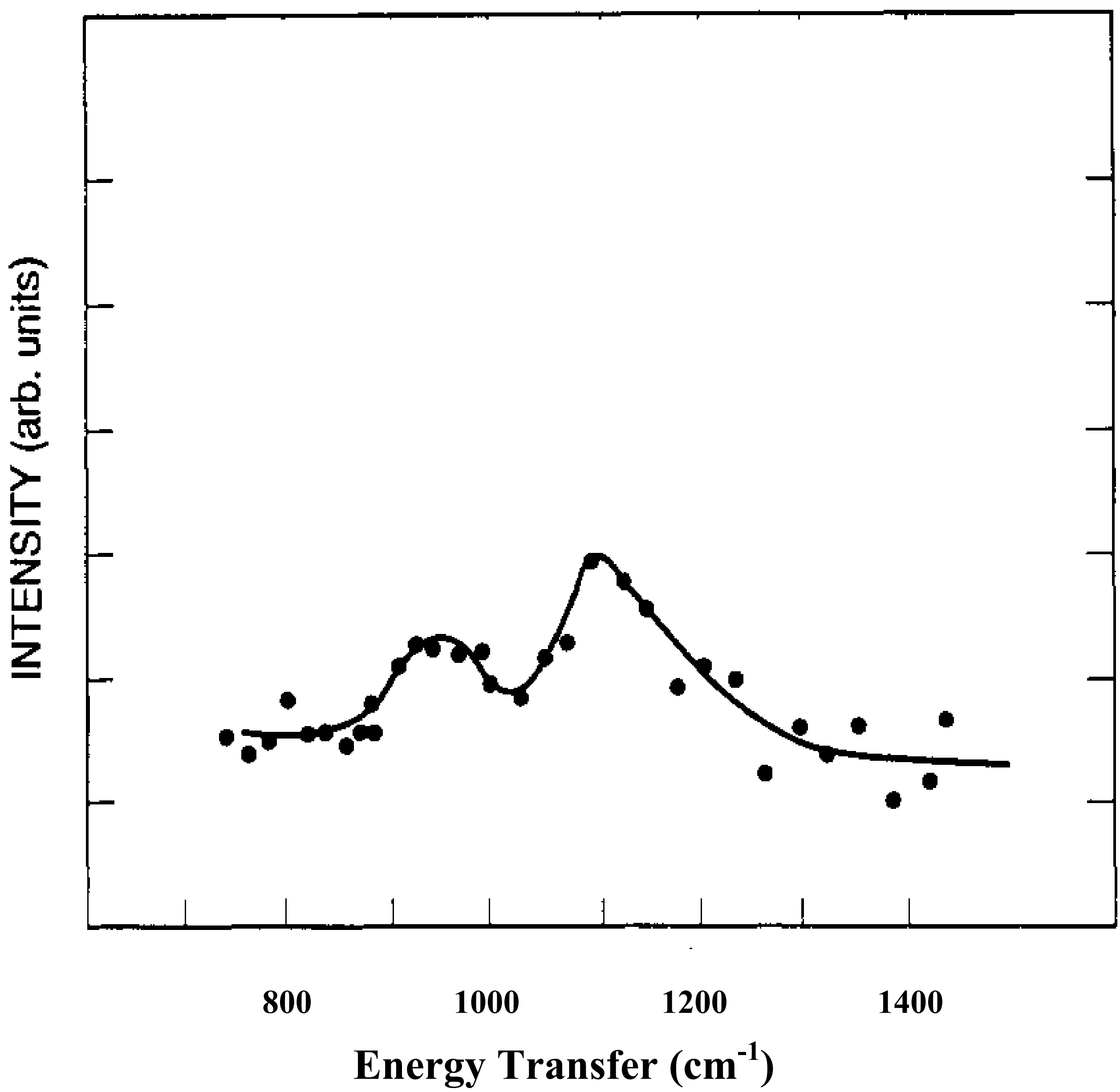


INS Spectrum of $Cs[HCo_6(CO)_{15}]$

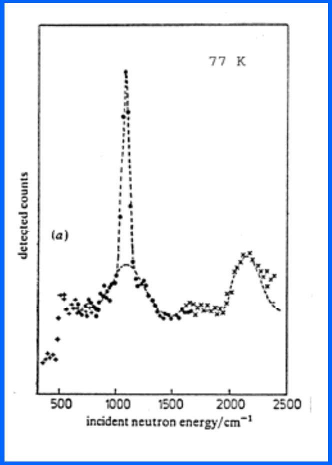


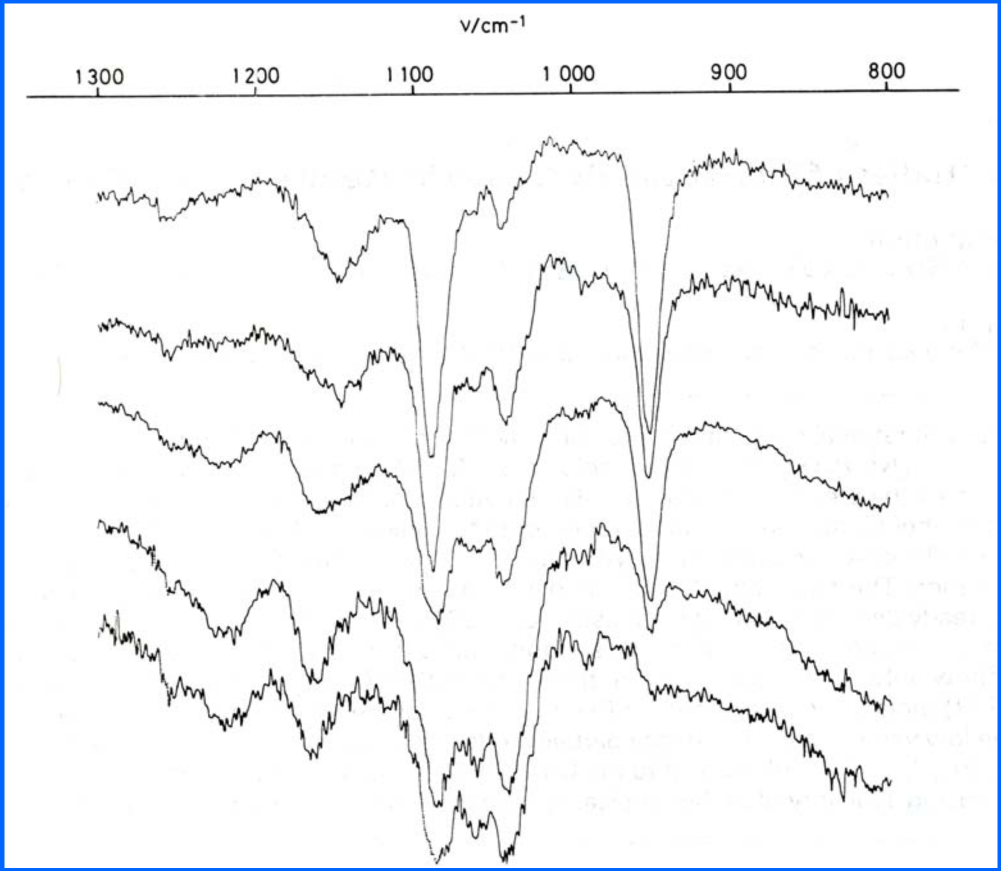
Graham, Howard, Waddington
J.C.S. Faraday Trans. B79B, 1713 (1983)

INS Spectrum of $K[HCo_6(CO)_{15}]$
FDS @15K



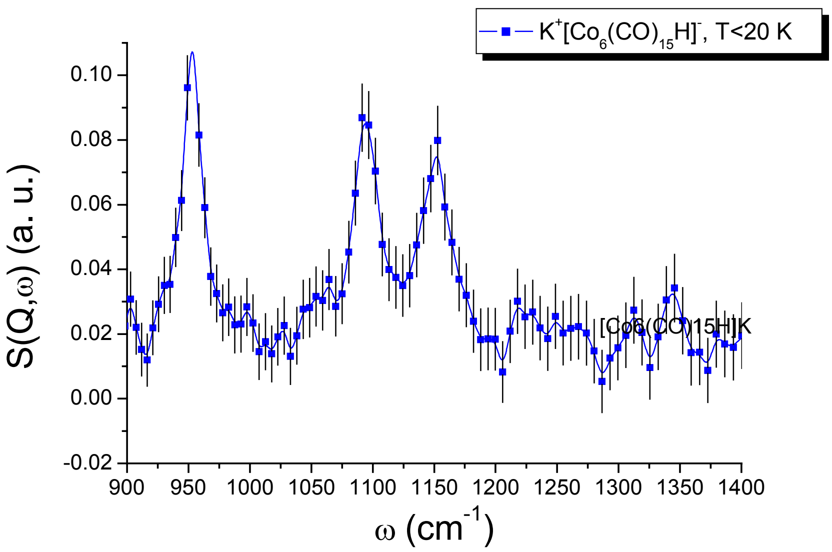
Series of I.R. Spectra of K[$Co_6(CO)_{15}H$] in CsI

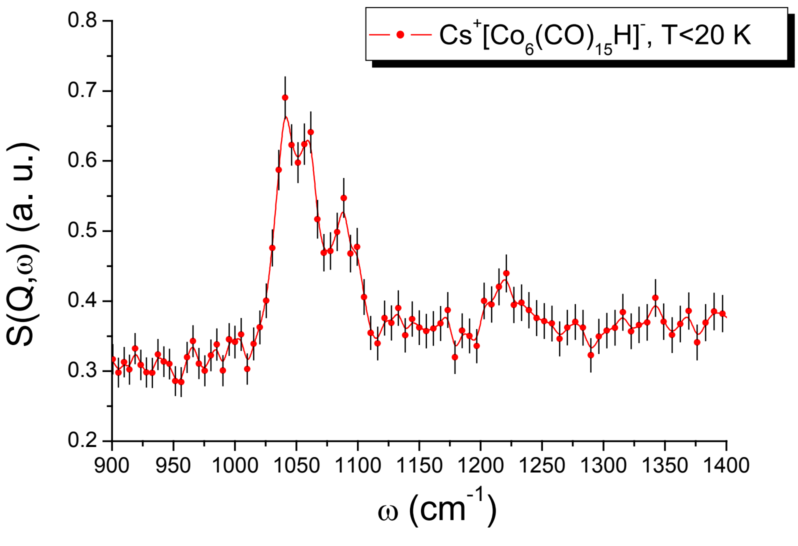




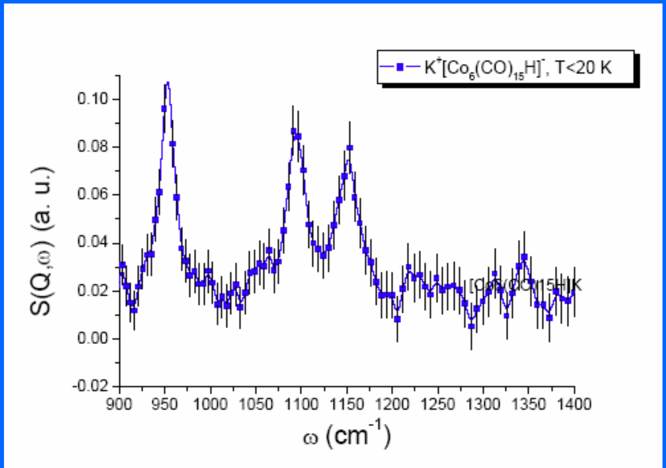
T = 110K

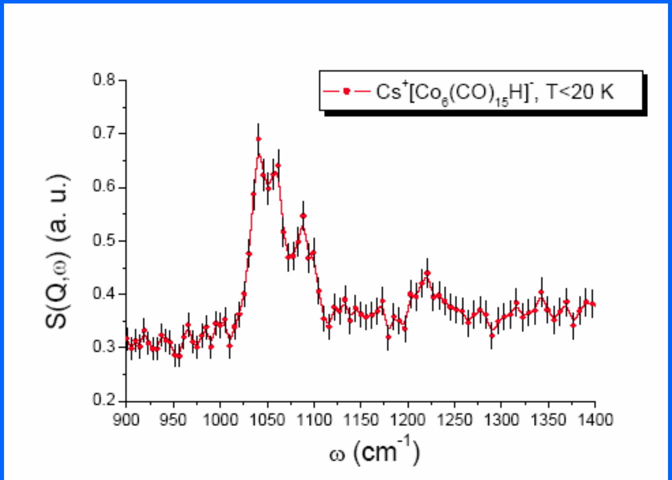
$[Co_6(CO)_{15}H]K$ and $[Co_6(CO)_{15}H]Cs$ TOSCA Spectra

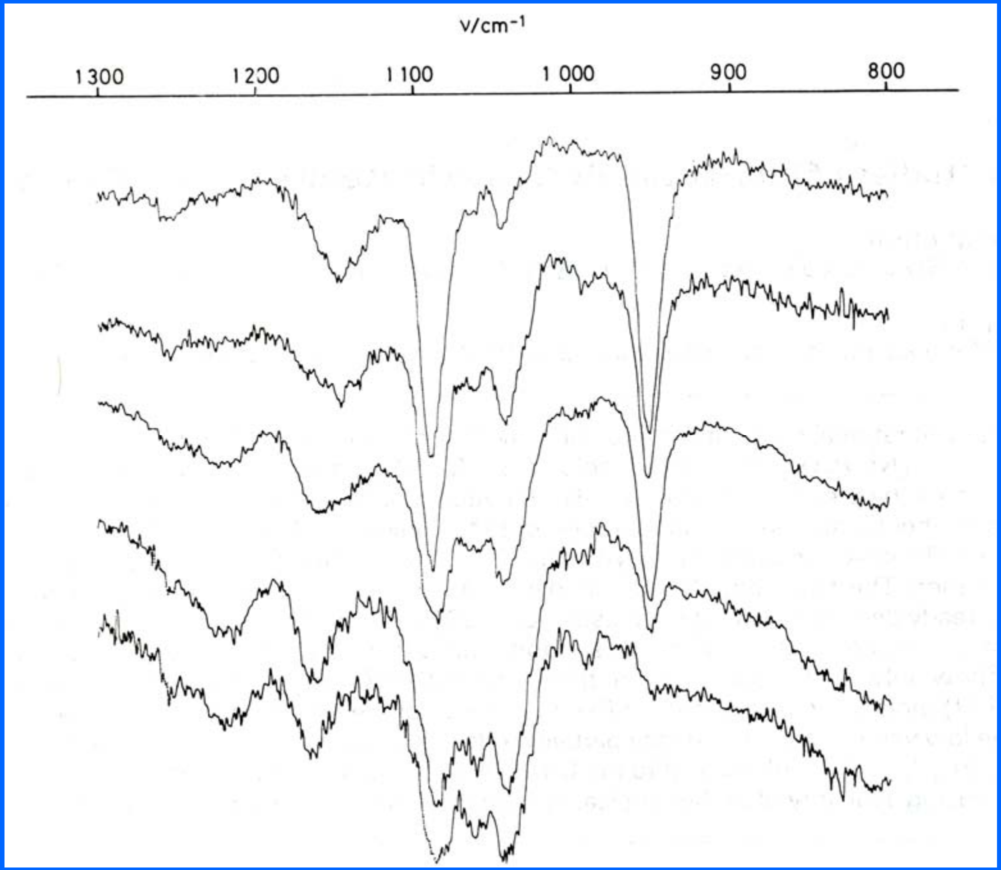




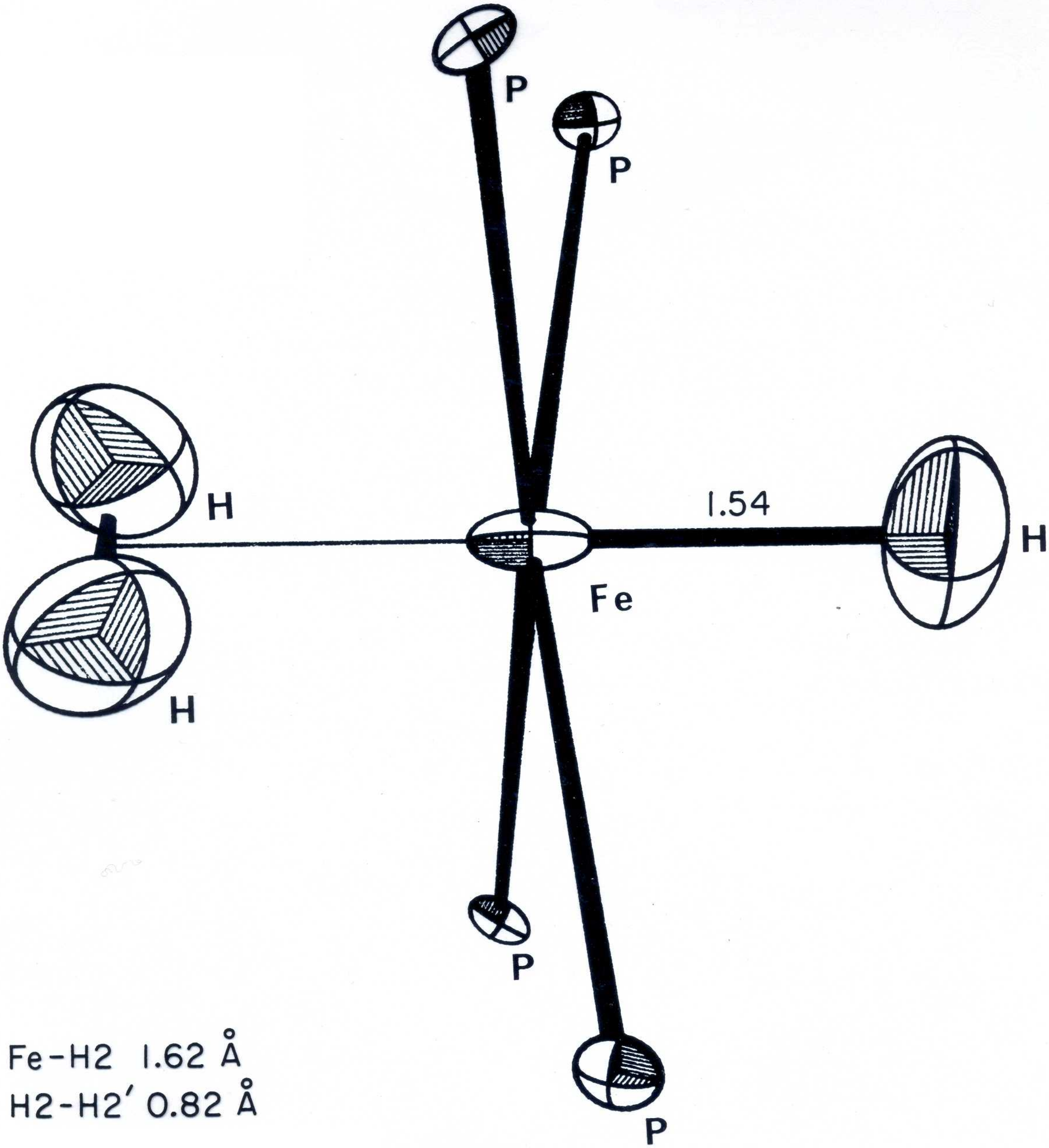
INS vs. I.R. Spectra of $K[Co_6(CO)_{15}H]$ in CsI







T = 110K



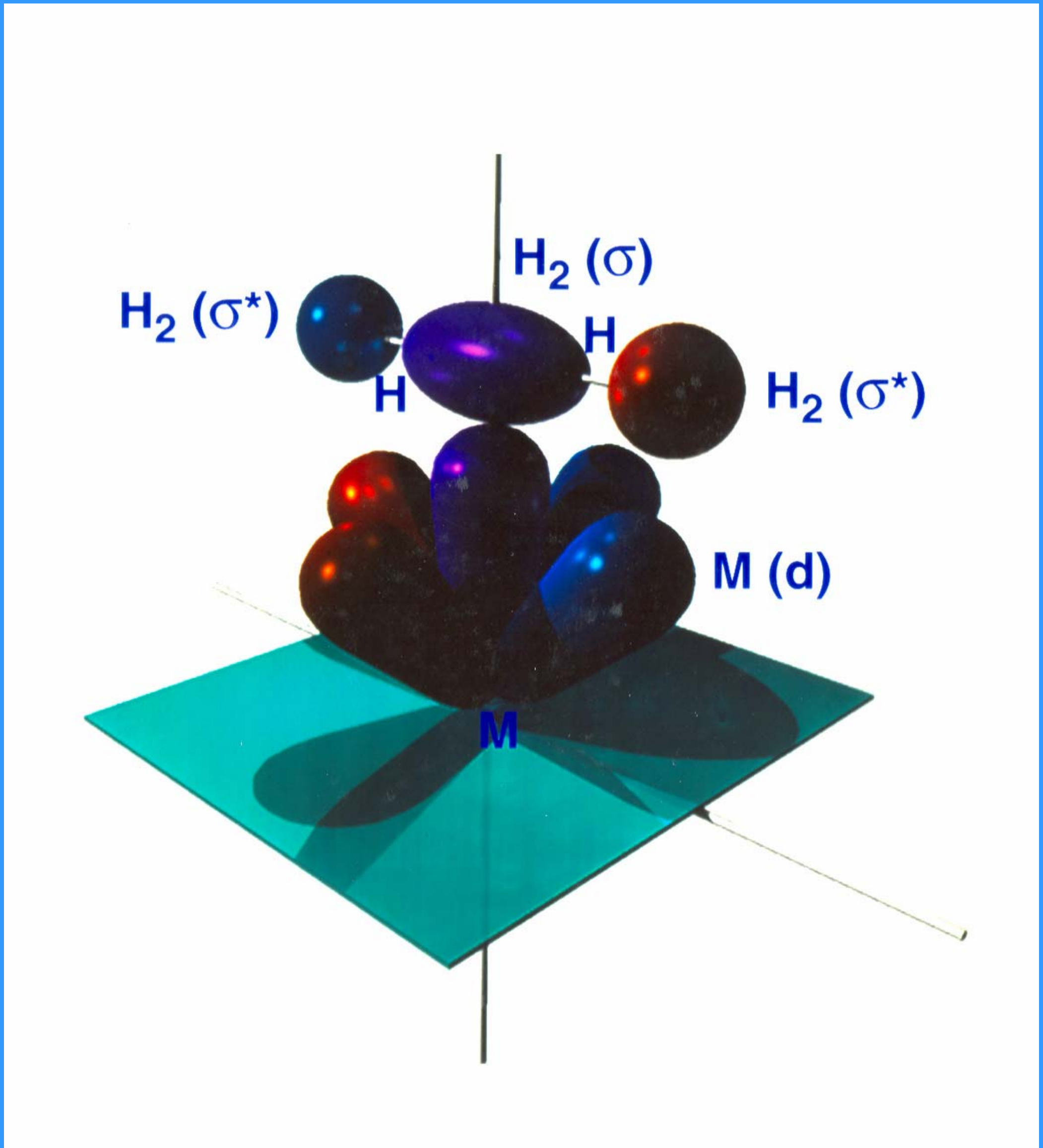
Fe-H2 1.62 Å
H2-H2′ 0.82 Å

$[Fe(dppe)_2(\eta^2\text{-}H_2)(H)]^+$

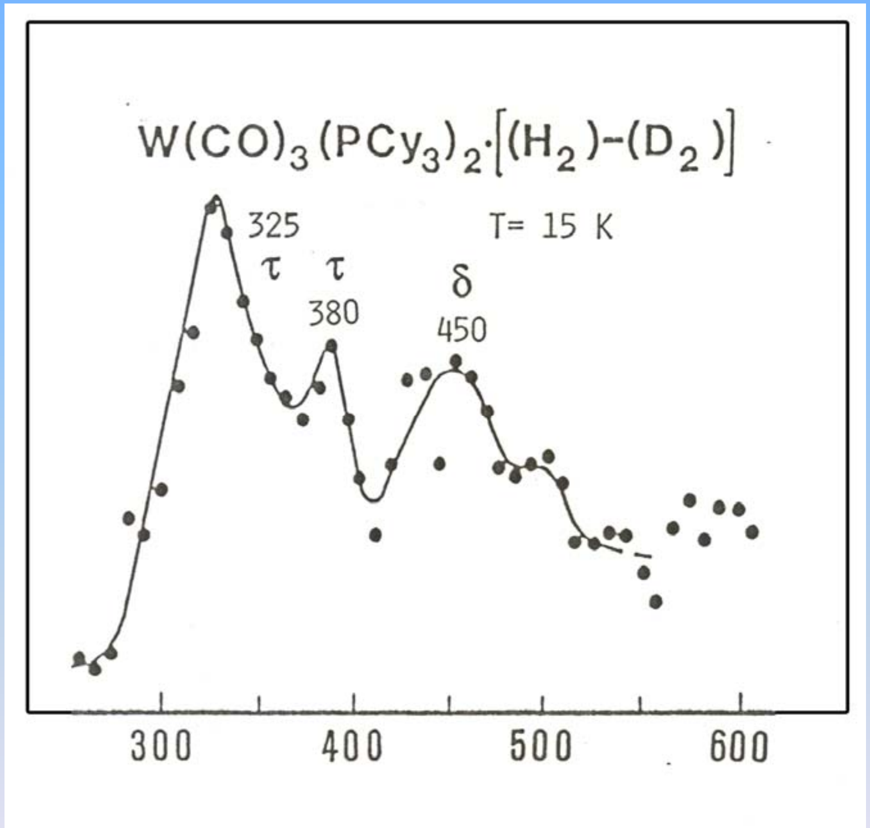
H-H Bond Lengths (Neutron Diffraction) and Coupling Constants (NMR).

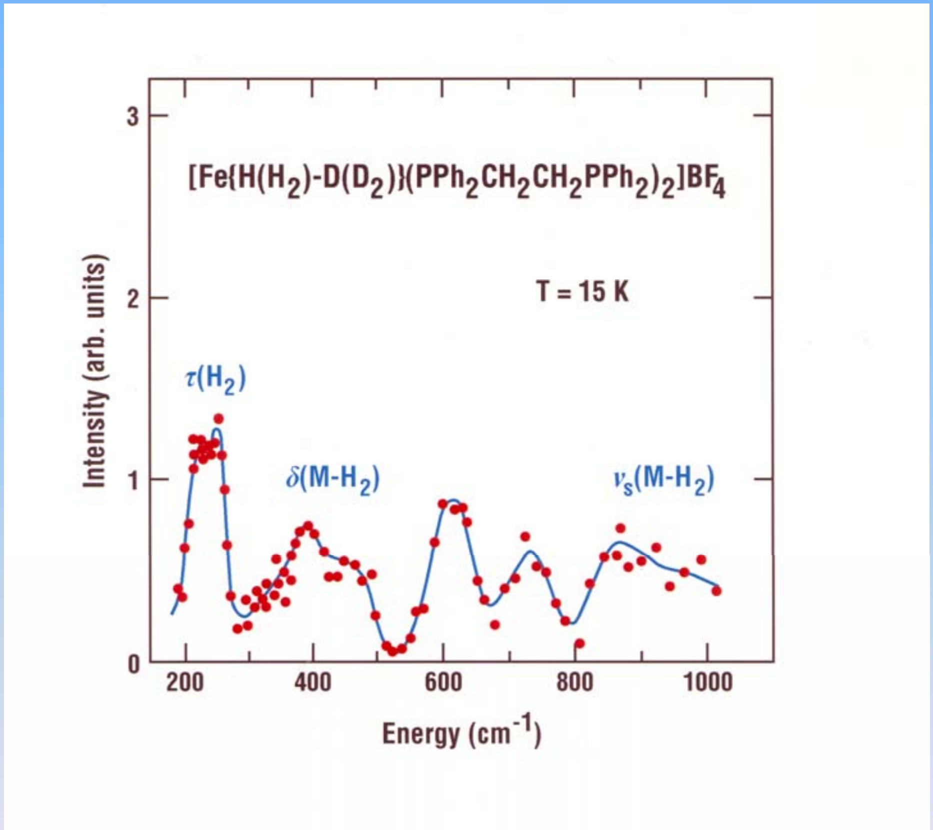
Compound	H-H (Å)	$J_{(HD)}$ (Hz)
$W(CO)_3(P\,^iPr_3)_2(H_2)$	0.82 (1)	34
$[Fe(dppe)_2(H)(H_2)]^+$	0.82 (2)	32.5
$[Os(dppe)_2(H)(H_2)]^+$	0.79 (2)	26.5
$[Rucp^*(dppm)_2(H_2)]^+$	1.08 (3)	20.9

M-(η^2-H_2) Bonding

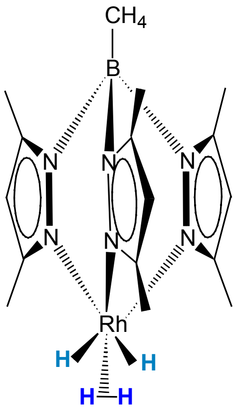


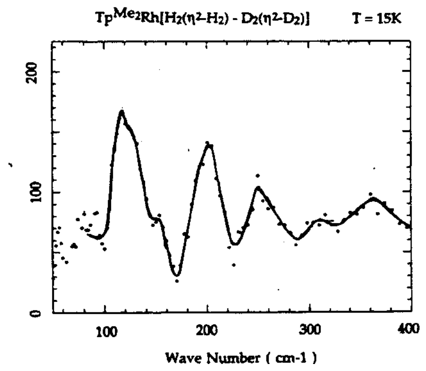
INS Spectra of M-(H_2) Complexes

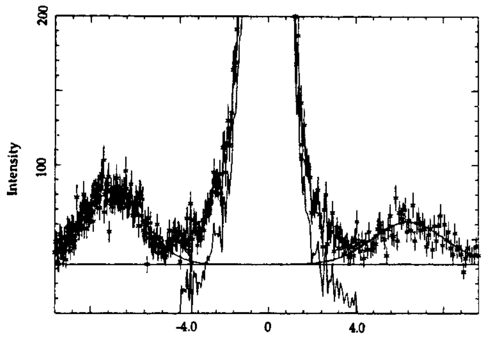




Tunnelling Frequencies, Rotational Transitions and Barrier Heights in $\{Tp^{3,5\text{-}Me}\}Rh(H)_2(H_2)$







$$\left[-B\left(\frac{\partial^2}{\partial\phi^2}\right)+\sum_{2n}V_n(1-\cos n\phi)\right]\Psi = E\Psi$$

B = 49.7 cm-1 $\quad$ $d_{(H\text{-}H)}$ = 0.81Å $\quad$ V_2 = 1.1

ω (cm^{-1})	τ_{calc} (cm^{-1})	τ_{obs} (cm^{-1})
6.7(5)	118, 126	
	194	188
	203	255

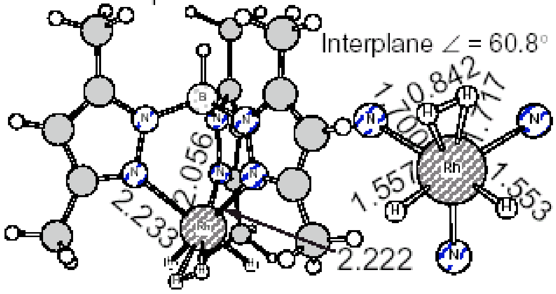
B = 37.1 cm-1 $\quad$ $d_{(H\text{-}H)}$ = 0.94Å $\quad$ V_2 = 0.68

V_2 = 0.60 V_4 = 0.26

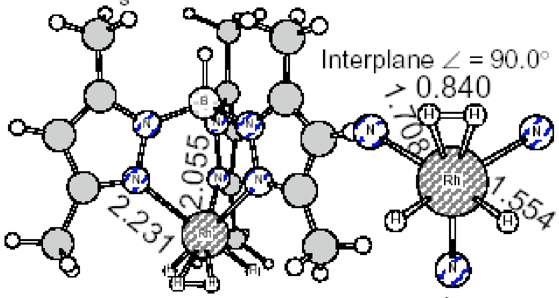
ω (cm^{-1})	τ_{calc} (cm^{-1})	τ_{obs} (cm^{-1})	
		V_2	$V_2 + V_4$
6.7(5)	118, **126**	121	**124**
	194	180	**195**
	203	219	**204**

B3LYP Calculated Structures for {$Tp^{3,5\text{-}Me}$}$Rh(H)_2(H_2)$

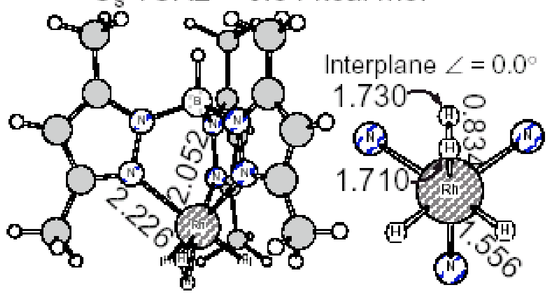
C_1 MIN 0.0 kcal mol^{-1}



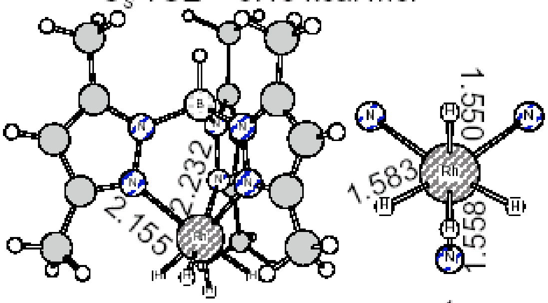
C_s TSR1 +0.04 kcal mol^{-1}



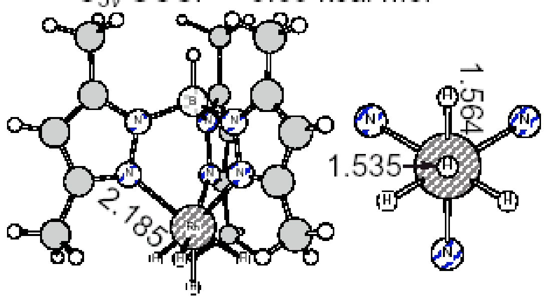
C_s TSR2 +0.34 kcal mol^{-1}



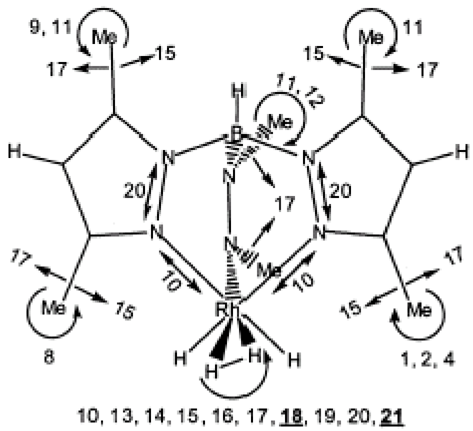
C_s TSE +6.18 kcal mol^{-1}



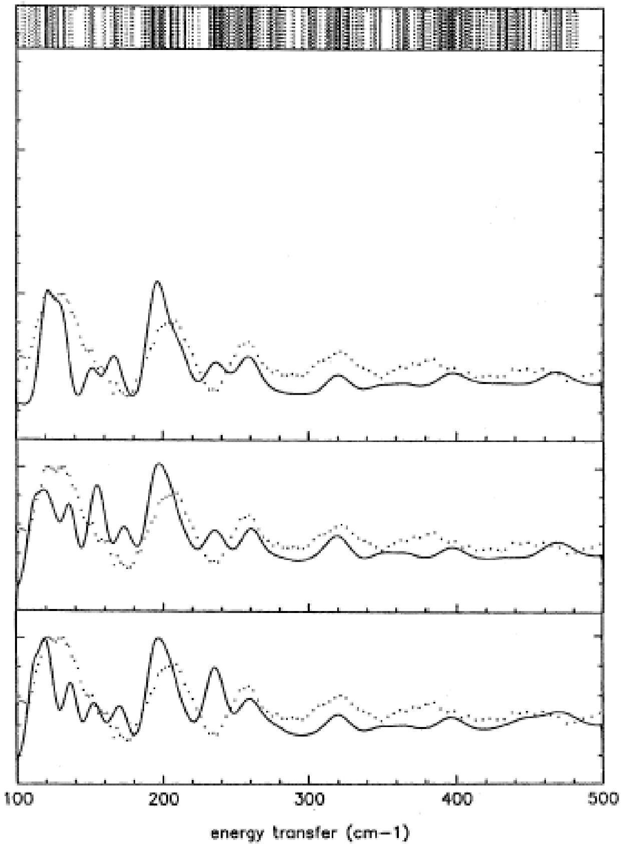
C_{3v} SOSP +9.89 kcal mol^{-1}



The INS Vibrational Spectrum of $Tp^{3,5\text{-}Me}Rh(H)_2(H_2)$

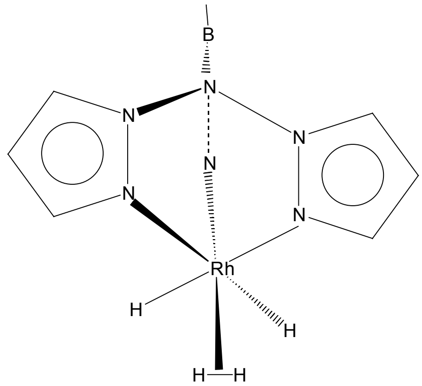


Several of the first 27 B3LYP vibrational modes



Calculated and observed INS spectra for the C_1(Min), C_s (TSR1) and C_s(TSR2) structures.

The INS Vibrational Spectrum of $\{Tp^{3,5-Me}\}Rh(H)_2(H_2)$



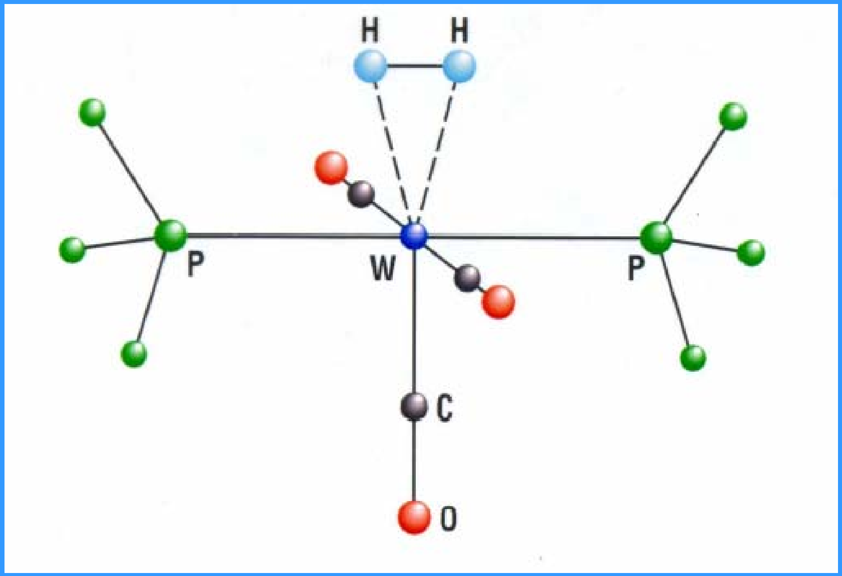
Rotational potential parameters and transitions

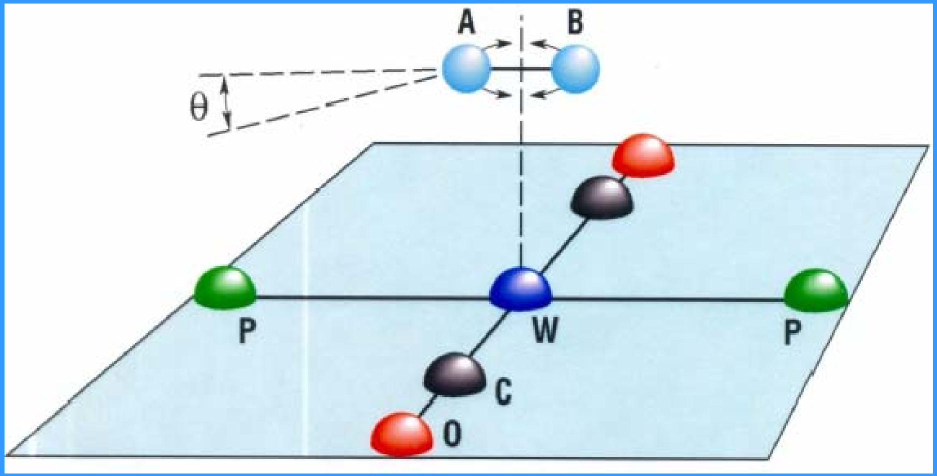
	d(HH) (Å)	V_2 (kcal mol^{-1})	V_4 (kcal mol^{-1})	ω_t	Torsional transitions (cm^{-1})	
Experimental (Ref. [5])	–			6.7(5)	118, 126	194, 203
V adj. (Ref. [5])	0.94	0.6	0.26	6.7	123	195, 204
Fit 1, using $d(HH)_{B3LYP}$	0.842	1.1	−0.4	6.7	150	195
Fit 2, using $d(HH)_{B3LYP}$	0.842	0.44	1.5	6.7	128	176
Fit 1, using $d(HH)_{BP86}$	0.898	0.78	0	6.7	138	199
Fit 2, using $d(HH)_{BP86}$	0.898	0.92	−0.46	6.7	122	160
Calculated V B3LYP	0.842	0.35	−0.1	23	80	202
Calculated $V_{scaled\text{-}B3LYP}$	0.842	1.05	0.28	6.7	157	207
Calculated V BP86	0.898	0.01	1.49	26, 30	67	321
Calculated $V_{scaled\text{-}BP86}$	0.898	0.04	4.4	6.7	13	732

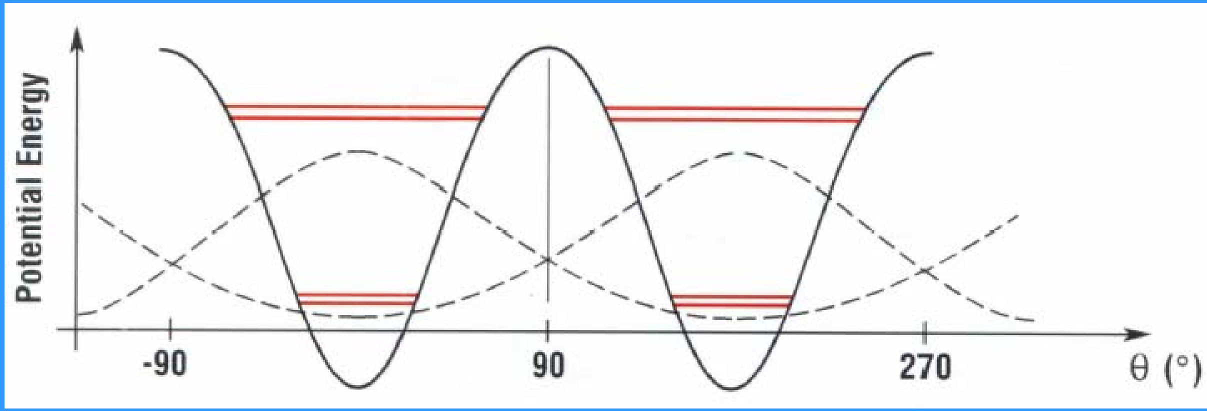
$\tau_{(H\text{-}H)}$	200 cm^{-1} (210 cm^{-1} B3LYP)	125 and 200 cm^{-1}
$d_{(H\text{-}H)}$	0.842 -. 0.898 Å (B3LYP)	0.94 Å
ΔE_{rot}	~ 1 kcal mol^{-1}	

INS spectra result from a quantum averaged ground state encompassing, at least two, low energy structures.

Non-classical Hydrides and Rotational Tunnelling Spectroscopy

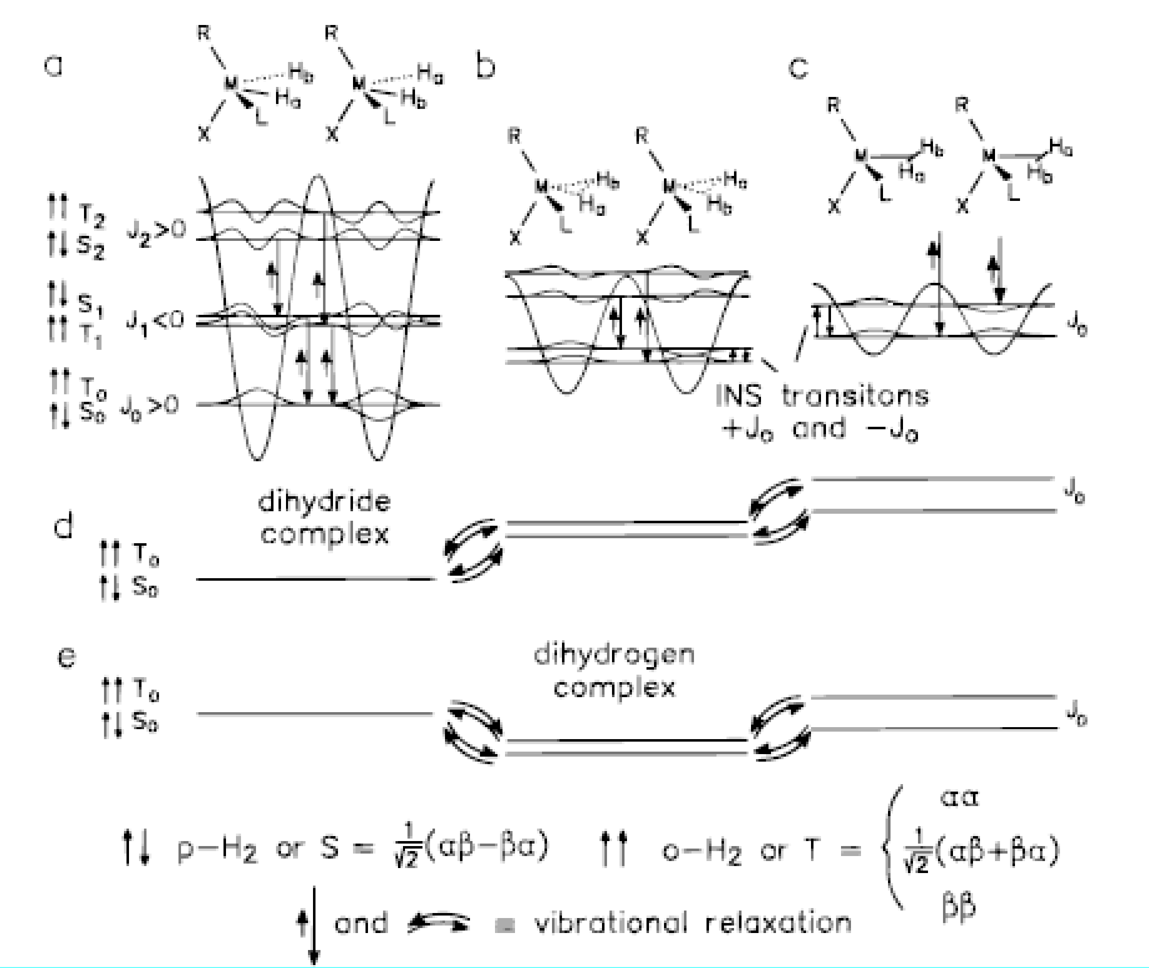




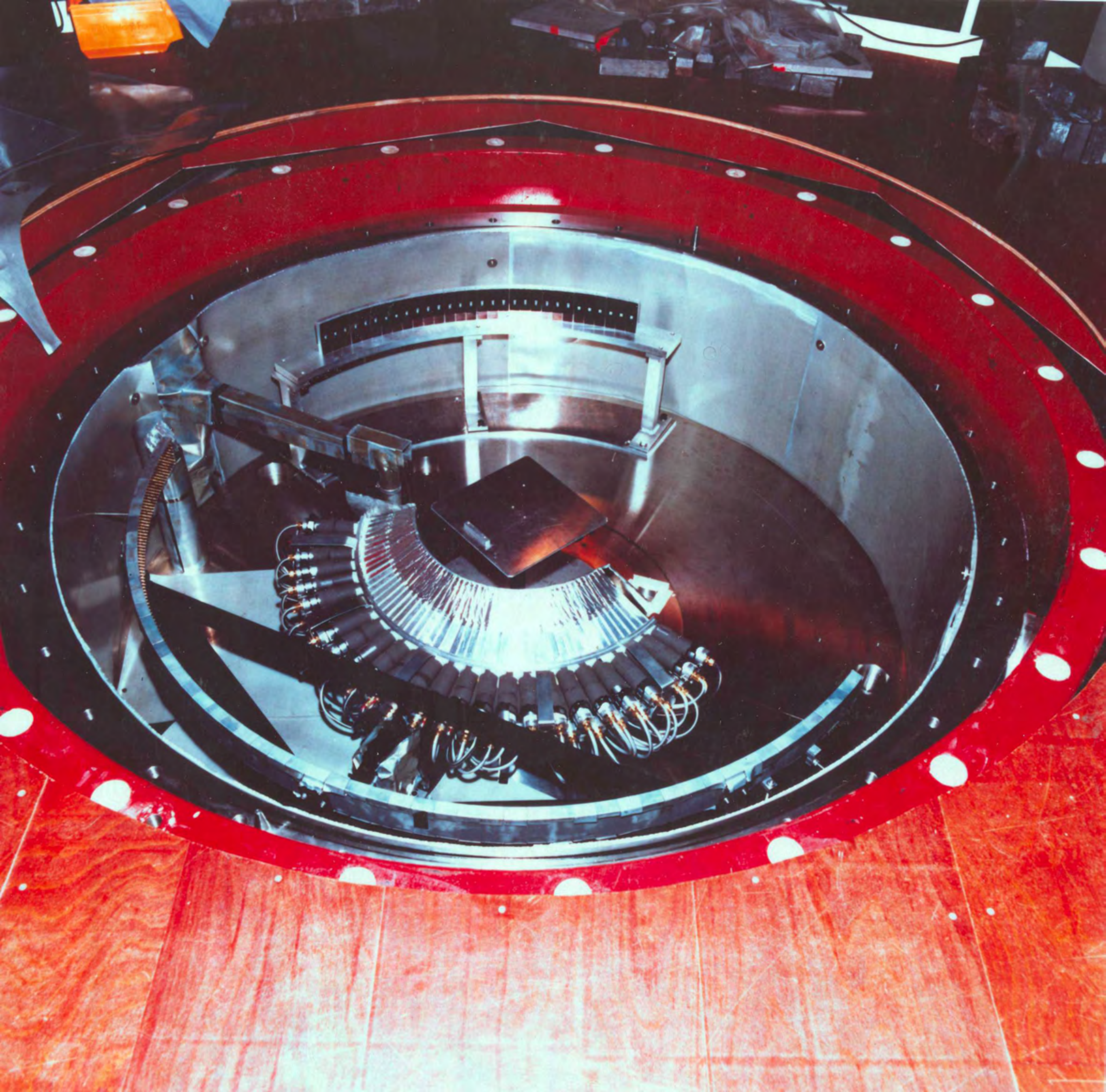


Energy Eigenstates of the H_a– H_b System in a Two-fold Potential

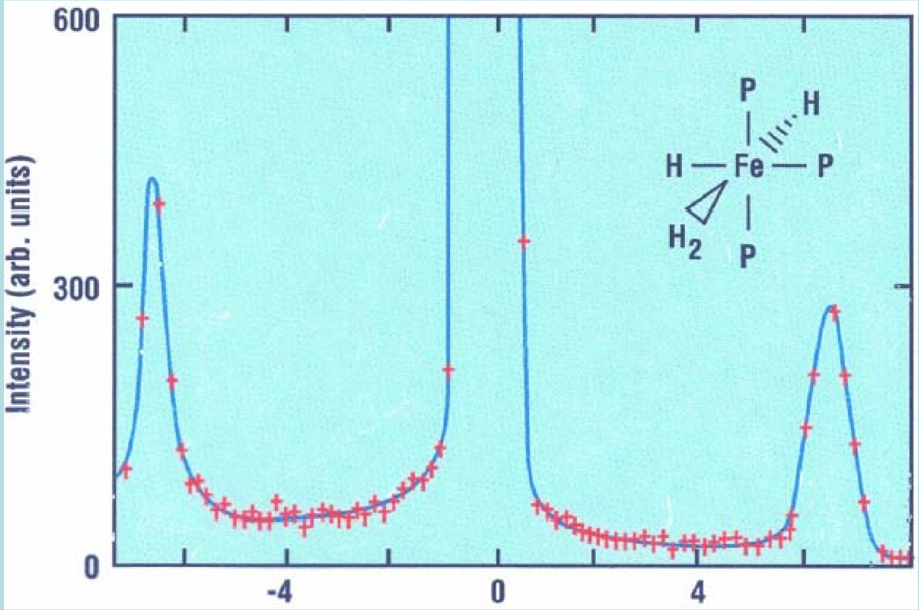
(one dimensional rotation)

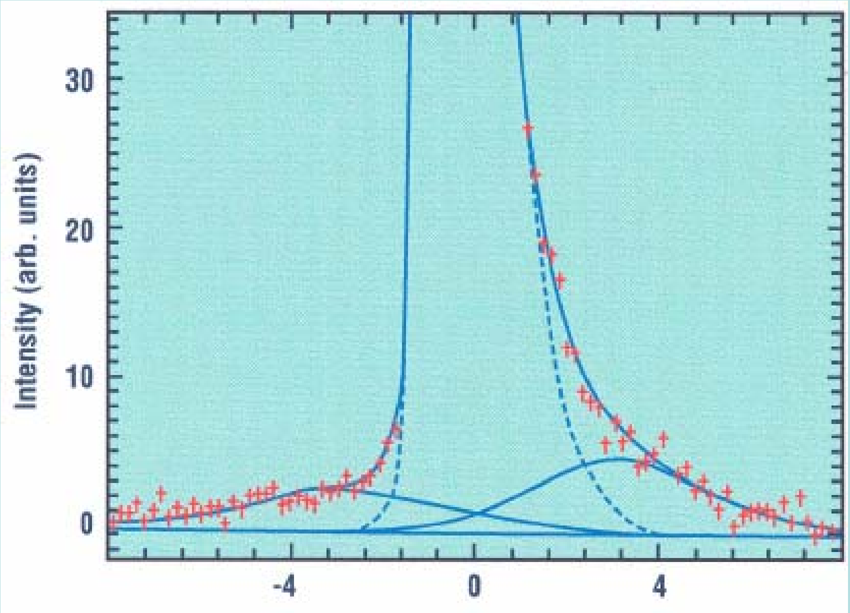


H. Limbach & al. *JACS* **1998**, *120*, 7929



Rotational Tunnelling in $[Fe(H)_2(H_2)L_3]$ and $[Ru(H_2)(H)(dppe)_2]^+$



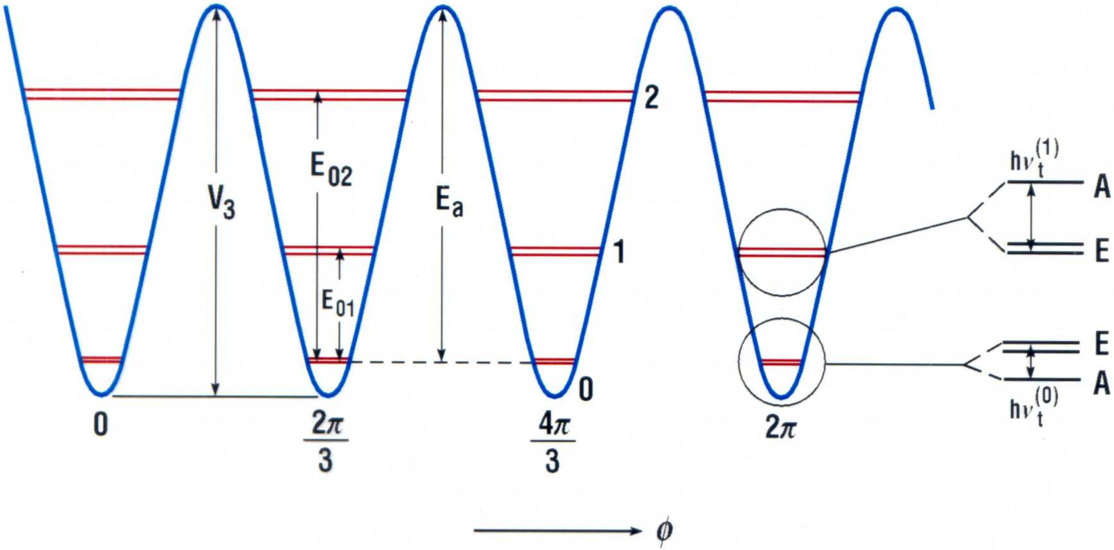


Energy Transfer (cm^{-1})

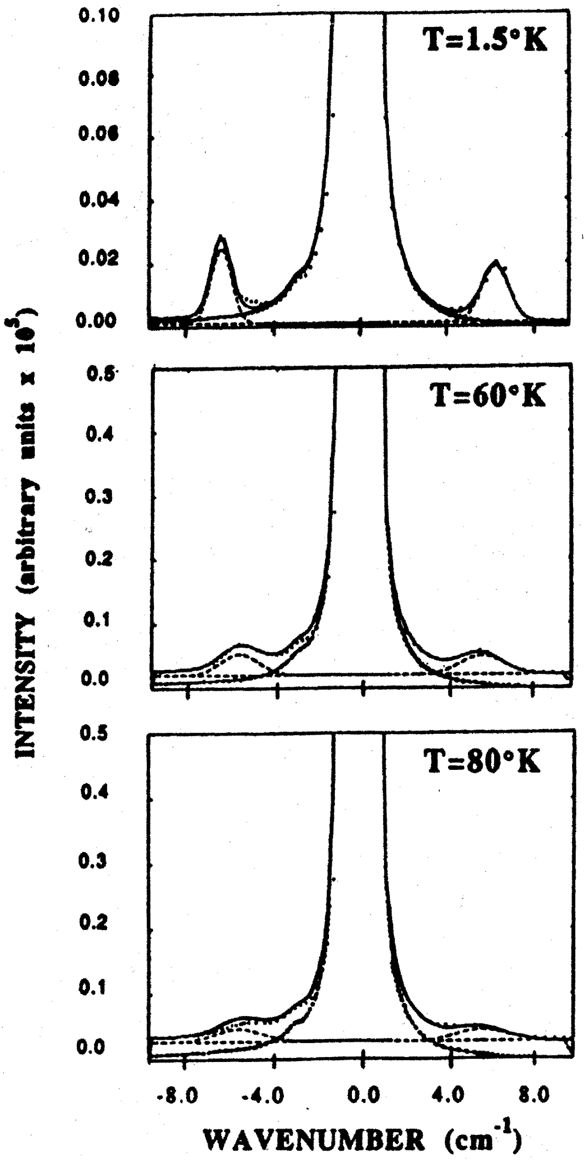
VIBRATIONAL FREQUENCIES and TUNNEL SPLITTINGS for M-H_2 COMPLEXES

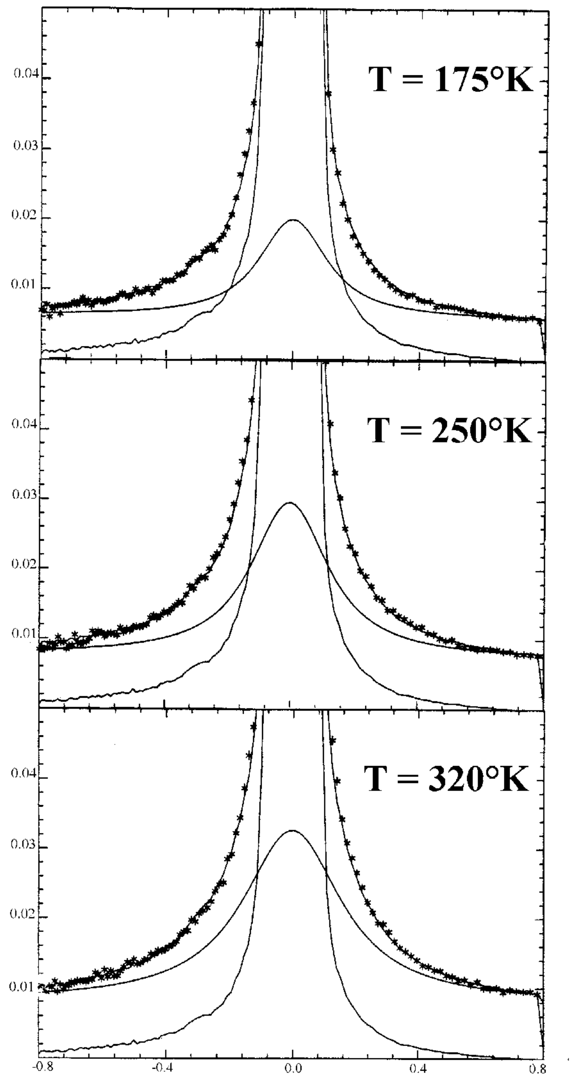
Compound	ν(H-H) [cm^{-1}] (IR)	τ(H-H) [cm^{-1}]	ω_t [cm^{-1}]	V_t [kcal/m]
$W(CO)_3(P\,^iPr_3)_2(H)_2$	2695	370 - 340	0.73	2.4
$W(CO)_3(PCy_3)_2(H)_2$	2690	380 - 325	0.89	2.2
$[Fe(dppe)_2(H)(H_2)]^+$	2973	255 - 225	2.10	1.8
$[Ru(dppe)_2(H)(H_2)]^+$			3.2	1.0
$[Fe(PR'R_2)_3(H)_2(H_2)]$	2380	252 - 170	6.40	1.1
$[Fe(PPPP)(H)(H_2)]^+$		276 - 259	1.15	1.9
$[Ru(PPPP)(H)(H_2)]^+$		225 - 184	2.58	1.6
$IrBr(P\,^iPr_3)_2(H)_2(H_2)$			18.9	0.53
$IrI(P\,^iPr_3)_2(H)_2(H_2)$			9.8	0.98
$Rh(TpMe_2)(H)_2(H_2)$	2238	203 -118	6.72	0.9

A Schematic Diagram of the Energy Levels of a Methyl Rotor In a Three-Fold Potential



$FeH_2(H_2)(PEtPh_2)_3$. Temperature Dependence of the INS Spectra: *from Tunnelling to QENS*

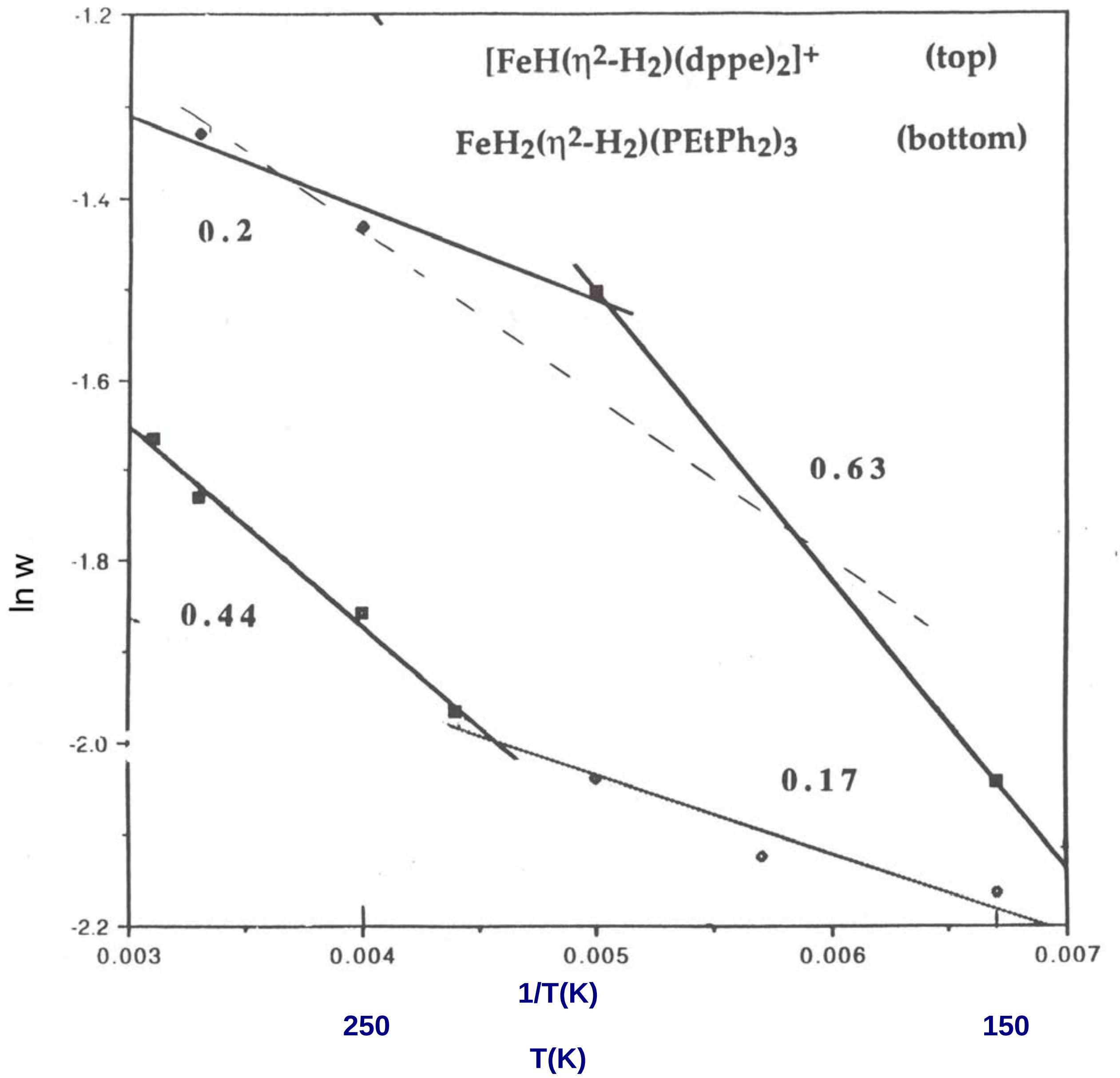




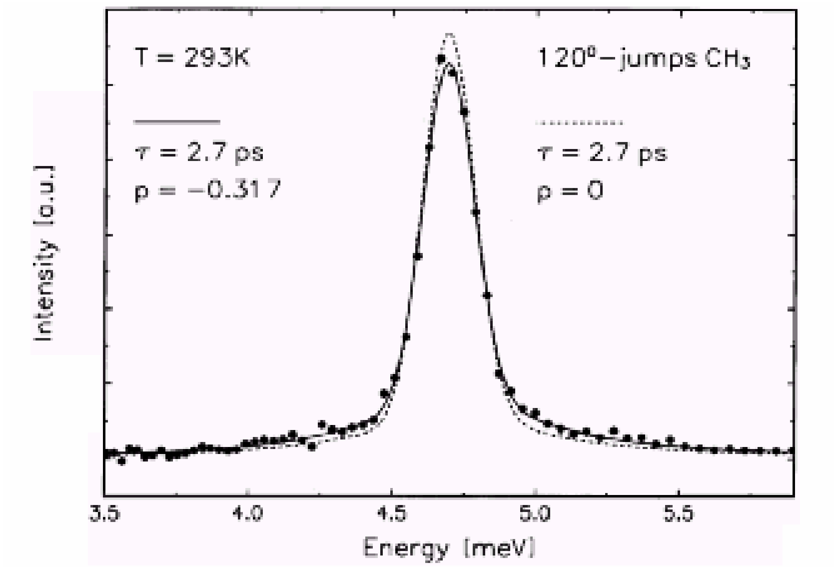
$$\boxed{\Gamma(\mathrm{T}) = \Gamma_0 e^{-\left(\frac{\mathrm{E}^*(\Gamma)}{\mathrm{kT}}\right)}}$$

$$\Delta\left(\hbar\omega(\mathrm{T})\right) = \hbar\omega_0 e^{-\left(\frac{\mathrm{E}(\Gamma)}{\mathrm{kT}}\right)}$$

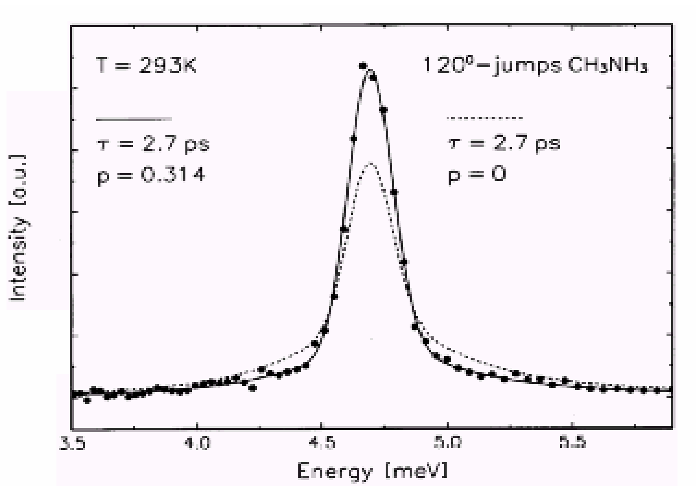
Activation Energies (*kcal/mol*) for the Dihydrogen Rotation in Fe(η-H_2) Complexes from QENS



QENS Study of the Cation $(CH_3NH_3)^+$



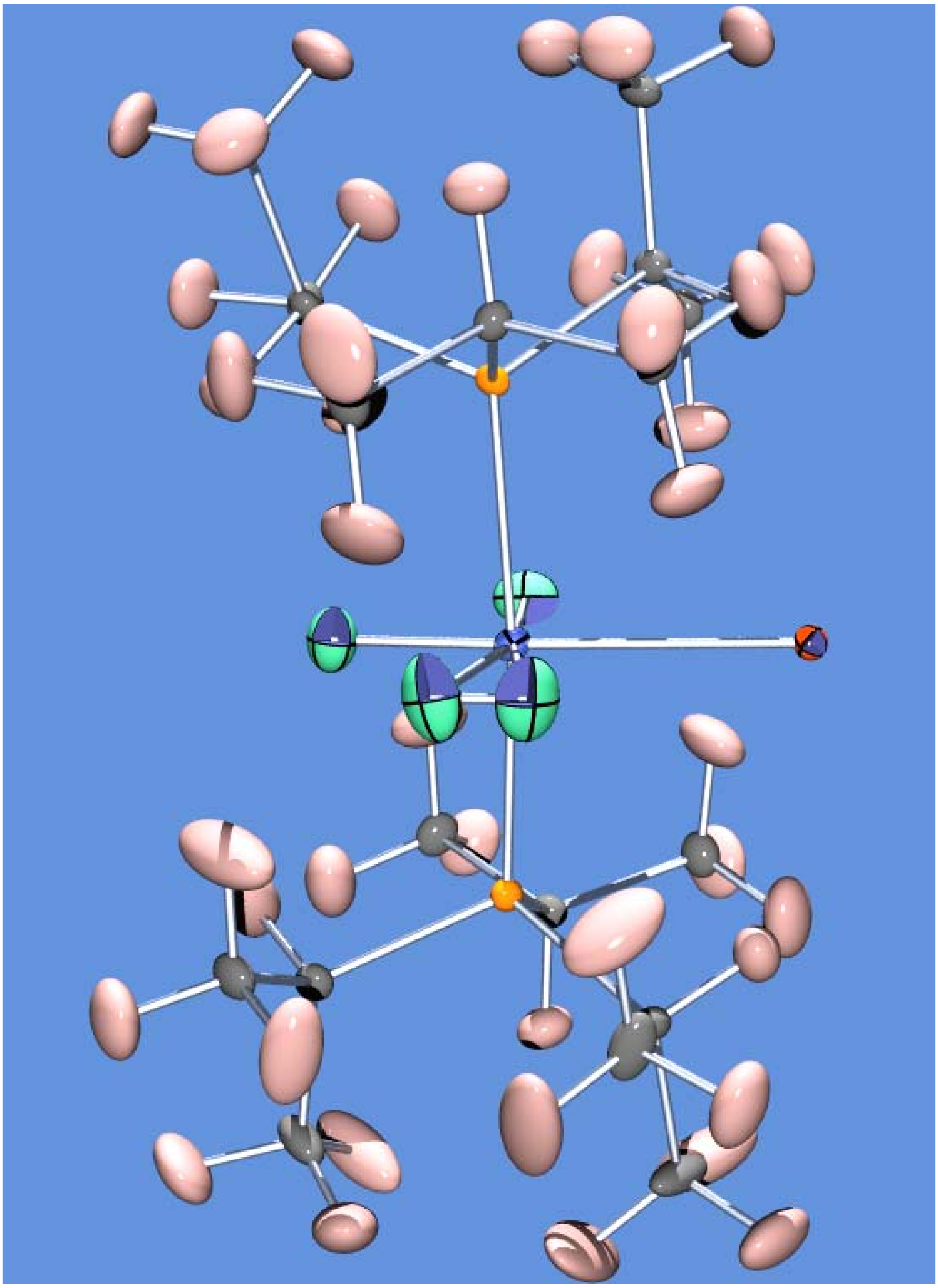
Uniaxial 120° jumps of all CH_3 groups: rotation around the C-N axis



Rotation of all CH_3NH_3 as a whole around the C-N axis

R. Jakubas & al. Physica *B 241- 243,* 481 (1998)

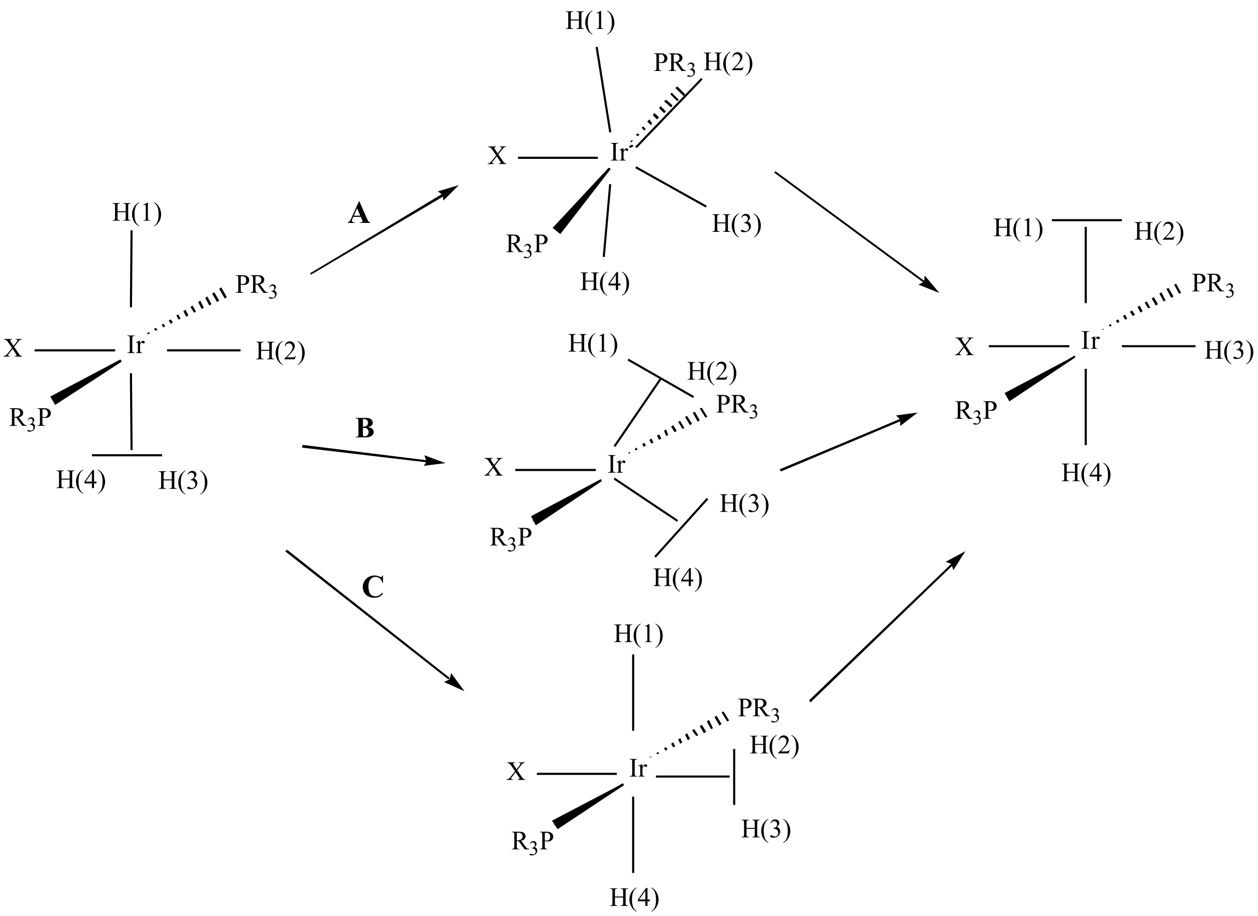
$Ir(H_2)(H)_2Br(P^iPr3)_2$



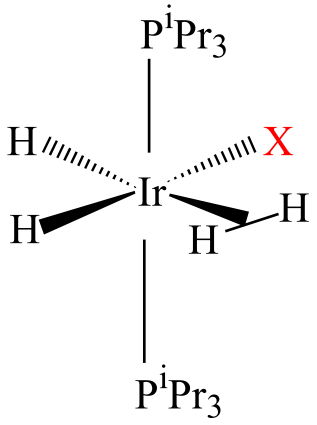
H – H 0.819(8) Å

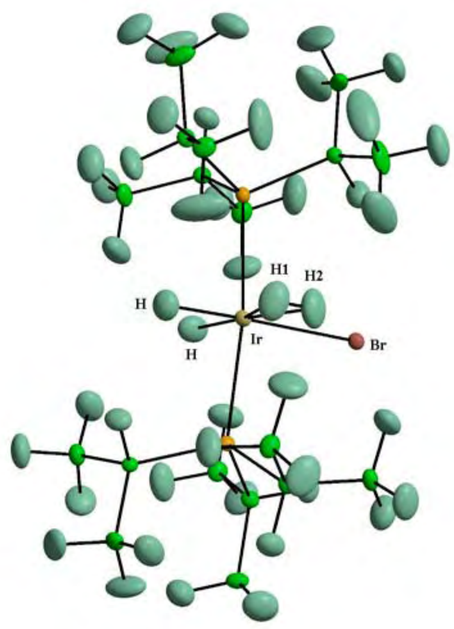
Ir – H_t 1.585 (5) Å
Ir – H_t 1.602 (6) Å *trans* to Br

Dihydrogen-Hydride Exchange in $IrX(H)_2(H_2)(PR_3)_2$:
Possible Reaction-Mechanisms.



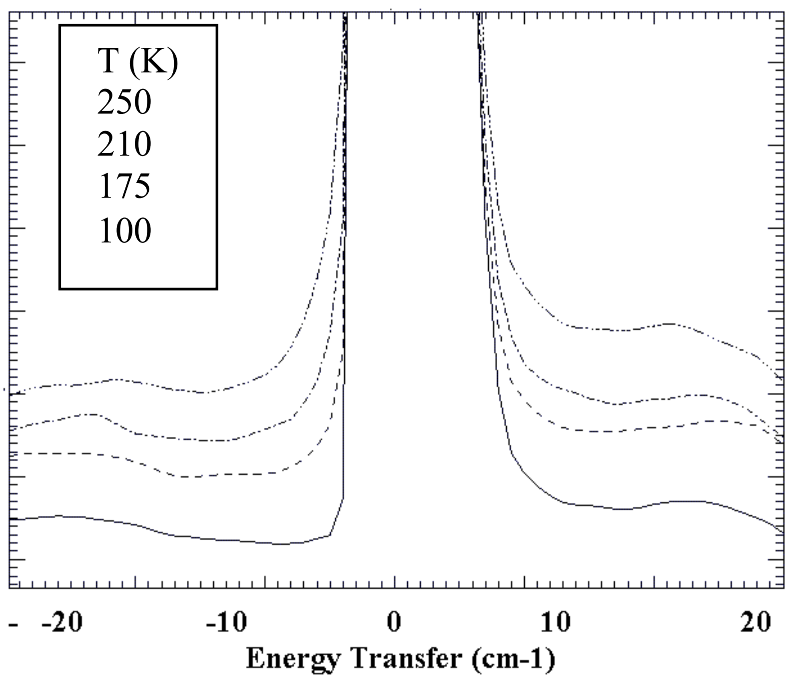
$(P\,^{i}Pr_3)_2IrX(H)_2(H_2)$ Complexes:
Effect of the *cis*-Halide Ligand

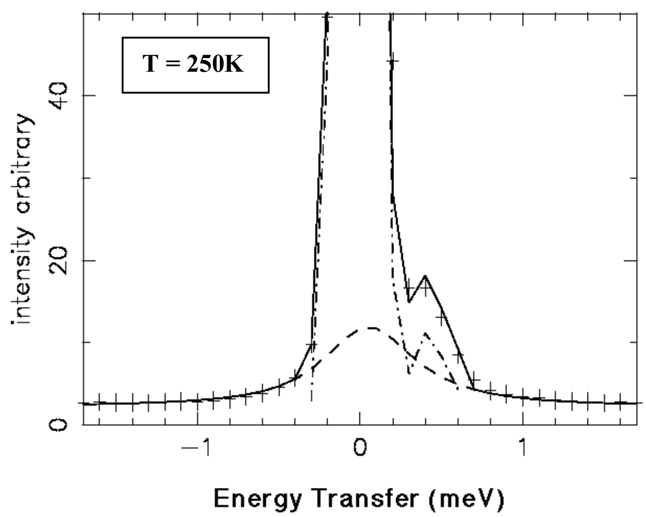




	X = Cl	X = Br	X = I
Rotat. tunnelling freq. (ω, cm^{-1})	**20**	**19**	**6**
Rotat. Barrier **V_2^{exp}** (kcal/mole)	**0.51(3)**	**0.48(3)**	**1.00(4)**
Rotat. Barrier **V^{calc}** (PMe_3 / PH_3 kcal/mole)	**0.37 (2.04)**	**0.42 (2.11)**	**0.66 (2.32)**
$d_{(H\text{-}H)exp}$ (Å)	*0.78* (INS)	**0.819(8)**	**0.856(9)**
$d_{(H\text{-}H)calc}$	0.853	0.857	0.862

QENS in $IrCl(H)_2(H_2)(PPr^i_3)_2$

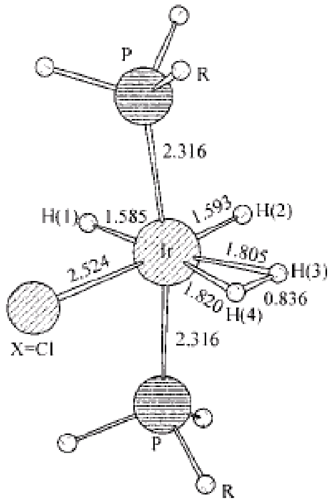




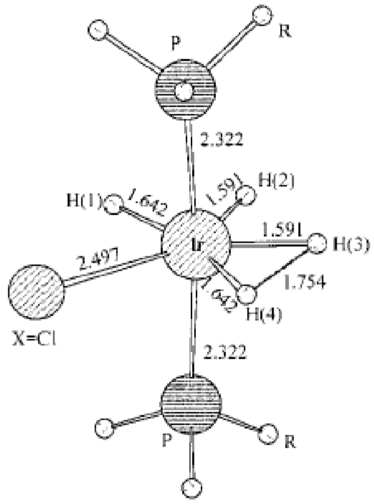
$$\Gamma(T) = \Gamma_0 e^{-\left(\frac{E_a(\Gamma)}{kT}\right)}$$

$\boxed{\Delta E_a = 1.5(2)\ \text{kcal/mol}}$

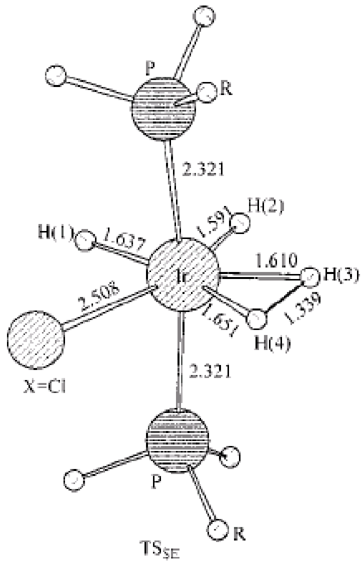
B3LYP/BS4 Optimized Structures and Energies for the H_2/H Exchange in $IrCl(H)_2(H_2)(PPr^i_3)_2$



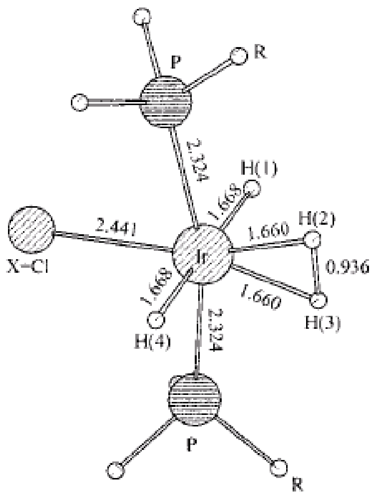
Reactant



Intermediate



TS_{SE}

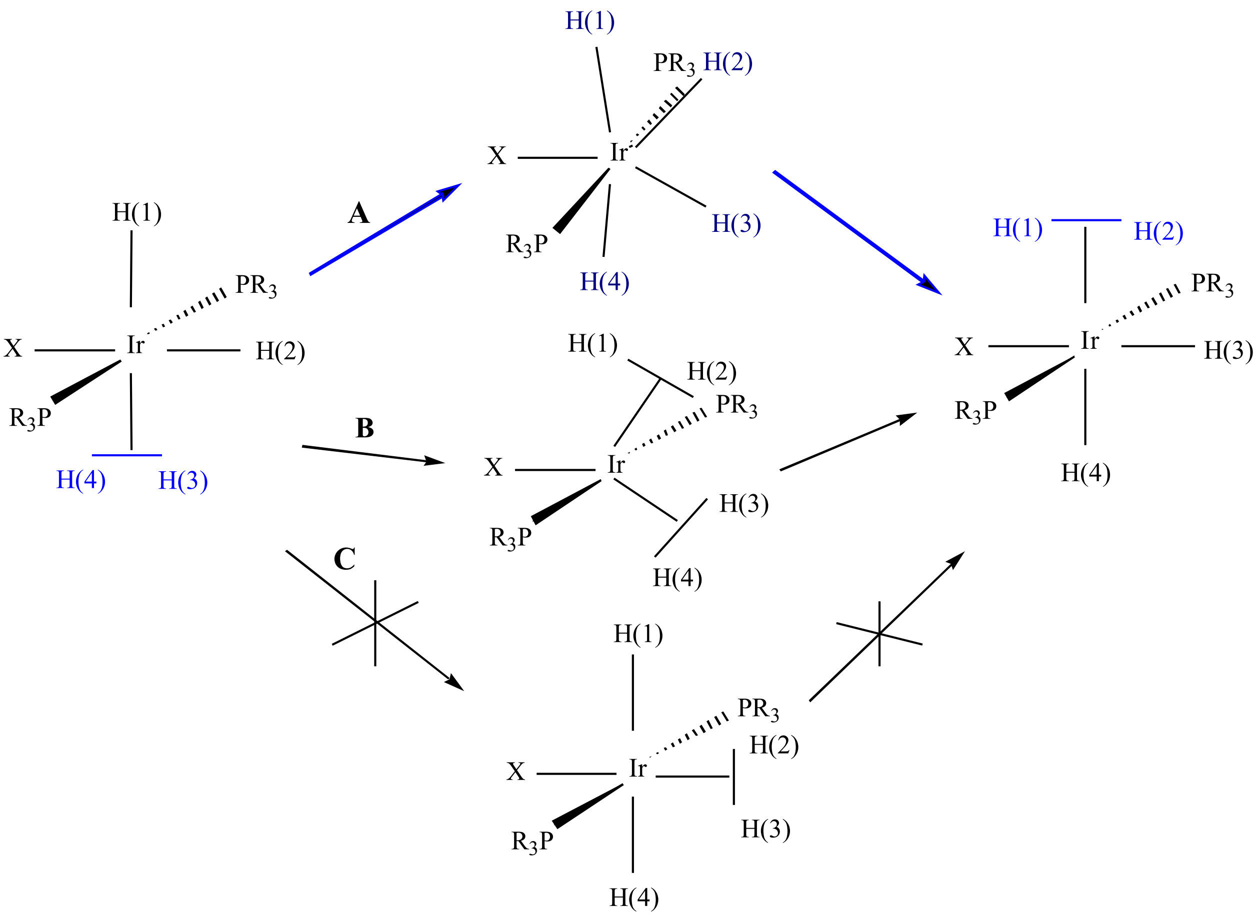


TS_{HE}

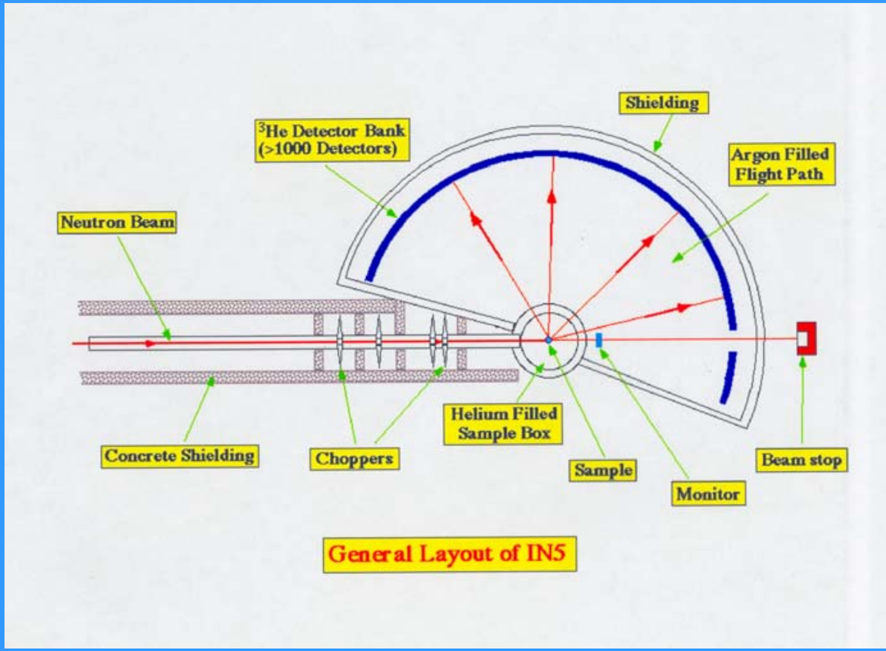
$\Delta E^*_a = 1.5(2)$ **$\Delta E_{int} = 1.40$** **$\Delta E^*_{TS} = 1.87$**

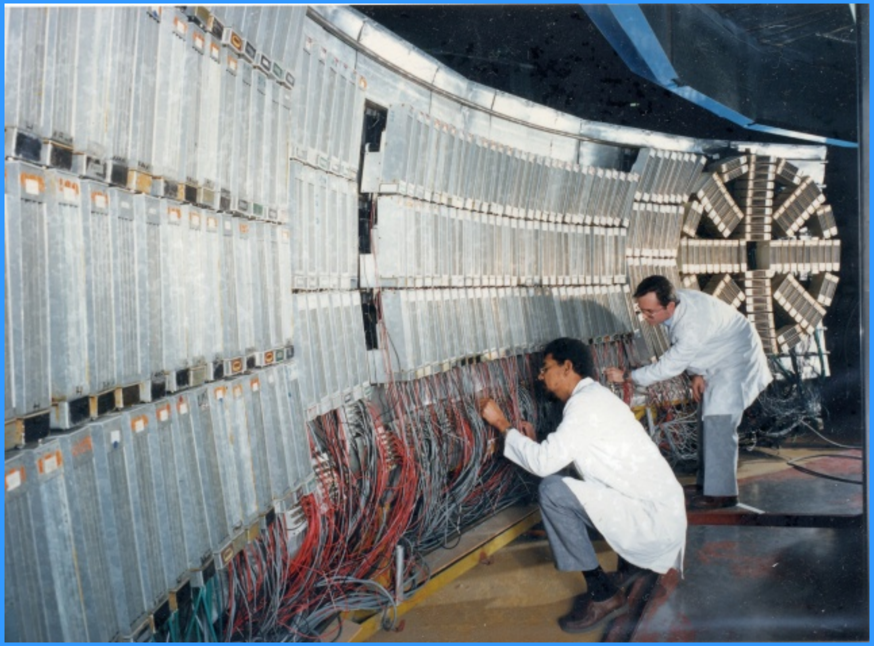
$E \equiv [kcal][mol]^{-1}$

Dihydrogen-Hydride Exchange in $IrX(H)_2(H_2)(PR_3)_2$:
Possible Reaction-Paths.



The IN5 Spectrometer at ILL





...sooner or later you will end up

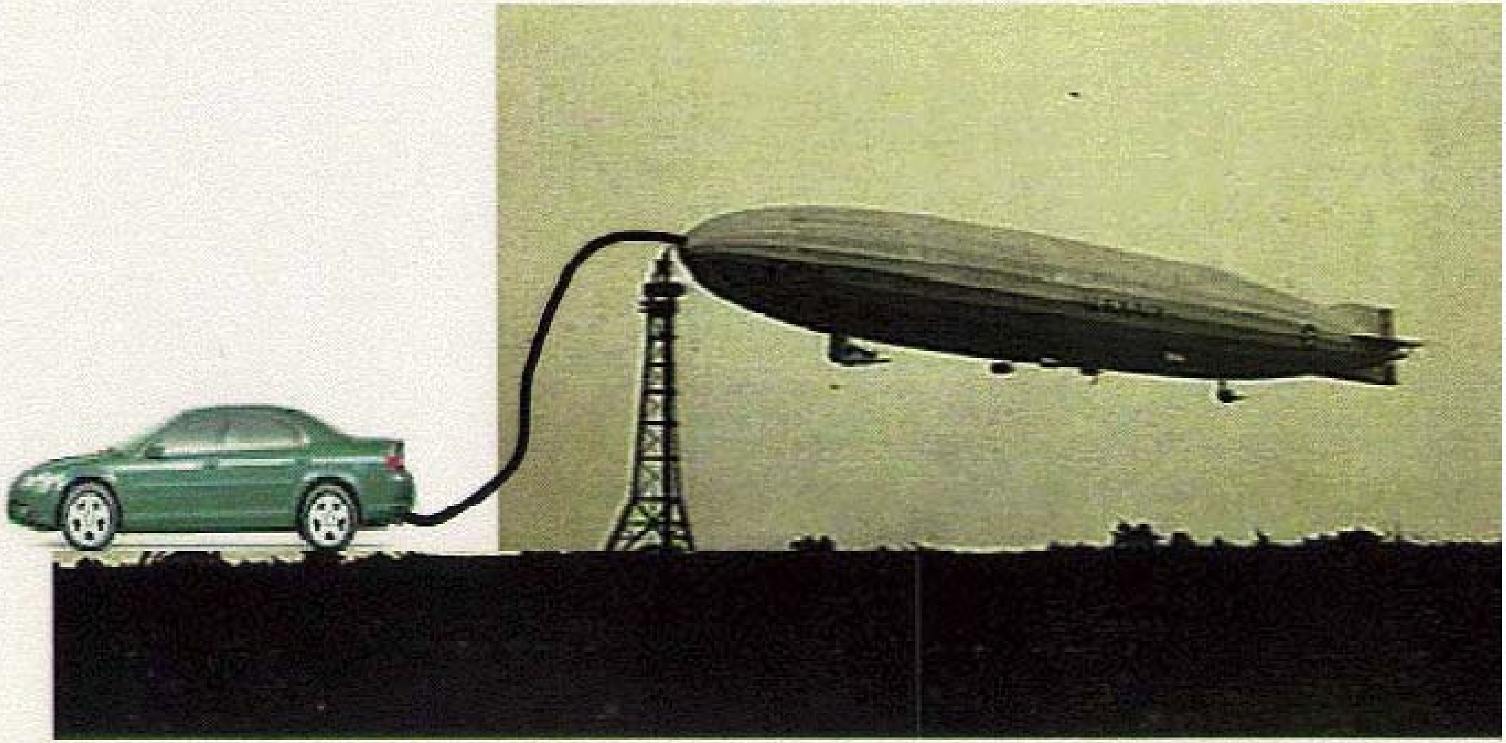
studying

the Hydrogen Storage

problem...

U.S. Department of Energy
Energy Efficiency and Renewable Energy

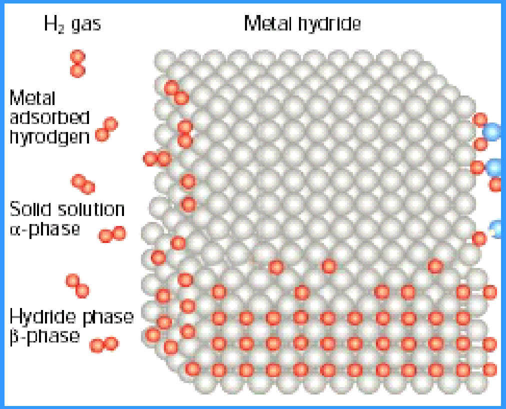
Proposed H_2 Storage Concept

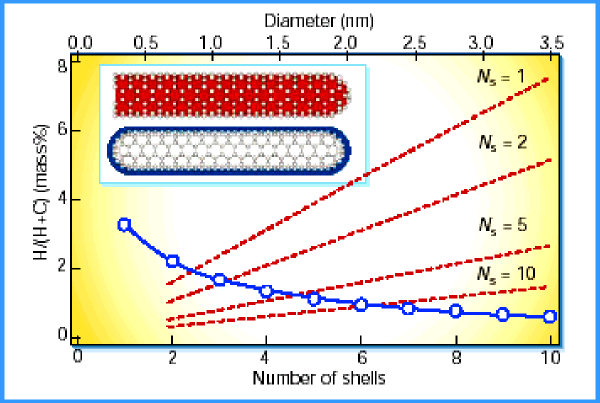


Proposed H_2 Storage Materials

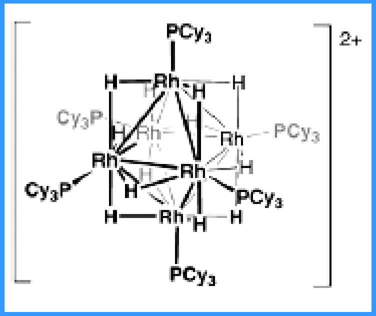
Mg_2NiH_4 $LaNi_5H_6$ $H_2(l)$ H_2 *(200 atm)*

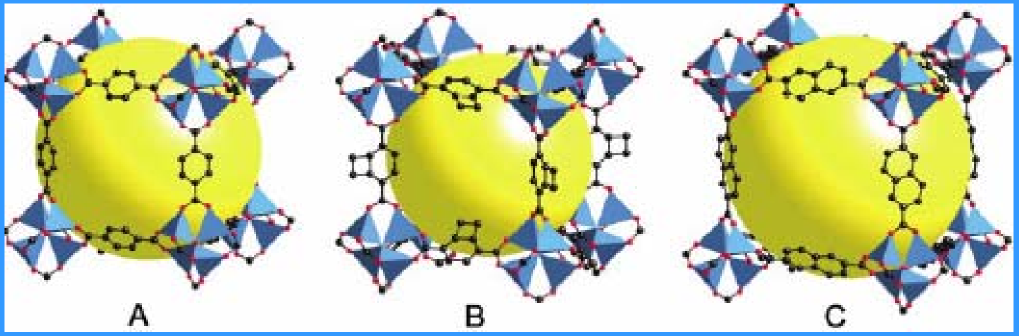
4Kg Hydrogen





$$2NaAlH_4 \rightleftarrows 2NaH + 2Al + 3H_2\uparrow$$





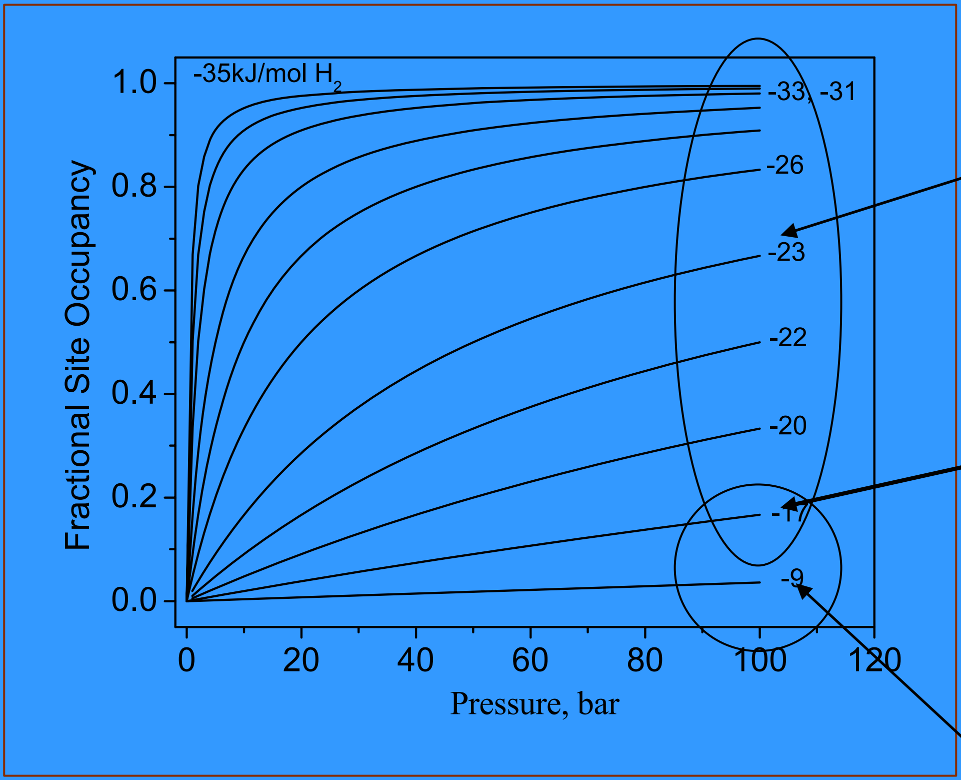
[Weller (2006)]

[Yaghi (2001)]

Parameters, Values and Methods

- Capacity >6% wt, 60kg H_2/m^3 at RT, P<100 bar. This includes the weight of all tank associated details and heat management system. : i.e. ~ 10% wt , at least, for the bare storage material itself.
- Thermodynamics and kinetics of the adsorption /desorption process. $-20 < Q_{st}(\Delta H) < -40$ kJ/mol H_2; $D_{chem} > 10^{-9} cm^2/s$
- Structural stability upon cycling/activation; Resistance against poisoning agents -H_2O, CO, CO2, N_2, etc. Cost and Environment safety
- To experimentally probe the interactions between H_2 and adsorption sites at the molecular level: Inelastic Neutron Scattering.

Expected Interactions and Associated Thermodynamics



Interstitial hydrides-$LaNi_5$, Non-classical hydrides: M-(η^2-H_2) complexes of Transition Metals

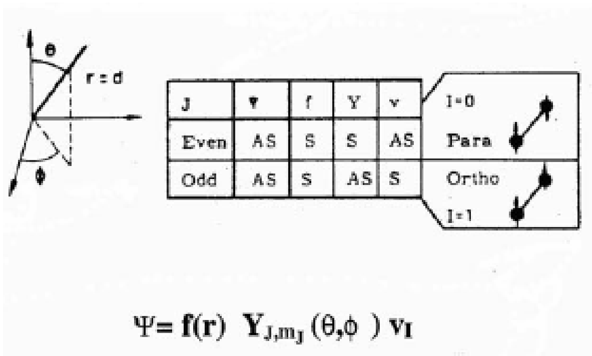
Very likely a combination of electronic and dispersive interactions. Most challenging to model and characterize. It was hoped that MOF's would fall here.

Van der Waals–a few kJ, electrostatic -<10 kJ/mol H_2

Graphite, activated carbons, Carbon Nanotubes, Na^+ , Li^+… -exchanged Zeolites

Rotational Energy Levels of the Hydrogen Molecule

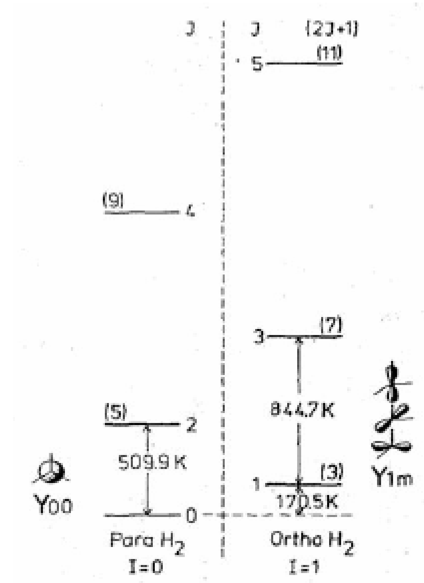
Symmetry Properties



Molecular wave function is AS with respect to particle exchange (rotation): fermions

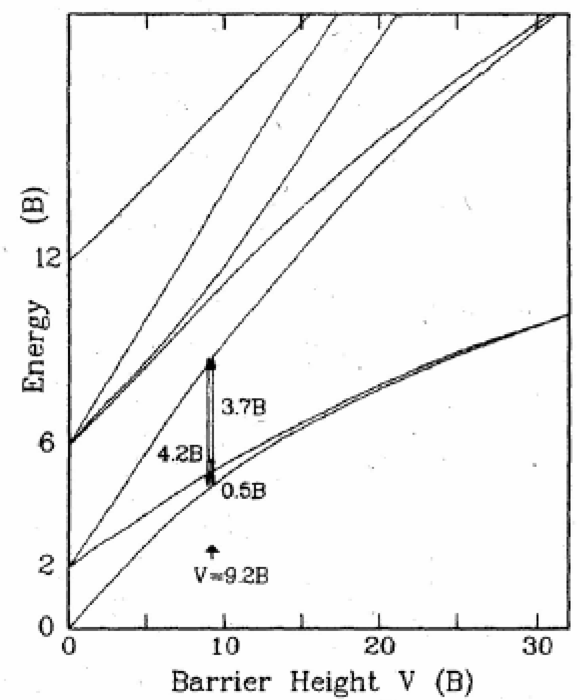
Rotational Energy Levels

$$E = BJ(J+1)$$



Rotational transition between odd(ortho) and even (para) J requires $\Delta I = 1$

Introduction of a Barrier to Rotation of the H_2 Molecule

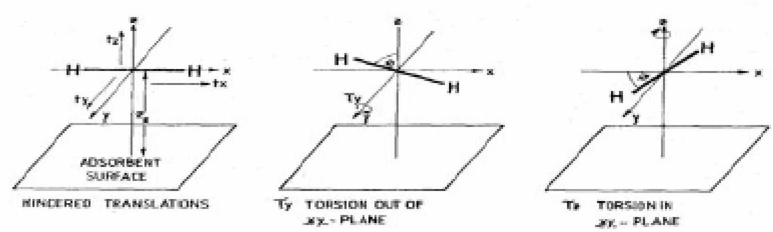


Some degeneracy in J levels is lifted

Note sensitivity to V of "0-1" transition
Levels depends on the form of the barrier

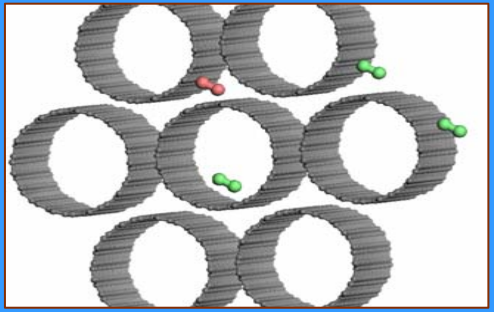
Transitions can be observed by neutron scattering - deduce barrier height V (as shown)

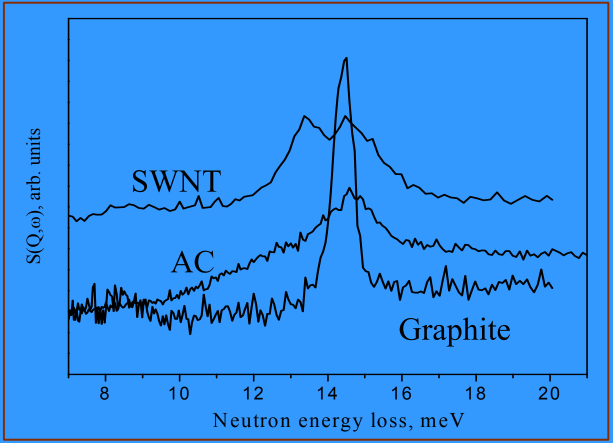
Barrier height can be compared with computational studies

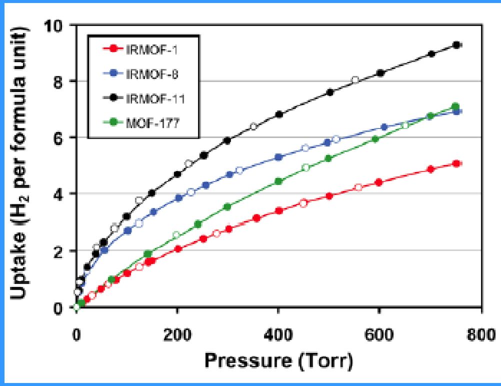


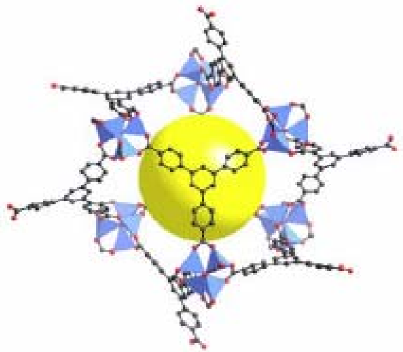
H_2 Absorption in Nanoporous Materials

SWCNT

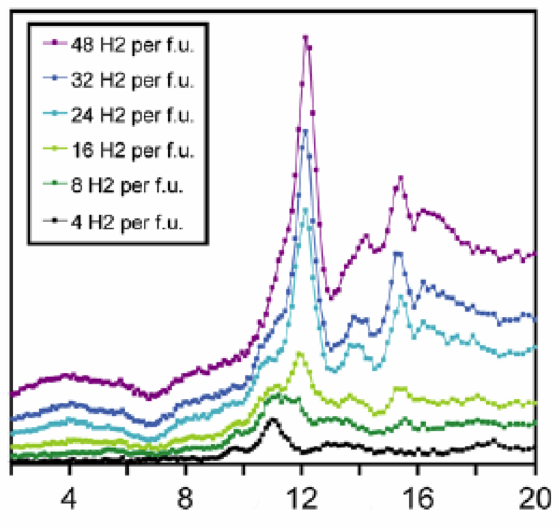


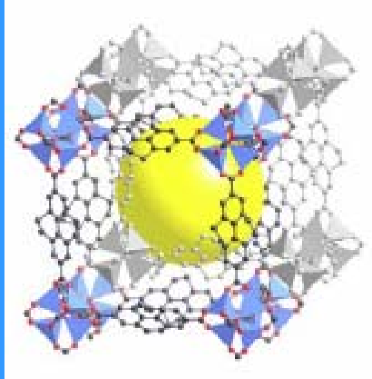




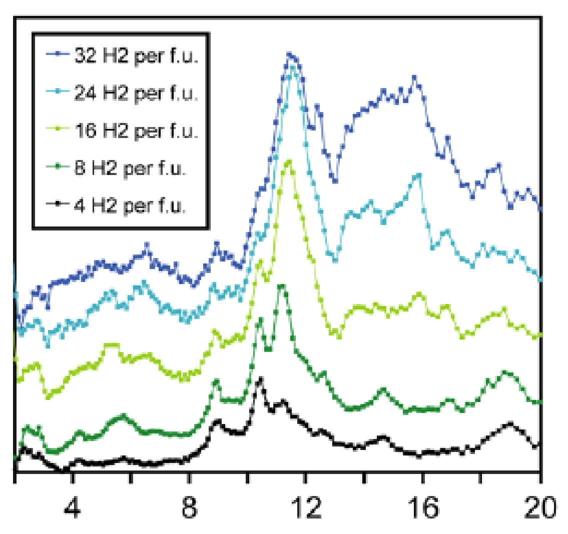


MOF-177
$Zn_4O(BTB)_2$



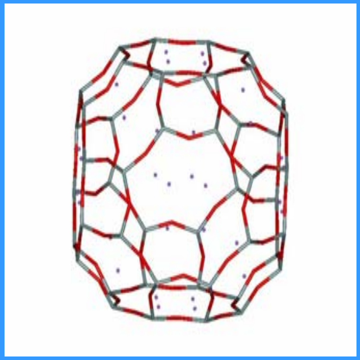


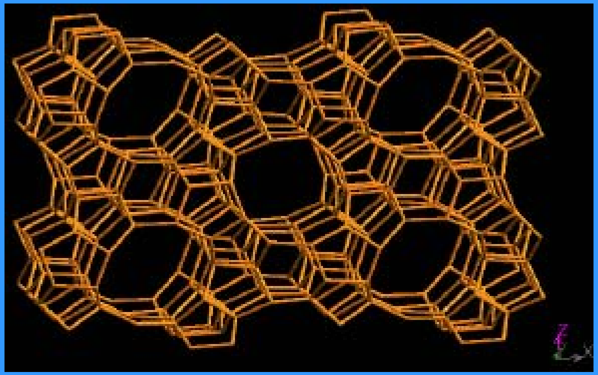
IRMOF-11
$Zn_4O(HPDC)_3$

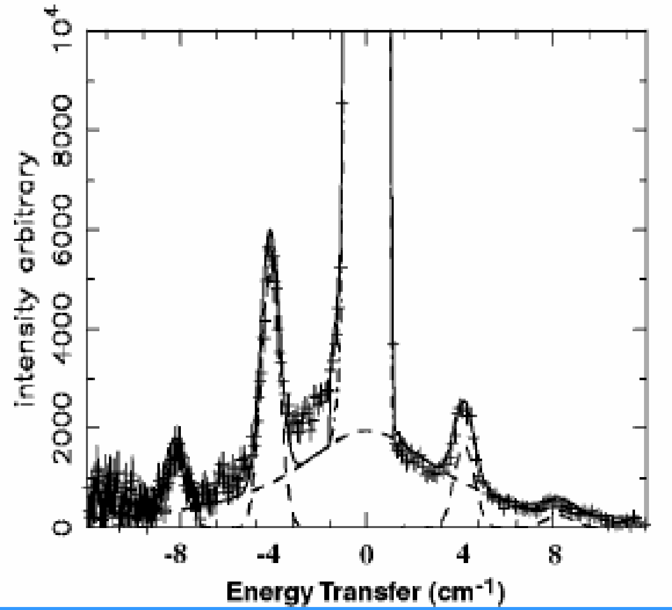


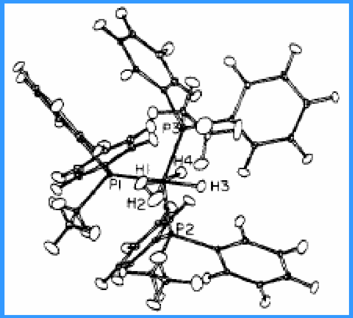
J. Eckert & al. JACS (2005)

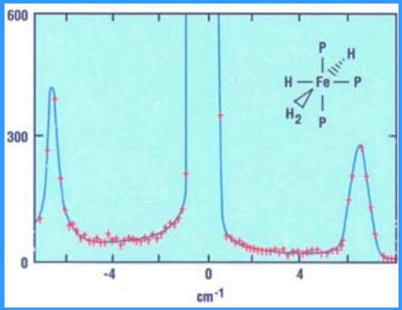
Chemisorption of H_2 in Fe -ZSM-5









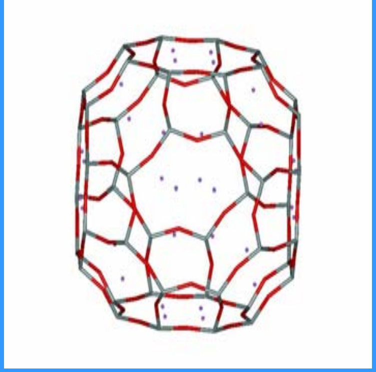


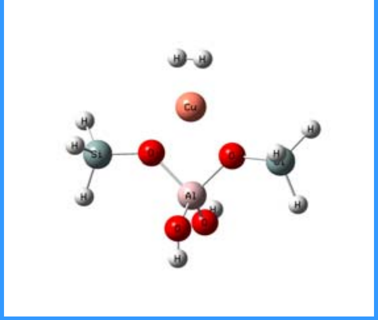
ω = 4.2(2) cm^{-1} 8.3(2) cm^{-1}

NEAT @5K - λ = 5.1Å

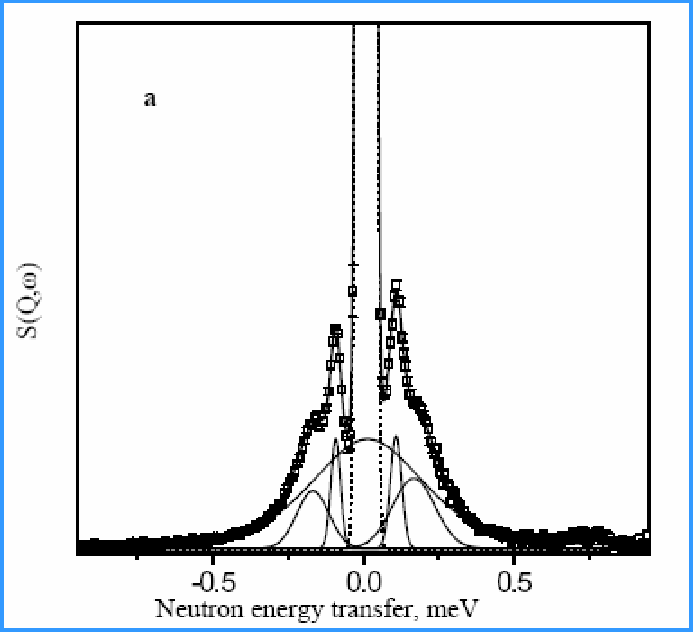
Van der Sluys & al. *JACS* **1990**, *112*, 4831

Chemisorption of Molecular Hydrogen in: Cu–ZSM5

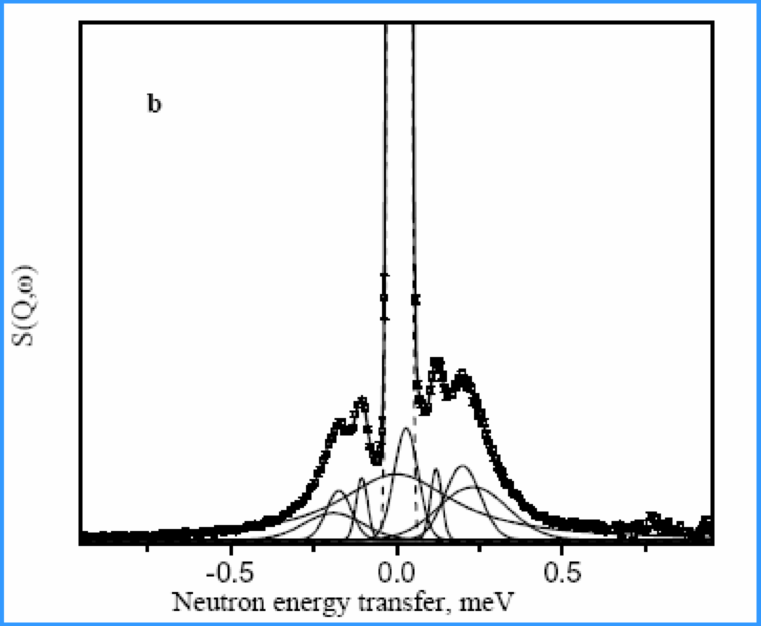




H_2/Cu 0.4

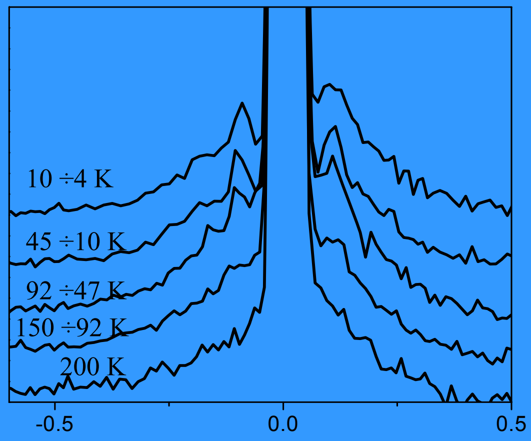


H_2/Cu 2.0



ω_τ $\pm 0.80\ cm^{-1}$ $\pm 1.37\ cm^{-1}$

IN5 @4K - $\lambda = 7.0Å$



Time-Energy Scales in Neutron Scattering

Hydrogen in Metals

optic phonons *(local modes at low H conc.)*	~100 meV	~20 THz
acoustic phonons	≤ 30 meV	~7 THz
jump diffusion *(width)*	0.1-10 μeV	~10^{-5}-10^{3} THz

Molecular Crystals (e.g.: Benzene)

Internal modes (vibrations)	≥ 50 meV	~12 THz
phonons	≤ 10 meV	~2 THz

Adsorbates

guest - host	≤ 15 meV	~4 THz
rotational diffusion (e.g. liquids)	~ 0.5 meV	~0.1 THz
translational diffusion	~ 1 μeV	~10^{-4} THz

Inelastic and Quasielastic Neutron Spectroscopy

$$\boxed{\Delta E \tau \approx h/2\pi}$$

Time Scale τ	Resolution ΔE	Spectroscopic Technique
10^{-11} sec	10 - 100 μeV	Direct Geometry TOF
10^{-9} sec	0.3 - 20 μeV	Backscattering Crystal Analyzer
10^{-7} sec	5 neV - 1 μeV	Spin Echo

Momentum Transfer Q ($Å^{-1}$)	Distance (Å)	Regime
0.05	100	Continous or Macrospic Diffusion
5	1	Atomic or Microscopic Diffusion