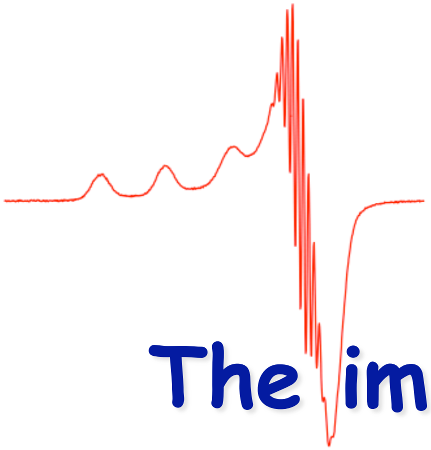

Beyond XAS –
The importance of other techniques

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Cornell University
July 9, 2009

2009 APS XAFS School

"Science without contact with experiments is an enterprise which is likely to go completely astray into imaginary conjecture." — Hannes Alfven

Reminder: Please avoid "imaginary conjecture" in your beam time proposals!

Characterize your samples by as many techniques as you can!

Explore new methods to find the answers to tough questions.

Other Methods of Characterizing your samples…

1) Laboratory spectroscopic methods (before, after or even during your synchrotron experiments)

2) Advanced Synchrotron methods

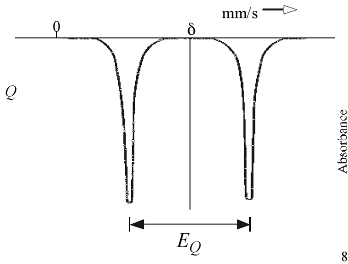
Additional spectroscopic data:

- provides complementary information
- provides a check sample integrity/ radiation damage
- helps constrain possible models/ parameters
- arrive at a more detailed understanding

Spectroscopic Techniques

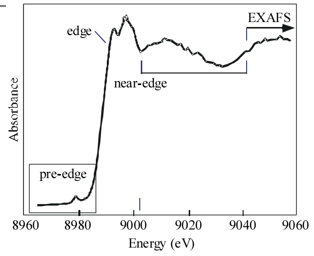
	Gamma	X-Ray	UV/vis	Infrared	Microwave	Radiowave
eV	14000	8000 2000	4 - 1	0.1-0.01	10^{-4} -10^{-5}	10^{-6} -10^{-7}

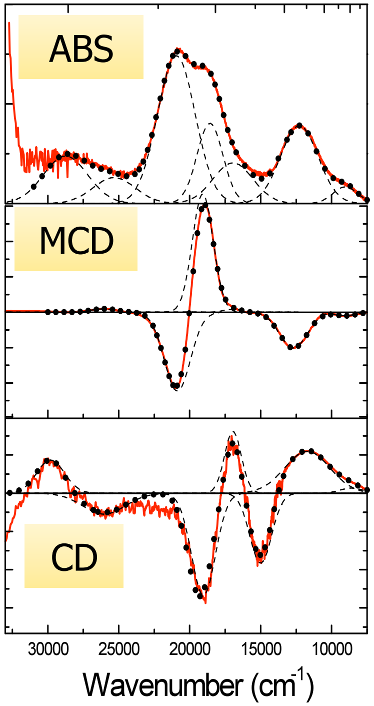
Möss-bauer



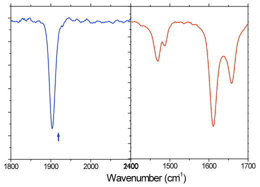
XAS

EXAFS

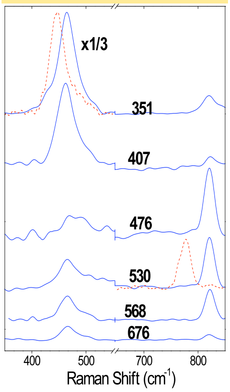




IR

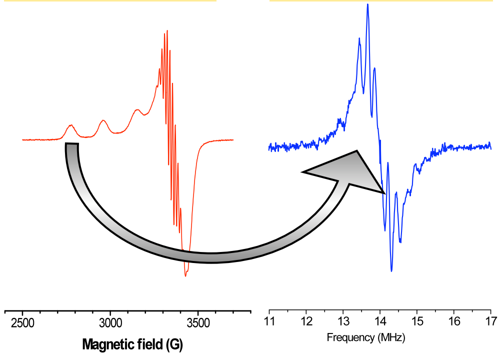


Raman



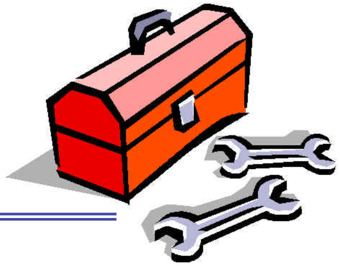
EPR

ENDOR



NMR

The Spectroscopy Toolbox



- **Mössbauer** - recoilless emission and absorption of high energy gamma photons, primarily applies to Fe (Sb, Sn, Ru, Au, I, Ir also possible)

- **UV-Vis** – low energy electronic excitations. Applies to anything with a chromophore! Useful tool for quantitation, kinetics. Possible in situ (at synchrotron).
- **CD** – Circular dichorism – differential absorption of left and right circularly polarized light (ideal for chiral chromophores)
- **MCD** – magnetic CD – add optical probe of paramagnetism

- **Vibrational Spectroscopy**
  - Infared – requires a change in dipole
  - Raman – requires a change in polarization, enhances through resonace excitation

What is EPR?

- Electron Paramagnetic Resonance

- EPR is a spectroscopic technique that detects:
  - unpaired electrons (electron spins : ESR)
  - identity of the paramagnetic molecule
  - Information about the molecular structure (structure, dynamics, bonding)
  - the molecular environment (local and long-range (< 0.8 nm for nuclear spins and up to 5 nm for other electron spins))

Applicability of EPR

Which Substances can be Studied by EPR ?

All Substances which contain unpaired electrons

Including:

1. Most Transition Metals (Cu^{II},$Ni^{I,III}$,Co^{II},Fe^{III},Mn^{II},V^{IV},Mo^{V})
2. Radicals in proteins ($Tyr^{\cdot}$,$Trp^{\cdot}$,$Gly^{\cdot}$,$Cys^{\cdot}$) or small molecules ($NO^{\cdot}$,$O2^{\cdot-}$,....)
3. Transient Paramagnetic Species in Light Driven Processes

Information Content of EPR

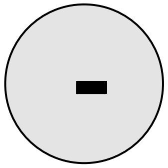
1. Is the Substance Paramagnetic ?
   ... But watch out – some Integer Spin Systems are EPR inactive!
2. Which type of Paramagnet is present ?
   ... Fingerprinting! Metal, Radical, Interacting system, ...
3. How much Paramagnet is present?
   ... Quantification! **Complements XAS edges!!**
4. Information about Geometric and Electronic Structure of the Paramagnet.
5. In Transition Metals - Qualitative Information about type and number of Ligands (**Constraint for EXAFS**)
6. In Interacting Systems – Information about Distances, Coupling between metal centers

Elementary Properties of Electrons

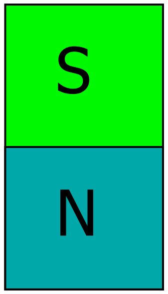
An Electron has the following properties:

- Mass m_e
- Charge $-e_0$
- Spin → Magnetic Dipole Moment m

$$\mu = -\underbrace{g_e}_{2.002319\ldots}\ \underbrace{\beta}_{\text{Bohr Magneton}}$$

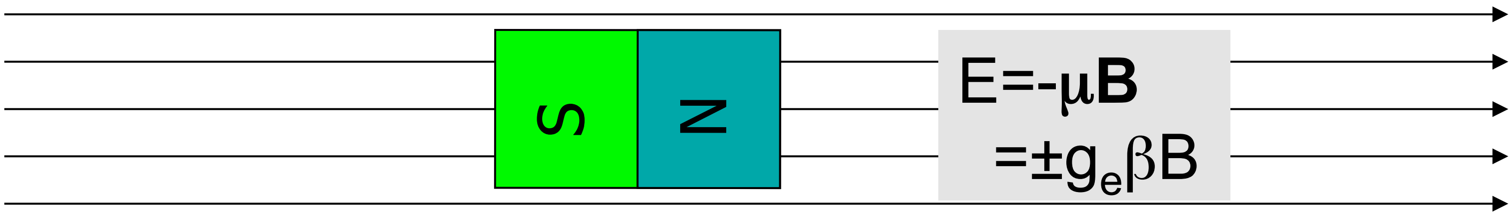


Electric monopole



Magnetic Dipole

The Magnetic Dipole in a Magnetic Field:



$E = -\mu \mathbf{B}$

$= \pm g_e \beta B$

Field **B**

An Electron in a Magnetic Field

Energy of an Electron in a Magnetic Field:

$$E=-\mu \mathbf{B} = \pm g_e \beta\ |B|\ \cos(\theta)$$

In Quantum Mechanics:

Only Orientations with $\cos(\theta)=\pm 1/2$ are possible

Thus, the Electron can have only two states:

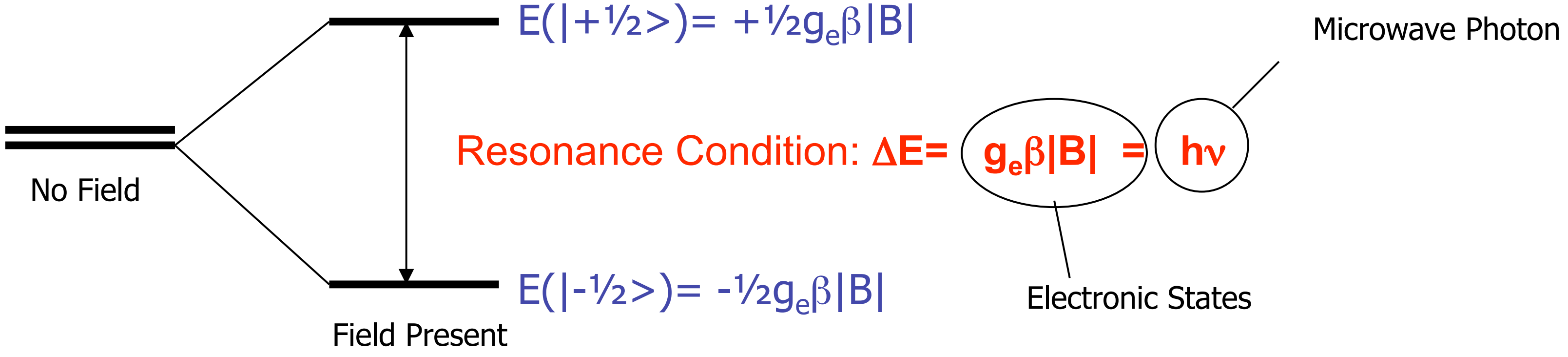
$|+1/2\rangle$ and $|-1/2\rangle$

„up“ „down“

An EPR Transition

In order to change the orientation of the electronic magnetic dipole moment in the presence of a magnetic field we need to apply a force (energy).

A suitable energy is provided by a Microwave Photon which induces a transition Between the $|-\frac{1}{2}>$ and $|+\frac{1}{2}>$ Levels.



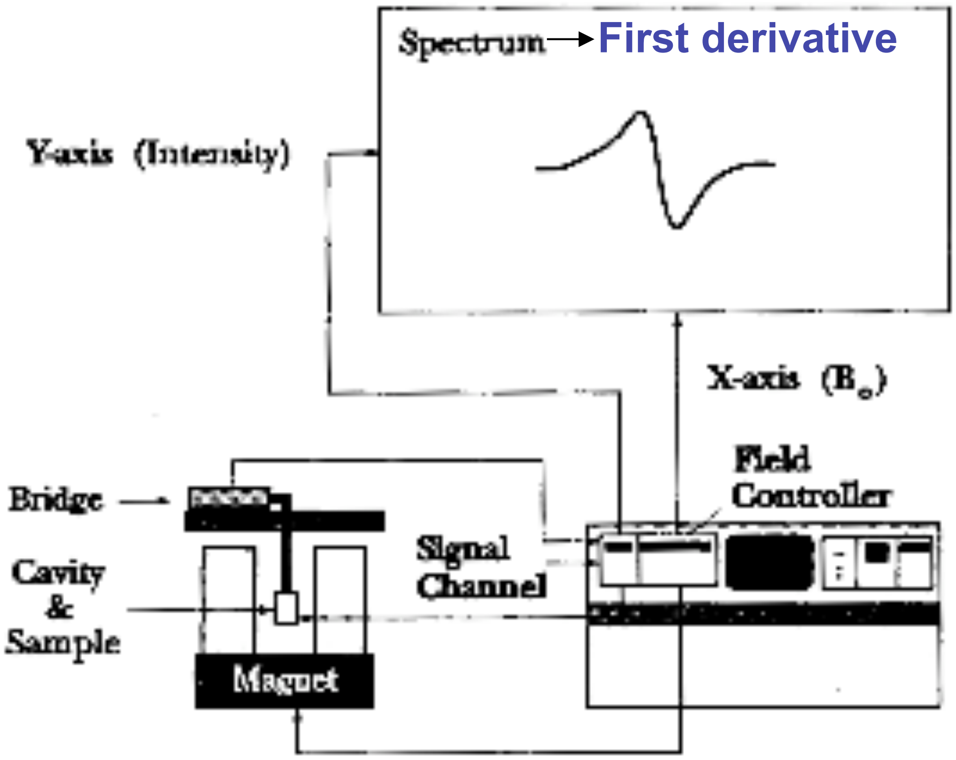
$E(|+½>) = +½g_e\beta|B|$

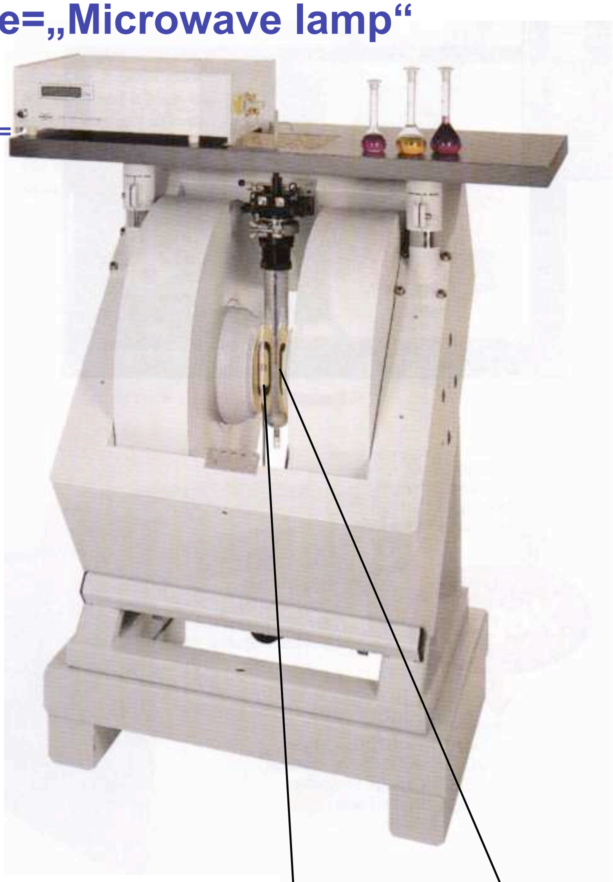
Resonance Condition: $\Delta E = g_e\beta|B| = h\nu$

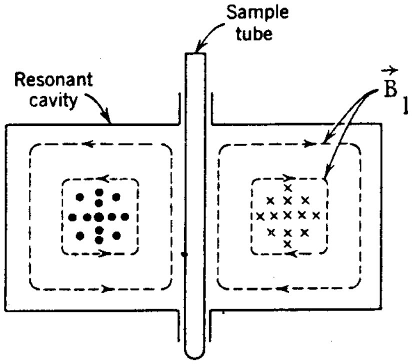
$E(|-½>) = -½g_e\beta|B|$

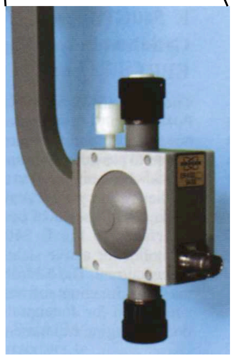
EPR Spectrometer

Bridge=„Microwave lamp“







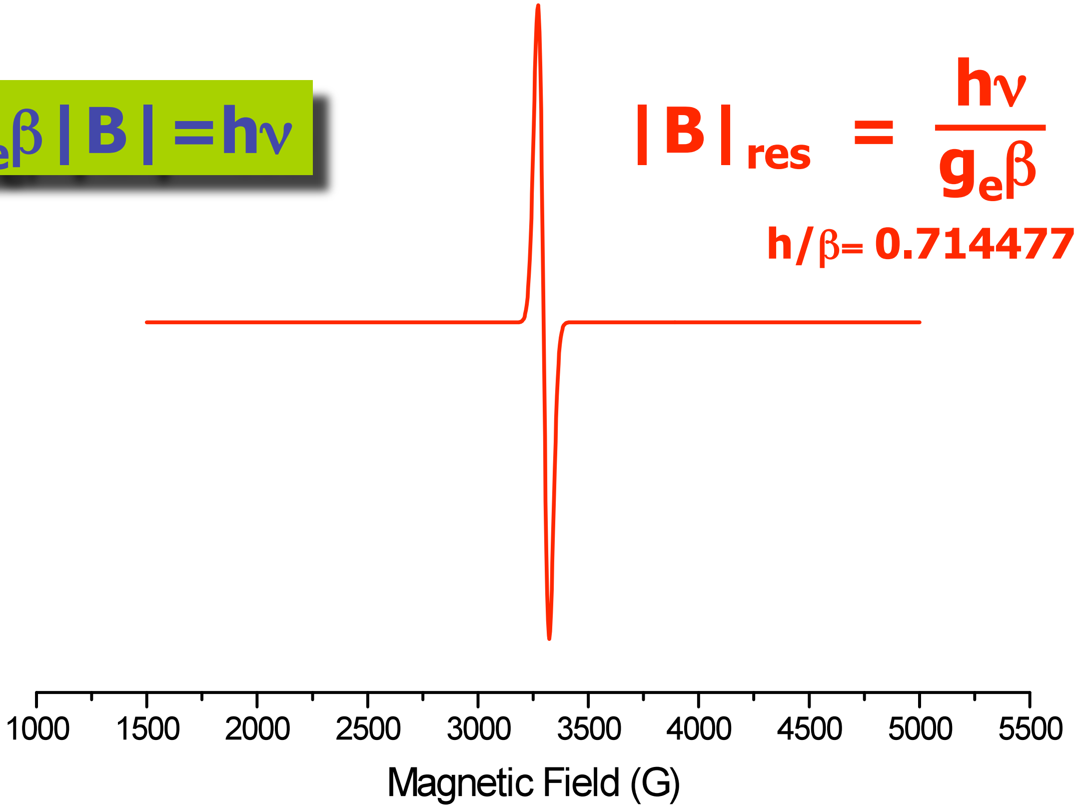


Sample Cavity

Experimental Observation of Resonance

Experimentally we record the spectrum on a Magnetic Field scale at fixed microwave frequency.

$\Delta E = g_e \beta |B| = h\nu$

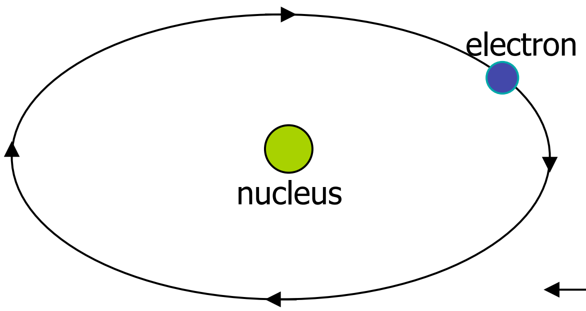


$$|B|_{res} = \frac{h\nu}{g_e \beta}$$

$h/\beta = 0.7144775$ Gauss/GHz

Bound Electrons

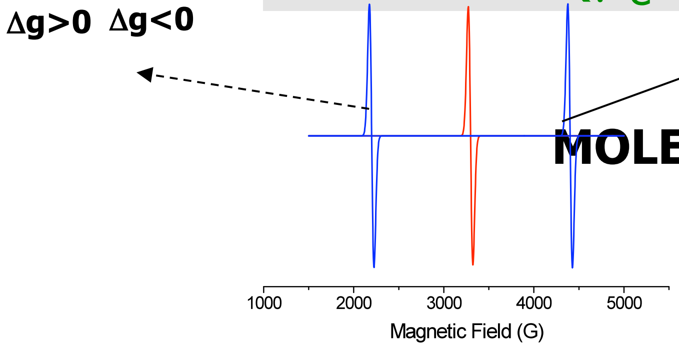
In Reality Resonance does NOT Always Occur at the same Field Because bound Electrons also carry some ORBITAL ANGULAR MOMENTUM (l) in addition to their SPIN ANGULAR MOMENTUM (s).



Additional Magnetic Moment $\mu_L \propto \mathbf{l}=\mathbf{r} \times \mathbf{p}$

Modification of Resonance Condition:

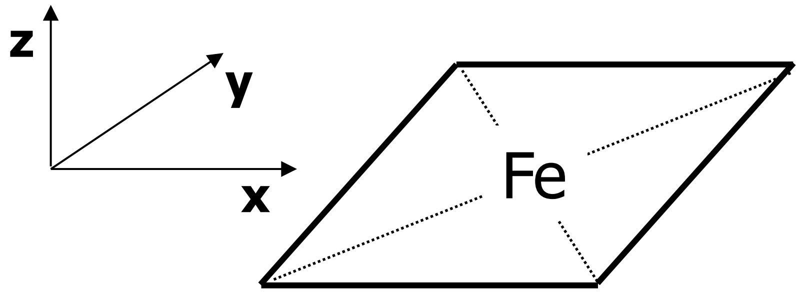
$$\Delta E = h\nu = -B(\mu_e+\mu_L) = \beta|B|\, g_{eff}$$



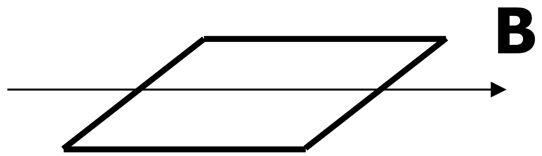
MOLECULAR Quantity=ge+Δg

Anisotropic Electron Movement

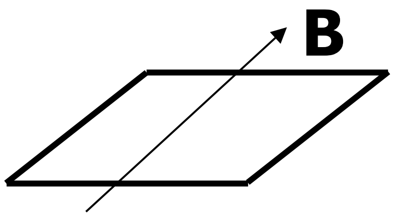
The relative orientations of **B** and $\mu= \mu_e+\mu_L$ matter a lot!



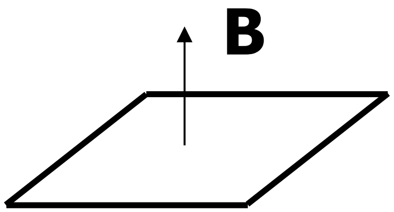
There are three extreme possibilities:



$h\nu=-B_x\mu_x=\beta B_x\mathbf{g_x}$



$h\nu=-B_y\mu_y=\beta B_y\mathbf{g_y}$



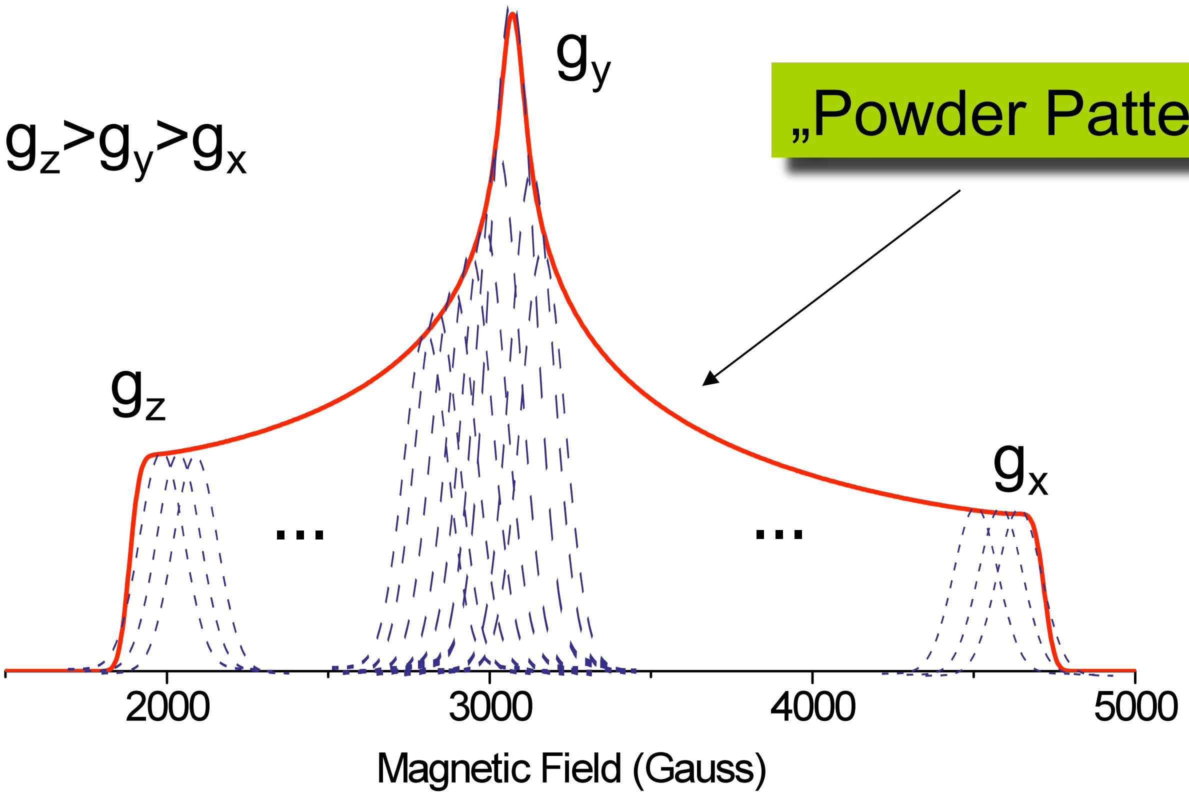
$h\nu=-B_z\mu_z=\beta B_z\mathbf{g_z}$

Thus, g-becomes anisotropic: the „g-Tensor“

Consequences for the Spectrum

In Frozen Solutions one has Randomly Oriented Molecules and thus we have to Integrate Over All Possible Orientations!

Assume $g_z > g_y > g_x$



„Powder Pattern“

Nomenclature for Powder Patterns

RHOMBIC

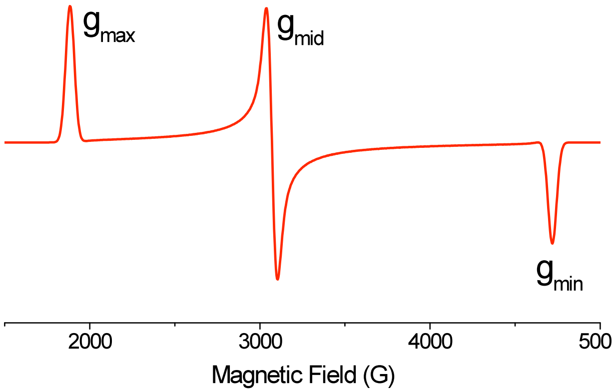
$g_x \neq g_y \neq g_z$

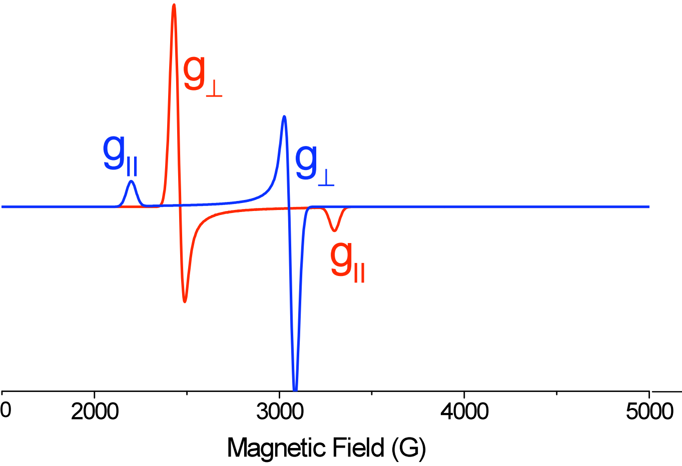
AXIAL

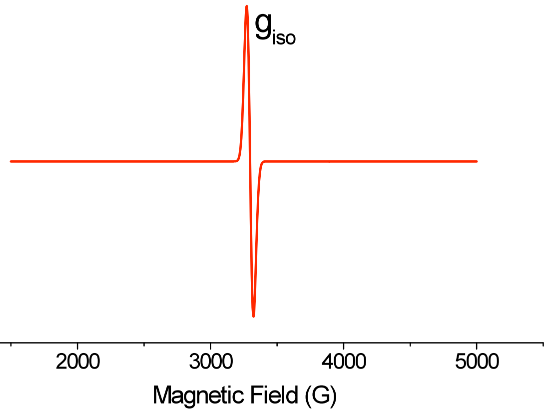
$g_x = g_y (= g_\perp) \neq g_z\ (= g_{||})$

ISOTROPIC

$g_x = g_y = g_z$



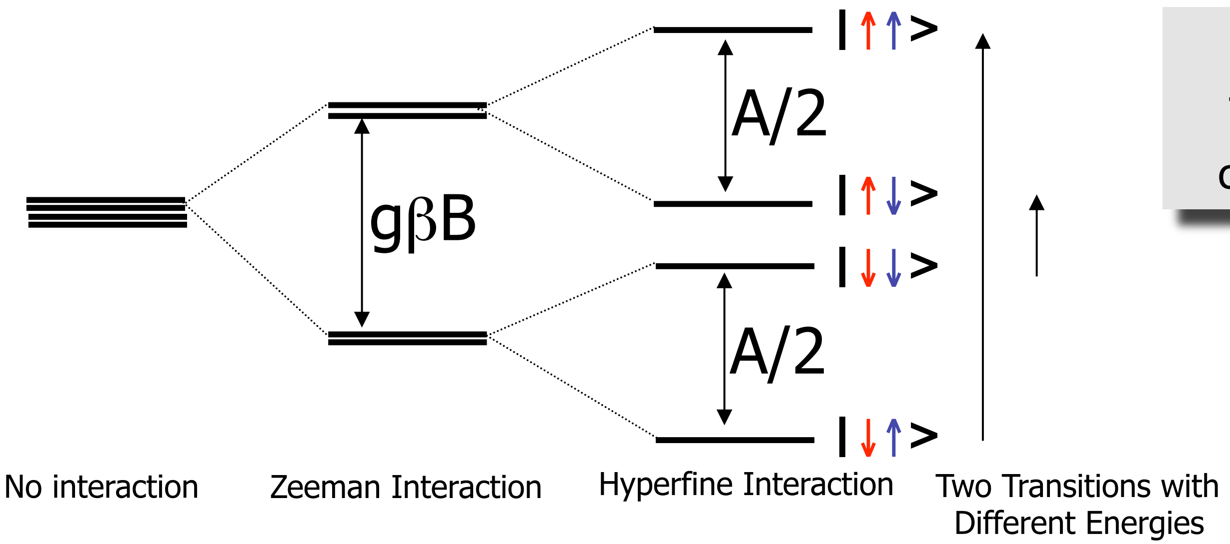




The Hyperfine Interaction

Some Nuclei are also Little Bar Magnets (→NMR Spectroscopy).

- The Condition is that the Nuclei have Nonzero Spin I.
  (i.e. ^{14,15}N, ^{17}O, ^{19}F, ^{63,65}Cu, ^{61}Ni, ...)
- The Magnetic Interaction between the Nuclei and the Unpaired Electrons is Called Hyperfine Interaction (Symbol *A*)
- The Hyperfine Interaction Leads to a Splitting of EPR Lines

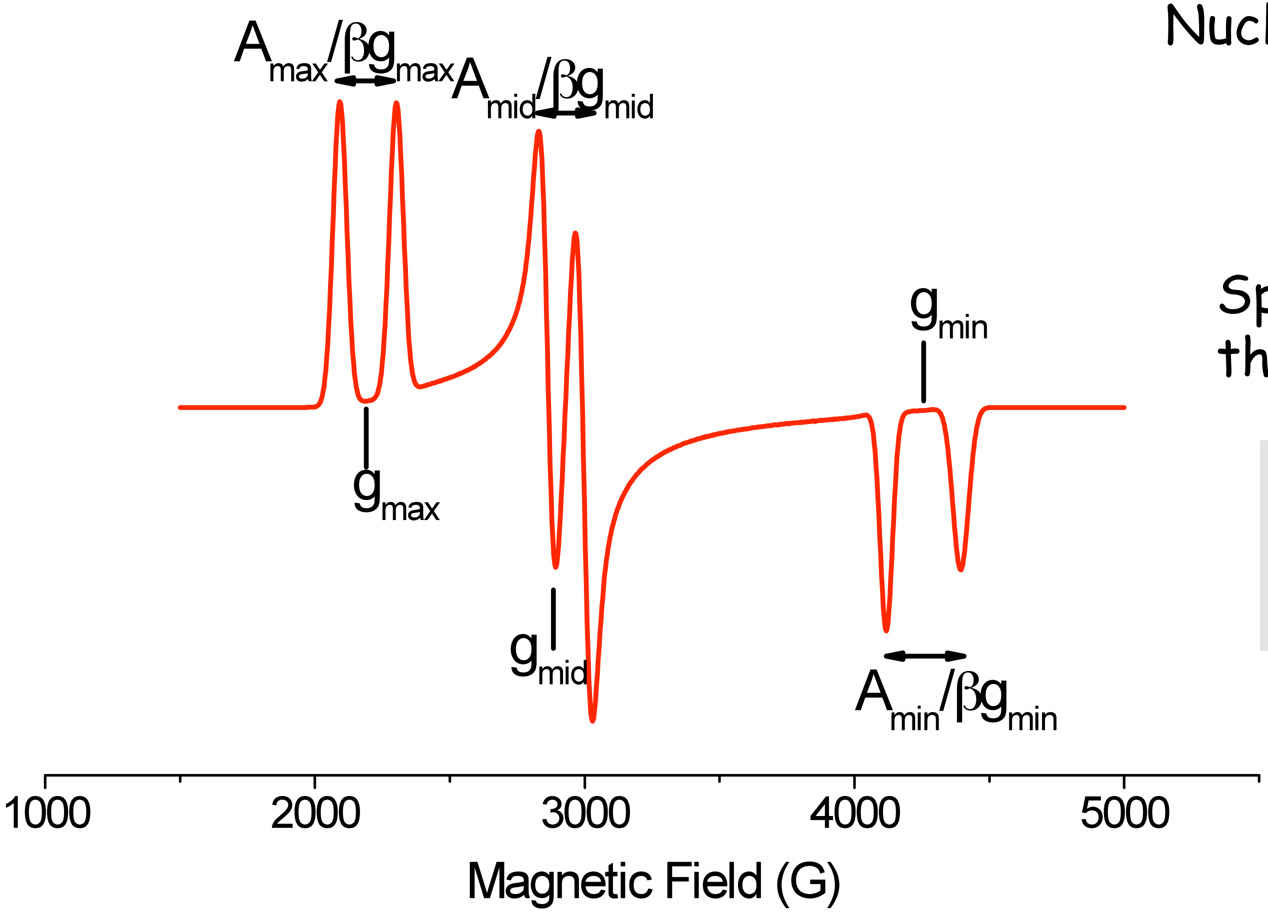


Selection Rule:
The Nuclear Spin must not change in an EPR Transition

↑ Electron Spin

↑ Nuclear Spin

The EPR Spectrum with Hyperfine Structure



Nucleus with Spin I:

2I+1 Lines

Splitting Depends on the Orientation

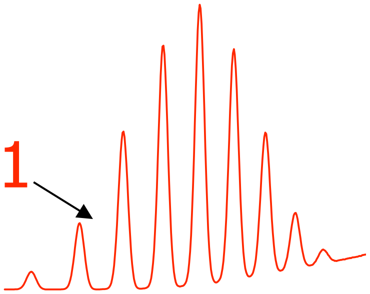
A is different for Each g-direction → „A-Tensor“

Further splitting sue to the ligand Nuclei = superhyperfine

Equivalent Nuclei

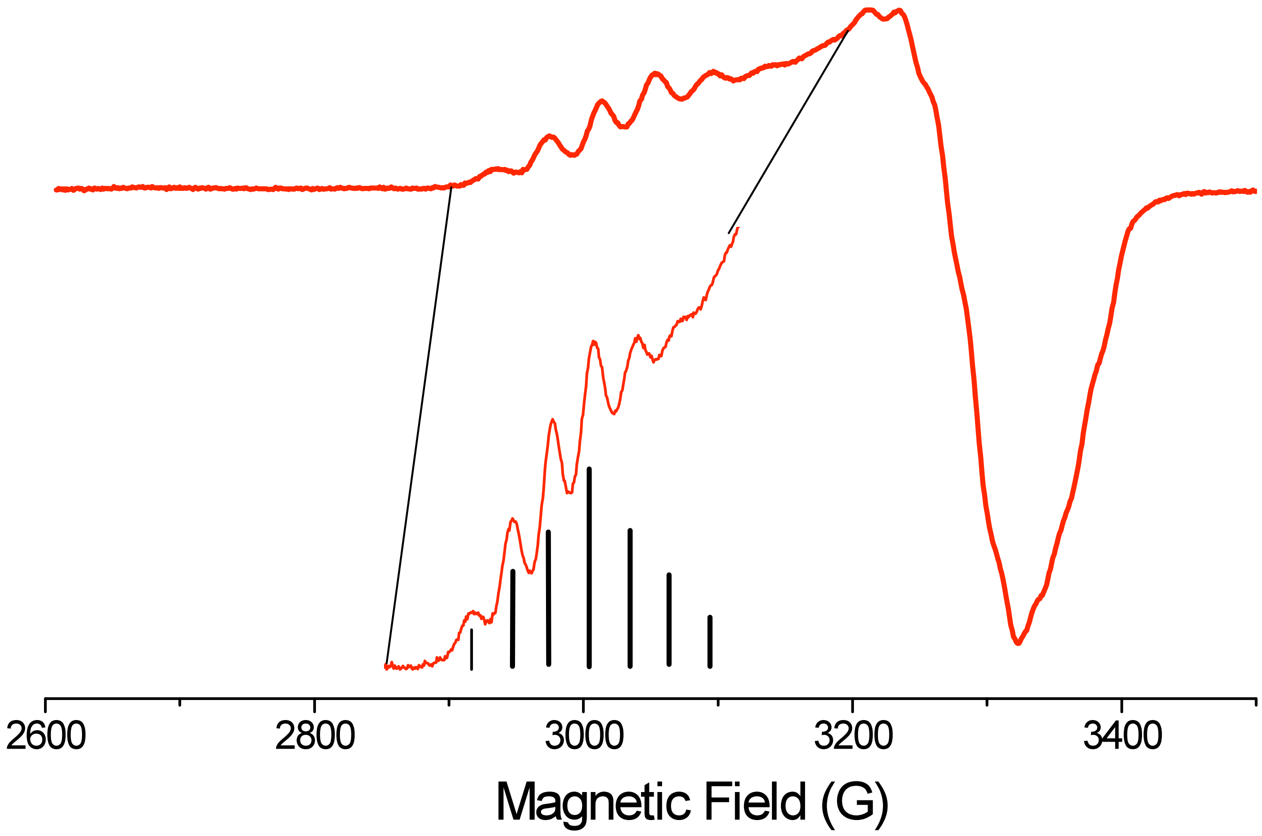
In the case of n equivalent Nuclei with Spin I one Obtains a Hyperfine Pattern with 2nI+1 Lines and a Binomial Intensity Distribution

	I=1/2	I=1
n=1	1:1	1:1:1
n=2	1:2:1	1:2:3:2:1
n=3	1:2:2:1	1:2:3:4:3:2:1
n=4	1:2:3:2:1	1:2:3:4:5:4:3:2:1



Example of Hyperfine Structure

Cu_A in Nitrous Oxide Reductase



I_{Cu}=3/2

7-Lines Observed

#Lines=2nI+1
→ n=2
2x2x3/2+1=7√

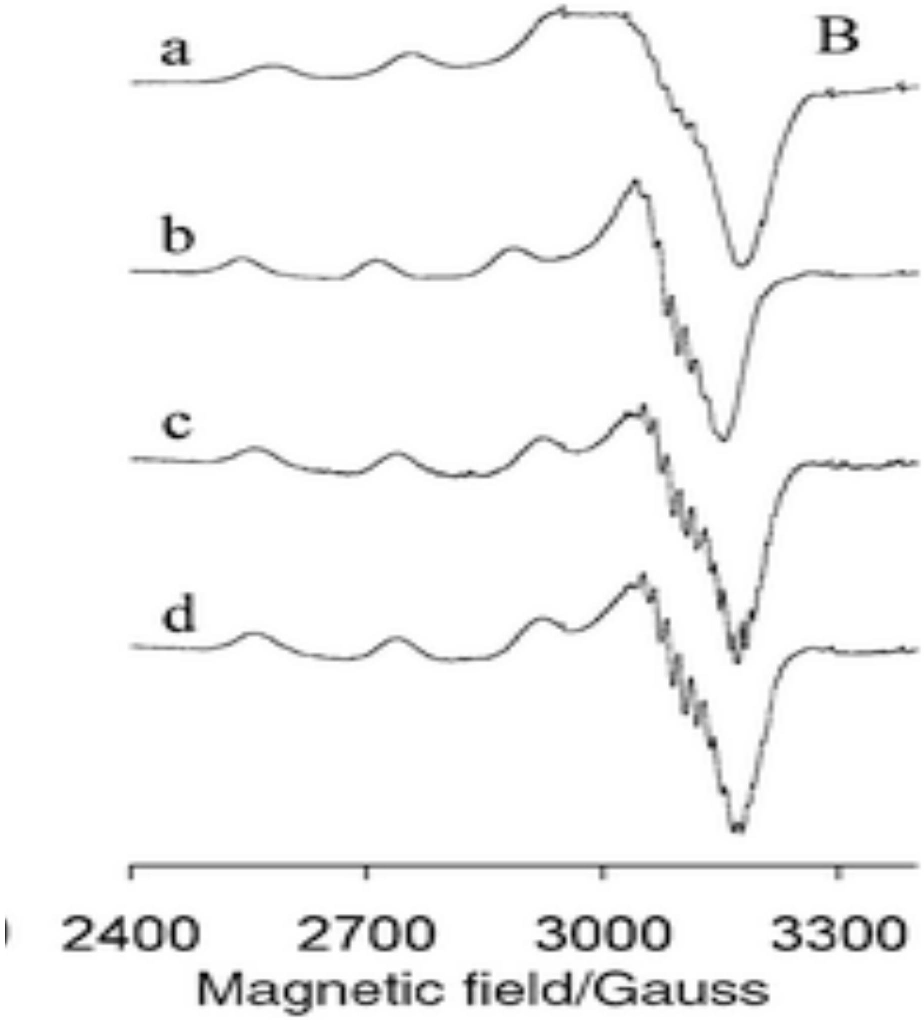
→1:2:3:4:3:2:1
Expec-
ted and Observed

→2 Equivalent
Cu predicted

MV Cu(1.5)-Cu(1.5)

What would the EPR for two interacting Cu(II)-Cu(II) sites look like? One Cu(II)? Two non-interacting Cu(II)s?

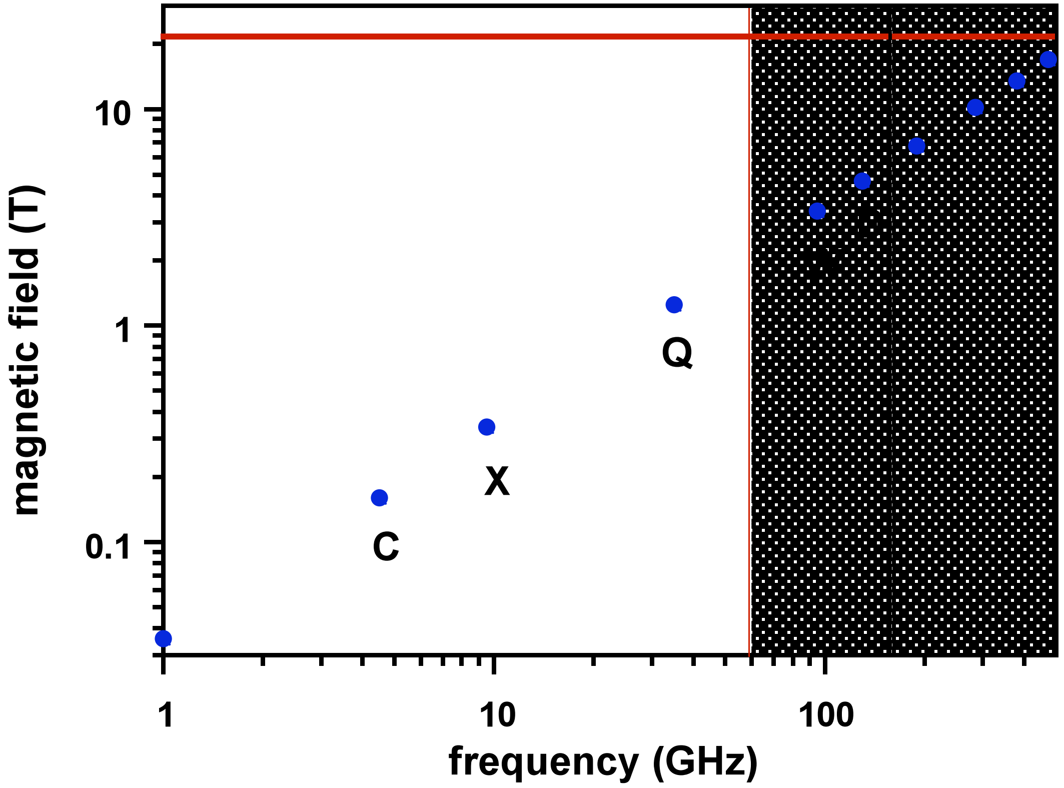
Mononuclear Cu(II) EPR



Mutlifrequency EPR

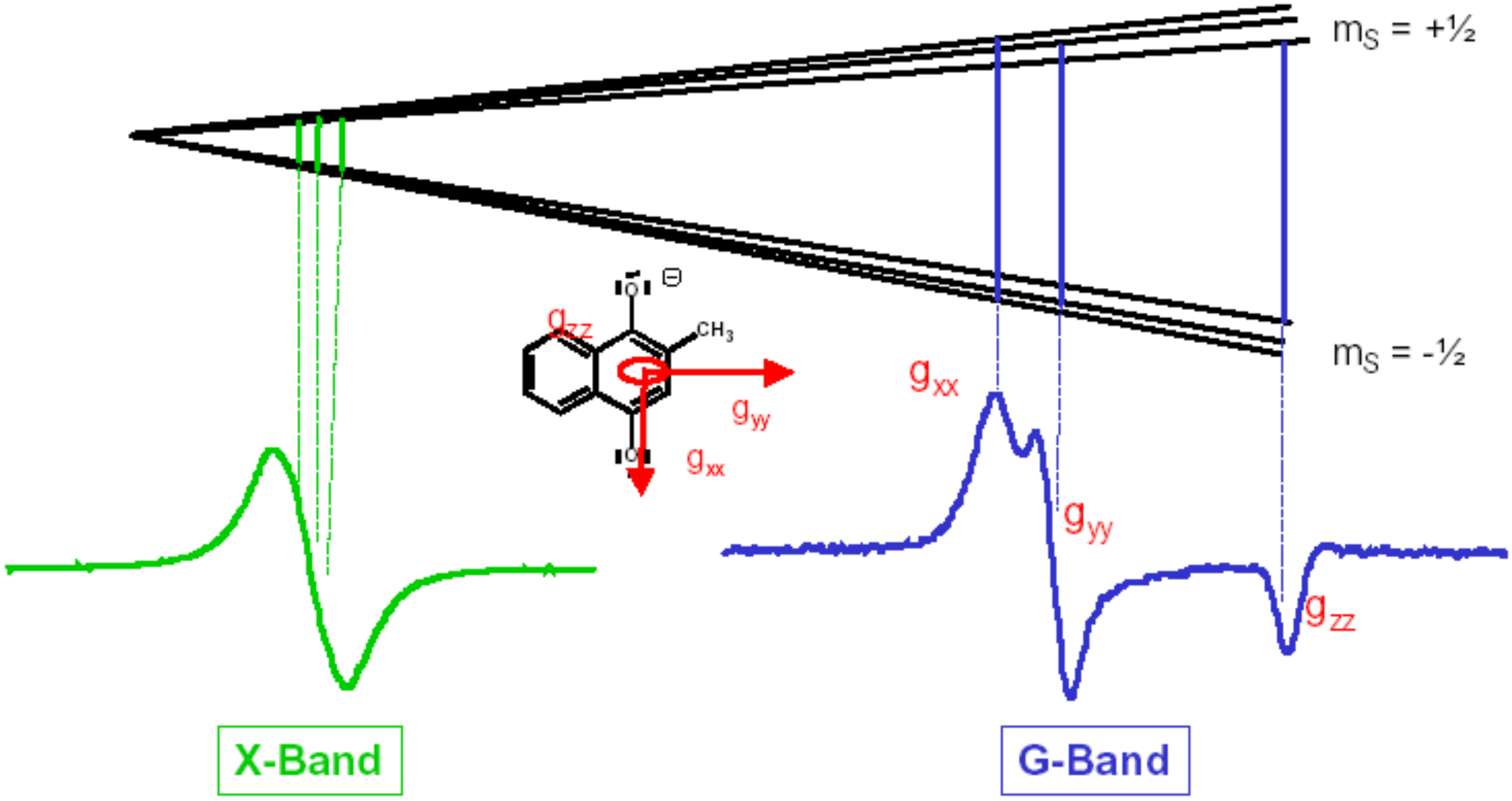
band	GHz	mm
S	2	120
C	4	60
X	10	30
Q	35	10
W	95	3
D	130	2
G	180	1.5

Resonant magnetic field
for a S=1/2 system (g=2.0023)



High Field EPR

Resolution of G-anisotropy: Orientation selection



Other Methods of Characterizing your samples…

1) Laboratory spectroscopic methods (before, after or even during your synchrotron experiments)

2) Advanced Synchrotron methods

Additional spectroscopic data:

- provides complementary information
- provides a check sample integrity/ radiation damage
- helps constrain possible models/ parameters
- arrive at a more detailed understanding

Synchrotron Radiation

Properties of the ring and the insertion device determine the types of experiments that are possible

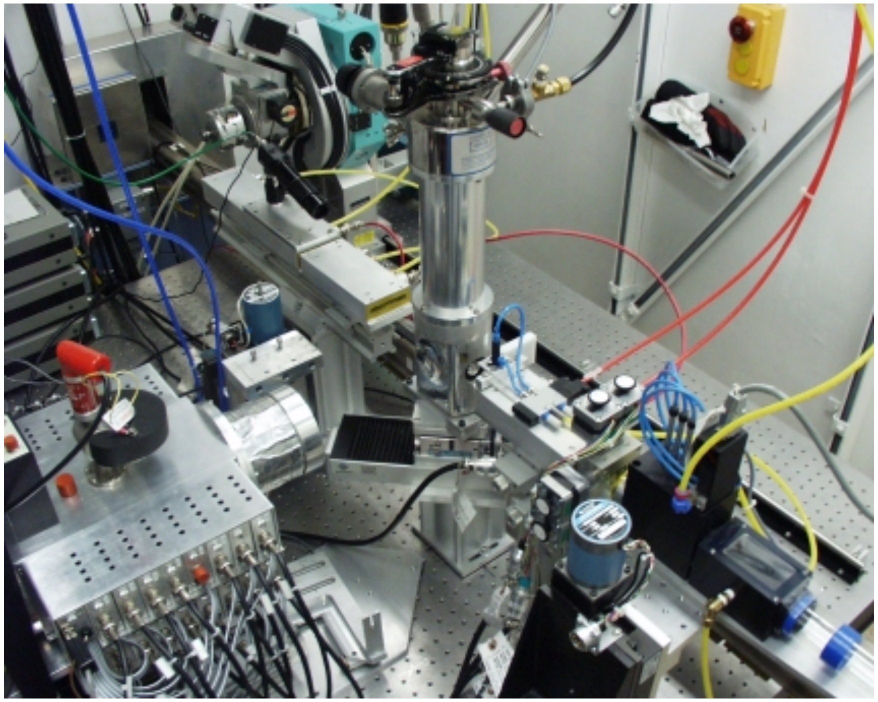
All synchrotron radiation is:

1) pulsed in nature (10-20 psec, with 2nsec + separation)

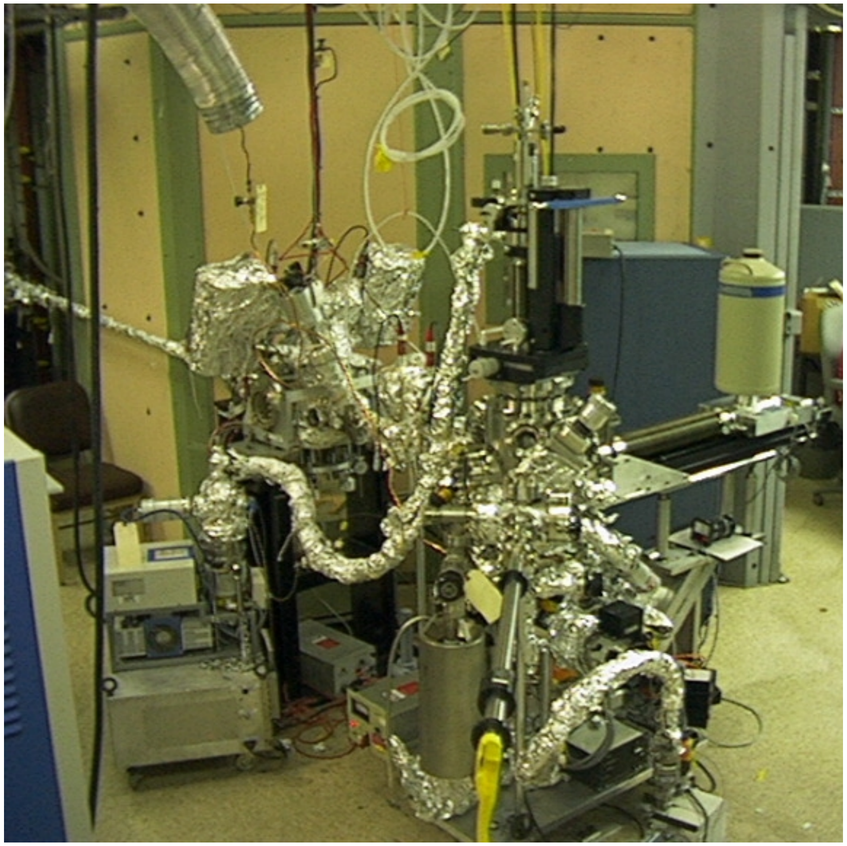
2) polarized

3) highly collimated

Beam Lines



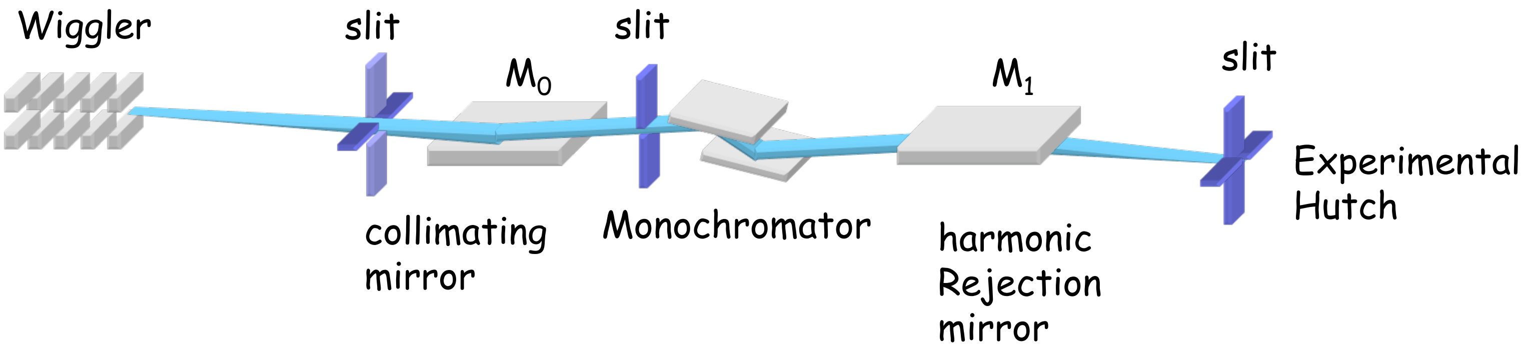
5000-30000 eV



200-1200 eV

Beam line optics and experimental setup are tailored for the energy range of interest.

Beam Line Resolution

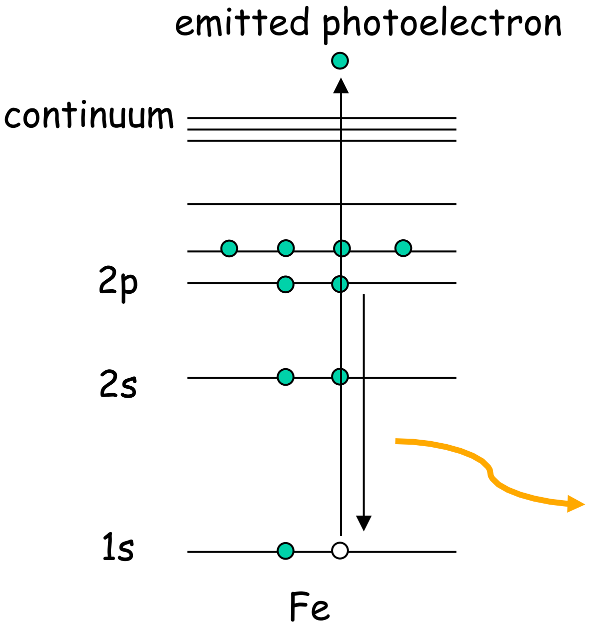


Upstream optics determine beam line resolution

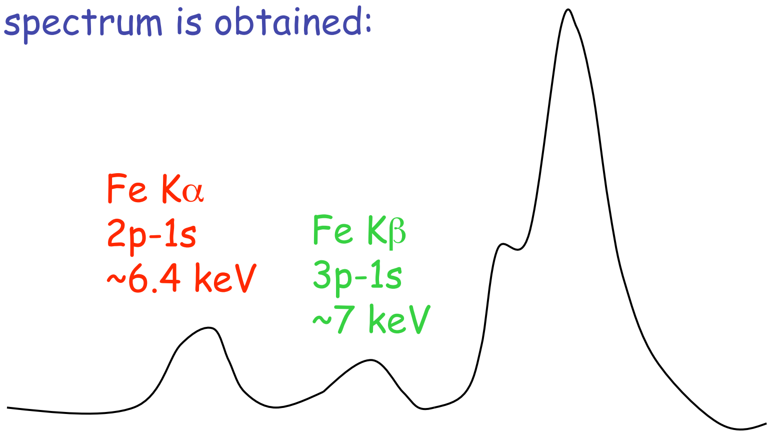
Monochromator crystal choice is a flux vs. resolution issue

For a “typical” XAS setup, best $E/\Delta E = 10^4$ (i.e. ~1eV at 10 keV)

Fluorescence Detection & Resolution



Using a solid state Ge Detector, an XES spectrum is obtained:



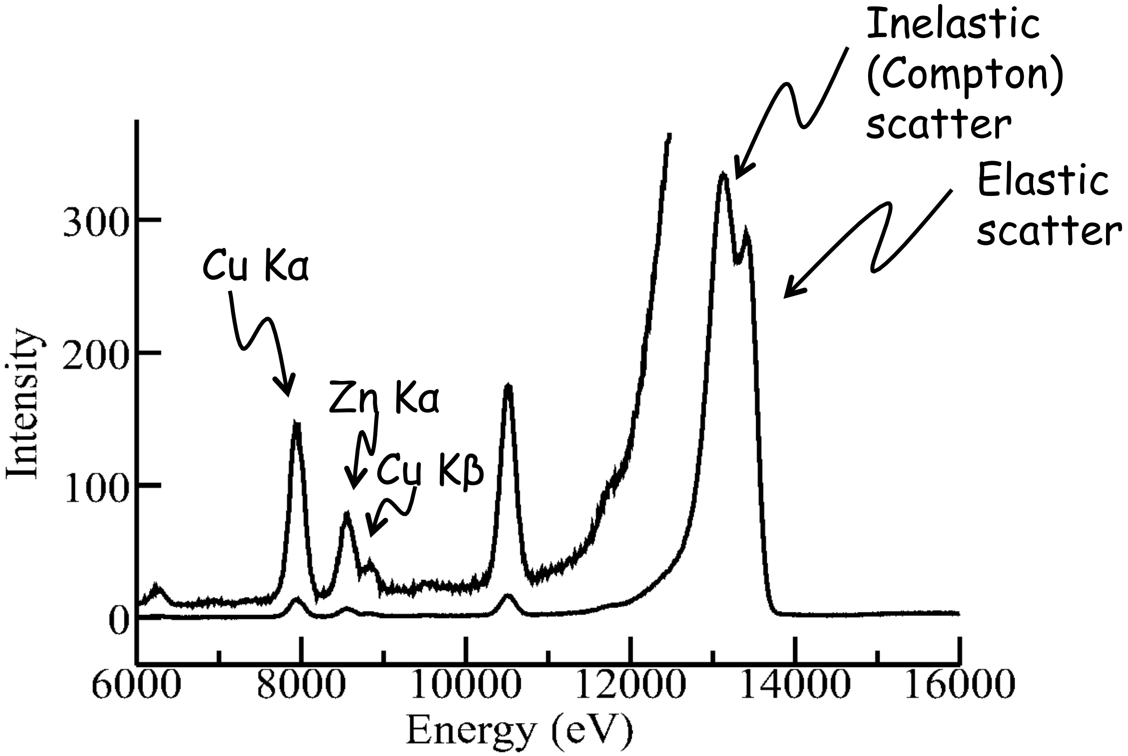
A solid state Ge Detector consists of an a array of reverse bias diodes.

X-rays entering the diode produce a cloud of electron pair holes, and the number of these is proportional to the x-ray energy.

Typically, E/ΔE ~40, so at 7 keV, resolution is ~175 eV.

Therefore no fine structure is apparent on Kα or Kβ emission lines.

Effect of Detector Resolution on XAS data



Cannot separate metals of different oxidation states (Cu(I) vs Cu(II) just contribute to total average).

Z+1 metals can contribute to EXAFS (i.e. Zn to Cu, Fe to Mn)

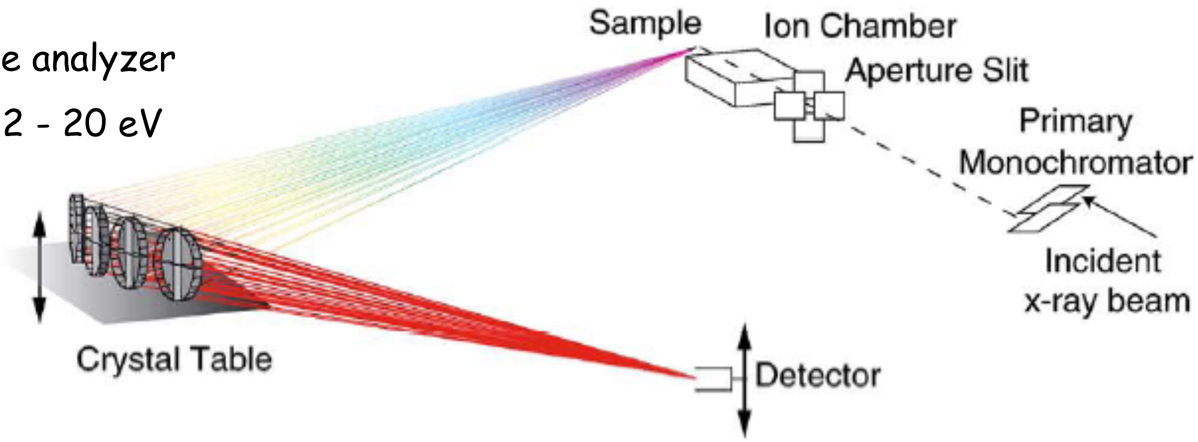
Understanding the emission spectrum allows for new experiments…

Separation of similar ligands (N/O)
"Polarized" data on isotropic samples

High Resolution X-ray Spectrometer

tunable analyzer

$\Delta E = 0.2 - 20$ eV

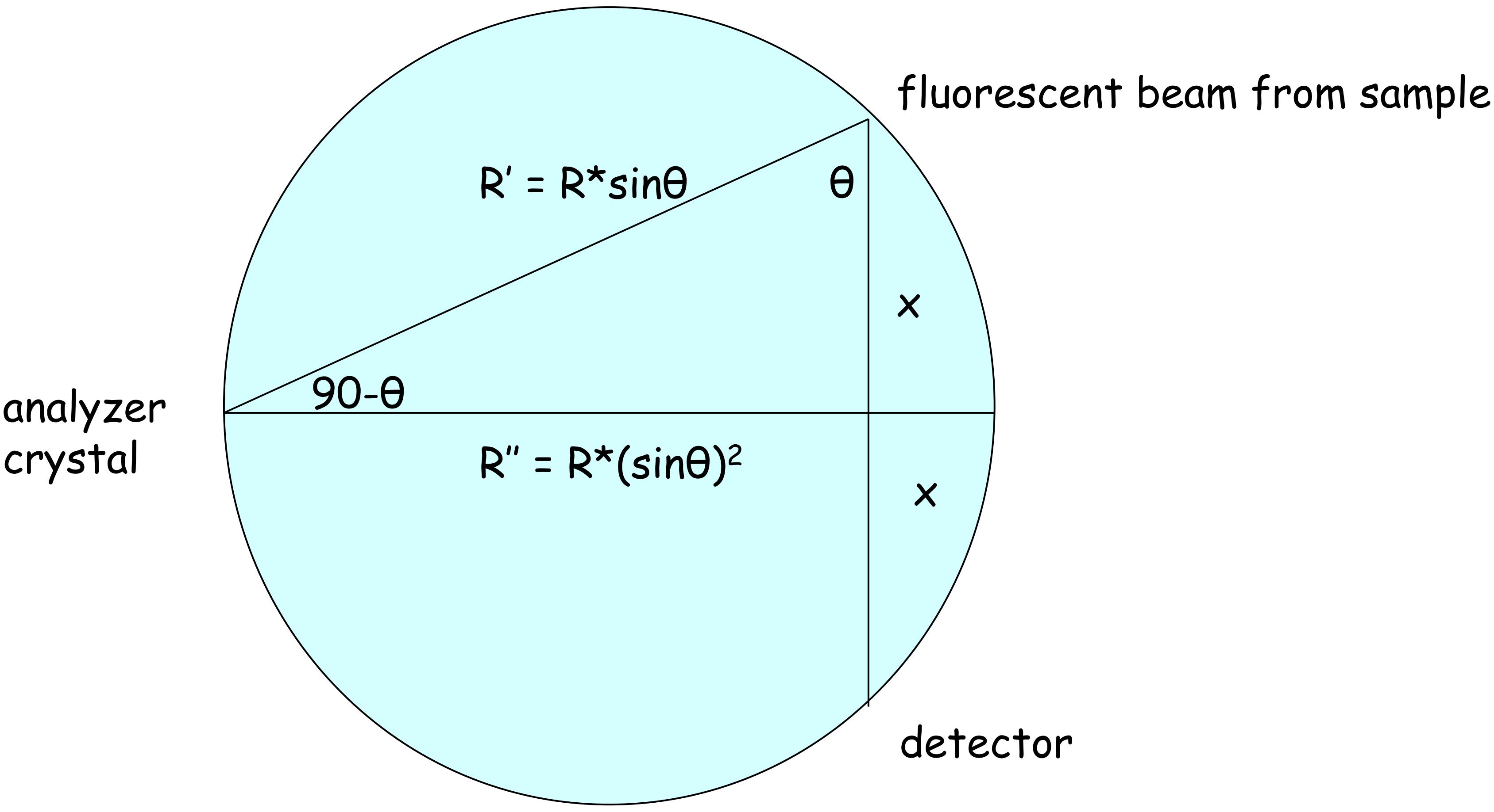


Emission Spectrometer is a Bragg Crystal that spectrally analyzes the fluorescence and reflects it on to a photon detector.

Crystal required therefore depends on the x-ray energy of the experiment. Absorption by crystals also means high flux is required.

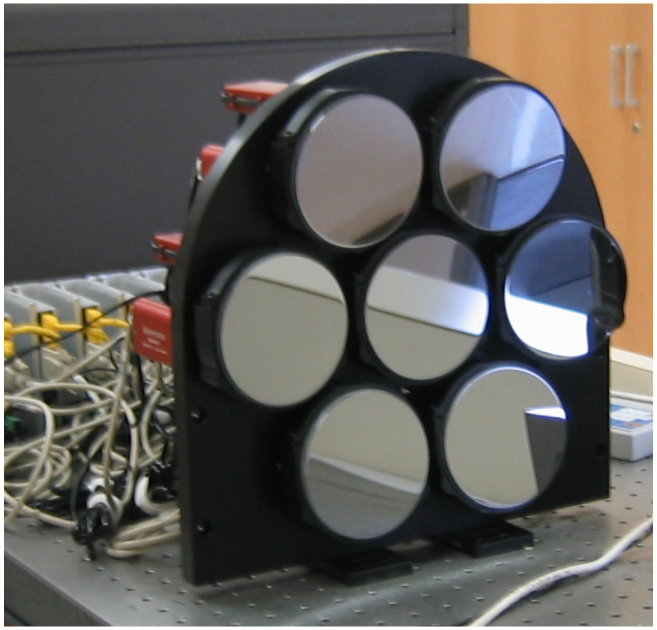
However, an $E/\Delta E > 5000$ or ~1.4 eV resolution at 7 keV can be achieved.

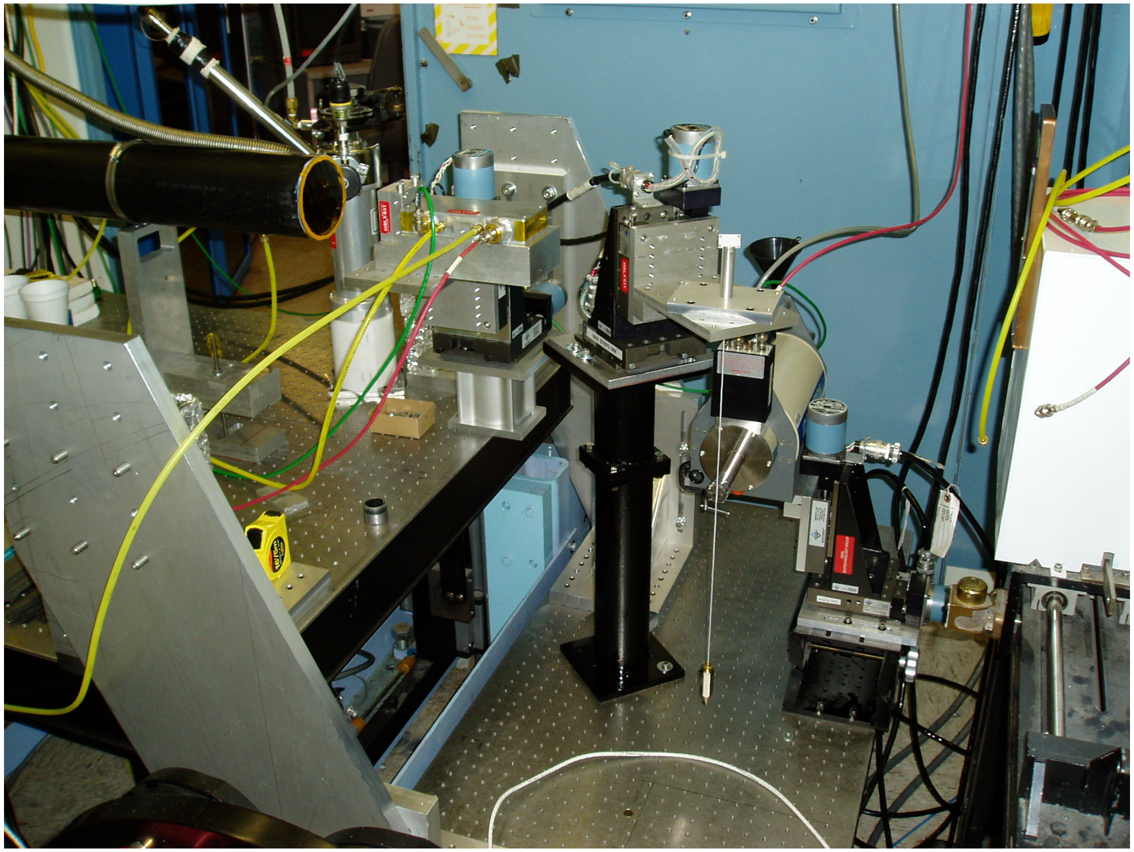
Rowland Geometry



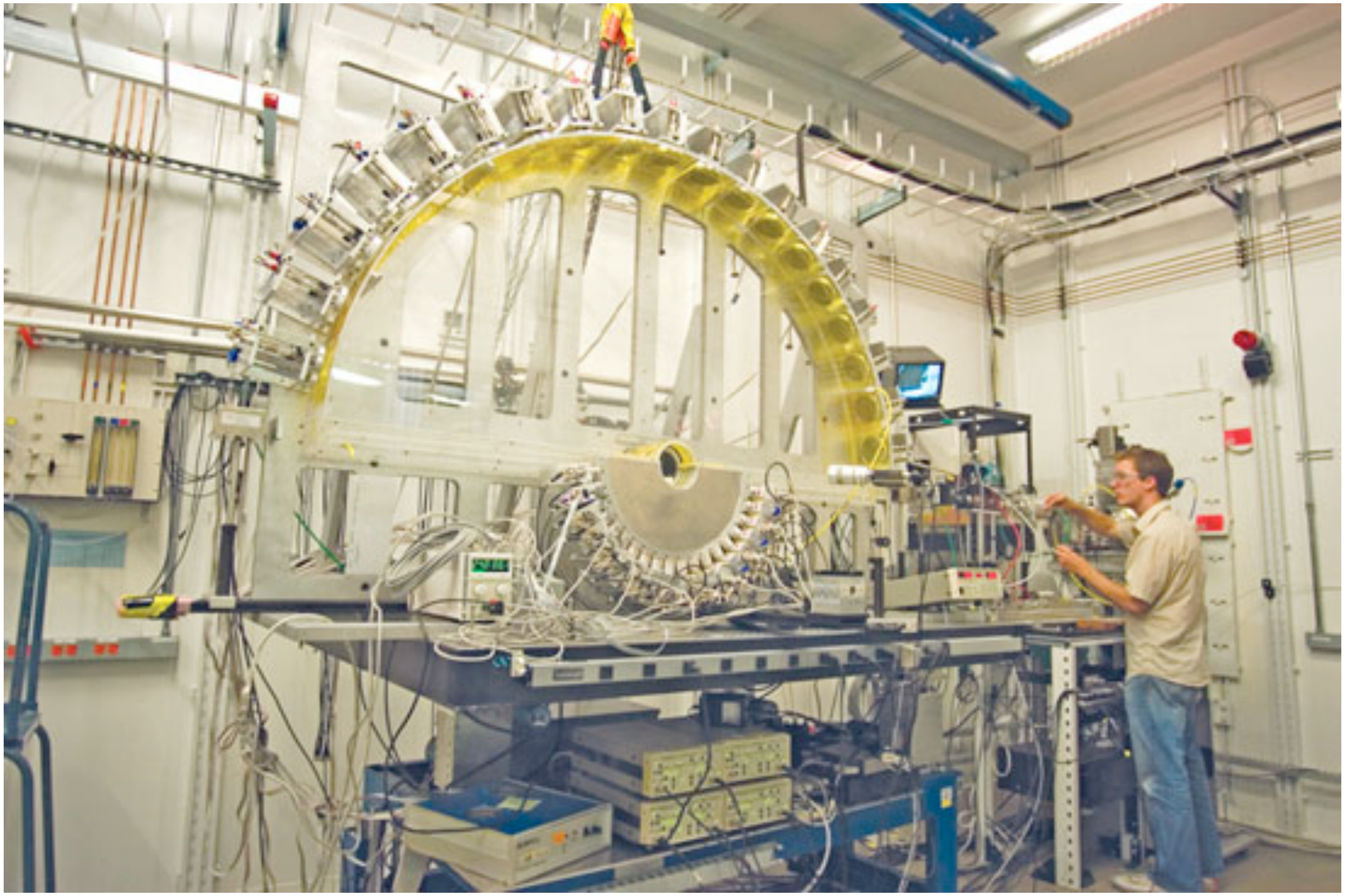
R = the focal length of the analyzer crystal

Setup at SSRL BL6-2



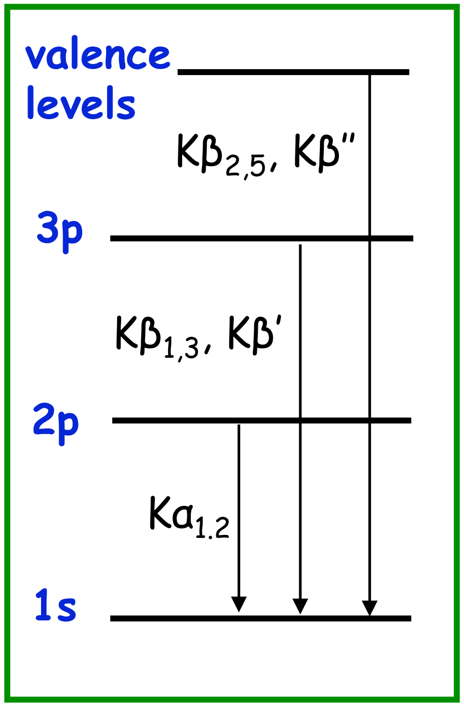


LERIX detector installed on the XOR/PNC 20 I-D-B beam line, APS



X-ray Emission Lines

level diagram



valence levels

$K\beta_{2,5}$, $K\beta''$

3p

$K\beta_{1,3}$, $K\beta'$

2p

$K\alpha_{1,2}$

1s

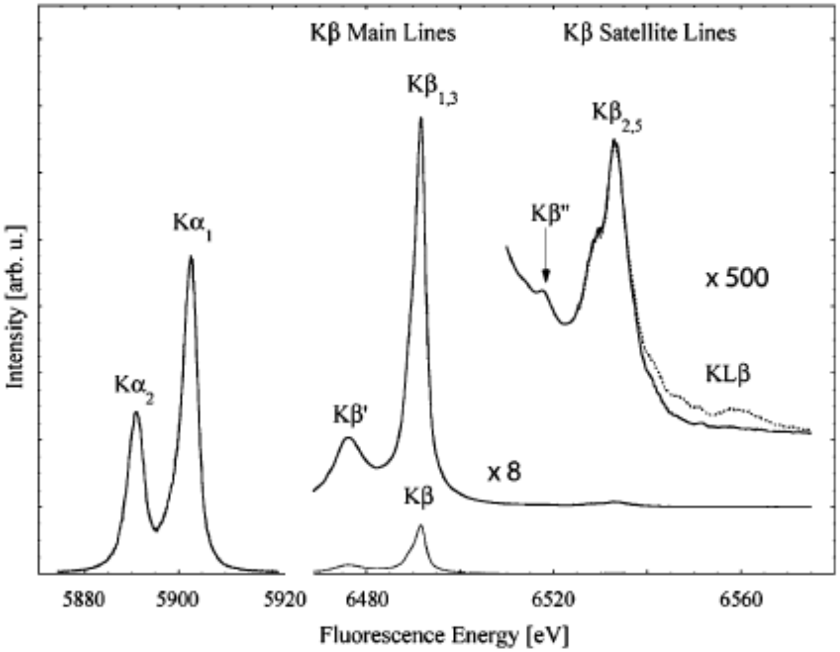
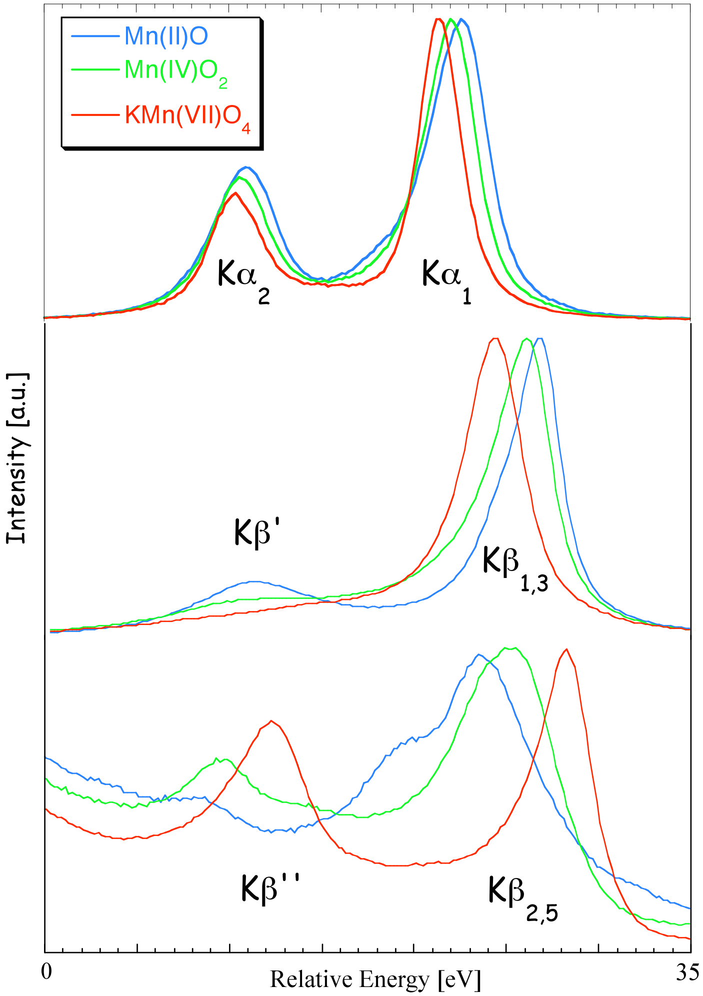


Fig. 3. K shell emission lines in MnO. The final state configurations are given in Fig. 2. The Kβ satellite lines are shown for excitation energies below and above the KL edge, where a 2p electron is excited together with a 1s electron (multiple electron excitation) [24]. The KLβ structure (dotted line) thus arises from doubly ionised final states. The magnification factors for the Kβ main and satellite spectra are given.

X-ray Emission Lines



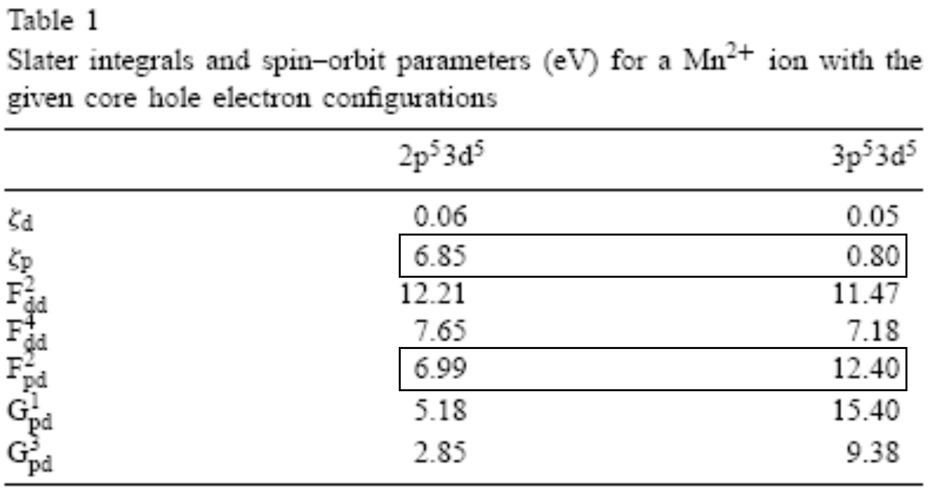
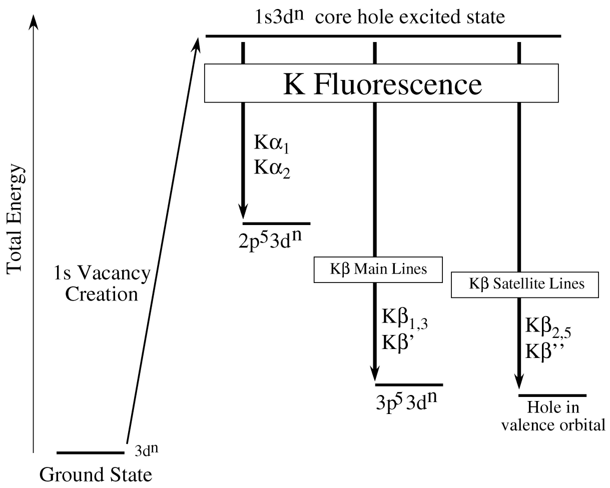


Table 1

Slater integrals and spin–orbit parameters (eV) for a Mn^{2+} ion with the given core hole electron configurations

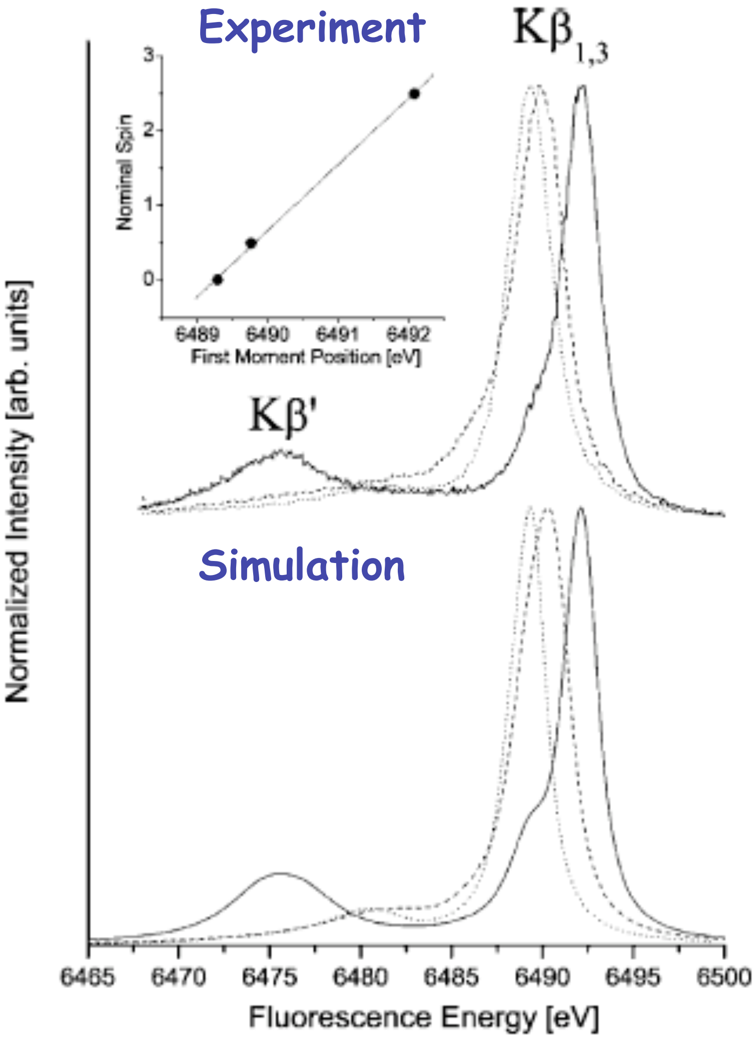
	$2p^5 3d^5$	$3p^5 3d^5$
ζ_d	0.06	0.05
ζ_p	6.85	0.80
F^2_{dd}	12.21	11.47
F^4_{dd}	7.65	7.18
F^2_{pd}	6.99	12.40
G^1_{pd}	5.18	15.40
G^3_{pd}	2.85	9.38



Kβ lines and sensitivity to spin state

$K_4Fe(CN)_6$, $K_3Fe(CN)_6$, Fe_2O_3

S=0 to S=1/2 to S=5/2



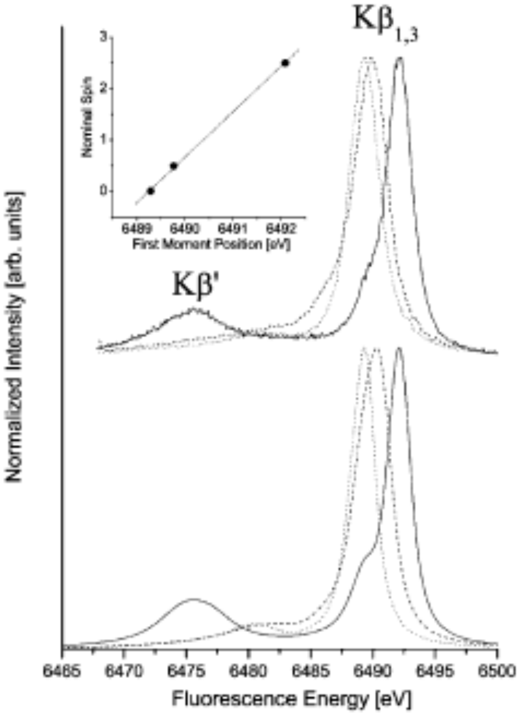
Kβ lines dominated by 3p-3d exchange interaction

Kβ' assignment ambiguous (CT?)

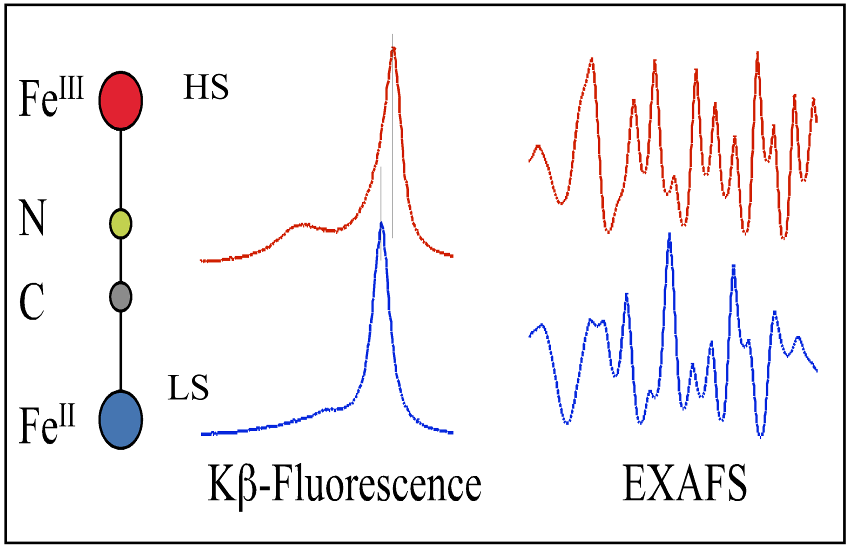
$K\beta_{1,3}$ and Kβ' move closer together with decreasing spin state (i.e as 3p-3d exchange interaction decreases)

Kβ lines reflect number of unpaired d electrons

Site-Selective EXAFS



Application to Prussian Blue $Fe_4(Fe(CN)_6)_3{*}15H_2O$



The Kβ emission line is sensitive to oxidation and spin state.

This results from 3p,3d exchange interaction. After a 3p-1s transition occurs a 3d electron will respond to the change in electron configuration.

Allows for separation of EXAFS for atoms of different spin/oxidation state.

Site-Selective XAS: Possible Applications

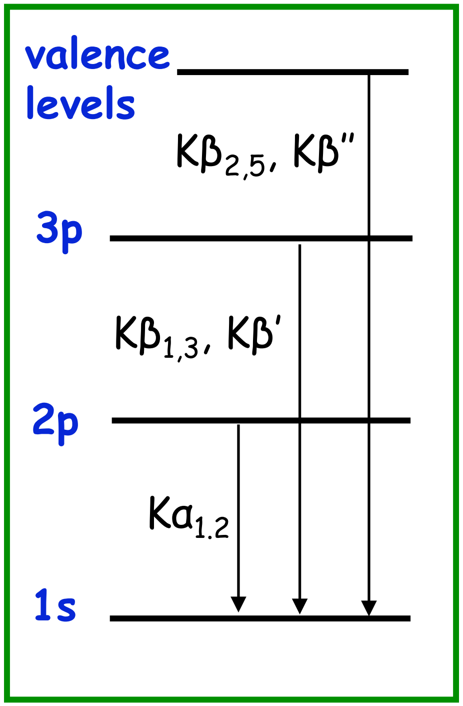
Characterization of different metal sites (edges and EXAFS) in multinuclear clusters (provided shifts in Kβ lines are large enough)

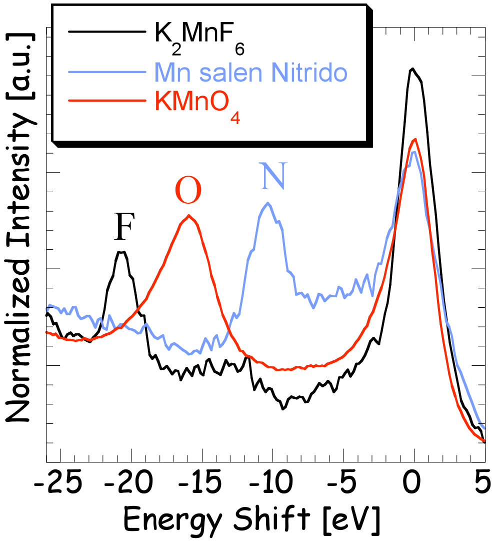
Characterization of intermediates that cannot be obtained in high yield.

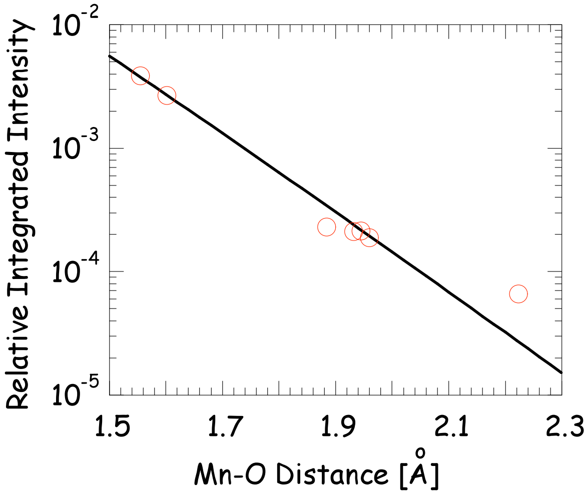
May allow for a way to examine degree of delocalization in mixed-valent systems.

Kβ" crossover peaks

level diagram





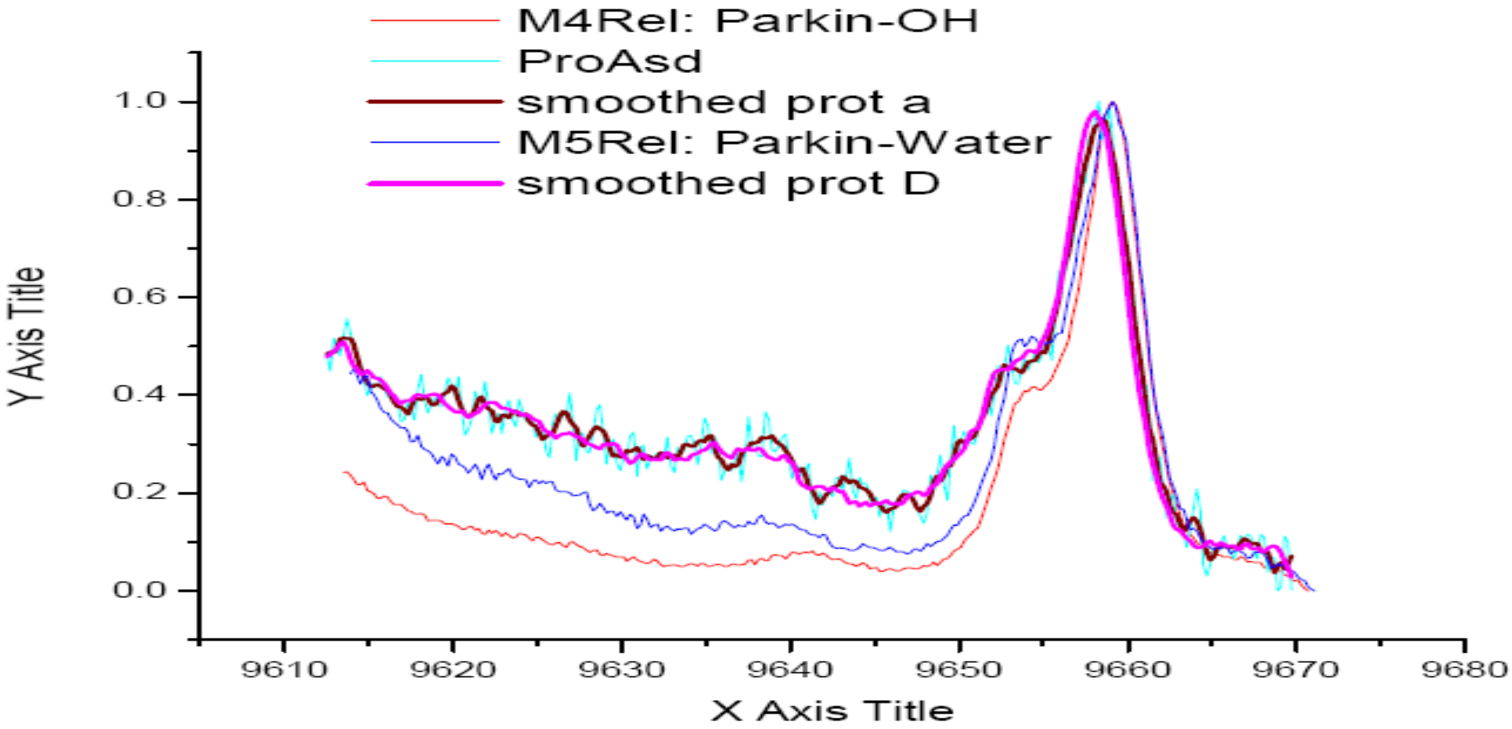


Kβ" crossover peaks are sensitive to ligand type and M-L distance.

Formally a ligand 2s to metal 1s transition, which gains intensity through metal character mixed into the ligand 2s orbitals.

Allows for N/O to be distinguished.

Kβ" crossover peaks

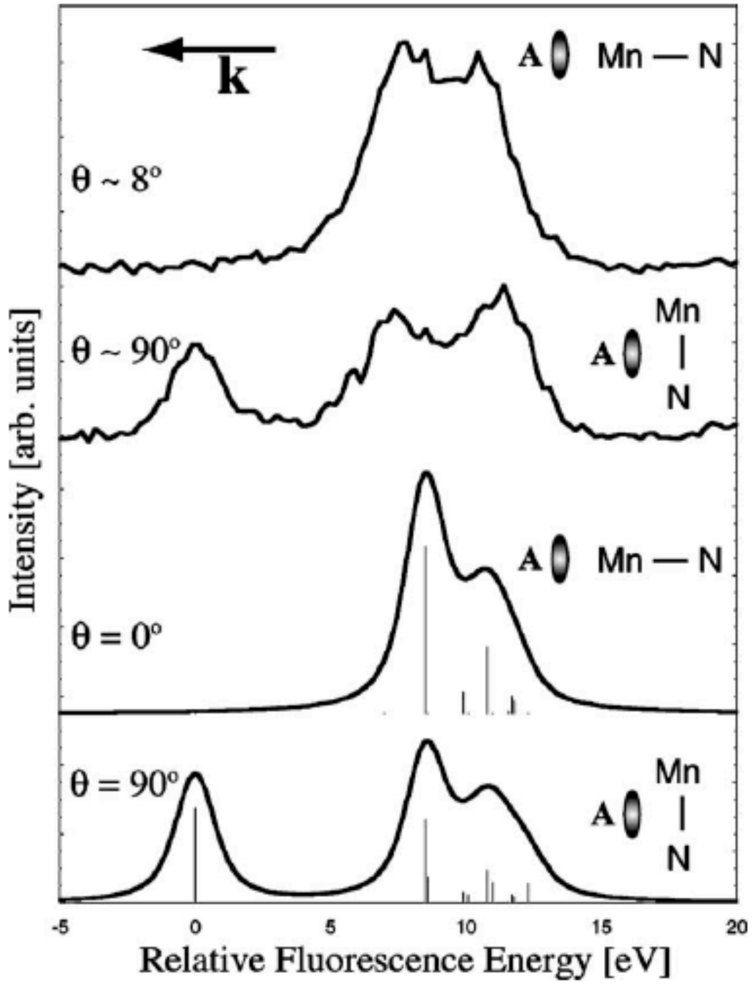


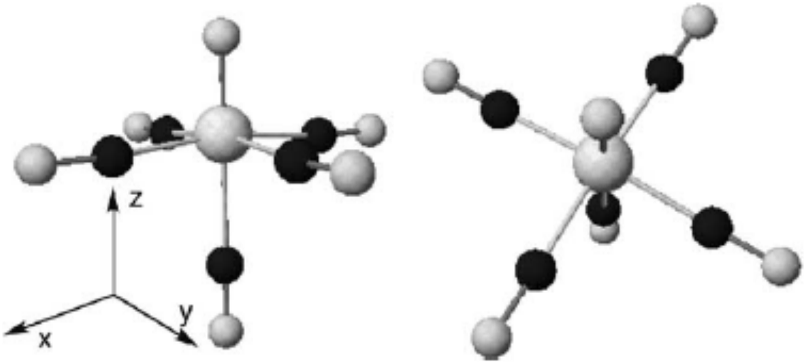
Allows for OH-/H_2O or different O_2 binding modes to be distinguished

Correlates to ligand 2s binding energies (from XPS)

Kβ" crossover peaks: Ligand Selective EXAFS

Polarized Mn XES



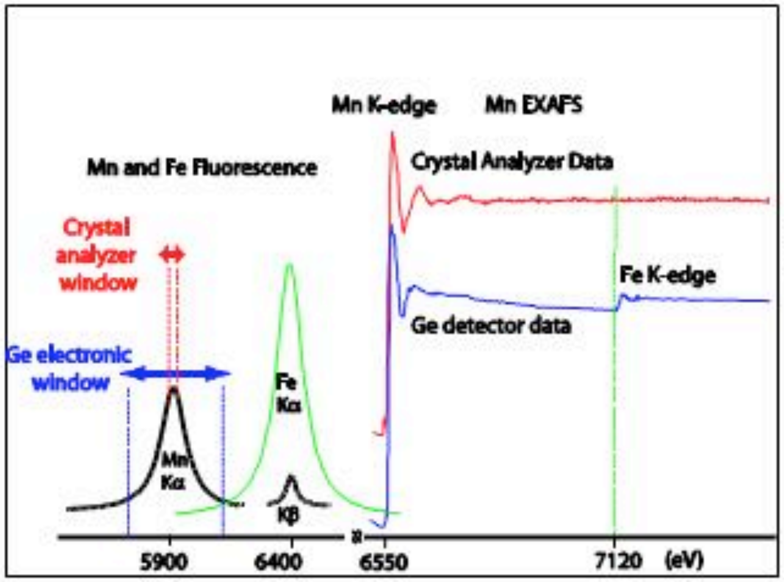


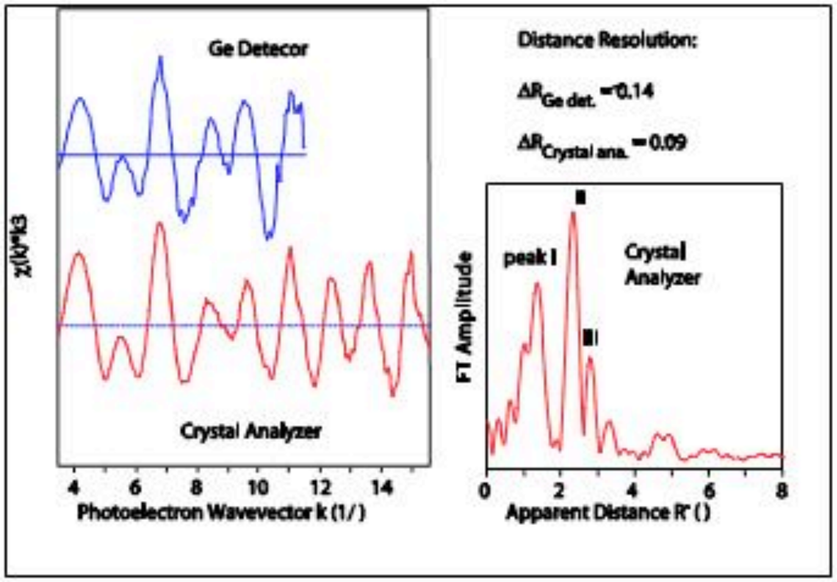
$[Mn(N)(CN)_5](H_2O)$

EXAFS: of Mn-N(nitrido) vector only

Allows for "artificially polarized" XES
- Independent of crystal packing!

Extended-Range EXAFS



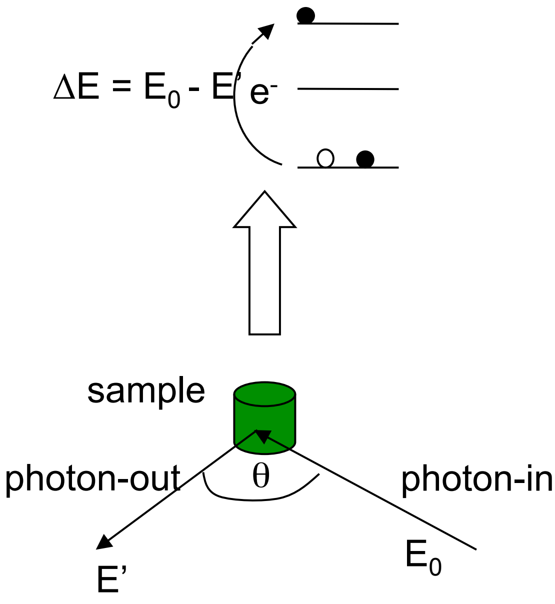


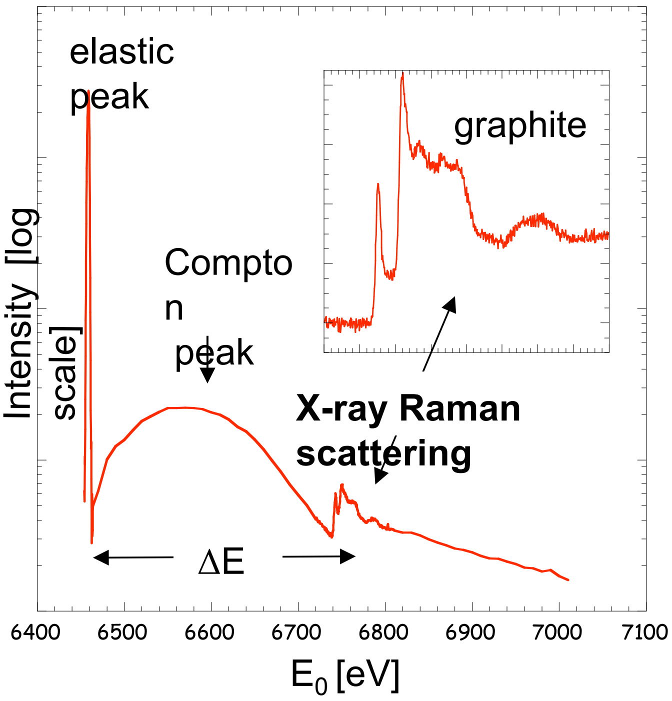
Using a standard solid state detector, fluorescence lines of neighboring atoms will overlap.

This means that the Mn EXAFS will often be cut off due to presence of a small amount of Fe and the Cu EXAFS will be truncated due to the presence of Zn.

A high resolution detector set-up allow this problem to be overcome improving the resolution of the data, but at the cost of counts.

Non-resonant Inelastic X-ray Scattering





Ability to obtain soft x-ray information, with a hard x-ray probe! (less damaging)

Monitors a scattering process, not an absorption.

NO Vacuum requirements!

Scattering probability (w):

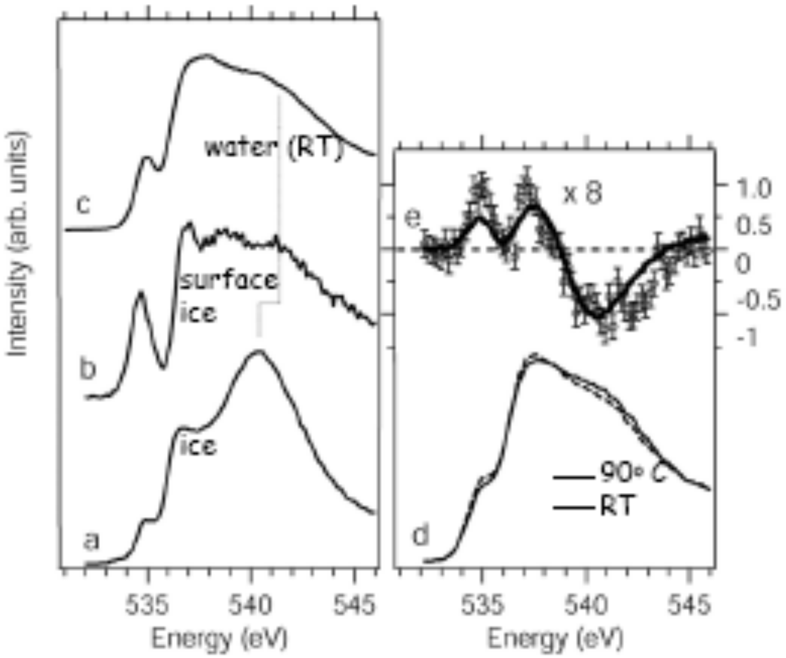
w ∝ Z^{-4}, therefore high Z elements in sample will limit scattering probability

w ∝ ΔE^{-1}, therefore lower energy edges are easier

Use a fixed incident energy and scan the analyzer.

IXS: XAS ofH_2O

O K-edges



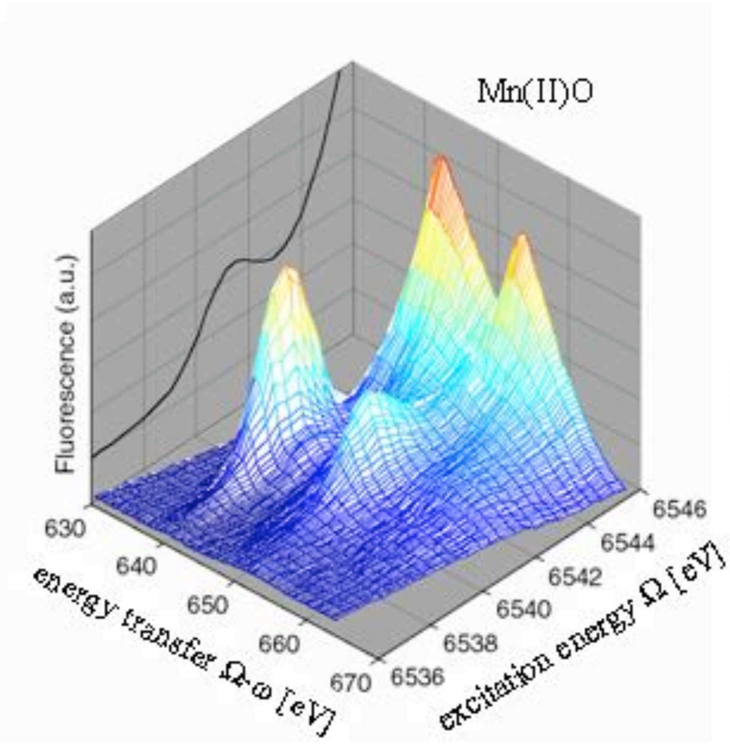
Allows for measurements of O K-edge and EXAFS of solutions.

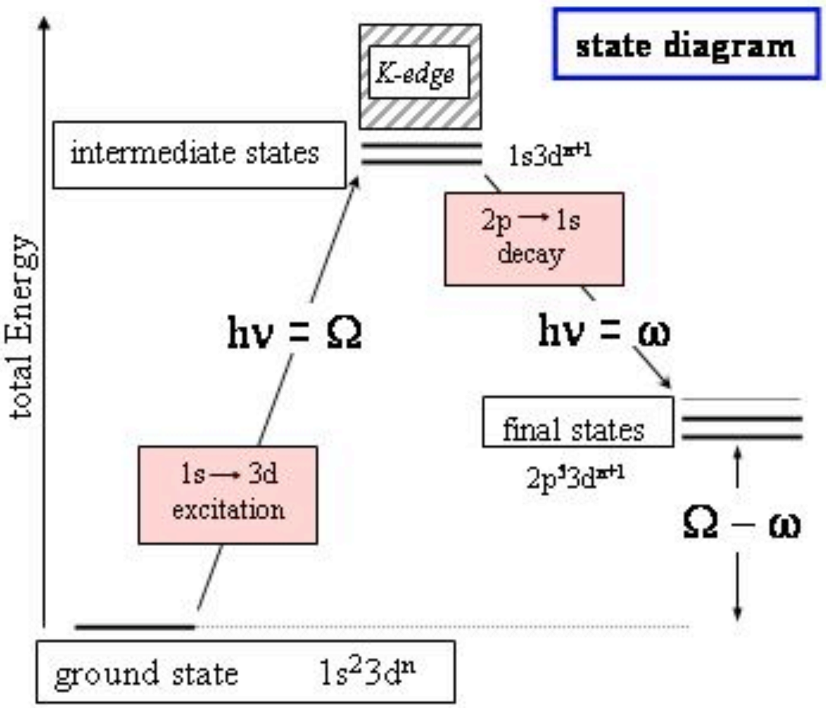
Very limited application to proteins.

Application to models in non-oxygen containing solvents.

Carbon and Nitrogen K-edges also accessible.

Resonant Inelastic X-ray Scattering





Inelastic scattering of the incident photon at the atom of interest

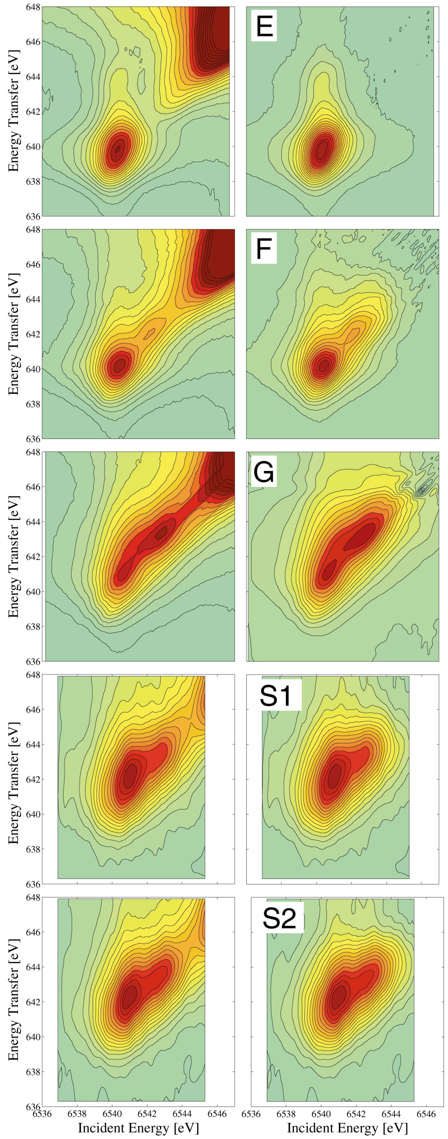
Similar to non-resonant methods, but the incident energy is close to an absorption edge (analogous to resonance Raman)

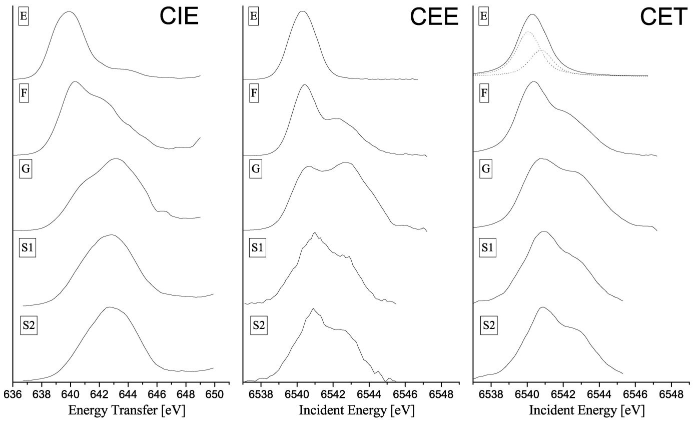
Scan both the incident energy and the analyzer.

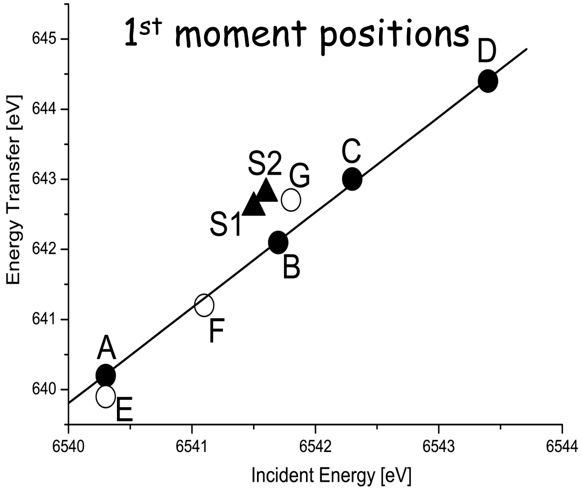
L-edge information from a high energy x-ray probe.

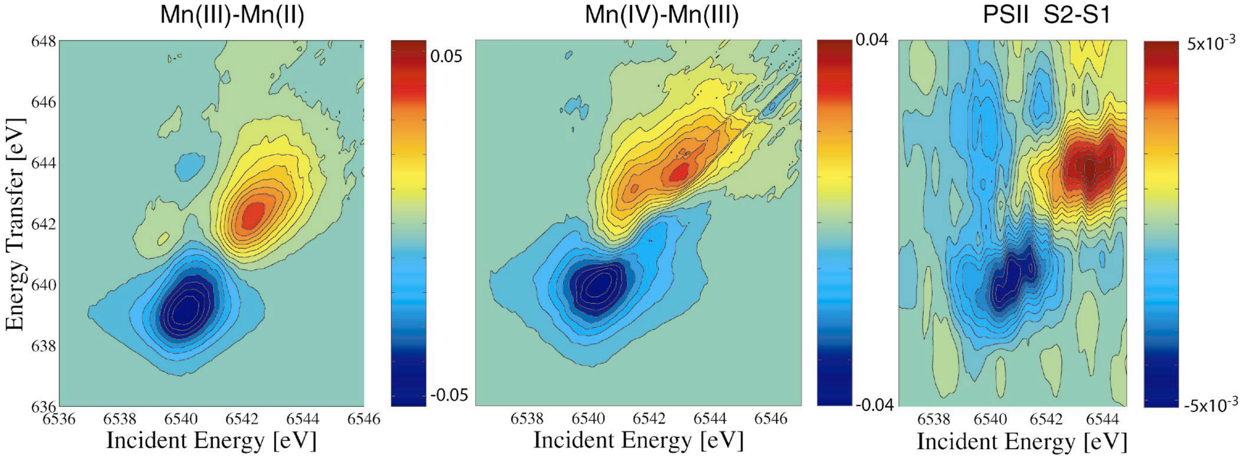
RIXS Spectra of Mn models and PSII

E: MnII(acac)$_2$(H2O)$_2$ F: MnIII(acac)$_3$ G: MnIV(sal)$_2$(bipy)









Glatzel et al, JACS.

Inelastic X-ray Scattering

IXS, both resonant and non-resonant, allows for new probes of solution chemistry that was not previously accessible using conventional vacuum measurements.

Allows for combined metal L- and ligand K- information using a hard x-ray probe on the same beam line with the same setup.

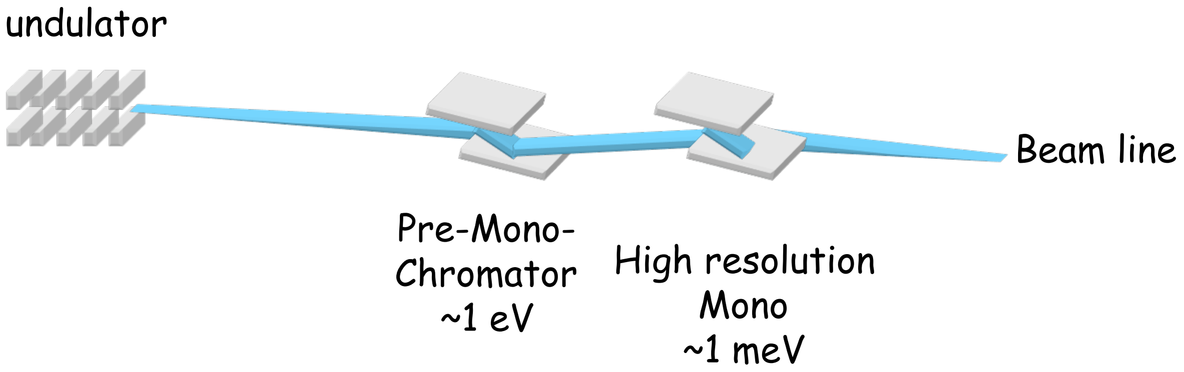
Applications of non-resonant methods to obtain O K-, N K-, and C K- can be limiting.

RIXS provides resonance signal enhancement and added dimension. Interpretation is less straightforward.

Experiments require appropriate analyzer crystals…

Element	Emission	Energy [keV]	Analyzer	Bragg angle	Resolution (eV)	Radius [mm]/ aperture [mm]
Mn	Kα_1	5.899	Ge(333)	74.8	0.22	1500/50
	Kα_2	5.888	Ge(333)	75.3	0.21	1500/50
	K$\beta_{1,3}$	6.491	Si(440)	84.2	0.2	1000
	Kβ”	6.519	Si(440)	82.1	0.25	1000
Fe	Kα_1	6.404	Si(333)	67.8	0.35	1500/50
	Kα_2	6.391	Si(333)	68.1	0.35	1500/50
	K$\beta_{1,3}$	7.058	Ge(620)	79.1	0.5	1000
	Kβ”	7.092	Ge(620)	77.8	0.6	1000
Cu	Kα_1	8.048	Si(444)	79.3	0.28	1500
	Kα_2	8.028	Si(444)	80.1	0.25	1500
	K$\beta_{1,3}$	8.905	Si(553)	79.9	0.6	1000
	Kβ”	8.959	Si(553)	78.1	0.7	1000
Zn	Kα_1	8.639	Si(642)	81.4	0.2	1500
	Kα_2	8.616	Si(642)	82.5	0.2	1500
	K$\beta_{1,3}$	9.572	Ge(555)	82.5	0.4	1000
	Kβ”	9.639	Ge(555)	79.9	0.6	1000

High Resolution Beam Lines



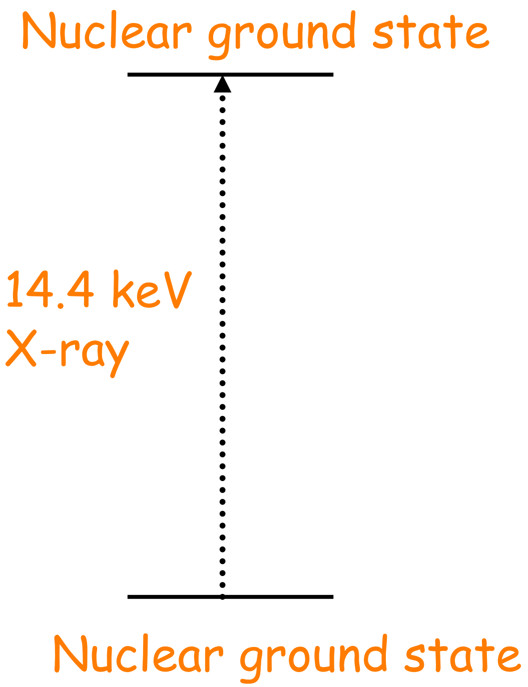
Pre-monochromator reduces power load on high res. mono (1000 to 0.1 W)

High res. mono – 4 crystal diamond mono

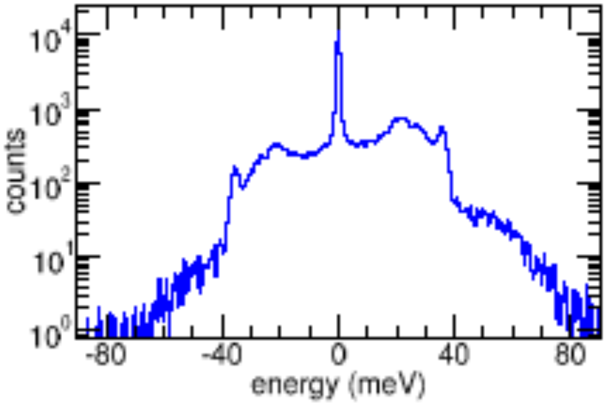
Flux “loss” ~10^6 photons

Tunable range of high res. mono is small (a few hundered meV)

Nuclear Resonant Vibrational Spectroscopy



NRVS (or NRIXS) spectrum of ^{57}Fe foil



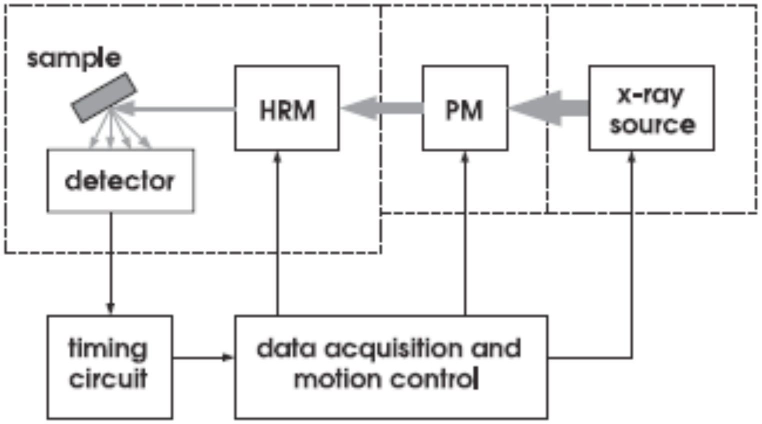
W. Sturhahn, *J. Phys. Cond. Matt.* 16, **2004**, S497.

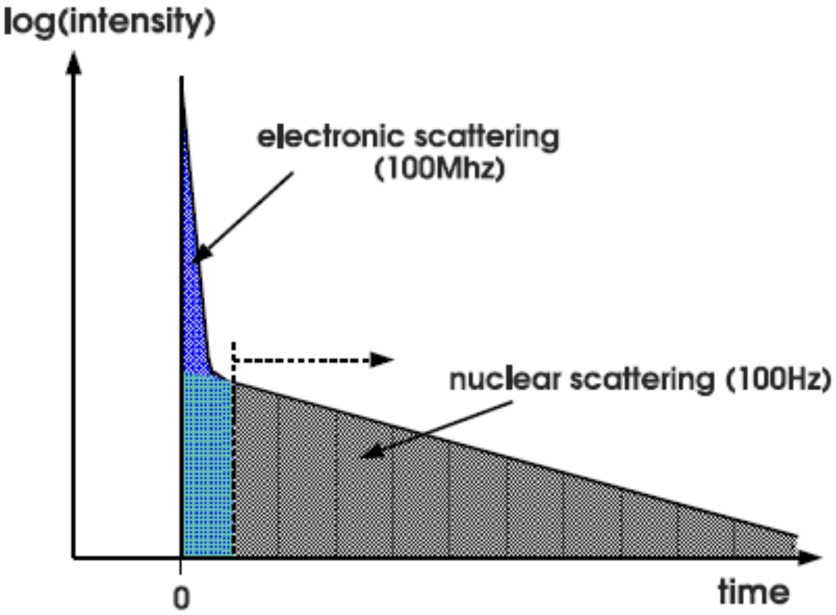
Spectrum is dominated by Mössbauer resonance (at E=0, cross-section at E≠0 order of magnitude weaker)

Additional transition correspond to nuclear excitation in combination with excitation (Stokes) or de-excitation (Anti-Stokes) of vibrational modes.

Selection is based on motion of resonant nucleus.

NRVS: Detection





Monitor all processes following nuclear excitation: : i.e. 14.4 keV emission, transfer of excitation energy to electron shell

Average delay – from nuclear excitation to decay ~141 ns (^{57}Fe)

Scattering from electrons – femtosecond time scale

Use timing difference to see events associated with nuclear excitation only

NRVS: Vibrational Density of States

$E_{x\text{-}ray} = E_{nuc\ trans} + E_{vib}$

w [illegible] ΔE^{-1}

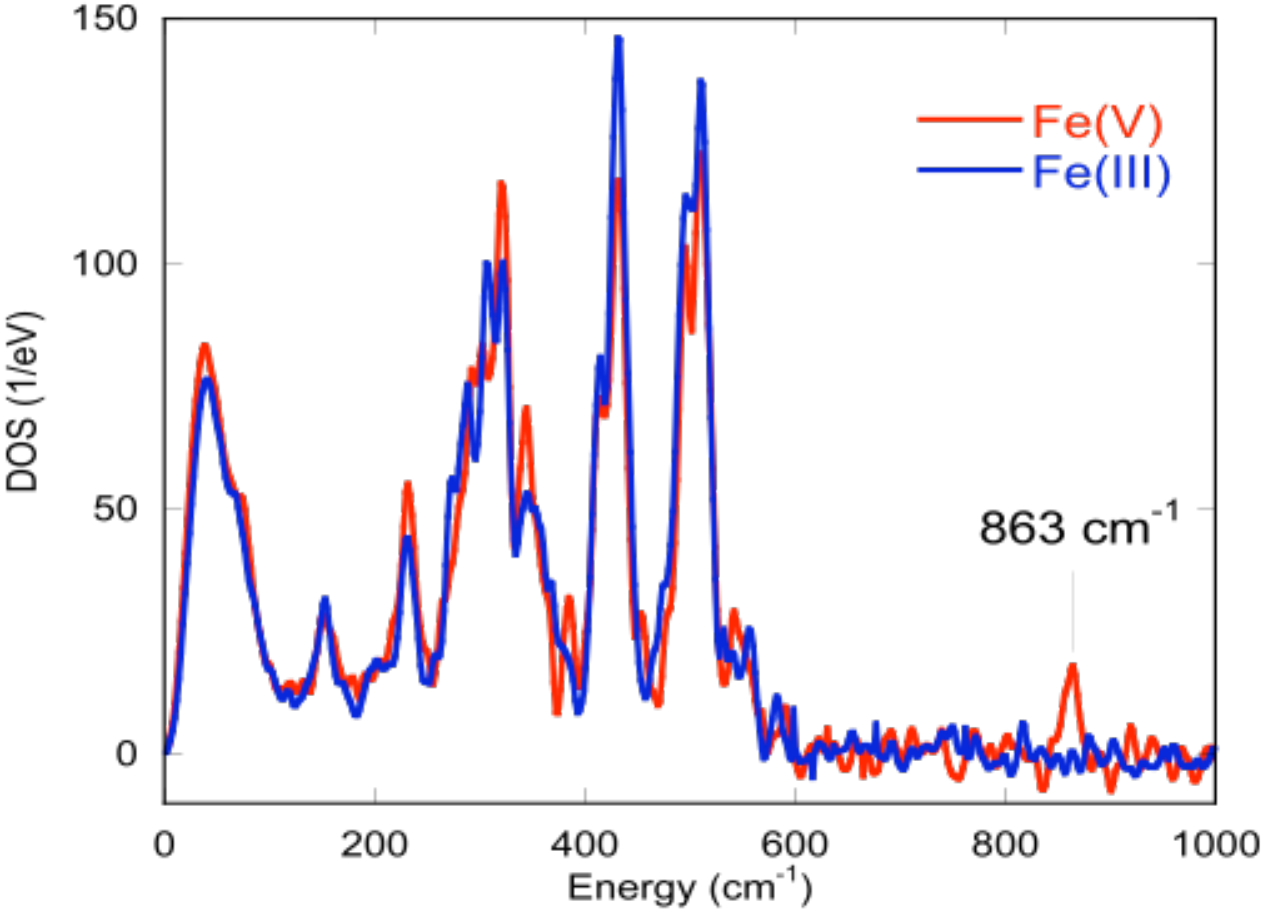
Fe mode composition factor:

$$e^2_{Fe,\alpha} = \frac{m_{Fe} r_{Fe,\alpha}{}^2}{\sum_j m_j r^2_{j,\alpha}}$$

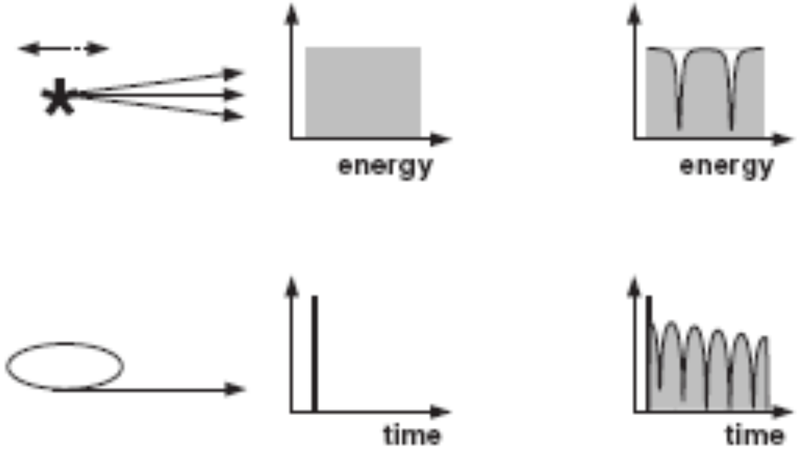
m = mass of atom; r^2 = mean square motion

Selection rule: Movement of resonant nucleus along direction of incident beam (polarized measurements possible)

NRVS of Fe(V)-nitrido and Fe(III)-azide



Synchrotron Mössbauer Spectroscopy (SMS)



Conventional Mössbauer

Synchrotron Mössbauer

J. Jackson et al, Amer. Miner., ***2005****, 90, 199.*

SMS utilizes pulsed nature of synchrotron beam

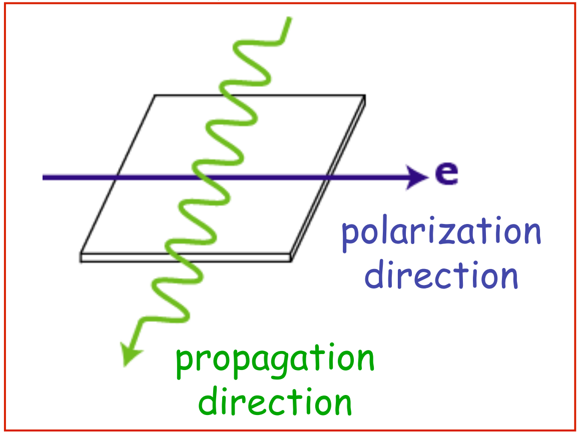
Resonantly excite all Fe nuclei and follow time-dependent transmission.

FT of time spectrum is energy. Both give quadrupole splitting.

Isomer shift in conventional Mössbauer relative to source in SMS (relative to reference absorber).

Polarized XAS

Synchrotron radiation is polarized



X-ray absorption cross section (σ) is related to polarization vector (**e**) in dipole approximation by:

$$\sigma \propto \sum \left|\langle f|\mathbf{e}\cdot\mathbf{r}|i\rangle\right|^2$$

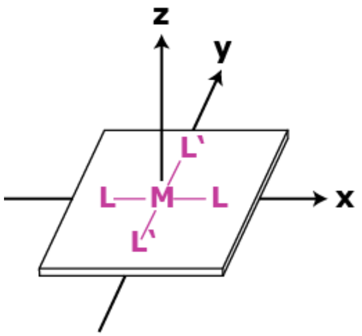
For a 1s initial state (K-shell):

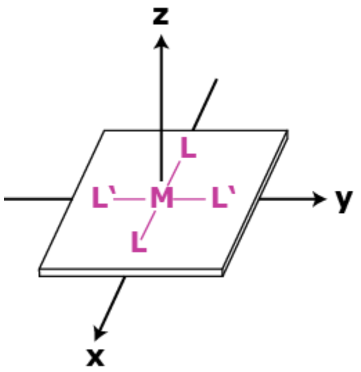
$$\sigma \propto \sum \cos^2\theta \left|\langle f|\mathbf{r}|i\rangle\right|^2$$

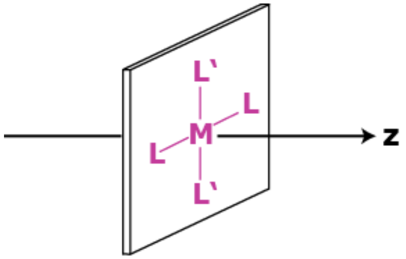
where θ = ∠ between **e** and **r**

In isotropic systems, polarized spectral features of the molecular dipoles (x, y, z) are averaged over all orientations → 1/3 polarized intensity

With anisotropic crystals, polarization vector can be aligned along molecular vectors to selectively enhance specific features

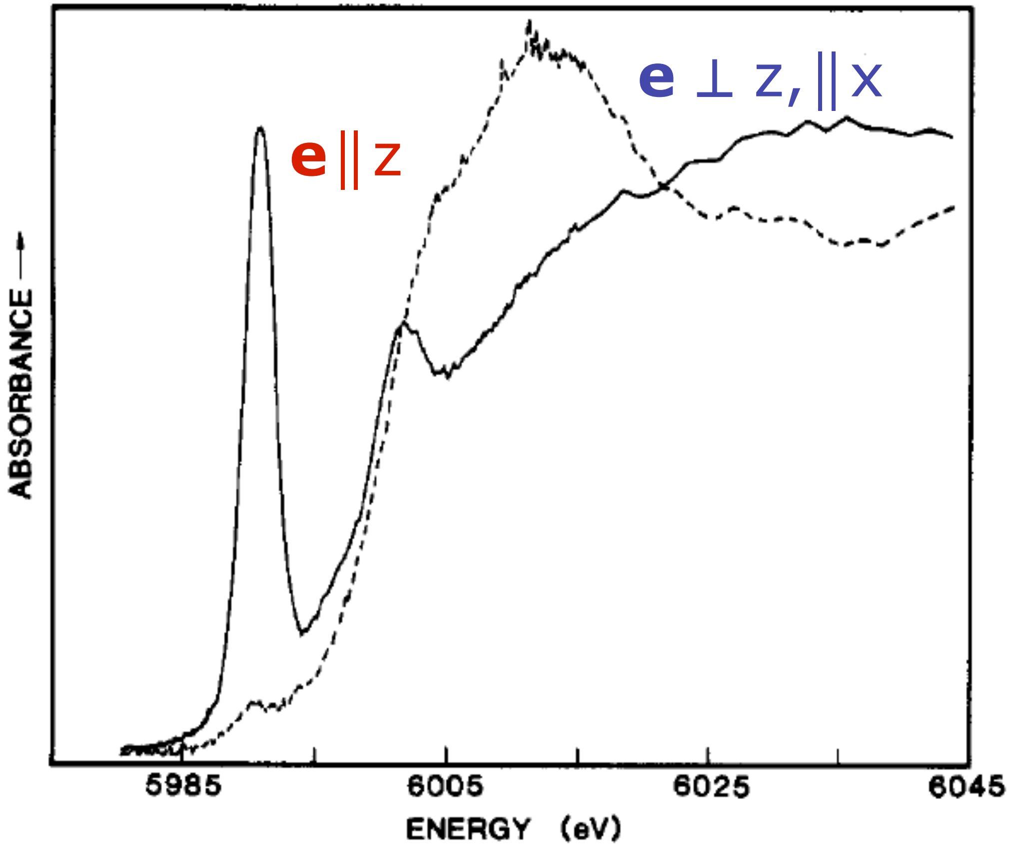


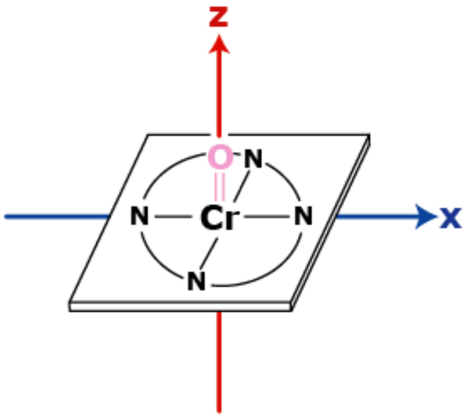




Polarized XAS: Edges

Polarized Cr K-edge XAS spectra of $\mathrm{Cr^{IV}}$(TPP)O crystal in two pre-aligned orientations



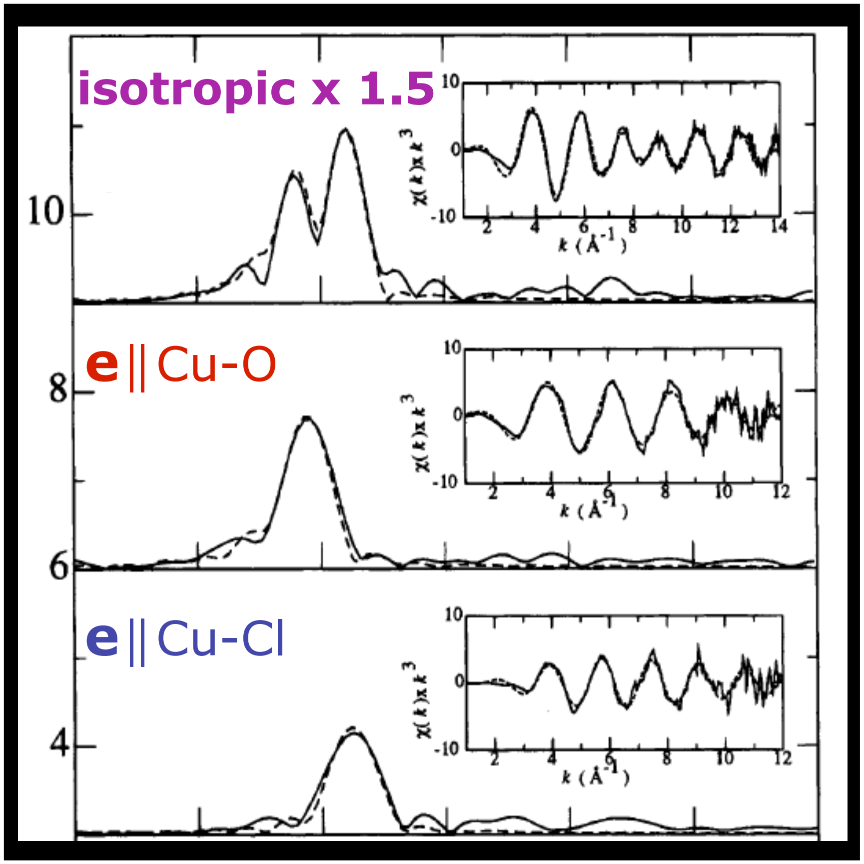


Pre-edge intensity in z-parallel orientation indicates significant amount of ligand p_z mixing into metal 3*d* orbitals

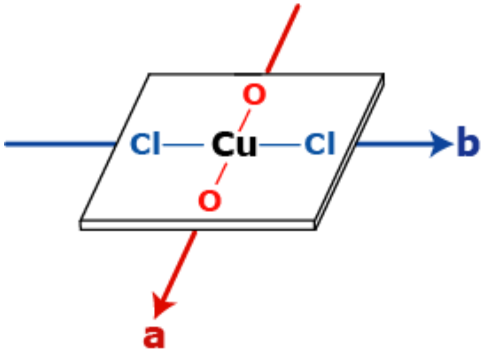
Penner-Hahn, Benfatto, Hedman, Takahashi, Doniach, Groves, Hodgson (1986) *Inorg Chem* **25**, 2255.

Polarized XAS: EXAFS

Cu K-edge EXAFS spectra and FTs of $CuCl_2 \cdot H_2O$
powder and oriented single crystal

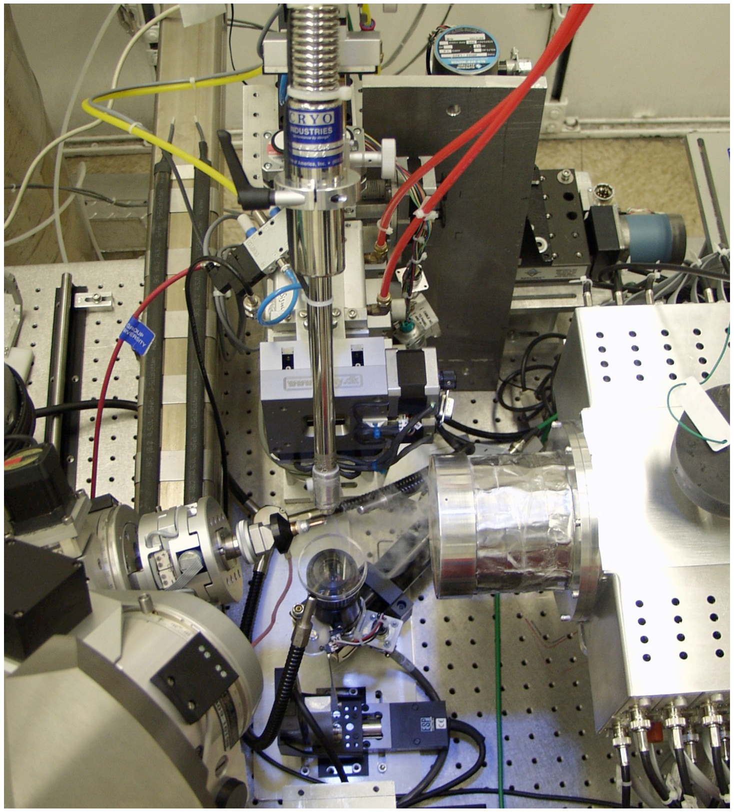


Pickering & George (1995) *Inorg Chem* **34**, 3142.



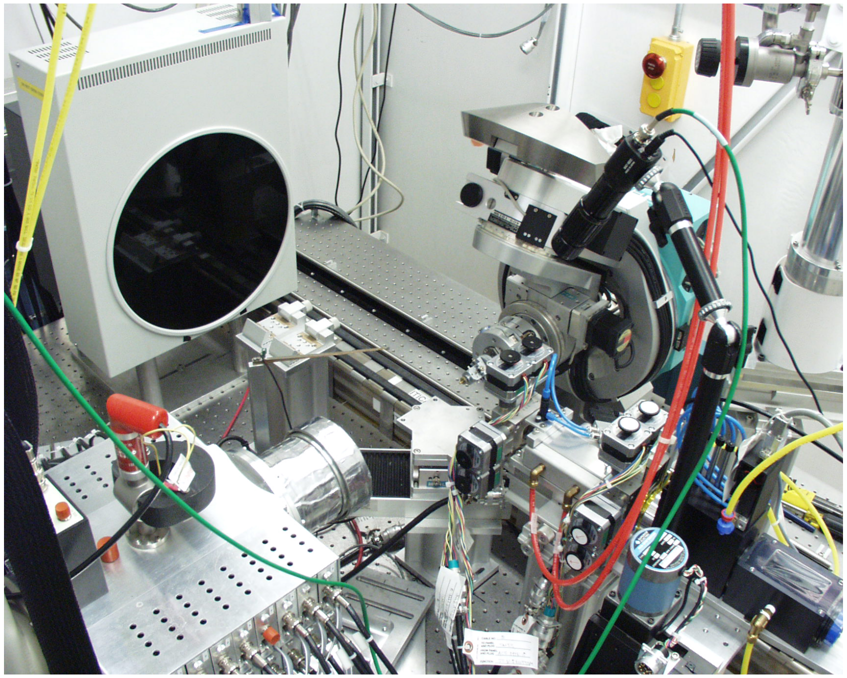
Polarization provides both differentiation and enhancement of structural features

SSRL BL9-3 – Combined Capabilities for XAS and PX



LHe cryo cooler in use

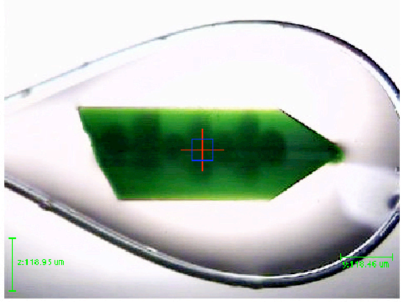
mar345 imaging plate detector also used for diffraction measurements

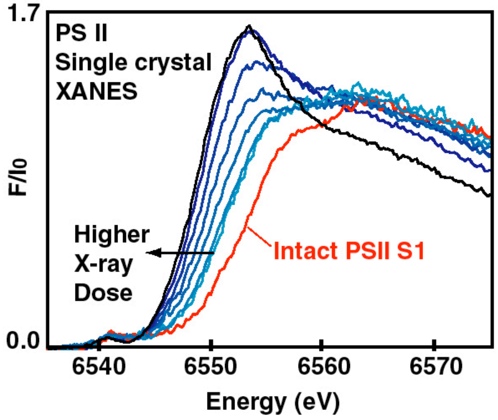


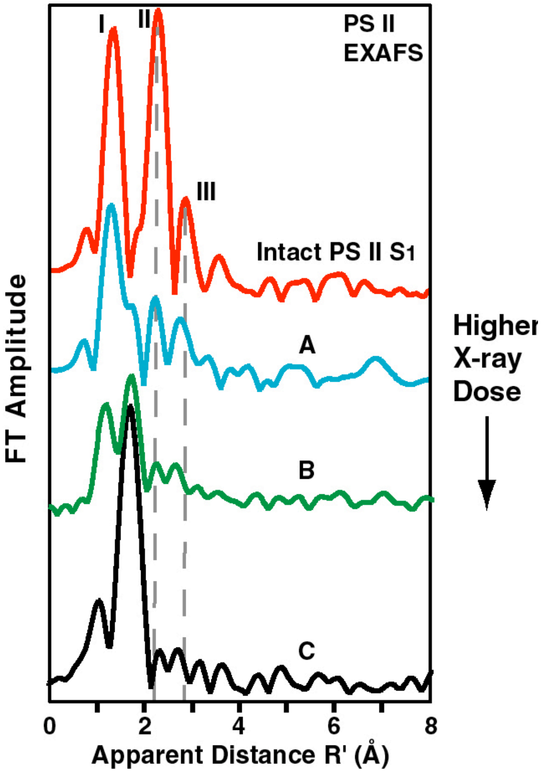
"X-ray Damage to the Mn4Ca Complex in Single Crystals of Photosystem II Studied Using *In Situ* X-ray Spectroscopy: A Case Study for Metallo-Protein Crystallography"

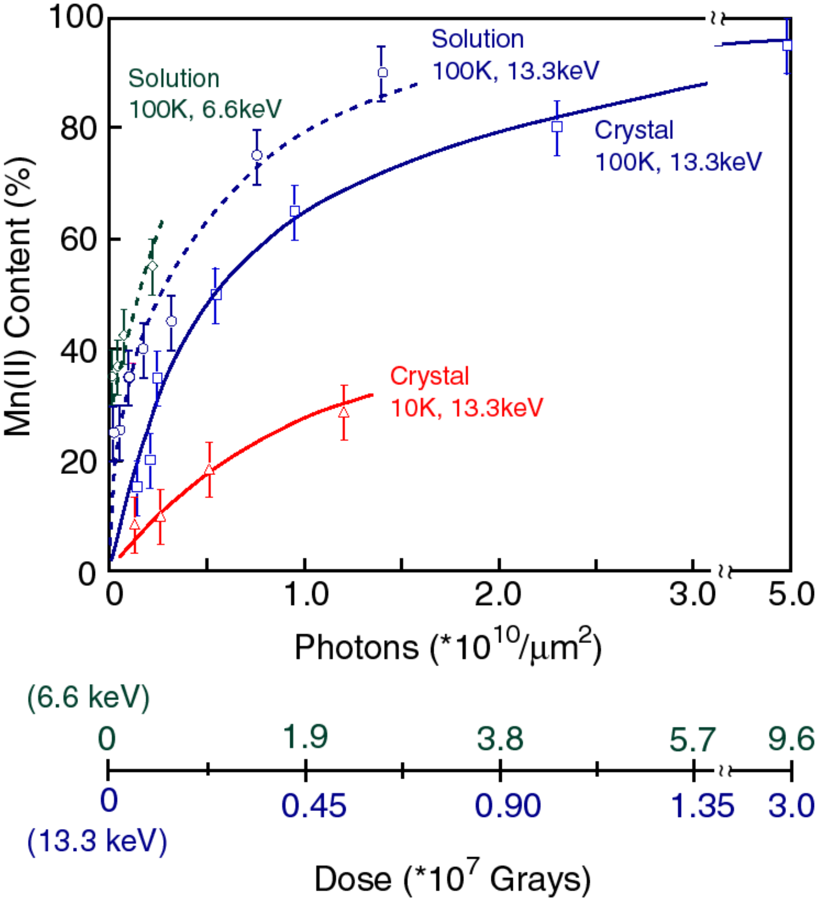
Yano, J et al. *Proc. Natl. Acad. Sci. USA* **2005**, *102*, 12047.

PS II Crystal









XAS Imaging

Uses very small beams to raster samples and obtain spatial resolution

- elemental distribution (fluorescent microprobe, micro-XF, SRIXE)
- chemical distribution (micro-XAS)

Use particular fluorescent emission line or edge feature to create a "distribution map"

Spot size depends on method used:

	spot size (microns)
aperture	20
capillary	5
KB optics	1
zone plates	0.1

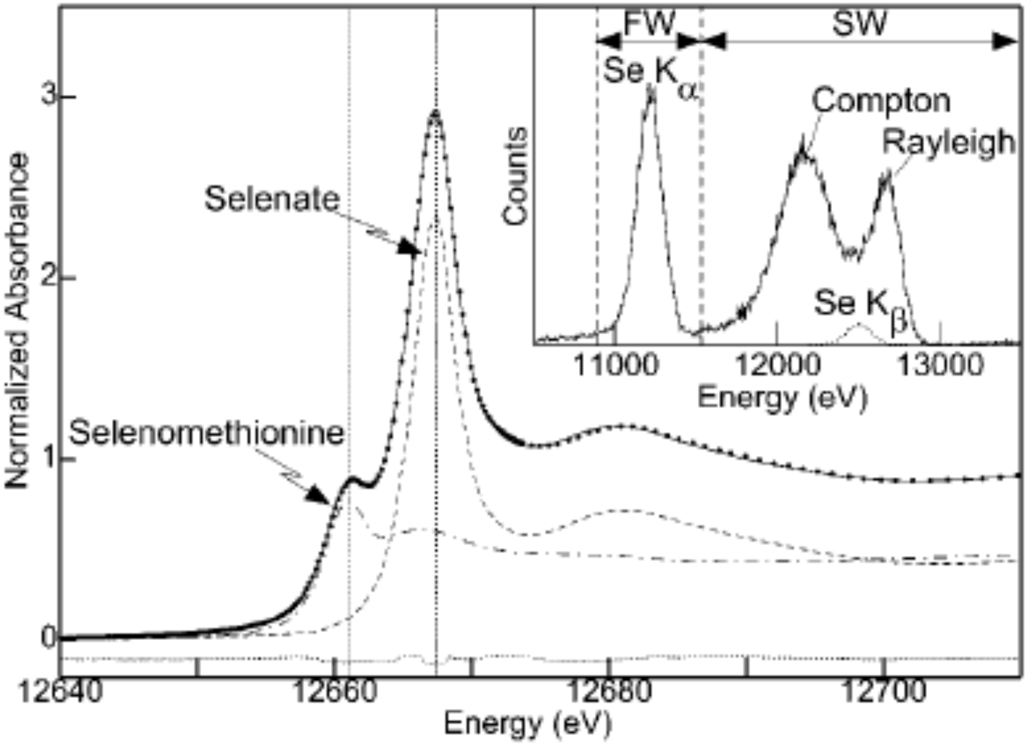
XAS Imaging: Selenium Transformation in Plants

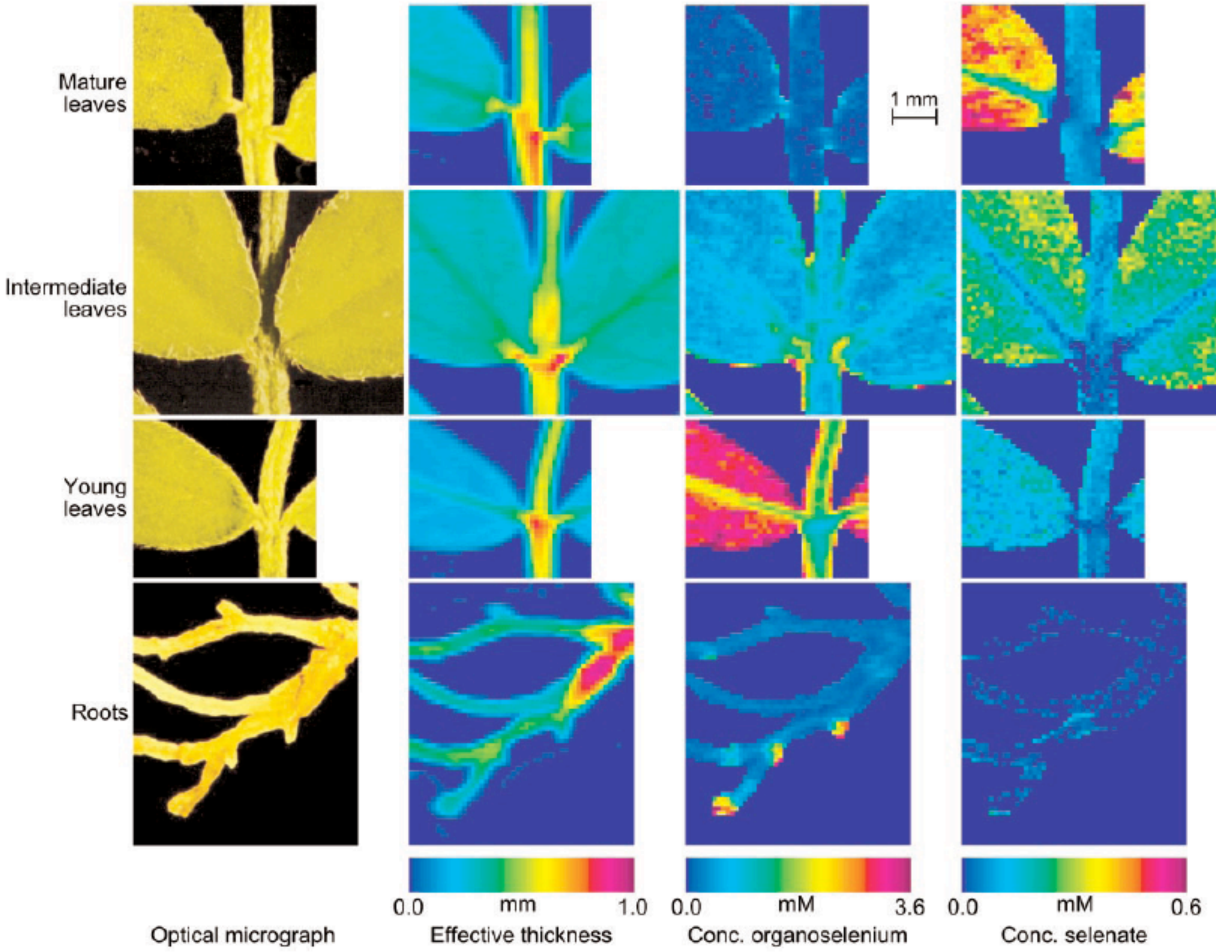
*Pickering et al. PNAS, **2000**, 97, 10717*

Application to *Astragalus bisulcatus,* A selenium hyperaccumulating plant

Tune X-ray energy to different chemically specific features in rising edge

Determine relative change in fluorescent intensities and generate intensity maps





100 micron resolution

Mature leave-
Selenate in leaves

Young leaves-
organoselenium

Possible insight into biochemical transformation of selenium

Conclusions

Using additional laboratory and synchrotron based spectroscopy methods allows for a more detailed understanding of sample geometric and electronic parameters.

Using high resolution detection methods allows us to extend the information we can get from XAS (site-selective and ligand-selective XAS)

High resolution detection also allows for measurement of XES spectra, and IXS (both resonant and non-resonant)

High-resolution beam lines allow for NRVS and SMS

Time structure, polarization, and beam collimation also allow for extended capabilities

Acknowledgements

Special thanks to Frank Neese, Uwe Bergmann, Mary Corbett, and Britt Hedman!