实用中子衍射晶体学

Practical Neutron Diffraction Crystallography

(I)

粉末衍射和材料科学

Powder Diffraction and Materials Science

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中国散裂中子源

China Spallation Neutron Source

China Spallation Neutron Source (CSNS)

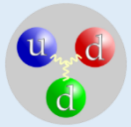
In different periods, the design and construction of different instruments and equipment must be based on needs of national and/or reginal science and technology and economic development.

第一期

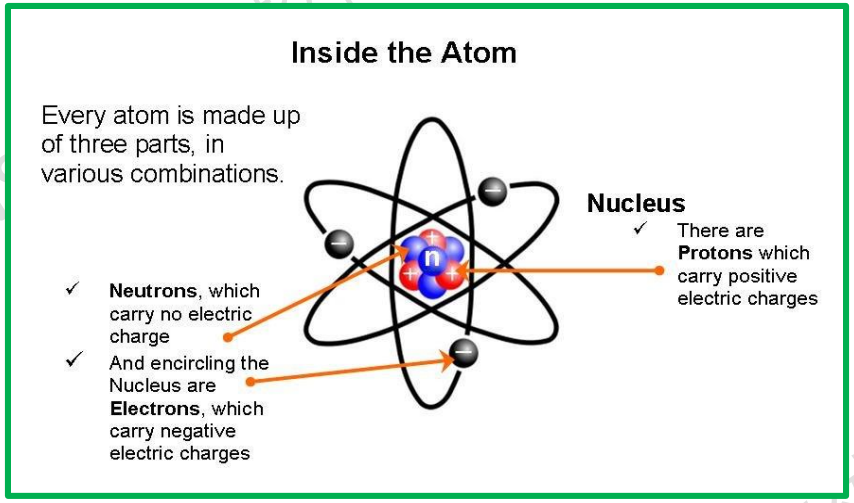
BL18: General-Purpose Powder Diffractometer
BL02: Multi-Purpose Reflectometer
BL01: Small-Angle Neutron Scattering
BL16: Multi-Physics Instrument
BL11: Atmospheric Neutron Irradiation Spectrometer
BL05: High-Energy Direct-Geometry Inelastic Spectrometer
BL13: Energy-Resolved Neutron Imaging Instrument
BL14: Very Small-Angle Neutron Scattering
BL15: High-Pressure Neutron Diffractometer
BL09: High-Resolution Neutron Diffractometer
BL08A: Engineering Material Neutron Diffractometer

第二期

BL20: Direct-Geometry Polarized Inelastic Spectrometer
BL12: Neutron Physics and Application Spectrometer
BL19: Macromolecular Single-Crystal Neutron Diffractometer
BL17: Elastic Diffuse Scattering Neutron Diffractometer
BL10: Neutron Backscattering Spectrometer
BL04: Cold Neutron Inelastic Spectrometer
BL08B: Neutron Technology Development
BL03: Liquid Reflectometer
BL06: Indirect-Geometry Molecular Vibrational Spectrometer



Neutron, A Subatomic Particle

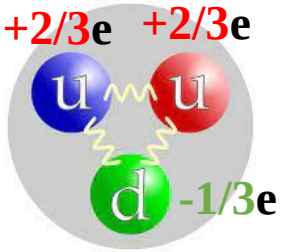


All matters are composed of tiny particles call atom. Every atom is made up of three types of smaller subatomic particles, electron, neutron, and proton. Proton and neutron make up nucleus, surrounded by electrons.

Proton

two “up” quarks (charge +4/3 *e*)

one “down” quark (charge -1/3 *e*)



+e

Proton

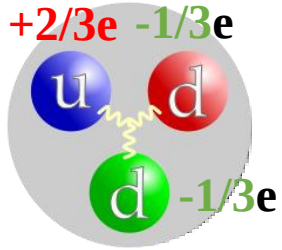
U = "up" quark $+\frac{2}{3}$ e

D = "down" quark $-\frac{1}{3}$ e

Neutron

one “up” quark (charge +2/3*e*)

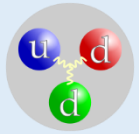
two “down” quarks (charge −2/3 *e*)



0e

Neutron

The proton carries two “up” quarks and one “down” quark, while the neutron carries one “up” quark and two ‘down” quarks. The “up” quark have +2/3 e, and the “down quark has -1/3 e. So that the proton carries +e, and the neutron is a neutral particle.



Intrinsic Properties of Neutron, Wave-particle Duality

中子的本征性质， 波粒二象性

Theorized	Ernest Rutherford (1920)
Discovered	James Chadwick (1932)
Mass	$1.67492749804(95)\times10^{-27}$ kg, 939.56542052(54) MeV/c^2, 1.00866491588(49) Da
Mean lifetime	879.4(6) s (free)
Electric charge	0 e $(-2\pm8)\times10^{-22}$ e (experimental limits)
Electric dipole moment	$< 2.9\times10^{-26}$ e·cm (experimental upper limit)
Electric polarizability	$1.16(15)\times10^{-3}$ fm^3
Magnetic moment	$-1.04187563(25)\times10^{-3}\mu_B$, $-1.91304273(45)\ \mu_N$
Magnetic polarizability	$3.7(20)\times10^{-4}$ fm^3
Spin	1/2
Wavevector	Magnitude $2\pi / \lambda$
Wavelength	h/mv
Energy (E)	$(1/2)mv^2=h^2/2m\lambda^2$

1. The most mass of an atom comes from proton and neutron. The mass of a neutron （$1.67492749804(95)\times10^{-27}$ kg） is slightly greater than a proton.
2. Neutrons accompany protons in nucleus. When neutrons leave nucleus become free, the average lifetime of a free neutron is about 14.66 minutes.
3. Although neutron is a neutral particle, it carries zero electric charge. The magnetic moment of neutron is not zero.
4. It has spin ½ with moment of -0.001042 μ_B.
5. This is an indication of its quark substructure and internal charge distribution.
6. Energy $E= \frac{1}{2} mv^2=h^2/2m\lambda^2$, that is the lower v the lower E or the shorter λ the higher E.
7. Neutrons move in a wave mode; the wavelength $\lambda=h/mv$, *i.e.* the higher v the shorter λ.
8. The magnitude of wavevector ($2\pi / \lambda$) is a function of wavelength.
9. Neutrons possess wave-particle duality.

Neutron, Wave-Particle Duality

Wave Neutron diffraction is a form of elastic scattering where the neutrons exiting the experiment have the same energy as the incident neutrons. This technique can be used to study the atomic and magnetic structures of a material, such as crystalline solids, amorphous, liquids, and gasses.

中子衍射类似X-射线衍射，是一种弹性散射，即实验中的入射与散射的中子具有相同的能量。但不同的辐射所得到的信息具有互补性.中子衍射用于分析晶体结构/磁结构，适用研究结晶固体，气体，液体以及非晶材料。

Particle Inelastic scattering occurs because the atoms in a solid are of finite mass and they can gain or loss energy when neutrons, or any kind of radiation, collide with them. It can used to study the atomic dynamics of the sample, such as quantum materials, energy-related materials, soft matter, complex fluids, biology, magnetic excitations, vibrational and rotational， diffusional processes and quantum tunnelling.

非弹性散射发生在当中子或任何类型的辐射与固体中的原子碰撞时获得或损失能量。用来研究量子材料，能量相关材料，软物质，复合流体，生物学，磁激发，振动和旋转光谱，扩散过程和量子隧道等。

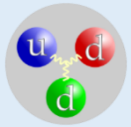
Elastic and Inelastic Scattering

Table 1.1.1

Types of scattering from a sample

Type of scattering	Coherent	Incoherent
Elastic **Wave** Neutrons scattering from a sample have the same energy as the incident neutrons.	Bragg scattering Magnetic Bragg scattering Bragg scattering from ferroelectric/magnetic order Diffuse scattering from static defects Diffuse signal from small nanoparticles (<10 nm) Scattering from amorphous material (except excitations) Multiple scattering (coherent)	Laue monotonic diffuse scattering Neutron incoherent scattering Multiple scattering (incoherent)
Inelastic **Particle** The neutrons gain or lose some energy as scattering from a sample.	Thermal diffuse scattering Spin-wave scattering Paraelectric/paramagnetic scattering Scattering from liquids	Compton scattering Fluorescence Incoherent scattering from hydrogen

When atoms in a solid are of finite mass and they do or don't gain or loss energy when neutrons, or any kind of radiation, collide with them.



中子的优势特点

为什么用中子？中子有揭示了其他探针无法获得的特性的能力。它可以像波一样衍射或反射，或者像粒子在运动过程中与物质碰撞时获得或失去能量。

波长 从0.1A到100A不等，允许它们测量从像原子一样小到蛋白质一样大的结构。

能量 在毫电子伏特量级，与固体或液体中原子运动，磁性材料中的波或分子振动的能量相同。可以检测的小的纳米电子伏特和十分之一电子伏特的中子与物质之间的能量交换。

散射本领 几乎随机地因原子核而异。有利于对探测轻的原子，同位分离等。

磁性 使得中子对原子中的电子自旋和电子的轨道自旋的有序度都很敏感。

穿透能力强 中性的中子使得其能够深入样品，更容易穿过极端条件环境设备壁达到样品，深入测量工程部件中的应力应变。

Table 2.3.5
Advantages of CW and TOF instruments (modified from Kisi & Howard, 2008)

CW	TOF
(1) Incident beam may be essentially monochromatic, in which case the spectrum is well characterized 入射中子基本单一波长，谱图特性好	(1) The whole incident spectrum is utilized, but it needs to be carefully characterized if intensity data are to be used 运用全入射谱，强度数据需仔细进行刻度校正。
(2) Large *d*-spacings are easily accessible for study of complex magnetic and large-unit-cell structures 能测量大d值晶面间距，有利于分析复杂磁结构和大晶胞晶体结构	(2) Data are collected to very large *Q* values (small *d*-spacings) 能测量非常大Q值数据 (小晶面间距*d*)
(3) Can fine tune the resolution during an experiment 在实验过程中能调整分辨率	(3) Few cold neutron instruments are available for study of complex magnetic and large-unit-cell structures 冷中子谱议可用于研究磁结构和大晶胞结构。
(4) More common 更通用	(4) Resolution is constant across the whole pattern 整个谱图的分辨率不变
(5) Peak shapes are simpler to model 峰型简单更容易拟合	(5) Very high resolution is readily attained by using long flight paths 用长的飞行管道可达到非常高的分辨率
(6) Absorption and extinction corrections are relatively straightforward 吸收和消光校正相对简单	(6) Complex sample environments are very readily used if 90° detector banks are available 复杂的样品环境可用于90度的探测器组。
(7) Data storage and reduction is simpler 数据存储和简化简单	(7) Simpler to intersect a large proportion of the Debye–Scherrer cones with large detector banks 用大的探测器组对横切大比例Debye-Scherrer锥更为简单。
(8) Extremely rapid data collection and stroboscopic measurements are feasible 可进行极快的数据收集和频闪测量	(8) Very fast data collection is feasible 数据采集非常快捷。
(9) Engineering diffractometers are very well suited for strain scanning in complex objects 工程衍射仪非常适合复杂构件的应变扫描	(9) Engineering diffractometers use an extended diffraction pattern, ideal for *in situ* loading and/or heating 工程谱议适合原位加载和/或加热，连续采集衍射谱。
(10) Texture is straightforward to measure on engineering diffractometers 工程衍射仪对织构测量简单容易	(10) Texture can be measured on universal instruments 通用谱议可测织构。

Table 2.3.6
Suitability of problems to high-resolution or high-intensity diffractometers

Reproduced from Kisi & Howard (2008) by permission of Oxford University Press.

Problem	High resolution	High intensity (medium resolution)
Solve a complex crystal or magnetic structure 分析复杂晶体结构或磁结构	Essential, especially in the presence of pseudo-symmetry	Not usually suitable†‡
Refine a complex crystal or magnetic structure 精化复杂晶体结构或磁结构	Essential. Will benefit from a high Q-range if available	Not usually suitable†‡
Solve or refine small inorganic structures 解析或精化小分子无机晶体结构	Beneficial, but not usually essential unless pseudosymmetry is present	Usually adequate
Quantitative phase analysis 定量相分析	Only required when peaks from the different phases are heavily overlapped	Usually adequate. Allows phase quantities to be tracked in fine environmental variable steps (T, P, E, H *etc.*) during *in situ* experiments
Phase transitions 相转变	Depends on the nature of the transition and complexity of the structures. Essential for transitions involving subtle unit-cell distortions and pseudosymmetry	Often adequate for small inorganic structure transitions and order–disorder transitions. Allows fine steps in an environmental variable (T, P, E, H *etc.*)
Line-broadening analysis 线-宽分析	Essential for complex line broadening such as from a combination of strain and particle size, dislocations, stacking faults *etc.*	Adequate for tracking changes in severe line broadening as a function of an environmental variable (T, P *etc.*) especially if the pure instrumental peak shape is well characterized
Rapid kinetic studies 快速动力学研究	Not appropriate	Essential

† In some cases the symmetry and lattice parameters are such that the diffraction peaks are well spaced and not severely overlapped even at modest resolution. ‡ May be necessary to supplement high-resolution data to observe weak superlattice reflections in the presence of very subtle or incomplete order–disorder transitions.

International Tables for Crystallography (2018). Vol. H, Chapter 2.3, p92.

Table 2.3.7
Guidance on choice of wavelength/detector bank

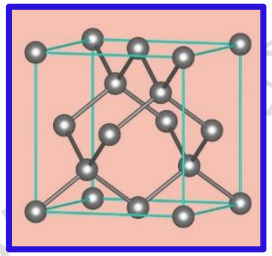
Reproduced from Kisi & Howard (2008) by permission of Oxford University Press.

Problem	Choice	Reasons
Solve complex or low-symmetry structures 分析复杂或低对称性的结构	Longer wavelength	Increase *d*-spacing resolution to allow correct symmetry and space group to be assigned
Refine a large or complex crystal structure 精修大的或复杂的晶体结构	Shorter wavelength	Ensure that the number of peaks greatly exceeds the number of parameters. Improve determination of site occupancies and displacement parameters
Solve or refine magnetic structures 解磁结构或精修磁结构	Longer wavelength	Ensure that large *d*-spacing peaks are observed. Spread the magnetic form factor over the entire diffraction pattern
Quantitative phase analysis 定量相分析	Usually shorter wavelength	Improve the accuracy of the determination. Longer wavelengths only required if peak overlap is severe
Phase transitions 相转变分析	Shorter wavelength	Ensures adequate data for order–disorder or other unit-cell-enlarging transitions
	Longer wavelength	Subtle unit-cell distortion or pseudosymmetric structures

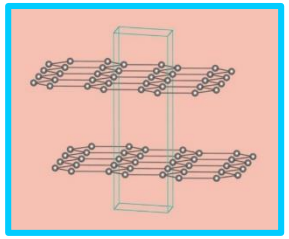
International Tables for Crystallography (2018). Vol. H, Chapter 2.3, p92.

结构与性能
Structure and Property

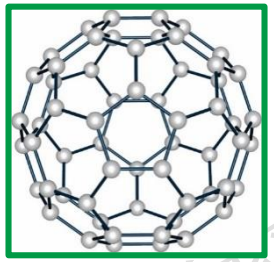
材料科学: 一级学科，包括金属材料，无机非金属材料，有机材料，有机高分子材料等。
主要研究: 材料成分，组织结构，制备工艺与材料性能及应用之间相互关系。
核心问题: 结构与性能。



Diamond

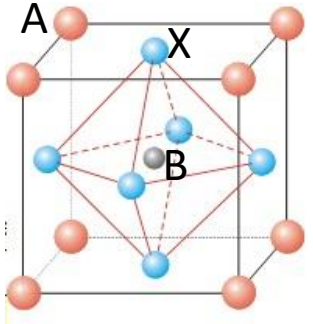


Graphite



C60

(A) 同质异构
性能不同



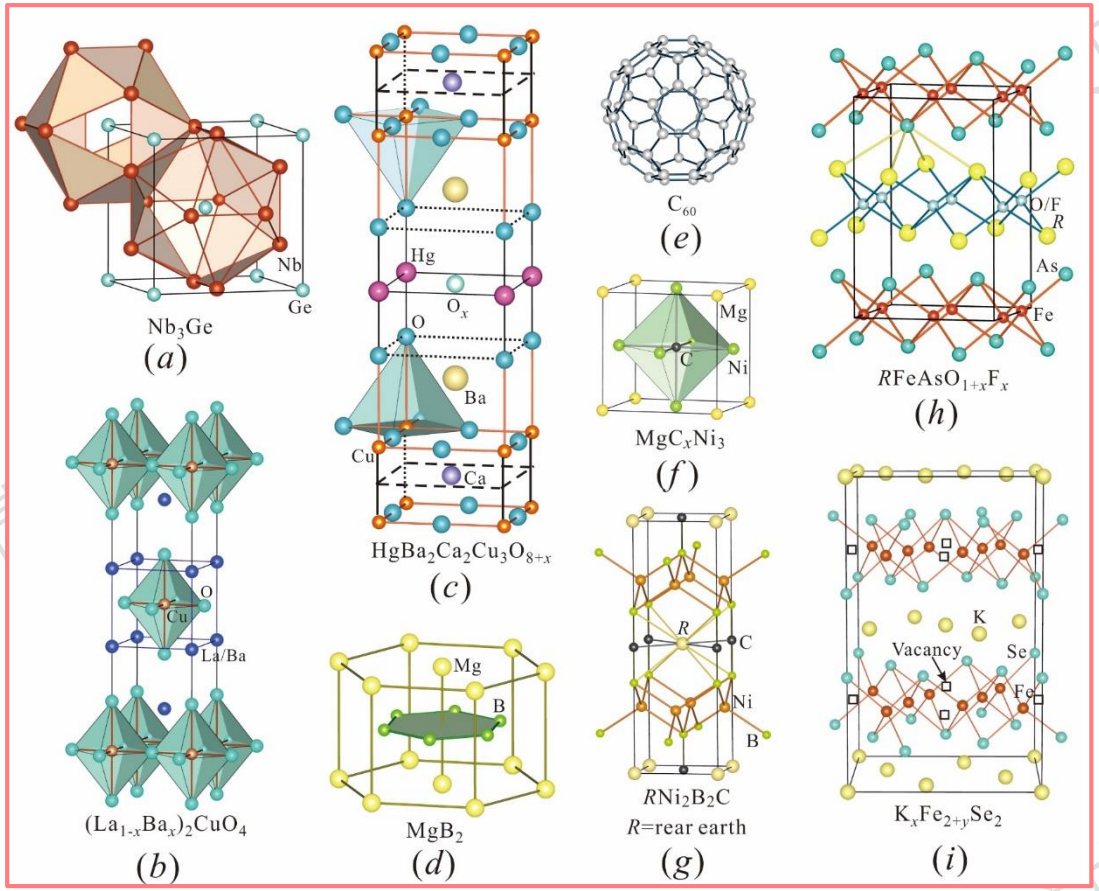
ABX_3

Ba Ti O_3

Mg C Ni_3

Zn N Mn_3

(B) 异质同构
性能不同



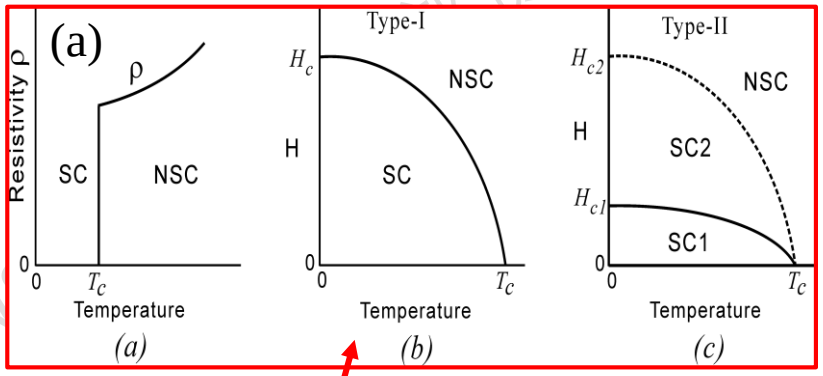
(C) 异质异构　同种性能

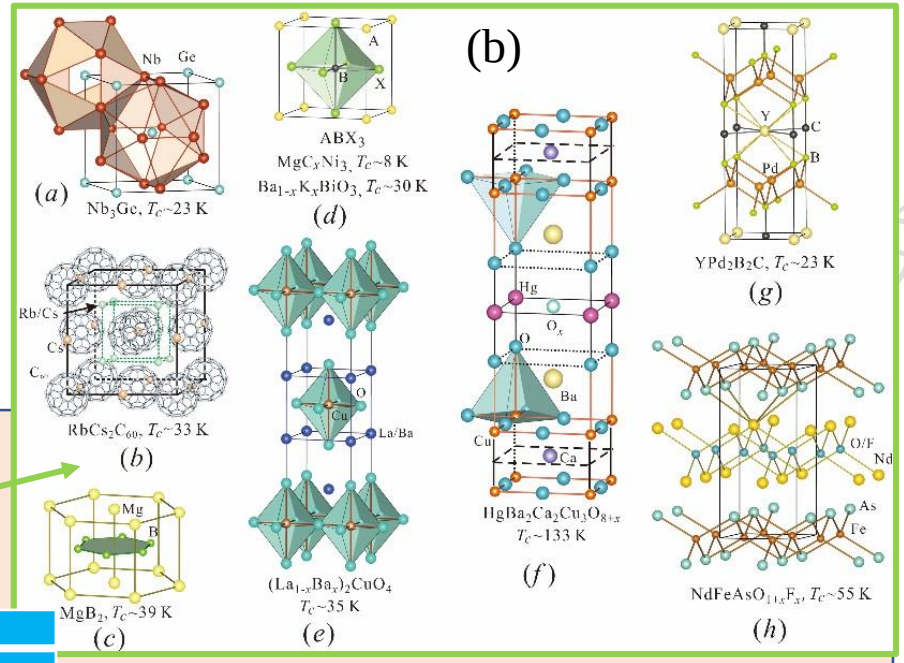
在材料科学中，性能是由结构和结构中的成分及其分布决定，例如:

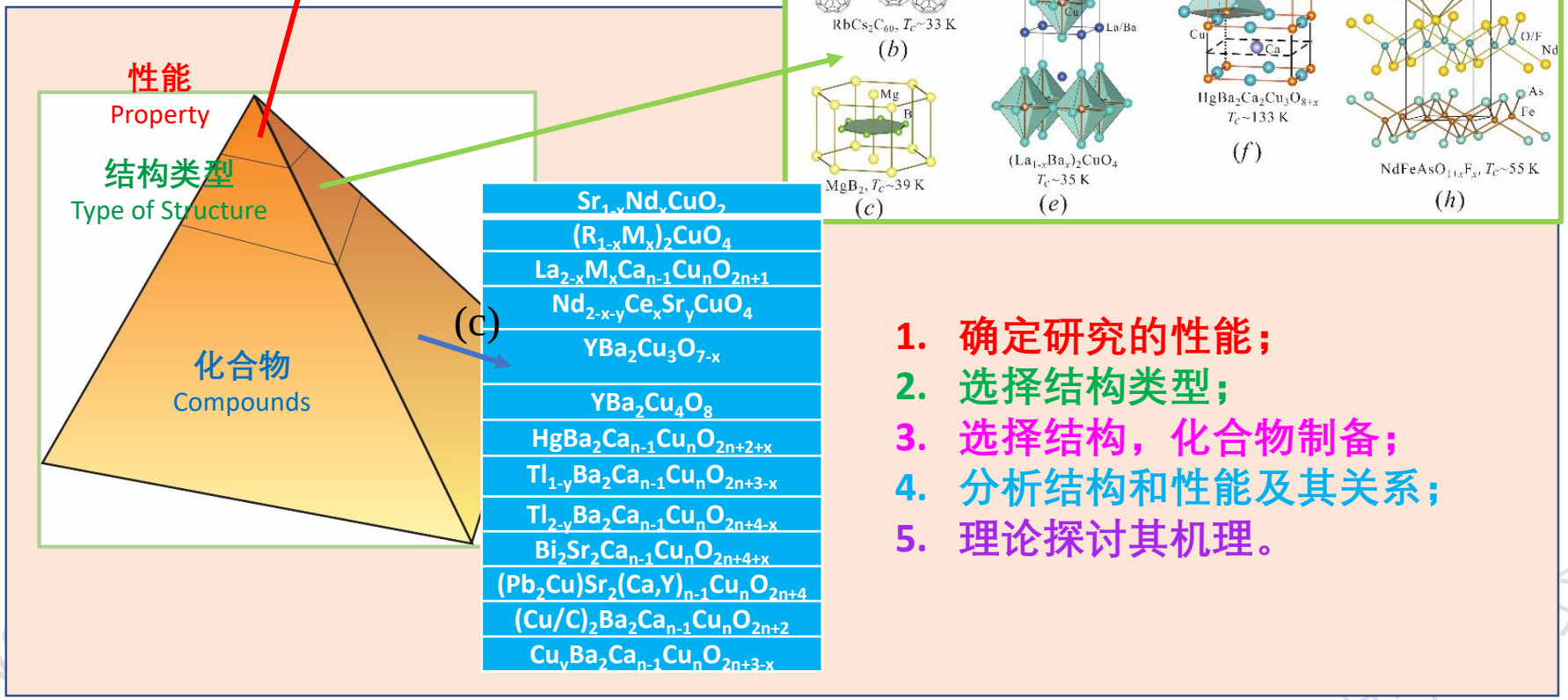
1. 图(A)中的三种不同的结构都由碳元素组成，但它们具由不同的特性。
2. 图(B)列出的三种化合物都具有相同的结构，但它们的性能完全不同。
3. 图(C)所示的所有的结构和成分都不相同，但它们都可能具有超导性能。其超导性能也随着部分改变其中的组分而变化。

结构材料也与功能材料类似，性能与结构紧密关联。因此在材料科学中，结构的研究是建立材料基因库的重中之重。

功能材料探索中的重要步骤
Search for new Functional Materials







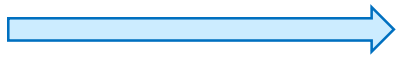
1. **确定研究的性能；**
2. **选择结构类型；**
3. **选择结构，化合物制备；**
4. **分析结构和性能及其关系；**
5. **理论探讨其机理。**

在新材料的探索研究过程中一般有以下几个过程:

1. 首先选择要研究材料的性能, 例如选择研究图(a)超导性能。
2. 选择可能具有超导性能的已知的结构类型（如图(b)）或根据经验和理论推测一种新的结构模型。
3. 设计切合该结构的化合物。
4. 化合物制备并进行性能测试和结构分析。
5. 结果分析。

Powder diffraction: a useful toll for revealing
the most important structural information in materials science

Powder Diffraction Structures Analysis



X-ray
Neutron
Electron
} Diffraction

Rietveld 方法和相应的峰型分析软件的发展
Development of Rietveld method and related software for profile analysis

粉末样品制备简易
Easy to prepare powder sample

困难或不可能生长足够大的单晶体
Difficulty or impossible to grow single crystal

使用特殊的环境条件方便
Convenient for using special environmental condition

容易中子衍射研究磁结构和性能
Easy for studying magnetic structure and properties by NPD

…

定量物相分析 Quantitative phase analysis
结构精化 Structure refinement
化学成分确定 Chemical composition
对称性分析 Symmetry analysis
分析元素分布 Element distribution
织构，应变等研究 Texture, stress …
二维结构测定 2-D structure
局域结构等 Local structure…
有序度研究 Order degree
磁结构和性能 Magnetic structure & properties (NPD only)

多晶衍射方法的广泛应用

Macromolecules 大分子
Zeolites 沸石
Minerals and Mining 矿物和采矿
Inorganic Structures 无机结构
Glass Ceramics 玻璃陶瓷
Ceramic Materials (incl medicals) 陶瓷材料
Metals and Alloys 金属和合金
Cement 水泥
Polymers and Fibers 聚合物和纤维
Pharmaceuticals 制药
Forensic Science 法医科学
Materials for Energy Storage and Conversion 能源储存和转换材料
Magnetic Materials 磁性材料
Catalysis 催化
Peroleum and Petrochemicals 石油和石化产品
Superconductivity 超导
Composites 复合材料
Paint and Pigments 油漆和颜料
Piezo Ceramics 压电陶瓷
Aeronautics and Space Materials 航空航天材料
Metal-Organic Framework 金属有机框架
。。。。。。

X射线和中子粉末衍射峰的位置，强度和结构因子

Powder diffraction positions, intensity, and structural factors for XRPD & NPD

Peaks Position: $2d\sin\theta = n\lambda$

where ***l*** is the incident beam wavelength, ***d*** and θ are the distance between successive *hkl* planes and Bragg angles of reflections, respectively.

Diffraction Intensity: $I_{hkl} = C|F_{hkl}|^2$

where $|F_{hkl}|^2$ is the *hkl* reflection amplitude of the diffracted X-ray, or neutron, or magnetic, and **C** is all others.

X-ray: $|F_{hkl}|^2 = |\sum f_j \exp(2\pi i (hx + ky + lz))|^2 e^{-2W}$

where f_j is the X-ray atomic scattering factor of atom *j* for X-ray.

Neutron: $|F_{hkl}|^2 = \sum b_j \exp(2\pi i (hx + ky + lz))|^2 e^{-2W}$

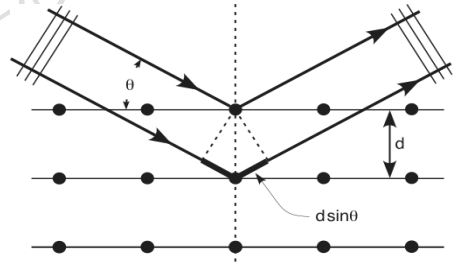
where b_j is the neutron scattering length for atom *j*.

Magnetic: $|F_{hkl}|^2 = \sum q_j f_{Mj} \exp(2\pi i (hx + ky + lz))|^2 e^{-2W}$

where q_j and f_{Mj} are the magnetic interaction vector and the magnetic form factor for atom *j*, respectively.

X-射线衍射与中子衍射具有许多共同点。峰的位置都遵循Bragg方程:

$2d\sin\theta = n\lambda$



衍射峰的强度:

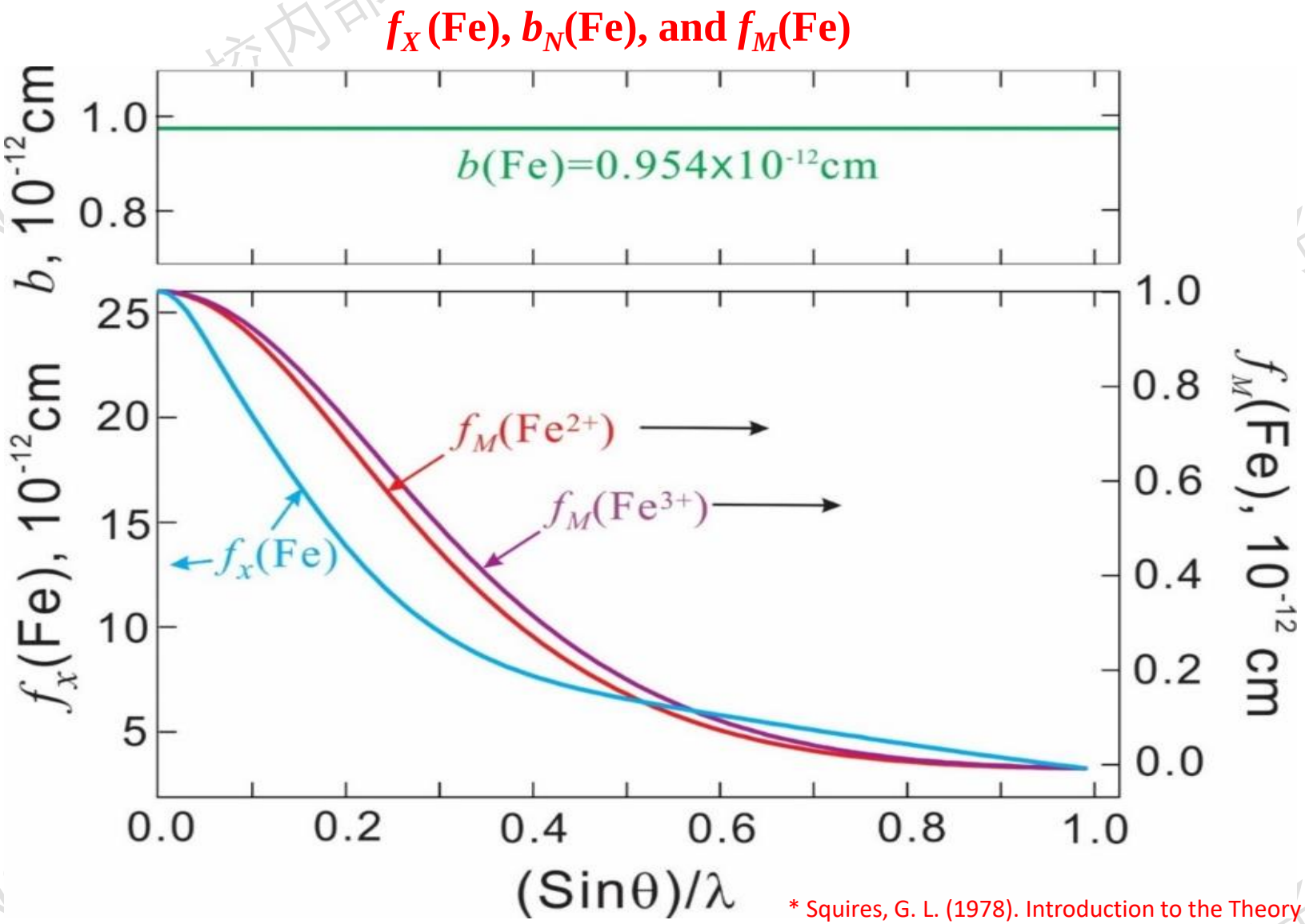
$I_{hkl} = C|F_{hkl}|^2$

式中 C 是与晶体结构无关的参数, F_{hkl} 是结构因子。

（1）在结构因子中，除了由于元素的散射因子差异使得衍射峰强度不同外，其它与结构有关的参数都一样。

（2）在中子衍射中，磁有序的衍射谱图是一套独立于晶体结构的衍射图，因此磁相可作为一个独立的相精化得到磁结构信息。

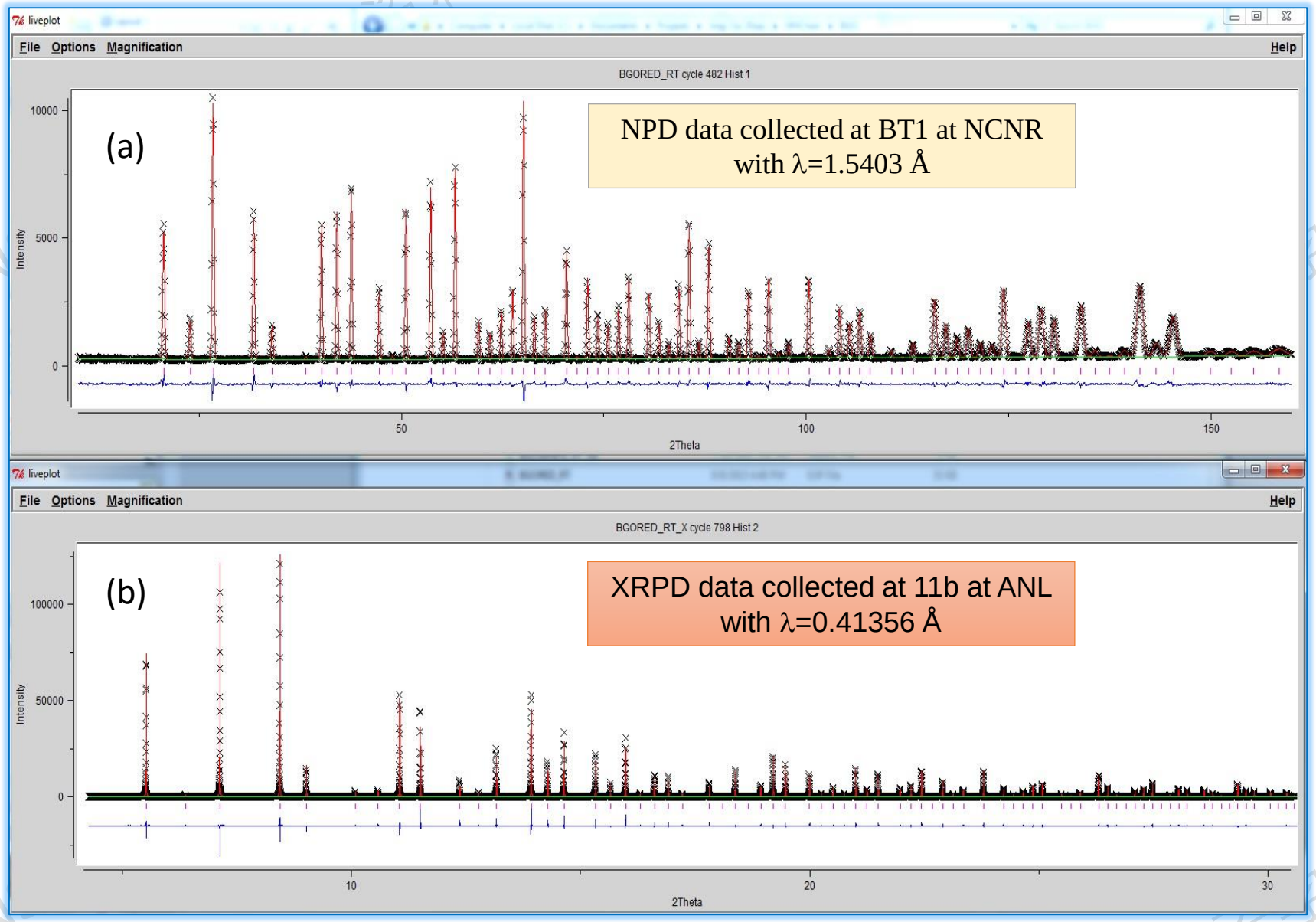
中子, X射线和粉末衍射峰的位置，强度和结构因子
Powder diffraction positions, intensity, and structural factors for XRPD & NPD



X-射线的电子散射因子（f_x）和磁形状因子（f_M）都是衍射角和波长（sinθ/λ)的函数，数值随着sinθ/λ增大而减小，因而其衍射峰强度随着sinθ/λ增大而衰减。而中子散射因子(b*)和磁矩(μ_B)是常数，不随sinθ/λ变化而变化，因此中子衍射在高角度仍然有强峰。

* Squires, G. L. (1978). Introduction to the Theory of Thermal Neutron Scattering. Cambridge University Press.

X射线与中子衍射谱图 XRPD& NPD diffraction patterns

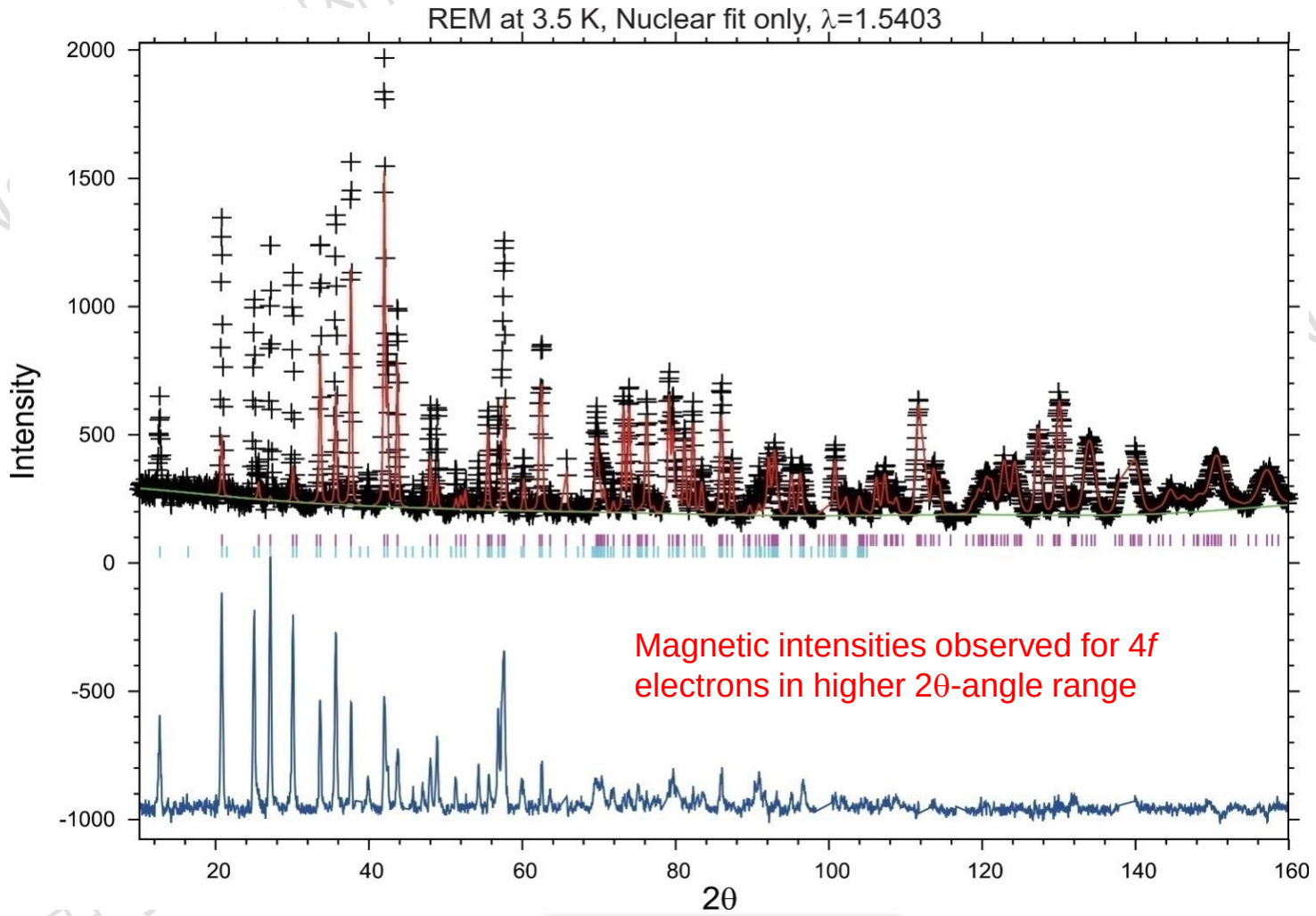


XRPD and NPD patterns for $Bi_4Ge_3O_{12}$， *Sample comes from Jintai Zhao's group*

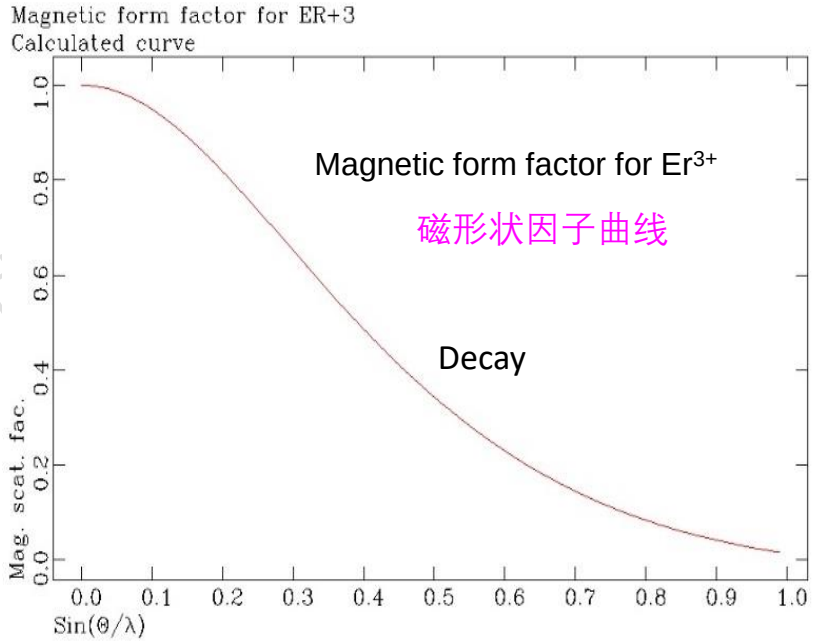
左图所示的是$Bi_4Ge_3O_{12}$的中子(a) 和X射线(b)在相同Q范围的粉末衍射精修谱。该化合物为立方晶系，样品由单晶体研磨并过300目筛，衍射数据在室温收集。可以看到：

1. 衍射峰没有重叠现象；
2. 图(a)的中子衍射在整给角度范围内强度都比较均匀，高Q的峰强没有明显的减小，这是因为中子的散射振幅是常数；
3. 图(b)的XRPD的衍射谱图随着角度的增大强度迅速减弱，这是由于X射线衍射中的电子散射振幅随着角度增大而减小，最终趋近零。

磁有序, 磁晶胞, 磁对称性，磁结构及性能
Spins order, magnetic cell, magnetic symmetry, and structure & properties

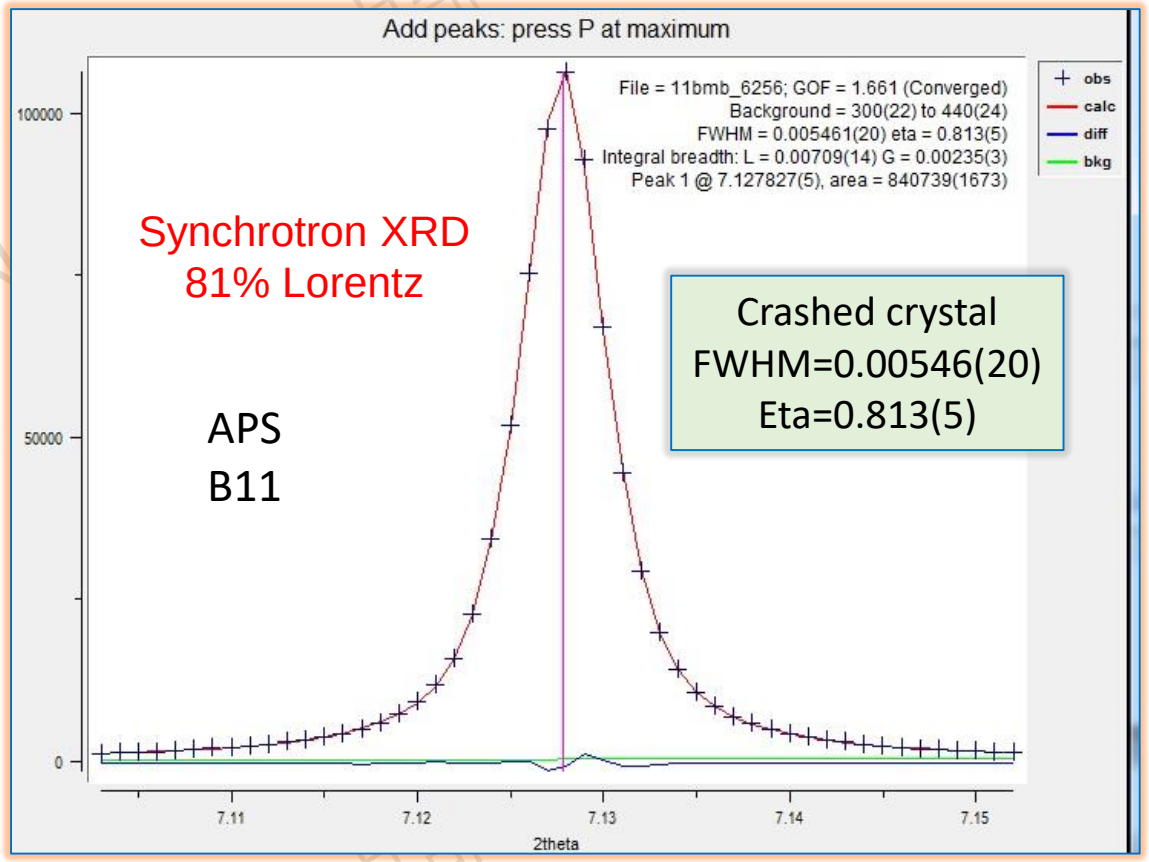


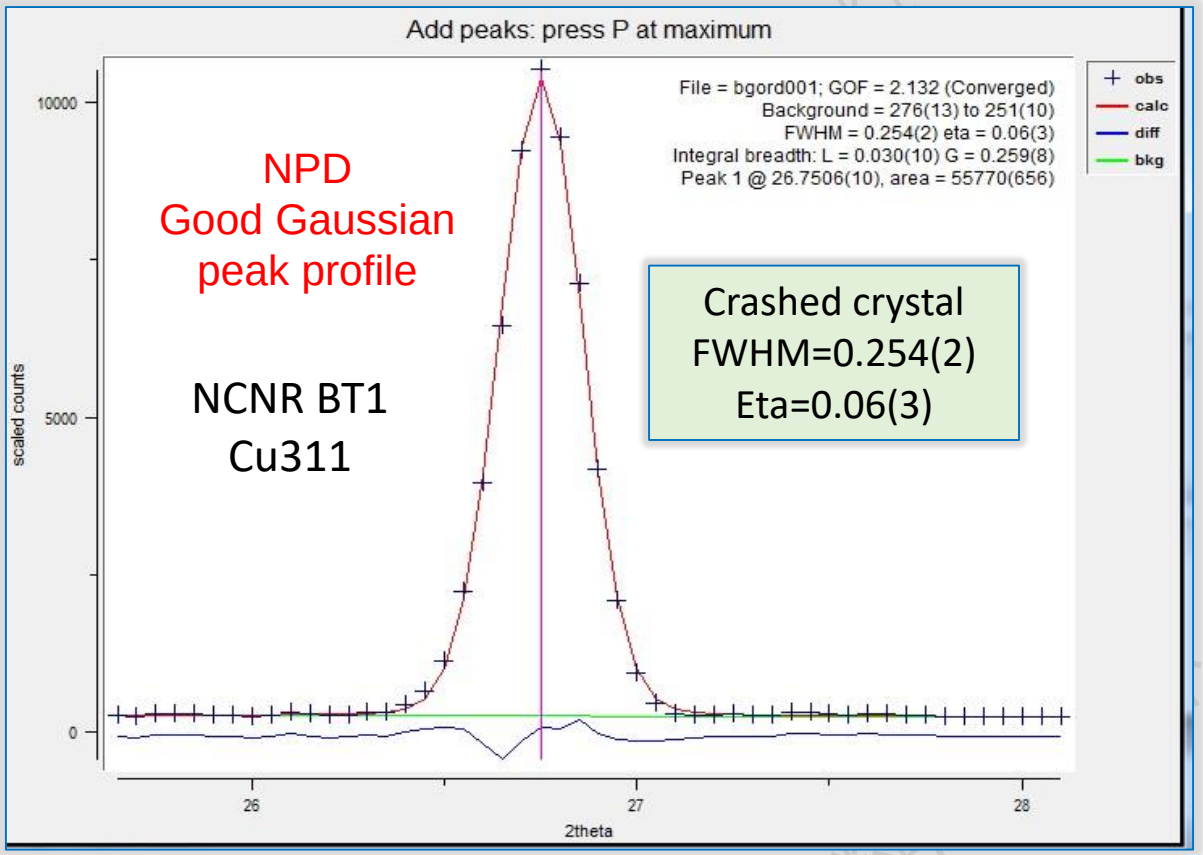
磁峰出现在低角度范围



含重稀土Er^{3+} 合金的中子衍射谱图。图中红线是以晶体结构拟合曲线，图的下部观察数据与计算数据的差值是Er^{3+}的有序的磁衍射峰。

X射线和中子衍射峰的峰型剖面
Diffraction Peak Profile of XRPD and NPD





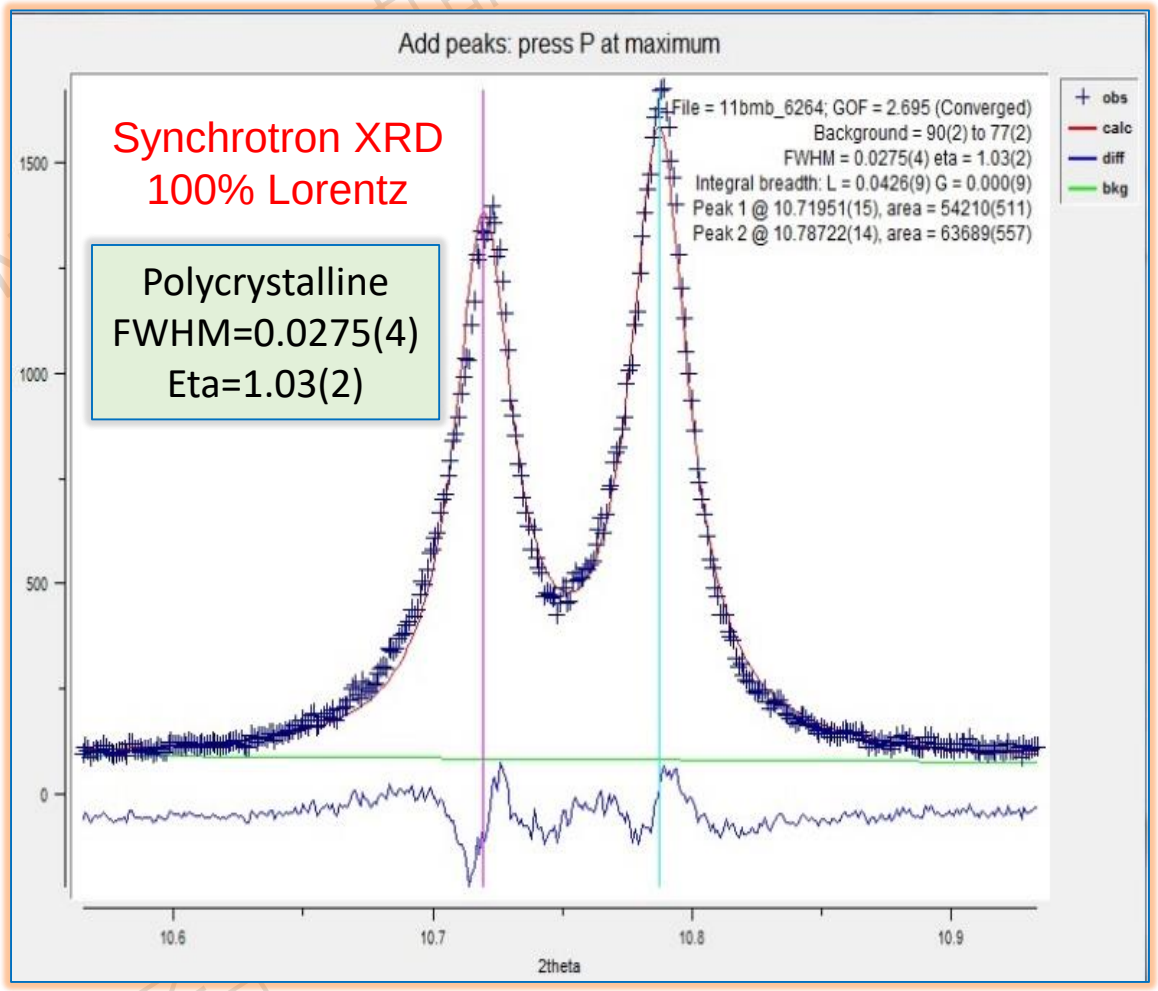
$$L(2\theta - 2\theta_{hkl}) = \frac{1}{2\pi}\left(\frac{\mathrm{FWHM}}{(2\theta - 2\theta_{hkl}) + \mathrm{FWHM}^2/4}\right)$$

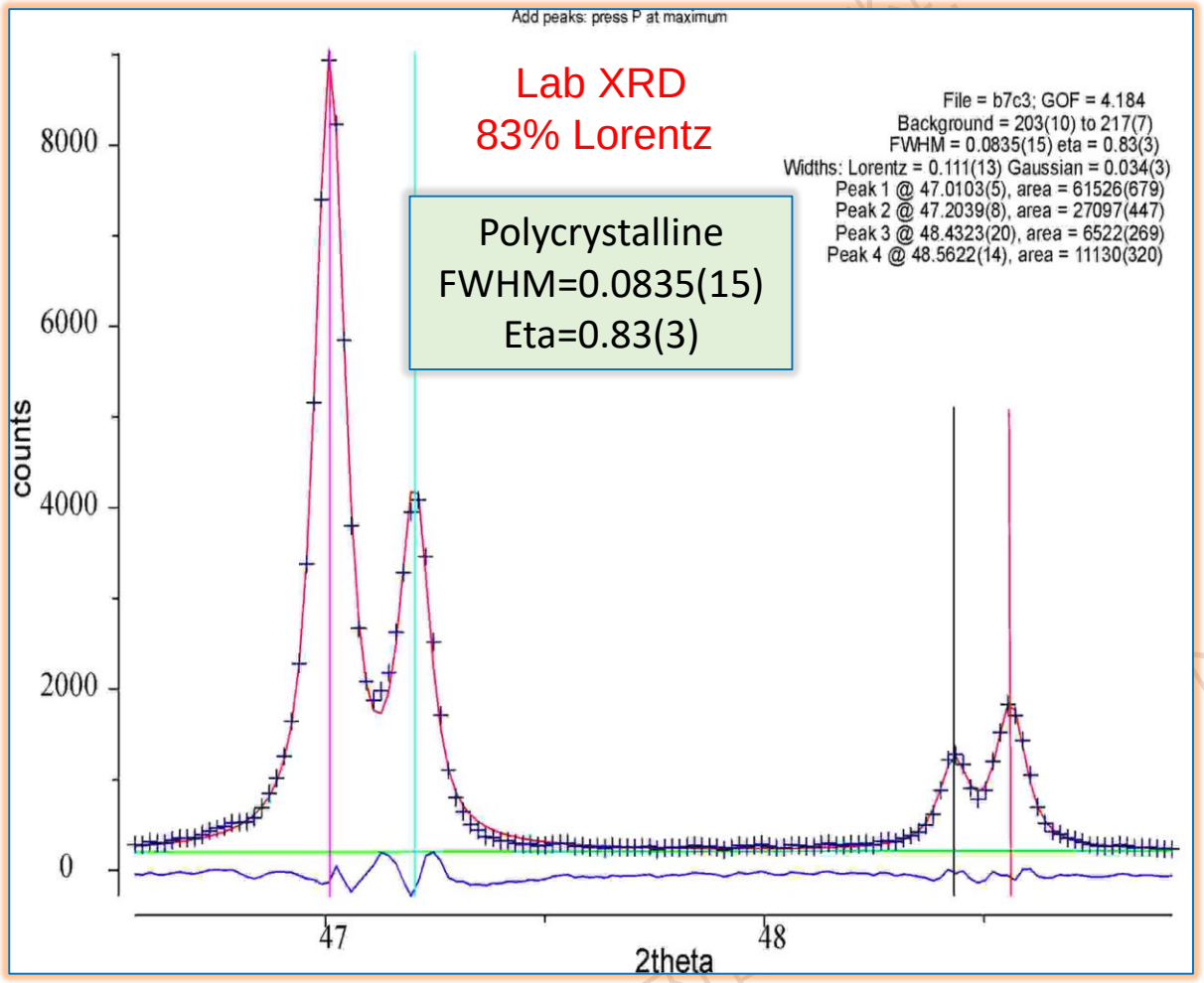
理想的X射线衍射的峰型可用洛伦兹函数描述

$$G(2\theta - 2\theta_{hkl}) = \left(\frac{2\sqrt{\ln(2)/\pi}}{\mathrm{FWHM}}\right)\exp\left(\frac{-4\ln(2)(2\theta - 2\theta_{hkl})^2}{\mathrm{FWHM}^2}\right)$$

反应堆单色波中子衍射的峰型函数则是高斯函数

X射线和中子衍射峰的峰型剖面
Diffraction Peak Profile of XRPD and NPD



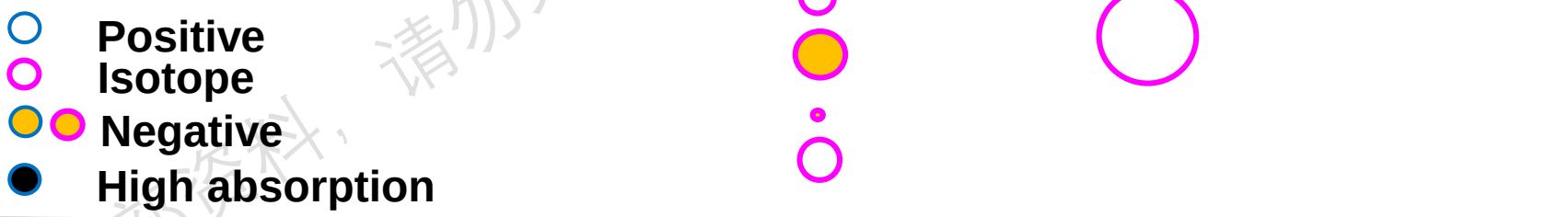


对于一般合成的粉末样品，由于晶粒大小不均匀因而引起衍射峰的展宽，特别是高分辨衍射仪尤其明显。

部分X射线散射和中子散线截面

Some scattering cross section of x-ray and neutron

	H	B	C	O	Ti	V	Cu	Zn	Pb
f_x	·	o	o						
#	1	5	6	8	22	23	29	30	82
b_N (fm)	-0.374	0.535	0.665	0.581	-0.334	-0.038	0.772	0.580	0.940



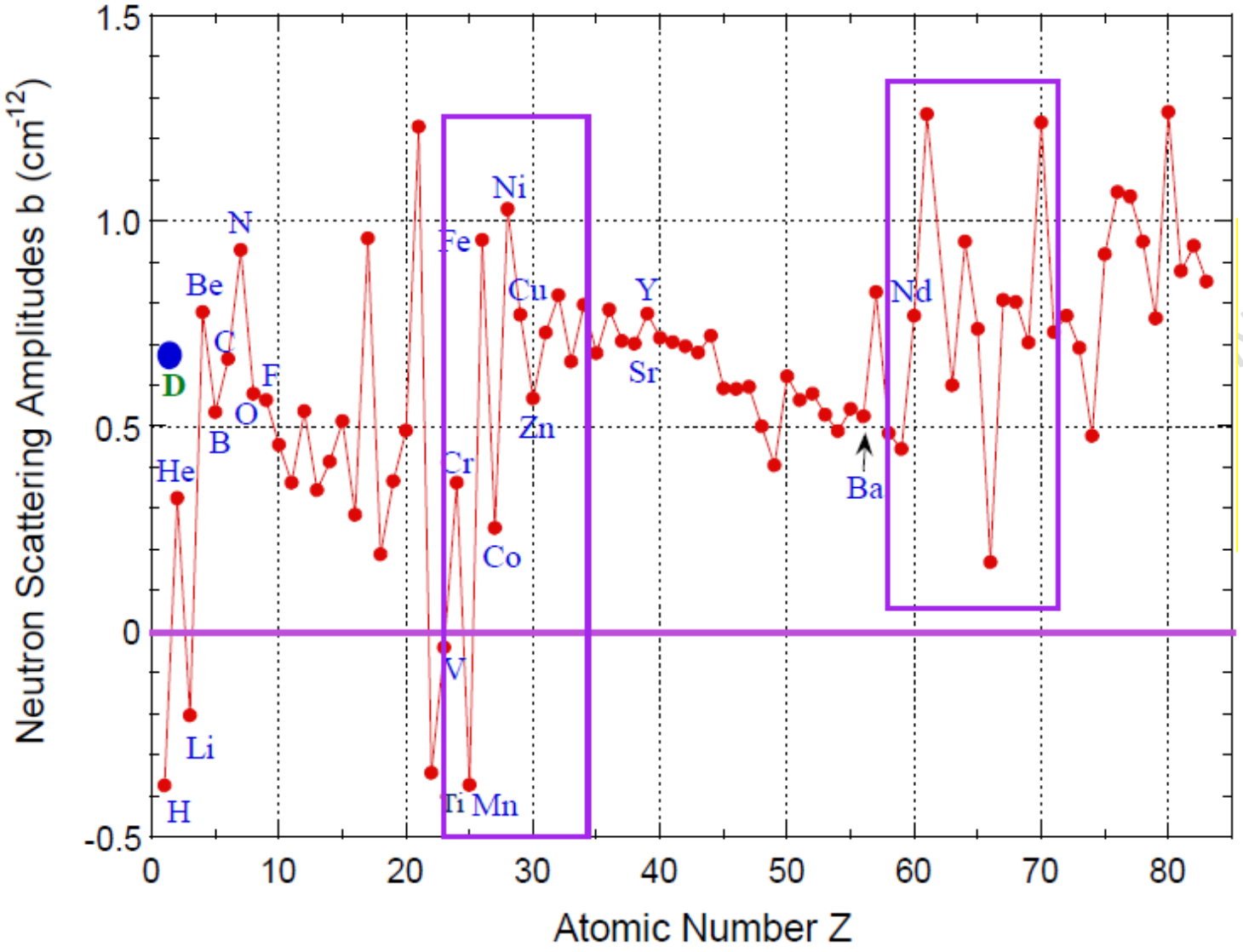
部分X射线散射和中子散线截面（以图中的圆圈的面积表示）

1. X射线衍射的强度随着元素内部的电子数目的增加而增强，即X射线散射的截面随着原子序数增大而增加，因此对原子序数低的元素不敏感。
2. 中子散射截面不随原子序数的规律变化，对原子序数小的元素也可能有较大的散射截面。而且对非相干散射大和吸收大的元素可以用相应的同位素替代。

Representations of the scattering of X-rays and neutrons by selected elements. The scattering cross sections are proportional to the areas of the circles shown. For the neutron case, separate entries appear for the different isotopes and negative scattering lengths are indicated by shading.

部分元素的中子散射因子

Representations of the neutron scattering amplitudes of selected elements



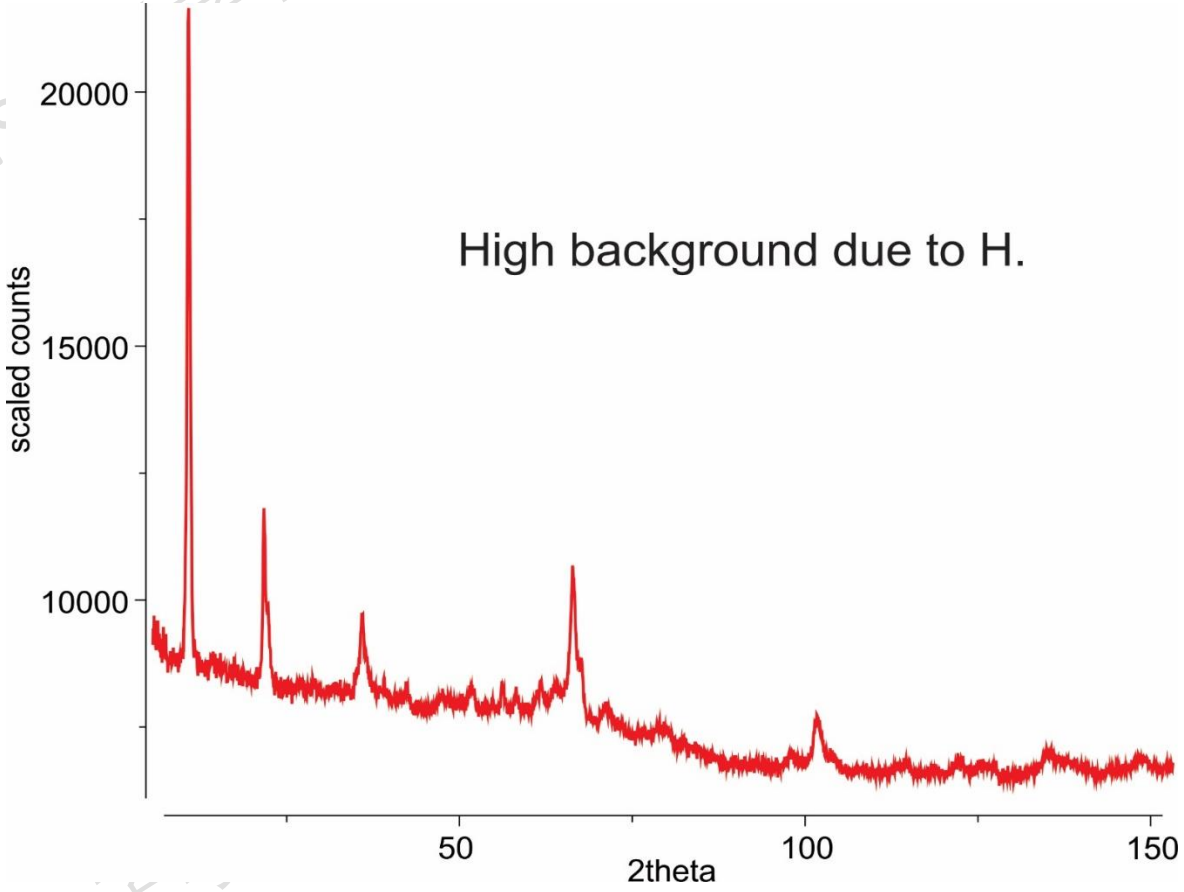
Atom	Atomic #	b(cm^{-12})
Ti	22	-0.3438
V	23	-0.0382
Cr	24	0.3635
Mn	25	-0.373
Fe	26	0.954
Co	27	0.253
Ni	28	1.03
Cu	29	0.7718

与X射线散射因子不同，中子散射因子与原子序数无关，是常数，即不随衍射角变化，有正值也有负值等特点。因此在运用粉末衍射方法测定晶体结构上弥补了X射线衍射方法上一些不足。对序数是小的元素较敏感，如 H, D, Li, Be, ^{11}B, C, N, O 等，通常用来测定这类元素的位置和占有率。对过渡金属，稀土等相邻元素具有较强的分辨能力，常用来探测其在共占位中的比例。

应该指出不宜用中子测量含有大量高吸收元素，如 **B, Cd, Pm, Sm, Eu,** 和 **Gd**，有些可用同位素替代，如在中子测量**MgB_2**就是用**^{11}B**来替代 **B**。而对于**H**元素，由于非相干散射很强，用中子测量产生很高的背底，因此测量对大量含**H**的化合物，可以用同位素氘（**D**）替代。

由于元素的中子散射因子有负值，在与正值元素共占位，结果会相互抵消。

Higher background and absorption due to samples contain higher incoherent scattering elements



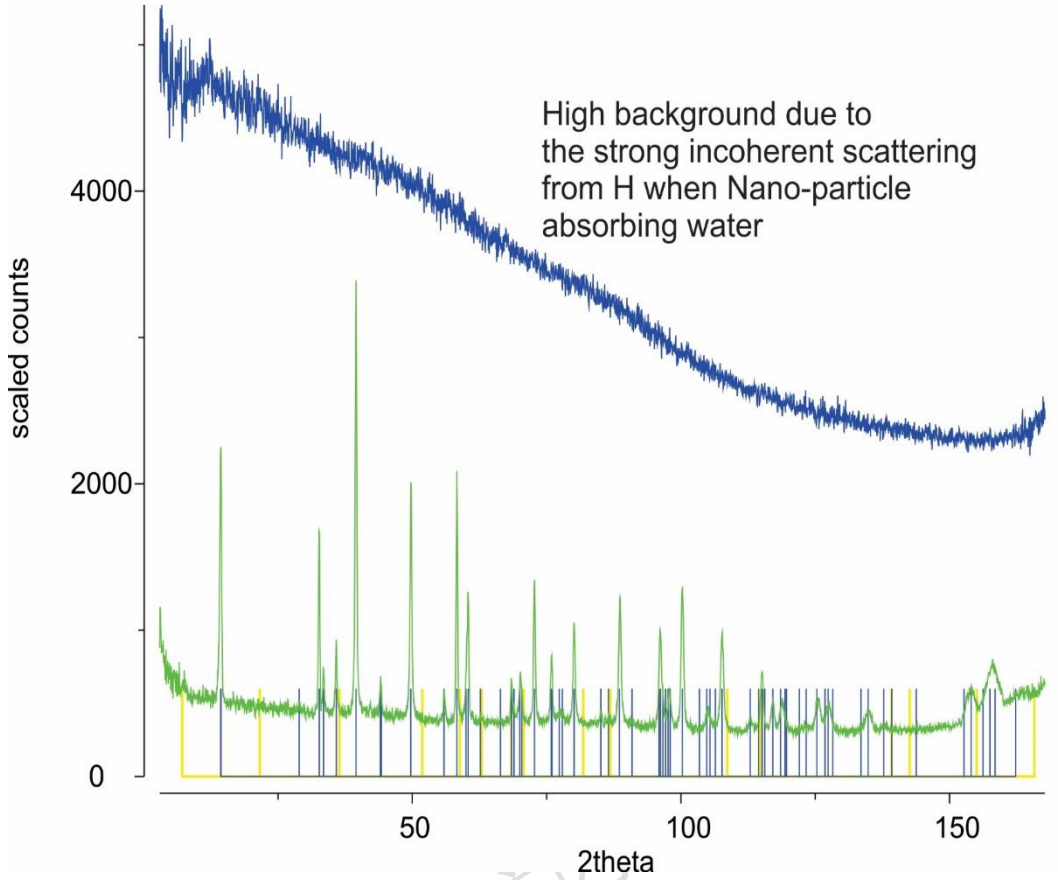


Table 4.4.4.1. *Bound scattering lengths, b, in fm and cross sections, σ, in barns (1 barn = 100 fm²) of the elements and their isotopes*

Z: atomic number; *A*: mass number; $I(\pi)$: spin (parity) of the nuclear ground state; *c*: % natural abundance (for radioisotopes, the half-life is given instead in annums); b_c: bound coherent scattering length; b_i: bound incoherent scattering length; σ_c: bound coherent scattering cross section; σ_i: bound incoherent scattering cross section; σ_s: total bound scattering cross section; σ_a: absorption cross section for 2200 m s^{-1} neutrons (E = 25.30 meV, k = 3.494 Å^{-1}, λ = 1.798 Å); $i = \sqrt{-1}$.

Element	Z	A	$I(\pi)$	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
H	1				−3.7390(11)		1.7568(10)	80.26(6)	82.02(6)	0.3326(7)
		1	1/2(+)	99.985	−3.7406(11)	25.274(9)	1.7583(10)	80.27(6)	82.03(6)	0.3326(7)
		2	1(+)	0.015	6.671(4)	4.04(3)	5.592(7)	2.05(3)	7.64(3)	0.000519(7)
		3	1/2(+)	(12.32a)	4.792(27)	−1.04(17)	2.89(3)	0.14(4)	3.03(5)	0
He	2				3.26(3)		1.34(2)	0.00	1.34(2)	0.00747(1)
		3	1/2(+)	0.00014	5.74(7)	−2.5(6)	4.42(10)	1.6(4)	6.0(4)	5333.(7.)
					−1.483(2)i	+2.568(3)i				
		4	0(+)	99.99986	3.26(3)	0	1.34(2)	0	1.34(2)	0
Li	3				−1.90(2)		0.454(14)	0.92(3)	1.37(3)	70.5(3)
		6	1(+)	7.5	2.00(11)	−1.89(5)	0.51(5)	0.46(2)	0.97(7)	940.(4.)
					−0.261(1)i	0.257(11)i				
		7	3/2(−)	92.5	−2.22(2)	−2.49(5)	0.619(11)	0.78(3)	1.40(3)	0.0454(3)
Be	4	9	3/2(−)	100	7.79(1)	0.12(3)	7.63(2)	0.0018(9)	7.63(2)	0.0076(8)
B	5				5.30(4)		3.54(5)	1.70(12)	5.24(11)	767.(8.)
					0.213(2)i					
		10	3(+)	20.0	−0.1(3)	−4.7(3)	0.144(8)	3.0(4)	3.1(4)	3835.(9.)
					1.066(3)i	1.231(3)i				
		11	3/2(−)	80.0	6.65(4)	−1.3(2)	5.56(7)	0.22(6)	5.78(9)	0.0055(33)
C	6				6.6460(12)		5.550(2)	0.001(4)	5.551(3)	0.00350(7)
		12	0(+)	98.90	6.6511(16)	0	5.559(3)	0	5.559(3)	0.00353(7)
		13	1/2(−)	1.10	6.19(9)	−0.52(9)	4.81(14)	0.034(12)	4.84(14)	0.00137(4)
N	7				9.36(2)		11.01(5)	0.50(12)	11.51(11)	1.90(3)
		14	1(+)	99.63	9.37(2)	2.0(2)	11.03(5)	0.5(1)	11.53(11)	1.91(3)
		15	1/2(−)	0.37	6.44(3)	−0.02(2)	5.21(5)	0.00005(10)	5.21(5)	0.000024(8)
O	8				5.803(4)		4.232(6)	0.000(8)	4.232(6)	0.00019(2)
		16	0(+)	99.762	5.803(4)	0	4.232(6)	0	4.232(6)	0.00010(2)
		17	5/2(+)	0.038	5.78(12)	0.18(6)	4.20(22)	0.004(3)	4.20(22)	0.236(10)
		18	0(+)	0.200	5.84(7)	0	4.29(10)	0	4.29(10)	0.00016(1)
F	9	19	1/2(+)	100	5.654(10)	−0.082(9)	4.017(17)	0.0008(2)	4.018(14)	0.0096(5)
Ne	10				4.566(6)		2.620(7)	0.008(9)	2.628(6)	0.039(4)
		20	0(+)	90.51	4.631(6)	0	2.695(7)	0	2.695(7)	0.036(4)
		21	3/2(+)	0.27	6.66(19)	±0.6(1)	5.6(3)	0.05(2)	5.7(3)	0.67(11)
		22	0(+)	9.22	3.87(1)	0	1.88(1)	0	1.88(1)	0.046(6)
Na	11	23	3/2(+)	100	3.63(2)	3.59(3)	1.66(2)	1.62(3)	3.28(4)	0.530(5)
Mg	12				5.375(4)		3.631(5)	0.08(6)	3.71(4)	0.063(3)
		24	0(+)	78.99	5.66(3)	0	4.03(4)	0	4.03(4)	0.050(5)
		25	5/2(+)	10.00	3.62(14)	1.48(10)	1.65(13)	0.28(4)	1.93(14)	0.19(3)
		26	0(+)	11.01	4.89(15)	0	3.00(18)	0	3.00(18)	0.0382(8)
Al	13	27	5/2(+)	100	3.449(5)	0.256(10)	1.495(4)	0.0082(7)	1.503(4)	0.231(3)
Si	14				4.1491(10)		2.1633(10)	0.004(8)	2.167(8)	0.171(3)
		28	0(+)	92.23	4.107(6)	0	2.120(6)	0	2.120(6)	0.177(3)
		29	1/2(+)	4.67	4.70(10)	0.09(9)	2.78(12)	0.001(2)	2.78(12)	0.101(14)
		30	0(+)	3.10	4.58(8)	0	2.64(9)	0	2.64(9)	0.107(2)
P	15	31	1/2(+)	100	5.13(1)	0.2(2)	3.307(13)	0.005(10)	3.312(16)	0.172(6)
S	16				2.847(1)		1.0186(7)	0.007(5)	1.026(5)	0.53(1)
		32	0(+)	95.02	2.804(2)	0	0.9880(14)	0	0.9880(14)	0.54(4)
		33	3/2(+)	0.75	4.74(19)	1.5(1.5)	2.8(2)	0.3(6)	3.1(6)	0.54(4)
		34	0(+)	4.21	3.48(3)	0	1.52(3)	0	1.52(3)	0.227(5)
		36	0(+)	0.02	3.(1.) *E*	0	1.1(8)	0	1.1(8)	0.15(3)

Table 4.4.4.1. *Bound scattering lengths (cont.)*

Element	Z	A	$I(\pi)$	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
Cl	17				9.5770(8)		11.526(2)	5.3(5)	16.8(5)	33.5(3)
		35	3/2(+)	75.77	11.65(2)	6.1(4)	17.06(6)	4.7(6)	21.8(6)	44.1(4)
		37	3/2(+)	24.23	3.08(6)	0.1(1)	1.19(5)	0.001(3)	1.19(5)	0.433(6)
Ar	18				1.909(6)		0.458(3)	0.22(2)	0.683(4)	0.675(9)
		36	0(+)	0.337	24.90(7)	0	77.9(4)	0	77.9(4)	5.2(5)
		38	0(+)	0.063	3.5(3.5)	0	1.5(3.1)	0	1.5(3.1)	0.8(2)
		40	0(+)	99.600	1.830(6)	0	0.421(3)	0	0.421(3)	0.660(9)
K	19				3.67(2)		1.69(2)	0.27(11)	1.96(11)	2.1(1)
		39	3/2(+)	93.258	3.74(2)	1.4(3)	1.76(2)	0.25(11)	2.01(11)	2.1(1)
		40	4(−)	0.012	3.(1.) *E*		1.1(8)	0.5(5)	1.6(9)	35.(8.)
		41	3/2(+)	6.730	2.69(8)	1.5(1.5)	0.91(5)	0.3(6)	1.2(6)	1.46(3)
Ca	20				4.70(2)		2.78(2)	0.05(3)	2.83(2)	0.43(2)
		40	0(+)	96.941	4.80(2)	0	2.90(2)	0	2.90(2)	0.41(2)
		42	0(+)	0.647	3.36(10)	0	1.42(8)	0	1.42(8)	0.68(7)
		43	7/2(−)	0.135	−1.56(9)	0.31(4)	0.5(5) *E*		0.8(5)	6.2(6)
		44	0(+)	2.086	1.42(6)	0	0.25(2)	0	0.25(2)	0.88(5)
		46	0(+)	0.004	3.6(2)	0	1.6(2)	0	1.6(2)	0.74(7)
		48	0(+)	0.187	0.39(9)	0	0.019(9)	0	0.019(9)	1.09(14)
Sc	21	45	7/2(−)	100	12.29(11)	−6.0(3)	19.0(3)	4.5(5)	23.5(6)	27.5(2)
Ti	22				−3.370(13)		1.427(11)	2.63(3)	4.06(3)	6.43(6)
		46	0(+)	8.2	4.725(5)	0	2.80(6)	0	2.80(6)	0.59(18)
		47	5/2(−)	7.4	3.53(7)	−3.5(2)	1.57(6)	1.5(2)	3.1(2)	1.7(2)
		48	0(+)	73.8	−5.86(2)	0	4.32(3)	0	4.32(3)	8.30(9)
		49	7/2(−)	5.4	0.98(5)	5.1(2)	0.12(1)	3.3(3)	3.4(3)	2.2(3)
		50	0(+)	5.2	5.88(10)	0	4.34(15)	0	4.34(15)	0.179(3)
V	23				−0.3824(12)		0.01838(12)	5.08(6)	5.10(6)	5.08(2)
		50	6(+)	0.250	7.6(6)		7.3(1.1)	0.5(5) *E*	7.8(1.0)	60.(40.)
		51	7/2(−)	99.750	−0.402(2)	6.435(4)	0.0203(2)	5.07(6)	5.09(6)	4.9(1)
Cr	24				3.635(7)		1.660(6)	1.83(2)	3.49(2)	3.05(8)
		50	0(+)	4.35	−4.50(5)	0	2.54(6)	0	2.54(6)	15.8(2)
		52	0(+)	83.79	4.920(10)	0	3.042(12)	0	3.042(12)	0.76(6)
		53	3/2(−)	9.50	−4.20(3)	6.87(10)	2.22(3)	5.93(17)	8.15(17)	18.1(1.5)
		54	0(+)	2.36	4.55(10)	0	2.60(11)	0	2.60(11)	0.36(4)
Mn	25	55	5/2(−)	100	−3.750(18)	1.79(4)	1.77(2)	0.40(2)	2.17(3)	13.3(2)
Fe	26				9.45(2)		11.22(5)	0.40(11)	11.62(10)	2.56(3)
		54	0(+)	5.8	4.2(1)	0	2.2(1)	0	2.2(1)	2.25(18)
		56	0(+)	91.7	9.94(3)	0	12.42(7)	0	12.42(7)	2.59(14)
		57	1/2(−)	2.2	2.3(1)	0.66(6)		0.3(3) *E*	1.0(3)	2.48(30)
		58	0(+)	0.3	15.(7.)	0	28.(26.)	0	28.(26.)	1.28(5)
Co	27	59	7/2(−)	100	2.49(2)	−6.2(2)	0.779(13)	4.8(3)	5.6(3)	37.18(6)
Ni	28				10.3(1)		13.3(3)	5.2(4)	18.5(3)	4.49(16)
		58	0(+)	68.27	14.4(1)	0	26.1(4)	0	26.1(4)	4.6(3)
		60	0(+)	26.10	2.8(1)	0	0.99(7)	0	0.99(7)	2.9(2)
		61	3/2(−)	1.13	7.60(6)	±3.9(3)	7.26(11)	1.9(3)	9.2(3)	2.5(8)
		62	0(+)	3.59	−8.7(2)	0	9.5(4)	0	9.5(4)	14.5(3)
		64	0(+)	0.91	−0.37(7)	0	0.017(7)	0	0.017(7)	1.52(3)
Cu	29				7.718(4)		7.485(8)	0.55(3)	8.03(3)	3.78(2)
		63	3/2(−)	69.17	6.43(15)	0.22(2)	5.2(2)	0.006(1)	5.2(2)	4.50(2)
		65	3/2(−)	30.83	10.61(19)	1.79(10)	14.1(5)	0.40(4)	14.5(5)	2.17(3)
Zn	30				5.60(5)		4.054(7)	0.077(7)	4.131(10)	1.11(2)
		64	0(+)	48.6	5.22(4)	0	3.42(5)	0	3.42(5)	0.93(9)
		66	0(+)	27.9	5.97(5)	0	4.48(8)	0	4.48(8)	0.62(6)
		67	5/2(−)	4.1	7.56(8)	−1.50(7)	7.18(15)	0.28(3)	7.46(15)	6.8(8)
		68	0(+)	18.8	6.03(3)	0	4.57(5)	0	4.57(5)	1.1(1)
		70	0(+)	0.6	6.(1.) *E*	0	4.5(1.5)	0	4.5(1.5)	0.092(5)

Table 4.4.4.1. *Bound scattering lengths (cont.)*

Element	Z	A	I(π)	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
Ga	31				7.288(2)		6.675(4)	0.16(3)	6.83(3)	2.75(3)
		69	3/2(−)	60.1	7.88(2)	−0.85(5)	7.80(4)	0.091(11)	7.89(4)	2.18(5)
		71	3/2(−)	39.9	6.40(3)	−0.82(4)	5.15(5)	0.084(8)	5.23(5)	3.61(10)
Ge	32				8.185(20)		8.42(4)	0.18(7)	8.60(6)	2.20(4)
		70	0(+)	20.5	10.0(1)	0	12.6(3)	0	12.6(3)	3.0(2)
		72	0(+)	27.4	8.51(10)	0	9.1(2)	0	9.1(2)	0.8(2)
		73	9/2(+)	7.8	5.02(4)	3.4(3)	3.17(5)	1.5(3)	4.7(3)	15.1(4)
		74	0(+)	36.5	7.58(10)	0	7.2(2)	0	7.2(2)	0.4(2)
		76	0(+)	7.8	8.21(1.5)	0	8.(3.)	0	8.(3.)	0.16(2)
As	33	75	3/2(−)	100	6.58(1)	−0.69(5)	5.44(2)	0.060(10)	5.50(2)	4.5(1)
Se	34				7.970(9)		7.98(2)	0.33(6)	8.30(6)	11.7(2)
		74	0(+)	0.9	0.8(3.0)	0	0.1(6)	0	0.1(6)	51.8(1.2)
		76	0(+)	9.0	12.2(1)	0	18.7(3)	0	18.7(3)	85.(7.)
		77	1/2(−)	7.6	8.25(8)	±0.6(1.6)	8.6(2)	0.05(26)	8.65(16)	42.(4.)
		78	0(+)	23.5	8.24(9)	0	8.5(2)	0	8.5(2)	0.43(2)
		80	0(+)	49.6	7.48(3)	0	7.03(6)	0	7.03(6)	0.61(5)
		82	0(+)	9.4	6.34(8)	0	5.05(13)	0	5.05(13)	0.044(3)
Br	35				6.795(15)		5.80(3)	0.10(9)	5.90(9)	6.9(2)
		79	3/2(−)	50.69	6.80(7)	−1.1(2)	5.81(12)	0.15(6)	5.96(13)	11.0(7)
		81	3/2(−)	49.31	6.79(7)	0.6(1)	5.79(12)	0.05(2)	5.84(12)	2.7(2)
Kr	36				7.81(2)		7.67(4)	0.01(14)	7.68(13)	25.(1.)
		78	0(+)	0.35		0		0		6.4(9)
		80	0(+)	2.25		0		0		11.8(5)
		82	0(+)	11.6		0		0		29.(20.)
		83	9/2(+)	11.5		185(30.)				
		84	0(+)	57.0		0		0		0.113(15)
		86	0(+)	17.3	8.1(2)	0	8.2(4)	0	8.2(4)	0.003(2)
Rb	37				7.09(2)		6.32(4)	0.5(4)	6.8(4)	0.38(4)
		85	5/2(−)	72.17	7.03(10)	6.2(2)	0.5(5)	*E*	6.7(5)	0.48(1)
		87	3/2(−)	27.83	7.23(12)	6.6(2)	0.5(5)	*E*	7.1(5)	0.12(3)
Sr	38				7.02(2)		6.19(4)	0.06(11)	6.25(10)	1.28(6)
		84	0(+)	0.56	7.(1.) *E*	0	6.(2.)	0	6.(2.)	0.87(7)
		86	0(+)	9.86	5.67(5)	0	4.04(7)	0	4.04(7)	1.04(7)
		87	9/2(+)	7.00	7.40(7)	6.88(13)	0.5(5)	*E*	7.4(5)	16.(3.)
		88	0(+)	82.58	7.15(6)	0	6.42(11)	0	6.42(11)	0.058(4)
Y	39	89	1/2(−)	100	7.75(2)	1.1(3)	7.55(4)	0.15(8)	7.70(9)	1.28(2)
Zr	40				7.16(3)		6.44(5)	0.02(15)	6.46(14)	0.185(3)
		90	0(+)	51.45	6.4(1)	0	5.1(2)	0	5.1(2)	0.011(5)
		91	5/2(+)	11.32	8.7(1)	−1.08(15)	9.5(2)	0.15(4)	9.7(2)	1.17(10)
		92	0(+)	17.19	7.4(2)	0	6.9(4)	0	6.9(4)	0.22(6)
		94	0(+)	17.28	8.2(2)	0	8.4(4)	0	8.4(4)	0.0499(24)
		96	0(+)	2.76	5.5(1)	0	3.8(1)	0	3.8(1)	0.0229(10)
Nb	41	93	9/2(+)	100	7.054(3)	−0.139(10)	6.253(5)	0.0024(3)	6.255(5)	1.15(5)
Mo	42				6.715(2)		5.67(3)	0.04(5)	5.71(4)	2.48(4)
		92	0(+)	14.84	6.91(8)	0	6.00(14)	0	6.00(14)	0.019(2)
		94	0(+)	9.25	6.80(7)	0	5.81(12)	0	5.81(12)	0.015(2)
		95	5/2(+)	15.92	6.91(6)	6.00(10)	0.5(5)	*E*	6.5(5)	13.1(3)
		96	0(+)	16.68	6.20(6)	0	4.83(9)	0	4.83(9)	0.5(2)
		97	5/2(+)	9.55	7.24(8)	6.59(15)	0.5(5)	*E*	7.1(5)	2.5(2)
		98	0(+)	24.13	6.58(7)	0	5.44(12)	0	5.44(12)	0.127(6)
		100	0(+)	9.63	6.73(7)	0	5.69(12)	0	5.69(12)	0.4(2)
Tc	43									
		99	9/2(+)	$(2.13\times10^5$a)	6.8(3)	5.8(5)	0.5(5)	*E*	6.3(7)	20.(1.)

Table 4.4.4.1. *Bound scattering lengths (cont.)*

Element	Z	A	I(π)	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
Ru	44				7.03(3)		6.21(5)	0.4(1)	6.6(1)	2.56(13)
		96	0(+)	5.5	0	0	0.28(2)			
		98	0(+)	1.9	0	0	<8.0			
		99	5/2(+)	12.7	6.9(1.0)					
		100	0(+)	12.6	0	0	4.8(6)			
		101	5/2(+)	17.0	3.3(9)					
		102	0(+)	31.6	0	0	1.17(7)			
		104	0(+)	18.7	0	0	0.31(2)			
Rh	45	103	1/2(−)	100	5.88(4)	4.34(6)	0.3(3)	*E*	4.6(3)	144.8(7)
Pd	46				5.91(6)		4.39(9)	0.093(9)	4.48(9)	6.9(4)
		102	0(+)	1.02	7.7(7) *E*	0	7.5(1.4)	0	7.5(1.4)	3.4(3)
		104	0(+)	11.14	7.7(7) *E*	0	7.5(1.4)	0	7.5(1.4)	0.6(3)
		105	5/2(+)	22.33	5.5(3)	−2.6(1.6)	3.8(4)	0.8(1.0)	4.6(1.1)	20.(3.)
		106	0(+)	27.33	6.4(4)	0	5.1(6)	0	5.1(6)	0.304(29)
		108	0(+)	26.46	4.1(3)	0	2.1(3)	0	2.1(3)	8.5(5)
		110	0(+)	11.72	7.7(7)*E*	0	7.5(1.4)	0	7.5(1.4)	0.226(31)
Ag	47				5.922(7)		4.407(10)	0.58(3)	4.99(3)	63.3(4)
		107	1/2(−)	51.839	7.555(11)	1.00(13)	7.17(2)	0.13(3)	7.30(4)	37.6(1.2)
		109	1/2(−)	48.161	4.165(11)	−1.60(13)	2.18(1)	0.32(5)	2.50(5)	91.0(1.0)
Cd	48				4.87(5) −0.70(1)*i*		3.04(6)	3.46(13)	6.50(12)	2520.(50.)
		106	0(+)	1.25	5.(2.) *E*	0	3.1(2.5)	0	3.1(2.5)	1.
		108	0(+)	0.89	5.4(1)	0	3.7(1)	0	3.7(1)	1.1(3)
		110	0(+)	12.51	5.9(1)	0	4.4(1)	0	4.4(1)	11.(1.)
		111	1/2(+)	12.81	6.5(1)	5.3(2)	0.3(3)	*E*	5.6(4)	24(3.)
		112	0(+)	24.13	6.4(1)	0	5.1(2)	0	5.1(2)	2.2(5)
		*113	1/2(+)	12.22	−8.0(2) −5.73(11)*i*	12.1(4)	0.3(3) *E*	12.4(5)		20600(400.)
		114	0(+)	28.72	7.5(1)	0	7.1(2)	0	7.1(2)	0.34(2)
		116	0(+)	7.47	6.3(1)	0	5.0(2)	0	5.0(2)	0.075(13)
In	49			4.065(20)	2.08(2) −0.0539(4)*i*	0.54(11)	2.62(11)	193.8(1.5)		
		113	9/2(+)	43	5.39(6)	±0.017(1)	3.65(8)	0.000037(5)	3.65(8)	12.0(1.1)
		115	9/2(+)	957	4.01(2) −0.0562(6)*i*	−2.1(2)	2.02(2)	0.55(11)	2.57(11)	202(2.)
Sn	50				6.225(2)		4.870(3)	0.022(5)	4.892(6)	0.626(9)
		112	0(+)	1.0	6.1(1.) *E*	0	4.5(1.5)	0	4.5(1.5)	1.01(11)
		114	0(+)	0.7	6.2(3)	0	4.8(5)	0	4.8(5)	0.114(30)
		115	1/2(+)	0.4	6.(1.) *E*	4.5(1.5)	0.3(3) *E*	4.8(1.5)	30(7.)	
		116	0(+)	14.7	5.93(5)	0	4.42(7)	0	4.42(7)	0.14(3)
		117	1/2(+)	7.7	6.48(5)	5.28(8)	0.3(3) *E*	5.6(3)	2.3(5)	
		118	0(+)	24.3	6.07(5)	0	4.63(8)	0	4.63(8)	0.22(5)
		119	1/2(+)	8.6	6.12(5)	4.71(8)	0.3(3) *E*	5.0(3)	2.2(5)	
		120	0(+)	32.4	6.49(5)	0	5.29(8)	0	5.29(8)	0.14(3)
		122	0(+)	4.6	5.74(5)	0	4.14(7)	0	4.14(7)	0.18(2)
		124	0(+)	5.6	5.97(5)	0	4.48(8)	0	4.48(8)	0.133(5)
Sb	51				5.57(3)		3.90(4)	0.00(7)	3.90(6)	4.91(5)
		121	7/2(+)	57.3	5.71(6)	−0.05(15)	4.10(9)	0.0003(19)	4.10(9)	5.75(12)
		123	5/2(+)	42.7	5.38(7)	−0.10(15)	3.64(9)	0.001(4)	3.64(9)	3.8(2)
Te	52				5.80(3)		4.23(4)	0.09(1)	4.32(4)	4.05(5)
		120	0(+)	0.096	5.3(5)	0	3.5(7)	0	3.4(7)	2.3(3)
		122	0(+)	2.60	3.8(2)	0	1.8(2)	0	1.8(2)	3.4(5)
		123	1/2(+)	0.908	−0.05(25) −0.116(8)*i*	−2.04(9)	0.002(3)	0.52(5)	0.52(5)	418(30.)
		124	0(+)	4.816	7.96(10)	0	8.0(2)	0	8.0(2)	6.8(1.3)
		125	1/2(+)	7.14	5.02(8)	−0.26(13)	3.17(10)	0.008(8)	3.18(10)	1.55(16)
		126	0(+)	18.95	5.56(7)	0	3.88(10)	0	3.88(10)	1.04(15)
		128	0(+)	31.69	5.89(7)	0	4.36(10)	0	4.36(10)	0.215(8)
		130	0(+)	33.80	6.02(7)	0	4.55(11)	0	4.55(11)	0.29(6)

Table 4.4.4.1. *Bound scattering lengths (cont.)*

Element	Z	A	I(π)	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
I	53	127	5/2(+)	100	5.28(2)	1.58(15)	3.50(3)	0.31(6)	3.81(7)	6.15(6)
Xe	54				4.92(3)		3.04(4)			23.9(1.2)
		124	0(+)	0.10		0		0		165.(20.)
		126	0(+)	0.09		0		0		3.5(8)
		128	0(+)	1.91		0		0		< 8.
		129	1/2(+)	26.4						21.(5.)
		130	0(+)	4.1		0		0		< 26.
		131	3/2(+)	21.2						85.(10.)
		132	0(+)	26.9		0		0		0.45(6)
		134	0(+)	10.4		0		0		0.265(20)
		136	0(+)	8.9		0		0		0.26(2)
Cs	55	133	7/2(+)	100	5.42(2)	1.29(15)	3.69(3)	0.21(5)	3.90(6)	29.0(1.5)
Ba	56				5.07(3)		3.23(4)	0.15(11)	3.38(10)	1.1(1)
		130	0(+)	0.11	−3.6(6)	0	1.6(5)	0	1.6(5)	30(5.)
		132	0(+)	0.10	7.8(3)	0	7.6(6)	0	7.6(6)	7.0(8)
		134	0(+)	2.42	5.7(1)	0	4.08(14)	0	4.08(14)	2.0(1.6)
		135	3/2(+)	6.59	4.67(10)		2.74(12)	0.5(5) *E*	3.2(5)	5.8(9)
		136	0(+)	7.85	4.91(8)	0	3.03(10)	0	3.03(10)	0.68(17)
		137	3/2(+)	11.23	6.83(10)		5.86(17)	0.5(5) *E*	6.4(5)	3.6(2)
		138	0(+)	71.70	4.84(8)	0	2.94(10)	0	2.94(10)	0.27(14)
La	57				8.24(4)		8.53(8)	1.13(19)	9.66(17)	8.97(5)
		138	5(+)	0.09	8.(2.) *E*	8.(4.)	0.5(5) *E*	8.5(4.0)	57.(6.)	
		139	7/2(+)	99.91	8.24(4)	3.0(2)	8.53(8)	1.13(15)	9.66(17)	8.93(4)
Ce	58				4.84(2)		2.94(2)	0.00(10)	2.94(10)	0.63(4)
		136	0(+)	0.19	5.80(9)	0	4.23(13)	0	4.23(13)	7.3(1.5)
		138	0(+)	0.25	6.70(9)	0	5.64(15)	0	5.64(15)	1.1(3)
		140	0(+)	88.48	4.84(9)	0	2.94(11)	0	2.94(11)	0.57(4)
		142	0(+)	11.08	4.75(9)	0	2.84(11)	0	2.84(11)	0.95(5)
Pr	59	141	5/2(+)	100	4.58(5)	−0.35(3)	2.64(6)	0.015(3)	2.66(6)	11.5(3)
Nd	60				7.69(5)		7.43(10)	9.2(8)	16.6(8)	50.5(1.2)
		142	0(+)	27.16	7.7(3)	0	7.5(6)	0	7.5(6)	18.7(7)
		143	7/2(−)	12.18	14.2(5) *E*	±21.1(6)	25.(7.)	55.(7.)	80.(2.)	334.(10.)
		144	0(+)	23.80	2.8(3)	0	1.0(2)	0	1.0(2)	3.6(3)
		145	7/2(−)	8.29	14.2(5)	*E*	25.(7.)	5.(5.) *E*	30.(9.)	42.(2.)
		146	0(+)	17.19	8.7(2)	0	9.5(4)	0	9.5(4)	1.4(1)
		148	0(+)	5.75	5.7(3)	0	4.1(4)	0	4.1(4)	2.5(2)
		150	0(+)	5.63	5.3(2)	0	3.5(3)	0	3.5(3)	1.2(2)
Pm	61									
		147	7/2(+)	(2.62a)	12.6(4)	±3.2(2.5)	20.0(1.3)	1.3(2.0)	21.3(1.5)	168.4(3.5)
Sm	62				0.80(2) −1.65(2)*i*		0.422(9)	39.(3.)	39.(3.)	5922.(56.)
		144	0(+)	3.1	−3.(4.) *E*	0	1.(3.)	0	1.(3.)	0.7(3)
		147	7/2(−)	15.1	14(3.)	±11.(7.)	25.(11.)	14.(19.)	39(16.)	57(3.)
		148	0(+)	11.3	−3.(4.) *E*	0	1.(3.)	0	1.(3.)	2.4(6)
		*149	7/2(−)	13.9	−19.2(1) −11.7(1)*i*	±31.4(6) −10.3(1)*i*	63.5(6)	137.(5.)	200.(5.)	42080.(400.)
		150	0(+)	7.4	14(3.)	0	25(11.)	0	25(11.)	104(4.)
		152	0(+)	26.6	−5.0(6)	0	3.1(8)	0	3.1(8)	206.(6.)
		154	0(+)	22.6	9.3(1.0)	0	11.(2.)	0	11.(2.)	8.4(5)
Eu	63				7.22(2) −1.26(1)*i*		6.75(4)	2.5(4)	9.2(4)	4530.(40.)
		*151	5/2(+)	47.8	6.13(14) −2.53(3)*i*	±4.5(4) −2.14(2)*i*	5.5(2)	3.1(4)	8.4(4)	9100(100.)
		153	5/2(+)	52.2	8.22(12)	±3.2(9)	8.5(2)	1.3(7)	9.8(7)	312.(7.)

Table 4.4.4.1.*Bound scattering lengths (cont.)*

Element	Z	A	I(π)	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
Gd	64				6.5(5) −13.82(3)*i*		29.3(8)	151.(2.)	180.(2.)	49700.(125.)
		152	0(+)	0.2	10.(3.) *E*	0	13.(8.)	0	13.(8.)	735.(20.)
		154	0(+)	2.1	10.(3.) *E*	0	13.(8.)	0	13.(8.)	85.(12.)
		*155	3/2(−)	14.8	6.0(1) −17.0(1)*i*	±5.(5.) *E* −13.16(9)*i*	40.8(4.)	25.(6.)	66.(6.)	61100.(400.)
		156	0(+)	20.6	6.3(4)	0	5.0(6)	0	5.0(6)	1.5(1.2)
		*157	3/2(−)	15.7	−1.14(2) −71.9(2)*i*	±5.(5.) *E* −55.8(2)*i*	650(4.)	394.(7.)	1044.(8.)	259000.(700.)
		158	0(+)	24.8	9.(2.)	0	10.(5.)	0	10.(5.)	2.2(2)
		160	0(+)	21.8	9.15(5)	0	10.52(11)	0	10.52(11)	0.77(2)
Tb	65	159	3/2(+)	100	7.38(3)	−0.17(7)	6.84(6)	0.004(3)	6.84(6)	23.4(4)
Dy	66				16.9(2) −0.276(4)*i*		35.9(8)	54.4(1.2)	90.3(9)	994.(13.)
		156	0(+)	0.06	6.1(5)	0	4.7(8)	0	4.7(8)	33.(3.)
		158	0(+)	0.10	6.(4.) *E*	0	5.(6.)	0	5.(6.)	43.(6.)
		160	0(+)	2.34	6.7(4)	0	5.6(7)	0	5.6(7)	56.(5.)
		161	5/2(+)	19.0	10.3(4)	±4.9(8)	13.3(1.0)	3.(1.)	16.(1.)	600.(25.)
		162	0(+)	25.5	−1.4(5)	0	0.25(18)	0	0.25(18)	194.(10.)
		163	5/2(−)	24.9	5.0(4)	1.3(3)	3.1(5)	0.21(10)	3.3(5)	124.(7.)
		164	0(+)	28.1	49.4(5) −0.79(1)*i*	0	307.(3.)	0	307.(3.)	2840.(40.)
Ho	67	165	7/2(−)	100	8.01(8)	−1.70(8)	8.06(16)	0.36(3)	8.42(16)	64.7(1.2)
Er	68				7.79(2)		7.63(4)	1.1(3)	8.7(3)	159.(4.)
		162	0(+)	0.14	8.8(2)	0	9.7(4)	0	9.7(4)	19.(2.)
		164	0(+)	1.56	8.2(2)	0	8.4(4)	0	8.4(4)	13.(2.)
		166	0(+)	33.4	10.6(2)	0	14.1(5)	0	14.1(5)	19.6(1.5)
		167	7/2(+)	22.9	3.0(3)	1.0(3)	1.1(2)	0.13(8)	1.2(2)	659.(16.)
		168	0(+)	27.1	7.4(4)	0	6.8(7)	0	6.9(7)	2.74(8)
		170	0(+)	14.9	9.6(5)	0	11.6(1.2)	0	11.6(1.2)	5.8(3)
Tm	69	169	1/2(+)	100	7.07(3)	0.9(3)	6.28(5)	0.10(7)	6.38(9)	100.(2.)
Yb	70				12.43(3)		19.42(9)	4.0(2)	23.05(18)	34.8(8)
		168	0(+)	0.14	−4.07(2) −0.62(1)*i*	0	2.13(2)	0	2.13(2)	2230.(40.)
		170	0(+)	3.06	6.77(10)	0	5.8(2)	0	5.8(2)	11.4(1.0)
		171	1/2(−)	143	9.66(10)	−5.59(17)	11.7(2)	3.9(2)	15.6(3)	48.6(2.5)
		172	0(+)	21.9	9.43(10)	0	11.2(2)	0	11.2(2)	0.8(4)
		173	5/2(−)	16.1	9.56(7)	−5.3(2)	11.5(2)	3.5(3)	15.0(4)	17.1(1.3)
		174	0(+)	31.8	19.3(1)	0	46.8(5)	0	46.8(5)	69.4(5.0)
		176	0(+)	12.7	8.72(10)	0	9.6(2)	0	9.6(2)	2.85(5)
Lu	71				7.21(3)		6.53(5)	0.7(4)	7.2(4)	74.(2.)
		175	7/2(+)	97.39	7.24(3)	±2.2(7)	6.59(5)	0.6(4)	7.2(4)	21.(3.)
		*176	7(−)	2.61	6.1(1) −0.57(1)*i*	±3.0(4) +0.61(1)*i*	4.7(2)	1.2(3)	5.9(4)	2065.(35.)
Hf	72				7.77(14)		7.6(3)	2.6(5)	10.2(4)	104.1(0.5)
		174	0(+)	0.2	10.9(1.1)	0	15.(3.)	0	15.(3.)	561.(35.)
		176	0(+)	5.2	6.61(18)	0	5.5(3)	0	5.5(3)	23.5(3.1)
		177	7/2(−)	18.6	0.8(1.0) *E*	±0.9(1.3)	0.1(2)	0.1(3)	0.2(2)	373.(10.)
		178	0(+)	27.1	5.9(2)	0	4.4(3)	0	4.4(3)	84.(4.)
		179	9/2(+)	13.7	7.46(16)	±1.06(8)	7.0(3)	0.14(2)	7.1(3)	41.(3.)
		180	0(+)	35.2	13.2(3)	0	21.9(1.0)	0	21.9(1.0)	13.04(7)
Ta	73				6.91(7)		6.00(12)	0.01(17)	6.01(12)	20.6(5)
		*180	9(−)	0.012	7.(2.) *E*	6.2(3.5)	0.5(5)	*E*	7.(4.)	563.(60.)
		181	7/2(+)	99.988	6.91(7)	−0.29(3)	6.00(12)	0.011(2)	6.01(12)	20.5(5)

Table 4.4.4.1. *Bound scattering lengths (cont.)*

Element	Z	A	I(π)	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
W	74				4.86(2)		2.97(2)	1.63(6)	4.60(6)	18.3(2)
		180	0(+)	0.1	5.(3.) *E*	0	3.(4.)	0	3.(4.)	30.(20.)
		182	0(+)	26.3	6.97(14)	0	6.10(7)	0	6.10(7)	20.7(5)
		183	1/2(−)	14.3	6.53(4)		5.36(7)	0.3(3) *E*	5.7(3)	10.1(3)
		184	0(+)	30.7	7.48(6)	0	7.03(11)	0	7.03(11)	1.7(1)
		186	0(+)	28.6	−0.72(4)	0	0.065(7)	0	0.065(7)	37.9(0.6)
Re	75				9.2(2)		10.6(5)	0.9(6)	11.5(3)	89.7(1.0)
		185	5/2(+)	37.40	9.0(3)	±2.0(1.8)	10.2(7)	0.5(9)	10.7(6)	112.(2.)
		187	5/2(+)	62.60	9.3(3)	±2.8(1.1)	10.9(7)	1.0(8)	11.9(4)	76.4(1.0)
Os	76				10.7(2)		14.4(5)	0.3(8)	14.7(6)	16.0(4)
		184	0(+)	0.02	10.(2.) *E*	0	13.(5.)	0	13.(5.)	3000.(150.)
		186	0(+)	1.58	11.6(1.7)	0	17.(5.)	0	17.(5.)	80.(13.)
		187	1/2(−)	1.6	10.(2.) *E*	13.(5.)	0.3(3)	*E*	13.(5.)	320(10.)
		188	0(+)	13.3	7.6(3)	0	7.3(6)	0	7.3(6)	4.7(5)
		189	3/2(−)	16.1	10.7(3)		14.4(8)	0.5(5) *E*	14.9(9)	25(4.)
		190	0(+)	26.4	11.0(3)	0	15.2(9)	0	15.2(8)	13.1(3)
		192	0(+)	41.0	11.5(4)	0	16.6(1.2)	0	16.6(1.2)	2.0(1)
Ir	77				10.6(3)		14.1(8)	0.(3.)	14.(3.)	425.3(2.4)
		191	3/2(+)	37.3						954.(10.)
		193	3/2(+)	62.7						111.(5.)
Pt	78				9.60(1)		11.58(2)	0.13(11)	11.71(11)	10.3(3)
		190	0(+)	0.01	9.0(1.0)	0	10.(2.)	0	10.(2.)	152.(4.)
		192	0(+)	0.79	9.9(5)	0	12.3(1.2)	0	12.3(1.2)	10.0(2.5)
		194	0(+)	32.9	10.55(8)	0	14.0(2)	0	14.0(2)	1.44(19)
		195	1/2(−)	33.8	8.83(9)	−1.00(17)	9.8(2)	0.13(4)	9.9(2)	27.5(1.2)
		196	0(+)	25.3	9.89(8)	0	12.3(2)	0	12.3(2)	0.72(4)
		198	0(+)	7.2	7.8(1)	0	7.7(2)	0	7.6(2)	3.66(19)
Au	79	197	3/2(+)	100	7.63(6)	−1.84(10)	7.32(12)	0.43(5)	7.75(13)	98.65(9)
Hg	80				12.692(15)		20.24(5)	6.6(1)	26.8(1)	372.3(4.0)
		196	0(+)	0.2	30.3(1.0)	0	115(8.)	0	115(8.)	3080(180.)
		198	0(+)	10.1		0		0		2.0(3)
		199	1/2(−)	17.0	16.9(4)	±15.5(8)	36.(2.)	30.(3.)	66.(2.)	2150.(48.)
		200	0(+)	23.1		0		0		< 60.
		201	3/2(−)	13.2			7.8(2.0)			
		202	0(+)	29.6		0		0		4.89(5)
		204	0(+)	6.8		0		0		0.43(10)
Tl	81				8.776(5)		9.678(11)	0.21(15)	9.89(15)	3.43(6)
		203	1/2(+)	29.524	6.99(16)	1.06(14)	6.14(28)	0.14(4)	6.28(28)	11.4(2)
		205	1/2(+)	70.476	9.52(7)	−0.242(17)	11.39(17)	0.007(1)	11.40(17)	0.104(17)
Pb	82				9.405(3)		11.115(7)	0.0030(7)	11.118(7)	0.171(2)
		204	0(+)	1.4	9.90(10)	0	12.3(2)	0	12.3(2)	0.65(7)
		206	0(+)	24.1	9.22(5)	0	10.68(12)	0	10.68(12)	0.0300(8)
		207	1/2(−)	22.1	9.28(4)	0.14(6)	10.82(9)	0.002(2)	10.82(9)	0.699(10)
		208	0(+)	52.4	9.50(2)	0	11.34(5)	0	11.34(5)	0.00048(3)
Bi	83	209	9/2(−)	100	8.532(2)	0.259(15)	9.148(4)	0.0084(10)	9.156(4)	0.0338(7)
Po	84									
At	85									
Rn	86									
Fr	87									
Ra	88									
		226	0(+)	$(1.60\times10^3$a)	10.0(1.0)	0	13.(3.)	0	13.(3.)	12.8(1.5)

Table 4.4.4.1. *Bound scattering lengths (cont.)*

Element	Z	A	I(π)	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
Ac	89									
Th	90	232	0(+)	100	10.31(3)	0	13.36(8)	0	13.36(8)	7.37(6)
Pa	91									
		231	3/2(−)	$(3.28\times10^4$a)	9.1(3)	1	0.4(7)	0.1(3.3)	10.5(3.2)	200.6(2.3)
U	92				8.417(5)		8.903(11)	0.005(16)	8.908(11)	7.57(2)
		233	5/2(+)	$(1.59\times10^5$a)	10.1(2)	±1.(3.)	12.8(5)	0.1(6)	12.9(3)	574.7(1.0)
		234	0(+)	0.005	12.4(3)	0	19.3(9)	0	19.3(9)	100.1(1.3)
		235	7/2(−)	0.720	10.47(3)	±1.3(6)	13.78(11)	0.2(2)	14.0(2)	680.9(1.1)
		238	0(+)	99.275	8.402(5)	0	8.871(11)	0	8.871(11)	2.68(2)
Np	93									
		237	5/2(+)	$(2.14\times10^6$a)	10.55(10)		14.0(3)	0.5(5)*E*	14.5(6)	175.9(2.9)
Pu	94									
		238	0(+)	(87.74a)	14.1(5)	0	25.0(1.8)	0	25.0(1.8)	558.(7.)
		239	1/2(+)	$(2.41\times10^4$a)	7.7(1)	±1.3(1.9)	7.5(2)	0.2(6)	7.7(6)	1017.3(2.1)
		240	0(+)	$(6.56\times10^3$a)	3.5(1)	0	1.54(9)	0	1.54(9)	289.6(1.4)
		242	0(+)	$(3.76\times10^5$a)	8.1(1)	0	8.2(2)	0	8.2(2)	18.5(5)
Am	95									
		243	5/2(−)	$(7.37\times10^3$a)	8.3(2)	±2.(7.)	8.7(4)	0.3(2.6)	9.0(2.6)	75.3(1.8)
Cm	96									
		244	0(+)	(18.10a)	9.5(3)	0	11.3(7)	0	11.3(7)	16.2(1.2)
		246	0(+)	$(4.7\times10^3$a)	9.3(2)	0	10.9(5)	0	10.9(5)	1.36(17)
		248	0(+)	$(3.5\times10^5$a)	7.7(2)	0	7.5(4)	0	7.5(4)	3.00(26)

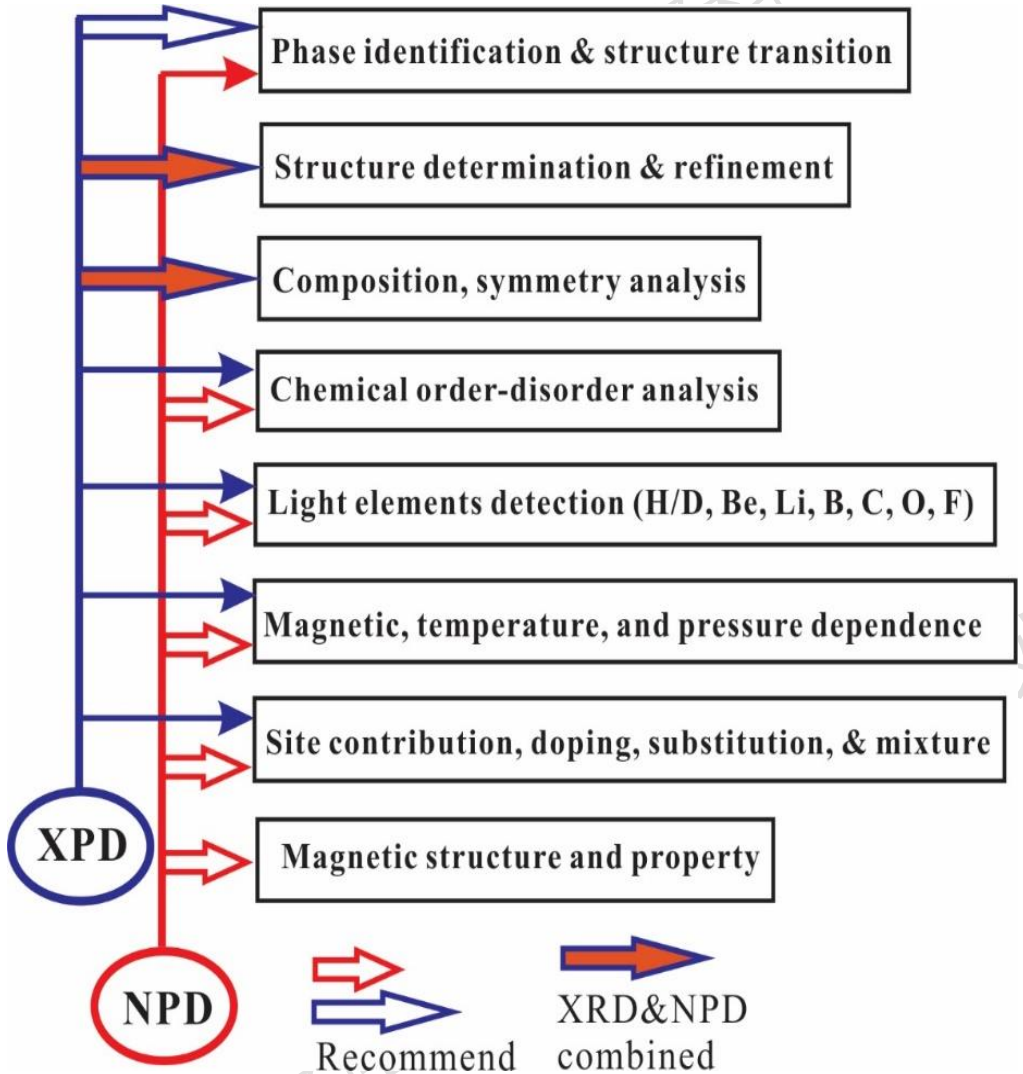
比较X射线衍射与中子衍射的应用
Comparison the Application of XRPD and NPD

中子相对优势 (Neutron Advantage)

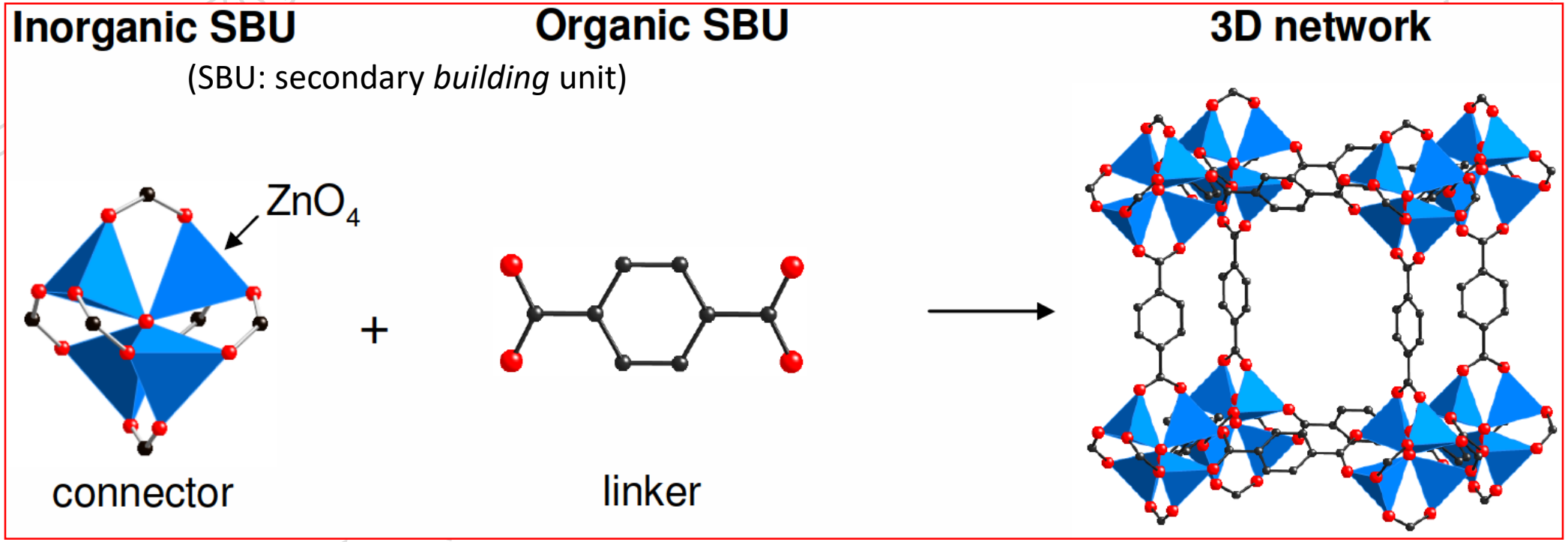
- 保持高角度峰强 (Comparable intensity at High-Q)
- 轻元素位置和占有率(Position & occupancy for Light elements)
- 近邻过渡族金属元素分布与共占位 (Distinguishing neighbor transition & rear-earth elements)
- 占有率与温度因子的相关性小 (Smaller correlation between occupancy and temperature factor)
- 有序磁对称性，磁结构及性能 (Ordered magnetic symmetry & structure and properties)
- 穿透力强 (Strong penetration)

中子相对劣势 (Neutron Disadvantage)

- 衍射强度低 (Lower intensity)
- 角分辨率低 (Lower Resolution)
- 要求样品量多 (Larger sample required)
- 中子源少 （High cost)



Metal-organic frameworks (MOFs)

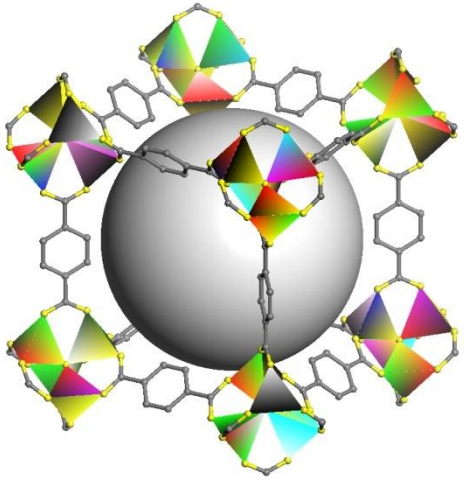


- Modular synthesis: hydrothermal or solvothermal methods
- Well-defined structure: crystal with uniform pore geometry
- Versatile chemistry: various metal clusters and organic linkers possible
  - → Tunable pore size
  - → Tunable functionality
- Gas-adsorption related applications: gas storage, gas separation etc.

*Omar M. Yaghi et al., ***Nature*** 402, 276 (1999).

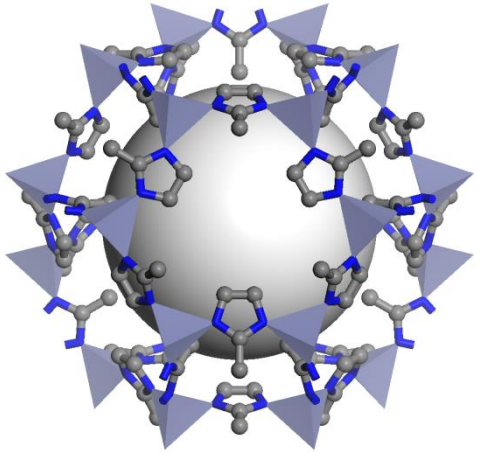
Some prototypical MOFs

MOF-5
(Metal Organic Framework-5)



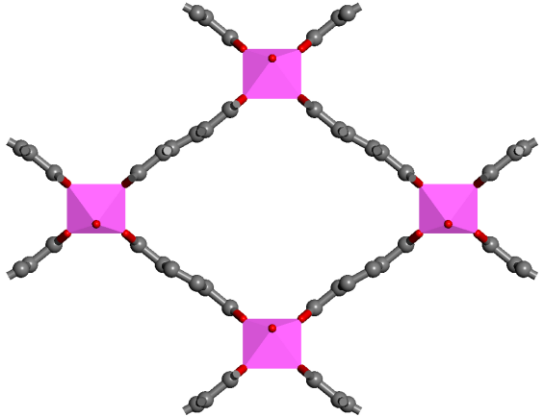
$ZnO_4+(C_6H_4)-(CO_2)_2$
(Yaghi's group)

ZIF-8
(Zeolitic Imidazolate Framework-8)

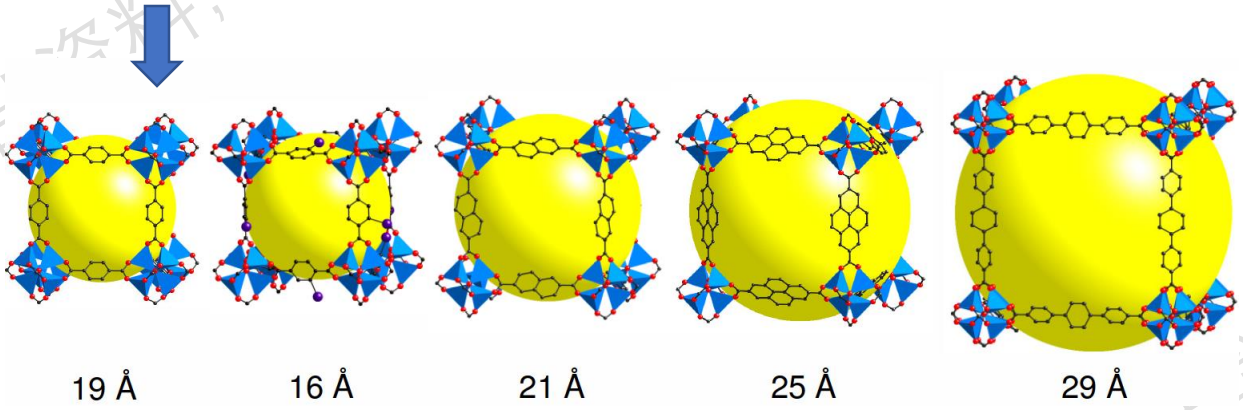


$ZnN_4+(C_3N_2H_2)-CH_3$
(Yaghi's group)

MIL-53
(Materials of Institut Lavoisier-53)



$AlO_6+(C_6H_4)-(CO_2)_2$
(Férey's group)

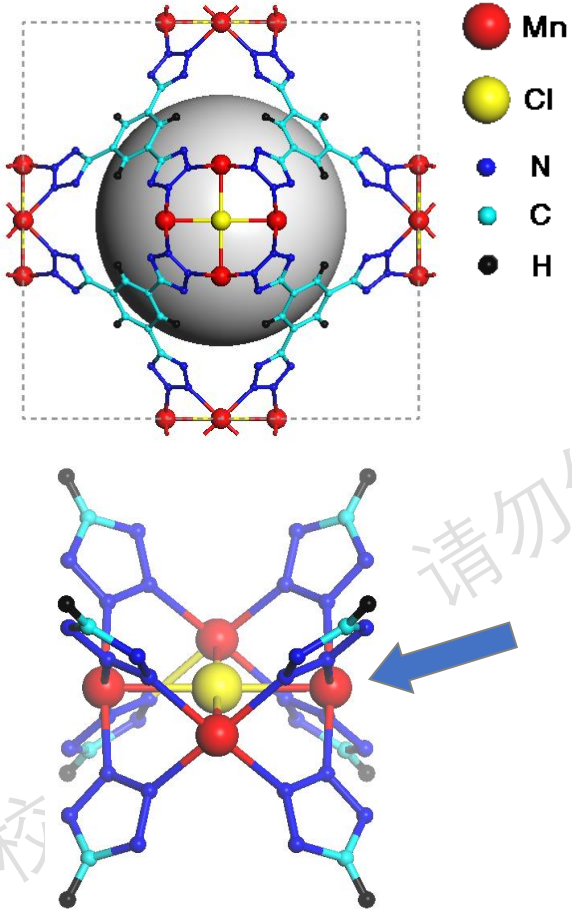


Large sphere:
the void/pore
in the structure

MOFs with open M coordination sites

Mn_4Cl-MOF

$(Mn_4Cl)_3(btt)_8$ / $Mn_4ClC_{24}H_8N_{32}$

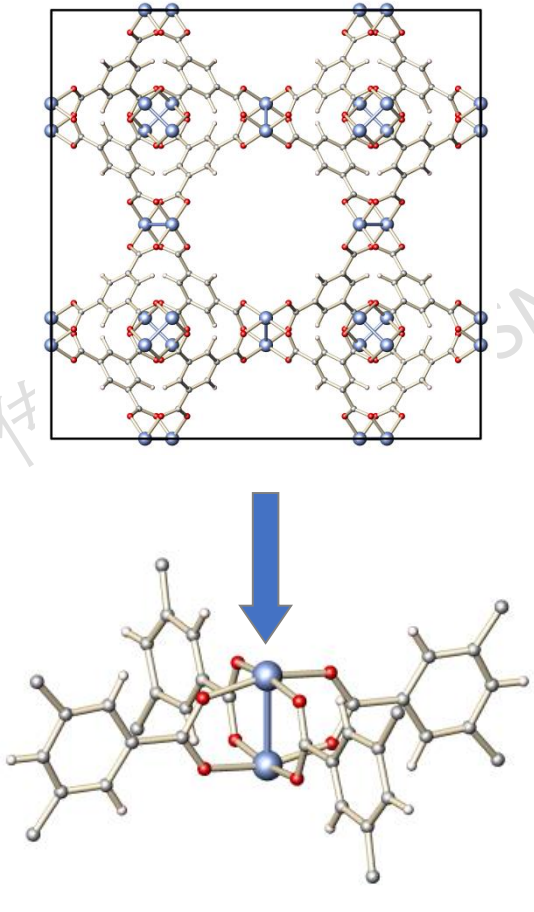


Mn: unsaturated

(Long's group)

HKUST-1

$Cu_3(btc)_2$ / $Cu_3C_{12}H_4O_8$

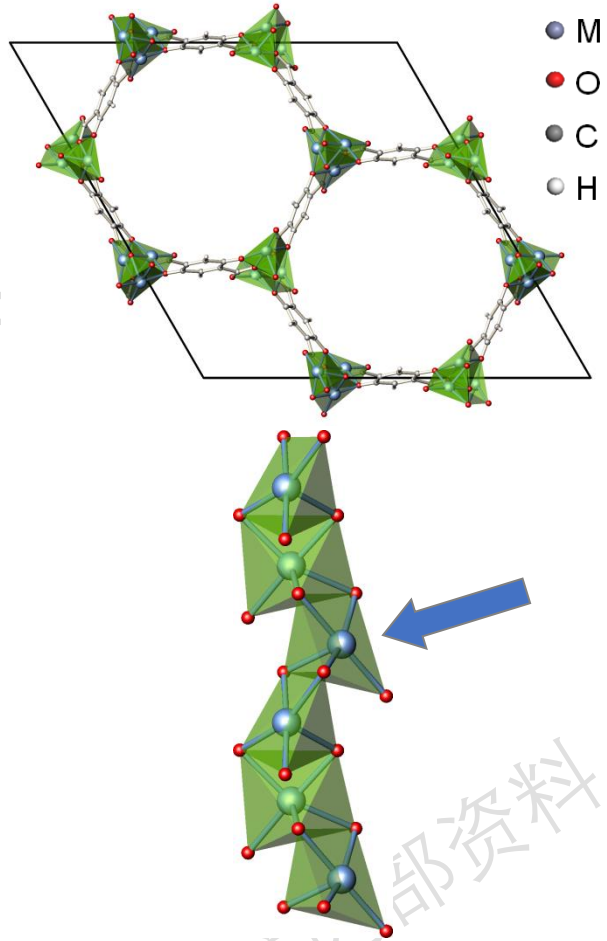


Cu: unsaturated

(Williams's group)

MOF-74

$Zn_2(dhtp)$ / $Zn_2C_8H_2O_6$



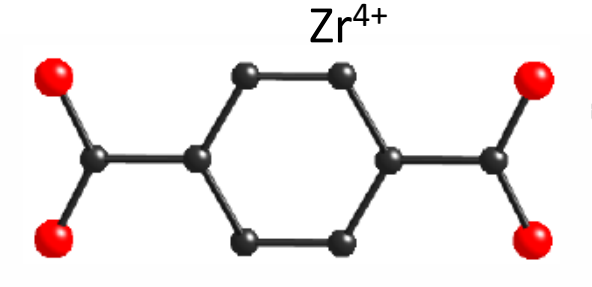
Zn: unsaturated

(Yaghi's group)

MOF结构中缺陷的研究
Study of Vacancy in MOF

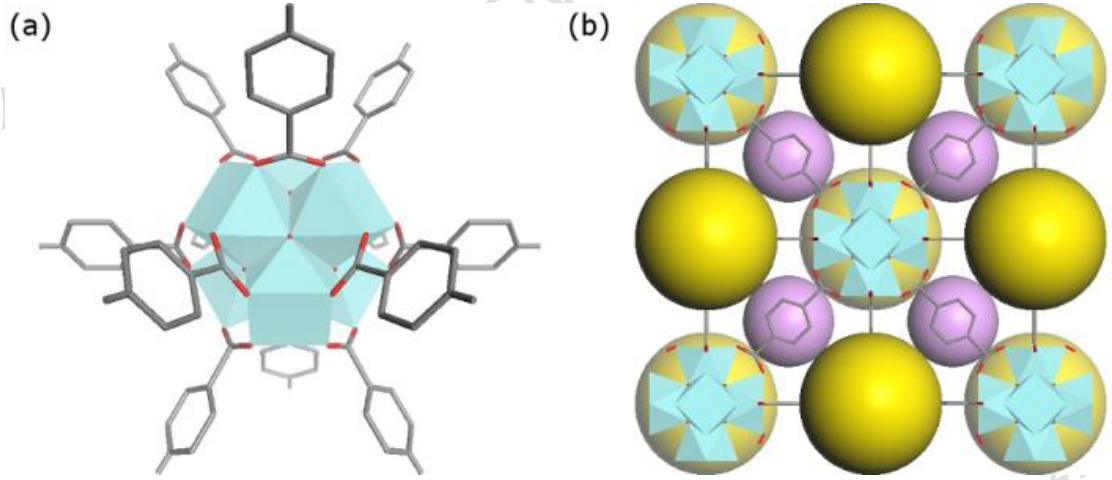
一个典型的Zr基MOF，能连接多个有机单元，具有其它一般的MOF所不具备的不寻常的化学，热学性质以及框价结构的稳定性。实验得到的空隙容积比理论值大20%，暗示这种MOF结构中可能有大量的空位。但同步辐射X射线衍射并没有发现空位的存在。

♦ Zr-UIO-66: an important prototypical Zr-based MOF; each metal center connected to 12 linkers. Because of its high framework connectivity, it exhibits exceptional chemical, thermal, and mechanical stabilities not commonly found in other MOFs.



BDC linker

(Lillerud's group)

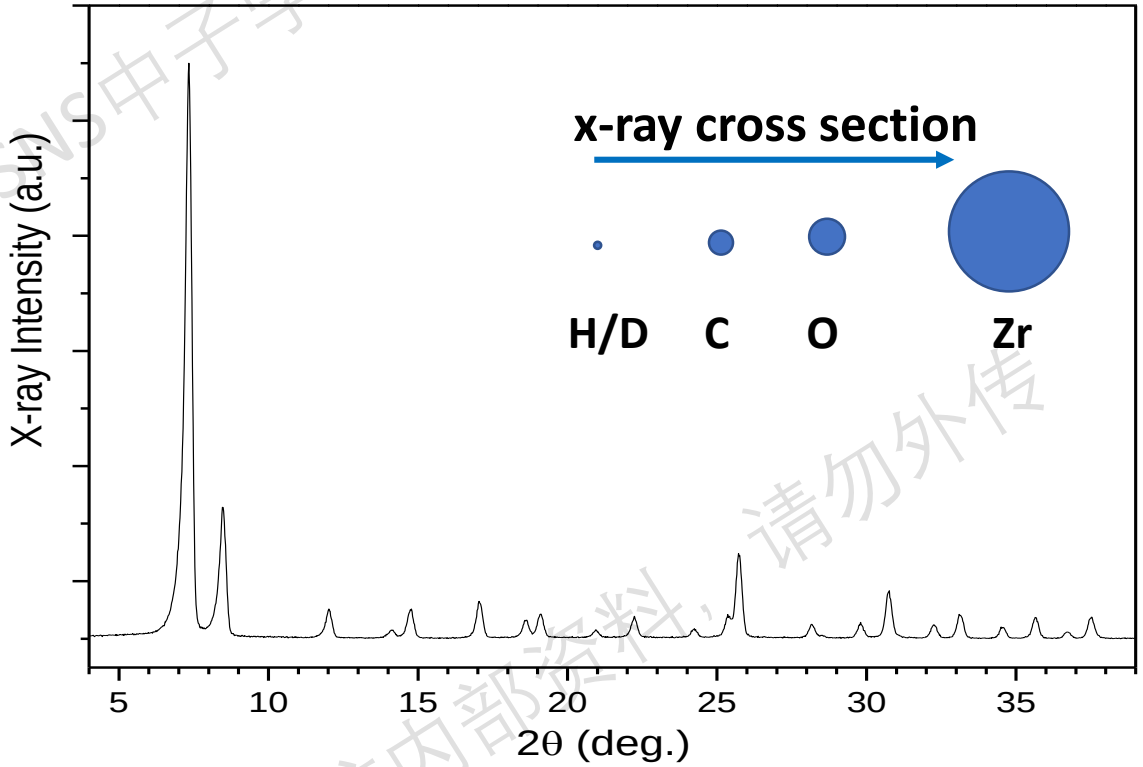


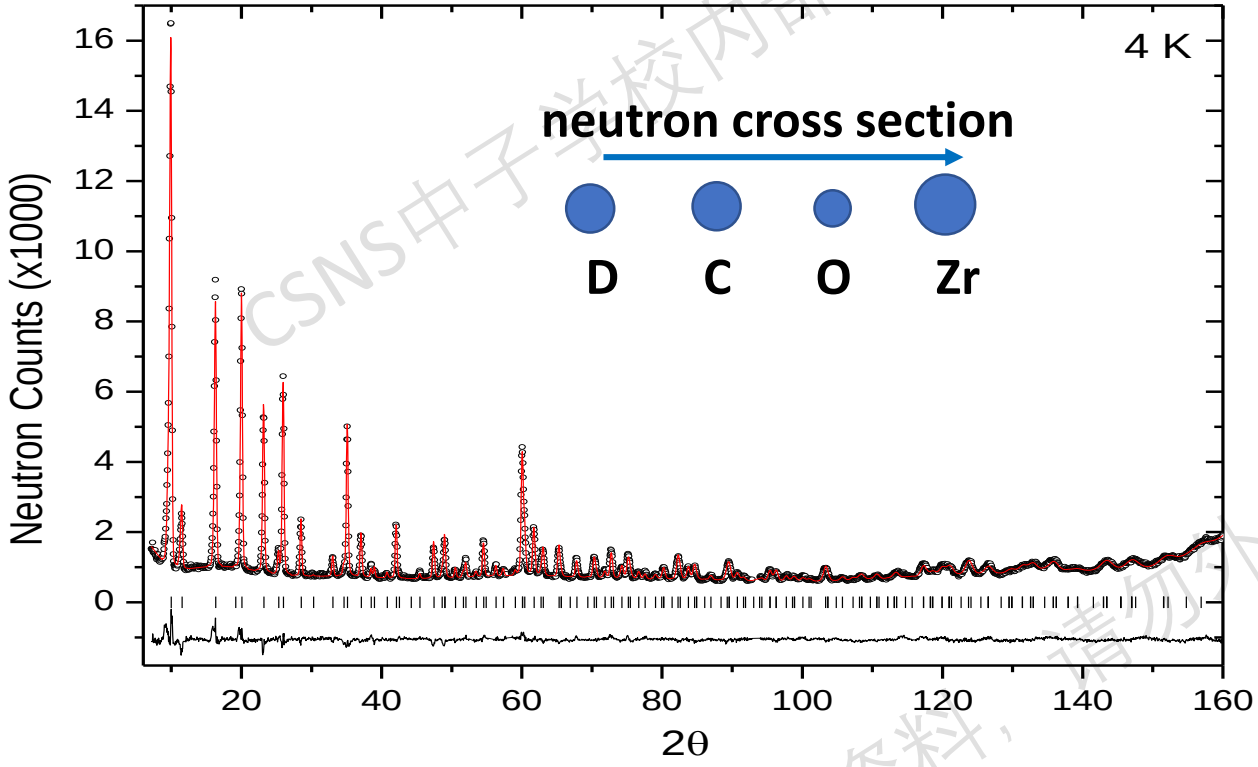
♦ A long-standing myth about this MOF: The experimental pore volume is ~20% higher than the theoretical value, suggesting that this MOF might contain significant amount of vacancy defects. However, synchrotron XRD data fit nicely with the ideal crystal structure.

H. Wu, T. Yildirim, W. Zhou*, ***J. Phys. Chem. Lett.***, 4, 925–930 (2013).

X-射线比较中子粉末衍射

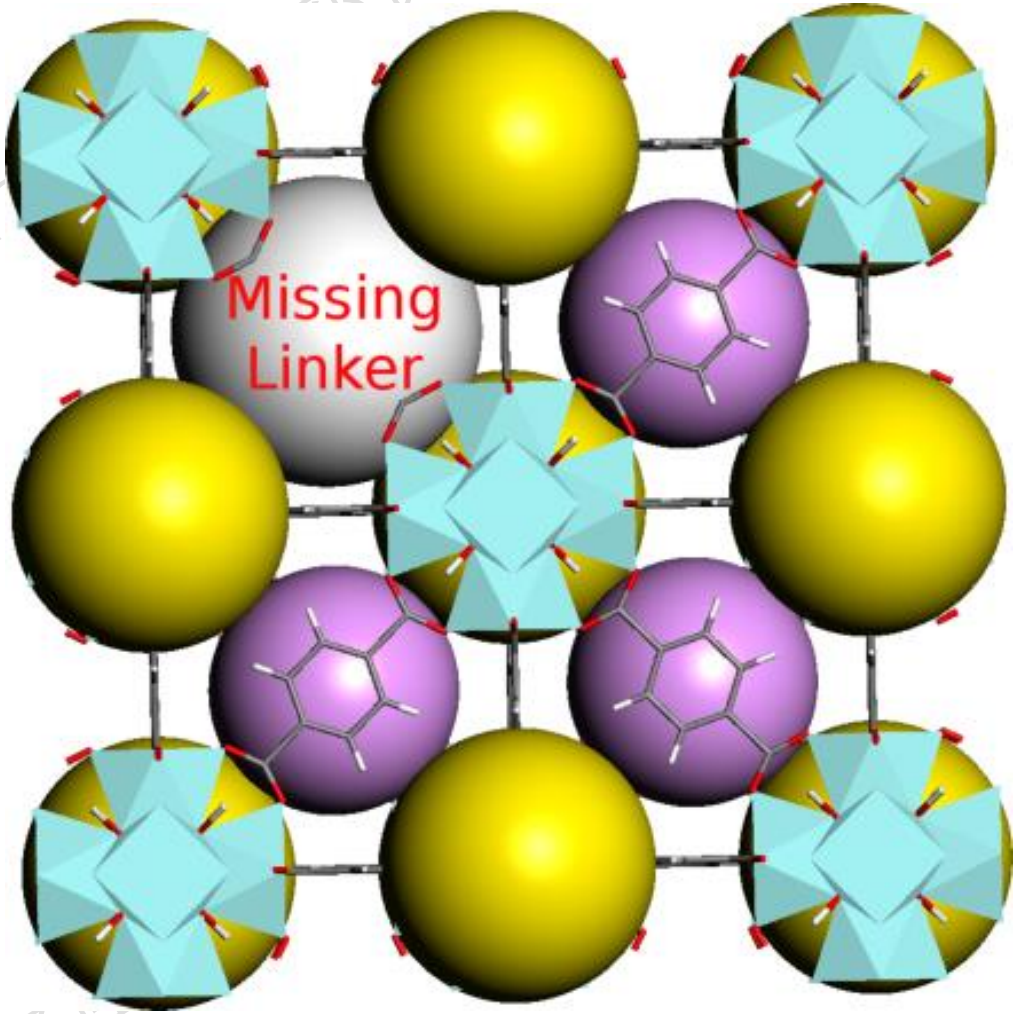
Neutron solved the myth in Zr-UiO-66





H. Wu, Y. S. Chua, V. Krungleviciute, M. Tyagi, P. Chen, T. Yildirim, W. Zhou*, ***J. Am. Chem. Soc.***, *135* , 10525 (2013).

Neutron solved the myth in Zr-UiO-66



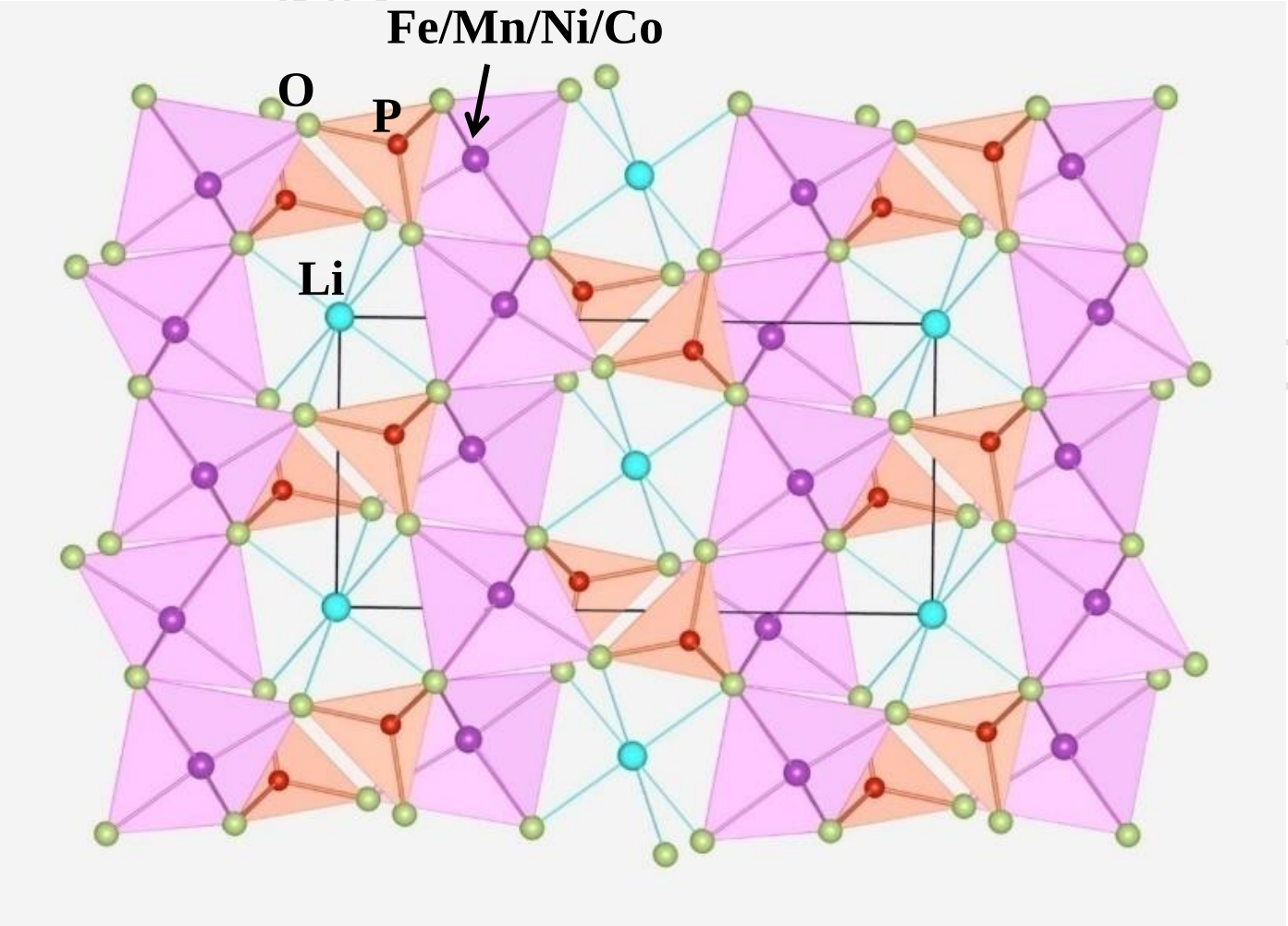
中子粉末衍射方法分析发现框架网络中只有连接有11个有机单元而不是理论的12个。而由于X射线衍射强度中重元素Zr占主导地位，因此没能发现丢了一个不敏感的较轻元素组成的有机单元。

Neutron diffraction shows that Zr-UiO-66 contains significant amount of **missing-linker defects**, which effectively reduce the framework connection from 12 to 11. (In contrast, x-ray diffraction is dominated by scattering from heavy element Zr, and thus is much less sensitive to linker vacancies.)

H. Wu, Y. S. Chua, V. Krungleviciute, M. Tyagi, P. Chen, T. Yildirim, W. Zhou*, ***J. Am. Chem. Soc.,*** *135* , 10525 (2013).

锂离子电极材料$Li^{+}_{x}(Fe/Ni)^{2+\sim3+}P^{5+}O^{2-}_{4}$结构分析及讨论

Discussion of Structure of electrode material $Li^{+}_{x}Fe^{2+\sim3+}P^{5+}O^{2-}_{4}$



价态变化

x=1： $Li^{1+}_{x}M^{2+}P^{5+}O^{2-}_{4}$

x=0-1： $Li^{1+}_{x}M^{2+}_{1-x}M^{3+}_{x}P^{5+}O^{2-}_{4}$

x~0： $Li^{1+}_{x}M^{3+}P^{5+}O^{2-}_{4}$

Neutron scattering amplitude

b_{Fe} =0.954　　b_{Ni} =1.03

b_{Li} = -0.203　　b_{O} =0.5805

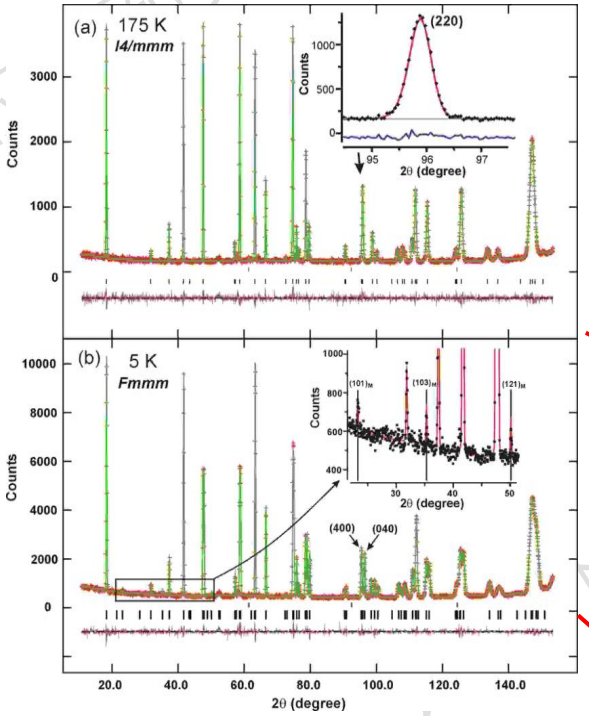
b_{P} =0.513　　b_{Mn} = -0.373

b_{Co} =0.254

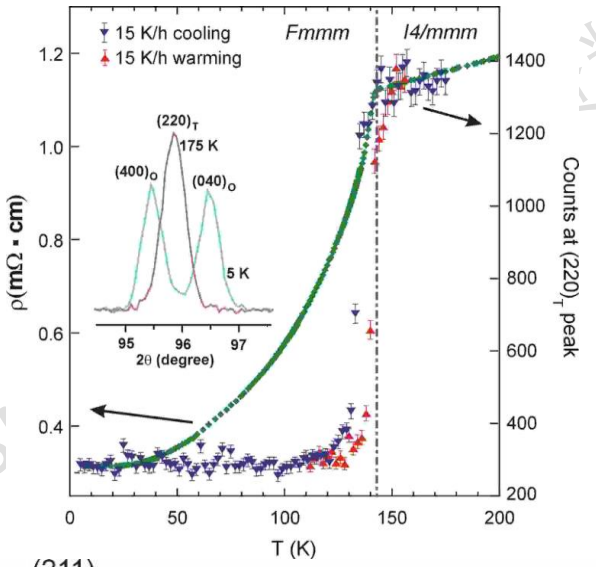
中子测定锂电池电极材料$Li^{+}_{x}Fe^{2+\sim3+}P^{5+}O^{2-}_{4}$中离子通道中Li含量和混合占位引起的结构和性能变化，因为X射线对轻元素Li极不敏感，很难测出准确的Li的占位率以及不同Li离子占位率对结构的影响。在充放电过程中，由于Li离子占位率变化，Fe和Ni的价态发生变化而伴随的晶胞体积的变化可能对电池的运用受到影响。

$BaFe_2As_2$晶体结构和磁结构,相转变与性能

Crystal & Magnetic Structure, Phase Transformation, and properties of $BaFe_2As_2$

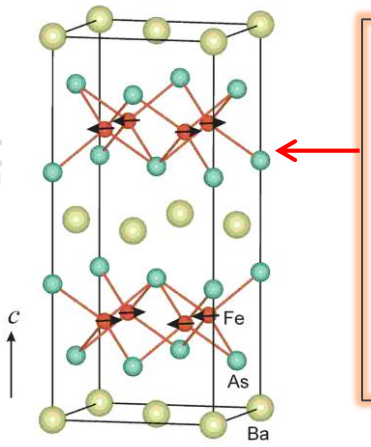


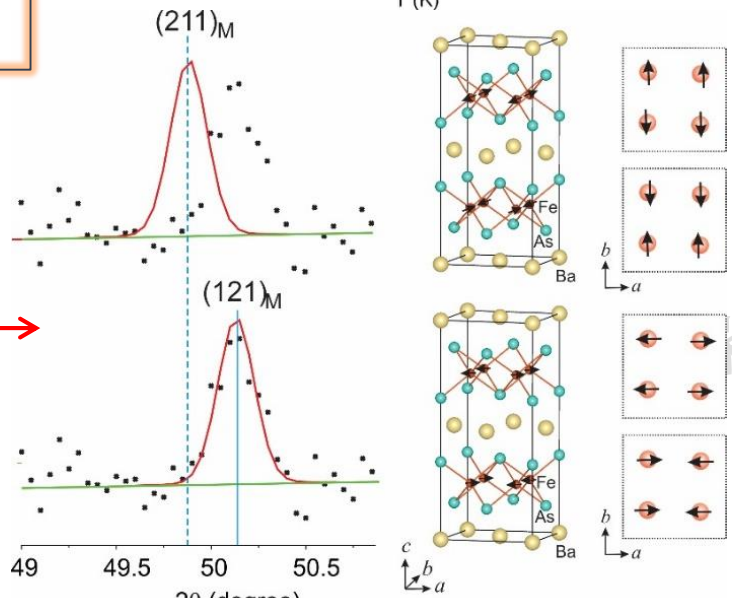
化合物$BaFe_2As_2$在~142 K经历由高温*I4/mmm*到低温*Fmmm*的一级晶体结构相变，伴随着从顺磁到反铁磁的磁有序转变和电阻急剧下降的突变。



Relationships between structure and properties …

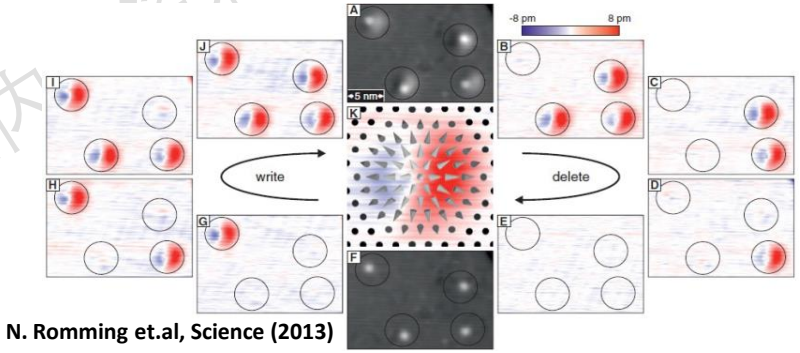
Determine and refine crystal and magnetic structures:
Chemical & symmetry
Atomic distribution
Magnetic order-disorder
Spin arrangement
…



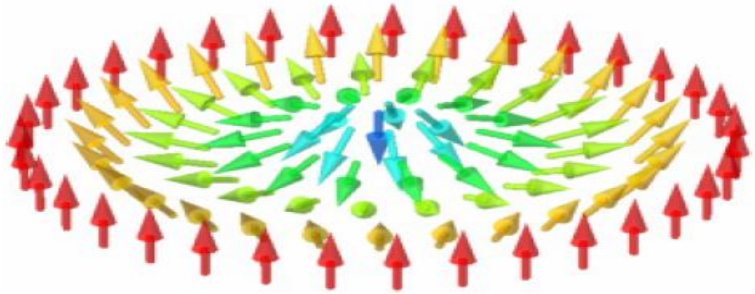


Huang, Q ., Qiu, Y., Bao, W ., et.al. PRL,101, 257003 (2008)

Magnetic Skyrmions

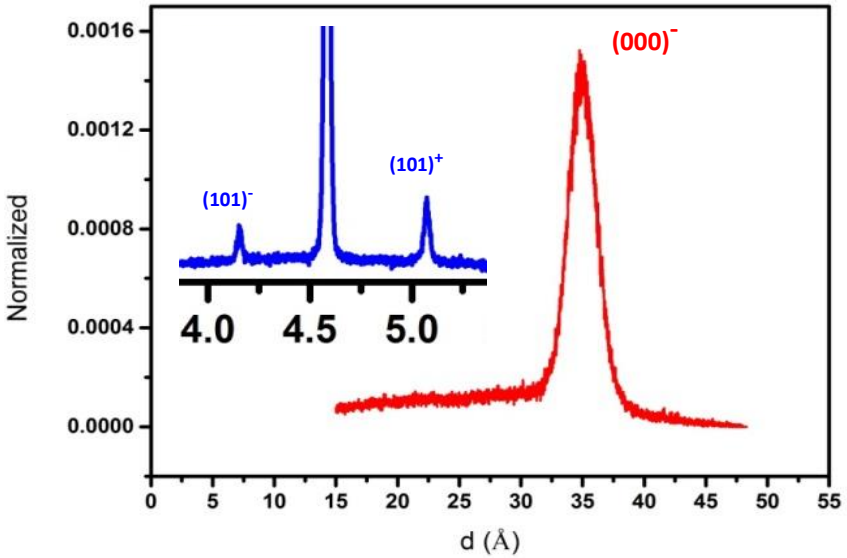


N. Romming et.al, Science (2013)



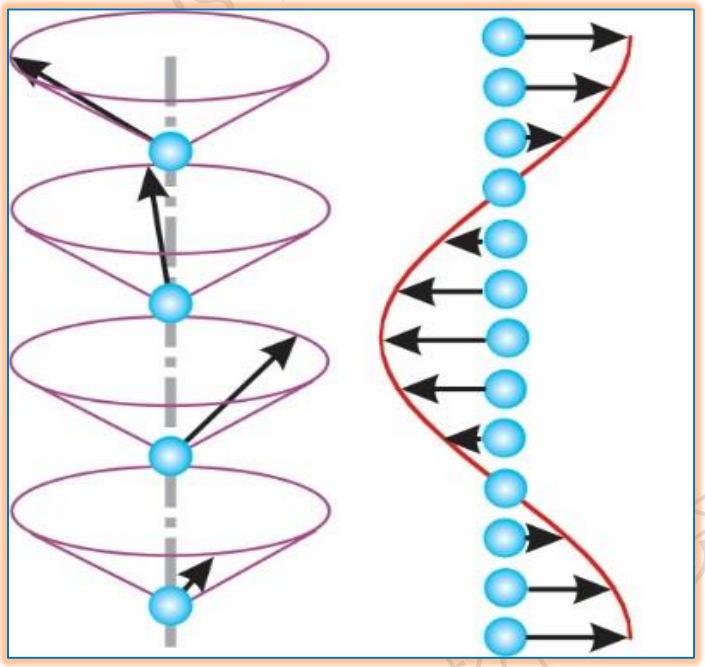
C. Pfleiderer, Nature Physics (2011)

Skyrmions has a potential applications



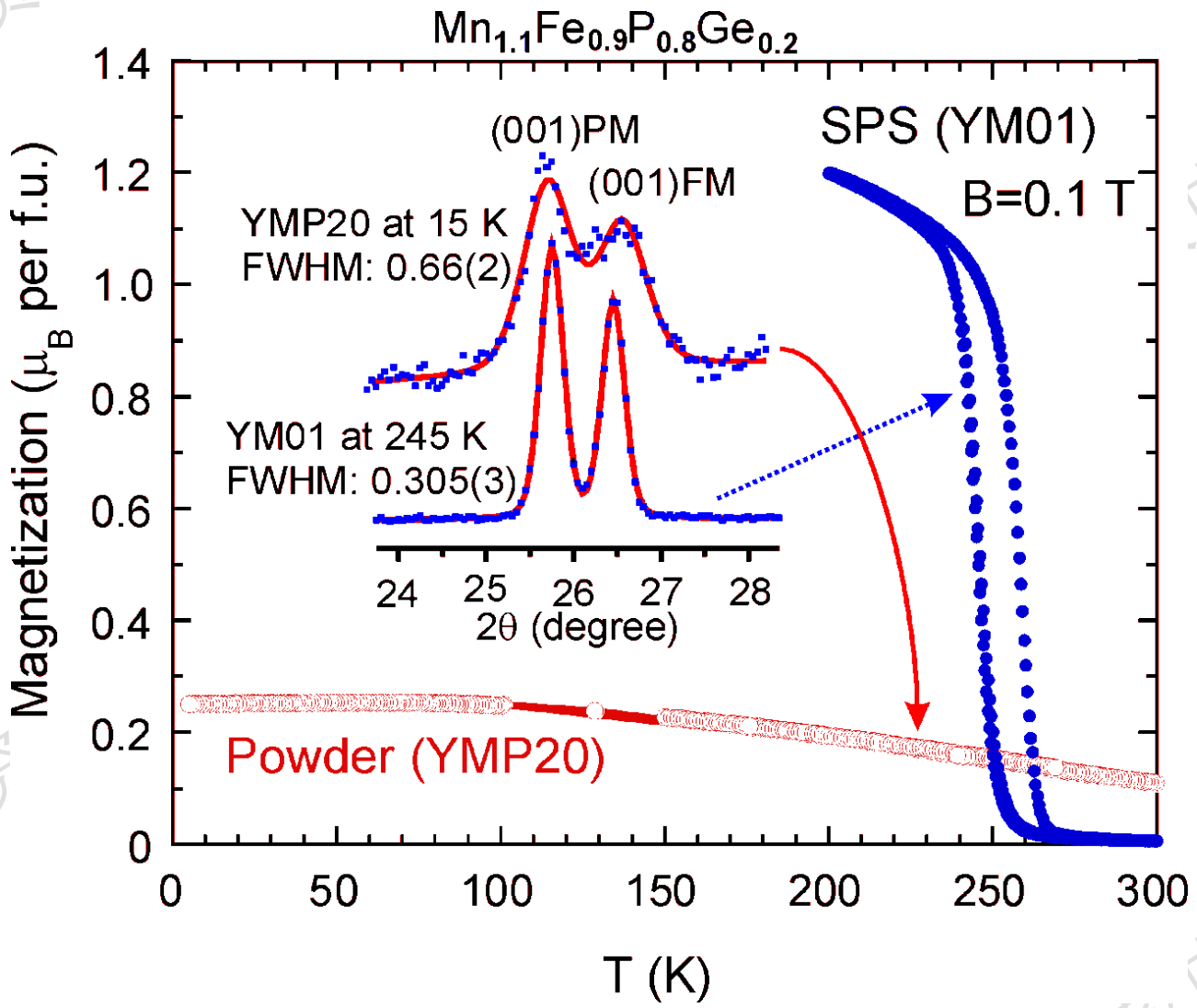
Satellite peaks of incommensurate magnetic ordering observed at GPPD

在中国散裂源GPPD探测到的无公度磁有序卫星峰



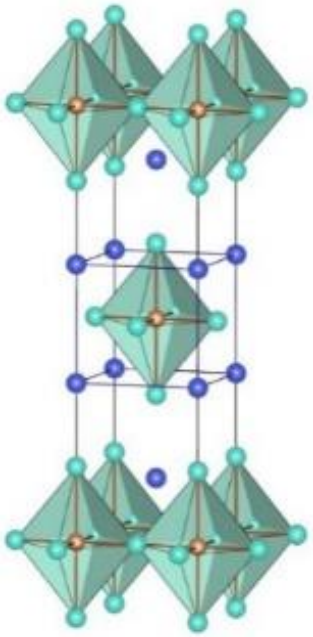
Incommensurate magnetic

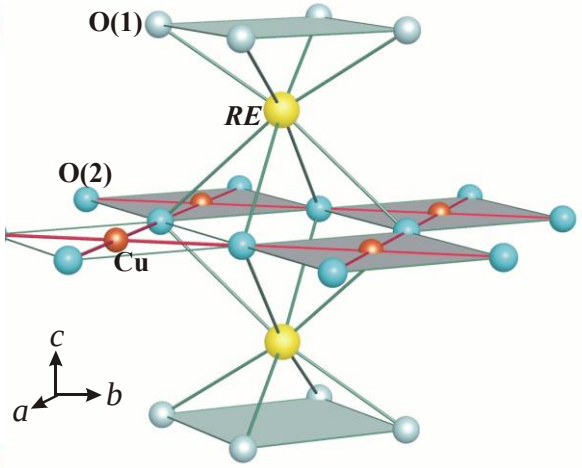
晶粒尺度对铁磁有序度的影响



Small crystalline size inhibits the magnetic order

结构中得到$LaPr_{0.88}Ce_{0.12}CuO_{4+\delta}$是E-doping超导体的证据





Hole doping

$La_{1.88}^{3+}Ba_{0.12}^{2+}Cu^{2.12+}O_4$

Electron doping

$La^{3+}Pr_{0.88}^{3+}Ce_{0.12}^{4+}Cu^{1.88+}O_4$

	SC crystal	*As-grown powder*	*SC powder*	*NSC powder*
n(La)	0.481(4)	0.489(4)	0.479(4)	0.480(4)
n(Cu)	1.001(6)	0.977(6)	1.001(6)	0.988(5)
n(O2)	0.974(5)	0.988(6)	0.972(5)	0.986(5)
Ratio(Cu:O)	**1:3.94**	**1:4.07**	**1:3.94**	**1:4.02**
RE-O(1)	2.3640(3)	2.3609(3)	2.3636(3)	2.3615(3)
***RE*-O(2)**	**2.6922(4)**	**2.6948(4)**	**2.6933(4)**	**2.6952(4)**
O(1)-O(1)	2.81995(3)	2.81921(3)	2.82001(2)	2.81923(2)
O(2)-O(2)	3.07875(4)	3.07805(3)	3.07940(3)	3.07980(3)
***V*(REO_8)**	**24.4826(6)**	**24.4642(5)**	**24.4888(5)**	**24.4781(5)**
Cu-O(2)	1.99401(2)	1.99348(2)	1.99405(1)	1.99350(2)
$\mathcal{V}$(Cu)* (e.u.)	**1.661**	**1.729**	**1.658**	**1.706**

根据实验测得的键长，用表中的数据计算离子的价态

$V_i=\sum_j v_{ij}$, $v_{ij}=\exp[(R_{ij}-d_{ij})/b]$, e=2.71828, b=0.37, d_{ij} is bond distance

Recommended bond-valence parameters for oxides, fluorides and chlorides

Cation	O	F	Cl
Ac^{III}	2·24	*2·13*	*2·63*
Ag^{I}	1·805	1·80	2·09
Al^{III}	1·651	1·545	2·03
Am^{III}	2·11	*2·00*	*2·48*
As^{III}	1·789	1·70	2·16
As^{V}	1·767	1·62	*2·14*
Au^{III}	1·833	1·81	2·17
B^{III}	1·371	1·31	1·74
Ba^{II}	2·29	2·19	2·69
Be^{II}	1·381	1·28	*1·76*
Bi^{III}	2·09	1·99	2·48
Bi^{V}	2·06	1·97	*2·44*
Bk^{III}	2·08	*1·96*	*2·46*
Br^{VII}	1·81	*1·72*	*2·19*
C^{IV}	1·39	1·32	1·76
Ca^{II}	1·967	1·842	2·37
Cd^{II}	1·904	1·811	2·23
Ce^{III}	2·151	2·036	2·52
Ce^{IV}	2·028	1·995	*2·41*
Cf^{III}	2·07	1·95	2·45
Cl^{VII}	1·632	*1·55*	*2·00*
Cm^{III}	2·23	*2·12*	*2·62*
Co^{II}	1·692	1·64	2·01
Co^{III}	1·70	*1·62*	2·05
Cr^{II}	*1·73*	1·67	2·09
Cr^{III}	1·724	1·64	2·08
Cr^{VI}	1·794	1·74	2·12
Cs^{I}	2·42	2·33	2·79
Cu^{I}	1·593	*1·6*	1·85
Cu^{II}	1·679	1·60	2·00

Cation	O	F	Cl
Mn^{IV}	1·753	1·71	*2·13*
Mn^{VII}	1·79	1·72	*2·17*
Mo^{VI}	1·907	*1·81*	2·28
N^{III}	1·361	1·37	1·75
N^{V}	1·432	*1·36*	*1·80*
Na^{I}	1·80	1·677	2·15
Nb^{V}	1·911	1·87	2·27
Nd^{III}	2·117	2·008	2·492
Ni^{II}	1·654	1·599	2·02
Os^{IV}	1·811	*1·72*	*2·19*
P^{V}	1·604	1·521	1·99
Pb^{II}	2·112	2·03	2·53
Pb^{IV}	2·042	*1·94*	2·43
Pd^{II}	1·792	1·74	2·05
Pr^{III}	2·135	2·022	2·50
Pt^{II}	1·768	*1·68*	2·05
Pt^{IV}	1·879	1·759	2·17
Pu^{III}	2·11	2·00	2·48
Rb^{I}	2·26	2·16	2·65
Re^{VII}	1·97	1·86	2·23
Rh^{III}	1·791	1·71	*2·17*
Ru^{IV}	1·834	1·74	2·21
S^{IV}	1·644	1·60	*2·02*
S^{VI}	1·624	1·56	2·03
Sb^{III}	1·973	1·90	2·35
Sb^{V}	1·942	1·80	2·30
Sc^{III}	1·849	1·76	*2·23*
Se^{IV}	1·811	1·73	2·22
Se^{VI}	1·788	1·69	*2·16*
Si^{IV}	1·624	1·58	2·03

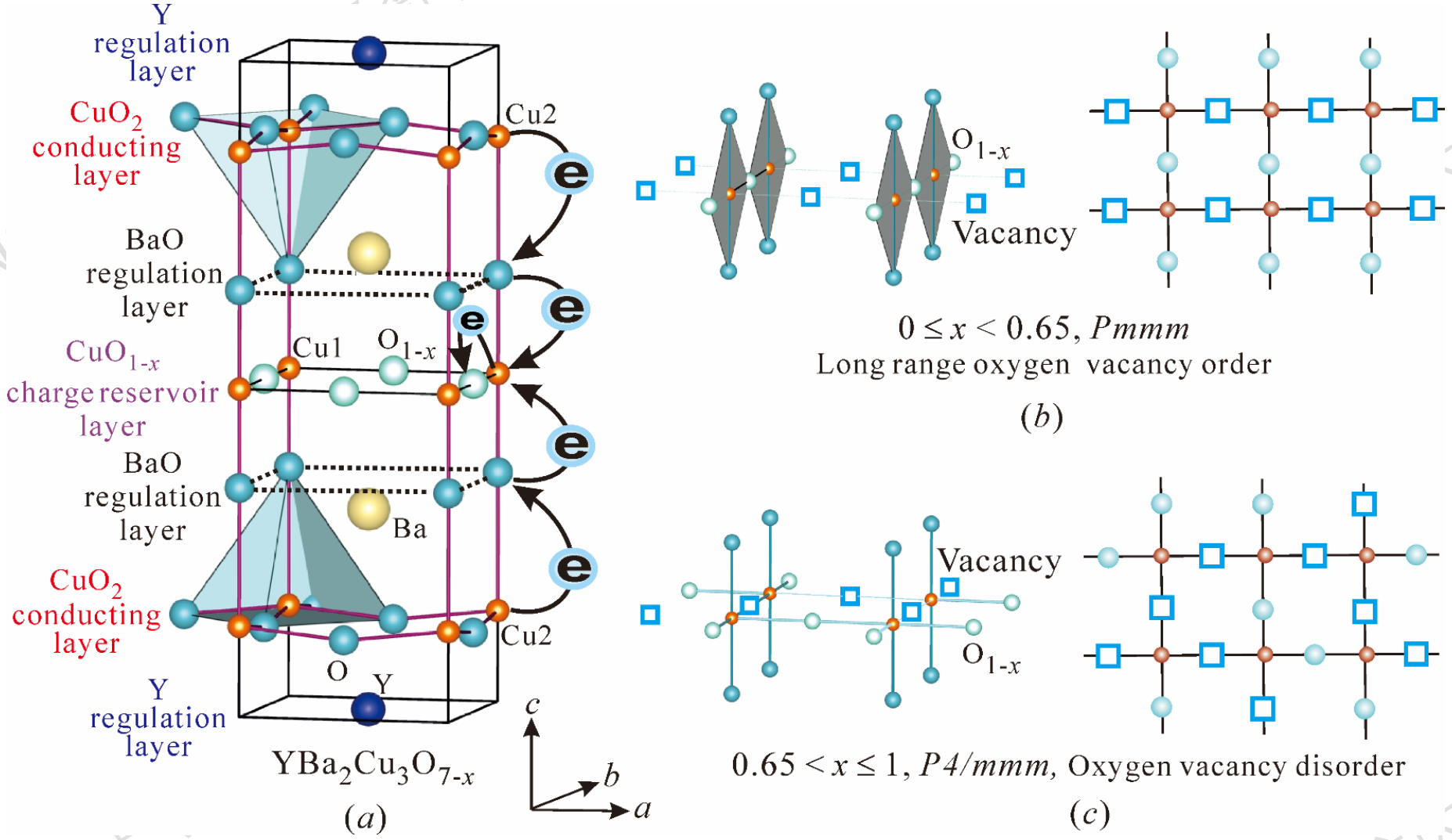
Cation	O	F	Cl
Dy^{III}	2·036	1·922	2·41
Er^{III}	2·010	1·906	2·39
Eu^{II}	2·147	2·04	2·53
Eu^{III}	2·076	1·961	2·455
Fe^{II}	1·734	1·65	2·06
Fe^{III}	1·759	1·67	2·09
Ga^{III}	1·730	1·62	2·07
Gd^{III}	2·065	1·95	2·445
Ge^{IV}	1·748	1·66	2·14
H^{I}	0·95	0·92	1·28
Hf^{IV}	1·923	1·85	*2·30*
Hg^{I}	1·90	*1·81*	*2·28*
Hg^{II}	1·93	1·90	2·25
Ho^{III}	2·023	1·908	2·401
I^{V}	2·00	*1·90*	*2·38*
I^{VII}	1·93	1·83	*2·31*
In^{III}	1·902	1·79	*2·28*
Ir^{V}	1·916	1·82	2·30
K^{I}	2·13	1·99	2·52
La^{III}	2·172	2·057	2·545
Li^{I}	1·466	1·360	1·91
Lu^{III}	1·971	1·876	2·361
Mg^{II}	1·693	1·581	2·08
Mn^{II}	1·790	1·698	2·13
Mn^{III}	1·760	1·66	*2·14*

Cation	O	F	Cl
Sm^{III}	2·088	1·977	2·466
Sn^{II}	1·984	1·925	*2·36*
Sn^{IV}	1·905	1·84	2·28
Sr^{II}	2·118	2·019	2·51
Ta^{V}	1·920	1·88	2·30
Tb^{III}	2·049	1·936	2·427
Te^{IV}	1·977	1·87	2·37
Te^{VI}	1·917	1·82	*2·30*
Th^{IV}	2·167	2·07	*2·55*
Ti^{III}	1·791	1·723	*2·17*
Ti^{IV}	1·815	1·76	*2·19*
Tl^{I}	2·172	2·15	*2·56*
Tl^{III}	2·003	1·88	2·32
Tm^{III}	2·000	1·842	2·38
U^{IV}	2·112	2·034	2·48
U^{VI}	2·075	1·966	2·46
V^{III}	1·743	1·702	*2·19*
V^{IV}	1·784	1·70	*2·16*
V^{V}	1·803	1·71	2·16
W^{VI}	1·921	1·83	2·27
Y^{III}	2·014	1·904	2·40
Yb^{III}	1·985	1·875	2·371
Zn^{II}	1·704	1·62	2·01
Zr^{IV}	1·937	1·854	2·33

Cu^{III}-O, R=1.724; Co^{IV}-O, R=1.75; Fe^{IV}-O, R=1.78;
Ni^{III}-O, R=1.68; Ni^{IV}-O, R=1.72

N.E.Brese and M.O'Keefe. Bond-Valence Parameters for Solids. Acta Cryst., B47, 192-197(1991)

化学成分，结构对称性 & 元素分布与性能的关系



Schematic view of charge transfer between conduction layer and charge reservoir layer in superconducting and related compounds. Electron transfer from the conducting layer to the charge reservoir layer is known as "hole doping" and moving electrons from the charge reservoir layer to the conducting layer is known as "electron doping".

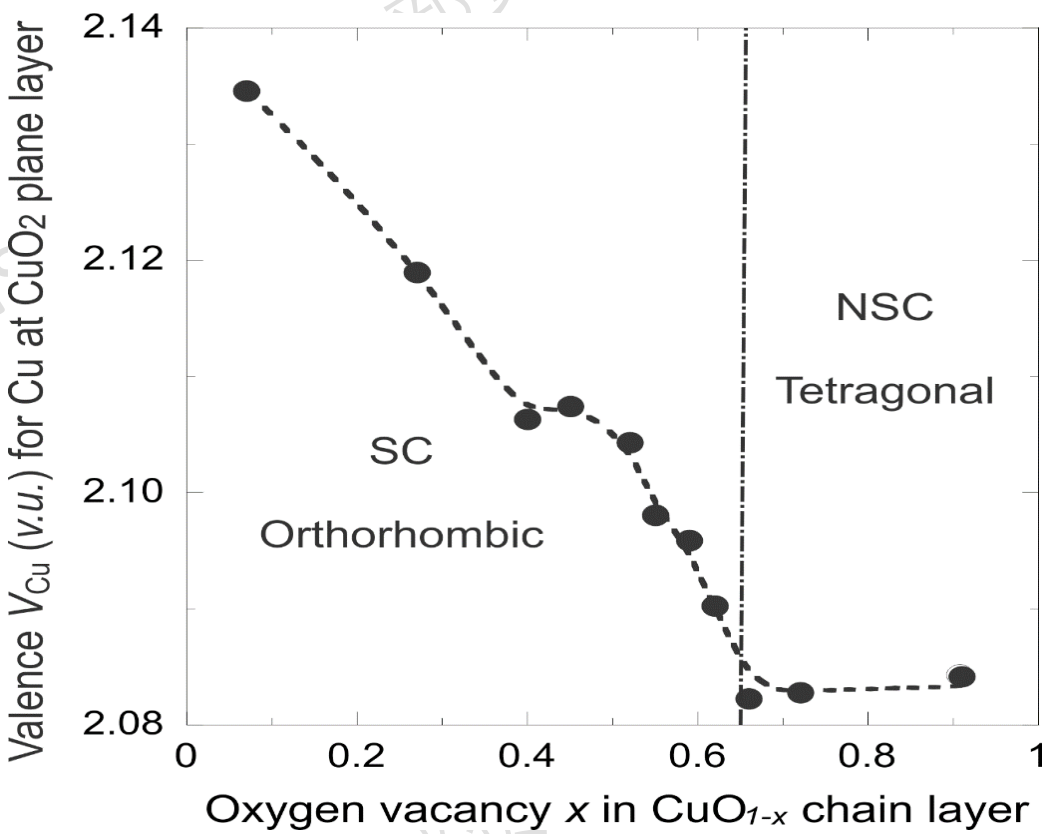
$YBa_2Cu_3O_{7-x}$是第一个被发现T_C在液氮以下的高温超导体。研究发现：

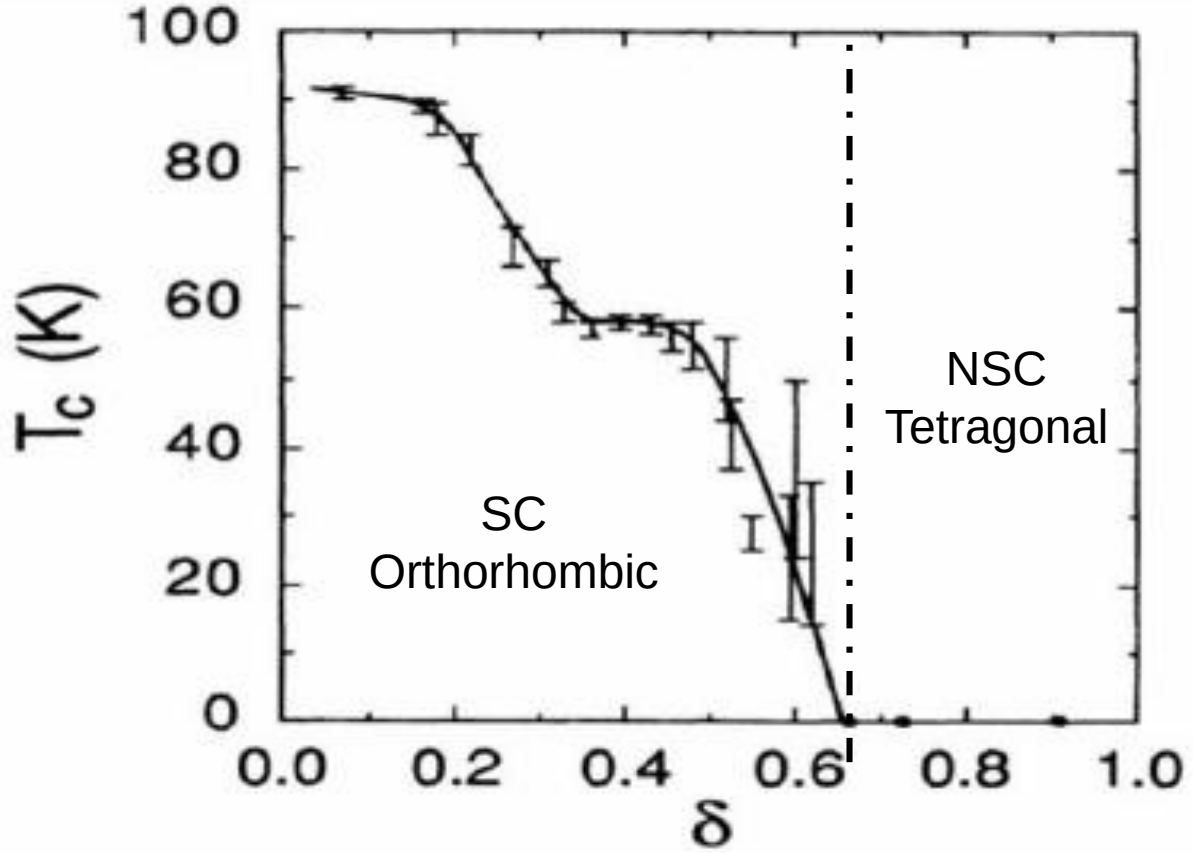
1）O1位置的占有率高于35%时为有序占有，结构变为正交*Pmmm*对称性，化合物超导。

2）O1位置的占有率低于35%时为无序占有，结构为四方*P4/mmm*对称性，不超导。

3）超导温度随着O1的占有率增加上升到91 K。

$YBa_2Cu_3O_{7-x}$超导温度T_C和对应的价态$\mathcal{V}_{Cu(plane)}$随氧空位δ(O1) 的变化





(a) Calculated bond-valence for Cu in the CuO_2 plane layer versus oxygen content in the chain layer of $YBa_2Cu_3O_{7-x}$. The data of bond distances used in the calculation are based on the structure information reported by Jorgensen *et al.* (1990). (b) T_C versus oxygen content in the chain layer of $YBa_2Cu_3O_{7-x}$.

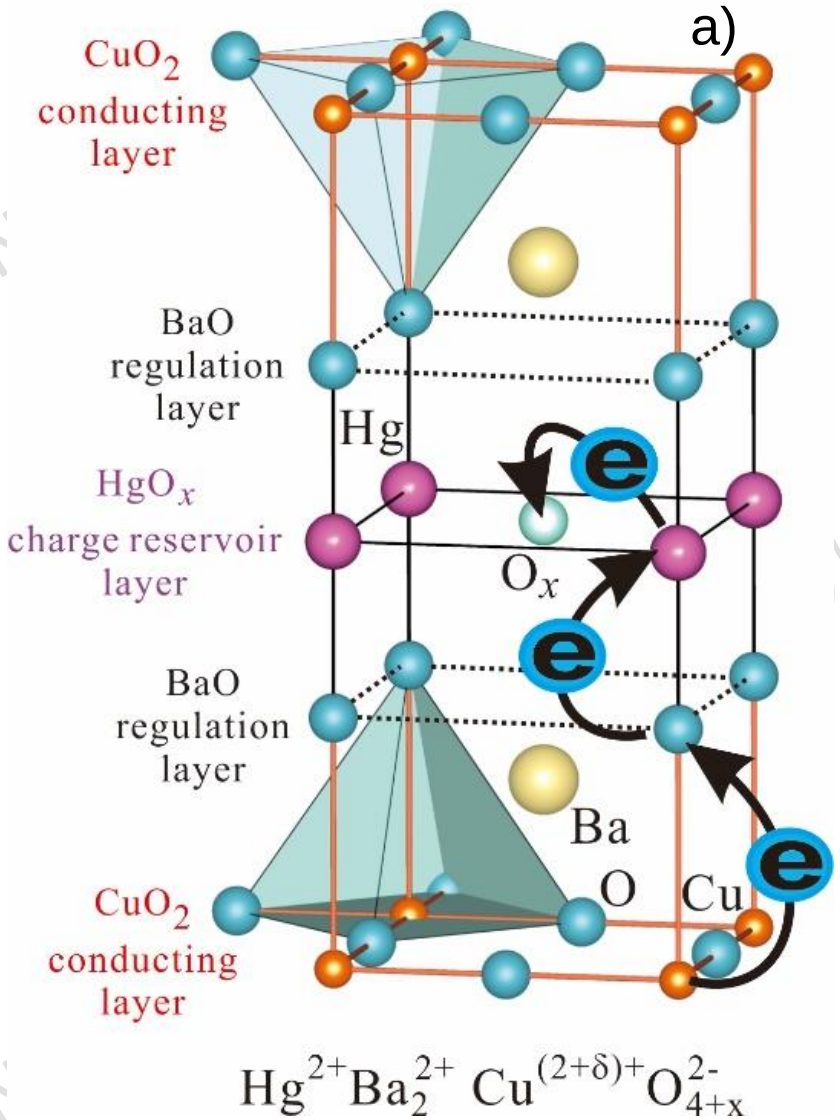
$\mathcal{V} = \sum v_{ij}$, $v_{ij} = \exp[(R_{ij} - d_{ij})/b]$, $e = 2.71828$, b = 0.37, d_{ij} is observed interatomic distance.

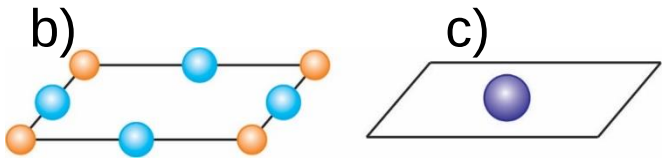
N. E. Brese and M. O'Keeffe. Bond-Valence Parameters for Solid. Acta Cryst. B47, 192-197(1991).

Bond Valence Wizard http://orlov.ch/bondval/

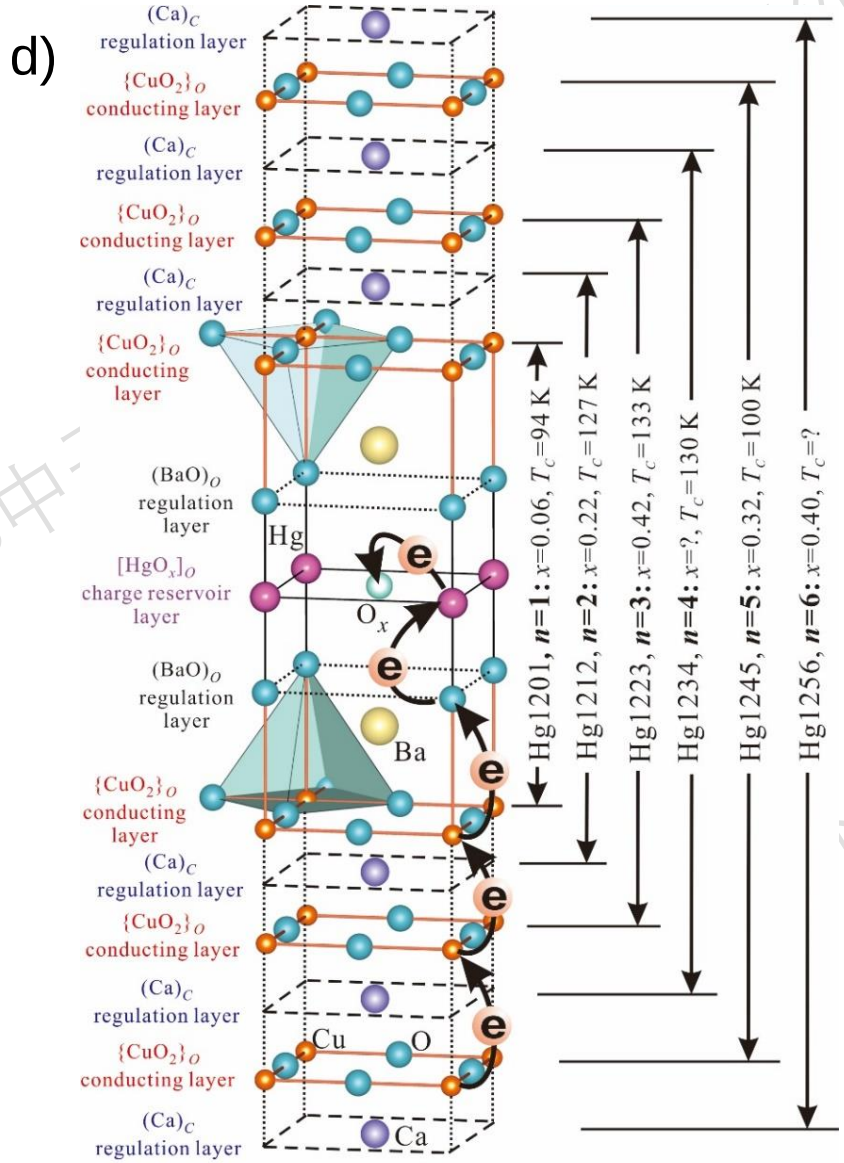
层状汞系铜基高温超导体$HgBa_2Ca_{n-1}Cu_nO_{(2n+2)+x}$结构分析

Analysis of High-T_c superconductors $HgBa_2Ca_{n-1}Cu_nO_{(2n+2)+x}$





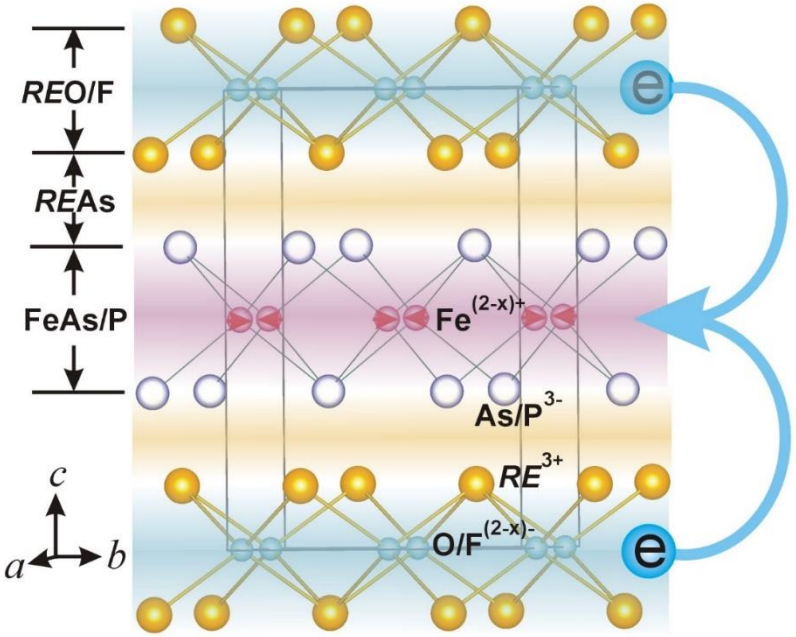
以图**a**的$HgBa_2CuO_{4+x}$的结构为基础，在***c***轴方向叠加图**b**和**c**的平面构成图d的三维层状结构层状汞系铜基高温超导系列化合物$HgBa_2Ca_{n-1}Cu_nO_{(2n+2)+x}$是。最高超导温度达到133 K. 如图所示的电荷转移示意。当HgO_x层的X=0时，化合物不超导。因此，准确测定HgO_x层中的O的占有率是研究化合物结构与性能的关系的关键。电荷转移可以用半经验方法计算Cu的价态得以估计。同时可以根据层间距估计化合物晶胞***c***轴的长度。



P4/mmm

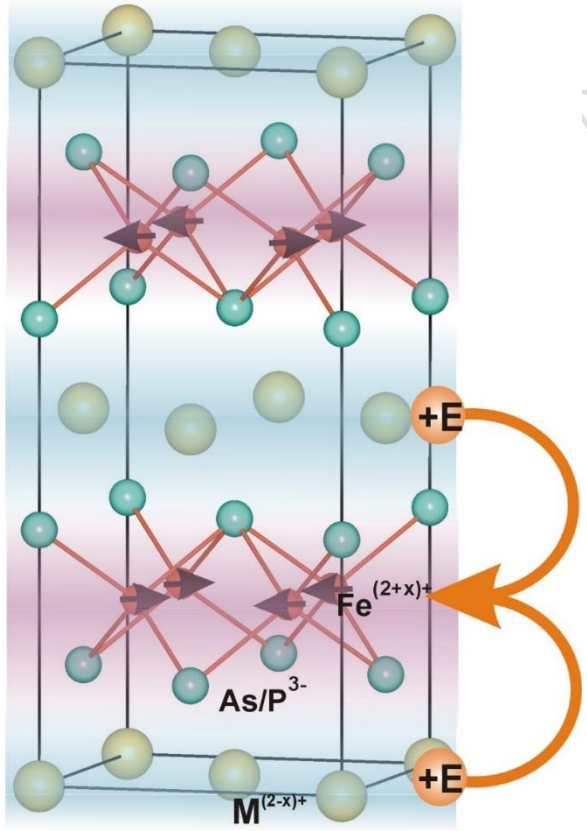
$HgBa_2Ca_{n-1}Cu_nO_{(2n+2)+x}$

铁基超导机理研究



$RE^{3+}O^{2-}Fe^{2+}As^{3-}$

(1111)



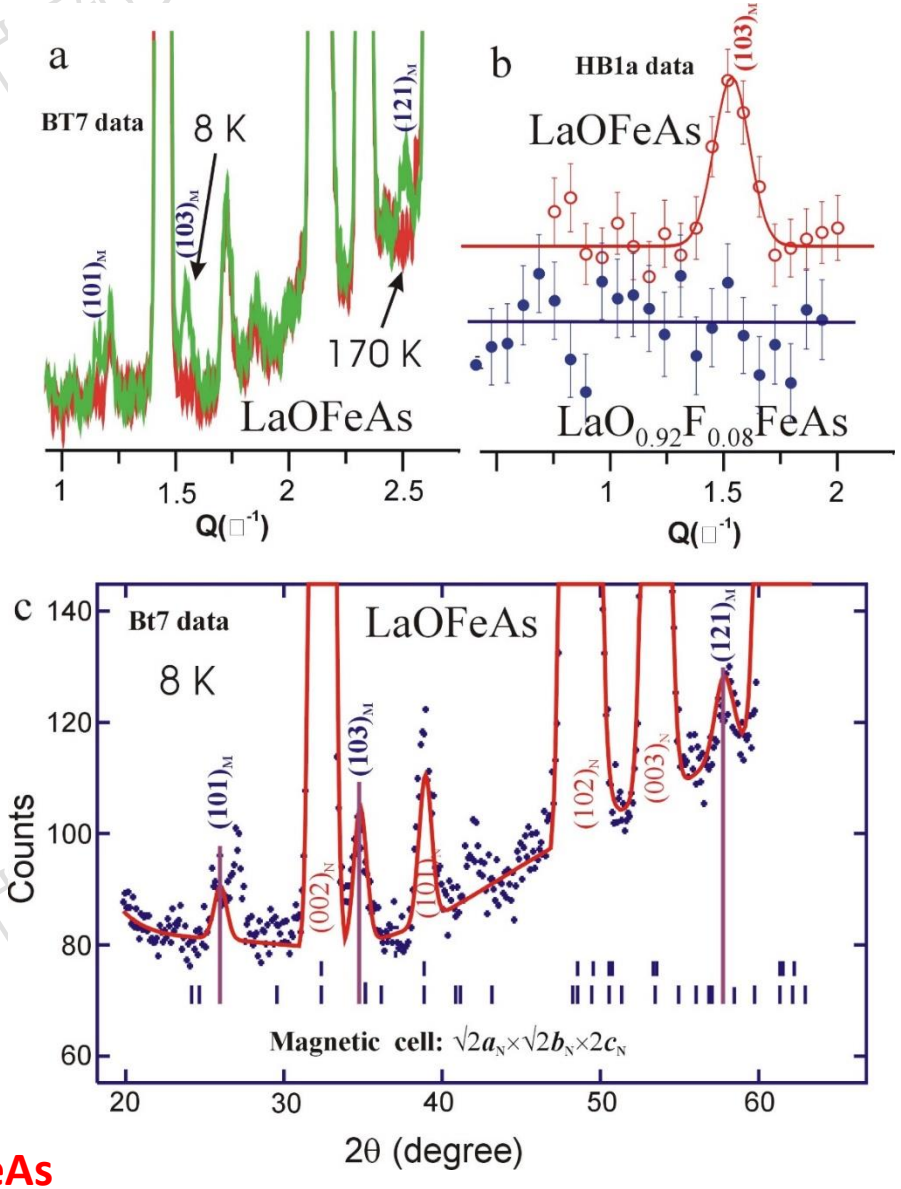
$Ba^{2+}Fe^{2+}{}_2As^{3-}{}_2$

(122)

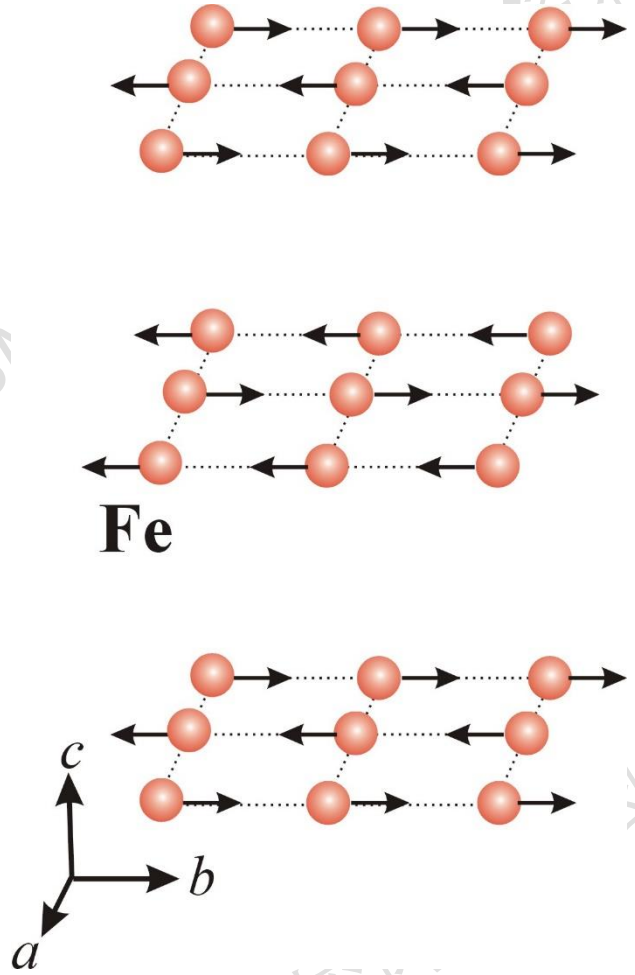
Fe-As~2.4 Å; *RE*-As~3.4 Å; *RE*-O/F~2.4 Å; M-As~3.3 Å.

Charge Transforms

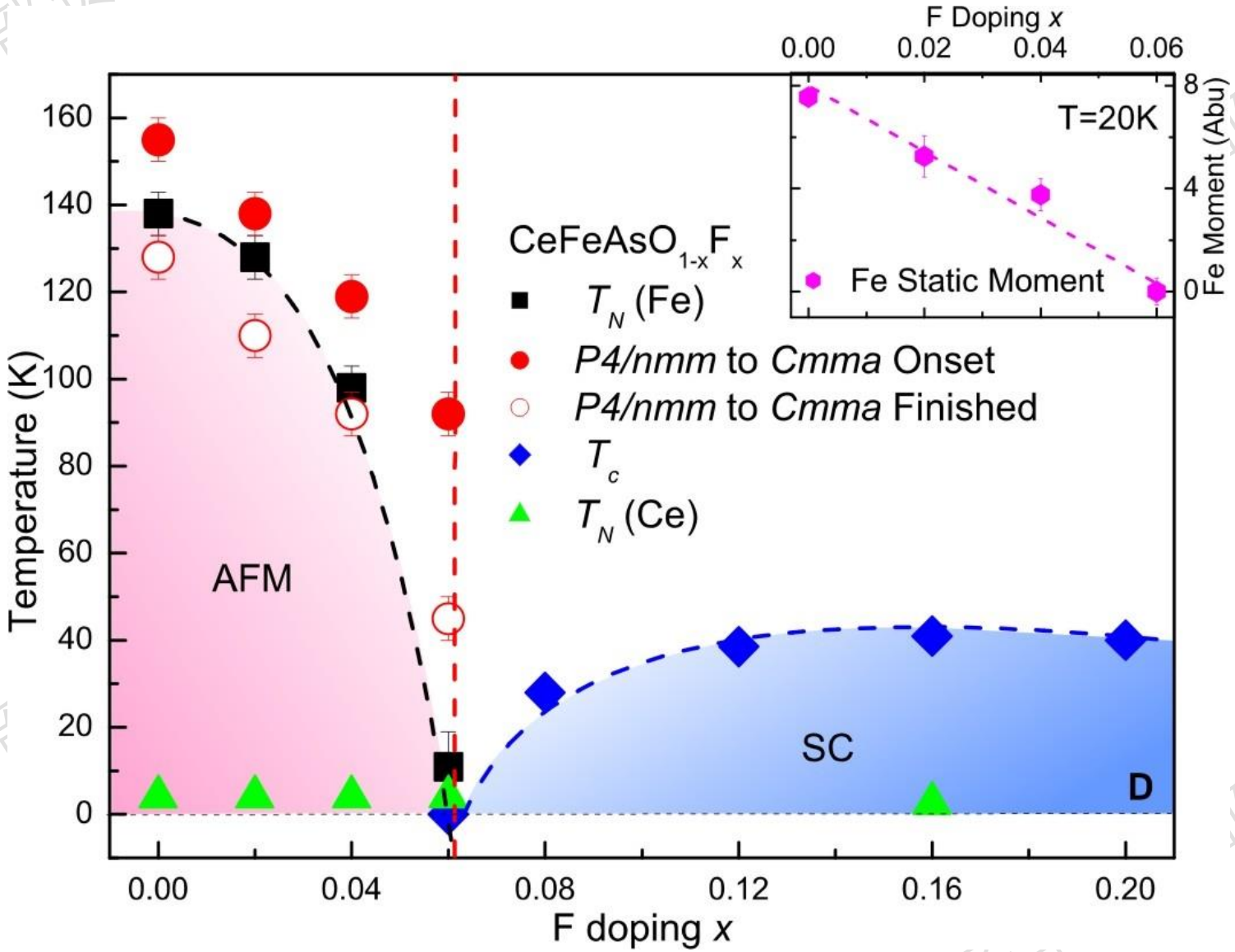
铁基超导机理研究



LaOFeAs



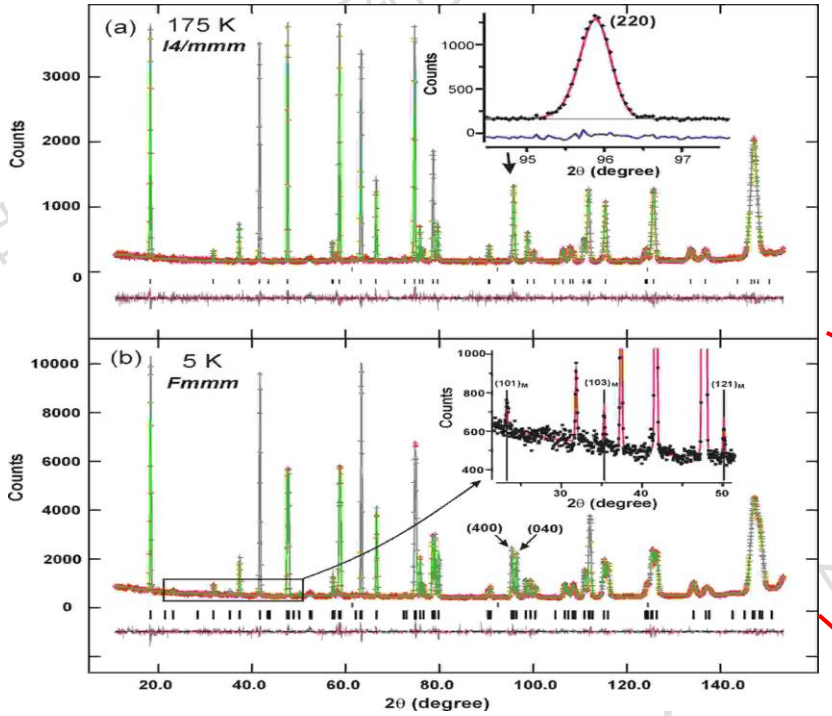
铁基超导机理研究



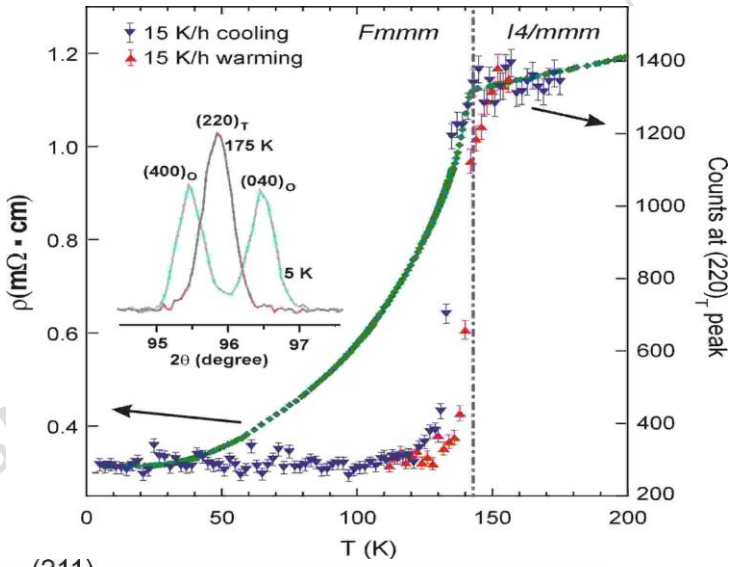
$CeO_{1-x}F_xFeAs$

$BaFe_2As_2$晶体结构和磁结构,相转变与性能

Crystal & Magnetic Structure, Phase Transformation, and properties of $BaFe_2As_2$

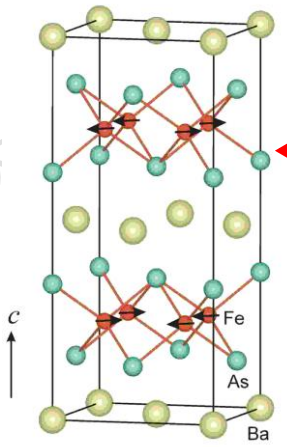


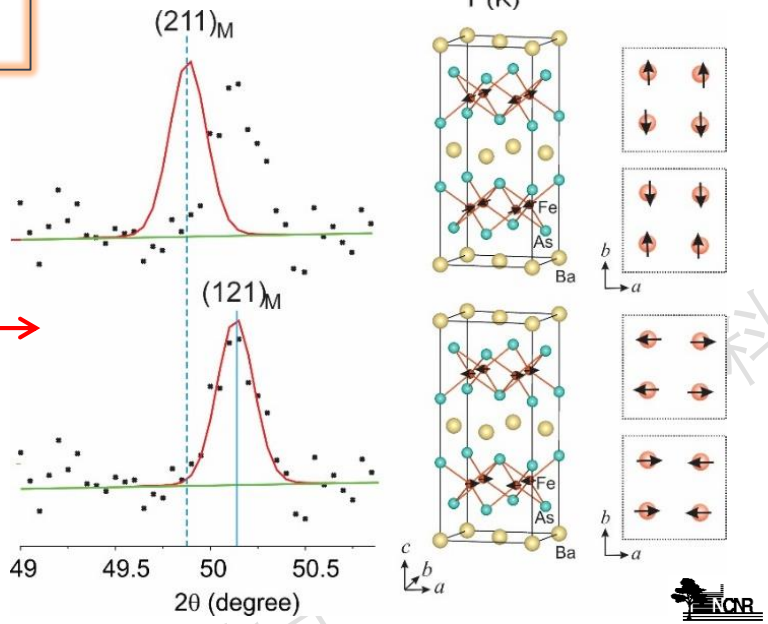
化合物$BaFe_2As_2$在~142 K经历由高温*I4/mmm*到低温*Fmmm*的一级晶体结构相变，伴随着从顺磁到反铁磁的磁有序转变和电阻急剧下降的突变。



Relationships between structure and properties …

Determine and refine crystal and magnetic structures:
Chemical & symmetry
Atomic distribution
Magnetic order-disorder
Spin arrangement
…

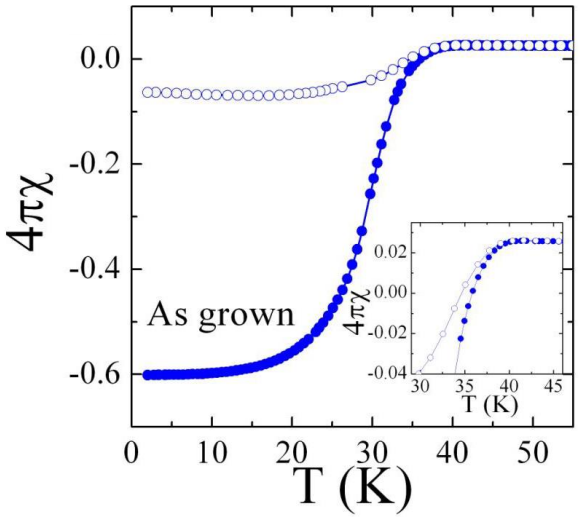


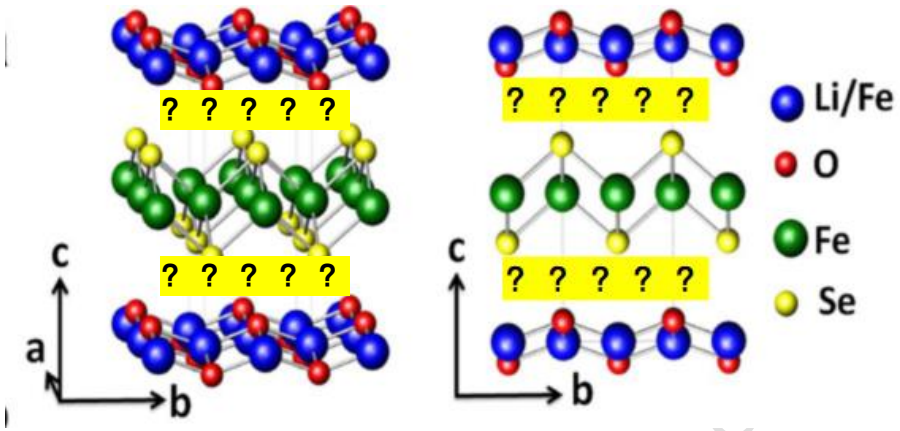


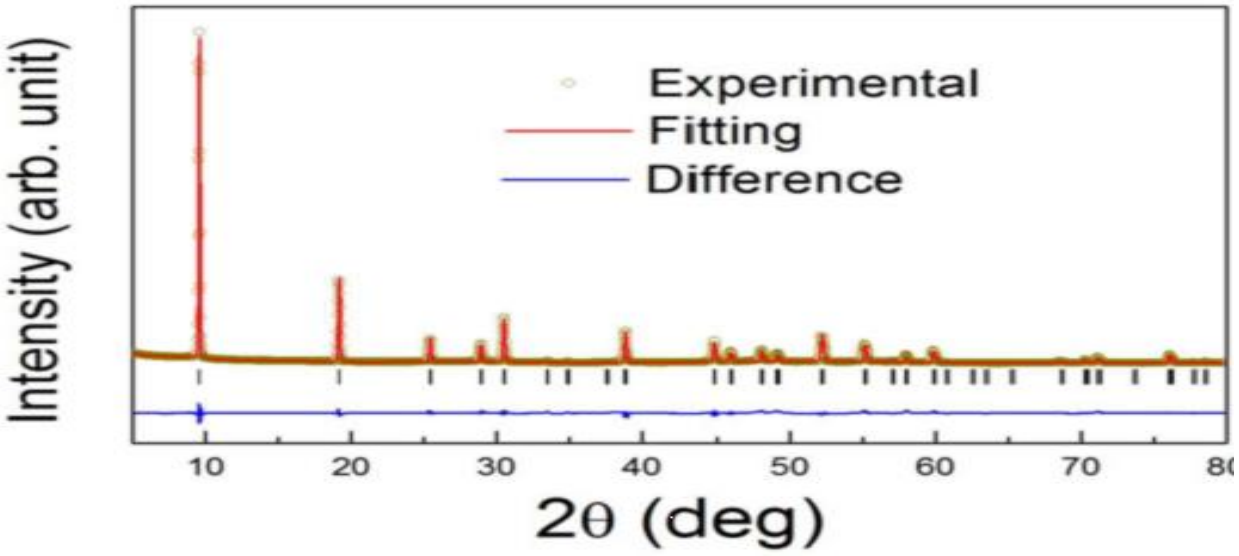
Huang, Q ., Qiu, Y., Bao, W ., et.al. PRL,101, 257003 (2008)

超导化合物(Li/Fe)OH-FeSe 的晶体结构测定

Structure Determination of (Li/Fe)OH-FeSe Superconductor, T_c=43 K







X.F.Lu *et al.* PHYSICAL REVIEW B. **89**, 020507(R) (2014)

利用中子对元素H和Li敏感优势，准确地测定了(Li/Fe)OH-FeSe的晶体结构。化合物具有43K的超导温度使得铁基超导体进入高温超导行列。由于X射线对H和Li的不敏感，先前的X射线粉末衍射工作未能发现H的位置和确定Fe/Li混合占位的比例。可以假定结构中，FeSe层与(Li/Fe)O层之间是通过Se与O存在有Van der Waals 键连接，结构也合理。

铁基超导化合物 (Li/Fe)OH-FeSe 的X射线与中子衍射谱图

XRPD & NDP pattern of superconductor (Li/Fe)OH-FeSe

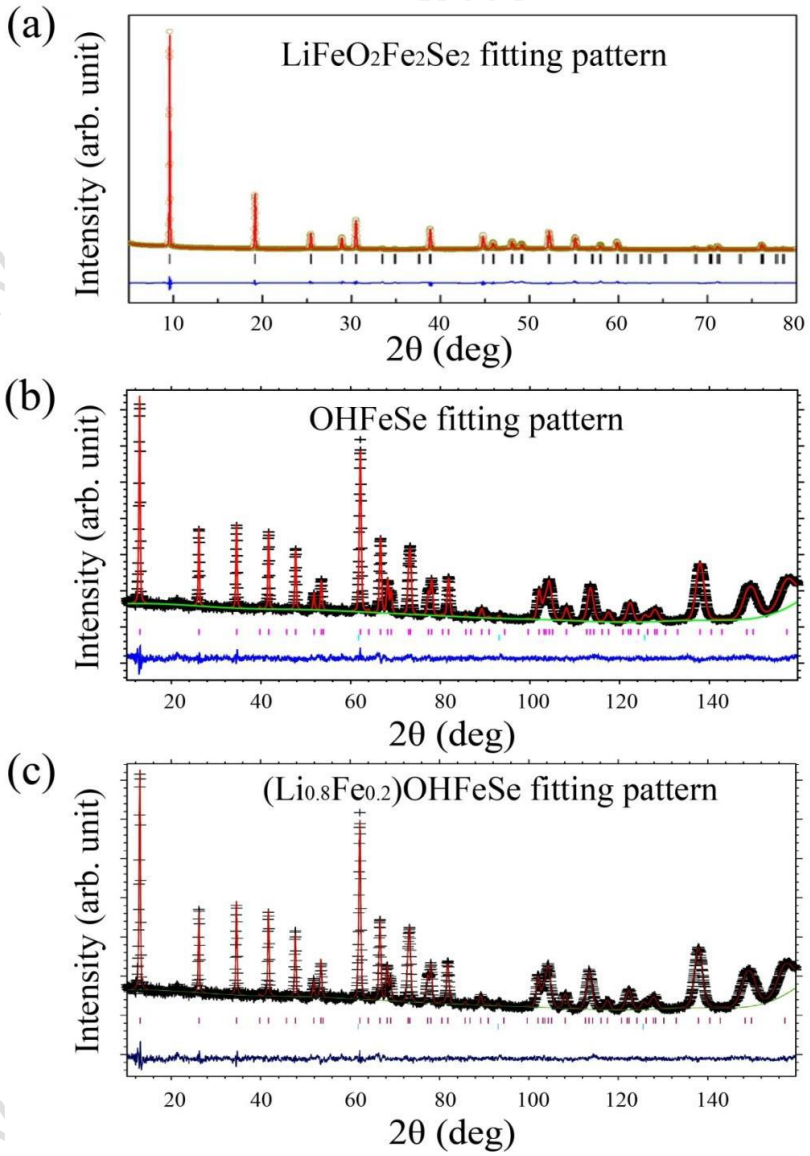


Figure S2:
(a): Rietveld refinement on XRD data collected at 298 K for the structural model of $LiFeO_2Fe_2Se_2$ which was shown in Fig. S1(a).

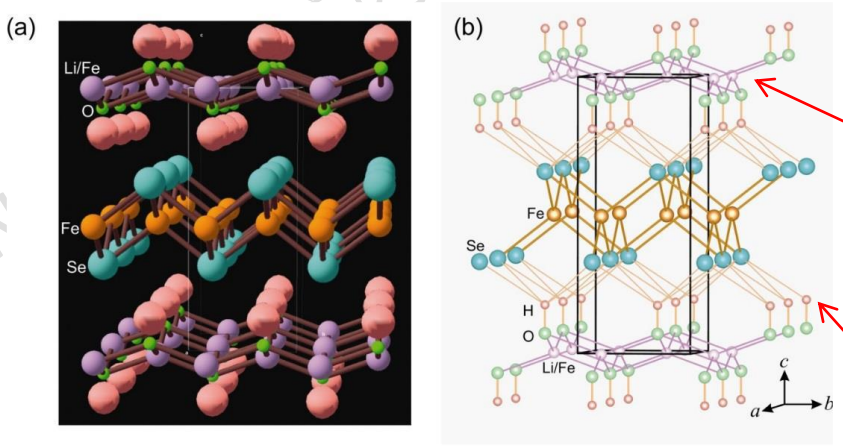
(b): Rietveld refinement on NPD data with the structural model of OHFeSe shown in Fig. S1(b). The NPD data was collected over the 2-Theta range of 1.3-166.3° using Ge311 (λ=2.0775Å) monochromator at 4 K.

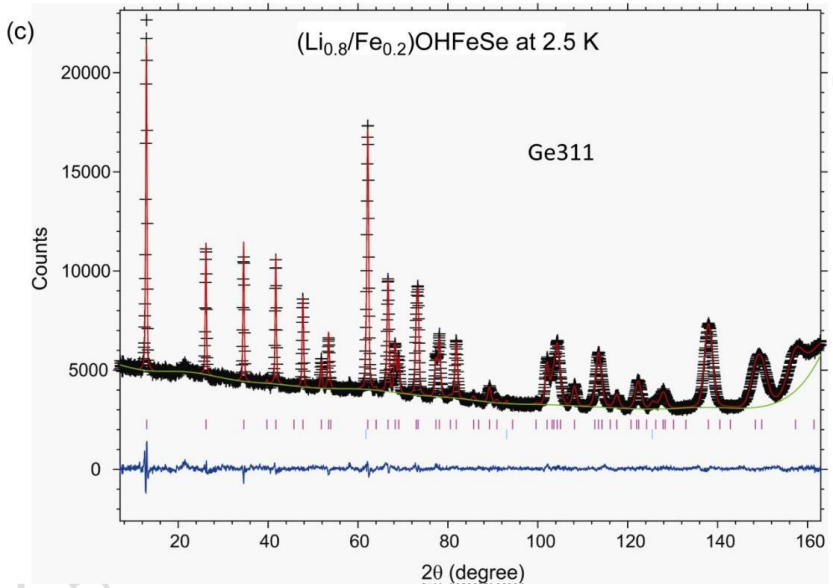
(c): Rietveld refinement on NPD pattern which was collected at 4 K using Ge311 (λ=2.0775Å) monochromator with the structural model of $(Li_{0.8}Fe_{0.2})OHFeSe$ shown in Fig. S1(c).

Name	X,#	N, *b*
H	1	-0.3741
Li	3	-0.203
O	8	0.5805
Fe	26	0.954
Se	34	0.797

图a和b分别是XRPD和NPD的谱图。对于XRPD，衍射峰的强度随着衍射角的增大而迅速衰减。而在NPD图中，由于中子散射因子是常数，高角度衍射峰并没有明显减弱。再比较X射线和中子散射因子，H和Li的原子序数为1和3，X射线的散射本领极低。而H和Li的中子分别为-0.3741和-0.203，对NPD的贡献要比XRPD大的多。

超导化合物(Li/Fe)OH-FeSe晶体结构测定
Structure determination of (Li/Fe)OH-FeSe superconductor





? at (0 0 0) Neutron cross section

b(H)= -0.374

b(Fe)=0.954

b(Li)= -0.203

***b*(0.814Li+0.186Fe)=0.012**

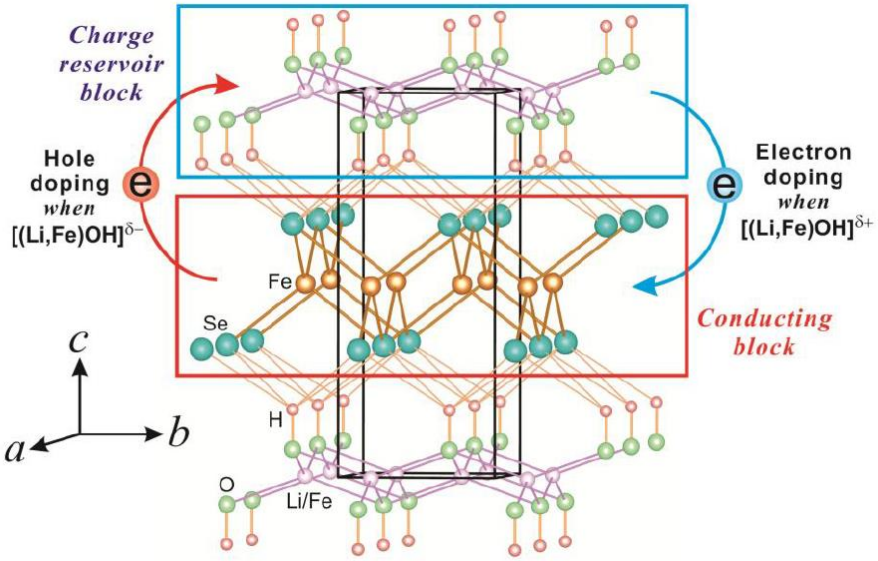
DELF: H at (3/4,3/4,0.175)

a, Neutron scattering Fourier difference analysis using NPD data. Fourier difference contours are highlighted in pink. Oxygen atoms (green), Li/Fe atoms (purple).

b, A schematic view of the structure of $(Li_{0.8}Fe_{0.2})OHFeSe$.

c, Observed (crosses) and calculated (red solid line) NPD pattern for $(Li_{0.8}Fe_{0.2})OHFeSe$ (λ = 2.0775 Å) at 2.5 K.

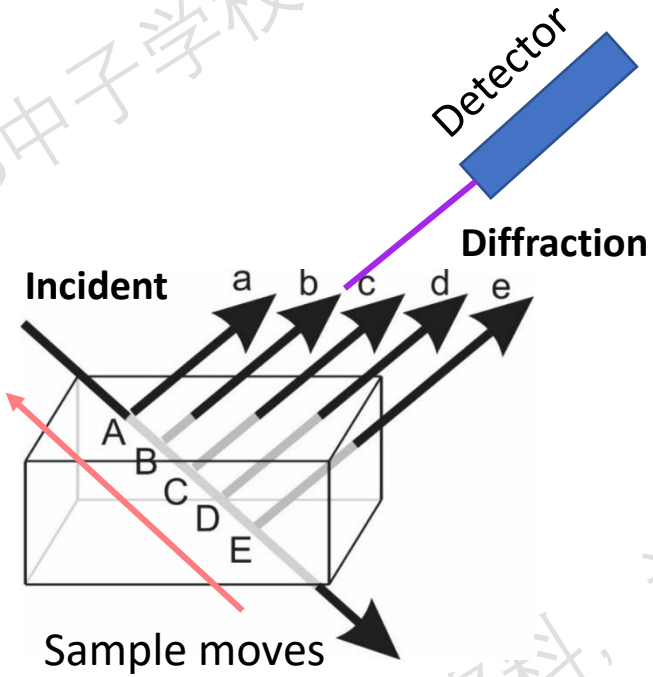
用中子粉末衍射数据进行差傅里叶分析发现了夹层中存在H，同时中子数据分析最后确认，在(000)的位置上$Fe_{0.186}$和$Li_{0.814}$共同占位。最后确定以H-O和H-Se连接FeSe和(Fe/Li)O形成三维结构。



A schematic view of the structure of $(Li_{0.8}Fe_{0.2})OHFeSe$. The FeSe layer, which acts as the conducting block, alternately stacks with the charge reservoir block $(Li_{0.8}Fe_{0.2})OH$ layer in this model.

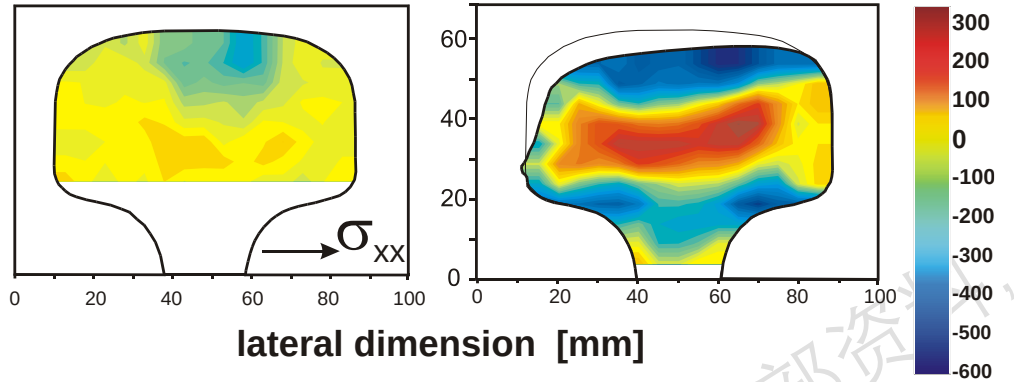
Strong penetration

When there is stress in solid materials, lattice deformation causes diffraction peak displacement.



To study residual stresses in steel, aluminum, superalloys, and other such structural materials. Elastic strain in these materials can be determined by measuring their interplanar atomic spacing, and the instrument should be designed to use the high-penetration power of neutrons to generate “maps” of the strain resulting from residual or applied stresses in bulk materials.

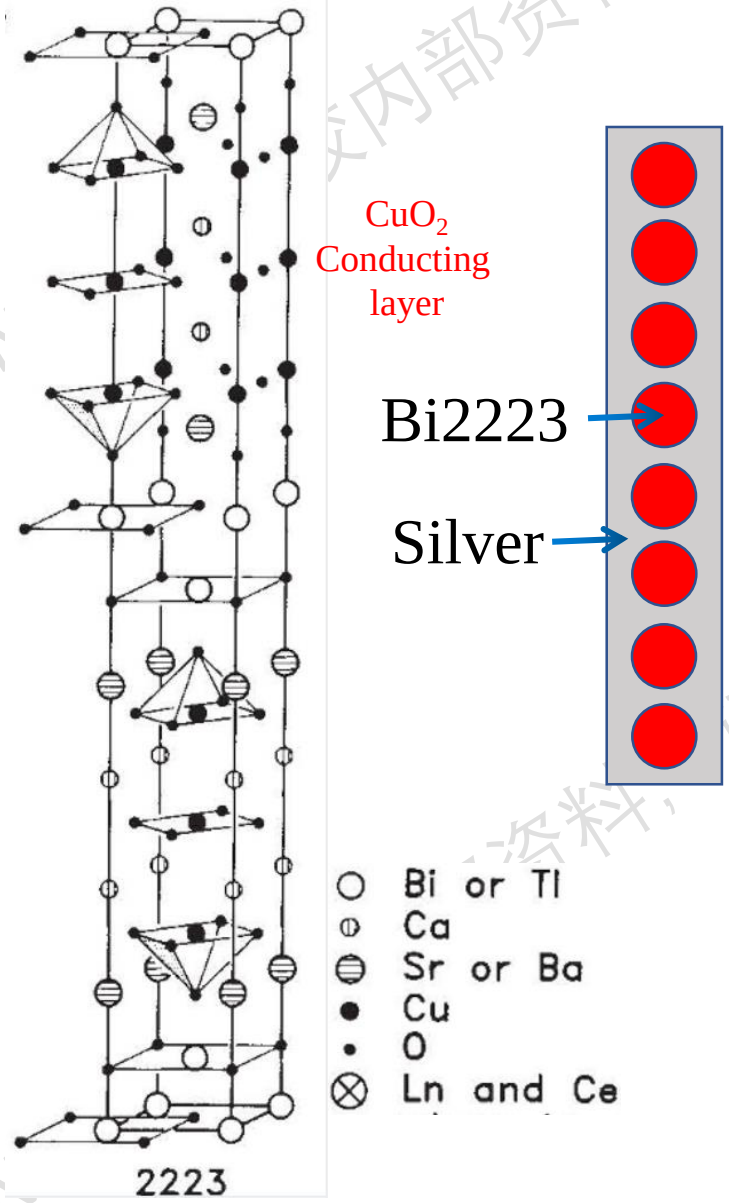
Neutrons can penetrate deeply without destroying samples, and pass through walls controlling a sample's environment allowing measurements under extreme conditions. Non-destructive residual stress, texture, and microstructure investigation in engineering components.

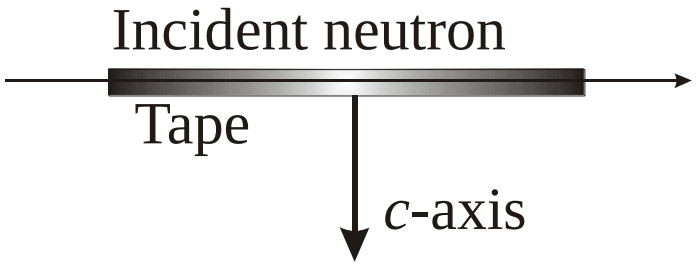


Neutron Diffraction Residual Stress Measurement: Stresses in Railroad Rails before and after Service

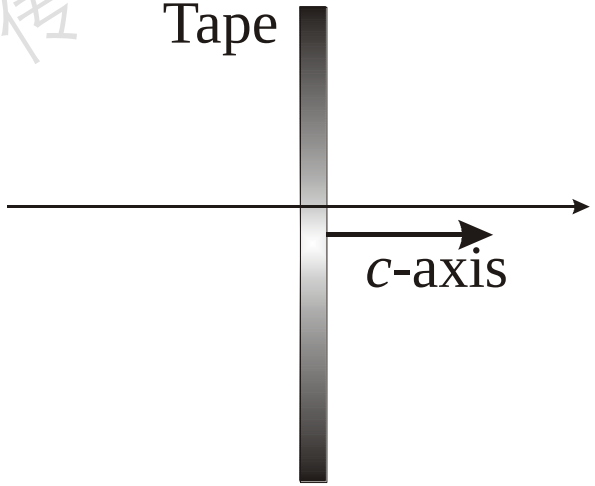
NCNR - Thomas Gnäupel-Herold

Bi2223 超导带中晶粒取向

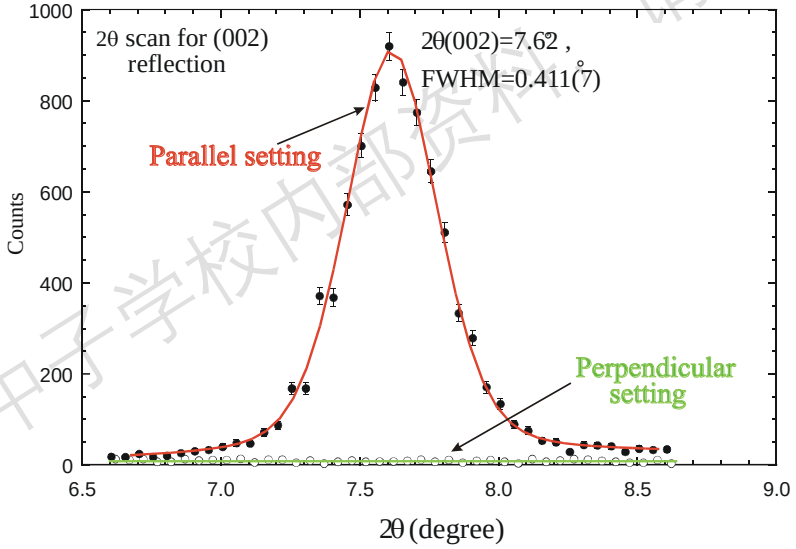


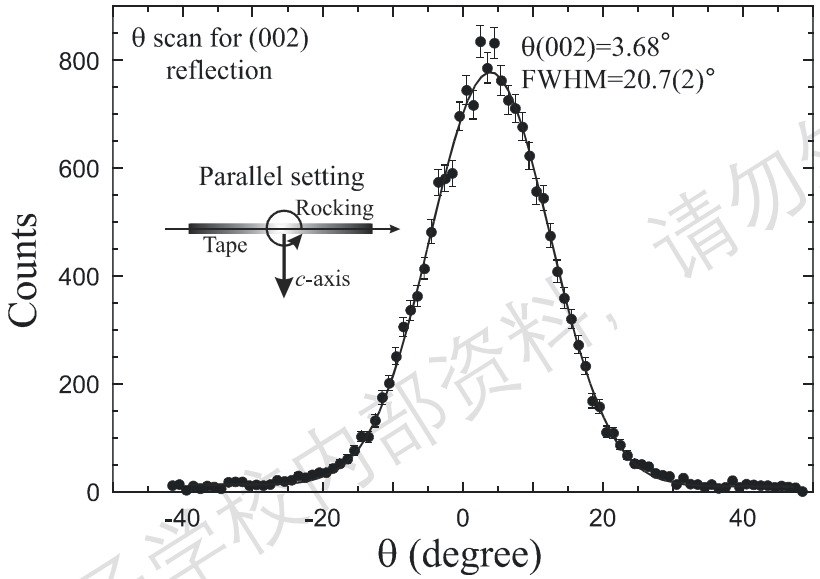


(a) Parallel setting



(b) Perpendicular setting





中子的性质，波粒二象性 Wave-particle Duality

Table 2.3.1
Properties of the neutron (adapted from Kisi & Howard, 2008)

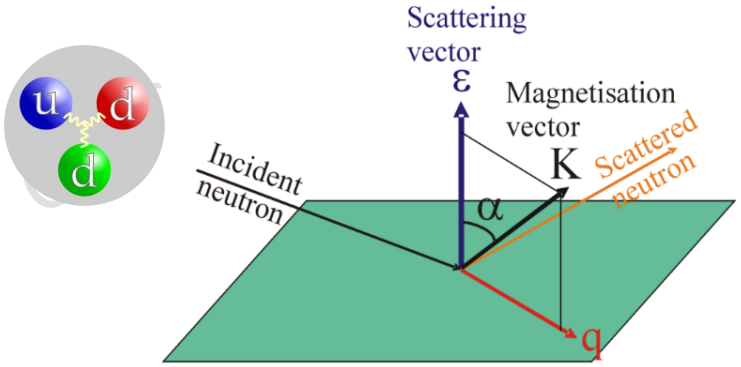
Mass (m)	1.675×10^{-27} kg
Charge	0
Spin	$\frac{1}{2}$
Magnetic moment (μ_n)	$-1.913\ \mu_N$
Wavelength (λ)	h/mv
Wavevector (**k**)	Magnitude $2\pi/\lambda$
Momentum (**p**)	$\hbar\mathbf{k}$
Energy (E)	$(1/2)mv^2 = h^2/2m\lambda^2$

Although the neutron is a neutral particle, the magnetic moment of a neutron is not zero. It has spin ½ and a moment of -0.001042 μ_B, an indication of its quark substructure and internal charge distribution. It can be modeled as a sum of the magnetic moments of the constituent quarks. The calculation assumes that the quarks behave like pointlike Dirac (迪拉克An English physicist) particles, each having their own magnetic moment. Simplistically, the magnetic moment of the neutron can be viewed as resulting from the vector sum of the three quark magnetic moments, plus the orbital magnetic moments caused by the movement of the three charged quarks within the neutron.

The neutron contains one “up” quark (charge +2/3 *e*) and two “down” quarks (charge −1/3 *e*). Neutron is a neutral particle.

Magnetic interaction vector

$q=\varepsilon(\varepsilon\cdot K)-K$



$|q|=\sin\alpha$

Definition of the vectors relevant in the evaluation of factor (Bacon, G. E. (1962)). **ε** and **K** are unit vectors in the directions of the scattering and magnetic moment, respectively. The magnetic interaction vector **q** is always perpendicular to the scattering vector.

根据微观粒子的波粒二象性，中子具有波动性，慢中子的波长约10^{-10}米，与晶体内原子间距相当。中子衍射是研究晶体结构的重要技术。中子是不带电的基本粒子，静止质量为1.6748×10^{-27}kg，它的半径约为0.8×10^{-15}m，与质子大小类似。

Magnetic Intensity

Peaks Position: $2d\sin\theta = n\lambda$

where λ is the incident beam wavelength, d and θ are the distance between successive *hkl* planes and Bragg angles of reflections, respectively.

Diffraction Intensity: $I_{hkl} = C|F_{hkl}|^2$

where F_{hkl} is the amplitude of the diffracted X-ray or neutron *hkl* reflection, and **C** is all others.

X-ray: $F_{hkl} = \sum f_j \exp(2\pi i (hx + ky + lz)) e^{-2W}$

where f_j is the X-ray atomic scattering factor of atom *j* for X-ray.

Neutron: $F_{hkl} = \sum b_j \exp(2\pi i (hx + ky + lz)) e^{-2W}$

where b_j is the neutron scattering length for atom *j*.

Magnetic: $F_{hkl} = \sum q_j f_{Mj} \exp(2\pi i (hx + ky + lz)) e^{-2W}$

where q_j and f_{Mj} are the magnetic interaction vector and the magnetic form factor for atom *j*, respectively.

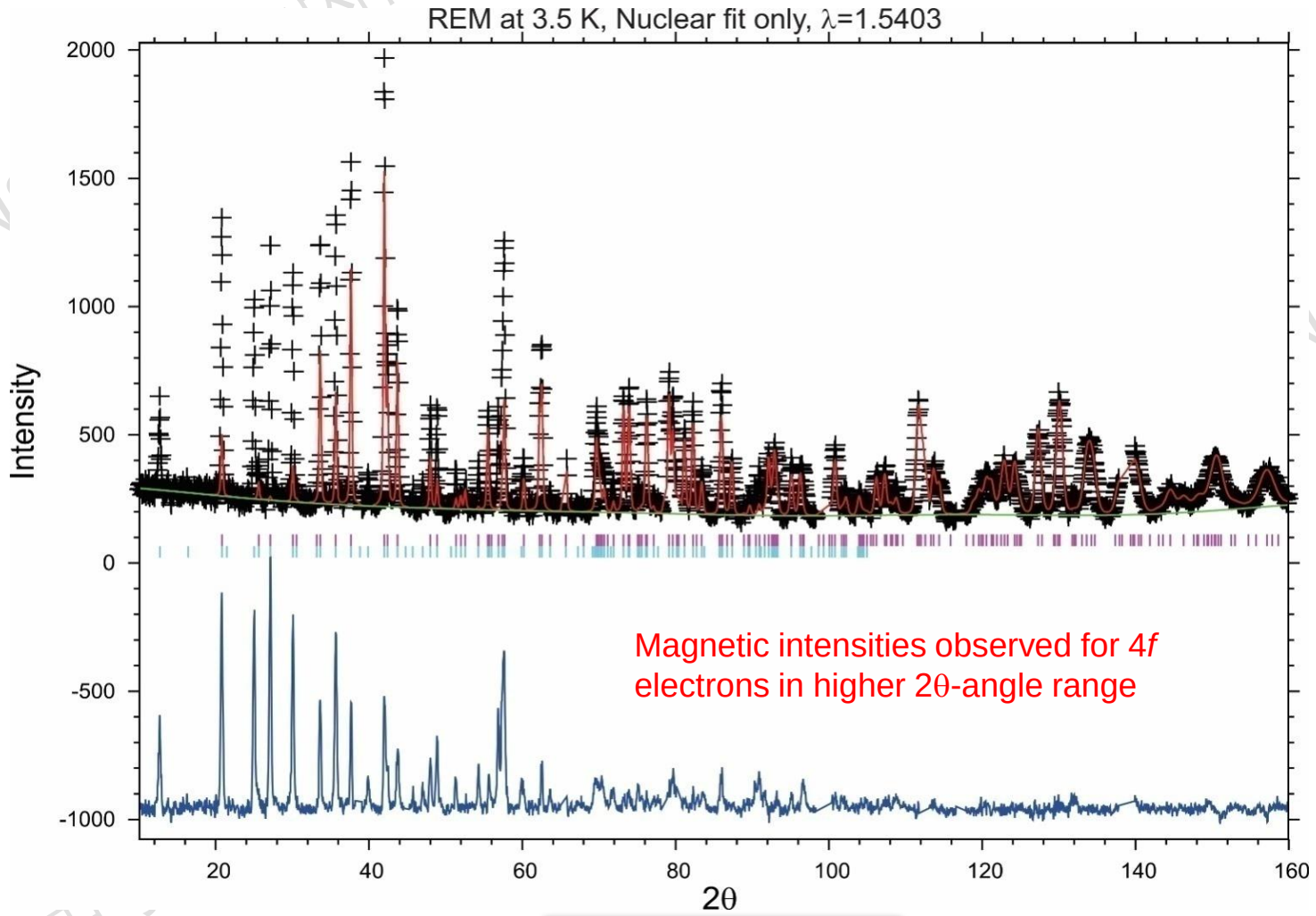
$$I_M = C\,\mathscr{M}_T\,A(\theta_B)\,[(\gamma e^2)/(2mc^2)]^2\,\langle 1-(\tau\cdot M)^2\rangle\,|F_M|^2$$

C- Instrumental constant
$\mathscr{M}_T$- Multiplicity (for powder)
$A(\theta_B)$- angular factor, $1/(\sin\theta\,\underline{\sin 2\theta})$
$[(\gamma e^2)/(2mc^2)]$=-0.27 - neutron-electron coupling
$\langle 1-(\tau\cdot M)^2\rangle$-orientation factor
F_M- Magnetic structure factor

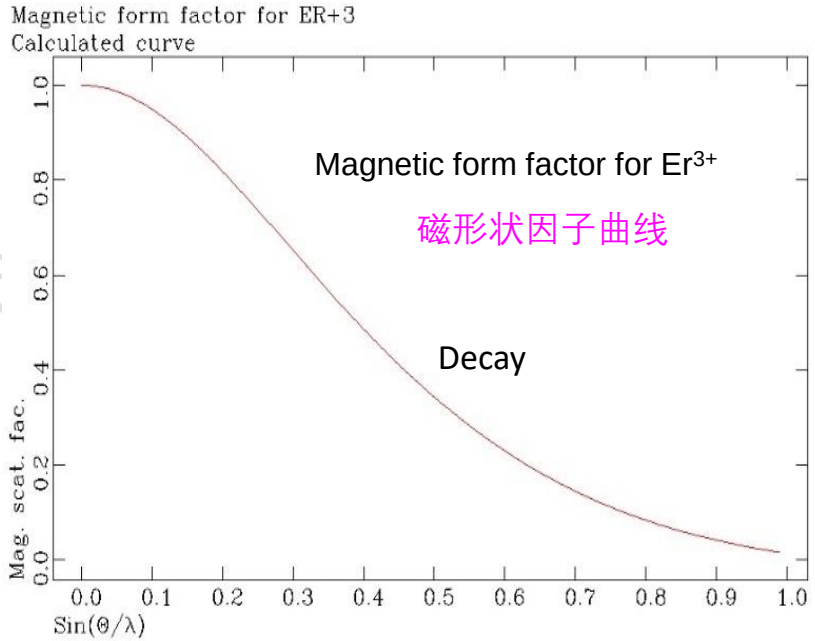
$$F_M = \sum \mu f \exp(2\pi i(hx + ky + lz))\, e^{-W}$$

μ- magnetic moment
f- magnetic form factor
W-Debye Waller factor

磁有序, 磁晶胞, 磁对称性，磁结构及性能
Spins order, magnetic cell, magnetic symmetry, and structure & properties



磁峰出现在低角度范围

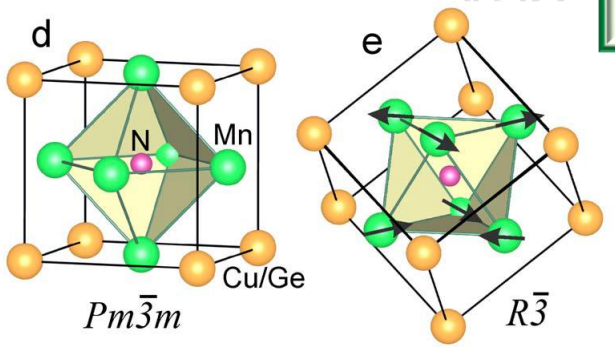


含重稀土Er^{3+} 合金的中子衍射谱图。图中红线是以晶体结构拟合曲线，图的下部观察数据与计算数据的差值是Er^{3+}的有序的磁衍射峰。

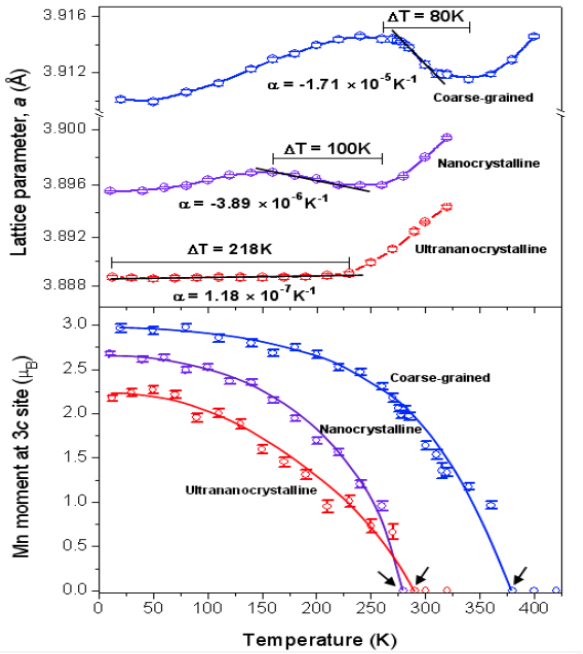
具有反钙钛矿结构$Mn_3Cu_{0.5}Ga_{0.5}N$的零热膨胀研究

Zero Thermal Expansion in Antiperovskite $Mn_3Cu_{0.5}Ga_{0.5}N$

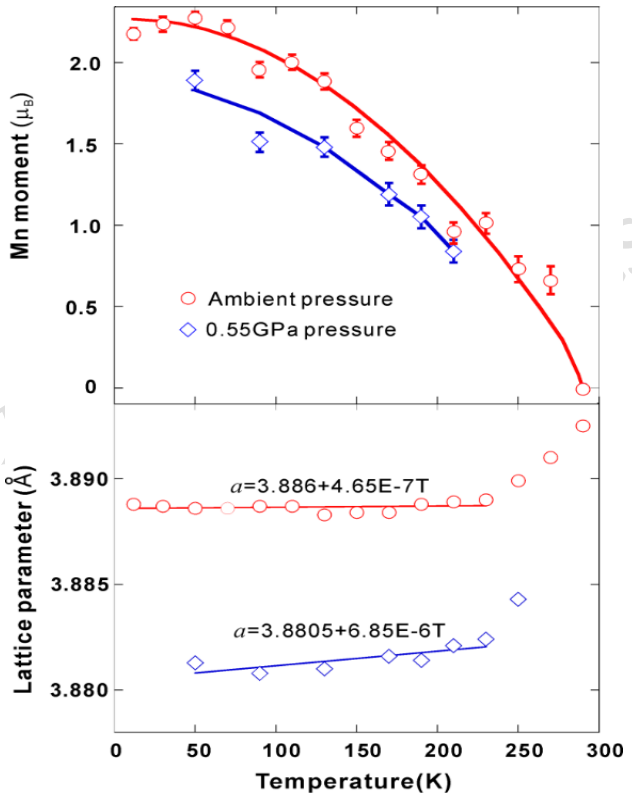
Mean grain size (nm)	>1000	~30	~12
Refined occupancy n_{Mn}	1	0.878	0.787
a (Å) at 295 K	3.90077(6)	3.90021(4)	3.89891(1)
M_{Mn} (μ_B) at Mn site	2.970(5)	2.71(2)	2.22(3)



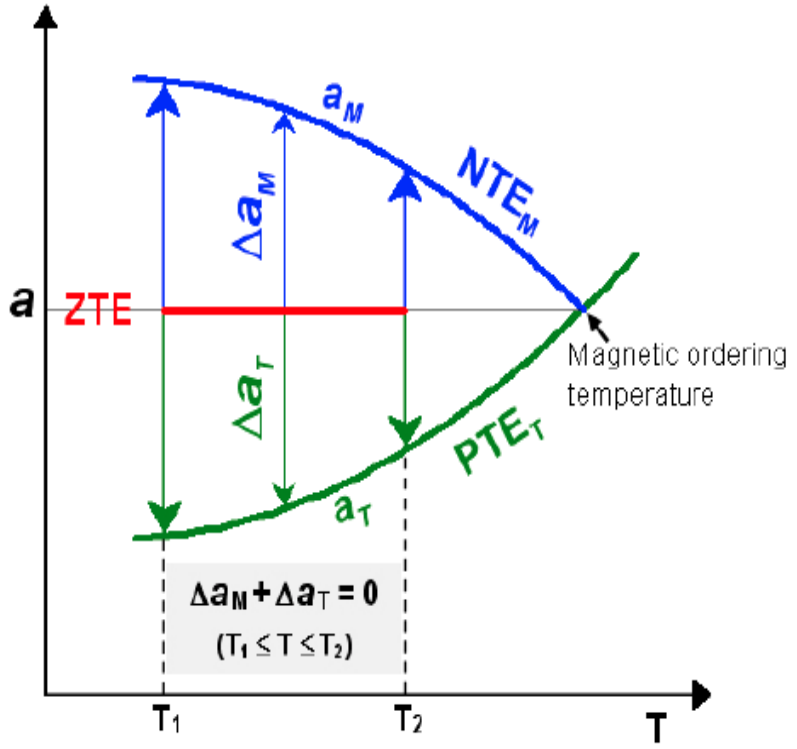
晶体结构和磁结构



磁有序度引起的负膨胀与温度引起的正膨胀完全抵消时，材料呈现零膨胀。



负膨胀与磁有序度有密切关联，样品的结晶晶粒大小也直接影响磁有序行为。



磁有序度引起的负膨胀与温度引起的正膨胀完全抵消时，材料呈现零膨胀。

Xiaoyan Song, *et al.*, *Adv. Mater*. 2011, **23**, 4690

元素周期表（二）

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB			IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIIA
H 六方H 0.32 2.1 — 0.108 2.08(−1) 0.014 — — 14.1 0.004 313 3.45																	He 六方H 0.93 — — 0.020 — 0.005 — — 31.8 .0003 567 1.25
Li 立方I 1.23 1.0 1.55 32.46 0.60(+1) 0.72 — 0.108 13.1 0.17 124 0.79	Be 六方H 0.90 1.5 1.12 73.9 0.31(+2) 2.8 — 0.25 5.0 0.38 215 0.45											B 六方H 0.82 2.0 0.92 128 0.20(+3) 5.3 — 10^{-13} 4.6 — 191 0.309	C 六方H 0.77 2.5 0.914 171.7 2.60(−4) — 0.15(+4) .0007 5.3 0.057 260 0.165	N 六方H 0.75 3.0 0.92 0.666 1.71(−3) 0.086 0.11(+5) — 17.3 .00006 336 0.247	O 立方P 0.73 3.5 — 0.815 1.40(−2) 0.053 0.09(+6) — 14.0 .00006 314 0.218	F 0.72 4.0 — 0.755 1.36(−1) 0.061 0.07(+2) — 17.1 — 402 0.18	Ne 立方F 0.71 — — 0.422 — 0.080 — — 16.8 .0001 497 —
Na 立方I 1.54 0.9 1.90 24.12 0.95(+1) 0.62 — 0.216 23.7 0.32 119 0.295	Mg 六方H 1.36 1.2 1.60 32.517 0.65(+2) 2.14 — 0.224 14.0 0.38 176 0.25											Al 立方F 1.18 1.5 1.43 67.9 0.50(+3) 2.55 — 0.382 10.0 0.50 138 0.215	Si 金刚石型 1.11 1.8 1.32 (40.6) 2.71(−1) 11.1 0.41(+4) 0.10 12.1 0.20 188 0.162	P 立方P 1.06 2.1 1.28 2.97 2.12(−3) 0.15 0.34(+5) 10^{-17} 17.0 — 254 0.177	S 正交P 1.02 2.5 1.27 3.01 1.84(−2) 0.34 0.29(+6) 10^{-18} 15.5 .0007 239 0.175	Cl 四方P 0.99 3.0 — 2.44 1.81(−1) 0.77 0.26(+7) — 18.7 .00002 300 0.116	Ar 立方F 0.98 — — 1.50 — 0.281 — — 24.2 .00004 363 0.125
K 立方I 2.03 0.8 2.35 18.9 1.33(+1) 0.55 — 0.143 45.3 0.23 100 0.177	Ca 立方F 1.74 1.0 1.97 36.74 0.99(+2) 2.1 — 0.216 26.9 0.3 141 0.149	Sc 六方H 1.44 1.3 1.62 81 0.81(+3) 3.8 — 0.015 15.0 0.015 151 0.13	Ti 六方H 1.32 1.5 1.47 106.5 0.90(+2) 3.7 0.68(+4) 0.024 10.6 — 158 0.126	V 立方I 1.22 1.6 1.34 106 0.74(+3) 4.2 0.59(+5) 0.04 8.35 — 156 0.120	Cr 立方I 1.18 1.6 1.30 72.97 0.63(+3) 3.3 0.52(+6) 0.076 7.23 0.16 156 0.11	Mn 立方P 1.17 1.5 1.35 50.7 0.80(+2) 2.50 0.46(+7) 0.084 7.39 — 171 0.15	Fe 立方I 1.17 1.8 1.26 84.6 0.76(+2) 3.67 0.64(+3) 0.10 7.1 0.18 182 0.11	Co 六方H 1.16 1.8 1.25 93 0.74(+2) 3.64 0.63(+3) 0.16 6.7 0.16 181 0.099	Ni 立方F 1.15 1.8 1.25 91.0 0.72(+2) 4.21 0.62(+3) 0.145 6.6 0.22 176 0.105	Cu 立方F 1.17 1.9 1.28 72.8 0.96(+1) 3.11 0.69(+2) 0.593 7.1 0.94 178 0.092	Zn 六方H 1.25 1.6 1.38 27.4 0.74(+2) 1.76 — 0.167 9.2 0.27 216 0.0915	Ga 正交P 1.26 1.8 1.41 — 1.13(+1) 1.34 0.62(+3) 0.058 11.8 — 138 0.079	Ge 金刚石型 1.22 1.8 1.37 68 0.93(+2) 7.6 0.53(+4) 0.022 13.6 0.14 187 0.073	As 三方R 1.20 2.0 1.39 7.75 2.22(−3) 6.62 0.47(+5) 0.029 13.1 — 231 0.082	Se 六方H 1.16 2.4 1.40 3.34 1.98(−2) 1.25 0.42(+6) 0.08 16.5 .00001 225 0.084	Br 正交P 1.14 2.8 — 3.58 1.95(−1) 1.26 0.39(+7) 10^{-18} 23.5 — 273 0.070	Kr 立方F 1.12 — — 2.16 — 0.39 — — 32.2 .00002 323 —
Rb 立方I 2.16 0.8 2.48 18.1 1.48(+1) 0.55 — 0.080 55.9 — 96 0.080	Sr 立方F 1.91 1.0 2.15 33.8 1.13(+2) 2.1 — 0.043 33.7 — 131 0.176	Y 六方H 1.62 1.3 1.78 93 0.93(+3) 2.7 — 0.019 19.8 0.035 152 0.071	Zr 六方H 1.45 1.4 1.60 120 0.80(+4) 4.0 — 0.024 14.1 — 166 0.066	Nb 立方I 1.34 1.6 1.46 — 0.70(+5) 6.4 — 0.080 10.8 0.125 156 0.065	Mo 立方I 1.30 1.8 1.39 128 0.68(+4) 6.6 0.62(+6) 0.19 9.4 0.35 166 0.061	Tc 1.27 1.9 1.36 120 — 5.5 — — — — 167 —	Ru 六方H 1.25 2.2 1.34 143 0.69(+3) 6.1 0.67(+4) 0.10 8.3 — 173 0.057	Rh 立方F 1.25 2.2 1.34 127 0.86(+2) 5.2 — 0.22 8.3 0.21 178 0.059	Pd 立方F 1.28 2.2 1.37 90 0.86(+2) 4.0 — 0.093 8.9 0.17 192 0.058	Ag 立方F 1.34 1.9 1.44 60.7 1.26(+1) 2.70 — 0.616 10.3 0.98 175 0.056	Cd 六方H 1.48 1.7 1.54 23.9 0.97(+2) 1.46 — 0.146 13.1 0.22 207 0.055	In 四方P 1.44 1.7 1.66 53.7 1.32(+1) 0.78 0.81(+3) 0.111 15.7 0.057 133 0.057	Sn 四方P 1.41 1.8 1.62 70 1.12(+2) 1.72 0.71(+4) 0.088 16.3 0.16 169 0.054	Sb 三方R 1.40 1.9 1.59 46.6 2.45(−3) 4.74 0.62(+5) 0.026 18.4 0.05 199 0.049	Te 六方H 1.36 2.1 1.60 11.9 2.21(−2) 4.28 0.56(+6) 10^{-6} 20.5 0.014 208 0.047	I 正交P 1.33 2.5 — 5.2 2.16(−1) 1.87 0.50(+7) 10^{-16} 25.7 0.001 241 0.052	Xe 立方F 1.31 — — 3.02 — 0.55 — — 42.9 .0001 280 —
Cs 立方I 2.35 0.7 2.67 16.3 1.69(+1) 0.50 — 0.052 70 — 90 0.052	Ba 立方I 1.98 0.9 2.22 35.7 1.35(+2) 1.83 — 0.018 39 — 120 0.068	La* 六方H 1.69 1.1 1.87 96 1.15(+3) 1.5 — 0.017 22.5 0.033 129 0.045	Hf 六方H 1.44 1.3 1.67 155 0.81(+4) 5.2 — 0.031 13.6 0.22 127 0.035	Ta 立方I 1.34 1.5 1.49 180 0.73(+5) 6.8 — 0.081 10.9 0.13 138 0.036	W 立方I 1.30 1.7 1.41 185 0.64(+4) 8.05 0.68(+6) 0.151 9.53 0.40 184 0.032	Re 六方H 1.28 1.9 1.37 152 — 7.9 — 0.051 8.85 0.17 182 0.03	Os 六方H 1.26 2.2 1.35 162 0.69(+4) 6.4 — 0.11 8.43 — 201 0.031	Ir 立方F 1.27 2.2 1.36 152 0.66(+4) 6.6 — 0.189 8.54 0.14 212 0.031	Pt 立方F 1.30 2.2 1.39 122 0.96(+2) 4.7 — 0.095 9.10 0.17 207 0.032	Au 立方F 1.34 2.4 1.46 81.8 1.37(+1) 3.03 — 0.42 10.2 0.71 213 0.031	Hg 三方R 1.49 1.9 1.57 13.9 1.10(+2) 0.56 — 0.011 14.8 0.02 241 0.033	Tl 六方H 1.48 1.7 1.71 38.8 1.40(+1) 1.02 0.95(+3) 0.055 17.2 0.093 141 0.031	Pb 立方F 1.47 1.8 1.75 42.4 1.20(+2) 1.22 0.84(+4) 0.046 18.3 0.083 171 0.031	Bi 三方R 1.46 1.9 1.70 42.7 1.20(+3) 2.6 0.74(+5) 0.009 21.3 0.02 185 0.034	Po 单斜P 1.46 2.0 1.76 29 — — — 0.02 22.7 — — —	At (1.45) 2.2 — 8 — — — — — — — —	Rn 立方F — — — 3.92 — 0.69 — — — — 248 —
Fr 立方I — 0.7 — — 1.76(+1) — — — — — — —	Ra — 0.9 — 27.4 1.40(+2) 2.4 — — 45 — — —	Ac** — 1.1 1.88 — 1.18(+3) — — — — — — —															

★	Ce 立方F	Pr 六方H	Nd 六方H	Pm 六方H	Sm 三方R	Eu 立方I	Gd 六方H	Tb 六方H	Dy 六方H	Ho 六方H	Er 六方H	Tm 六方H	Yb 立方F	Lu 六方H
	1.65 1.1 1.81 95 1.11(+3) 1.2 1.03(+4) 0.013 21.0 0.026 159 0.042	1.65 1.1 1.82 79 1.09(+3) 1.60 0.92(+4) 0.015 20.8 0.028 133 0.048	1.64 1.2 1.82 69 1.08(+3) 1.70 — 0.013 20.6 0.031 145 0.045	— — — — 1.06(+3) — — — — — 133 —	1.62 1.2 1.81 46 1.04(+3) 2.1 — 0.011 19.9 — 129 0.042	1.85 — 1.99 42 1.12(+2) 2.2 — 0.012 28.9 — 131 0.039	1.61 1.1 1.79 72 1.02(+3) 3.70 — 0.007 19.9 0.021 142 0.071	1.59 1.2 1.80 70 1.00(+3) 3.9 — 0.009 19.2 — 155 0.044	1.59 — 1.80 67 0.99(+3) 4.1 — 0.011 19.0 0.024 157 0.041	1.58 1.2 1.79 67 0.97(+3) 4.1 — 0.011 18.7 — — 0.039	1.57 1.2 1.78 67 0.96(+3) 4.1 — 0.012 18.4 0.023 — 0.040	1.56 1.2 1.77 59 0.95(+3) 4.4 — 0.011 18.1 — — 0.038	— 1.1 1.94 38 1.13(+2) 1.8 0.94(+3) 0.035 24.8 — — 0.035	1.56 1.2 1.75 90 0.93(+3) 4.6 — 0.015 17.8 — 115 0.037
★★	Th 立方F	Pa	U 正交P	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lw
	1.65 1.3 1.80 — 1.14(+3) 4.6 0.95(+4) 0.055 19.9 — — 0.034	— 1.5 1.61 130 1.12(+3) — 0.98(+4) — 15.0 — — —	1.42 1.7 1.38 110 1.11(+3) 2.7 0.97(+4) .034 12.5 0.064 — 0.028	— 1.3 1.3 94.3 1.09(+3) — 0.95(+4) — 21.1 — — —	— 1.3 1.73 87.2 1.07(+3) — 0.93(+4) — — — — —	— 1.3 1.73 60.2 1.06(+3) — 0.92(+4) 0.007 20.8 — — 0.033								

元素名称
共价半径Å
原子半径Å(6)
原子半径Å(5)
原子体积
厘米³/克原子
第一电离能
(千卡/克原子)

Zn 六方H
1.25 1.6
1.38* 27.4
0.74(+2) 1.76
9.2 0.167
216 0.0915

晶体结构(1)
电负性
蒸发热(千卡/克·原子)(3)
熔化热(千卡/克·原子)
电导(微欧)⁻¹(4)
导热率(卡/厘米/℃/秒)(2)
比热(卡/克/℃)

注：(1) 立方F：立方面心；立方I：立方体心；立方P：简单立方；单[illegible]P：简单单斜；六方H：简单六方；三方R：简单三方；四方P：简单四方；正交P：简单正交
(2) 在室温 (3) 在沸点 (4) 从0°到20°C (5) 配位数为6的离[illegible]子(晶体)半径 (6) 配位数为12的金属半径

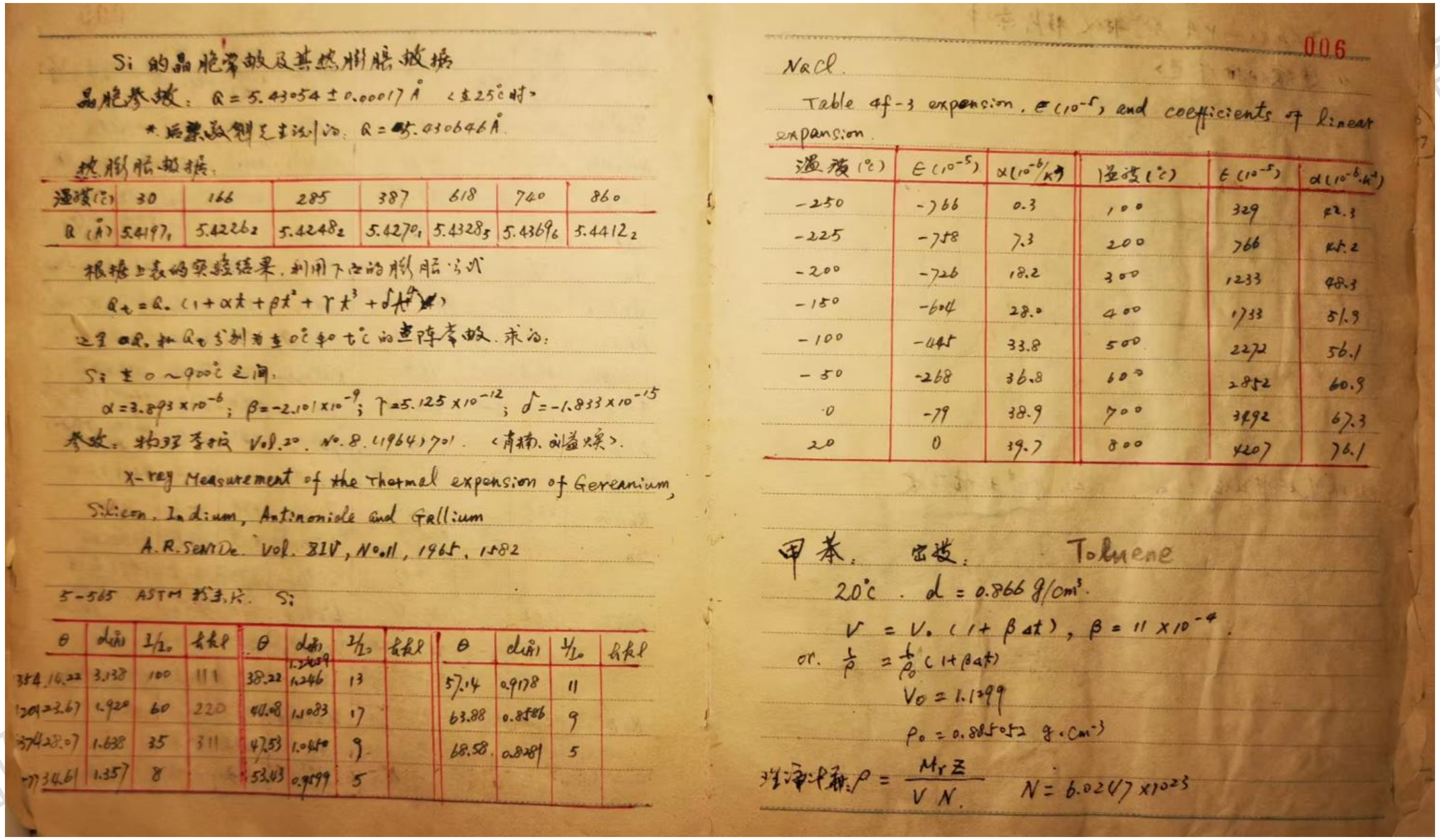
元素周期表(一)

IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB		IB	IIB	IIIA	IVA	VA	VIA	VIIA	VIIIA
1 1.00797 −252.7 1 −259.2 H 0.071 1s¹ Hydrogen 氢																2 4.0026 −268.9 −269.7 0.126 He 1s² Helium 氦
3 6.941 1330 1 180.5 Li 0.53 1s²2s¹ Lithium 锂	4 9.0122 2970 2 1277 Be 1.85 1s²2s² Beryllium 铍															
11 22.9898 892 1 97.8 Na 0.97 [Ne]3s¹ Sodium 钠	12 24.305 1107 2 650 Mg 1.74 [Ne]3s² magnesium 镁										13 26.9815 2450 3 660 Al 2.70 [Ne]3s²3p¹ Aluminium 铝	14 28.086 2680 4 1410 Si 2.33 [Ne]3s²3p² Silicon 硅	15 30.9738 280白 ±3,5,4 44.2白 P 1.82白 [Ne]3s²3p³ Phosphorus 磷	16 32.064 444.6 ±2,4,6 119.0 S 2.07 [Ne]3s²3p⁴ Sulphur 硫	17 35.453 −34.7 ±1,3,5,7 −101.0 Cl 1.56 [Ne]3s²3p⁵ Chlorine 氯	18 39.948 −185.8 −189.4 Ar 1.40 [Ne]3s²3p⁶ Argon 氩
19 39.102 760 1 63.7 K 0.86 [Ar]4s¹ Potassium 钾	20 40.08 1487 2 838 Ca 1.55 [Ar]4s² Calcium 钙	21 44.956 2730 3 1539 Sc 3.0 [Ar]3d¹4s² Scandium 钪	22 47.90 3260 4,3 1668 Ti 4.51 [Ar]3d²4s² Titanium 钛	23 50.942 3450 5,4,3,2 1900 V 6.1 [Ar]3d³4s² Vanadium 钒	24 51.996 2665 6,3,2 1875 Cr 7.19 [Ar]3d⁵4s¹ Chromium 铬	25 54.938 2150 7,6,4,2,3 1245 Mn 7.43 [Ar]3d⁵4s² Magnese 锰	26 55.847 3000 2,3 1536 Fe 7.86 [Ar]3d⁶4s² Iron 铁	27 58.93 2900 2,3 1495 Co 8.9 [Ar]3d⁷4s² Cobalt 钴	28 58.71 2730 2,3 1453 Ni 8.9 [Ar]3d⁸4s² Nickel 镍	29 63.54 2595 2,1 1083 Cu 8.96 [Ar]3d¹⁰4s¹ Copper 铜	30 65.37 906 2 419.5 7.14 [Ar]3d¹⁰4s² Zinc 锌	31 69.72 2237 3 29.8 Ga 5.91 [Ar]3d¹⁰4s²4p¹ Gallium 镓	32 72.59 2830 4 937.4 Ge 5.32 [Ar]3d¹⁰4s²4p² Germanium 锗	33 74.922 613 ±3,5 817 As 5.72 [Ar]3d¹⁰4s²4p³ Arsenic 砷	34 78.96 685 −2,4,6 217 Se 4.79 [Ar]3d¹⁰4s²4p⁴ Selenium 硒	35 79.904 58 ±1,5 −7.2 Br 3.12 [Ar]3d¹⁰4s²4p⁵ Bromine 溴	36 83.80 152 157.3 Kr 2.6 [Ar]3d¹⁰4s²4p⁶ Krypton 氪
37 85.47 688 1 38.9 Rb 1.53 [Kr]5s¹ Rubidium 铷	38 87.62 1380 2 768 Sr 2.6 [Kr]5s² Strontium 锶	39 88.905 2927 3 1509 Y 4.47 [Kr]4d¹5s² Yttrium 钇	40 91.22 3580 4 1852 Zr 6.49 [Kr]4d²5s² Zirconium 锆	41 92.906 3300 5,3 2468 Nb 8.4 [Kr]4d⁴5s¹ Niobium 铌	42 95.94 5560 6,5,4,3,2 2610 Mo 10.2 [Kr]4d⁵5s¹ Molybdenum 钼	43 98.906 — 7 2140 Tc 11.5 [Kr]4d⁵5s² Technetium 锝	44 101.07 4900 2,3,4,6,8 2500 Ru 12.2 [Kr]4d⁷5s¹ Ruthenium 钌	45 102.90 4500 2,3, 1966 Rh 12.4 [Kr]4d⁸5s¹ Rhodium 铑	46 106.4 3980 2,4 1552 Pd 12.0 [Kr]4d¹⁰5s⁰ Palladium 钯	47 107.870 2210 1 960.8 Ag 10.5 [Kr]4d¹⁰5s¹ Silver 银	48 112.40 765 2 320.9 Cd 8.65 [Kr]4d¹⁰5s² Cadmium 镉	49 114.82 2000 3 156.2 In 7.31 [Kr]4d¹⁰5s²5p¹ Indium 铟	50 118.69 2270 4,2 231.9 Sn 7.30 [Kr]4d¹⁰5s²5p² Tin 锡	51 121.75 1380 ±3,5 630.5 Sb 6.68 [Kr]4d¹⁰5s²5p³ Antimony 锑	52 127.60 989.8 2,4,6 449.5 Te 6.24 [Kr]4d¹⁰5s²5p⁴ Tellurium 碲	53 120.904 183 ±1,5,7 113.7 I 4.94 [Kr]4d¹⁰5s²5p⁵ Iodine 碘	54 131.30 −108.0 −111.9 Xe 3.06 [Kr]4d¹⁰5s²5p⁶ Xenon 氙
55 132.905 690 1 28.7 Cs 1.90 [Xe]6s¹ Cæsium 铯	56 137.34 1640 2 714 Ba 3.5 [Xe]6s² Barium 钡	57 138.91 3470 3 920 La* 6.17 [Xe]5d¹6s² Lanthanum 镧	72 178.49 5400 4 2222 Hf 13.1 [Xe]4f¹⁴5d²6s² Hafnium 铪	73 180.948 5425 5 2996 Ta 16.6 [Xe]4f¹⁴5d³6s² Tantalum 钽	74 183.85 5930 6,5,4,3,2 3410 W 19.3 [Xe]4f¹⁴5d⁴6s² Tungsten 钨	75 186.2 5900 7,6,4,2,1 3180 Re 21.0 [Xe]4f¹⁴5d⁵6s² Rhenium 铼	76 190.2 5500 2,3,4,6,8 3000 Os 22.6 [Xe]4f¹⁴5d⁶6s² Osmium 锇	77 192. 5300 2,3,4 2454 Ir 22.5 [Xe]4f¹⁴5d⁷6s² Iridium 铱	78 195.09 4530 2,4 1769 Pt 21.4 [Xe]4f¹⁴5d⁹6s¹ Platinum 铂	79 196.967 2970 3,1 1063 Au 19.3 [Xe]4f¹⁴5d¹⁰6s¹ Gold 金	80 200.59 357 2,1 −38.4 Hg 13.6 [Xe]4f¹⁴5d¹⁰6s² Mercury 汞	81 204.37 1457 3,1 303 Tl 11.85 [Xe]4f¹⁴5d¹⁰6s²6p¹ Thalium 铊	82 207.19 1725 4,2 327.4 Pb 11.4 [Xe]4f¹⁴5d¹⁰6s²6p² Lead 铅	83 208.980 1560 3,5 271.3 Bi 9.8 [Xe]4f¹⁴5d¹⁰6s²6p³ Bismuth 铋	84 (210) 962 2,4 254 Po (9.2) [Xe]4f¹⁴5d¹⁰6s²6p⁴ Polonium 钋	85 (210) 334 ±1,3,5,7 302 At — [Xe]4f¹⁴5d¹⁰6s²6p⁵ Astatin 砹	86 (222) (−61.8) (−71) Rn — [Xe]4f¹⁴5d¹⁰6s²6p⁶ Radon 氡
87 (223) — (27) Fr — [Rn]7s¹ Francium 钫	88 226.025 — 700 Ra 5.0 [Rn]7s² Radium 镭	89 (227) — 1050 Ac** — [Rn]6d¹7s² Actinium 锕	104													

★	58	59	60	61	62	63	64	65	66	67	68	69	70	71
	140.12 3468 3,4 795 Ce 6.67 [Xe]4f¹5d¹6s² Cerium 铈	140.9077 3127 3,4 935 Pr 6.77 [Xe]4f³6s² Praseodymium 镨	144.24 3027 3 1024 Nd 7.00 [Xe]4f⁴6s² Neodymium 钕	(147) — (1027) Pm — [Xe]4f⁵6s² Promethium 钷	150.35 1900 1072 Sm 7.54 [Xe]4f⁶6s² Samarium 钐	151.96 1439 3,2 826 Eu 5.26 [Xe]4f⁷6s² Europium 铕	157.25 3000 3 1312 Gd 7.89 [Xe]4f⁷5d¹6s² Gadolinium 钆	158.925 2800 3,4 1356 Tb 8.27 [Xe]4f⁹6s² Terbium 铽	162.50 2600 3 1407 Dy 8.54 [Xe]4f¹⁰6s² Dysprosium 镝	164.930 2600 3 1461 Ho 8.80 [Xe]4f¹¹6s² Holmium 钬	167.26 2900 3 1497 Er 9.05 [Xe]4f¹²6s² Erbium 铒	168.934 1727 3,2 1545 Tm 9.33 [Xe]4f¹³6s² Thulium 铥	173.04 1427 3,2 824 Yb 6.98 [Xe]4f¹⁴6s² Ytterbium 镱	174.97 3327 3 1652 Lu 9.84 [Xe]4f¹⁴5d¹6s² Lutetium 镥
★★	90 232.038 3850 4 1750 Th 11.7 [Rn]5f⁰6d²7s² Thorium 钍	91 231.036 — 5,4 (1230) Pa 15.4 [Rn]5f²6d¹7s² Protactinium 镤	92 238.03 3818 6,5,4,3 1132 U 19.07 [Rn]5f³6d¹7s² Uranium 铀	93 237.048 — 6,5,4,3 637 Np 19.5 [Rn]5f⁴6d¹7s² Neptunium 镎	94 (242) 3235 (6,4,3 640 Pu — [Rn]5f⁶7s² Plutonium 钚	95 (243) — 6,5,4,3 — Am 11.7 [Rn]5f⁷6d⁰7s² Americium 镅	96 (247) — 3 — Cm — [Rn]5f⁷6d¹7s² Curium 锔	97 (247) — 4,3 — Bk — [Rn]5f⁹6d⁰7s² Berkelium 锫	98 (249) — 3 — Cf — [Rn]5f¹⁰6d⁰7s² Californium 锎	99 (254) — — — Es — [Rn]5f¹¹6d⁰7s² Einsteinium 锿	100 (253) — — — Fm — [Rn]5f¹²6d⁰7s² Fermium 镄	101 (256) — — — Md — [Rn]5f¹³6d⁰7s² Mendele-vium 钔	102 (254) — — — No — [Rn]5f¹⁴6d⁰7s² Nobelium 锘	103 (257 — — — Lw — [Rn]5f¹⁴6d¹ Laurea-cium 铹

原子序数 — 30 65.37 — 原子量
熔点℃ — 906 2 — 氧化态
沸点℃ — 419.5
密度 — 7.14 Zn — 元素符号(1)
(克/厘米³)(3) — [Ar]3d¹⁰4s² 锌 — 元素名称
电子构型

注：(1) 93号元素以后为人工合成的元素　(2) 以碳12为基准　(3) 气体元素的数值为沸点时液体的数值



Si 的晶胞常数及其热膨胀数据

晶胞参数：$a = 5.43054 \pm 0.00017$ Å 〈在25°C时〉

*后来最新测定[illegible]：$a = 5.430646$ Å

热膨胀数据：

温度(°C)	30	166	285	387	618	740	860
a (Å)	5.4197_1	5.4226_2	5.4248_2	5.4270_1	5.4328_5	5.4369_6	5.4412_2

根据上表的实验结果，利用下面的膨胀公式

$$a_t = a_0 (1 + \alpha t + \beta t^2 + \gamma t^3 + \delta t^4)$$

这里 a_0 和 a_t 分别为在0°C和t°C的点阵常数。求得：

Si 在 0～900°C 之间：

$\alpha = 3.893 \times 10^{-6}$; $\beta = -2.101 \times 10^{-9}$; $\gamma = 5.125 \times 10^{-12}$; $\delta = -1.833 \times 10^{-15}$

参考：物理学报 Vol.20, No.8 (1964) 701.〈肖[illegible]、刘益焕〉

X-ray Measurement of the Thermal expension of Gereanium, Silicon, Indium, Antinomide and Gallium

A.R. SenDe Vol. 31V, No.11, 1965, 1582

5-565 ASTM 卡片. Si

θ	$d_{(Å)}$	I/I_0	hkl	θ	$d_{(Å)}$	I/I_0	hkl	θ	$d_{(Å)}$	I/I_0	hkl
354 14.22	3.138	100	111	38.22	1.2459 1.246	13		57.14	0.9178	11	
1209 23.67	1.920	60	220	40.08	1.1083	17		63.88	0.8586	9	
374 28.07	1.638	35	311	47.53	1.0450	9		68.58	0.8281	5	
77 34.61	1.357	8		53.43	0.9599	5					

006

NaCl.

Table 4f-3 expension, ε (10^{-5}), and coefficients of linear expansion.

温度(°C)	ε (10^{-5})	α (10^{-6}/K)	温度(°C)	ε (10^{-5})	α (10^{-6}·K^{-1})
−250	−766	0.3	100	329	42.3
−225	−758	7.3	200	766	45.2
−200	−726	18.2	300	1233	48.3
−150	−604	28.0	400	1733	51.9
−100	−445	33.8	500	2272	56.1
−50	−268	36.8	600	2852	60.9
0	−79	38.9	700	3492	67.3
20	0	39.7	800	4207	76.1

甲苯：密度： Toluene

20°C. $d = 0.866$ g/cm³.

$V = V_0 (1 + \beta \Delta t)$, $\beta = 11 \times 10^{-4}$.

or. $\frac{1}{\rho} = \frac{1}{\rho_0}(1 + \beta \Delta t)$

$V_0 = 1.1299$

$\rho_0 = 0.885052$ g·cm^{-3}

X射线密度：$\rho = \frac{M_r Z}{V N}$. $N = 6.02417 \times 10^{23}$

CSNS中子学校内部资料，请勿外传

有机标准物质相变温度 (°C) [13]

化合物	相变性质	标称相变温度	峰值温度
对氧苯甲酸	固—液	51.5	51.5
六氯乙烷	固—固	71.4	
萘	固—液	80.3	80.4
六甲苯苯	固—固	110.2	
苯甲酸	固—液	122.4	122.1
己二酸	固—液	151.4	151.0
茴香醇	固—液	183.0	183.1
2-氯蒽醌	固—液	209.1	209.4
联二苯	固—液	245.3	245.2
蒽醌	固—液	280.6	283.9

不同温度校正热量的物质和焓变值 [14]

物质	相变温度 (°C)	相变性质	热焓变化 (J/g)	物质	相变温度 (°C)	相变性质	热焓变化 (J/g)
H_2O	0	S-L	333.89	联苯	69.8	S-L	120.11
NH_4NO_3	32	S-S	19.87	萘	80.3	S-L	149
CBr_4	47	S-S	20.13	蒽	99.3	S-L	104.63
二苯酮	48.2	S-L	93.35	邻二硝基苯	114	S-L	135.18
硬脂酸	69	S-L	198.79	安息香酸	121.8	S-L	141.87

物质	相变温度 (°C)	相变性质	热焓变化 (J/g)	物质	相变温度 (°C)	相变性质	热焓变化 (J/g)
苯甲酸	122.4	S-L	148	$KClO_3$	299.8	S-S	99.18
NH_4NO_3	125	S-S	52.74	$NaNO_3$	306.2	S-L	194.7; 194.98
KNO_3	129	S-S	49.47; 53.83	Cd	320.9	S-L	53.99; 54.49; 55.96; 56.90; 57.00
AgI	154	S-S	26.21				
In	157	S-L	28.5	Pb	327.5	S-L	22.6; 23.02; 24.69
$AgNO_3$	160	S-S	14.65; 15.02	KNO_3	335	S-L	98.25; 117.60
$RbNO_3$	166	S-S	26.96	$Na_2Cr_2O_7$	355	S-L	134.97
NH_4NO_3	169.6	S-L	79.78	$K_2Cr_2O_7$	395	S-L	137.28
季戊四醇	187.8	S-L	322.66	Zn	419.4	S-L	102.13; 108.90; 113
NH_4Cl	196	S-S	83.71	Ag_2SO_4	427	S-S	52.84; 54.82; 56.85
$AgNO_3$	211	S-L	67.87; 71.46	CsCl	~440	S-S	16.82; 17.16
$RbNO_3$	228	S-S	18.45	$PbCl_2$	498	S-L	87.47
Sn	231.9	S-L	59.00; 59.70 59.99, 60.23, 60.69	LiBr	553	S-L	150.66
				SiO_2	573	S-S	5.99; 6.58
$LiNO_3$	252	S-L	37.37	Li_2SO_4	575	S-S	299.47; 307.41
Bi	271	S-L	50.22, 52.00 50.20, 53.79	Na_2WO_4	588.8	S-S	118.57
				Al	660	S-L	396; 400.9
$RbNO_3$	278	S-S	9.93	K_2CrO_4	667.3	S-S	35.62
				Ag	960.8	S-L	105
				Au	1063.0	S-L	62.8

标准物质相变温度 (°C) [12]

标准物质	相变性质	平衡相变温度	ICTA 标准试验	
			外推始偏点	峰值
KNO_3	固—固	127.7	128±5	135
In	固—液	157	154±6	159
Sn	固—液	231.9	230±5	237
$KClO_4$	固—固	299.5	299±6	309
Pb	固—液	327.5		
Zn	固—液	419.6		
Ag_2SO_4	固—固	424	424±7	433
SiO_2	固—固	573	571±5	574
K_2SO_4	固—固	583	582±7	588
Al	固—液	660.4		
K_2CrO_4	固—固	665	665±7	673
$BaCO_3$	固—固	810	808±8	819
$SrCO_3$	固—固	925	928±7	938
Ge	固—液	937.4		
Ag	固—液	961.9		
Au	固—液	1060.4		
Cu	固—液	1083.4		
Si	固—液	1410		
Ni	固—液	1453		
Fe	固—液	1535		

Magnetic moment calculation:

$$I_N = C\frac{m_{hkl}A_{hkl}}{\sin\theta\sin 2\theta}|F_N(\tau)|^2$$

$$F_N = \sum_{j=1}^{N} b_j e^{i\tau r_j} e^{-W_j} = \sum_{j=1}^{N} b_j \exp(2\pi i(hx_j + ky_j + lz_j))$$

$$I_M = C\left(\frac{re^2}{2mc^2}\right)^2 \frac{m_{hkl}A_{hkl}}{\sin\theta\sin 2\theta}|F_M(\tau)|^2\langle 1-(\hat{\tau}\cdot\hat{M})^2\rangle$$

$$F_M = \sum_{j=1}^{N}\langle\mu\rangle_j f_j(\tau)\exp(2\pi i(hx_j + ky_j + lz_j))$$

Method 1: $\langle\mu_j f_j\rangle^2 = \dfrac{I_M \cdot m_{hkl}\cdot F_N^2}{(0.27\times 10^{12})^2 m_{hkl}\cdot(\sum F_M)^2\cdot\langle 1-(\hat{\tau}\cdot\hat{M})^2\rangle\cdot I_N}$

Method 2. ① $C = I_N\sin\theta\sin 2\theta / m_{hkl}A_{hkl}F_N^2$

② $\langle Mf\rangle^2 = \dfrac{1}{\dfrac{I_N\sin\theta\sin 2\theta}{m_{hkl}A_{hkl}F_N^2}\left[\dfrac{I_M\sin\theta\sin 2\theta}{\left(\frac{re^2}{2mc^2}\right)^2\langle 1-\langle\tau\cdot M\rangle^2\rangle\sum F_M\cdot m\cdot A\cdot\sin\theta\sin 2\theta}\right]}$

$$= \frac{m_{hkl}A_{hkl}F_N^2\cdot I_M\sin\theta\sin 2\theta}{\left(\frac{re^2}{2mc^2}\right)^2\cdot\langle 1-(\tau\cdot M)^2\rangle\sum F_M\cdot m\cdot A\cdot\sin\theta\sin 2\theta\cdot I_N}$$

$$= \frac{I_M F_N^2 m_{hkl}}{\left(\frac{re^2}{2mc^2}\right)^2\cdot\langle 1-(\tau\cdot M)^2\rangle\cdot\sum F_m\cdot I_N}$$

$\langle 1-(\tau\cdot M)^2\rangle = \sin^2 2\theta$

$(0.27)^2 = 0.729$

* In GSAS. $F_{calc}^2 = \left(\frac{re^2}{2mc^2}\right)^2|F_M(\tau)|^2\langle 1-(\hat{\tau}\cdot\hat{M})^2\rangle$

化合物的折射率计算经验公式

$n = 1 + d\sum j k$. j为分子数. k为种类系数, d为密度.

氧化物	分子量	k_i	氧化物	分子量	k_i
H_2O	18	0.34	Y_2O_3	226	0.14
Li_2O	30	0.31	La_2O_3	326	0.15
Na_2O	62	0.18	Bi_2O_3	466	0.16
K_2O	94	0.19	Cl_2	44	0.22
BeO	25	0.24	SiO_2	60	0.21
MgO	40	0.20	TiO_2	80	0.40
CaO	56	0.23	ZrO_2	123	0.20
SrO	104	0.14	SnO_2	151	0.15
BaO	153	0.13	N_2O_5	108	0.24
PbO	223	0.15	P_2O_5	142	0.19
B_2O_3	70	0.22	Nb_2O_5	268	0.30
Al_2O_3	102	0.20	SO_3	80	0.18

The probable error for the value of weight w_j is

$$p_{w_j} = \pm 0.6745\sqrt{\frac{\sum w_i d_i^2}{(n-1)w_j}}$$

and for the weighted average

$$P_w = \pm 0.6745\sqrt{\frac{\sum w_i d_i^2}{(n-1)\sum w_i}}$$

It is possible to determine the relative weights to be attached to the individual measurements since the weight w_j is inversely proportional to $p_{w_j}^2$. The usual custom is to assign weights arbitrarily.

13.35. Probable Error of a Function.—In general the results of several independently measured quantities are combined to give the final value of the physical constant desired. Suppose $X, Y, \cdots$ have been obtained as the average value of certain quantities with probable errors $P_X, P_Y, \cdots$. If they are combined to give Z, where

$$Z = f(X,Y,\cdots)$$

then its probable error is

$$P = \sqrt{(P_X \partial Z/\partial X)^2 + (P_Y \partial Z/\partial Y)^2 + \cdots}$$

We record a few special cases for convenience of reference.

1. $Z = X \pm Y$; $P = \pm\sqrt{P_X^2 + P_Y^2}$

2. $Z = XY$; $P = \pm\sqrt{(XP_Y)^2 + (YP_X)^2}$

3. $Z = X/Y$; $P = \pm\frac{1}{Y^2}\sqrt{Y^2P_X^2 + X^2P_Y^2}$

4. $Z = a + bX$. Suppose we know the value Z_1 with its probable error p_1 at the point $X = X_1$ and Z_2 with error p_2 at $X = X_2$. We wish to fit the two points to a linear equation. Then

$$P_a = \sqrt{\left(\frac{X_2 p_1}{X_2 - X_1}\right)^2 + \left(\frac{X_1 p_2}{X_1 - X_2}\right)^2}$$

$$P_b = \sqrt{\left(\frac{p_1}{X_1 - X_2}\right)^2 + \left(\frac{p_2}{X_2 - X_1}\right)^2}$$

$$P_Z = \sqrt{\left(\frac{p_1(X_2 - X)}{(X_2 - X_1)}\right)^2 + \left(\frac{p_2(X_1 - X)}{(X_1 - X_2)}\right)^2}$$

where P_a, P_b and P_Z are the probable errors in a, b and Z, respectively.

Table I (*cont.*)

ION	EC	CN	SP	CR	*IR*	
NB+1	2P	6	IV	1.13	.99	
			V	1.14	1.00	
			VI	1.16	1.02	
			VII	1.26	1.12	
			VIII	1.32	1.18	
			IX	1.38	1.24	C
			XII	1.53	1.39	
NB+3	4D	2	VI	.86	.72	
NB+4	4D	1	VI	.82	.68	RE
			VIII	.93	.79	
NB+5	4P	6	IV	.62	.48	C
			VI	.78	.64	
			VII	.83	.69	C
			VIII	.88	.74	
MO+2	4F	4	VIII	1.43	1.29	
			IX	1.49	1.35	
MO+3	4F	3	VI	1.123	.983	R
			VIII	1.249	1.109	RR
			IX	1.303	1.163	R
			XII	1.41	1.27	E
N1+2	3D	8	IV	.69	.55	
			1VSQ	.83	.69	
			V	.77	.63	E
			VI	.830	.690	RR
N1+3	3D	7	VI	LS .70	.56	RR
				MS .74	.60	E
N1+4	3D	6	VI	LS .62	.48	R
MO+2	5F	14	VI	1.24	1.1	E
NP+2	5F	5	VI	1.24	1.10	
NP+3	5F	4	VI	1.15	1.01	R
NP+4	5F	3	VI	1.01	.87	R
			VIII	1.12	.98	R
NP+5	5F	2	VI	.89	.75	
NP+6	5F	1	VI	.86	.72	R
NP+7	6P	6	VI	.85	.71	R
D +2	2P	6	II	1.21	1.35	?
			III	1.22	1.36	
			IV	1.24	1.38	
			VI	1.26	1.40	
			VIII	1.28	1.42	
D+1			II	1.18	1.32	
			III	1.20	1.34	
			IV	1.21	1.35	E
			VI	1.23	1.37	E
DS+4	5D	4	VI	.770	.630	RR
DS+5	5D	3	VI	.715	.575	E
DS+6	5D	2	V	.63	.49	
			VI	.685	.545	E
DS+7	5D	1	VI	.665	.525	E
DS+8	5P	6	IV	.53	.39	
P +3	3S	2	VI	.58	.44	A
P +5	2P	6	IV	.31	.17	*
			V	.43	.29	
			VI	.52	.38	C
PA+3	5F	2	VI	1.18	1.04	E
PA+4	6D	1	VI	1.04	.90	R
			VIII	1.15	1.01	
PA+5	6P	6	VI	.92	.78	
			VIII	1.05	.91	
			IX	1.09	.95	
PB+2	6S	2	1VPY	1.12	.98	C
			VI	1.33	1.19	
			VII	1.37	1.23	C
			VIII	1.43	1.29	C
			IX	1.49	1.35	C
			X	1.54	1.40	C
			XI	1.59	1.45	C
			XII	1.63	1.49	
PB+4	5D10		IV	.79	.65	E
			V	.87	.73	E
			VI	.915	.775	R
			VIII	1.08	.94	R
PD+1	4D	9	II	.73	.59	
PD+2	4D	8	1VSQ	.78	.64	
			VI	1.00	.86	
PD+3	4D	7	VI	.90	.76	
PD+4	4D	6	VI	.755	.615	R
PM+3	4F	4	VI	1.11	.97	R
			VIII	1.233	1.093	R
			IX	1.284	1.144	R
PD+4	6S	2	VI	1.08	.94	R
			VIII	1.22	1.08	R
PD+6	5D10		VI	.81	.67	A
PR+3	4F	2	VI	1.13	.99	R
			VIII	1.286	1.126	R
			IX	1.319	1.179	R
PR+4	4F	1	VI	.99	.85	R
			VIII	1.10	.96	R
PT+2	5D	8	1VSQ	.74	.60	
			VI	.94	.80	A
PT+4	5D	6	VI	.765	.625	R
PT+5	5D	5	VI	.71	.57	ER
PU+3	5F	5	VI	1.14	1.00	R
PU+4	5F	4	VI	1.00	.86	R
			VIII	1.10	.96	
PU+5	5F	3	VI	.88	.74	E
PU+6	5F	2	VI	.85	.71	R
RA+2	6P	6	VIII	1.62	1.48	R
			VII	1.84	1.70	R
RB+1	4P	6	VI	1.66	1.52	
			VII	1.70	1.56	
			VIII	1.75	1.61	
			IX	1.77	1.63	E
			X	1.80	1.66	
			XI	1.83	1.69	
			XII	1.86	1.72	
			XIV	1.97	1.83	
RE+4	5D	3	VI	.77	.63	RR
RE+5	5D	2	VI	.72	.58	E
RE+6	5D	1	VI	.69	.55	E
RE+7	5P	6	IV	.52	.38	
			VI	.67	.53	
RH+3	4D	8	VI	.805	.665	R
RH+4	4D	5	VI	.74	.60	RR
RH+5	4D	4	VI	.69	.55	
RU+3	4D	5	VI	.82	.68	
RU+4	4D	4	VI	.760	.620	RR
RU+5	4D	3	VI	.705	.565	ER
RU+6	4D	2	VI	.65	.51	
RU+7	4D	1	IV	.52	.38	
RU+8	4P	6	IV	.50	.36	
S -2	3P	6	VI	1.75	1.84	P
S +4	3S	2	VI	.51	.37	A
S +6	2P	6	IV	.26	.12	*
			VI	.43	.29	C
SB+3	5S	2	1VPY	.90	.76	
			V	.94	.80	
			VI	.90	.76	A
SB+5	4D10		VI	.74	.60	*
SC+3	3P	6	VI	.885	.745	RR
			VIII	1.010	.870	RR
SE-2	4P	6	VI	1.84	1.98	P
SE+4	4S	2	VI	.64	.50	A
SE+6	3D10		IV	.42	.28	*
			VI	.56	.42	C
SI+4	2P	6	IV	.40	.26	*
			VI	.540	.400	RR
SM+2	4F	6	VII	1.36	1.22	
			VIII	1.41	1.27	
			IX	1.46	1.32	
SM+3	4F	5	VI	1.098	.958	R
			VII	1.16	1.02	E
			VIII	1.219	1.079	R
			IX	1.272	1.132	R
			XII	1.38	1.24	C
SN+4	4D10		IV	.69	.55	R
			V	.76	.62	C
			VI	.830	.690	RR
			VII	.89	.75	
			VIII	.96	.82	C
SR+2	4P	6	VI	1.32	1.18	
			VII	1.35	1.21	
			VIII	1.40	1.26	
			IX	1.45	1.31	
			X	1.50	1.36	C
			XII	1.58	1.44	C
TA+3	5D	2	VI	.86	.72	E
TA+4	5D	1	VI	.82	.68	E
TA+5	5P	6	VI	.78	.64	
			VII	.83	.69	
			VIII	.88	.74	
TB+3	4F	8	VI	1.063	.923	R
			VII	1.12	.98	E
			VIII	1.180	1.040	R
			IX	1.235	1.095	R
TB+4	4F	7	VI	.90	.76	R
			VIII	1.02	.88	
TC+4	4D	1	VI	.785	.645	RR
TC+5	4D	2	VI	.74	.60	ER
TC+7	4P	6	IV	.51	.37	
			VI	.70	.56	R
TE-2	5P	6	VI	2.07	2.21	P
TE+4	5S	2	VIII	.66	.52	
			IV	.80	.66	
			VI	1.11	.97	
TE+6	4D10		IV	.57	.43	C
			VI	.70	.56	*
TM+4	6P	6	VI	1.08	.94	C
			VIII	1.19	1.05	RC
			IX	1.23	1.09	*
			X	1.27	1.13	E
			XI	1.32	1.18	C
			XII	1.35	1.21	C
TI+2	3D		VI	1.00	.86	E
TI+3	3D		VI	.810	.673	RR
TI+4	3P		IV	.56	.42	C
			V	.65	.51	C
			VI	.745	.605	RR
			VIII	.88	.74	C
TL+1	6S		VI	1.64	1.50	R
			VIII	1.71	1.59	R
			XII	1.84	1.70	RE
TL+3	5D1		IV	.69	.75	
			VI	1.025	.885	R
TM+2	4F1		VI	1.17	1.03	
			VII	1.23	1.09	
TM+3	4F1		VI	1.020	.880	R
			VIII	1.134	.994	R
			IX	1.192	1.052	R
U +3	5P		VI	1.165	1.025	R
U +4	5P		VI	1.03	.89	
			VII	1.09	.95	E
			VIII	1.14	1.30	RR
			IX	1.19	1.05	
			XII	1.31	1.17	E
U +5	5P		VI	.90	.76	
U +6	6P		VII	.98	.84	E
			II	.59	.45	
			IV	.66	.52	
			VI	.87	.73	*
			VII	.95	.81	E
			VIII	1.30	.86	
V +2	3D		VI	.93	.79	
V +3	3D		VI	.780	.640	RR
V +4	3D		V	.67	.53	
			VI	.72	.58	RR
			VIII	.86	.72	E
V +5	3P		IV	.495	.355	RR
			V	.60	.46	*
			VI	.68	.54	
W +4	5D	2	VI	.80	.66	RR
W +5	5D	1	VI	.76	.62	R
W +6	5P	6	IV	.56	.42	*
			V	.65	.51	
			VI	.74	.60	*
XE+6	4D	0	IV	.54	.40	
			VI	.62	.48	
Y +3	4P	6	VI	1.040	.900	RR
			VII	1.10	.96	
			VIII	1.159	1.019	RR
			IX	1.215	1.075	R
			X	1.27	1.13	
			XI	1.22	1.08	E
			VIII	1.28	1.14	
YB+3	4F	3	VI	1.008	.868	RR
			VII	1.065	.925	E
			VIII	1.125	.985	R
			IX	1.182	1.042	R
ZN+2	3D	10	IV	.74	.60	*
			V	.62	.48	*
			VI	.840	.746	RR
			VIII	1.04	.90	C
ZR+4	4P	6	IV	.73	.59	R
			V	.80	.66	C
			VI	.86	.72	RR
			VII	.92	.78	*
			VIII	.98	.84	*
			IX	1.03	.89	

标准物质相变温度(°C)[12]

标准物质	相变性质	平衡相变温度	ICTA标准试验	
			外推始偏点	峰值
KNO_3	固—固	127.7	128±5	135
In	固—液	157	154±6	159
Sn	固—液	231.9	230±5	237
$KClO_4$	固—固	299.5	299±6	309
Pb	固—液	327.5		
Zn	固—液	419.6		
Ag_2SO_4	固—固	424	424±7	433
SiO_2	固—固	573	571±5	574
K_2SO_4	固—固	583	582±7	588
Al	固—液	660.4		
K_2CrO_4	固—固	665	665±7	673
$BaCO_3$	固—固	810	808±8	819
$SrCO_3$	固—固	925	928±7	938
Ge	固—液	937.4		
Ag	固—液	961.9		
Au	固—液	1060.4		
Cu	固—液	1083.4		
Si	固—液	1410		
Ni	固—液	1453		
Fe	固—液	1535		

有机标准物质相变温度 (°C)[13]

化合物	相变性质	标称相变温度	熔融点温度
对氧基苯酚	固—液	51.5	51.5
六氯乙烷	固—固	71.4	
萘	固—液	80.3	80.4
六甲基苯	固—固	110.2	
苯甲酸	固—液	122.4	122.1
己二酸	固—液	151.4	151.0
茴香醇	固—液	183.0	183.1
2-氯蒽醌	固—液	209.1	209.4
联苯	固—液	245.3	245.2
蒽醌	固—液	280.6	283.9

不同温度校正质量的物质和焓变值[10]

物质	相变温度 (°C)	相变性质	热焓变化 (J/g)	物质	相变温度 (°C)	相变性质	热焓变化 (J/g)
H_2O	0	S-L	333.89	联苯	68.8	S-L	120.11
NH_4NO_3	32	S-S	19.87	萘	80.3	S-L	149
CBr_4	47	S-S	20.13	蒽	99.3	S-L	104.63
二苯酮	48.2	S-L	98.35	邻二硝基苯	114	S-L	135.18
硬脂酸	69	S-L	198.79	安息香酸	121.8	S-L	141.87

物质	相变温度 (°C)	相变性质	热焓变化 (J/g)	物质	相变温度 (°C)	相变性质	热焓变化 (J/g)
苯甲酸	122.4	S-L	148	$KClO_3$	299.8	S-S	99.18
NH_4NO_3	125	S-S	52.74	$NaNO_3$	306.2	S-L	184.7; 184.98
KNO_3	129	S-S	69.47; 53.83	Cd	320.9	S-L	53.99; 54.49; 55.96; 56.90; 57.00
AgI	154	S-S	26.21				
In	157	S-L	28.5	Pb	327.5	S-L	22.6; 23.02; 24.69
$AgNO_3$	160	S-S	14.65; 15.02	KNO_3	335	S-L	98.25; 117.60
$RbNO_3$	166	S-S	26.96	$Na_2Cr_2O_7$	355	S-L	134.97
NH_4NO_3	169.6	S-L	79.78	$K_2Cr_2O_7$	395	S-L	137.28
季戊四醇	187.8	S-L	322.66	Zn	419.4	S-L	102.13; 108.90; 113
NH_4Cl	196	S-S	83.71	Ag_2SO_4	427	S-S	52.84; 54.82; 56.85
$AgNO_3$	211	S-L	67.87; 71.46	CsCl	~440	S-S	16.82; 17.16
$RbNO_3$	228	S-S	18.45	$PbCl_2$	498	S-L	87.47
Sn	231.9	S-L	59.00; 59.70 59.99, 60.21, 60.69	LiBr	553	S-L	150.66
				SiO_2	573	S-S	5.99; 6.58
$LiNO_3$	252	S-L	37.37	Li_2SO_4	575	S-S	249.67; 307.41
Bi	271	S-L	50.22, 52.00 50.20, 53.79	Na_2WO_4	588.8	S-S	119.57
				Al	660	S-L	396; 400.9
$RbNO_3$	278	S-S	9.93	K_2CrO_4	667.3	S-S	35.60
				Ag	960.8	S-L	105
				Au	1063.0	S-L	62.8

Ir^{4+}	6	76.5
Ir^{5+}	6	71
K^{1+}	4	151
	6	152
	7	160
	8	165
	9	169
	10	173
	12	178
La^{3+}	6	117.2
	7	124
	8	130
	9	135.6
	10	141
	12	150
Li^{1+}	4	73
	6	90
	8	106
Lu^{3+}	6	110.1
	8	111.7
	9	117.2
Mg^{2+}	4	
	5	80
	6	86
	8	103
Mn^{2+}	4HS	80
	5HS	89
	6LS	81
	HS	97
	7HS	104
	8	110
Mn^{3+}	5	72
	6LS	72
	HS	78.5
Mn^{4+}	4	53
	6	67
Mn^{5+}	4	47
Mn^{6+}	4	39.5
Mn^{7+}	4	39
	6	60
Mo^{3+}	6	83
Mo^{4+}	6	79
Mo^{5+}	4	60
	6	75
	6	73
	7	87
N^{3-}	4	132
N^{3+}	6	30
N^{5+}	3	4.4
	6	27
Na^{1+}	4	113
	5	114
	6	116
	7	126
	8	132
	9	138
	12	153
Nb^{3+}	6	86
Nb^{4+}	6	82
	8	93
Nb^{5+}	4	62
	6	78
	7	83
	8	88
Nd^{3+}	8	143
	9	149
Nd^{3+}	6	112.3
	8	124.9
	9	130.3
	12	141
Ni^{2+}	4	69
	4SQ	63
	5	77
	6	83
Ni^{3+}	6LS	70
	HS	74
Ni^{4+}	6LS	62
NO^{3+}	6	124
Np^{3+}	6	124
Np^{3+}	6	115
Np^{4+}	6	101
	8	112
Np^{5+}	6	89
Np^{6+}	6	86
Np^{7+}	6	85
O^{2-}	2	121
	3	122
	4	124
	6	126
	8	128
OH^-	2	118
	3	120
	4	121
	6	123
Os^{4+}	6	77
Os^{5+}	6	71.5
Os^{6+}	5	63
	6	68.5
Os^{7+}	6	66.5
Os^{8+}	4	53
P^{3+}	6	58
P^{5+}	4	31
	5	43
	6	52
Pa^{3+}	6	118
Pa^{4+}	6	104
	8	115
Pa^{5+}	6	92
	8	105
	9	109
Pb^{2+}	4PY	112
	6	133
	7	137
	8	143
	9	149
	10	154
	11	159
	12	163
Pb^{4+}	4	79
	5	87
	6	91.5
	8	108
Pd^{1+}	2	73
Pd^{2+}	4SQ	78
	6	100
Pd^{3+}	6	90
Pd^{4+}	6	75.5
Pm^{3+}	6	111
	8	123.3
	9	129.4
Po^{4+}	6	
	8	78

Pt (铂) 的热膨胀参数.

$a = 3.9160\ kX \qquad 1\ kX = 1.00203\ \text{Å}$

$\Delta a/a = 7.543\times10^{-6}(T-291) + 2.362\times10^{-9}(T-291)^2$

T(K)	a (Å)	T(K)	a (Å)	T(K)	a (Å)
291	3.9240	[illegible]	3.9779	1770	3.9883 ?
1140	3.9564	1705	3.9827	1890	3.9957
1335	3.9660	1770	3.9877	2005	4.0023

T(°C)	a (kX)	T(°C)	a (kX)	T(°C)	a (kX)
15	3.9161	256	3.9247	504	3.9347
56	3.9172	302	3.9264	539	3.9354
102	3.9192	351	3.9286	543	3.9359
150	3.9208	402	3.9309	595	3.9382
208	3.9231	453	3.9326	600	3.9380

以上引自. A Handbook of Lattice Spacings and Structures of Metals and Alloys. W. B. Pearson; (D.F.C. M.A. D.Phil.)

Pt: 0—1000°C.

$l_t = l_0(1+\alpha t+\beta t^2) \qquad \alpha = 0.0868\times10^{-4},\ \beta = 0.013\times10^{-7}$

Ref. Handbook of Chemistry and Physics. 37th Edition. P2086.

Pt. 膨胀系数. $9.1\times10^{-6}/°C$.

BBO: 11. $\Delta a/a = 4\times10^{-6}/K$. 33 $\Delta c/c = 36\times10^{-6}/K$.

BBO Pt 热导. Thermal conductivity.

11. 0.08 W/m/K, 33, 0.8 W/m/K

有效离子半径(a)

离子	配位数	半径 pm	离子	配位数	半径 pm	离子	配位数	半径 pm
Ac^{3+}	6	126	As^{5+}	4	47.5		6	117
Ag^{1+}	2	81		6	60		8	131
	4	114	At^{7+}	6	76	Bi^{5+}	6	90
	4SQ(b)	116	Au^{1+}	6	151	Bk^{3+}	6	110
	5	123	Au^{3+}	4SQ	82	Bk^{4+}	6	97
	6	129		6	99		8	107
	7	136	Au^{5+}	6	71	Br^{1-}	6	182
	8	142	B^{3+}	3	15	Br^{3+}	4SQ	73
Ag^{2+}	4SQ	93		4	25	Br^{5+}	3PY(c)	45
	6	108		6	41	Br^{7+}	4	39
Ag^{3+}	4SQ	81	Ba^{2+}	6	149		6	53
	6	89		7	152	C^{4+}	3	6
Al^{3+}	4	53		8	156		4	29
	5	62		9	161		6	30
	6	67.5		10	166	Ca^{2+}	6	114
Am^{2+}	7	135		11	171		7	120
	8	140		12	175		8	126
	9	145	Be^{2+}	3	30		9	132
Am^{3+}	6	111.5		4	41		10	137
	8	123		6	59		12	148
As^{3+}	6	72	Bi^{3+}	5	110	Cd^{2+}	4	92

B^{5+} 6 77

V^{4+}	5	67		8	112.5
	6	72		9	118.2
	8	85	Zn^{2+}	4	74
V^{5+}	4	49.5		5	82
	5	60		6	88
	6	68		8	104
W^{4+}	6	80	Zr^{4+}	4	73
W^{5+}	6	76		5	80
W^{6+}	4	56		6	86
	5	65		7	92
	6	74		8	98
Xe^{8+}	4	54		9	103.
	6	62			
Y^{3+}	6	104			
	7	110			
	8	114.9			
	9	121.5			
Yb^{2+}	6	116			
	7	122			
	8	128			
Yb^{3+}	6	100.8			
	7	106.5			

数据 R. D. Shannon, Acta Crystallogr., A32, 751 (1976). (b). SQ表示平面四方, (c) PY表示三角锥, (d). HS表示高自旋状态, (e) LS表示低自旋状态.

哥希密德(G), 鲍林(P)和拉德(L)对各种离子半径.

012

离子	G	P	L	离子	G	P	L
H^-	1.54	2.08	1.39	O^{2-}	1.32	1.40	1.24
F^-	1.33	1.36	1.19	S^{2-}	1.74	1.84	1.70
Cl^-	1.81	1.81	1.70	Se^{2-}	1.91	1.98	1.81
Br	1.96	1.95	1.87	Te^{2-}	2.11	2.21	1.97
I^-	2.20	2.16	2.12				
Li^+	0.78	0.60	0.86	Co^{2+}	0.82	0.74	0.88
Na^+	0.98	0.95	1.12	Ni^{2+}	0.68	0.69	—
K^+	1.33	1.33	1.04	Cu^{2+}	0.72	—	—
Rb^+	1.49	1.48	1.58	Bi^{3+}	0.2	0.2	—
Cs^+	1.65	1.69	1.84	Ai^{3+}	0.45	0.40	—
Cu^+	0.95	0.96	—	Sc^{3+}	0.68	0.83	—
Ag^+	1.13	1.26	1.27	Y^{3+}	0.90	0.93	—
Au^+		1.37	—	La^{3+}	1.04	1.15	—
Tl^+	1.49	1.40	1.54	Ga^{3+}	0.60	0.62	—
NH^+		1.48	1.66	Zn^{3+}	0.81	0.81	—
Be^{2+}	0.34	0.31	—	Tl^{3+}	0.91	0.95	—
Mg^{2+}	0.78	0.65	0.87				
Ca^{2+}	1.06	0.99	1.18				
Sr^{2+}	1.27	1.13	1.32	Fe^{3+}	0.53	—	—
Ba^{2+}	1.43	1.35	1.49	Cr^{3+}	0.53	—	—
Ra^{2+}		1.40	1.57				
Zn^{2+}	0.69	0.74	—	C^{4+}	0.15	0.15	
Cd^{2+}	1.03	0.97	1.14	Si^{4+}	0.38	0.41	
Hg^{2+}	0.93	1.10	—	Ti^{4+}	0.60	0.68	
				Zr^{4+}	0.77	0.86	
Pb^{2+}	1.17	1.21	—	Ce^{4+}	0.87	1.01	
Mn^{2+}	0.91	0.80	0.93	Ge^{4+}	0.44	0.53	
Fe^{2+}	0.83	0.76	0.90	Sn^{4+}	0.71	0.71	
				Pb^{4+}	0.81	0.84	