# Mössbauer Effect Reference and Data Journal

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# Mössbauer Effect Reference and Data Journal



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#### On the cover:

This issue is the first one published by MEDC at the new location. The host of the Center – Dalian Institute of Chemical Physics provides all help in establishing working facilities. "*The road ahead will be long and our climb will be steep, but our goal is clear and determination is strong*."

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### **Greeting from Editor**

Hello, all colleagues around the world! The Mössbauer Effect Data Center (MEDC) was officially moved to Dalian Institute of Chemical Physics (DICP), Chinese Academy of Sciences in July of 2010. We greet you from a beautiful harbor city of Dalian in the northeastern China, ready to welcome international visitors. The Center continues to offer the publications and services to the Mössbauer Community. This year issues of the journal will come in a traditional format and we hope you can use them as before.

In the current issue of the *Mössbauer Effect Reference and Data Journal*, we feature the Mössbauer research in DICP, its development history, main achievements, active researchers, and much more (see the *NewsLetter*). One can also take a look at the opening ceremony of MEDC in Dalian and the Symposium on Applications of the Mössbauer Spectroscopy, held at DICP June, 21-24. We believe the images included in the *NewsLetter* will provide a lively overview of the Institute and its Mössbauer group. We hope that this would help you know us better and could be a good start for closer cooperation in coming years.

Our approach includes a heavy emphasis on photos to provide an overview of our institute and its Mössbauer research. We believe this approach fairly make you know us much more.

Please join us!

Tao Zhang Director Volume 33, Number 7

#### MÖSSBAUER CENTURY CLUB

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10A015	A.Allanore, H.Lavelaine, G.Valentin, J.P.Birat, P.Delcroix, and F.Lapicque, <i>Electrochim. Acta</i> <b>55</b> (12),4007-13(2010) Observation and modeling of the reduction of hematite particles to metal in alkaline solution by electrolysis.
10B015	I.Bsoul, S.H.Mahmood, and A.F.D.Lehlooh, <i>J. Alloys Compd.</i> <b>498</b> (2),157-61(2010) Structural and magnetic properties of BaFe <sub>12-2x</sub> Ti <sub>x</sub> Ru <sub>x</sub> O <sub>19</sub> .
10B016	F.Bosi, T.Balic-Zunic, and A.A.Surour, <i>Am. Mineral.</i> <b>95</b> (4),510-8(2010) Crystal structure analyses of four tournaline specimens from the Cleopatra's Mines (Egypt) and Jabal Zalm (Saudi Arabia), and the role of Al in the tournaline group.
10B017	R.Blinc, P.Cevc, A.Potocnik, B.Zemva, E.Goreshnik, D.Hanzel, A.Gregorovic, Z.Trontelj, Z.Jaglicic, V.Laguta, M.Perovic, N.S.Dalal, and J.F.Scott, <i>J. Appl. Phys.</i> <b>107</b> (4),043511-1-5(2010) Magnetic properties of multiferroic K <sub>3</sub> Cr <sub>2</sub> Fe <sub>3</sub> F <sub>15</sub> .
10B018	W.Bodnar, M.Szklarska-Lukasik, P.Stoch, P.Zachariasz, J.Pszczola <sup>*</sup> , and J.Suwalski, <i>J. Alloys Compd.</i> <b>496</b> (1-2),37-42(2010) Hyperfine interactions and electronic band structure in Tb $_{0.27}$ Dy $_{0.73}$ (Fe $_{1-x}$ Co $_x$ ) $_2$ compounds.
10B019	A.A.Borisov, and C.A.McCammon, <i>Am. Mineral.</i> <b>95</b> (4),545-55(2010) The effect of silica on ferric/ferrous ratio in silicate melts: an experimental study using Mössbauer spectroscopy.
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10D010	C.Desvaux, P.Lecante, M.Respaud, and B.Chaudret*, J. Mater. Chem. <b>20</b> (1),103-9(2010) Structural and magnetic study of the annealing of Fe-Co nanoparticles.
10D011	K.Duerr, J.Olah, R.M.Davydov, M.Kleimann, J.Li, N.lang, R.Puchta, E.Hübner, T.Drewello, J.N.Harvey, N.Jux, and I.Ivanovic-Burmazovic <sup>*</sup> , <i>Dalton Trans.</i> <b>39</b> (8),2049-56(2010) Studies on an iron(iii)-peroxo porphyrin. Iron(iii)-peroxo or iron(ii)-superoxo?.
10E002	A.Ertl, G.R.Rossman, J.M.Hughes, D.London, Y.Wang, J.A.O'leary, M.D.Dyar, S.Prowatke, T.Ludwig, and E.Tillmanns, <i>Am. Mineral.</i> <b>95</b> (1),24-40(2010) Tourmaline of the elbaite-schorl series from the Himalaya Mine, Mesa Grande, California: a detailed investigation.
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105019	F.Suzuki, T.Honma, T.Ishibashi, T.Komatsu <sup>*</sup> , Y.Doi, and Y.Hinatsu, J. Phys. Chem. Solids <b>71</b> (6),906-12(2010) Synthesis and laser patterning of Bi-doped $Y_3Fe_5O_{12}$ crystals in germanosilicate glasses.
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#### Mössbauer Employment Positions Available

Mössbauer Effect Data Center (MEDC), Dalian Institute of Chemical Physics (DICP), Chinese Academy of Sciences (CAS)

Mössbauer Effect Data Center (MEDC) was moved to Dalian Institute of Chemical Physics (DICP) within Chinese Academy of Sciences (CAS) on July 1, 2010. To enhance further its development and Mössbauer research in DICP, we cordially invite senior professors, young scientists and post doctors excellent to work with us. The hosts are Prof. Tao Zhang (http://www.taozhang.dicp.ac.cn/english/Member/zhangtao.htm) and Prof. Junhu Wang (http://www.taozhang.dicp.ac.cn/english/Member/Wangjh.htm). Prof. Tao Zhang is the current director of DICP and MEDC. If you are interested in these positions, please send us your curriculum vitae and publication lists. After careful reviewing, we will recommend a suitable position to apply for, officially offered by CAS. You also welcome to introduce your colleagues, students and friends to apply for these positions. Here please note that you have two chances for applying for positions per year.

Below are our favorite research topics:

In situ Mössbauer investigation combined with other spectroscopic studies (such as XAFS and so on) on the structural properties and mechanism of iron and/or tin containing  $TiO_2$  photocatalytic materials;

Development and characterization of novel catalytic materials and catalytic reactions;

Development and characterization of apatite-based nano-composite materials, especially applied for catalysis and biomedicine;

Database research and journal publication, especially Mössbauer database & Mössbauer Effect Reference and Data Journal (MERDJ) (http://www.medc.dicp.ac.cn/)

Further information of CAS fellowships, see http://english.bic.cas.cn/AF/Fe/, and Prof. Tao Zhang's group is http://www.taozhang.dicp.ac.cn/.

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#### DATA LISTING

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Source	Temp	Absorber	Temp	IS	QS	Comments	Code
<u>Eu-151 21.60 keV T</u> EuF <sub>3</sub>	<u>Transition</u>	$Eu_5Zr_3S_{12}$	v			mixed-valence of Eu <sup>2+</sup> and Eu <sup>3+</sup> , T=4.2&77K	09J009
<u>Fe-57 14.40 keV Tra</u> Rh(IS/Fe)	ansition: B	<u>iological Compounds</u> CS-co-AAc magnetic hydrogel	300	.33	.93	magnetic and structural information	09P034
Fe-57 14.40 keV Tra	ansition: C	atalysts		10	1.74	1 .1 .1	00 4 020
XX Dd/IS / Eq)		$(FePctBu)_2N$	77	10	1.64	two iron ions have identical sites	09A020
Pu(15/Fe)		$100 \text{Fe}/3\text{K}/65 \text{IO}_2$			1.00	inagnetic property and particle size characterization	0910015
RI(15/Fe)	200	$Ce_2 \Sigma I_{1.5} Fe_5 O_{(8-d)}$	200	.55	1.09	after reaction structural information	107004
RI(15/Fe)	200	$IFeO_x/SiO_2$	200			aller reaction, structural information	10Z004
Rh(IS/Fe)	300	$IFFeO_x/SIO_2$	300	.32	.00	Ea <sup>4+</sup> onin state	102004
Rh(IS/Fe)		$[FePc(5O_2C_6H_{13})_4]_2N_4$	77	11	1.33	Fe , spin state	091002
Kn(IS/Fe)		[FePCSO <sub>2</sub> CBu <sub>4</sub> ] <sub>2</sub> N	//	03	1.47	Fe <sup>-</sup> , spin state	091002
<u>Fe-57 14.40 keV Tra</u> Rh(IS/Fe)	ansition: Fi	<u>ine Arts</u> pottery (Tascany, Italy)	300			oxidizing firing condition	08B083
Fe-57 14.40 keV Tra Rh(IS/Fe)	ansition: Fi	<u>rozen Solutions</u> green rust	80			carbon number=12, coordination of iron in metal hydroxide	10A013
Rh(IS/Fe)		water (Iron Mountain.	v			rhomboclase, spin state of hexaguairon(III), T=6&15K	09B057
141(10/10)		California)	·				0,200,
<u>Fe-57 14.40 keV Tra</u> Pd(IS/Fe)	ansition: G	ilasses and Amorphous Su 23Na <sub>2</sub> O-12Y <sub>2</sub> O <sub>3</sub> -25Fe <sub>2</sub> O <sub>3</sub> - 40SiO	<u>bstances</u> 300	.258	1.076	Fe <sup>3+</sup> predominant valence state	105019
Rh(IS/Fe)		Ferry Co Nh-BCu	300			Co raises mean hyperfine field of amorphous state	10T003
Rh(IS/Fe)		Fe/B/Ag multilaver	v			broad bimodal concentration distribution at interface. 12 <t<300k< td=""><td>09B053</td></t<300k<>	09B053
xx(IS/Fe)		silicate melts-Fe	300			$Fe^{3+}/Fe^{2+}$ ratio	10B019
Fo 57 14 40 koV Tr	ancition: Ir	organic Halidas					
xx	ansmon. n	K <sub>3</sub> Cr <sub>2</sub> Fe <sub>3</sub> F <sub>15</sub>	v			electronic structure of Fe, 4 <t<300k< td=""><td>10B017</td></t<300k<>	10B017
xx		$K_3Cu_3Fe_2F_{15}$	v			two magnetic and one nonmagnetic Fe sites, T=10&87K	09B054
<u>Fe-57 14.40 keV Tra</u> Pd(IS/Fe)	ansition: Ir	norganic Oxides 100Fe/3K/6SiO <sub>2</sub>				magnetic property and particle size characterization	09W015
Pd(IS/Fe)		23Na <sub>2</sub> O-12Y <sub>2</sub> O <sub>3</sub> -25Fe <sub>2</sub> O <sub>3</sub> -	300	.258	1.076	Fe <sup>3+</sup> predominant valence state	10S019
Rh(IS/Fe)	300	$a$ -Fe <sub>2</sub> $\Omega_{2}$ -Fe <sub>2</sub> $\Omega_{1}$	V			phase composition with thermal treatment 80 <t<300k< td=""><td>091.031</td></t<300k<>	091.031
Rh(IS/Fe)	500	$\alpha = Fe_2O_3 = FO_3O_4$	300			Fe phase composition	104011
Rh(IS/Fo)		amphiholos (Biancavilla	300			$E_0^{3+}/E_0$ ratio	094.018
10(10/10)		Italy)	500				071010
xx		$BaFe_{\scriptscriptstyle (12\text{-}2x)}Ti_{\scriptscriptstyle x}Ru_{\scriptscriptstyle x}O_{\scriptscriptstyle 19}$	300			dopant site distribution	10B015
Rh		basalt glass	295			Fe <sup>2+</sup> /Fe <sup>3+</sup> ratio in synthetic basalt glasses	09D021
Rh(IS/Fe)		bentonite				$\mathrm{Fe}^{^{2+}}/\mathrm{Fe}^{^{3+}}$ , with or without thiocompound absorbed, pH=8.00	10S021
xx(IS/Fe)		bentonite (Slovak Rep.)	80			Fe charge state, mineral composition	09O012
Rh(IS/Fe)		$Ce_{2}Zr_{1.5}Fe_{.5}O_{(8\text{-}d)}$		.33	1.09	iron state determination	09N021
Rh(IS/Fe)		CoFe <sub>2</sub> O <sub>4</sub>	300			diminution of population of core iron for cycled electrodes	10V007
Rh(IS/Fe)		CoFe <sub>2</sub> O <sub>4</sub>	300			bulk and surface iron locations	09L030
Rh(IS/Fe)		CuFe <sub>2</sub> O <sub>4</sub> -CuO	300			thermal degradation product, structural characterization	10T004
Rh(IS/Fe)		$\epsilon$ -Fe <sub>2</sub> O <sub>3</sub> /SiO <sub>2</sub>				iron oxide phase identification	09B052
Rh(IS/Fe)		erionite (Oregon, USA)	v			Fe <sup>3+</sup> in two octahedral sites, T=77&298K	09B055
Rh		Fe-Fe <sub>3</sub> O <sub>4</sub> -Fe <sub>2</sub> O <sub>3</sub>	300			phase analysis	10A015
Rh		$Fe/Lu_2O_3$	300			Fe phase state at interface	09M042
xx(IS/Fe)		Fe <sub>2</sub> O <sub>3</sub> /Si		.37	.71	phase identification	09P035
Rh(IS/Fe)		Fe <sub>3</sub> O <sub>4</sub>	v			canting angles of magnetic moments of Fe	09R039
Rh		Fe <sub>3</sub> O <sub>4</sub>	300			Fe charge state and site occupation affected by milling	10K009
xx		Fe <sub>3</sub> O <sub>4</sub>	77	.32	.02	HI=50 T, morphology and structure of nanosized magnetite, T=77&300K	10S017
Rh(IS/Fe)		Fe <sub>3</sub> O <sub>4</sub> -C	300			Fe phase composition	10A011
xx(IS/Fe)		Fe <sub>3</sub> O <sub>4</sub> -TMAOH/beta- cyclodextrin	v			superparamagnetic character	10S020
Rh(IS/Fe)	300	IrFeO <sub>x</sub> /SiO <sub>2</sub>	300			after reaction, structural information	10Z004

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Source	Temp	Absorber	Temp	IS	QS	Comments	Code
Rh(IS/Fe)	300	IrFeO <sub>x</sub> /SiO <sub>2</sub>	300	.32	.88	calcination, structural information	10Z004
Rh(IS/Fe)		$La_{(1-x)}Sr_{x}Fe_{.8}Cr_{.2}O_{(3-y)}$	v			co-existence of different Fe valence states, 4.2 <t<343k< td=""><td>10C018</td></t<343k<>	10C018
Rh(IS/Fe)		$La_{0.8}Sr_{1.2}Co_{0.5}Fe_{0.5}O_{3.65}$	16	.44	64	$Fe^{3+}$ in less than six-fold coordination, HI=50.1T	09E006
Rh(IS/Fe)		$La_{0.8}Sr_{1.2}Co_{0.5}Fe_{0.5}O_{3.65}$	298	.31	1.43	Fe <sup>3+</sup> in less than six-fold coordination	09E006
Rh(IS/Fe)		$La_{0.8}Sr_{1.2}Co_{0.5}Fe_{0.5}O_{4}$	v			Intermadiate charge between six-fold Fe <sup>3+</sup> and Fe <sup>4+</sup>	09E006
Rh(IS/Fe)		${\rm Li}_{2}{\rm FeTiO}_{4}$	300			evolution of charge state and local environment of Fe during discharge	09K039
Pd		MC-3-750	300			magnetic mesoporous carbon composies, phase compositions analysis	09G023
Pd		MC-3-850	300			magnetic mesoporous carbon composies, phase compositions analysis	09G023
Rh(IS/Fe)		$MgFe_2O_4$	300			ferrimagnetic behavior	10A014
Rh		MgFe <sub>2</sub> O <sub>4</sub>	v			determination of nanoparticle size	09S059
Rh(IS/Fe)		morillonite				$\mathrm{Fe}^{2+}/\mathrm{Fe}^{3+}$ , with or without thiocompound absorbed, pH=8.00	10S021
XX		Nickel ferrite/maghemite	4.2			core-shell structure is field dependent	095060
Rh(IS/Fe)		NiCrxFe <sub>(2-x)</sub> O <sub>4</sub>	300			Fe charge state and site occupation	09P033
xx(IS/Fe)		olivine	300			ratio of Fe <sup>3+</sup>	09F018
Rh(IS/Fe)		olivine	v			Fe charge state and site occupation in synthetic samples, 4 <t<293k< td=""><td>09D020</td></t<293k<>	09D020
xx		post-perovskite				Fe <sup>3+</sup> in bipolar prismatic and octahedral sites, 0 <p<136gpa< td=""><td>10C017</td></p<136gpa<>	10C017
Rh(IS/Fe)		pottery (Tascany, Italy)	300			oxidizing firing condition	08B083
Pd		R-3-700	300			magnetic mesoporous carbon composies, phase compositions analysis	09G023
xx(IS/Fe)		SrFe <sub>12</sub> O <sub>19</sub>	300			structural characteirzation, iron in five sites	10J009
Rh(IS/Fe)		tourmaline (Egypt)	300			Fe <sup>3+</sup> /Fe ratio	10B016
Rh(IS/Fe)		tourmaline (San Diego, California)	300			Fe charge state and site occupation	10E002
xx(IS/Fe)		wadsleyite	300			ratio of Fe <sup>3+</sup>	09F018
<u>Fe-57 14.40 keV 7</u> Rh(IS/Fe)	Fransition: Ir	organic Sulfides FeCe, Al S.	v			TDebve=247K. Fe <sup>2+</sup> valence state, 4.2 <t<300k< td=""><td>10K008</td></t<300k<>	10K008
Rh(IS/Fe)		FeCe <sub>1</sub> , In <sub>2</sub> S <sub>4</sub>	v			TDebye=239K, $Fe^{2+}$ valence state, 4.2 <t<300k< td=""><td>10K008</td></t<300k<>	10K008
Rh(IS/Fe)		FeCe <sub>1</sub> Al <sub>1</sub> S	4.2		2.54	HI=139 kOe, Fe <sup>2+</sup> valence state, 4.2 <t<300k< td=""><td>10K008</td></t<300k<>	10K008
Rh(IS/Fe)		FeCe <sub>1</sub> Al <sub>1</sub> S	300	.50		TDebye=299K, Fe <sup>2+</sup> valence state, 4.2 <t<300k< td=""><td>10K008</td></t<300k<>	10K008
Rh(IS/Fe)		FeCe <sub>1 a</sub> In <sub>1</sub> S <sub>4</sub>	4.2		2.64	HI=126 kOe, $Fe^{2+}$ valence state, 4.2 <t<300k< td=""><td>10K008</td></t<300k<>	10K008
Rh(IS/Fe)		FeCe <sub>1.9</sub> In <sub>.1</sub> S <sub>4</sub>	300	.50		TDebye=257K, Fe <sup>2+</sup> valence state, 4.2 <t<300k< td=""><td>10K008</td></t<300k<>	10K008
<u>Fe-57 14.40 keV 7</u> xx	Transition: M	letals and Alloys (Fe <sub>50</sub> Co <sub>50</sub> ) <sub>97</sub> V <sub>2</sub> Nb	300			Fe site occupation and phase analysis	10J010
Rh(IS/Fe)		$Cu_{s_0}Fe_{1_0}Ni_{1_0}$	300			phase evolution by annealing	09C025
Rh(IS/Fe)		Fe-C	300			Fe phase composition	10A011
Rh(IS/Fe)		FeCo	80			FeCo phase after annaling	10D010
Rh(IS/Fe)		FeCo	80			impurity exist before annaling	10D010
Rh(IS/Fe)		Fe@APTES	4.2			three iron sites	09G024
xx		Sm(Fe,Mo) <sub>12</sub>	293	099		Fe sites assigment	09K040
xx		Sm <sub>2</sub> (Fe,Mo) <sub>17</sub>	293	109		Fe sites assigment	09K040
xx		Sm <sub>3</sub> (Fe,Mo) <sub>29</sub>	293	101		Fe sites assigment	09K040
Pd(IS/Fe)		$Tb_{.27}Dy_{.73}Fe_{(2\text{-}2x)}Co_{2x}$	4.2			easy axis of magnetization	10B018
<u>Fe-57 14.40 keV 7</u> Rh(IS/Fe)	Transition: N	liscellaneous Inorganic C Fe <sub>(77 v</sub> )Co,Nb <sub>7</sub> B <sub>15</sub> Cu	ompounds 300			Co raises mean hyperfine field of amorphous state	10T003
Rh(IS/Fe)		Fe/B/Ag multilaver	v			broad bimodal concentration distribution at interface. 12 <t<300k< td=""><td>09B053</td></t<300k<>	09B053
Rh		Fe <sub>so</sub> Nb <sub>2</sub> Cu <sub>1</sub> B <sub>16</sub>	300			change of microstructure	101011
xx		La(Fe <sub>ss</sub> Si <sub>12</sub> ) <sub>12</sub>	4.2	01		isotropic volume expansion by hydrogenation. 4.2 <t<333k< td=""><td>09F016</td></t<333k<>	09F016
xx		La(FeSi)H.	4.2	.12		isotropic volume expansion by hydrogenation, 4.2 <t<333k< td=""><td>09F016</td></t<333k<>	09F016
Rh(IS/Fe)		$Li_{0.07}Fe_{0.07}PO_{4}$	300			Fe(III), different annealing Temperatures	09H022
Rh(IS/Fe)		LiFePO <sub>4</sub>	300	1.22	2.95	Fe(III)	09H022
<u>Fe-57 14.40 keV</u>	Transition: O	rganic Compounds	77	- 10	1.64	two iron ions have identical sites	00 4 0 2 0
Rh(IS/Ea)		(mana)Ea (m O)	80	10	1.04	Fo(III) high spin state	09A020
MI(10/1°C)		(	00	.57	.75	i c(iii) ingii spii suite	070020

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#### DATA LISTING

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Source 7	Гетр	Absorber	Temp	IS	QS	Comments	Code
		Fe(mana)					
Rh(IS/Fe)		(NCH <sub>2</sub> CH <sub>2</sub> NCHCNHCH CHN) <sub>3</sub> Fe(BF <sub>4</sub> ) <sub>2</sub>	77	.37	.36	Fe charge and spin state, T=77&295K	09A019
Rh(IS/Fe)		(NCH <sub>2</sub> CH <sub>2</sub> NCHCNHCH CHN) <sub>3</sub> FeK(BF <sub>4</sub> ) <sub>3</sub>	295	.29	.37	Fe(II) low spin state	09A019
Rh(IS/Fe)		(NCH <sub>2</sub> CH <sub>2</sub> NCHCNHCH CHN) <sub>3</sub> FeNa(BF <sub>4</sub> ) <sub>3</sub>	295	.22	.40	Fe(II) low spin state	09A019
Rh(IS/Fe)		(NCH <sub>2</sub> CH <sub>2</sub> NCHCNHCH CHN) <sub>3</sub> FeNH <sub>4</sub> (BF <sub>4</sub> ) <sub>3</sub>	295	.22	.39	Fe(II) low spin state	09A019
XX		$Bu_2NH_2Cr_7Fe_8(O_2CCMe_3)$	2.1	1.29	-2.67	mean spin value of Fe	10C016
Pd(IS/Fe)		$C_4N_3H_{16}(C_4N_3H_{15})_5Fe_2B_4P_7O_{26}(OH)_4$	300			mixed-valent state iron	09Y012
Rh(IS/Fe)		CS-co-AAc magnetic hydrogel	300	.33	.93	magnetic and structural information	09P034
Rh(IS/Fe)		Cu(apet)Fe(CN) <sub>5</sub> NO- H <sub>2</sub> O	300		.95	diamagnetic low-spin Fe(III) complexes, higher symmetry iron vicinity	10T004
Rh(IS/Fe)		Cu(hto)Fe(CN)5NO-2H2O	25	17	.89	Doppler and temperature effect	10T004
Rh(IS/Fe)		Cu(hto)Fe(CN)₅NO- 2H₂O	300		.88	diamagnetic low-spin Fe(III) complexes, higher symmetry iron vicinity	10T004
Rh(IS/Fe)		Cu(nme) <sub>2</sub> Fe(CN) <sub>5</sub> NO- H <sub>2</sub> O	25	16	.94	Doppler and temperature effect	10T004
Rh(IS/Fe)		Cu(nme) <sub>2</sub> Fe(CN) <sub>5</sub> NO- H <sub>2</sub> O	300		.93	diamagnetic low-spin Fe(III) complexes, higher symmetry iron vicinity	10T004
xx(IS/Fe)		Fe(3py-im) <sub>2</sub> (NCS) <sub>2</sub> -7H <sub>2</sub> O	v			Fe high spin to low spin ratio, 9 <t<300k< td=""><td>10Y001</td></t<300k<>	10Y001
Rh(IS/Fe)		Fe(5-Cl-qsal)₂Ni(α- tpdt)₂-MeCN	v			incomplete spin-crossover, 4 <t<295k< td=""><td>09N020</td></t<295k<>	09N020
Pd(IS/Fe)		Fe(mnt)(phen)(t-BuNC) <sub>2</sub>	80	.26	.56	configuration of octahedral complexes	09M041
Rh(IS/Fe)		Fe(salen)(atz)	300	.407	1.518	high spin state of Fe(III), 2 <t<300k< td=""><td>09H021</td></t<300k<>	09H021
Rh(IS/Fe)		Fe(salen)(bimz)	300	.417	1.35	high spin state of Fe(III)	09H021
Rh(IS/Fe)		Fe(salen)(btriz)	300	.397	1.458	high spin state of Fe(III)	09H021
Rh(IS/Fe)		Fe(salen)(imz)	300	.394	1.109	high spin state of Fe(III)	09H021
Rh(IS/Fe)		Fe(salen)(mtz)	300	.402	1.725	high spin state of Fe(III)	09H021
Rh(IS/Fe)		Fe(salen)(triz)	300	.392	1.243	high spin state of Fe(III)	09H021
Rh(IS/Fe)		FePyCHNNHCOC <sub>6</sub> H <sub>4</sub> O H-5H <sub>2</sub> O	v			Fe valence and spin state, 3 <t<286k< td=""><td>10Z005</td></t<286k<>	10Z005
Rh(IS/Fe)		FePyCMeNNHCOC <sub>6</sub> H <sub>4</sub> OH	3	.349	1.22	Fe(II) low spin state, 3 <t<286k< td=""><td>10Z005</td></t<286k<>	10Z005
Rh(IS/Fe)		Fe@APTES	4.2			three iron sites	09G024
Rh(IS/Fe)		green rust	80			carbon number=12, coordination of iron in metal hydroxide	10A013
xx		Me <sub>2</sub> NH <sub>2</sub> Fe <sub>2</sub> (HCOO) <sub>6</sub>	298			Fe charge state and coordination	09H020
Rh(IS/Fe)		[FePc(SO <sub>2</sub> C <sub>6</sub> H <sub>13</sub> ) <sub>4</sub> ] <sub>2</sub> N <sub>4</sub>	77	11	1.33	Fe <sup>4+</sup> , spin state	09I002
Rh(IS/Fe)		[FePcSO <sub>2</sub> CBu <sub>4</sub> ] <sub>2</sub> N	77	03	1.47	Fe <sup>3.5+</sup> , spin state	091002
xx		${[Fe(H_2O)_2]_2Nb(CN)_8-4H_2O]_n}$	v			Fe(II) high spin state, 4.2 <t<300k< td=""><td>09P036</td></t<300k<>	09P036
<u>Fe-57 14.40 keV Trans</u> Rh(IS/Fe)	ition: Te	errestrial and Extraterrestri amphiboles (Biancavilla,	<u>al Mineral</u> 300	<u>ls</u> 		Fe <sup>3+</sup> /Fe ratio	09A018
xx		basaltic rocks (Gusev crater of mars)	v			surface and interior, 235 <t<275k< td=""><td>09G025</td></t<275k<>	09G025
xx(IS/Fe)		bentonite (Slovak Rep.)	80			Fe charge state, mineral composition	090012
Rh(IS/Fe)		erionite (Oregon, USA)	v			Fe <sup>3+</sup> in two octahedral sites, T=77&298K	09B055
Rh(IS/Fe)		olivine	v			Fe charge state and site occupation in synthetic samples. 4 <t<293k< td=""><td>09D020</td></t<293k<>	09D020
XX		post-perovskite	-			$Fe^{3*}$ in bipolar prismatic and octahedral sites $0 < P < 136 GPa$	10C017
Rh(IS/Fe)		tourmaline (Egypt)	300			$Fe^{3+}/Fe$ ratio	10B016
Rh(IS/Fe)		tourmaline (San Diego	300			Fe charge state and site occupation	10E002
Rh(IS/Fe)		California) water (Iron Mountain	v			rhomboclase spin state of hexaguairon(III) $T=68-15K$	09B057
		California)	·			nonsection opinious of restauguaron(in), r-ocross	072007
<u>Sb-121 37.20 keV Tran</u> CaSnO <sub>3</sub>	<u>sition</u> 300	Ba <sub>2</sub> SbEuO <sub>6</sub>		02		hybridized-orbital behavior	10W006

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Source	Temp	Absorber	Temp	IS	QS	Comments	Code
CaSnO <sub>3</sub>	300	Ba <sub>2</sub> SbNdO <sub>6</sub>		24		hybridized-orbital behavior	10W006
CaSnO <sub>3</sub>	300	$Ba_2SbPrO_6$		76		hybridized-orbital behavior	10W006
CaSnO <sub>3</sub>	300	Ba <sub>2</sub> SbSmO <sub>6</sub>		06		hybridized-orbital behavior	10W006

#### ABBREVIATION LISTING

alv	alloy	hmpab	2-[(E)-2-(2-hydroxy-5-methylphenyl)-1-	nme	N-methylethylenediamine
anot	N N'-bis(3-		diazenyi]benzoate	PDVB	poly(divinylbenzene)
aper	aminopropyl)ethylenediamine	hto	1,3,6,9,11,14- hexaazatricyclo[12.2.1.1(6,9)]octadecan	PFC	potassium ferrocyanide
Bu	butyl		e	Ph	phenyl
code	reference code	Hx	hexyl	Pr	propyl
Ср	cyclopentadienyl	info	information	Ру	pyridine
EFG	electric field gradient	IS	isomer shift	py-im	4-pyridyl-imidazole
EQ	e2qQ(quadrupole coupling constant)	IS/	isomer shift relative to	QS	quadrupole splitting
Et	ethyl	mana	2,2'-(1,5-dimethyl-3,7-	R	room temperature
eta	asymmetry parameter		diazabicyclo[3.3.1]nonan-3,7- diyl)diacetate	SNP	sodium nitroprusside
fhpab	2-[(E)-3-formyl-4hydroxyphenyl)-	Me	methyl	SS	stainless steel
	diazenyijbenzoate	MNT	cis-1,2-dicyanoethylenedithiolate	struc	structure
FUA	Fusidate	mopag	5-[(E)-2-(4-methoxyphenyl)-1- diazenyl]quinolin-8-ol	Т	temperature or Tesla
hcpab	2-{(E)-4-hydroxy-3-[((E)-4- chlorophenyliminomethyl]-	1.1		Temp	temperature(Kelvin)
	phenyldiazenyl}benzoate	mpahb	(E)-2-(4-methylphenyl)-1-diazenyl]-2-	v	variable
He	liquid helium temperature(4.2 K)	NT		xx	material not reported
HI	internal magnetic field	IN	liquid nitrogen temperature		
			ISOTOPE INDEX		

#### Eu-151: 09J009 Sb-121: 10W006 Sn-119: 09B056 10A012 10B020 10C019 10N005 10S018

#### International Symposium on the Industrial Applications of the Mössbauer Effect (ISIAME 2012)

Dear Colleagues,

As all of you know, during ISIAME'08 in Budapest the decision was made for ISIAME 2012 conference to be held in Asheville under the Professor John Stevens leadership. However, last summer, the University of North Carolina at Asheville made the decision to close MEDC, precluding also any possibility to host ISIAME 2012.

MEDC moved to the Dalian Institute of Chemical Physics in China, under the direction of Professors Zhang and Wang, which also expressed their interest in hosting ISIAME 2012.

The Dalian Institute has the needed infrastructure to organize ISIAME, Dalian is an outstanding city and DICP has many connections with industry as witnessed by its projects and patents.

Considering also that the time till the conference is relatively short, the ISIAME Scientific Executive Committee has decided to award ISIAME 2012 to Dalian under the Professors Zhang and Wang leadership.

Professor Massimo Carbucicchio Chair, ISIAME Scientific Executive Committee

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Carbonyl Comj 10K010	plexes:		
Catalysts:			
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# Mössbauer Effect Data Center

is pleased to offer these publications and services to the international Mössbauer community...

Mössbauer Effect Reference and Data Journal



It's all about the battery ...

# Mössbauer Effect Reference and Data Journal

The *Journal* reports as thoroughly as possible all published information on Mössbauer spectroscopy. An annual subscription includes ten issues plus an index issue. Each issue includes a Reference Listing, a Data Listing, an Abbreviation Listing, an Isotope Index, a Subject Index, and the *Mössbauer Spectroscopy Newsletter*.

# Mössbauer Web Sites ON THE WORLD WIDE WEB



The Mössbauer Effect Data Center developed and administers two separate Web sites for the Mössbauer community

(<WWW.mossbauer.org> and <WWW.medc.dicp.ac.cn> These sites provide Mössbauer researchers with pertinent and timely information, free of charge. Included on the sites are general information pertinent to the Mössbauer community, news items, regional lab information, position postings, information on upcoming conferences, the most recent *Mössbauer Spectroscopy Newsletter*, IBAME information, an E-Mail and Fax Directory of Mössbauer Authors, links to Mössbauer instrument and source suppliers, and further information regarding the Center's products and services. Access to the MEDC Web-Access Database is also provided through the MEDC site. Researchers may now access and search the MEDC database *from their computers* via the MEDC Web site. The MEDC Database contains both a Reference and a Data file, and includes search, sort, and print functions.

For further information about these and our many other publications and services for the Mössbauer community, please visit us at our Web site

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# MÖSSBAUER SPECTROSCOPY NEWSLETTER

#### SEPTEMBER 2010

#### **Passing the Baton**

John Stevens, Airat Khasanov, Nina Hall, Irina Khasanova



The Mössbauer Community is a global circle of over 3,400 active researchers from more than 1,300 institutions around the world. The scientific tool they utilize relates scientists from 118 countries and appeals for closer ties and collaboration.

The Mössbauer Effect Data Center (MEDC) has evolved as central to this international community, through its activities in four interlocking areas: (1) the publication of the Mössbauer Effect Reference and Data Journal (MERDJ), a scientific reference journal now in its 33rd volume year; (2) the development, creation, and hosting of two Web sites (http://www. mossbauer.org/ and http://www.medc.dicp.ac.cn/ index.html); (3) support of the global community through e-mail and personal contact; and (4) the Mössbauer Research Laboratory.

John Stevens, the long standing Director of MEDC, continued the Mössbauer Effect Data Index, which had been started in 1966 by Muir, Ando and Coogan, and pushed it to a status of a monthly journal, published since 1975 with the help of various co-editors. Under his leadership the journal added a regular newsletter section, special front covers and various analytical pieces.

The newsletter covers many areas, featuring research laboratories in a selected country, topical articles in the hot fields of research, celebrating outstanding members of the Mössbauer Community, information about upcoming conferences and reports from the past ones, and other valuable information.

The Center scientists are reviewing published scientific papers, extracting experimental data and adding it to the MEDC database. This database is used to publish digests of data on various topics from general reviews to a popular mineral handbook. MEDC is also helping individual researchers with special requests. Many researchers visited the Center during these years and used its facilities.

The Center is maintaining two websites aimed at providing researchers with detailed information on Mössbauer spectroscopy and facilitating communication between scientists. The site provides basic introduction to the Mössbauer effect for newcomers, as well as information on upcoming conferences, instrument and source suppliers, reporting methods, news of interest to the community (such as job openings, major events within the community), a listing of major books related to the subject, a listing of laboratories world-wide, and regional information on Mössbauer research.

MEDC has taken a strong leadership position with international Mössbauer conferences. In 1993, John Stevens was the Conference Chair for the International Conference on the Applications of the Mössbauer Effect (ICAME), held in Vancouver, Canada. The staff of the Center was vital for the organization of this highly successful conference, attended by 349 international participants. He also spearheaded the first International Symposium on the Industrial Applications of the Mössbauer Effect in 1984.

The Director of the Center holds a Permanent Guest Membership at the International Board on the Applications of the Mössbauer Effect (IBAME), the governing body of the Community with 40 elected members.

A 20 member International Advisory Board for MEDC helped further strengthening the ties between the Center and the Community. We enjoyed the assistance of 11 Associate Editors of the Journal who aided us in collecting reprints.

The new century brings new challenges and we see them clearly – faster, more comprehensive information sources, sophisticated search engines, new ideas in communication, new areas of research. These challenges will be tackled by a new generation of scientists. MEDC has been following the advancement of young scientists and emerging centers of research. We observed Dalian Institute of Chemical Physics under the leadership of Tao Zhang being a fast accelerating research center and Junhu Wang was on the Center's list of most active scientists. So it came as no surprise to us that these two scientists stepped up to the challenges of steering the leadership of the community and bringing to life all necessary innovations.

Two of us (JS and AK) visited Dalian this year and were very much impressed by the energy and resources put into action by Tao Zhang and Junhu Wang. Their colleagues Duorong Liu, Changzi Jin, Xin Liu, and Hui Sun form a very impressive team ready to solve many technical problems that followed the relocation of the Center and they will lead the Mössbauer Effect Data Center to new levels in the best interest of the Mössbauer Community. Long discussions confirmed our belief that the good traditions of MEDC will be kept strong and many new ideas will be implemented.

We wish the greatest success to the MEDC Dalian and join colleagues around the world expressing our full support to its staff in their commitment to serve the Mössbauer Community.

#### **Dalian Institute of Chemical Physics, CAS**



Dalian Institute of Chemical Physics

Dalian Institute of Chemical Physics (DICP), Chinese Academy of Sciences (CAS) was founded in March 1949. It is a multidisciplinary institute engaging in both fundamental and applied research of chemistry and chemical engineering, especially with strengths in technological development. It is one of the academic divisions of the CAS, the national highest and leading academic body in science and technology in China.

DICP, as one of China's top ten academic institutions in natural sciences and high-tech innovation, has conducted researches of many fields. It has developed its own features in catalytic chemistry, engineering chemistry, organic synthetic chemistry, chemical lasers and molecular reaction dynamics. It has strong abilities in technology development and is a well-known research and development center in chemistry and chemical engineering. The mainstay is to undertake key research projects contracted by government sectors and industrial enterprises.

Aiming at building a world-wide reputation for outstanding academic and research achievements, DICP is making unprecedented efforts to promote the academic exchange and international cooperation at all levels (for more on DICP, visit www.dicp.cas.cn/)

#### History of Mössbauer Research in DICP

**T**rom the early years of 1980s, DICP started the Mössbauer spectroscopic studies. Prof. Liwu Lin (Member of Chinese Academy of Sciences) and Prof. Su Zhang played the central roles on the DICP's Mössbauer related researches. The research activities were initially focused on the study of catalytic materials. Importantly, at that time, a fruitful international collaboration had been established between DICP in China and The University of Birmingham in United Kingdom. Prof. Frank Berry (immediate past chairman of IBAME) was one of the most active members for the fruitful collaboration. Since then, the Mössbauer technique always played an important role in the development and characterization of novel iron and/or tin containing catalytic materials at DICP. Prof. Tao Zhang (present Director of DICP and MEDC) was a representative at that time. Prof. Tao Zhang began his Mössbauer related research works in 1989 when he was a doctoral student under supervisor by Prof. Liwu Lin.

In 2004, based on the urgent needs of the spectroscopic characterization of advanced catalysis in China, Prof. Tao Zhang, decided to further enhance In-Situ Mössbauer spectroscopic studies at DICP. Prof. Junhu Wang was invited to return to China from Japan, and was appointed as the team leader of the new Mössbauer research laboratory in 2007. Recently, over again, a well-equipped Mössbauer laboratory has been built.



In-Situ Catalytic Mössbauer Setup in DICP



Prof. Linli Wu just started collaboration with Frank Berry in '80s.



*Prof. Su Zhang wrote a chapter on Mössbauer Spectroscopy in 1996.* 



Prof. Chengyu Wang visited Birmingham University



Prof. Hongzhang Du visited Birmingham University



Dr. Yunfu Sun, Mr. Lijin Pan and Prof. Changyu Wang in Mössbauer Laboratory



Prof. Frank Berry visited DICP in '80s



Prof. Su Zhang visited Birmingham University



Prof. Changhai Xu visited Birmingham University 139



Prof. Wenzhao Li and Dr. Tao Zhang visited Birmingham University



Old friends reunited in Dalian in 2010

#### Mössbauer Effect Data Center

s you know, the MEDC has been located for the past 40 years at the University of North Carolina at Asheville in the United States and has been relocated to the DICP since 1 July 2010. The events of "Opening Ceremony of Mössbauer Effect Data Center (MEDC) and International Symposium on Mössbauer Spectroscopy" were held at DICP on 23-25 June, 2010. More than 70 Mössbauer scientists from abroad and China participated in this event.

On the opening ceremony, welcome speech was made by Prof. Tao Zhang, Director of DICP, CAS. Congratulation messages were separately given by Prof. Frank Berry, past Chairman of IBAME, Prof. Michael Reissner, Secretary of IBAME, Prof. John Stevens, past Director of MEDC, Prof. Elisa Baggio Saitovitch, past Vice-Chairman of IBAME, Prof. Zhifang Chai, Member of CAS and from Institute of High Energy Physics, CAS and Prof. Shengyun Zhu, General Secretary of Chinese Nuclear Physics Society.

Among others are included the following distinguished guests and specialists: Vice-Director of DICP (Prof. Zhongmin Liu), three Academicians of CAS from DICP (Prof. Liwu Lin, Prof. Can Li, and Prof. Xinhe Bao), Chairman of Chinese Mössbauer Community (Prof. Fashen Li), Vice-Chairmen of Chinese Mössbauer Community (Prof. Guilin Zhang and Prof. Xielong Yang), Members of IBAME representing Japan (Prof. Yutaka Yoshida) and Spain (Dr. J. F. Marco), past Deputy Director of MEDC (Prof. Clive Wynter), and representative of WissEl Mössbauer Company (Dr. Horst Engelmann).

The mission of MEDC is to provide information needs to the international scientific community in the field of Mössbauer spectroscopy. It is well known that the role of MEDC within the international Mössbauer community is vitally important. MEDC was founded in 1969 at the University of North Carolina at Asheville in the United States. Since the founding of the Center, headed by Prof. John Stevens, it has made great achievements. Presently, MEDC is the world's sole central repository for the more than 50,000 published papers on the Mössbauer effect, dating back to 1958.

MEDC is relocated in DICP since 1 July 2010. Prof. Tao Zhang, Director of DICP, takes the responsibility of Director of MEDC. Prof. Junhu Wang was appointed the Executive Secretary of MEDC. Prof. John Stevens and Prof. Frank Berry were recommended as two Honorary Directors of MEDC in view of their great achievements to host and operate MEDC and reputation within the international Mössbauer community. Essentially, the new Center at DICP keeps firmly the existing mission of past MEDC headed by Prof. John Stevens. It will as always aim to provide the international Mössbauer research community with a variety of information needs, including the maintaining of bibliographical and data computer databases. Data and information are routinely disseminated via Internet-accessible databases, printed handbooks, a monthly data journal, the Center's Web pages and e-mail. In addition, MEDC will continuously assist the organizers of international, national, and regional Mössbauer conferences in their planning and communications and provide support to the IBAME, the governing body of the international Mössbauer research community.

The Center also continuously acts as an information center for international Mössbauer researchers on a regional basis, such as those groups working in Latin America, Europe, Russia, Japan, China and other countries. The Center's objectives are as bellows: we will listen very carefully to the international Mössbauer community for their suggestions, fully develop and promote the international Mössbauer community, timely update the database, create innovative tools and resources, and reach a more global audience – all toward the goal of ensuring that scientific knowledge relating to the Mössbauer effect is available to all scientists, students, and research groups. As known, International Symposium on the Industrial Applications of the Mössbauer Effect (ISIAME) is an international conference series, held every four years since 1984, and provides a major forum for scientists of various disciplines who deal with the industrial applications of the Mössbauer spectroscopy. Originally, the next ISIAME, in 2012, was awarded to be hosted at Asheville under the leadership of Prof. John Stevens. While the MEDC was officially moved to Dalian, the ISIAME 2012 was decided to be held at Dalian under leaderships of Prof. Tao Zhang and Prof. Junhu Wang.



Opening ceremony of MEDC in Dalian: Zhaohua Cheng



Opening ceremony of MEDC in Dalian: Tao Zhang, Frank Berry, F.J. Marco



*Opening ceremony of MEDC in Dalian: Michael Reissner* 



Opening ceremony of MEDC in Dalian from left to right: Junhu Wang, Tao Zhang, Shenyun Zhu, Zhifang Chai, Guilin Zhang, Fashen Li, Xielong Yang

#### **Current Mössbauer Research in MEDC**

In our group, the Mössbauer technique is mainly applied for: 1) Identification of catalyst components in terms of active phase or active sites and search for correlations between these components and one or more of the catalytic properties; 2) Investigations of catalysts under working conditions and analysis of activation or deactivation processes; 3) Development & characterization of novel iron and / or tin containing functional materials mainly applied for the heterogeneous catalytic and photo-catalytic research fields to address energy related issues. The chemical reactions include preferential CO oxidation in rich H<sub>2</sub> atmosphere (PROX), oxidative bromination of methane (OBM), iron interaction with ammonia borane novel hydrogen storage material, etc.

# 1) Investigate the Active Site of Ir-Fe/SiO<sub>2</sub> Catalyst under PROX

The newly developed Ir-Fe/SiO<sub>2</sub> catalyst has been systematically investigated under different treatment conditions through quasi in situ <sup>57</sup>Fe Mössbauer spectroscopy. It is found that in PROX reaction, CO was activated on the Ir sites, whereas O<sub>2</sub> was activated on Fe. The catalytic performance could be reasonably correlated with the Fe<sup>2+</sup> concentration. (K. Liu, A. Wang, W. Zhang, J. Wang, Y. Huang, T. Zhang, J. Phys. Chem. C114, 8533-8541, 2010)

#### 2) <sup>57</sup>Fe Mössbauer Spectroscopic Studies on Silica Supported FePO<sub>4</sub> for OBM Reaction

The Mössbauer spectroscopic studies have been conducted on the iron phosphate catalyst for the oxidative bromination of methane. It is found that the FePO<sub>4</sub> fresh catalyst transformed quickly to stable active species during the induction period, and the active components of the stable catalyst are identified as near-equimolar  $\alpha$ -Fe<sub>3</sub>(P<sub>2</sub>O<sub>7</sub>)<sub>2</sub> and Fe<sub>2</sub>P<sub>2</sub>O<sub>7</sub>. This work is a collaboration with Prof. Yunjie Ding and Dr. Ronghe Lin. (R. Lin, Y. Ding, L. Gong, W. Dong, J. Wang, T. Zhang, J. Catal. 272, 65-73, 2010)

#### 3) <sup>57</sup>Fe Mössbauer and XAFS Studies on Novel Hydrogen Storage Material of Fe-Modified Ammonia Borane

Quasi in situ <sup>57</sup>Fe Mössbauer and X-ray adsorption fine structure (XAFS) techniques are employed to identify the changes of Fe chemical environment during dehydrogenation process. The experimental results show that FeB nanoalloy is formed upon mixing AB with FeCl<sub>3</sub> which probably functions as catalytic species in the dehydrogenation process. This work is a collaboration with Prof. Ping Chen and Mr. Teng He. (T. He, J. Wang, T. Liu, G. Wu, Z. Xiong, J. Yin, H. Chu, T. Zhang, Submitted to Catal. Today)

#### **Current Staff of MEDC**

#### Director: Prof. Tao Zhang



Prof. Zhang got his Ph.D. degree of DICP, CAS in 1989, and became a Professor in 1995. He is at present the Director of DICP. The main research area of Prof. Zhang is industrial catalysis. His recent research interests involve "catalytic decomposition technology for non-toxic propellants", "environmental catalysis" and "new catalytic materials". For more details, please see http://www.taozhang.dicp.cas.cn.

Prof. Zhang started his Mössbauer-related activities from the early years of 1980s. His doctoral dissertation titled as "study of carbon deposition on highly dispersed Pt/Al<sub>2</sub>O<sub>3</sub> and Pt-Sn/Al<sub>2</sub>O<sub>3</sub> catalysts for dehydrogenation of alkanes". <sup>119</sup>Sn Mössbauer technique was effectively applied to investigate the structural and properties of Pt-Sn catalytic materials. In order to promote his Mössbauer-related skills, he ever studied in Prof. Frank Berry's group at The University of Birmingham for one years as a visiting scholar. He conducted a fruitful international collaboration with Prof. Frank Berry.

Prof. Zhang always maintains a strong interest on Mössbauer applications in catalysis & materials. Recent years, in order to achieve world-class of the Mössbauer-related activities in DICP, he advocated further strengthening of Mössbauer research and communication.

Executive Secretary: Prof. Junhu Wang



Prof. Wang got his Ph. D. degree of Toho University (Supervisor: Prof. Masuo Takeda) in Japan in 2002, and became a Professor in 2008. His present main research lines at DICP involve "development and application of novel catalytic materials" and "in-situ Mössbauer characterization". He plays a central role on the research of in-situ Mössbauer spectroscopic characterization on catalysis and materials chemistry at DICP.

Prof. Wang graduated from Radiochemistry of Modern Physics Department at Lanzhou University in China in 1991. He started his Mössbauer-related activities since 1996. His doctoral thesis deals with Mössbauer spectroscopic studies on gadolinium, erbium and neptunium compounds. He investigated the structures and bonding of lanthanide and actinide compounds by using <sup>155</sup>Gd, <sup>166</sup>Er and <sup>237</sup>Np Mössbauer spectroscopies. Since that time, Mössbauer characterization is always his most main research field. He has been selected as one of the Emerging Scientists. He has published more than 30 Mössbauer-related papers up to now, including one chapter of book and one technical report. For more details, please see http://www. htch.dicp.cas.cn/english/Member/Wangjh.htm. Recently, Prof.Wang has been granted the outstanding scholarship foundation of CAS (100 Talents Program) for promoting the applications of in-situ Mössbauer technique on aerospace catalysis and new materials in China. He also has a dream that the Mössbauer technique can be applied to Chinese spaceflight exploration in the near future like the famous MIMOS II.

Honorary Director: Professor Frank Berry

Honorary Director: Professor John Stevens

Other staff:

Dr. Changzi Jin



Analysis of the current publications in the field of Mössbauer spectroscopy, extraction of data, MEDC database update.

#### Dr. Xin Liu



Analysis of the current publications in the field of Mössbauer spectroscopy, extraction of data, MEDC database update.

#### Ms. Duorong (Lucy) Liu



Communication with research groups around the world, publications management, general management.





Initial data entry and information verification.

General support group includes:

Dr. Yanjie Zhang



# Ms. Jie Yin

#### Ms. Kunfeng Zhao



Several scientists participated in collaboration with DICP researchers in the past and recently. Below are recollections and insights of some of them.

#### Reflections on Thirty Years of Interaction with Dalian Institute of Chemical Physics

Frank Berry

School of Chemistry, The University of Birmingham, United Kingdom



T is a great pleasure to have been invited to write an article for the first Newsletter of The Mössbauer Effect Data Center (MEDC) since its relocation to Dalian Institute of Chemical Physics (DICP) and I thought it appropriate that I might reflect on my interactions with DICP over the past thirty years.

My first visit to DICP was in 1981. It was a part of a memorable visit as one of the first British scientists to tour China under an agreement between The Chinese Academy of Sciences and The Royal Society. The itinerary involved giving lectures in various Institutes and Universities in Beijing, Shanghai, Lanzhou, Changchun, Xian and Dalian. It was in Dalian however that a special link was made, I remember well my first visit to Dalian in 1981. I have strong memories of talking science with Professor Liwu Lin who is now a long-term friend. In those days in 1981 English was not so widely spoken in China as it is now and those lectures in 1981 were translated sentence by sentence by Professor Su Zhang who was DICP's expert in Mössbauer spectroscopy and who I remember with much appreciation. These translated lectures used to last for four or five hours and tea was served two, three or four times during one lecture.

It was in Dalian in 1981 that a curious chance event occurred that had a significant bearing on my scientific work for the following twelve years. I was due to fly from Dalian to Lanzhou but when I arrived at the airport the flight had been delayed for six hours. Professor Liwu Lin suggested that he and I should visit a nice place by the sea. We had some drinks and talked about science and during those six hours we discovered mutual and complimentary scientific interests and we agreed to initiate a collaboration. Somehow, Professor Liwu Lin persuaded The Chinese Academy of Sciences and I obtained the support of The Royal Society to fund this collaboration for nine years and then the European Union supported it for another two years. It remains the longest formal collaboration of my career and during that time seven younger Chinese scientists worked with me in Birmingham, Professor Liwu Lin visited several times, Professor Su Zhang also visited and I visited China on many occasions.

The collaboration sought to link the expertise of Professor Liwu Lin's group in catalyst preparation and evaluation with my interests in in-situ characterization by Mössbauer spectroscopy. The first Chinese visitor to Birmingham was Chengyu Wang in 1983 and we worked on the influence of metal-support and metalmetal interactions on the activity and selectivity of iron-ruthenium catalysts. Hongzhang Du visited in 1985 to continue the work, especially the unusual and unexpected observation of the oxidation of iron in titania-supported iron-ruthenium catalysts under reducing conditions. This was developed during the visit of Changhai Xu in 1987 and 1988 to the iron-iridium catalyst system by the application of synchrotron EXAFS techniques to the characterization of the materials. Subsequent work by Jianyi Shen between 1988 and 1989 focused on highly dispersed iron on activated carbon catalysts for Fischer-Tropsch synthesis and on phase formation and dispersion properties which influence catalytic performance. In 1989 Weishen Yang and Tao Zhang (now Director of MEDC) opened up new work on the influence of preparative methods on supported platinum-tin catalysts for the dehydration of propene. The results of the collaboration were published in over twenty papers in high impact factor Journals including J Chem Soc Faraday1, Chemical Communications, Applied Catalysis and numerous presentations were made at international and national conferences. It is now pleasing to see that many of the younger scientists from Dalian who participated in the collaboration and exchange programme now hold senior positions within some of the most prestigious institutions within China. During the past twenty years I have kept in less close contact with DICP mainly by meeting colleagues at conferences and have enjoyed many conversations with Junhu Wang.

Hence it was a special privilege and pleasure to attend the Opening Ceremony of MEDC in DICP in June. DICP is undoubtedly a premier scientific institution performing work which is internationally leading. The scientific presentations made at the Symposium to celebrate the opening of MEDC demonstrated the enthusiasm, variety and depth of Mössbauer spectroscopy within China and, under the leadership of Professors Tao Zhang and Junhu Wang, MEDC now enters a new era in its distinguished history. For me, it has been a privilege and pleasure to have been closely associated with DICP during the years between 1981 and 1992 and I look forward to seeing the development of both MEDC and DICP which, I think, will bring distinction to both our technique and to China.

For more information about publications of the Mössbauer Effect Data Center visit us at our web site:

www.medc.dicp.ac.cn

#### My work with Mössbauer spectroscopy

#### Jianyi Shen

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was delighted when I heard that the Mössbauer Effect Data Center (MEDC) would be relocated to Dalian Institute of Chemical Physics (DICP). Unfortunately, I was unable to attend the ceremony for the event in last June since I was visiting Lyon, France then.

I remember that I was trained to work with Mössbauer spectroscopy when I joined Prof. Liwu Lin's lab in DICP as a graduate student in 1980s. I was taught to use the Mössbauer spectrometer and clean the floor for the apparatus by Mr. Lijin Pan who was then a technician in charge of it. Profs. Liwu Lin and Su Zhang advised me when I began my research on highly dispersed iron on activated carbon (Fe/AC) for Fischer-Tropsch (FT) synthesis. The catalysts were black and difficult to characterize with other techniques. Mössbauer spectroscopy was the best technique that time to trace the valent states and phases of iron in Fe/AC catalysts treated in situ at various conditions.

The in situ technique for Mössbauer measurements in DICP was probably first used by Prof. Chengyu Wang. The key of the technique was an in situ cell, which was made of glass or quartz in the shape similar to  $\eta$  and could be sealed with valves. The longer tube contained a catalyst and could be heated at high temperatures. After cooled down to room temperature, the catalyst was transferred to the shorter tube with two plastic windows. The  $\gamma$  ray and detector were arranged in vertical mode so that powdered catalysts could be placed flatly on a plastic window for Mössbauer mea-

surements. Researchers in DICP enjoyed the technique and collected useful data.

Prof. Renyuan Tang got the idea to combine the in situ Mössbauer measurements with temperature programmed reduction (TPR). TPR usually produces a profile with several reduction peaks indicating the reduction processes. However, it is usually difficult to assign all the reduction peaks just according to the profile itself. Renyuan Tang designed an in situ cell that could be used for TPR and Mössbauer measurements. He monitored the TPR profile and measured Mössbauer spectrum after each TPR peak. In this way, he was able to describe every reduction peak in the TPR profiles of some supported iron catalysts. I brought the technique to Nanjing University (NJU) and some researchers in NJU studied iron molybdate catalysts for the selective oxidation of toluene with the technique.



Some researchers in DICP studied Fe/Al<sub>2</sub>O<sub>3</sub> and Fe/SiO<sub>2</sub> catalysts with Mössbauer spectroscopy. But these catalysts were not active for FT synthesis since the strong interactions between iron oxides and the supports. Iron was difficult to reduce due to the formation of iron aluminate and silicate. Soon, Profs. Liwu Lin and Su Zhang realized that Fe/AC might be good catalysts for FT synthesis since iron must be easier reduced when supported on AC.

For my PhD thesis, I studied Fe/AC catalysts with in-situ Mössbauer spectroscopy. Much work was accomplished in Prof. Frank Berry's lab in Birmingham University. Different promoters such as K, Mn, Cu and Mo were added into Fe/AC. The catalysts were reduced in H<sub>2</sub> and carburized in syngas at different temperatures and monitored by in situ Mössbauer spectroscopy. Although most iron could be reduced in H<sub>2</sub> at 773 K, there were always some unreduced iron species in the catalysts, indicating the strong interaction of iron species with carbon surfaces. Although such interaction was not as strong as those in Fe/Al<sub>2</sub> $O_3$ <u>146</u>

and Fe/SiO<sub>2</sub>, it was important for the high dispersion of iron on AC. The highly dispersed iron on AC was highly active for FT synthesis with high selectivity to gasoline and low selectivity to methane.

Since FT synthesis was performed under high pressures, the glass in situ cell could not be used to trace the iron phases during the FT synthesis. However, the catalysts after FT synthesis could be transferred into the in situ cell without exposing to air. Mössbauer measurements showed that mainly  $\varepsilon$ - and  $\chi$ -iron carbides were present in the Fe/AC catalysts during FT synthesis.



Trained as a researcher, I began my studies in NJU with Mössbauer spectroscopy in early 1990. Quite a few scientists in the Departments of Physics and Chemistry of NJU were working with Mössbauer spectroscopy that time. Profs. Yi Chen and Yuanfu Xia published textbooks on the Mössbauer effect and its applications then. Amorphous alloys were the main materials I studied with Mössbauer spectroscopy in NJU.

During my visit to Prof. Dumesic's lab in the Department of Chemical Engineering, UW-Madison in 1990s, I worked with Mössbauer spectroscopy of Sn and Eu. The surface acidity and basicity of  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> were found to be significantly inhibited by doped Sn(II) on the surface. The  $Eu_2O_2/SiO_2$  was found to be an acidic system which contained two oxides that individually did not possess acid sites for ammonia adsorption.

Recently, a collaboration work was performed on the Mössbauer spectroscopic studies of Fe-Ir/SiO<sub>2</sub> catalysts for PROX. Profs. Tao Zhang, Junhu Wang and I co-supervised a PhD student for the work. Fe(II) was found to play a key role for the preferential oxidation of CO in H<sub>2</sub> over the Fe-Ir/SiO<sub>2</sub> catalysts. Our collaboration will continue on the studies of iron catalysts. A new support  $(g-C_3N_4)$  synthesized in NJU will be used for iron catalysts.

#### New Perspectives on Collaboration between Dalian Institute of Chemical Physics and J. Heyrovský Institute of Physical Chemistry

#### Edyta Tabor

J. Heyrovský Institute of Physical Chemistry of the ASCR, v. v. i. Prague, Czech Republic



**F** rom 1st July 2010 Mössbauer Effect Data Center (MEDC) is located in Dalian Institute of Chemical Physics (DICP) in Dalian, China. It is the great honor and pleasure to be the first scholar in the research filed of Mössbauer spectroscopy in the Department of the Catalysis and New Materials for Aerospace since DICP presides over MEDC.

In our group at the Department of Structure and Dynamics in Catalysis, J. Heyrovský Institute of Physical Chemistry we successfully apply the Mössbauer spectroscopy to the characterization of active sites of mono- and bimetallic zeolitic catalysts, which are mainly employed in the decomposition of nitrous oxides.

One year ago I participated at the International Conference on the Application of the Mössbauer Effect, which was held in July 2009 in Vienna, Austria. During this conference I met Professor Junhu Wang. We talked about our scientific results and application of Mössbauer spectroscopy for the characterization of catalysts. At the end of the conversation with Prof. Wang we decided to try to initiate the collaboration between our groups. I wrote the proposal that was accepted by Professor Zdenek Sobalik, head of our Department, as well as by Professors Junhu Wang and Tao Zhang. After that I applied to the Czech Academy of Sciences for the support for our collaboration. Thanks to Bilateral Agreement between Czech Academy of Sciences and Chinese Academy of Sciences, I received two months fellowship in DICP.



I arrived to Dalian at the beginning of August 2010. Together with Professors Tao Zhang and Junhu Wang we elaborated the work schedule. The main goal of our project is to develop new efficient bimetallic catalysts for preferential oxidation of CO (PROX) and to determine the structure-activity relationships. In DICP we prepared a series of bimetallic catalyst supported on various carriers such as carbon materials and zeolites and we use them as catalyst in PROX reaction. We are optimizing the synthesis conditions in order to prepare improved catalysts for PROX reaction. The most active catalysts will be characterized by in- situ Mössbauer spectroscopy.



I hope that the results of our work will help to enlarge the knowledge about catalysts for PROX reaction. In-situ Mössbauer spectroscopy gives us a great possibility to investigate the nature of catalytically active species. I am convinced that the cooperation between our Institutes will be beneficial not only personally for us, but also for the Science we all serve.

#### In Memoriam Alexandr Afanasev

It is with deepest sadness to announce the passing of Professor Alexandr Mikhailovich Afanasev

Russian Academy of Sciences, Institute of Physics and Technology, Moscow

who died on 10 August 2010.

Alexandr (Sasha) Afanasev was born in Mnevniki near Moscow, Russia, on 8 June 1938. He graduated in 1960 from the Moscow National Research Nuclear University "MEPhI". From 1960 to 1963 he was a PhD student ("aspirant") at the Kurchatov Institute of Atomic Energy in Moscow and, until 1989, he remained a member of the same institute. In 1989 he became Head of the Laboratory "Physics of Surfaces and Microelectronic Structure" of the Institute of Physics and Technology of the Russian Academy of Sciences in Moscow.

Sasha obtained his PhD ("candidate of sciences") degree with his thesis "Theory of hyperfine structure of Mössbauer lines" in 1965 followed by a DSc ("doctor of sciences") degree with the thesis "Theory of dynamic interaction of radiation with matter". In 1976, he was awarded the State Prize of the Soviet Union. In 1984 he was elected as a corresponding member of the Academy of Sciences of his country.

Sasha was a distinguished member of the international Mössbauer community. His early works were devoted to the theory of spin-lattice relaxation, special cases of hyperfine interaction and, two decades before its realization at synchrotrons, to the coherent nuclear resonant scattering of X-rays. Later he became involved in Mössbauer studies on high-Tc superconductors, in elaborating mathematical methods for improving the resolution of Mössbauer spectroscopy and in further Mössbauer relaxation studies including those of cage diffusion, of rotational diffusion, of ferromagnetic nanoparticles under radio-frequency magnetic field excitation and many others. He was a frequent visitor and invited speaker of international Mössbauer conferences and an active part of international cooperation with groups in Germany, Hungary and other countries.

However, Sasha was much more than an exceptional theoretician in Mössbauer spectroscopy. He was

one of the most excellent solid-state theoreticians in Russia and beyond its borders having numerous important contributions in X-ray diffraction, X-ray optics, X-ray standing wave techniques and he also developed methods for X-ray surface analysis with nanometer resolution. He published more than 200 scientific papers including a monograph and four review articles.

Since 2002, Sasha has been fighting with serious health problems. He passed away on 10 August 2010 during these terrible three weeks with fires and smoke around and in Moscow.

We shall miss him. Our thoughts are with his family.

D.L. Nagy Chair, IBAME

(Reprinted from Mix Bulletin)

## Future Conferences, Symposia, and Workshops

November 7-12, 2010 **The XII Latin American Conference on the Application of Mössbauer Effect (LACAME2010);** Lima, Peru Web: web.lacame2010.org

December 15-20, 2010 Pacifichem 2010, Inorganic #2, Symposium # 275 (Pacifichem2010-NCFMNP); Hawaii, USA Web: www.pacifichem.orgsymposia/c\_symp\_275.htm

January 13-14, 2011 6th Nassau-Mössbauer Symposium; New York, USA Web: http://mossbauer.ncc.edu/

September 25-30, 2011 International Conference on the Applications of the Mössbauer Effect (ICAME2011); Tokyo, Japan http://www2.convention.co.jp/icame2011tokyo/index.html



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#### Mössbauer effect sources, absorbers

Mössbauer effect sources: serial, point & double sided sources



These sources are suitable for use in all Mössbauer spectrometers, and for practical applications in gamma-resonance field. Sources feature excellent spectral properties and reliable capsules suitable for cryogenic applications down to liquid He temperature.

Sources are certified on validated high-precision Mössbauer spectrometer with absolute velocity measurement method introduced to eliminate systematic errors.



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Line width:	0.110 ÷ 0.155 mm/s	$0.35\div0.48~\text{mm/s}$	3.2 mm/s
Туре:	serial, special, double	serial	serial
Window:	Be, 0.5 mm	Be, 0.5 mm	Be, 0.5 mm
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