

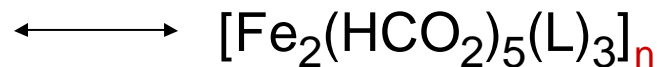
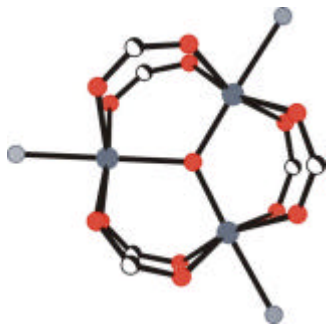
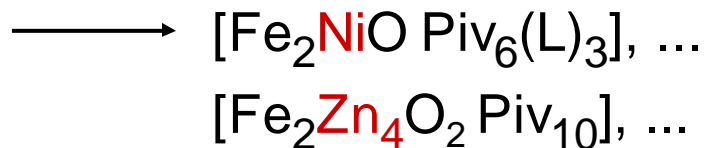
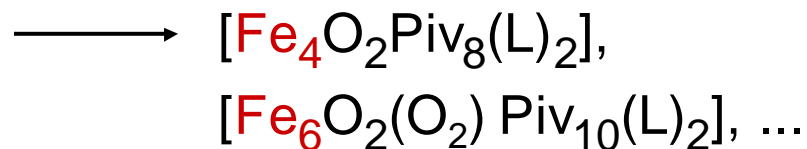
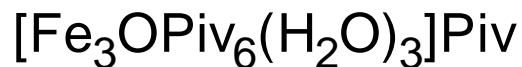
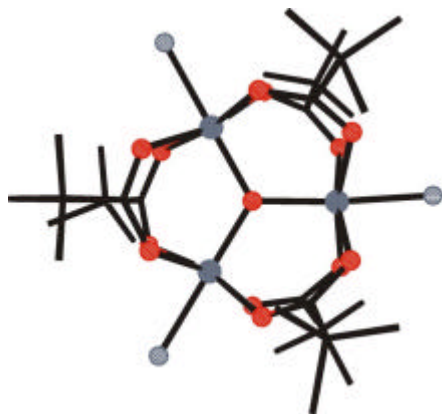
# The Mixed-Valence Iron(II/III) 2D-Layer Complex

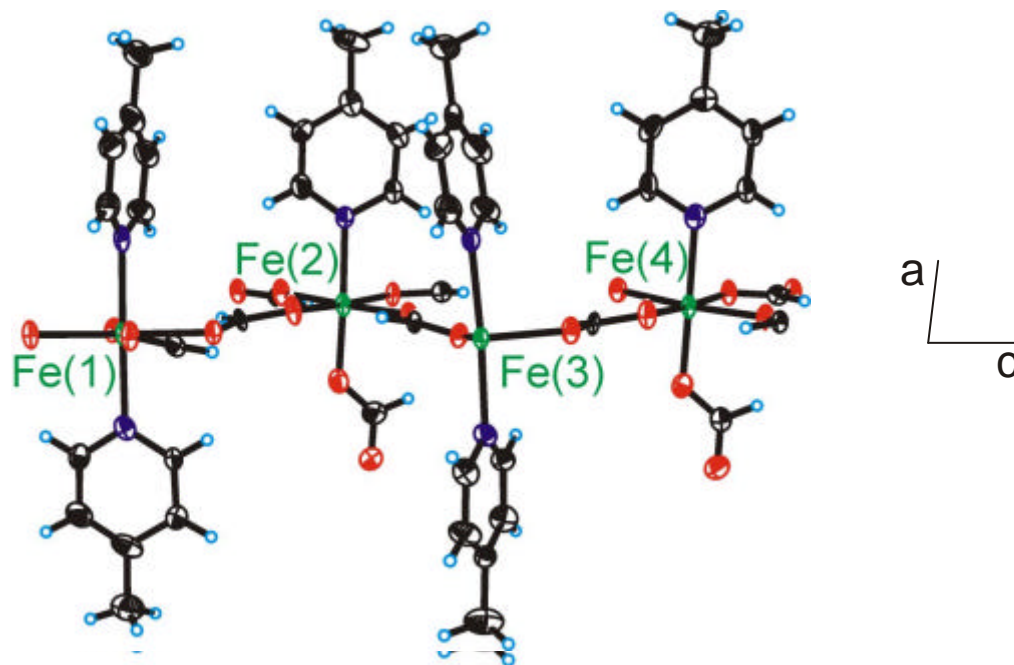


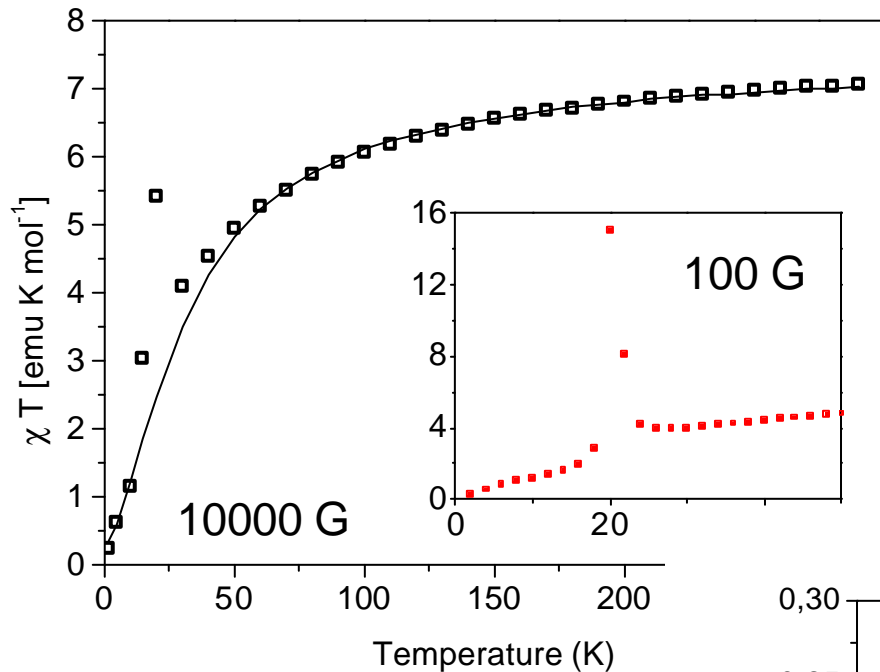
- Structural and Magnetic  
Investigations

Eva Rentschler, Jacob Overgaard,  
Grigore A. Timco, Finn K.Larsen

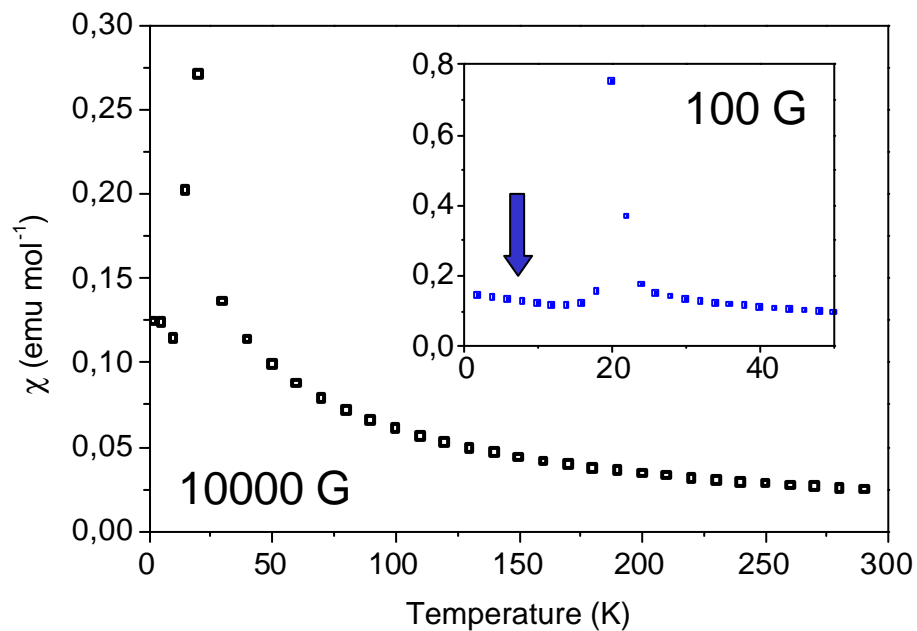
# $[\text{Fe}_3\text{O}]^{6+/7+}$ units as molecular building blocks

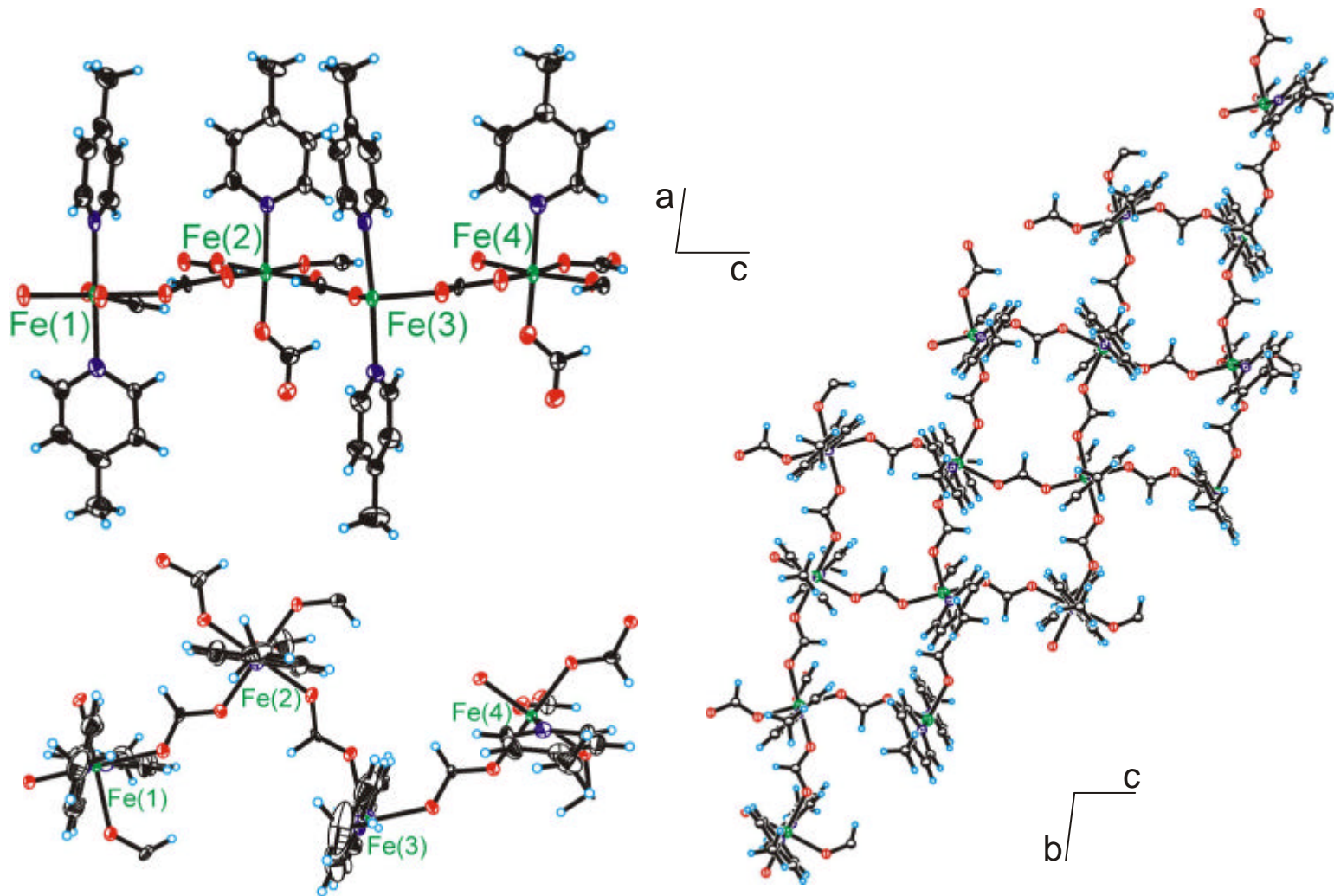


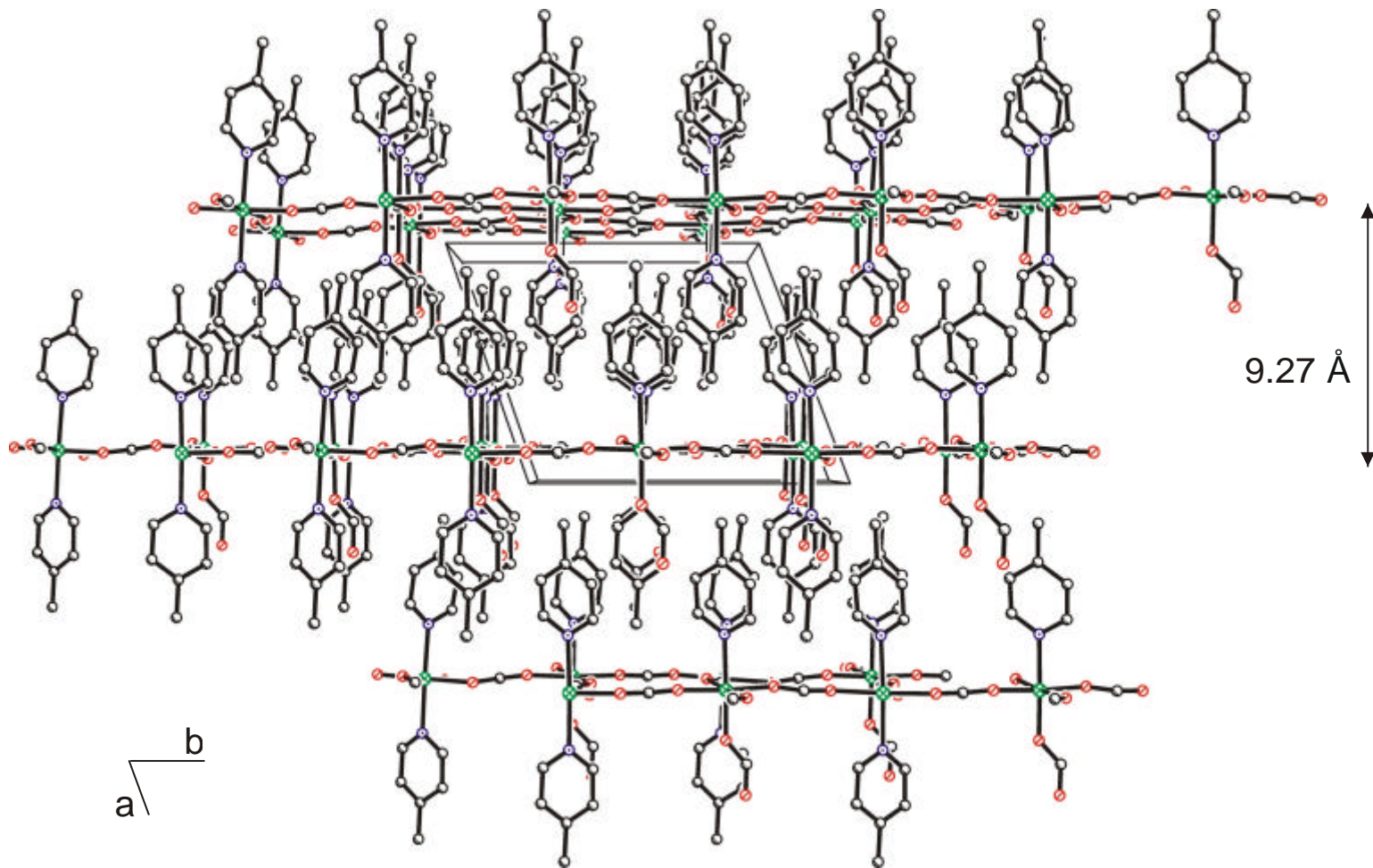


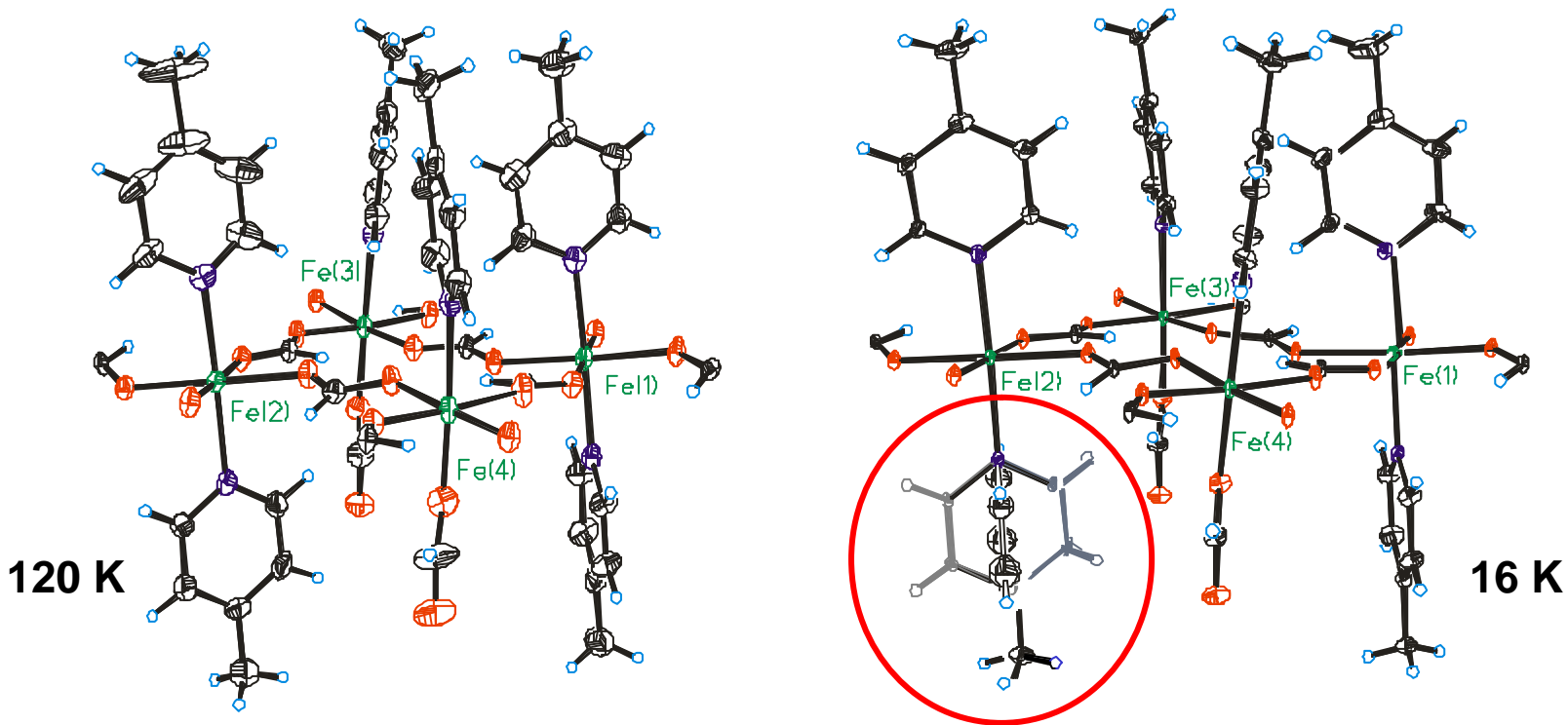


$g_{\text{Fe(III)}} 2.0$   
 $g_{\text{Fe(II)}} 2.04$   
 $J_{\text{Fe(III)-Fe(II)}} -2.76 \text{ cm}^{-1}$





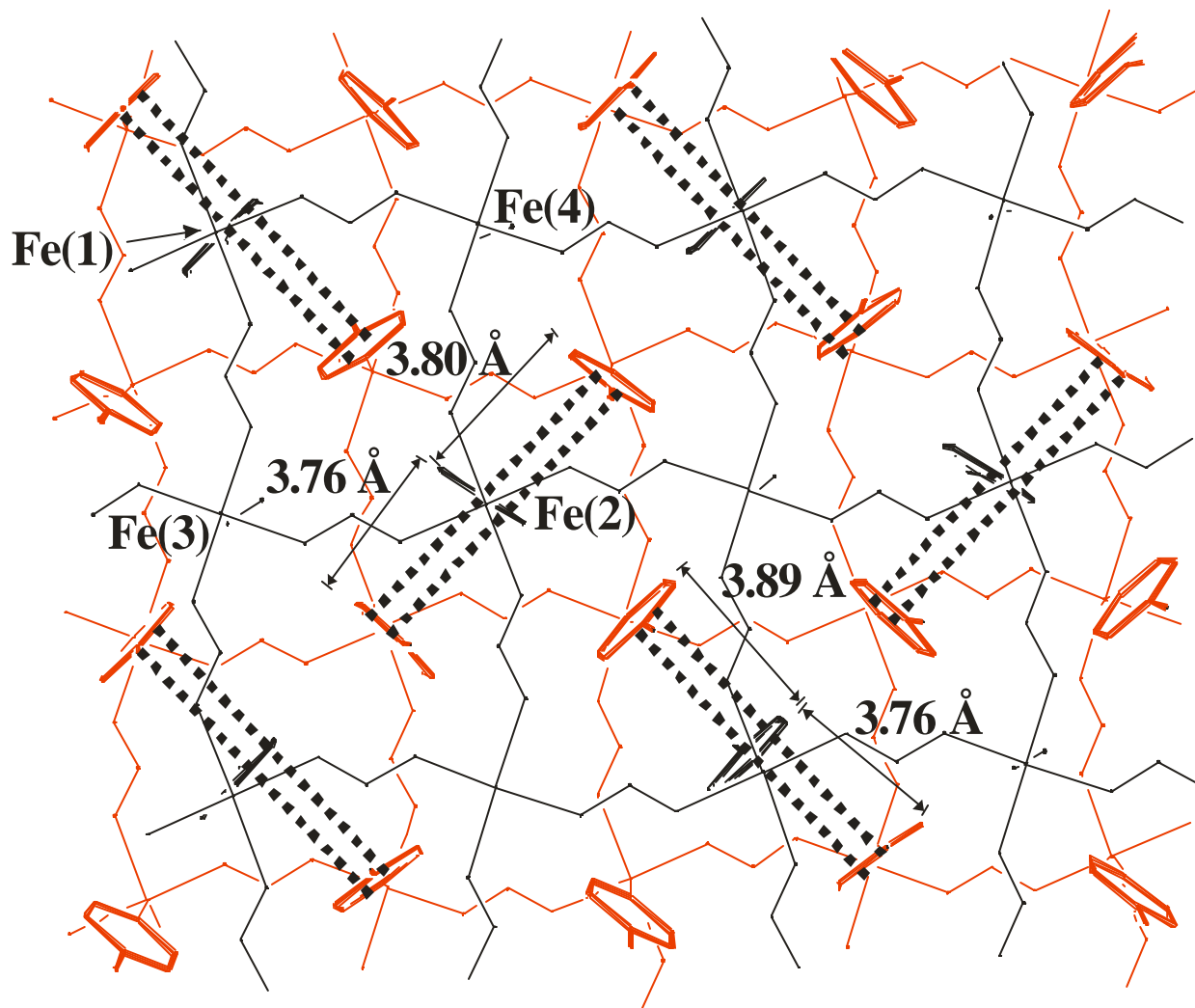




Temperature, K	297(1)	120(1)	16(5)
a, Å	10.3906(5)	10.245(1)	10.0920(6)
b, Å	12.1171(5)	12.090(1)	12.0948(7)
c, Å	12.1148(5)	12.090(1)	12.1096(7)

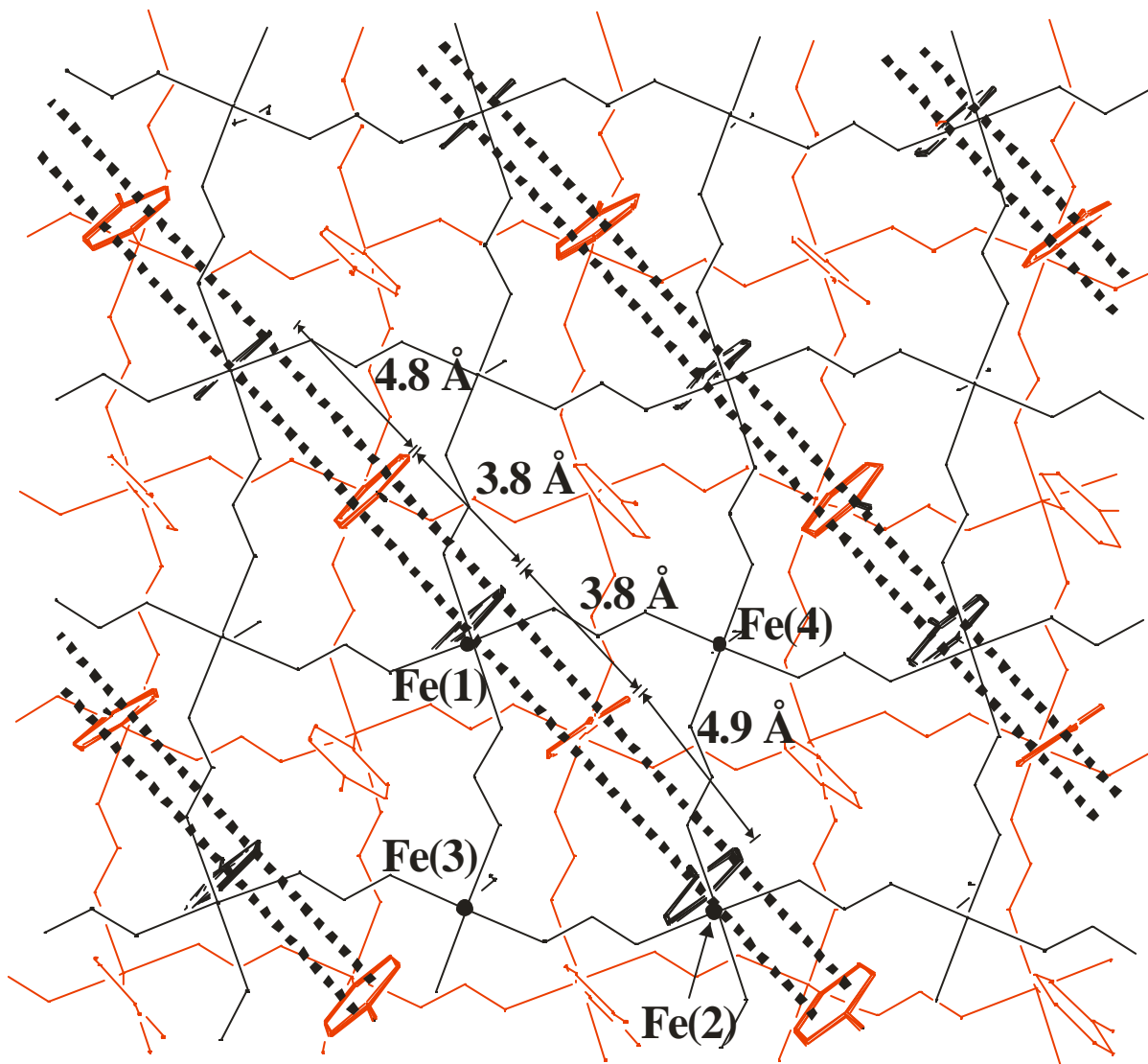
a  
c

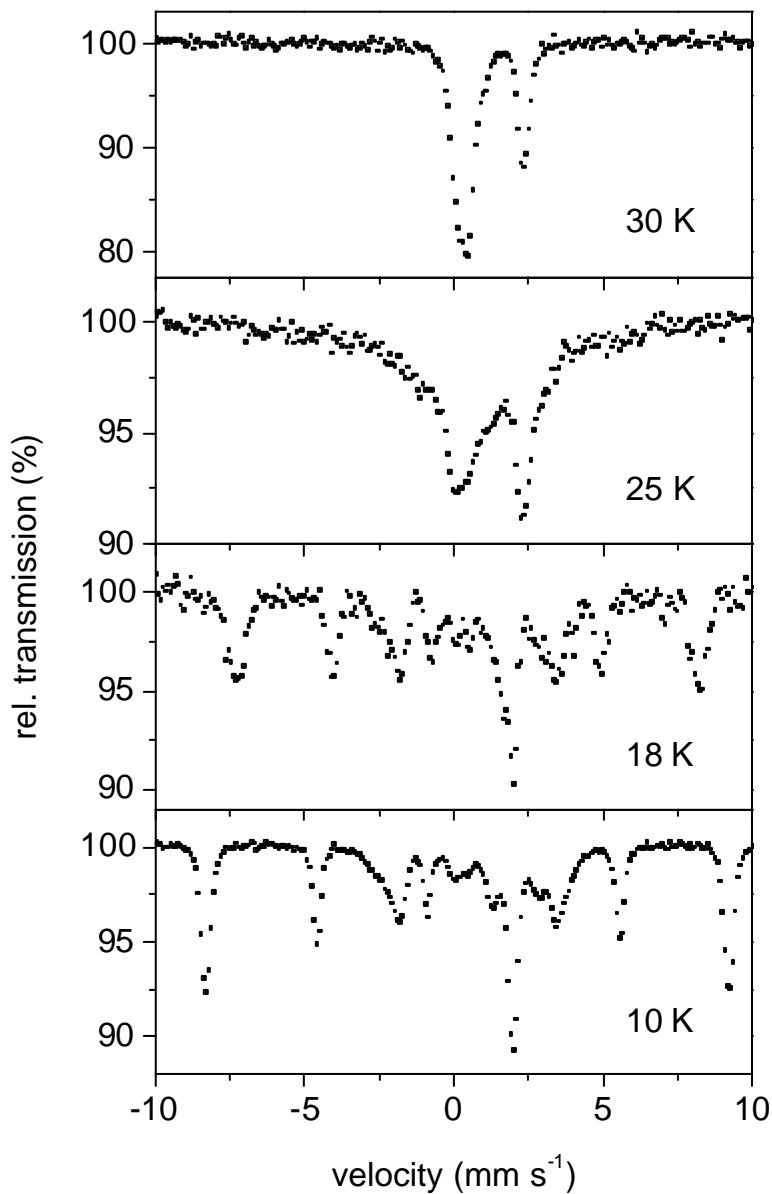
# HT phase





# LT phase

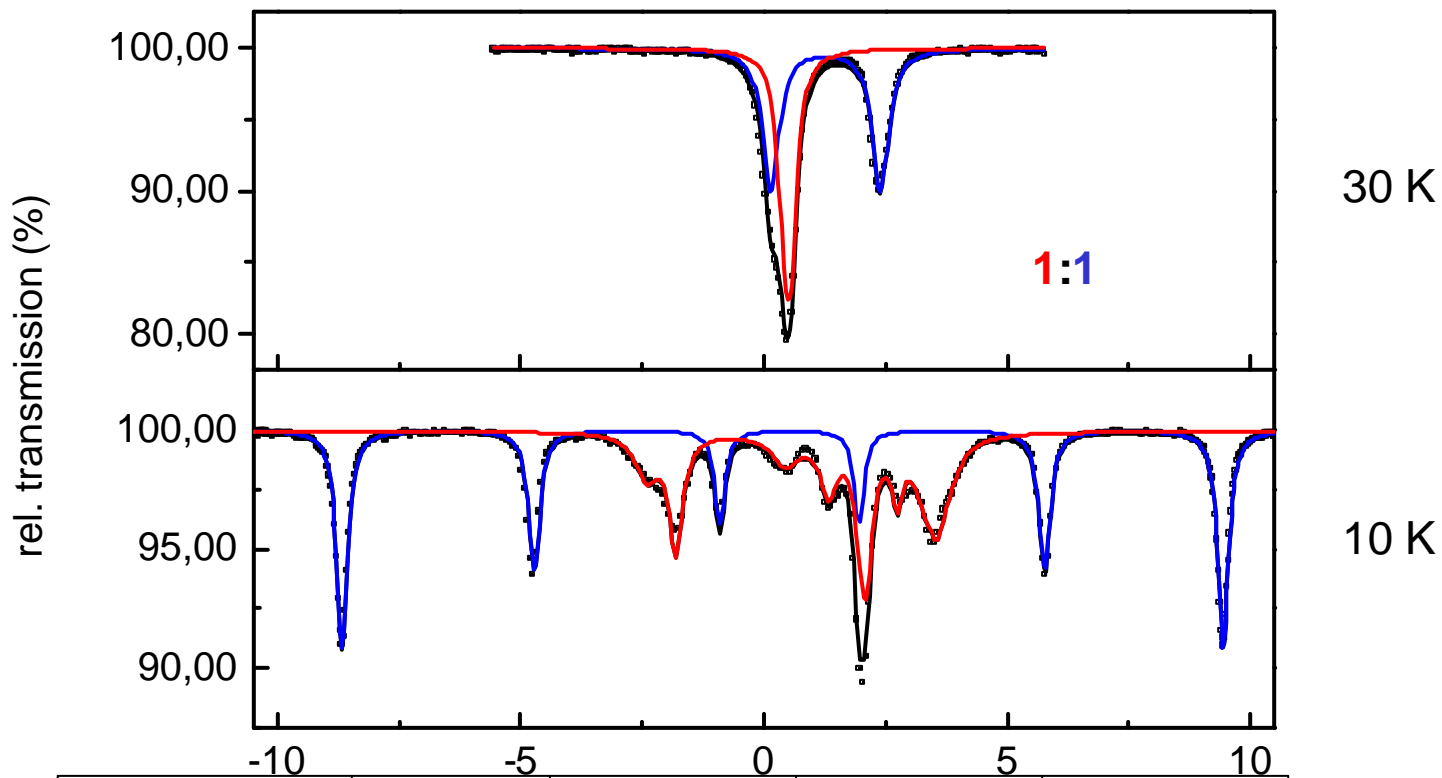




How does the iron centers feel like in

[Fe<sub>2</sub>(HCOO)<sub>5</sub>(g-pic)<sub>3</sub>]<sub>2</sub> ?

What about their valence state?



	<b>Fe(III) <sup>30K</sup></b>	<b>Fe(II) <sup>30K</sup></b>	<b>Fe(III) <sup>10K</sup></b>	<b>Fe(II) <sup>10K</sup></b>
$\delta / \text{mm s}^{-1}$	<b>0.498</b>	<b>1.241</b>	<b>0.499</b>	<b>1.269</b>
$\Delta E_Q / \text{mm s}^{-1}$	<b>0.154</b>	<b>2.238</b>	<b>0.151</b>	<b>-2.248 [a]</b>
$A_{xx} / \text{kG}$				<b>14.6</b>
$A_{yy} / \text{kG}$				<b>0</b>
$A_{zz} / \text{kG}$				<b>124.6</b>
$A / \text{kG}$			<b>545</b>	<b>125</b>

[a]  $V_{zz}$  negative  
 $\epsilon = 0.49$

