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Retraction: Detailed Mössbauer Characterization of Fe^{2+}Fur, the Active Form of the Ferric Uptake Regulation Protein from *E. coli* and Density Functional Calculations on Some Related Models

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The article "Detailed Mössbauer Characterization of Fe^{2+}Fur, the Active Form of the Ferric Uptake Regulation Protein from *E. coli* and Density Functional Calculations on Some Related Models" by Olivier Horner, Jean-Louis Oddou, Claudine Jeandey, Isabelle Michaud-Soret, Jean-Marie Mouesca, published online on June 3, 2009 in Wiley Interscience (www.interscience.wiley.com, 10.1002/ejic.200900091) and in print (*Eur. J. Inorg. Chem.* **2009**, 2959–2966), has been retracted (October 6, 2009) by the journal editor-in-chief, Dr Karen Hindson, and Wiley-VCH, in accordance with the "EUCheMS Ethical Guidelines for Publication in Journals and Reviews" adhered to by the journal (*EUCheMS Ethical Guidelines for Publication in Journals and Reviews*, **2006**, http://www.euchems.org/Publications/index.asp), due to lack of agreement among the authors regarding its publication.

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SUPPORTING INFORMATION

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Table S1. Coordinates in Å for model **4**, used for DFT calculations. The total charge is 0.

Atom	x	y	z
C	28.185	10.190	23.975
C	28.735	9.3600	23.053
N	28.046	9.4430	25.128
C	28.482	8.2140	24.903
N	28.904	8.1340	23.648
H	27.932	11.149	23.846
H	28.974	9.5980	22.112
H	27.675	9.7770	25.994
H	28.492	7.4680	25.569
C	33.221	6.4210	24.617
C	31.741	6.3290	24.231
O	30.895	6.2560	25.129
O	31.472	6.3310	23.073
H	33.779	6.4730	23.789
H	33.480	5.6100	25.142
H	33.371	7.2390	25.171
C	28.549	7.1900	18.973
C	28.441	6.6850	20.404
O	27.313	6.5280	20.912
O	29.503	6.4740	21.023
H	29.513	7.2610	18.716
H	28.118	8.0900	18.903
H	28.087	6.5510	18.358
C	26.504	3.9450	25.016
N	25.661	4.9090	24.548
C	26.426	5.8030	23.951
C	27.780	4.2700	24.693
N	27.716	5.4640	24.009
H	26.225	3.1270	25.519
H	24.665	4.9330	24.639
H	26.082	6.6320	23.510
H	28.604	3.7470	24.909
O	29.942	4.2600	22.633
H	29.746	3.8790	21.730
H	30.398	3.6980	23.324
Fe	29.406	6.2100	23.074

Table S2. Coordinates in Å for model **4bis**, used for DFT calculations. The total charge is 0.

Atom	x	y	z
Fe	0.000	0.000	0.000
C	-4.228	-0.056	-0.512
C	-3.107	0.708	-0.466
N	-3.837	-1.332	-0.159
C	-2.534	-1.336	0.075
N	-2.064	-0.109	-0.107
H	-5.152	0.246	-0.752
H	-3.052	1.687	-0.659
H	-4.440	-2.126	-0.091
H	-1.994	-2.133	0.346
C	0.073	0.304	4.109
C	0.000	0.000	2.609
O	-0.308	-1.141	2.246
O	0.247	0.885	1.854
H	0.333	1.259	4.244
H	0.756	-0.289	4.536
H	-0.820	0.140	4.526
C	-0.0340	3.472	-2.541
C	0.061	2.043	-2.027
O	-0.116	1.097	-2.818
O	0.290	1.883	-0.811
H	0.133	4.110	-1.790
H	-0.947	3.631	-2.917
H	0.649	3.615	-3.257
C	1.149	-3.552	-1.840
N	0.205	-3.200	-2.757
C	-0.358	-2.100	-2.297
C	1.147	-2.652	-0.826
N	0.174	-1.725	-1.132
H	1.750	-4.349	-1.904
H	-0.016	-3.680	-3.608
H	-1.095	-1.609	-2.762
H	1.733	-2.659	-0.016
O	2.061	0.002	0.195
H	2.619	0.581	-0.398
H	2.498	-0.577	0.884

Table S3. Eigenvalues and eigenvectors of the computed [g], [D] and [A_{orb}] tensors for models **1**, **2**, **3**, **4** and **4bis**.

	Model 1 (xy)			**Model 1 (yz)**		
	Eigenvalues			Eigenvalues		
[g]	2.198	2.168	2.054	2.289	2.223	2.028
[D] (cm^{-1})	-2.91	-1.43	4.34	-5.50	-2.19	7.69
[A_{orb}] (MHz)	5.05	2.48	-7.52	9.54	3.80	-13.34
	Eigenvectors			Eigenvectors		
x	0.617	0.765	-0.183	0.677	0.449	0.583
y	-0.521	0.572	0.633	-0.729	0.306	0.612
z	0.590	-0.296	0.752	-0.097	0.840	-0.534

	Model 2			**Model 3**		
	Eigenvalues			Eigenvalues		
[g]	2.238	2.124	2.040	2.169	2.116	2.011
[D] (cm^{-1})	-5.25	0.49	4.76	-3.56	-0.86	4.41
[A_{orb}] (MHz)	9.10	-0.86	-8.25	6.17	1.49	-7.65
	Eigenvectors			Eigenvectors		
x	0.714	-0.359	0.602	-0.391	0.763	0.514
y	-0.520	0.304	0.798	-0.066	-0.580	0.812
z	0.469	0.882	-0.031	0.918	0.284	0.277

	Model 4			**Model 4bis**		
	Eigenvalues			Eigenvalues		
[g]	2.169	2.061	2.031	2.153	2.065	2.037
[D] (cm^{-1})	4.145	-1.320	-2.824	3.432	-1.002	-2.431
[A_{orb}] (MHz)	7.189	-2.290	-4.900	5.954	-1.738	-4.216
	Eigenvectors			Eigenvectors		
x	0.964	0.145	-0.222	0.971	0.090	-0.2232
y	-0.113	0.982	0.148	-0.065	0.991	0.117
z	0.239	-0.118	0.964	0.231	-0.099	0.968

Table S4. Eigenvalues and eigenvectors of the computed [Q] tensor for models **4** and **4bis** (in mm/s).

		Model 4			**Model 4bis**	
		Eigenvalues			Eigenvalues	
[Q]	3.164	-1.536	-1.628	3.245	-1.440	-1.805
		Eigenvectors			Eigenvectors	
x	0.224	0.794	-0.565	0.199	-0.840	0.504
y	0.860	-0.434	-0.268	0.823	-0.135	-0.551
z	0.458	0.426	0.780	0.531	0.525	0.665

Table S5. Eigenvalues and eigenvectors of the computed [A_{dip}] tensors for models **4** and **4bis** (in MHz).

	Model 4			**Model 4bis**		
	Eigenvalues			Eigenvalues		
[A_{dip}] (MHz)	11.11	-5.07	-6.04	11.32	-4.80	-6.52
	Eigenvectors			Eigenvectors		
x	0.243	0.953	-0.180	0.213	0.906	0.365
y	0.856	-0.298	-0.423	0.820	0.037	-0.571
z	0.457	0.051	0.888	0.531	-0.421	0.736

Table S6. Eigenvectors of the computed [A_{tot}] tensor (sum of [A_{dip}] and [A_{orb}] tensors) for models **1**, **2** , **3**, **4** and **4bis** (in MHz).

	Model 1 (xy)			**Model 1 (yz)**		
	Eigenvalues			Eigenvalues		
[A_{tot}] (MHz)	14.4	-2.8	-11.6	16.6	6.9	-23.5
	Eigenvectors			Eigenvectors		
x	-0.024	0.990	-0.140	0.843	0.224	0.489
y	-0.562	0.102	0.821	-0.515	0.597	0.615
z	0.827	0.099	0.554	0.154	0.771	-0.619

	Model 2			**Model 3**		
	Eigenvalues			Eigenvalues		
[A_{tot}] (MHz)	19.2	-6.1	-13.1	9.2	7.9	-17.1
	Eigenvectors			Eigenvectors		
x	0.665	-0.297	0.685	0.901	0.141	0.410
y	-0.614	0.306	0.728	-0.303	-0.470	0.829
z	0.426	0.905	-0.021	-0.310	0.871	0.381

	Model 4			**Model 4bis**		
	Eigenvalues			Eigenvalues		
[A_{tot}] (MHz)	-10.3	9.5	0.8	10.0	-0.6	-9.4
	Eigenvectors			Eigenvectors		
x	-0.277	0.516	0.810	0.433	0.883	-0.184
y	-0.329	0.741	-0.585	0.761	-0.467	-0.450
z	0.903	0.429	0.035	0.483	-0.055	0.874

Table S7. Mononuclear iron complexes (column 1) used for establishing the linear correlation between calculated theoretical electron densities at the iron nucleus (column 3) and experimentally measured isomer shifts (column 4).

Compound	ref.	$\rho(o)$ (au^{-3})	$\delta_{/Fe}$ (mm/s)	ref.
$[Fe(H_2O)_6]^{2+}$	ICSD - 68452	24.037	1.39	[35]
$[L^8py_2Fe(O_2CCH_3)]^+$	[33]	24.833	1.06	[7][a]
$[FeCl_4]^{2-}$	[15][a]	24.645	1.01	[36]
$[L^8py_2Fe(SC_6H_4\text{-}m\text{-}CH_3)]^+$	[33]	24.946	0.93	[7][a]
$[L^8py_2Fe(SC_6H_{11})]^+$	[33]	24.976	0.93	[7][a]
$[Fe(SR)_4]^{2-}$	PDB – 1FHM	25.215	0.70	[37]
$[Fe(pyS_4)(NO)]$	CCDC-149006	26.427	0.33	[34]
trans-$[(cyclam)Fe(NO)Cl]^+$	[34]	26.294	0.27	[38], [39]
$[Fe(CN)_6]^{4-}$	ICSD - 23767	27.158	0.04	[7][a]

[a] These references are in the article.

References:

[33] J. A. Halfen, H. L. Moore, D. C. Fox, *Inorg. Chem.* **2002**, *41*, 3935–3943.

[34] C. Hauser, T. Glaser, E. Bill, T. Weyhermüller, K. Wieghardt, *J. Am. Chem. Soc.* **2000**, *122*, 4352–4365.

[35] R. W. Grant, H. Wiedersich, A. H. Muir Jr., U. Gonser, W. N. Delgass, *J. Chem. Phys.* **1966**, *45*, 1015–1019.

[36] P. R. Edwards, C. E. Johnson, R. J. P. Williams, *Chem. Phys.* **1967**, *47*, 2074–2082.

[37] C. Schultz, P. G. Debrunner, *J. de Physique C6* **1976**, *37*, C6153–C6158.

[38] M. Li, D. Bonnet, E. Bill, F. Neese, T. Weyhermüller, N. Blum, D. Sellmann, K. Wieghardt, *Inorg. Chem.* **2002**, *41*, 3444–3456.

[39] D. Sellmann, N. Blum, F. W. Heinemann, B. A. Hes, *Chem. Eur. J.* **2001**, *7*, 1874–1880.