

Supporting Material for

Vibrational properties of the polymeric spin crossover (SCO) Fe(II) complex [{Fe(4-amino-1,2,4-triazole)₃}X₂]_n: A nuclear inelastic scattering (NIS), Raman and DFT study.

Sergej Rackwitz, Kai Muffler, Klaus Achterhold, Rudolf Rüffer, Yann Garcia, Rolf Diller, Volker Schünemann and Juliusz A. Wolny

Sup. Mat. Table 1 Fe-Fe distances [Å] of the pentameric low-spin (LS) model (HLLH, spin multiplicity 9) and the corresponding high-spin (HS) model (HHHH, spin multiplicity 21) for [Fe₅(atr_z)₁₂(H₂O)₆]⁺¹⁰, [Fe₅(atr_z)₁₂(H₂O)₆](H₂O)₆⁺¹⁰ and [Fe₅(atr_z)₁₂(H₂O)₆]Cl₁₀ calculated by means of B3LYP/CEP-31G and TPSSh/TZVP. The last two columns contain the experimental data of [Fe(Htr_z)₂(tr_z)]BF₄.^{30,31,32}

[Å]	LS ^a	HS ^b	LS ^a	HS ^b	LS ^b	HS ^b	LS	HS	
	[Fe ₅ (atr _z) ₁₂ (H ₂ O) ₆] ⁺¹⁰		• 6 H ₂ O		• 10 Cl ⁻		[Fe(Htr _z) ₂ (tr _z)]BF ₄ ^c		
B3LYP	Fe ₁ -Fe ₂	4.022	4.078	3.991	4.125	3.766	3.810	-	-
CEP-31G	Fe ₂ -Fe ₃	3.982	4.355	3.936	4.240	3.688	3.900	-	-
TPSSh	Fe ₁ -Fe ₂	-	-	3.978	4.093	3.680	3.741	-	-
TZVP	Fe ₂ -Fe ₃	-	-	3.912	4.261	3.622	3.872	-	-
XRPD ³⁰	Fe-Fe	-	-	-	-	-	-	3.671	3.891
EXAFS ³¹	Fe-Fe	-	-	-	-	-	-	3.65	3.87
WAXS ³²	Fe-Fe	-	-	-	-	-	-	3.63	3.83

^a S₆ symmetry ^b C_i symmetry ^c Htr_z=1,2,4-4-H-triazole, tr_z=1,2,4-triazolate

Sup. Mat. Table 2 Fe-ligand distances [Å] of the pentameric low-spin (LS) model (HLLH, spin multiplicity 9) and the corresponding high-spin (HS) model (HHHH, spin multiplicity 21) for [Fe₅(atr_z)₁₂(H₂O)₆]⁺¹⁰, [{Fe₅(atr_z)₁₂(H₂O)₆](H₂O)₆]⁺¹⁰ and [Fe₅(atr_z)₁₂(H₂O)₆](Cl)₁₀. The distances were calculated by means of the metahybrid functional **TPSSh** and the triple zeta valence basis set **TZVP**.

	[Å]	LS ^a	HS ^b	LS ^b	HS ^b
	{[Fe ₅ (atr _z) ₁₂ (H ₂ O) ₆](H ₂ O) ₆] ⁺¹⁰			• 10 Cl ⁻	
1, 5	Fe-O	2.206	2.245	2.156	2.190
			2.219	2.141	2.152
	Fe-N	2.194	2.193	2.188	2.139
			2.227	2.161	2.184
			2.220	2.133	2.173
		2.203	2.143	2.157	
2, 4	Fe-N _{1,2}	2.080	2.304	1.975	2.178
			2.305	1.995	2.192
	Fe-N _{2,3}	2.042	2.308	1.987	2.175
			2.293	1.973	2.209
			2.301	1.976	2.189
		2.311	1.983	2.251	
3	Fe-N	2.049	2.299	1.973	2.192
			2.230	1.978	2.214
			2.230	1.972	2.190

^a S₆ symmetry ^b C_i symmetry

Sup. Mat. Table 3 Fe-ligand and Fe-Fe distances [Å] of the hexameric low-spin (LS) model (HLLLLH, spin multiplicity 9) and the corresponding high-spin (HS) model (HHHHHH, spin multiplicity 25) for [Fe₆(atrz)₁₅(H₂O)₆]Cl₁₂ calculated by means of B3LYP/CEP-31G.

	[Å]	LS	HS
[Fe ₆ (atrz) ₁₅ (H ₂ O) ₆]Cl ₁₂			
1	Fe ₁ -O	2.138	2.143
	Fe ₁ -N _{1,2}	2.165	2.179
	Fe ₁ -Fe ₂	3.749	3.776
2	Fe ₂ -N _{1,2}	1.992	2.158
	Fe ₂ -N _{2,3}	1.981	2.176
	Fe ₂ -Fe ₃	3.680	3.863
3	Fe ₃ -N _{2,3}	2.006	2.212
	Fe ₃ -N _{3,4}	1.995	2.171
	Fe ₃ -Fe ₄	3.695	3.877
4	Fe ₄ -N _{3,4}	1.995	2.241
	Fe ₄ -N _{4,5}	2.006	2.194
	Fe ₄ -Fe ₅	3.680	3.847
5	Fe ₅ -N _{4,5}	1.981	2.174
	Fe ₅ -N _{5,6}	1.992	2.146
	Fe ₅ -Fe ₆	3.749	3.782
6	Fe ₆ -O	2.138	2.147
	Fe ₆ -N _{5,6}	2.165	2.177

Sup. Mat. Table 4 Calculated frequencies **1-80** of the low-spin [Fe₅(atrz)₁₂(H₂O)₆]Cl₁₀ model system. E is the energy of the normal mode.

mode number	E [cm ⁻¹]	mode number	E [cm ⁻¹]	mode number	E [cm ⁻¹]	mode number	E [cm ⁻¹]
1	14	21	63	41	103	61	138
2	15	22	67	42	104	62	140
3	19	23	67	43	105	63	141
4	23	24	68	44	108	64	142
5	24	25	70	45	109	65	146
6	28	26	72	46	109	66	148
7	33	27	74	47	112	67	151
8	35	28	78	48	115	68	152
9	38	29	81	49	116	69	154
10	39	30	82	50	118	70	155
11	43	31	82	51	118	71	160
12	45	32	84	52	119	72	169
13	48	33	85	53	120	73	170
14	51	34	86	54	122	74	176
15	53	35	91	55	122	75	178
16	55	36	91	56	125	76	182
17	56	37	93	57	126	77	184
18	58	38	98	58	128	78	188
19	58	39	99	59	134	79	193
20	63	40	100	60	135	80	193

Sup. Mat. Table 5 Calculated frequencies **81-171** of the low-spin [Fe₅(atrz)₁₂(H₂O)₆]Cl₁₀ model system. E is the energy of the normal mode, Au or Ag defines whether it is an ungerade or gerade vibration. Fe central, neighbour or terminal defines a relative displacement vector for the iron ion (1-5) movement. **p** denotes a displacement “perpendicular” to the iron axis and **i** means “in iron axis” direction. The last column contains the information if there is a movie available in the supplementary materials.

mode number	E [cm ⁻¹]	symmetry	Fe 3 central	Fe 2 and 4 neighbour	Fe 1 and 5 terminal	movie
81	195	Ag	-	-	p	*
82	197					
83	203	Ag	-	-	-	*
84	207					
85	208					
86	212					
87	213					
88	214					
89	215					
90	216					
91	217					
92	217					
93	217					
94	218					
95	219					
96	223					
97	223					
98	225					

mode number	E [cm ⁻¹]	symmetry	Fe 3 central	Fe 2 and 4 neighbour	Fe 1 and 5 terminal	movie
99	225					
100	230					
101	231					
102	238	Ag	-	-	i	*
103	239					
104	243					
105	244					
106	245					
107	249					
108	250					
109	253					
110	254	Ag	-	i	-	*
111	264					
112	266					
113	268					
114	272					
115	272					
116	278					
117	279					
118	284					
119	287					
120	287					
121	291					
122	291					
123	298					
124	299					
125	299					
126	300					
127	305					
128	307					
129	311	Au	p	-p	-	*
130	311					
131	313					
132	314					
133	323					
134	323					
135	326	Au	p	-p	-	*
136	328					
137	328					
138	340					
139	341					
140	342					
141	344					
142	344	Au	p	-p	-	*
143	346					
144	347					
145	358					
146	359					
147	363					
148	365					
149	370	Au	p	-p	-p	*
150	373					
151	373					
152	374					
153	380	Au	i	-i	-	*
154	387	Ag	-	i/-i	-	*
155	389	Au	p/i	p/i	-	*
156	391	Ag	-	p/-p	p/-p	*
157	403	Ag	-	p/-p	p/-p	*
158	417	Au	p	p	p	*
159	419					
160	426	Ag	-	p/-p	-p/p	*
161	431	Ag	-	p/-p	-p/p	*
162	443					
163	444	Au	p	p	-	*
164	445					
165	449	Au	p/i	p/-i	-	*
166	457					
167	459					
168	467	Au	p	-p	-	*
169	473					
170	481					
171	498	Au	i	i	-	*

Sup. Mat. Table 6 Calculated frequencies **172-453** of the low-spin $[[\text{Fe}_5(\text{atrz})_{12}(\text{H}_2\text{O})_6]\text{Cl}_{10}]$ model system. E is the energy of the normal mode.

mode number	E [cm^{-1}]	mode number	E [cm^{-1}]	mode number	E [cm^{-1}]	mode number	E [cm^{-1}]
172	618	243	916	314	1242	385	1674
173	618	244	936	315	1242	386	1696
174	627	245	937	316	1245	387	1697
175	628	246	943	317	1245	388	1701
176	630	247	943	318	1254	389	1701
177	630	248	945	319	1255	390	1709
178	635	249	946	320	1268	391	1709
179	642	250	956	321	1268	392	1711
180	645	251	956	322	1276	393	1711
181	646	252	961	323	1276	394	2810
182	647	253	961	324	1292	395	2811
183	649	254	989	325	1292	396	2932
184	655	255	989	326	1303	397	2933
185	659	256	998	327	1303	398	2964
186	660	257	998	328	1339	399	2964
187	661	258	1002	329	1339	400	3130
188	663	259	1003	330	1352	401	3131
189	664	260	1006	331	1352	402	3153
190	664	261	1006	332	1368	403	3154
191	667	262	1007	333	1369	404	3164
192	667	263	1008	334	1373	405	3164
193	667	264	1008	335	1373	406	3199
194	669	265	1009	336	1373	407	3199
195	669	266	1010	337	1374	408	3225
196	673	267	1011	338	1379	409	3225
197	674	268	1012	339	1379	410	3237
198	675	269	1014	340	1392	411	3237
199	677	270	1019	341	1392	412	3249
200	680	271	1019	342	1397	413	3249
201	683	272	1021	343	1397	414	3344
202	684	273	1021	344	1404	415	3344
203	685	274	1022	345	1404	416	3346
204	686	275	1029	346	1410	417	3346
205	688	276	1031	347	1410	418	3348
206	691	277	1031	348	1411	419	3348
207	691	278	1039	349	1411	420	3351
208	695	279	1039	350	1415	421	3351
209	696	280	1082	351	1416	422	3352
210	697	281	1083	352	1464	423	3352
211	699	282	1087	353	1465	424	3353
212	721	283	1088	354	1468	425	3353
213	722	284	1088	355	1468	426	3401
214	756	285	1089	356	1468	427	3401
215	756	286	1090	357	1469	428	3423
216	816	287	1091	358	1469	429	3423
217	816	288	1094	359	1470	430	3429
218	844	289	1095	360	1474	431	3429
219	845	290	1095	361	1474	432	3438
220	850	291	1096	362	1490	433	3438
221	850	292	1204	363	1491	434	3474
222	856	293	1206	364	1532	435	3474
223	856	294	1207	365	1532	436	3569
224	858	295	1208	366	1535	437	3569
225	858	296	1208	367	1536	438	3591
226	863	297	1210	368	1536	439	3591
227	863	298	1210	369	1537	440	3599
228	866	299	1211	370	1539	441	3599
229	866	300	1214	371	1540	442	3614
230	869	301	1214	372	1542	443	3614
231	870	302	1221	373	1542	444	3626
232	887	303	1221	374	1543	445	3626
233	887	304	1222	375	1543	446	3664
234	896	305	1223	376	1633	447	3664
235	896	306	1226	377	1633	448	3811
236	907	307	1227	378	1643	449	3811
237	907	308	1229	379	1643	450	3814
238	910	309	1231	380	1648	451	3814
239	910	310	1234	381	1649	452	3815
240	913	311	1235	382	1667	453	3815
241	913	312	1240	383	1667		
242	916	313	1241	384	1674		

Sup. Mat. Table 7 Calculated frequencies **1-68** of the high-spin [Fe₅(atrz)₁₂(H₂O)₆]Cl₁₀ model system. E is the energy of the normal mode.

mode number	E [cm ⁻¹]	mode number	E [cm ⁻¹]	mode number	E [cm ⁻¹]	mode number	E [cm ⁻¹]
1	-6	18	48	35	85	52	110
2	9	19	52	36	86	53	110
3	14	20	54	37	87	54	114
4	17	21	55	38	88	55	115
5	18	22	59	39	89	56	117
6	20	23	61	40	89	57	119
7	21	24	64	41	91	58	120
8	23	25	68	42	94	59	121
9	30	26	71	43	96	60	121
10	31	27	71	44	98	61	122
11	36	28	75	45	100	62	123
12	36	29	75	46	100	63	123
13	38	30	78	47	103	64	127
14	43	31	78	48	103	65	128
15	43	32	79	49	104	66	129
16	45	33	80	50	105	67	129
17	48	34	82	51	108	68	131

Sup. Mat. Table 8 Calculated frequencies **69-142** of the high-spin [Fe₅(atrz)₁₂(H₂O)₆]Cl₁₀ model system. E is the energy of the normal mode, Au or Ag defines whether it is an ungerade or gerade vibration. Fe central, neighbour or terminal defines a relative displacement vector for the iron ion (1-5) movement. **p** denotes a displacement “perpendicular” to the iron axis and **i** means “in iron axis” direction. The last column contains the information if there is a movie available in the supplementary materials.

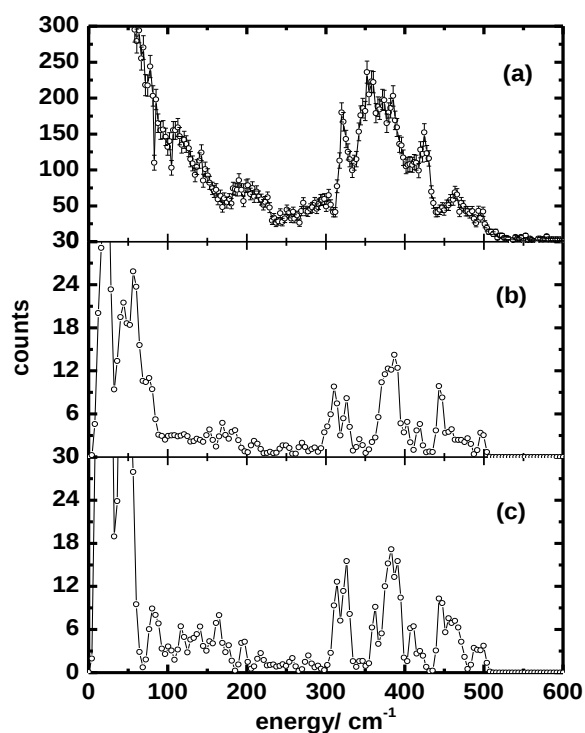
mode number	E [cm ⁻¹]	symmetry	Fe 3 central	Fe 2 and 4 neighbour	Fe 1 and 5 terminal	movie
69	132	Au	p/i	i	-	*
70	135					
71	137	Ag	-	p/-p	-p/p	*
72	140	Au	p/i	-	-p/-i	*
73	142	Ag	-	p/i//p/-i	-p/i//p/-i	*
74	144					
75	149	Ag	-	p/i//p/-i	-p/-i//p/i	*
76	150					
77	151	Au	p/i	-p/-i	p/-i	*
78	153					
79	153					
80	155					
81	156					
82	157					
83	158					
84	160					
85	162					
86	165					
87	166					
88	168					
89	170					
90	171	Ag	-	p/i	p/i	*
91	172					
92	178					
93	179					
94	191					
95	192	Au	p	-p	p	*
96	193					
97	195					
98	198	Au	p	-p	p	*
99	198					
100	205	Au	p/i	-p	p/-i	*
101	207	Au	p/i	-p/-i	p/-i	*
102	208					
103	213					
104	215	Au	p/i	-p/-i	-p/i	*
105	218					
106	221	Au	p/i	-p/-i	i	*
107	222	Au	p/i	-	-p/i	*
108	225					
109	227	Au	p	-p	-p/i	*
110	231	Au	p/i	-p/-i	p/i	*
111	233	Au	p	-p	-p	*
112	233					
113	238					
114	238	Au	p/i	-p/-i	-	*
115	240					

mode number	E [cm ⁻¹]	symmetry	Fe 3 central	Fe 2 and 4 neighbour	Fe 1 and 5 terminal	movie
116	242	Au	p/i	p/-i	-p/i	*
117	249	Au	p/i	-p	-p	*
118	249					
119	250					
120	254					
121	255	Au	p/i	-p/-i	-	*
122	261					
123	265	Au	p/i	p/i	-	*
124	266	Au	p	p/i	p/i	*
125	267					
126	267	Au	p/i	p	p/-i	*
127	267					
128	272	Au	p	p/i	-	*
129	272					
130	286					
131	287					
132	289					
133	289					
134	291					
135	294					
136	298					
137	299					
138	300					
139	303					
140	303					
141	306					
142	307	Au	p	p	-	*

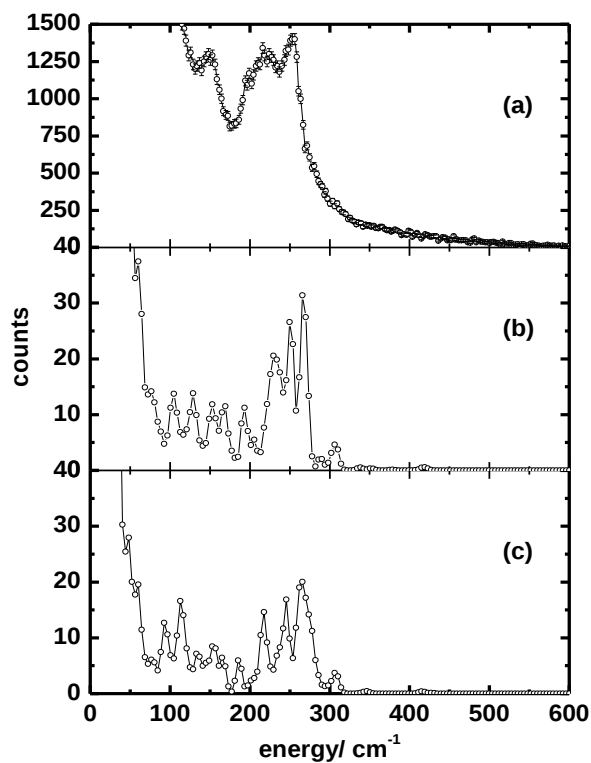
Sup. Mat. Table 9 Calculated frequencies **143-453** of the high-spin [Fe₅(atrz)₁₂(H₂O)₆]Cl₁₀ model system. E is the energy of the normal mode.

mode number	E [cm ⁻¹]	mode number	E [cm ⁻¹]	mode number	E [cm ⁻¹]	mode number	E [cm ⁻¹]
143	309	184	647	225	864	266	992
144	309	185	649	226	866	267	995
145	310	186	651	227	866	268	996
146	322	187	651	228	874	269	996
147	322	188	652	229	874	270	999
148	338	189	652	230	883	271	1000
149	338	190	657	231	883	272	1000
150	344	191	658	232	887	273	1001
151	345	192	662	233	887	274	1003
152	353	193	662	234	890	275	1004
153	353	194	663	235	890	276	1007
154	370	195	663	236	903	277	1007
155	371	196	667	237	903	278	1035
156	378	197	667	238	909	279	1035
157	378	198	671	239	909	280	1077
158	385	199	673	240	915	281	1077
159	385	200	675	241	915	282	1078
160	409	201	675	242	929	283	1079
161	411	202	679	243	929	284	1079
162	412	203	679	244	942	285	1079
163	415	204	683	245	942	286	1082
164	415	205	683	246	945	287	1082
165	416	206	686	247	945	288	1083
166	416	207	686	248	955	289	1084
167	420	208	688	249	956	290	1091
168	420	209	688	250	968	291	1091
169	420	210	690	251	968	292	1194
170	423	211	690	252	972	293	1196
171	423	212	719	253	973	294	1200
172	626	213	719	254	980	295	1201
173	626	214	787	255	980	296	1201
174	627	215	787	256	982	297	1202
175	627	216	840	257	982	298	1202
176	629	217	840	258	984	299	1203
177	630	218	848	259	986	300	1208
178	635	219	848	260	986	301	1208
179	636	220	854	261	987	302	1211
180	637	221	854	262	987	303	1211
181	638	222	858	263	990	304	1213
182	641	223	858	264	991	305	1214
183	642	224	864	265	991	306	1217

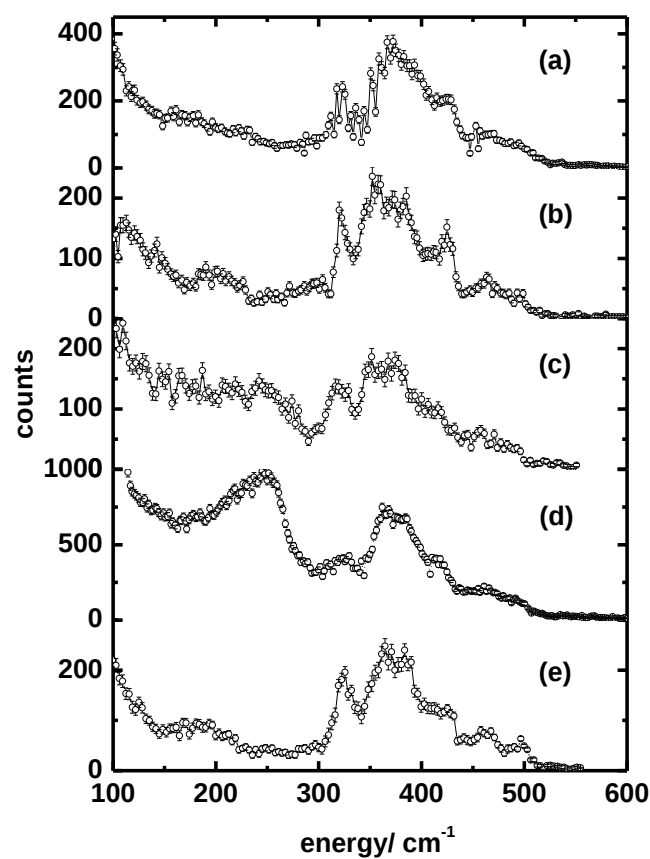
mode number	E [cm ⁻¹]	mode number	E [cm ⁻¹]	mode number	E [cm ⁻¹]	mode number	E [cm ⁻¹]
307	1217	344	1386	381	1659	418	3340
308	1220	345	1386	382	1676	419	3340
309	1220	346	1388	383	1676	420	3348
310	1227	347	1388	384	1681	421	3348
311	1227	348	1392	385	1681	422	3348
312	1234	349	1393	386	1681	423	3348
313	1234	350	1401	387	1681	424	3361
314	1234	351	1401	388	1697	425	3361
315	1235	352	1449	389	1697	426	3376
316	1236	353	1449	390	1710	427	3376
317	1236	354	1449	391	1710	428	3399
318	1244	355	1449	392	1719	429	3400
319	1244	356	1457	393	1719	430	3412
320	1263	357	1458	394	2832	431	3412
321	1263	358	1458	395	2833	432	3438
322	1270	359	1458	396	2866	433	3438
323	1270	360	1463	397	2867	434	3475
324	1284	361	1463	398	3025	435	3475
325	1284	362	1467	399	3025	436	3560
326	1311	363	1467	400	3126	437	3560
327	1311	364	1529	401	3126	438	3564
328	1342	365	1529	402	3153	439	3564
329	1342	366	1529	403	3154	440	3608
330	1358	367	1530	404	3162	441	3608
331	1359	368	1533	405	3163	442	3618
332	1365	369	1534	406	3164	443	3618
333	1365	370	1535	407	3165	444	3623
334	1369	371	1535	408	3171	445	3623
335	1369	372	1536	409	3171	446	3633
336	1371	373	1536	410	3255	447	3633
337	1371	374	1541	411	3255	448	3806
338	1378	375	1541	412	3314	449	3806
339	1378	376	1632	413	3315	450	3806
340	1380	377	1632	414	3328	451	3806
341	1380	378	1651	415	3328	452	3814
342	1383	379	1651	416	3338	453	3814
343	1383	380	1659	417	3338		



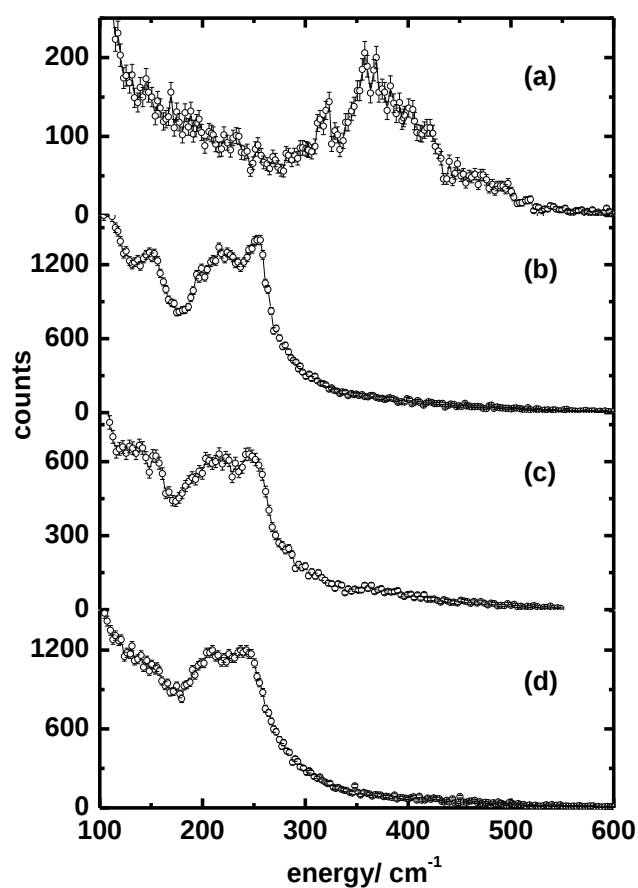
Sup. Mat. Fig. 1 Experimental NIS data of sample 2 at ca. 100 K (a) in comparison with the simulated low- spin (LS; S = 9) NIS data of the pentameric complex $[\text{Fe}_5(\text{atrz})_{12}(\text{H}_2\text{O})_6]\text{Cl}_{10}$ (b) and the simulated low- spin (LS; S = 9) NIS data of the hexameric complex $[\text{Fe}_6(\text{atrz})_{15}(\text{H}_2\text{O})_6]\text{Cl}_{12}$ (c).



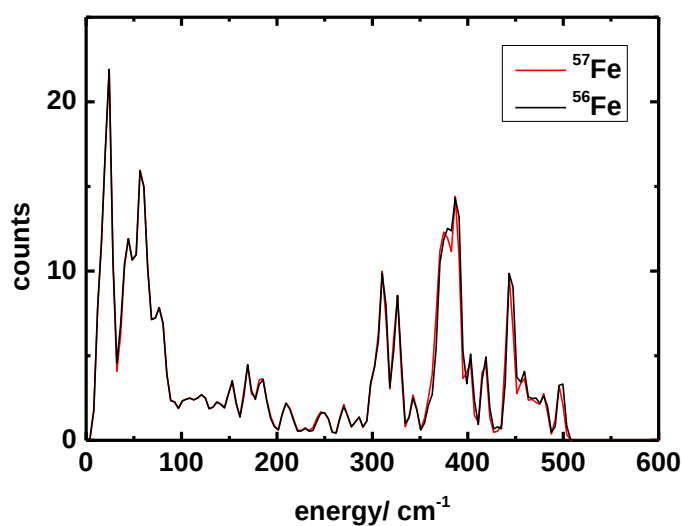
Sup. Mat. Fig. 2 Experimental NIS data of sample 2 at ca. 300 K (a) in comparison with the simulated high- spin (HS; S = 21) NIS data of the pentameric complex $[\text{Fe}_5(\text{atrz})_{12}(\text{H}_2\text{O})_6]\text{Cl}_{10}$ (b) and the simulated high- spin (HS; S = 21) NIS data of the hexameric complex $[\text{Fe}_6(\text{atrz})_{15}(\text{H}_2\text{O})_6]\text{Cl}_{12}$ (c).



Sup. Mat. Fig. 3 NIS spectra recorded at 100 K for $[\text{Fe}(\text{atrz})_3\text{X}_2]$; X = chlorine (a), methanesulfonate (b), 1-naphthalenesulfonate (c), perchlorate (d) and tosylate (e).



Sup. Mat. Fig. 4 NIS spectra recorded at 300 K for $[\text{Fe}(\text{atrz})_3\text{X}_2]$; X = chlorine (a), methanesulfonate (b), 1-naphthalenesulfonate (c) and perchlorate (d).



Sup. Mat. Fig. 5 Simulated NIS spectra of the pentameric low-spin (LS) model (HLLLH, spin multiplicity 9) with ^{56}Fe as well as ^{57}Fe . The energy differences between the calculated normal modes shift at most 2 cm^{-1} at 380 cm^{-1} and 378 cm^{-1} for ^{56}Fe and ^{57}Fe , respectively.

Geometries:

Sup. Mat. Table 10 Cartesian coordinates of the pentameric low-spin (LS) model (HLLH, spin multiplicity 9).

Fe	0.000000	0.000000	3.982367
Fe	0.000000	0.000000	0.000000
N	0.002803	-1.648753	2.726340
N	0.002600	-1.652598	1.273502
N	0.000000	-3.778735	2.007649
C	0.000993	-2.945208	0.900868
C	0.001034	-2.937151	3.115283
N	-0.001869	-5.183749	1.941388
H	0.000368	-3.332894	-0.109589
H	-0.000177	-3.296602	4.137548
H	0.881657	-5.661996	2.120339
H	-0.886261	-5.659734	2.122242
N	1.426460	0.826804	2.726340
N	1.429892	0.828551	1.273502
N	3.272481	1.889367	2.007649
C	2.550128	1.473464	0.900868
C	2.543130	1.469471	3.115283
N	4.490193	2.590256	1.941388
H	2.886187	1.666766	-0.109589
H	2.855030	1.648148	4.137548
H	4.462604	3.594535	2.120339
H	5.344604	2.062342	2.122242
N	-1.429263	0.821949	2.726340
N	-1.432492	0.824047	1.273502
N	-3.272481	1.889368	2.007649
C	-2.551121	1.471744	0.900868
C	-2.544164	1.467680	3.115283
N	-4.488324	2.593493	1.941388
H	-2.886555	1.666128	-0.109589
H	-2.854853	1.648454	4.137548
H	-5.344261	2.067461	2.120339
H	-4.458343	3.597392	2.122242
Fe	0.000000	0.000000	8.003963
N	-0.009277	1.712391	5.211500
N	0.003480	1.739188	6.657219
N	0.031622	3.852705	5.911855
C	0.030489	3.031731	7.033302
C	0.008362	3.001834	4.818879
N	0.054768	5.268832	5.789047
H	0.058794	3.401568	8.054630
H	0.007167	3.382331	3.805989
H	-0.808475	5.732762	6.089124
H	0.930903	5.704762	6.093591
N	-1.478336	-0.864230	5.211500
N	-1.507921	-0.866580	6.657219
N	-3.352351	-1.898967	5.911855
C	-2.640801	-1.489461	7.033302
C	-2.603846	-1.493675	4.818879
N	-4.590326	-2.586986	5.789047
H	-2.975241	-1.649867	8.054630
H	-2.932768	-1.684959	3.805989
H	-4.560480	-3.566541	6.089124
H	-5.405920	-2.046195	6.093591
N	1.487613	-0.848161	5.211500
N	1.504441	-0.872608	6.657219
N	3.320729	-1.953738	5.911855
C	2.610312	-1.542270	7.033302
C	2.595484	-1.508159	4.818879
N	4.535558	-2.681846	5.789047
H	2.916447	-1.751701	8.054630
H	2.925601	-1.697372	3.805989
H	5.368955	-2.166221	6.089124
H	4.475017	-3.658567	6.093591
Fe	0.000000	0.000000	-3.982367
N	-0.002803	1.648753	-2.726340
N	-0.002600	1.652598	-1.273502
N	0.000000	3.778735	-2.007649
C	-0.000993	2.945208	-0.900868
C	-0.001034	2.937151	-3.115283
N	0.001869	5.183749	-1.941388
H	-0.000368	3.332894	0.109589
H	0.000177	3.296602	-4.137548
H	-0.881657	5.661996	-2.120339

H	0.886261	5.659734	-2.122242
N	-1.426460	-0.826804	-2.726340
N	-1.429892	-0.828551	-1.273502
N	-3.272481	-1.889367	-2.007649
C	-2.550128	-1.473464	-0.900868
C	-2.543130	-1.469471	-3.115283
N	-4.490193	-2.590256	-1.941388
H	-2.886187	-1.666766	0.109589
H	-2.855030	-1.648148	-4.137548
H	-4.462604	-3.594535	-2.120339
H	-5.344604	-2.062342	-2.122242
N	1.429263	-0.821949	-2.726340
N	1.432492	-0.824047	-1.273502
N	3.272481	-1.889368	-2.007649
C	2.551121	-1.471744	-0.900868
C	2.544164	-1.467680	-3.115283
N	4.488324	-2.593493	-1.941388
H	2.886555	-1.666128	0.109589
H	2.854853	-1.648454	-4.137548
H	5.344261	-2.067461	-2.120339
H	4.458343	-3.597392	-2.122242
Fe	0.000000	0.000000	-8.003963
N	0.009277	-1.712391	-5.211500
N	-0.003480	-1.739188	-6.657219
N	-0.031622	-3.852705	-5.911855
C	-0.030489	-3.031731	-7.033302
C	-0.008362	-3.001834	-4.818879
N	-0.054768	-5.268832	-5.789047
H	-0.058794	-3.401568	-8.054630
H	-0.007167	-3.382331	-3.805989
H	0.808475	-5.732762	-6.089124
H	-0.930903	-5.704762	-6.093591
N	1.478336	0.864230	-5.211500
N	1.507921	0.866580	-6.657219
N	3.352351	1.898967	-5.911855
C	2.640801	1.489461	-7.033302
C	2.603846	1.493675	-4.818879
N	4.590326	2.586986	-5.789047
H	2.975241	1.649867	-8.054630
H	2.932768	1.684959	-3.805989
H	4.560480	3.566541	-6.089124
H	5.405920	2.046195	-6.093591
N	-1.487613	0.848161	-5.211500
N	-1.504441	0.872608	-6.657219
N	-3.320729	1.953738	-5.911855
C	-2.610312	1.542270	-7.033302
C	-2.595484	1.508159	-4.818879
N	-4.535558	2.681846	-5.789047
H	-2.916447	1.751701	-8.054630
H	-2.925601	1.697372	-3.805989
H	-5.368955	2.166221	-6.089124
H	-4.475017	3.658567	-6.093591
O	-1.305078	-1.054218	-9.406434
H	-0.950005	-1.356935	-10.275774
H	-2.265403	-1.270590	-9.379368
O	-0.260441	1.657340	-9.406434
H	-0.700138	1.501196	-10.275774
H	0.032338	2.597192	-9.379368
O	1.565519	-0.603122	-9.406434
H	1.650143	-0.144261	-10.275774
H	2.233065	-1.326602	-9.379368
O	1.305078	1.054218	9.406434
H	0.950005	1.356935	10.275774
H	2.265403	1.270590	9.379368
O	0.260441	-1.657340	9.406434
H	0.700138	-1.501196	10.275774
H	-0.032338	-2.597192	9.379368
O	-1.565519	0.603122	9.406434
H	-1.650143	0.144261	10.275774
H	-2.233065	1.326602	9.379368

Sup. Mat. Table 11 Cartesian coordinates of the pentameric low-spin (LS) model (HLLLH, spin multiplicity 9) surrounded by six water molecules.

Fe	0.000000	0.000000	3.936304
Fe	0.000000	0.000000	0.000000
N	-0.002053	-1.649133	2.698051
N	-0.008742	-1.646257	1.256102
N	-0.032065	-3.780440	1.974204
C	-0.007986	-2.940112	0.874682
C	-0.028622	-2.945249	3.082001
N	-0.015062	-5.190415	1.900113
H	0.006131	-3.314619	-0.139688
H	-0.035656	-3.308857	4.101686
H	0.681675	-5.739346	2.489754
H	-0.929698	-5.604708	1.709286
N	1.429218	0.822789	2.698051
N	1.430071	0.815558	1.256102
N	3.289990	1.862451	1.974204
C	2.550205	1.463140	0.874682
C	2.564971	1.447837	3.082001
N	4.502562	2.582163	1.900113
H	2.867479	1.662619	-0.139688
H	2.883382	1.623549	4.101686
H	4.629582	3.460021	2.489754
H	5.318669	1.997212	1.709286
N	-1.427165	0.826344	2.698051
N	-1.421329	0.830699	1.256102
N	-3.257925	1.917989	1.974204
C	-2.542219	1.476972	0.874682
C	-2.536349	1.497412	3.082001
N	-4.487500	2.608252	1.900113
H	-2.873610	1.652000	-0.139688
H	-2.847726	1.685308	4.101686
H	-5.311257	2.279325	2.489754
H	-4.388971	3.607496	1.709286
Fe	0.000000	0.000000	7.926909
N	0.000000	1.707420	5.154966
N	0.005635	1.742479	6.599518
N	0.049338	3.849521	5.840762
C	0.038666	3.036537	6.967512
C	0.026575	2.991495	4.752008
N	0.079119	5.263060	5.716129
H	0.064249	3.413761	7.985782
H	0.033995	3.359884	3.735146
H	-0.780352	5.733968	6.012456
H	0.961198	5.695594	6.003637
N	-1.478669	-0.853710	5.154966
N	-1.511849	-0.866359	6.599518
N	-3.358452	-1.882033	5.840762
C	-2.649051	-1.484783	6.967512
C	-2.603998	-1.472733	4.752008
N	-4.597503	-2.563011	5.716129
H	-2.988528	-1.651239	7.985782
H	-2.926742	-1.650501	3.735146
H	-4.575586	-3.542789	6.012456
H	-5.413128	-2.015375	6.003637
N	1.478669	-0.853710	5.154966
N	1.506214	-0.876120	6.599518
N	3.309114	-1.967488	5.840762
C	2.610385	-1.551754	6.967512
C	2.577423	-1.518762	4.752008
N	4.518384	-2.700049	5.716129
H	2.924279	-1.762522	7.985782
H	2.892747	-1.709383	3.735146
H	5.355938	-2.191179	6.012456
H	4.451930	-3.680219	6.003637
Fe	0.000000	0.000000	-3.936304
N	0.002053	1.649133	-2.698051
N	0.008742	1.646257	-1.256102
N	0.032065	3.780440	-1.974204
C	0.007986	2.940112	-0.874682
C	0.028622	2.945249	-3.082001
N	0.015062	5.190415	-1.900113
H	-0.006131	3.314619	0.139688
H	0.035656	3.308857	-4.101686
H	-0.681675	5.739346	-2.489754
H	0.929698	5.604708	-1.709286

N	-1.429218	-0.822789	-2.698051
N	-1.430071	-0.815558	-1.256102
N	-3.289990	-1.862451	-1.974204
C	-2.550205	-1.463140	-0.874682
C	-2.564971	-1.447837	-3.082001
N	-4.502562	-2.582163	-1.900113
H	-2.867479	-1.662619	0.139688
H	-2.883382	-1.623549	-4.101686
H	-4.629582	-3.460021	-2.489754
H	-5.318669	-1.997212	-1.709286
N	1.427165	-0.826344	-2.698051
N	1.421329	-0.830699	-1.256102
N	3.257925	-1.917989	-1.974204
C	2.542219	-1.476972	-0.874682
C	2.536349	-1.497412	-3.082001
N	4.487500	-2.608252	-1.900113
H	2.873610	-1.652000	0.139688
H	2.847726	-1.685308	-4.101686
H	5.311257	-2.279325	-2.489754
H	4.388971	-3.607496	-1.709286
Fe	0.000000	0.000000	-7.926909
N	0.000000	-1.707420	-5.154966
N	-0.005635	-1.742479	-6.599518
N	-0.049338	-3.849521	-5.840762
C	-0.038666	-3.036537	-6.967512
C	-0.026575	-2.991495	-4.752008
N	-0.079119	-5.263060	-5.716129
H	-0.064249	-3.413761	-7.985782
H	-0.033995	-3.359884	-3.735146
H	0.780352	-5.733968	-6.012456
H	-0.961198	-5.695594	-6.003637
N	1.478669	0.853710	-5.154966
N	1.511849	0.866359	-6.599518
N	3.358452	1.882033	-5.840762
C	2.649051	1.484783	-6.967512
C	2.603998	1.472733	-4.752008
N	4.597503	2.563011	-5.716129
H	2.988528	1.651239	-7.985782
H	2.926742	1.650501	-3.735146
H	4.575586	3.542789	-6.012456
H	5.413128	2.015375	-6.003637
N	-1.478669	0.853710	-5.154966
N	-1.506214	0.876120	-6.599518
N	-3.309114	1.967488	-5.840762
C	-2.610385	1.551754	-6.967512
C	-2.577423	1.518762	-4.752008
N	-4.518384	2.700049	-5.716129
H	-2.924279	1.762522	-7.985782
H	-2.892747	1.709383	-3.735146
H	-5.355938	2.191179	-6.012456
H	-4.451930	3.680219	-6.003637
O	-1.324462	-1.029265	-9.337461
H	-0.974873	-1.342205	-10.204669
H	-2.285476	-1.238448	-9.300651
O	-0.229139	1.661650	-9.337461
H	-0.674947	1.515367	-10.204669
H	0.070211	2.598504	-9.300651
O	1.553601	-0.632385	-9.337461
H	1.649820	-0.173162	-10.204669
H	2.215265	-1.360056	-9.300651
O	1.324462	1.029265	9.337461
H	0.974873	1.342205	10.204669
H	2.285476	1.238448	9.300651
O	0.229139	-1.661650	9.337461
H	0.674947	-1.515367	10.204669
H	-0.070211	-2.598504	9.300651
O	-1.553601	0.632385	9.337461
H	-1.649820	0.173162	10.204669
H	-2.215265	1.360056	9.300651
O	6.678492	-2.02312	-3.316637
O	5.091319	4.772184	3.316637
O	-1.587173	6.795304	-3.316637
O	-6.678492	2.02312	3.316637
O	-5.091319	-4.772184	-3.316637
O	1.587173	-6.795304	3.316637
H	7.446192	-1.55937	-2.911818
H	7.025482	-2.661599	-3.981042

H	-5.07355	-5.668906	-2.911818
H	-5.817753	-4.753446	-3.981042
H	-7.446192	1.55937	2.911818
H	-7.025482	2.661599	3.981042
H	5.817753	4.753446	3.981042
H	5.07355	5.668906	2.911818
H	1.207729	-7.415045	3.981042
H	2.372642	-7.228276	2.911818
H	-2.372642	7.228276	-2.911818
H	-1.207729	7.415045	-3.981042

Sup. Mat. Table 12 Cartesian coordinates of the pentameric low-spin (LS) model (HLLLH, spin multiplicity 9) surrounded by ten chlorine ions.

Fe	0.000000	0.000000	0.000000
Fe	0.001938	0.108143	3.685916
N	-0.036351	-1.559454	2.583943
N	-0.034220	-1.615398	1.164295
N	-0.241157	-3.681659	1.960207
C	-0.148273	-2.908491	0.823855
C	-0.165145	-2.819131	3.041286
N	-0.637493	-5.048627	1.930784
Cl	-3.631558	-3.429410	1.716723
H	-0.193845	-3.317264	-0.174062
H	-0.237213	-3.138963	4.085200
H	-0.131579	-5.594175	2.632199
H	-1.668420	-5.087282	1.986183
N	1.434706	0.905813	2.544393
N	1.433100	0.816340	1.124406
N	3.246594	1.930342	1.765568
C	2.546423	1.424664	0.686029
C	2.535809	1.596943	2.908918
N	4.411153	2.748234	1.702236
Cl	4.509253	-2.428728	1.727140
H	2.847007	1.607888	-0.341567
H	2.859363	1.809553	3.931914
H	4.423040	3.264243	0.810018
H	5.255819	2.205605	1.901269
N	-1.402646	0.958140	2.543476
N	-1.397402	0.867518	1.129549
N	-3.222578	1.969390	1.757686
C	-2.510558	1.476737	0.681090
C	-2.511146	1.647698	2.903133
N	-4.390574	2.784851	1.664441
H	-2.849623	1.608367	-0.346667
H	-2.798272	1.921413	3.919366
H	-5.161720	2.378800	2.201639
H	-4.608401	2.952542	0.665235
Fe	-0.001938	-0.108143	-3.685916
N	1.402646	-0.958140	-2.543476
N	1.397402	-0.867518	-1.129549
N	3.222578	-1.969390	-1.757686
C	2.510558	-1.476737	-0.681090
C	2.511146	-1.647698	-2.903133
N	4.390574	-2.784851	-1.664441
H	2.849623	-1.608367	0.346667
H	2.798272	-1.921413	-3.919366
H	5.161720	-2.378800	-2.201639
H	4.608401	-2.952542	-0.665235
N	0.036351	1.559454	-2.583943
N	0.034220	1.615398	-1.164295
N	0.241157	3.681659	-1.960207
C	0.148273	2.908491	-0.823855
C	0.165145	2.819131	-3.041286
N	0.637493	5.048627	-1.930784
Cl	3.631558	3.429410	-1.716723
H	0.193845	3.317264	0.174062
H	0.237213	3.138963	-4.085200
H	0.131579	5.594175	-2.632199
H	1.668420	5.087282	-1.986183
N	-1.434706	-0.905813	-2.544393
N	-1.433100	-0.816340	-1.124406
N	-3.246594	-1.930342	-1.765568
C	-2.546423	-1.424664	-0.686029
C	-2.535809	-1.596943	-2.908918
N	-4.411153	-2.748234	-1.702236

Cl	-4.509253	2.428728	-1.727140
H	-2.847007	-1.607888	0.341567
H	-2.859363	-1.809553	-3.931914
H	-4.423040	-3.264243	-0.810018
H	-5.255819	-2.205605	-1.901269
Fe	0.024183	-0.032466	7.449372
N	0.055836	1.751383	4.814202
N	0.214118	1.733331	6.224552
N	-0.035445	3.844476	5.567903
C	0.136012	2.993437	6.648807
C	-0.086207	3.031777	4.449617
N	-0.495702	5.184451	5.568735
Cl	3.730369	1.568254	6.336156
H	0.184641	3.310958	7.680158
H	-0.245745	3.417104	3.454015
H	-1.460471	5.220415	5.920796
H	0.178066	5.836994	5.969400
N	-1.486242	-0.694203	4.774023
N	-1.608255	-0.637627	6.184191
N	-3.256018	-1.895305	5.384397
C	-2.683821	-1.361855	6.518063
C	-2.490923	-1.461242	4.315789
N	-4.227119	-2.943485	5.403875
Cl	-3.026361	2.874577	6.516125
H	-3.043536	-1.545040	7.519849
H	-2.700811	-1.766412	3.294630
H	-3.725794	-3.825185	5.588869
H	-4.739850	-2.958848	4.515327
N	1.430688	-0.786997	4.754507
N	1.426375	-1.029068	6.148578
N	3.312971	-1.833329	5.293936
C	2.568309	-1.666202	6.441629
C	2.580426	-1.275263	4.263119
N	4.631212	-2.380283	5.229131
Cl	-0.870579	-4.054919	6.278409
H	2.885019	-1.991273	7.422118
H	2.923978	-1.303083	3.234210
H	5.309297	-1.629334	5.407253
H	4.767022	-2.822905	4.307519
Fe	-0.024183	0.032466	-7.449372
N	-1.430688	0.786997	-4.754507
N	-1.426375	1.029068	-6.148578
N	-3.312971	1.833329	-5.293936
C	-2.568309	1.666202	-6.441629
C	-2.580426	1.275263	-4.263119
N	-4.631212	2.380283	-5.229131
Cl	0.870579	4.054919	-6.278409
H	-2.885019	1.991273	-7.422118
H	-2.923978	1.303083	-3.234210
H	-5.309297	1.629334	-5.407253
H	-4.767022	2.822905	-4.307519
N	-0.055836	-1.751383	-4.814202
N	-0.214118	-1.733331	-6.224552
N	0.035445	-3.844476	-5.567903
C	-0.136012	-2.993437	-6.648807
C	0.086207	-3.031777	-4.449617
N	0.495702	-5.184451	-5.568735
Cl	-3.730369	-1.568254	-6.336156
H	-0.184641	-3.310958	-7.680158
H	0.245745	-3.417104	-3.454015
H	1.460471	-5.220415	-5.920796
H	-0.178066	-5.836994	-5.969400
N	1.486242	0.694203	-4.774023
N	1.608255	0.637627	-6.184191
N	3.256018	1.895305	-5.384397
C	2.683821	1.361855	-6.518063
C	2.490923	1.461242	-4.315789
N	4.227119	2.943485	-5.403875
Cl	3.026361	-2.874577	-6.516125
H	3.043536	1.545040	-7.519849
H	2.700811	1.766412	-3.294630
H	3.725794	3.825185	-5.588869
H	4.739850	2.958848	-4.515327
O	-1.754977	-0.712133	-8.433989
H	-2.024584	-0.805646	-9.368301
H	-2.482963	-1.049674	-7.783493
O	1.485989	-1.105835	-8.470936

H	1.794772	-1.108136	-9.398042
H	2.087102	-1.680139	-7.870455
O	0.221127	1.943005	-8.385412
H	0.117361	2.262221	-9.303310
H	0.397144	2.715936	-7.736805
O	-0.221127	-1.943005	8.385412
H	-0.117361	-2.262221	9.30331
H	-0.397144	-2.715936	7.736805
O	1.754977	0.712133	8.433989
H	2.024584	0.805646	9.368301
H	2.482963	1.049674	7.783493
O	-1.485989	1.105835	8.470936
H	-1.794772	1.108136	9.398042
H	-2.087102	1.680139	7.870455

Sup. Mat. Table 13 Cartesian coordinates of the pentameric high-spin (HS) model (HHHHH, spin multiplicity 21).

Fe	-0.000092	-0.000110	4.354838
Fe	0.000000	0.000000	0.000000
N	0.001090	1.800983	2.889621
N	-0.000972	1.802354	1.432571
N	0.002370	3.934519	2.162971
C	-0.000045	3.095171	1.058402
C	0.003100	3.091537	3.272067
N	0.003852	5.338658	2.099144
H	-0.000872	3.481270	0.045635
H	0.005704	3.457499	4.293405
H	-0.880362	5.817425	2.269549
H	0.889172	5.815586	2.268962
N	-1.560183	-0.899355	2.889598
N	-1.560237	-0.901847	1.432559
N	-3.408514	-1.964976	2.162811
C	-2.680267	-1.547453	1.058305
C	-2.678870	-1.542897	3.271968
N	-4.625309	-2.665676	2.098860
H	-3.014031	-1.741218	0.045477
H	-2.997150	-1.723625	4.293298
H	-4.597917	-3.670812	2.269276
H	-5.480943	-2.137340	2.268689
N	1.558914	-0.901347	2.889731
N	1.561127	-0.900233	1.432688
N	3.406055	-1.969095	2.163051
C	2.680288	-1.547387	1.058503
C	2.675584	-1.548342	3.272168
N	4.621402	-2.672310	2.099163
H	3.014968	-1.739670	0.045695
H	2.991200	-1.733565	4.293521
H	5.478050	-2.145828	2.269633
H	4.591893	-3.677499	2.268920
Fe	-0.000044	-0.000121	8.432447
N	0.022877	-1.837449	5.705869
N	0.001268	-1.795745	7.154001
N	-0.035717	-3.943183	6.504293
C	-0.035532	-3.069265	7.587869
C	-0.001057	-3.143895	5.373669
N	-0.066869	-5.360858	6.454459
H	-0.071922	-3.394995	8.623531
H	0.003990	-3.569587	4.377218
H	0.796328	-5.819640	6.759260
H	-0.948184	-5.781552	6.762019
N	1.579463	0.938512	5.705864
N	1.554682	0.898681	7.154019
N	3.432962	1.939976	6.503676
C	2.676325	1.503294	7.587520
C	2.722862	1.570702	5.373298
N	4.676516	2.621385	6.453452
H	2.977280	1.634618	8.623005
H	3.088499	1.787832	4.376660
H	4.642828	3.598208	6.758701
H	5.481448	2.068014	6.760297
N	-1.602613	0.898616	5.705803
N	-1.555963	0.896750	7.153955
N	-3.397093	2.002376	6.503521
C	-2.640623	1.565500	7.587399
C	-2.721938	1.572489	5.373179
N	-4.609232	2.738219	6.453280

H	-2.905108	1.760318	8.622848
H	-3.092694	1.780621	4.376511
H	-5.438228	2.220147	6.758009
H	-4.532941	3.711863	6.760671
Fe	0.000092	0.000110	-4.354838
N	-0.001090	-1.800983	-2.889621
N	0.000972	-1.802354	-1.432571
N	-0.002370	-3.934519	-2.162971
C	0.000045	-3.095171	-1.058402
C	-0.003100	-3.091537	-3.272067
N	-0.003852	-5.338658	-2.099144
H	0.000872	-3.481270	-0.045635
H	-0.005704	-3.457499	-4.293405
H	0.880362	-5.817425	-2.269549
H	-0.889172	-5.815586	-2.268962
N	1.560183	0.899355	-2.889598
N	1.560237	0.901847	-1.432559
N	3.408514	1.964976	-2.162811
C	2.680267	1.547453	-1.058305
C	2.678870	1.542897	-3.271968
N	4.625309	2.665676	-2.098860
H	3.014031	1.741218	-0.045477
H	2.997150	1.723625	-4.293298
H	4.597917	3.670812	-2.269276
H	5.480943	2.137340	-2.268689
N	-1.558914	0.901347	-2.889731
N	-1.561127	0.900233	-1.432688
N	-3.406055	1.969095	-2.163051
C	-2.680288	1.547387	-1.058503
C	-2.675584	1.548342	-3.272168
N	-4.621402	2.672310	-2.099163
H	-3.014968	1.739670	-0.045695
H	-2.991200	1.733565	-4.293521
H	-5.478050	2.145828	-2.269633
H	-4.591893	3.677499	-2.268920
Fe	0.000044	0.000121	-8.432447
N	-0.022877	1.837449	-5.705869
N	-0.001268	1.795745	-7.154001
N	0.035717	3.943183	-6.504293
C	0.035532	3.069265	-7.587869
C	0.001057	3.143895	-5.373669
N	0.066869	5.360858	-6.454459
H	0.071922	3.394995	-8.623531
H	-0.003990	3.569587	-4.377218
H	-0.796328	5.819640	-6.759260
H	0.948184	5.781552	-6.762019
N	-1.579463	-0.938512	-5.705864
N	-1.554682	-0.898681	-7.154019
N	-3.432962	-1.939976	-6.503676
C	-2.676325	-1.503294	-7.587520
C	-2.722862	-1.570702	-5.373298
N	-4.676516	-2.621385	-6.453452
H	-2.977280	-1.634618	-8.623005
H	-3.088499	-1.787832	-4.376660
H	-4.642828	-3.598208	-6.758701
H	-5.481448	-2.068014	-6.760297
N	1.602613	-0.898616	-5.705803
N	1.555963	-0.896750	-7.153955
N	3.397093	-2.002376	-6.503521
C	2.640623	-1.565500	-7.587399
C	2.721938	-1.572489	-5.373179
N	4.609232	-2.738219	-6.453280
H	2.905108	-1.760318	-8.622848
H	3.092694	-1.780621	-4.376511
H	5.438228	-2.220147	-6.758009
H	4.532941	-3.711863	-6.760671
O	1.350840	1.007210	-9.836678
H	1.027236	1.303487	-10.719809
H	2.310095	1.219887	-9.776885
O	0.196338	-1.673327	-9.836225
H	0.613934	-1.541537	-10.719776
H	-0.097808	-2.610724	-9.775168
O	-1.547437	0.666183	-9.837268
H	-1.642088	0.237721	-10.720381
H	-2.211651	1.390208	-9.777414
O	-1.350840	-1.007210	9.836678
H	-1.027236	-1.303487	10.719809

H	-2.310095	-1.219887	9.776885
O	-0.196338	1.673327	9.836225
H	-0.613934	1.541537	10.719776
H	0.097808	2.610724	9.775168
O	1.547437	-0.666183	9.837268
H	1.642088	-0.237721	10.720381
H	2.211651	-1.390208	9.777414

Sup. Mat. Table 14 Cartesian coordinates of the pentameric high-spin (HS) model (HHHHH, spin multiplicity 21) surrounded by six water molecules.

Fe	-4.240001	0.001462	-0.003711
Fe	0.000000	0.000000	0.000000
N	-2.855430	0.611736	-1.696146
N	-1.408868	0.621680	-1.684903
N	-2.122915	1.381322	-3.685691
C	-1.025915	1.069482	-2.898316
C	-3.232956	1.084685	-2.905060
N	-2.046224	1.854488	-5.013243
H	-0.009129	1.188326	-3.252104
H	-4.252026	1.214420	-3.251082
H	-2.627713	1.385123	-5.768461
H	-1.858509	2.856144	-5.085576
N	-2.856501	-1.771328	0.322478
N	-1.409960	-1.767655	0.307717
N	-2.125237	-3.879828	0.649596
C	-1.027712	-3.042783	0.525721
C	-3.234759	-3.054623	0.516693
N	-2.049565	-5.266281	0.903180
H	-0.011092	-3.409294	0.598540
H	-4.254026	-3.418811	0.576204
H	-2.630495	-5.684945	1.688030
H	-1.864023	-5.829766	0.071406
N	-2.854099	1.163816	1.373928
N	-1.407393	1.149660	1.377975
N	-2.122617	2.498421	3.038886
C	-1.025130	1.974213	2.374727
C	-3.232125	1.971640	2.389751
N	-2.046986	3.408156	4.115310
H	-0.008598	2.220519	2.656096
H	-4.251275	2.204844	2.676062
H	-2.624092	4.299538	4.086536
H	-1.863070	2.967219	5.018330
Fe	-8.364643	0.014770	-0.007775
N	-5.635190	-0.596319	1.722033
N	-7.081268	-0.574995	1.683069
N	-6.437506	-1.375030	3.675489
C	-7.519552	-1.047712	2.863255
C	-5.304324	-1.082079	2.933465
N	-6.398908	-1.899382	4.990811
H	-8.554376	-1.178932	3.163602
H	-4.306561	-1.243031	3.323476
H	-6.689633	-1.248414	5.724339
H	-6.704650	-2.871472	5.077148
N	-5.630112	1.802594	-0.334781
N	-7.075591	1.767655	-0.280540
N	-6.429960	3.889811	-0.601305
C	-7.512298	3.030068	-0.439164
C	-5.298021	3.093152	-0.525881
N	-6.389160	5.291756	-0.799888
H	-8.545953	3.361483	-0.432819
H	-4.300262	3.506105	-0.612890
H	-6.696664	5.606638	-1.723314
H	-6.676782	5.850516	0.006889
N	-5.617452	-1.188963	-1.384650
N	-7.063807	-1.160286	-1.369211
N	-6.394529	-2.511553	-3.030413
C	-7.487258	-1.958210	-2.365090
C	-5.271481	-2.010058	-2.395798
N	-6.340518	-3.403904	-4.129778
H	-8.518343	-2.154165	-2.642419
H	-4.268927	-2.272284	-2.711102
H	-6.641265	-4.359708	-3.923705
H	-6.635601	-3.003696	-5.023526
Fe	4.240001	-0.001462	0.003711
N	2.855430	-0.611736	1.696146

N	1.408868	-0.621680	1.684903
N	2.122915	-1.381322	3.685691
C	1.025915	-1.069482	2.898316
C	3.232956	-1.084685	2.905060
N	2.046224	-1.854488	5.013243
H	0.009129	-1.188326	3.252104
H	4.252026	-1.214420	3.251082
H	2.627713	-1.385123	5.768461
H	1.858509	-2.856144	5.085576
N	2.856501	1.771328	-0.322478
N	1.409960	1.767655	-0.307717
N	2.125237	3.879828	-0.649596
C	1.027712	3.042783	-0.525721
C	3.234759	3.054623	-0.516693
N	2.049565	5.266281	-0.903180
H	0.011092	3.409294	-0.598540
H	4.254026	3.418811	-0.576204
H	2.630495	5.684945	-1.688030
H	1.864023	5.829766	-0.071406
N	2.854099	-1.163816	-1.373928
N	1.407393	-1.149660	-1.377975
N	2.122617	-2.498421	-3.038886
C	1.025130	-1.974213	-2.374727
C	3.232125	-1.971640	-2.389751
N	2.046986	-3.408156	-4.115310
H	0.008598	-2.220519	-2.656096
H	4.251275	-2.204844	-2.676062
H	2.624092	-4.299538	-4.086536
H	1.863070	-2.967219	-5.018330
Fe	8.364643	-0.014770	0.007775
N	5.635190	0.596319	-1.722033
N	7.081268	0.574995	-1.683069
N	6.437506	1.375030	-3.675489
C	7.519552	1.047712	-2.863255
C	5.304324	1.082079	-2.933465
N	6.398908	1.899382	-4.990811
H	8.554376	1.178932	-3.163602
H	4.306561	1.243031	-3.323476
H	6.689633	1.248414	-5.724339
H	6.704650	2.871472	-5.077148
N	5.630112	-1.802594	0.334781
N	7.075591	-1.767655	0.280540
N	6.429960	-3.889811	0.601305
C	7.512298	-3.030068	0.439164
C	5.298021	-3.093152	0.525881
N	6.389160	-5.291756	0.799888
H	8.545953	-3.361483	0.432819
H	4.300262	-3.506105	0.612890
H	6.696664	-5.606638	1.723314
H	6.676782	-5.850516	-0.006889
N	5.617452	1.188963	1.384650
N	7.063807	1.160286	1.369211
N	6.394529	2.511553	3.030413
C	7.487258	1.958210	2.365090
C	5.271481	2.010058	2.395798
N	6.340518	3.403904	4.129778
H	8.518343	2.154165	2.642419
H	4.268927	2.272284	2.711102
H	6.641265	4.359708	3.923705
H	6.635601	3.003696	5.023526
O	9.808235	1.540575	-0.484919
H	10.637356	1.307265	-0.963960
H	9.816615	2.504943	-0.289553
O	9.784202	-0.337317	1.641913
H	10.656059	0.121998	1.665266
H	9.722778	-0.933189	2.422452
O	9.877081	-1.239025	-1.103619
H	10.662929	-1.613272	-0.641176
H	9.936577	-1.483753	-2.055283
O	-9.808235	-1.540575	0.484919
H	-10.637356	-1.307265	0.963960
H	-9.816615	-2.504943	0.289553
O	-9.784202	0.337317	-1.641913
H	-10.656059	-0.121998	-1.665266
H	-9.722778	0.933189	-2.422452
O	-9.877081	1.239025	1.103619
H	-10.662929	1.613272	0.641176

H	-9.936577	1.483753	2.055283
O	3.445898	-5.687245	-4.307775
O	-3.457418	-6.565801	2.778054
O	3.454424	-0.883613	7.07708
O	-3.445898	5.687245	4.307775
O	3.457418	6.565801	-2.778054
O	-3.454424	0.883613	-7.07708
H	3.040551	-6.563892	-4.121072
H	4.105894	-5.803228	-5.028742
H	3.055918	6.840401	-3.633079
H	4.118082	7.247478	-2.51791
H	-3.040551	6.563892	4.121072
H	-4.105894	5.803228	5.028742
H	-4.118082	-7.247478	2.51791
H	-3.055918	-6.840401	3.633079
H	-4.113695	1.450973	-7.537833
H	-3.053598	0.279635	-7.742074
H	3.053598	-0.279635	7.742074
H	4.113695	-1.450973	7.537833

Sup. Mat. Table 15 Cartesian coordinates of the pentameric high-spin (HS) model (HHHHH, spin multiplicity 21) surrounded by ten chlorine ions.

Fe	0.000000	0.000000	0.000000
Fe	-0.148169	0.239011	3.889610
N	-0.182903	-1.632427	2.706913
N	-0.099917	-1.757019	1.289655
N	-0.500909	-3.766301	2.160528
C	-0.290914	-3.052492	0.999553
C	-0.428343	-2.855801	3.205132
N	-1.003854	-5.099496	2.172258
Cl	-3.780917	-3.160339	1.861063
H	-0.309157	-3.503542	0.017169
H	-0.555180	-3.130743	4.257409
H	-0.578157	-5.643402	2.927144
H	-2.035791	-5.047148	2.189722
N	1.446380	1.132931	2.669599
N	1.503455	0.981325	1.250427
N	3.304649	2.104437	1.919605
C	2.639812	1.560902	0.832233
C	2.541523	1.823558	3.046684
N	4.491056	2.890499	1.874984
Cl	4.588966	-2.314147	1.927487
H	2.985294	1.695424	-0.194894
H	2.837794	2.056401	4.073806
H	4.575038	3.351302	0.960726
H	5.309610	2.350872	2.167571
N	-1.686814	1.128531	2.560944
N	-1.589071	0.952202	1.149501
N	-3.536726	1.933571	1.603264
C	-2.717486	1.436117	0.603577
C	-2.862915	1.739812	2.800057
N	-4.787361	2.609415	1.427325
H	-2.997097	1.488751	-0.449943
H	-3.247145	2.033958	3.769487
H	-5.558078	1.994117	1.711525
H	-4.867478	2.894295	0.432908
Fe	0.148169	-0.239011	-3.889610
N	1.686814	-1.128531	-2.560944
N	1.589071	-0.952202	-1.149501
N	3.536726	-1.933571	-1.603264
C	2.717486	-1.436117	-0.603577
C	2.862915	-1.739812	-2.800057
N	4.787361	-2.609415	-1.427325
H	2.997097	-1.488751	0.449943
H	3.247145	-2.033958	-3.769487
H	5.558078	-1.994117	-1.711525
H	4.867478	-2.894295	-0.432908
N	0.182903	1.632427	-2.706913
N	0.099917	1.757019	-1.289655
N	0.500909	3.766301	-2.160528
C	0.290914	3.052492	-0.999553
C	0.428343	2.855801	-3.205132
N	1.003854	5.099496	-2.172258
Cl	3.780917	3.160339	-1.861063
H	0.309157	3.503542	-0.017169

H	0.555180	3.130743	-4.257409
H	0.578157	5.643402	-2.927144
H	2.035791	5.047148	-2.189722
N	-1.446380	-1.132931	-2.669599
N	-1.503455	-0.981325	-1.250427
N	-3.304649	-2.104437	-1.919605
C	-2.639812	-1.560902	-0.832233
C	-2.541523	-1.823558	-3.046684
N	-4.491056	-2.890499	-1.874984
Cl	-4.588966	2.314147	-1.927487
H	-2.985294	-1.695424	0.194894
H	-2.837794	-2.056401	-4.073806
H	-4.575038	-3.351302	-0.960726
H	-5.309610	-2.350872	-2.167571
Fe	0.051149	-0.058954	7.682772
N	-0.175641	1.984328	5.184584
N	0.141528	1.807471	6.567608
N	-0.185829	3.979971	6.179626
C	0.124886	3.017559	7.131641
C	-0.373881	3.294395	4.990870
N	-0.620620	5.316568	6.411856
Cl	3.759880	1.569758	6.433399
H	0.319837	3.233034	8.170289
H	-0.648050	3.783869	4.065404
H	-1.415566	5.275781	7.073492
H	0.157108	5.916701	6.697435
N	-1.751261	-0.615000	5.105694
N	-1.741832	-0.577233	6.532750
N	-3.432107	-1.864479	5.862883
C	-2.768726	-1.327802	6.949920
C	-2.768029	-1.410775	4.732813
N	-4.360671	-2.940218	5.976934
Cl	-2.563510	3.515745	8.456101
H	-3.035725	-1.535579	7.976137
H	-3.041629	-1.716241	3.720836
H	-3.822036	-3.815243	6.061606
H	-5.029755	-2.926757	5.202906
N	1.414157	-0.786191	4.951187
N	1.434261	-1.035744	6.343179
N	3.337866	-1.770358	5.459492
C	2.600598	-1.637118	6.618953
C	2.574617	-1.228039	4.443418
N	4.681087	-2.252057	5.386693
Cl	-1.066825	-4.061652	6.450459
H	2.946760	-1.947749	7.594308
H	2.905135	-1.227250	3.409448
H	5.317711	-1.470037	5.586139
H	4.840092	-2.663378	4.453548
Fe	-0.051149	0.058954	-7.682772
N	-1.414157	0.786191	-4.951187
N	-1.434261	1.035744	-6.343179
N	-3.337866	1.770358	-5.459492
C	-2.600598	1.637118	-6.618953
C	-2.574617	1.228039	-4.443418
N	-4.681087	2.252057	-5.386693
Cl	1.066825	4.061652	-6.450459
H	-2.946760	1.947749	-7.594308
H	-2.905135	1.227250	-3.409448
H	-5.317711	1.470037	-5.586139
H	-4.840092	2.663378	-4.453548
N	0.175641	-1.984328	-5.184584
N	-0.141528	-1.807471	-6.567608
N	0.185829	-3.979971	-6.179626
C	-0.124886	-3.017559	-7.131641
C	0.373881	-3.294395	-4.990870
N	0.620620	-5.316568	-6.411856
Cl	-3.759880	-1.569758	-6.433399
H	-0.319837	-3.233034	-8.170289
H	0.648050	-3.783869	-4.065404
H	1.415566	-5.275781	-7.073492
H	-0.157108	-5.916701	-6.697435
N	1.751261	0.615000	-5.105694
N	1.741832	0.577233	-6.532750
N	3.432107	1.864479	-5.862883
C	2.768726	1.327802	-6.949920
C	2.768029	1.410775	-4.732813
N	4.360671	2.940218	-5.976934

Cl	2.563510	-3.515745	-8.456101
H	3.035725	1.535579	-7.976137
H	3.041629	1.716241	-3.720836
H	3.822036	3.815243	-6.061606
H	5.029755	2.926757	-5.202906
O	-1.883106	-0.594399	-8.588346
H	-2.066330	-0.880882	-9.504539
H	-2.578013	-0.962261	-7.922897
O	1.185882	-0.929973	-9.090104
H	1.407322	-0.605891	-9.985504
H	1.714566	-1.789834	-8.878941
O	0.220143	2.009429	-8.576940
H	-0.042085	2.372508	-9.446155
H	0.448273	2.756203	-7.919922
O	-0.220143	-2.009429	8.57694
H	0.042085	-2.372508	9.446155
H	-0.448273	-2.756203	7.919922
O	1.883106	0.594399	8.588346
H	2.06633	0.880882	9.504539
H	2.578013	0.962261	7.922897
O	-1.185882	0.929973	9.090104
H	-1.407322	0.605891	9.985504
H	-1.714566	1.789834	8.878941

Sup. Mat. Table 16 Cartesian coordinates of the hexameric low-spin (LS) model (HLLLLH, spin multiplicity 9) surrounded by twelve chlorine ions.

Fe	0.000000	0.000000	-1.847759
Fe	0.000000	0.000000	1.847467
N	-0.487707	-1.562543	0.706580
N	-0.488284	-1.562511	-0.707094
N	-1.264707	-3.522308	0.000139
C	-0.950005	-2.767761	-1.111788
C	-0.949025	-2.767643	1.111735
N	-1.755749	-4.854705	0.000741
H	-1.143880	-3.105824	-2.128206
H	-1.142225	-3.105561	2.128287
H	-2.247482	-5.058160	0.879996
H	-2.248078	-5.058719	-0.877923
N	-1.109349	1.203638	0.706580
N	-1.109032	1.204122	-0.707094
N	-2.418054	2.856423	0.000139
C	-1.921949	2.206609	-1.111788
C	-1.922336	2.205702	1.111735
N	-3.326423	3.947876	0.000741
H	-2.117782	2.543541	-2.128206
H	-2.118382	2.541976	2.128287
H	-3.256754	4.475457	0.879996
H	-3.256940	4.476252	-0.877923
N	1.597055	0.358905	0.706580
N	1.597316	0.358389	-0.707094
N	3.682762	0.665885	0.000139
C	2.871954	0.561152	-1.111788
C	2.871362	0.561941	1.111735
N	5.082172	0.906829	0.000741
H	3.261662	0.562282	-2.128206
H	3.260607	0.563585	2.128287
H	5.504236	0.582704	0.879996
H	5.505018	0.582467	-0.877923
Fe	0.000000	0.000000	-5.528032
N	1.098738	-1.210988	-4.409874
N	1.118461	-1.213417	-2.987912
N	2.645585	-2.651108	-3.735157
C	2.056233	-2.100377	-2.617623
C	2.033197	-2.077577	-4.838979
N	3.848801	-3.411033	-3.673475
Cl	4.999422	-0.245251	-3.556128
H	2.352790	-2.352258	-1.610980
H	2.254258	-2.334471	-5.882727
H	3.844053	-4.159894	-4.370422
H	4.643665	-2.751306	-3.727525
N	-1.598115	-0.346042	-4.409874
N	-1.610080	-0.361908	-2.987912
N	-3.618719	-0.965590	-3.735157
C	-2.847096	-0.730561	-2.617623
C	-2.815833	-0.722012	-4.838979

N	-4.878441	-1.627643	-3.673475
Cl	-2.712104	-4.207001	-3.556128
H	-3.213510	-0.861447	-1.610980
H	-3.148840	-0.785010	-5.882727
H	-5.524600	-1.249101	-4.370422
H	-4.704534	-2.645879	-3.727525
N	0.499377	1.557029	-4.409874
N	0.491619	1.575324	-2.987912
N	0.973134	3.616698	-3.735157
C	0.790863	2.830938	-2.617623
C	0.782636	2.799589	-4.838979
N	1.029640	5.038676	-3.673475
Cl	-2.287318	4.452252	-3.556128
H	0.860720	3.213705	-1.610980
H	0.894582	3.119480	-5.882727
H	1.680547	5.408995	-4.370422
H	0.060868	5.397185	-3.727525
Fe	0.000000	0.000000	5.527938
N	1.098985	-1.210717	4.409816
N	1.118727	-1.213141	2.987822
N	2.646068	-2.650612	3.735123
C	2.056788	-2.099784	2.617544
C	2.033545	-2.077114	4.838940
N	3.849302	-3.410500	3.673753
Cl	4.999506	-0.243706	3.554587
H	2.353356	-2.351701	1.610906
H	2.254798	-2.333954	5.882682
H	3.844415	-4.159335	4.370715
H	4.644245	-2.750877	3.727657
N	-1.598005	-0.346391	4.409816
N	-1.609974	-0.362275	2.987822
N	-3.618531	-0.966257	3.735123
C	-2.846861	-0.731339	2.617544
C	-2.815606	-0.722545	4.838940
N	-4.878231	-1.628343	3.673753
Cl	-2.710808	-4.207846	3.554587
H	-3.213311	-0.862215	1.610906
H	-3.148663	-0.785735	5.882682
H	-5.524298	-1.249693	4.370715
H	-4.704452	-2.646596	3.727657
N	0.499019	1.557108	4.409816
N	0.491247	1.575416	2.987822
N	0.972463	3.616868	3.735123
C	0.790072	2.831123	2.617544
C	0.782061	2.799659	4.838940
N	1.028929	5.038843	3.673753
Cl	-2.288698	4.451552	3.554587
H	0.859955	3.213917	1.610906
H	0.893865	3.119689	5.882682
H	1.679883	5.409029	4.370715
H	0.060207	5.397472	3.727657
Fe	0.000000	0.000000	-9.276936
N	-1.114732	1.245718	-6.610707
N	-1.083220	1.387865	-8.017555
N	-2.486797	2.893808	-7.183471
C	-1.908719	2.391243	-8.333078
C	-1.978658	2.152552	-6.131444
N	-3.413913	3.971708	-7.116509
Cl	2.388351	-3.279300	-8.074192
H	-2.108464	2.768358	-9.325513
H	-2.212637	2.372236	-5.096536
H	-3.168185	4.600476	-6.342249
H	-4.374674	3.618599	-7.080604
N	1.636189	0.342527	-6.610707
N	1.743536	0.244164	-8.017555
N	3.749509	0.706725	-7.183471
C	3.025237	0.457378	-8.333078
C	2.853494	0.637292	-6.131444
N	5.146556	0.970682	-7.116509
Cl	-4.034132	-0.428723	-8.074192
H	3.451701	0.441805	-9.325513
H	3.160735	0.730082	-5.096536
H	5.568222	0.443491	-6.342249
H	5.321135	1.979279	-7.080604
N	-0.521457	-1.588245	-6.610707
N	-0.660316	-1.632028	-8.017555
N	-1.262713	-3.600533	-7.183471

C	-1.116517	-2.848621	-8.333078
C	-0.874836	-2.789844	-6.131444
N	-1.732643	-4.942389	-7.116509
Cl	1.645781	3.708023	-8.074192
H	-1.343236	-3.210163	-9.325513
H	-0.948098	-3.102317	-5.096536
H	-2.400036	-5.043967	-6.342249
H	-0.946461	-5.597878	-7.080604
Fe	0.000000	0.000000	9.277172
N	-1.115099	1.245603	6.610706
N	-1.084634	1.386485	8.017728
N	-2.488037	2.892780	7.184046
C	-1.910673	2.389277	8.333587
C	-1.978892	2.152699	6.131646
N	-3.415504	3.970326	7.117854
Cl	2.391230	-3.277184	8.074085
H	-2.111635	2.765099	9.326261
H	-2.212348	2.373226	5.096769
H	-3.168072	4.602069	6.346574
H	-4.376083	3.617068	7.078365
N	1.636273	0.342903	6.610706
N	1.743048	0.246078	8.017728
N	3.749239	0.708313	7.184046
C	3.024511	0.460053	8.333587
C	2.853738	0.637421	6.131646
N	5.146155	0.97275	7.117854
Cl	-4.033739	-0.432274	8.074085
H	3.450463	0.44618	9.326261
H	3.161448	0.729336	5.096769
H	5.569544	0.442596	6.346574
H	5.320514	1.981265	7.078365
N	-0.521174	-1.588506	6.610706
N	-0.658414	-1.632563	8.017728
N	-1.261202	-3.601093	7.184046
C	-1.113838	-2.849329	8.333587
C	-0.874846	-2.790121	6.131646
N	-1.730651	-4.943076	7.117854
Cl	1.642509	3.709458	8.074085
H	-1.338828	-3.211279	9.326261
H	-0.949101	-3.102562	5.096769
H	-2.401473	-5.044665	6.346574
H	-0.944432	-5.598333	7.078365
O	-1.893594	-0.284451	-10.226945
H	-2.195426	-0.316261	-11.155576
H	-2.67662	-0.358574	-9.566792
O	0.700455	1.782125	-10.226945
H	0.823823	2.059426	-11.155576
H	1.027776	2.497308	-9.566792
O	1.193138	-1.497675	-10.226945
H	1.371603	-1.743165	-11.155576
H	1.648844	-2.138734	-9.566792
O	-1.893888	-0.283399	10.227219
H	-2.195041	-0.321439	11.155827
H	-2.676856	-0.358484	9.56702
O	0.701513	1.781855	10.227219
H	0.819146	2.061681	11.155827
H	1.027972	2.497467	9.56702
O	1.192375	-1.498456	10.227219
H	1.375895	-1.740242	11.155827
H	1.648884	-2.138983	9.56702

Sup. Mat. Table 17 Cartesian coordinates of the hexameric high-spin (HS) model (HHHHHH, spin multiplicity 25) surrounded by twelve chlorine ions.

Fe	0.000000	0.000000	1.959187
Fe	0.000000	0.000000	-1.918303
N	1.287738	1.250065	-0.697645
N	1.098335	1.488994	0.695554
N	2.332422	3.143041	-0.158964
C	1.728849	2.647745	0.993994
C	2.056498	2.245868	-1.175636
N	2.924329	4.419171	-0.328481
H	1.779540	3.155746	1.967724
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H	-3.727767	-4.465808	4.642408
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Fe	0.000000	0.000000	-9.557930
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N	1.177362	-3.743423	-7.643525
C	0.901251	-2.95777	-6.533963
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O	1.909634	-0.175236	10.553306
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H	-1.522184	-2.232018	9.889571
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O	1.871241	-0.397192	-10.524293
H	2.166317	-0.464446	-11.453205
H	2.643421	-0.545285	-9.862762
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H	-1.485381	-1.643862	-11.453205
H	-1.793942	-2.016627	-9.862762