Electronic Supplementary Material (ESI) for Dalton Transactions.
This journal is © The Royal Society of Chemistry 2021

Accurate calculation of spin-state energy gaps in Fe(III) Spin-Crossover systems using Density Functional Methods

Supporting Information

Daniel Vidal[1,2], Jordi Cirera[1] and Jordi Ribas-Arino[2]**

[1] Departament de Química Inorgànica i Orgànica and Institut de Recerca de Química Teòrica i Computacional, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Spain

[2] Departament de Ciència de Materials i Química Física and Institut de Recerca de Química Teòrica i Computacional, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Spain

e-mail: j.ribas@ub.edu
e-mail: jordi.cirera@qi.ub.es

DFT energies and lowest frequencies for all SCO studied systems	S1
Effect of the Hartree-Fock exchange on the spin-state energy gap	S8
Cartesian geometries for the B3LYP* optimized geometries	S9
Experimental data for the studied systems in bulk phase	S10
Experimental data for the studied systems in solution	S11

S-1 DFT energies and lowest frequencies for all SCO studied systems. Energies in atomic units, energy differences (ΔE) in kcal/mol and frequencies in cm^{-1}. L_{19} = (3-methoxysalicylideneaminopropyl)amine.

Method: **B3LYP**

System	*Refcode*	*E(S=5/2)*	*E(S=1/2)*	*ΔE*	*ν(S=5/2)*	*ν (S=1/2)*
1	ATOJUO01	-3158.09	-3158.08	-3.58946	11.95	18.52
2	TAMTEH02	-4399.51	-4399.50	-2.82083	14.75	18.82
3	SUPHUH	-2865.94	-2865.94	-0.38652	16.09	17.75
4	BIMZUU	-2718.59	-2718.58	-3.06256	13.11	17.83
5	GOWSES	-2708.57	-2708.57	-2.73144	16.82	22.18
6	DADFAR	-3113.66	-3113.66	-1.98547	12.01	14.32
7	DADFOF	-5117.03	-5117.03	-1.52971	10.11	12.17
8	DADGAS	-2790.70	-2790.70	-2.99520	12.90	15.59
9	FONNAZ	-3114.04	-3114.03	-3.49126	13.83	16.42
10	HAJLAH	-2718.57	-2718.57	-2.97758	15.69	21.51
11	PORBUV	-8013.11	-8013.11	-0.26565	09.08	9.37
12	LIGZUY	-4077.36	-4077.35	-3.28604	8.33	12.25
13	LIZZUR	-2672.91	-2672.90	-3.00024	16.63	20.94
14	XIZKEY	-3460.35	-3460.35	-0.28265	7.70	7.66
15	XUJDOX	-2901.99	-2901.99	-2.36507	14.08	18.69
16	DETBEJ	-2641.96	-2641.96	-1.84446	21.77	25.43
17	FEWVIM	-2444.15	-2444.16	1.42395	19.14	37.60
18	$[Fe(L_{19})py]^+$	-2831.73	-2831.72	-1.88160	22.82	24.99

Method: **TPSSh**

System	*Refcode*	*E(S=5/2)*	*E(S=1/2)*	*ΔE*	*ν(S=5/2)*	*ν (S=1/2)*
1	ATOJUO01	-3158.14	-3158.15	7.9633	12.35	17.47
2	TAMTEH02	-4399.59	-4399.60	9.3186	13.56	13.83
3	SUPHUH	-2866.03	-2866.05	11.3179	16.03	17.98
4	BIMZUU	-2718.65	-2718.67	8.8660	12.71	17.05
5	GOWSES	-2708.64	-2708.65	8.6627	16.20	21.54
6	DADFAR	-3113.74	-3113.76	9.6768	11.51	13.80
7	DADFOF	-5117.00	-5117.02	10.0961	9.44	12.43
8	DADGAS	-2790.78	-2790.79	8.4669	11.94	15.08
9	FONNAZ	-3114.10	-3114.12	8.0898	12.42	16.13
10	HAJLAH	-2718.64	-2718.65	9.0347	15.19	20.42
11	PORBUV	-8012.98	-8013.00	11.4401	09.03	9.40
12	LIGZUY	-4077.41	-4077.42	8.3045	8.41	11.58
13	LIZZUR	-2672.98	-2673.00	9.1638	13.99	18.19
14	XIZKEY	-3460.08	-3460.09	11.8423	6.15	7.96
15	XUJDOX	-2902.07	-2902.09	9.5018	12.47	17.46
16	DETBEJ	-2642.04	-2642.05	8.4216	20.47	22.03
17	FEWVIM	-2444.21	-2444.23	14.1331	14.91	38.22
18	$[Fe(L_{19})py]^{+}$	-2831.80	-2831.82	10.1615	21.66	22.13

Method: **M06L**

System	*Refcode*	*E(S=5/2)*	*E(S=1/2)*	*ΔE*	*ν(S=5/2)*	*ν (S=1/2)*
1	ATOJUO01	-3157.85	-3157.84	-8.72625	12.54	17.22
2	TAMTEH02	-4399.21	-4399.21	-3.47804	7.73	11.10
3	SUPHUH	-2865.69	-2865.68	-7.14870	14.33	12.88
4	BIMZUU	-2718.33	-2718.32	-8.90440	10.37	13.36
5	GOWSES	-2708.34	-2708.33	-9.37528	14.91	24.75
6	DADFAR	-3113.41	-3113.39	-9.57861	11.42	11.28
7	DADFOF	-5116.68	-5116.67	-9.07248	04.02	8.93
8	DADGAS	-2790.46	-2790.44	-10.72620	12.15	13.26
9	FONNAZ	-3113.78	-3113.76	-10.73816	13.99	10.13
10	HAJLAH	-2718.32	-2718.31	-7.92237	16.82	12.25
11	PORBUV	-8012.63	-8012.62	-6.83773	8.66	07.09
12	LIGZUY	-4077.09	-4077.08	-8.35673	11.40	11.44
13	LIZZUR	-2672.68	-2672.66	-9.01772	13.16	26.10
14	XIZKEY	-3460.25	-3460.24	-6.73197	07.02	5.66
15	XUJDOX	-2901.73	-2901.72	-8.19558	10.47	23.41
16	DETBEJ	-2641.73	-2641.72	-5.15064	12.37	22.60
17	FEWVIM	-2443.96	-2443.95	-3.63793	14.08	32.51
18	$[Fe(L_{19})py]^{+}$	-2831.47	-2831.46	-5.62529	17.47	22.33

Method: **B3LYP***

System	*Refcode*	*E(S=5/2)*	*E(S=1/2)*	*ΔE*	*ν(S=5/2)*	*ν (S=1/2)*
1	ATOJUO01	-3145.68	-3145.68	2.23979	12.09	18.66
2	TAMTEH02	-4383.00	-4383.01	3.670303	14.12	17.12
3	SUPHUH	-2852.44	-2852.45	5.98348	14.88	17.75
4	BIMZUU	-2706.13	-2706.13	2.85231	12.47	17.53
5	GOWSES	-2696.38	-2696.38	3.05123	16.26	21.88
6	DADFAR	-3099.88	-3099.89	3.79279	11.77	14.01
7	DADFOF	-5100.23	-5100.24	4.30647	9.94	12.01
8	DADGAS	-2777.76	-2777.77	2.80006	12.64	15.76
9	FONNAZ	-3100.41	-3100.41	2.28323	12.67	16.21
10	HAJLAH	-2706.11	-2706.11	2.98198	15.03	21.19
11	PORBUV	-7990.69	-7990.70	5.78267	9.21	9.34
12	LIGZUY	-4062.23	-4062.24	2.52559	8.60	12.29
13	LIZZUR	-2660.75	-2660.75	2.91777	16.13	20.14
14	XIZKEY	-3444.77	-3444.78	6.18430	6.13	7.72
15	XUJDOX	-2888.42	-2888.43	3.44719	13.67	18.34
16	DETBEJ	-2629.87	-2629.88	3.94010	20.97	25.42
17	FEWVIM	-2433.55	-2433.56	7.61202	17.92	36.59
18	$[Fe(L_{19})py]^{+}$	-2818.53	-2818.53	3.69018	21.88	25.28

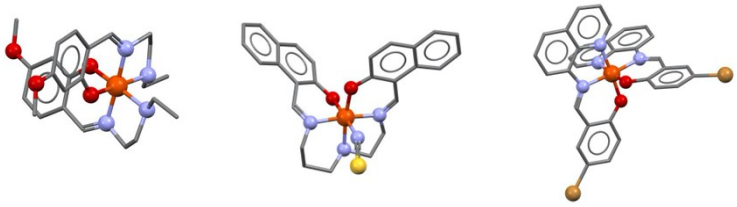
Method: **OPBE**

System	*Refcode*	*E(S=5/2)*	*E(S=1/2)*	*ΔE*	*ν(S=5/2)*	*ν (S=1/2)*
1	ATOJUO01	-3157.74	-3157.74	2.78935	13.16	20.92
2	TAMTEH02	-4399.00	-4399.00	0.02077	16.43	14.46
3	SUPHUH	-2865.42	-2865.43	2.37829	16.31	19.78
4	BIMZUU	-2718.11	-2718.10	-4.04334	12.54	18.75
5	GOWSES	-2708.11	-2708.11	-2.29771	16.80	24.01
6	DADFAR	-3113.16	-3113.16	-0.77115	12.76	15.14
7	DADFOF	-5117.23	-5117.22	-0.32357	11.03	13.88
8	DADGAS	-2790.21	-2790.20	-2.28512	13.13	16.14
9	FONNAZ	-3113.52	-3113.52	-2.14663	13.76	18.36
10	HAJLAH	-2718.09	-2718.09	-3.20042	15.48	23.22
11	PORBUV	-8014.04	-8014.04	1.99303	10.22	10.30
12	LIGZUY	-4076.94	-4076.95	3.19098	8.94	13.77
13	LIZZUR	-2672.48	-2672.47	-3.09089	13.65	23.84
14	XIZKEY	-3460.49	-3460.49	2.78306	7.30	8.66
15	XUJDOX	-2901.45	-2901.44	-3.85448	11.72	17.70
16	DETBEJ	-2641.53	-2641.52	-3.28918	6.26	16.53
17	FEWVIM	-2443.83	-2443.83	1.81802	18.06	39.68
18	$[Fe(L_{19})py]^{+}$	-2831.19	-2831.19	-3.67381	21.81	28.15

Method: **OLYP**

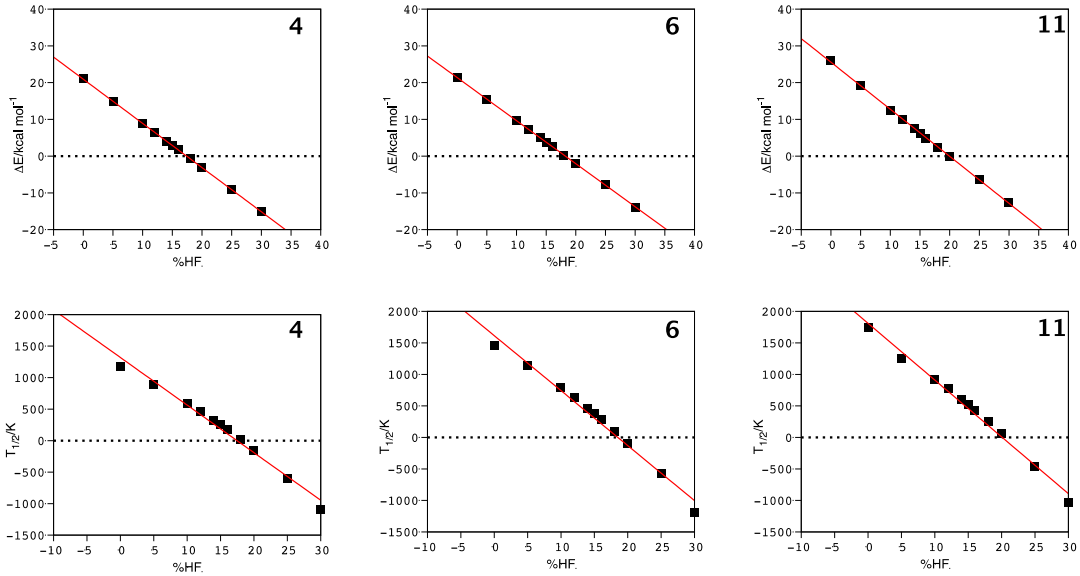
System	*Refcode*	*E(S=5/2)*	*E(S=1/2)*	*ΔE*	*ν(S=5/2)*	*ν (S=1/2)*
1	ATOJUO01	-3157.97	-3157.97	-1.75129	13.79	21.11
2	TAMTEH02	-4399.32	-4399.32	-2.46516	16.34	16.97
3	SUPHUH	-2865.62	-2865.62	-0.38274	15.74	19.54
4	BIMZUU	-2718.26	-2718.25	-6.17045	12.59	18.57
5	GOWSES	-2708.31	-2708.30	-4.84092	16.60	23.66
6	DADFAR	-3113.37	-3113.36	-3.81042	12.58	15.15
7	DADFOF	-5117.38	-5117.37	-3.42831	10.92	13.65
8	DADGAS	-2790.39	-2790.38	-4.90513	13.23	16.28
9	FONNAZ	-3113.73	-3113.73	-5.42070	12.82	17.27
10	HAJLAH	-2718.25	-2718.24	-5.62907	15.55	22.91
11	PORBUV	-8014.21	-8014.21	-0.92097	10.03	10.16
12	LIGZUY	-4077.27	-4077.26	-1.39940	9.59	13.87
13	LIZZUR	-2672.64	-2672.63	-6.18681	12.82	18.86
14	XIZKEY	-3460.42	-3460.42	-0.17500	6.95	8.49
15	XUJDOX	-2901.65	-2901.63	-6.43358	12.80	19.17
16	DETBEJ	-2641.67	-2641.66	-5.79526	14.31	15.49
17	FEWVIM	-2443.97	-2443.96	-1.21055	18.70	38.94
18	$[Fe(L_{19})py]^{+}$	-2831.37	-2831.36	-6.24158	21.15	27.94

S2 - Effect of the Hartree-Fock exchange mixing on the BLYP functional over the spin-state energy gap and computed $T_{1/2}$ for systems S4, S6 and S11



4 $[Fe(L_5)_2]^+$ **6** $[Fe(L_7)NCS]$ **11** $[Fe(L_{10})_2]^+$

L_5 = 2-(((2-(ethylamino)ethyl)imino)methyl)-5-methoxyphenolato L_7 = 1-(((3-((2-(((2-(Hydroxy)-1-naphthyl)methylene)amino)-ethyl)amino)propyl)imino)methyl)-2-naphtholato, L_{10} = 4-Bromo-2-(((quinolin-8-yl)imino)methyl)phenolato.



The amount of exact exchange Hartree-Fock to be mixed in the BLYP functional to match the experimental $T_{1/2}$ for systems S4, S6 and S11 (152, 151 and 298 K respectively) can be computed using the corresponding fitted models. These values will be 15.04%, 16.39% and 16.43% respectively for systems S4, S6 and S11.

S3. A data set collection of computational results is available in the ioChem-BD repository[1] and can be accessed via https://doi.org/10.19061/iochem-bd-6-108

[1] Álvarez-Moreno, M.; de Graaf, C.; Lopez, N.; Maseras, F.; Poblet, J.M.; Bo, C. J. Chem. Inf. Model. 2015, 55, 95,103.

Table S4: List of experimentally available data for the studied systems, including solvent and counterion when available, and the corresponding $T_{1/2}$, in bulk phase

System	*Refcode*	*Molecule*	*Solvent*	*Counterion*	$T_{1/2}$	*reference*
S1	ATOJUO01	[Fe(Hthsa)(thsa)]	H_2O	-	252	1
S2	TAMTEH02	$[(TPA)Fe(TCC)]^+$	-	$[PF_6]^-$	203-214	2
	CAMYAR	$[(TPA)Fe(TCC)]^+$	H_2O	ClO_4^-	253	3
	REWBAY	$[(TPA)Fe(TCC)]^+$		$[SbF_6]^-$	250	4
	TAMTEH	$[(TPA)Fe(TCC)]^+$	-	$[PF_6]^-$	204	3
	TAMTIL	$[(TPA)Fe(TCC)]^+$	H_2O	NO_3^-	245	3
S3	SUPHUH	$[Fe(qsal)_2]^+$	CH_3CN	$[Ni(dmise)_2]^-$	241-256	5
	VAWXIB	$[Fe(qsal)_2]^+$	CH_3CN	$[Ni(dmit)_2]^-$	194-231	6
	CIPVAB	$[Fe(qsal)_2]^+$	-	$[Ni(mnt)_2]^-$	35	7
	MUBPAA	$[Fe(qsal)_2]^+$	MeOH	$NCSe^-$	212-352	8
	MUBPEE	$[Fe(qsal)_2]^+$	CH_2Cl_2	$NCSe^-$	212-392	8
	QEDCUA	$[Fe(qsal)_2]^+$	MeCN	I^-	160	9
	QIXHIR	$[Fe(qsal)_2]^+$	-	$MeOSO_3$	402-414	10
	QIXJEP	$[Fe(qsal)_2]^+$	-	$[CF_3SO_3]^-$	361-365	10
	QORGUB	$[Fe(qsal)_2]^+$	MeOH	$[Fe(CN)_5(NO)]^-$	122	11
	QOYYEJ	$[Fe(qsal)_2]^+$	-	NCS^-	205-289	12
	QOYYOT	$[Fe(qsal)_2]^+$	-	$NCSe^-$	212-282	12
	RESZAT	$[Fe(qsal)_2]^+$	MeOH, H_2O	$[PhSO_3]^-$	195-205	13
	UVUTEL	$[Fe(qsal)_2]^+$	-	I_3^-	240	14
	WAWTAS	$[Fe(qsal)_2]^+$	-	Cl^-	268	15
S4	BIMZUU	$[Fe(4\text{-}OMe\text{-}salEen)_2]^+$	-	$[PF_6]^-$	225	16
	BINBEH	$[Fe(4\text{-}OMe\text{-}salEen)_2]^+$	-	NO_3^-	75.5-81	16
S5	GOWSES	$[Fe(salpet\text{-}Br)N_3]$	MeOH	-	140	17
S6	DADFAR	[Fe(napet)NCS]	MeCN	-	151	18
S7	DADFOF	[Fe(napet)NCSe]	MeCN	-	170	18
S8	DADGAS	[Fe(napet)NCO]	-	-	155	18
S9	FONNAZ	[Fe(salpet-3-OEt)NCS]	-	-	83	19
S10	HAJLAH	[Fe(3-OMe-salEen)2]+	-	$[PF_6]^-$	162.5-165.5	20
	ACOROA	[Fe(3-OMe-salEen)2]+	-	ClO_4^-	196	21
	GIRGOE	[Fe(3-OMe-salEen)2]+	MeOH	$[Ni(dmit)_2]^-$	345	22
	GIRGOE01	[Fe(3-OMe-salEen)2]+	-	$[Ni(dmit)_2]^-$	275	22
S11	PUGRIU	$[Fe(qsal\text{-}Br)_2]^+$	Acetone	$[Ni(dmit)_2]^-$	273-286	23
	JUGZUI	$[Fe(qsal\text{-}Br)_2]^+$	CH_2Cl_2	$[Ni(dmit)_2]^-$	250	23
	KORZAU	$[Fe(qsal\text{-}Br)_2]^+$	MeOH	NO_3^-	128-144, 229-234	24
	PORBUV	$[Fe(qsal\text{-}Br)_2]^+$	MeOH	NCS^-	340	25
	QOLPAL	$[Fe(qsal\text{-}Br)_2]^+$	H_2O	$[OTs]^-$	258-260	26
S12	LIGZUY	[Fe(5-Cl-Hthsa)(5-Cl-thsa)]	H_2O	-	230-231	1
S13	LIZZUR	$[Fe(Him)_2(hapen)]^+$	-	$[AsF_6]^-$	69.4-74.0	27
	GEWYEP	$[Fe(Him)_2(hapen)]^+$	-	$[SbF_6]^-$	105	28
	ZEWTIG	$[Fe(Him)_2(hapen)]^+$	H_2O	$[PF_6]^-$	78	29
	ZEWVAA	$[Fe(Him)_2(hapen)]^+$	H_2O	$CF_3SO_3^-$	50-200	29
S14	XIZKEY	$[Fe(Iqsal)_2]^+$	MeCN, H_2O	$[Ni(dmit)_2]^-$	150-156	30
	LECLUD	$[Fe(Iqsal)_2]^+$	-	$[NTf_2]^-$	244-278	31
	QOLPIT	$[Fe(Iqsal)_2]^+$	H_2O	$[OTs]^-$	298	26
	TAQZET	$[Fe(Iqsal)_2]^+$	EtOH	$[OTf]^-$	139-219	32
	TARBAS	$[Fe(Iqsal)_2]^+$	n-PrOH	$[OTf]^-$	199	32
	TARBAS02	$[Fe(Iqsal)_2]^+$	o-PrOH	$[OTf]^-$	251	32
	YICBIX	$[Fe(Iqsal)_2]^+$	MeOH	$[OTf]^-$	227-237	33
S15	XUJDOX	$[Fe(Him)_2(4\text{-}OMe\text{-}hapen)]^+$		$[PF_6]^-$	150	34
	PUKZIH	$[Fe(Him)_2(4\text{-}OMe\text{-}hapen)]^+$		$[MeSO_3]^-$	163-167	

	WUVRUC	$[Fe(Him)_2(4\text{-}OMe\text{-}hapen)]^+$		$[OTf]^-$	192-193	[35]
S16	DETBEJ	$[Fe(salten)(Pic)]^{2+}$	-	$[BPh_4]^-$	260	[36]
S17		$[Fe(acen)(Him)2]^+$	-	$[BPh_4]^-$	318	[37]
S18		$[Fe(py)(salten\text{-}3\text{-}OMe)]^+$		$[BPh_4]^-$	235-281	[38]

Table S5: List of experimentally available data for systems S11, S16, S17 and S18, including counterion when available, and the corresponding $T_{1/2}$, with measurements done in solution

System	***Molecule***	***Counterion***	***ΔH***	***ΔS***	***$T_{1/2}$***	***Reference***
S11	$[Fe(qsal\text{-}Br)_2]^+$				298[a]	[25]
S16	$[Fe(salten)(Pic)]^{2+}$	$[BPh_4]^-$	9.8	43.8	224	[37]
S17	$[Fe(acen)(Him)2]^+$	$[BPh_4]^-$	8.8	23.7	318	[37]
S18	$[Fe(py)(salten\text{-}3\text{-}OMe)]^+$	$[BPh_4]^-$	19.6	82.8	237	[38]

[a] The data in the SI of the publication indicates 49% of conversion at 298K, but no thermochemical data.

References:

1 E. W. T. Yemeli, G. R. Blake, A. P. Douvalis, T. Bakas, G. O. R. Alberda van Ekenstein and P. J. Koningsbruggen, *Chem. – A Eur. J.*, 2019, **25**, 16766–16776.

2 E. Collet, M.-L. Boillot, J. Hebert, N. Moisan, M. Servol, M. Lorenc, L. Toupet, M. Buron-Le Cointe, A. Tissot and J. Sainton, *Acta Crystallogr. Sect. B Struct. Sci.*, 2009, **65**, 474–480.

3 S. Floquet, A. J. Simaan, E. Rivière, M. Nierlich, P. Thuéry, J. Ensling, P. Gütlich, J.-J. Girerd and M.-L. Boillot, *Dalton Trans.*, 2005, 1734–1742.

4 A. Tissot, H. J. Shepherd, L. Toupet, E. Collet, J. Sainton, G. Molnár, P. Guionneau and M.-L. Boillot, *Eur. J. Inorg. Chem.*, 2013, **2013**, 1001–1008.

5 K. Takahashi, H. Mori, H. Kobayashi and O. Sato, *Polyhedron*, 2009, **28**, 1776–1781.

6 K. Takahashi, H. Cui, H. Kobayashi, Y. Einaga and O. Sato, *Chem. Lett.*, 2005, **34**, 1240–1241.

7 K. Takahashi, T. Sakurai, W.-M. Zhang, S. Okubo, H. Ohta, T. Yamamoto, Y. Einaga and H. Mori, *Inorganics*, 2017, **5**, 54.

8 S. Hayami, Z. Gu, H. Yoshiki, A. Fujishima and O. Sato, *J. Am. Chem. Soc.*, 2001, **123**, 11644–11650.

9 I.-R. Jeon, C. Mathonière, R. Clérac, M. Rouzières, O. Jeannin, E. Trzop, E. Collet and M. Fourmigué, *Chem. Commun.*, 2017, **53**, 10283–10286.

10 K. Takahashi, K. Yamamoto, T. Yamamoto, Y. Einaga, Y. Shiota, K. Yoshizawa and H. Mori, *Crystals*, 2019, **9**, 81.

11 T. Togo, S. A. Amolegbe, R. Yamaguchi, T. Kuroda-Sowa, M. Nakaya, K.

Shimayama, M. Nakamura and S. Hayami, *Chem. Lett.*, 2013, **42**, 1542–1544.
12 S. Hayami, K. Hiki, T. Kawahara, Y. Maeda, D. Urakami, K. Inoue, M. Ohama, S. Kawata and O. Sato, *Chem. - A Eur. J.*, 2009, **15**, 3497–3508.
13 A. Tsukiashi, M. Nakaya, F. Kobayashi, R. Ohtani, M. Nakamura, J. M. Harrowfield, Y. Kim and S. Hayami, *Inorg. Chem.*, 2018, **57**, 2834–2842.
14 K. Takahashi, T. Sato, H. Mori, H. Tajima and O. Sato, *Phys. B Condens. Matter*, 2010, **405**, S65–S68.
15 I.-R. Jeon, O. Jeannin, R. Clérac, M. Rouzières and M. Fourmigué, *Chem. Commun.*, 2017, **53**, 4989–4992.
16 A. Tissot, P. Fertey, R. Guillot, V. Briois and M.-L. Boillot, *Eur. J. Inorg. Chem.*, 2014, **2014**, 101–109.
17 C. Krüger, P. Augustín, L. Dlháň, J. Pavlik, J. Moncol', I. Nemec, R. Boča and F. Renz, *Polyhedron*, 2015, **87**, 194–201.
18 I. Nemec, R. Herchel, R. Boča, Z. Trávníček, I. Svoboda, H. Fuess and W. Linert, *Dalton Trans.*, 2011, **40**, 10090–10099.
19 P. Masárová, P. Zoufalý, J. Moncol, I. Nemec, J. Pavlik, M. Gembický, Z. Trávníček, R. Boča and I. Šalitroš, *New J. Chem.*, 2015, **39**, 508–519.
20 A. Tissot, R. Bertoni, E. Collet, L. Toupet and M.-L. Boillot, *J. Mater. Chem.*, 2011, **21**, 18347.
21 S. Hayami, S. Miyazaki, M. Yamamoto, K. Hiki, N. Motokawa, A. Shuto, K. Inoue, T. Shinmyozu and Y. Maeda, *Bull. Chem. Soc. Jpn.*, 2006, **79**, 442–450.
22 C. Faulmann, K. Jacob, S. Dorbes, S. Lampert, I. Malfant, M.-L. Doublet, L. Valade and J. A. Real, *Inorg. Chem.*, 2007, **46**, 8548–8559.
23 B. J. C. Vieira, J. C. Dias, I. C. Santos, L. C. J. Pereira, V. da Gama and J. C. Waerenborgh, *Inorg. Chem.*, 2015, **54**, 1354–1362.
24 D. J. Harding, W. Phonsri, P. Harding, K. S. Murray, B. Moubaraki and G. N. L. Jameson, *Dalton Trans.*, 2015, **44**, 15079–15082.
25 W. Phonsri, D. J. Harding, P. Harding, K. S. Murray, B. Moubaraki, I. A. Gass, J. D. Cashion, G. N. L. Jameson and H. Adams, *Dalton Trans.*, 2014, **43**, 17509–17518.
26 S. E. Lazaro, A. Alkaş, S. J. Lee, S. G. Telfer, K. S. Murray, W. Phonsri, P. Harding and D. J. Harding, *Dalton Trans.*, 2019, **48**, 15515–15520.
27 T. Fujinami, M. Koike, N. Matsumoto, Y. Sunatsuki, A. Okazawa and N. Kojima, *Inorg. Chem.*, 2014, **53**, 2254–2259.
28 T. Ueno, K. Miyano, D. Hamada, H. Ono, T. Fujinami, N. Matsumoto and Y. Sunatsuki, *Magnetochemistry*, 2015, **1**, 72–82.
29 M. Koike, K. Murakami, T. Fujinami, K. Nishi, N. Matsumoto and Y. Sunatsuki, *Inorganica Chim. Acta*, 2013, **399**, 185–192.
30 K. Fukuroi, K. Takahashi, T. Mochida, T. Sakurai, H. Ohta, T. Yamamoto, Y. Einaga and H. Mori, *Angew. Chemie Int. Ed.*, 2014, **53**, 1983–1986.
31 N. Phukkaphan, D. L. Cruickshank, K. S. Murray, W. Phonsri, P. Harding and D. J. Harding, *Chem. Commun.*, 2017, **53**, 9801–9804.
32 W. Phonsri, P. Harding, L. Liu, S. G. Telfer, K. S. Murray, B. Moubaraki, T. M. Ross, G. N. L. Jameson and D. J. Harding, *Chem. Sci.*, 2017, **8**, 3949–3959.
33 D. J. Harding, W. Phonsri, P. Harding, I. A. Gass, K. S. Murray, B. Moubaraki, J. D. Cashion, L. Liu and S. G. Telfer, *Chem. Commun.*, 2013, **49**, 6340.
34 T. Fujinami, M. Ikeda, M. Koike, N. Matsumoto, T. Oishi and Y. Sunatsuki, *Inorganica Chim. Acta*, 2015, **432**, 89–95.
35 K. Miyano, T. Nishida, H. Ono, D. Hamada, T. Fujinami, N. Matsumoto and Y. Sunatsuki, *Inorganica Chim. Acta*, 2016, **439**, 49–54.

36 N. Matsumoto, S. Ohta, C. Yoshimura, A. Ohyoshi, S. Kohata, H. Okawa and Y. Maeda, *J. Chem. Soc., Dalton Trans.*, 1985, 2575.
37 M. Y. Volkov, E. N. Frolova, L. V. Mingalieva, L. G. Gafiyatullin, O. A. Turanova, E. O. Milordova, I. V. Ovchinnikov and A. N. Turanov, *Polyhedron*, 2018, **154**, 407–410.
38 A. Ohyoshi, J. Honbo, N. Matsumoto, S. Ohta and S. Sakamoto, *Bull. Chem. Soc. Jpn.*, 1986, **59**, 1611–1613.