Electronic Supplementary Information

$Fe^{II/III}$ and Mn^{II} complexes based on 2,4,6-tris(2-pyridyl)-triazine: Synthesis, structures, magnetic and biological properties

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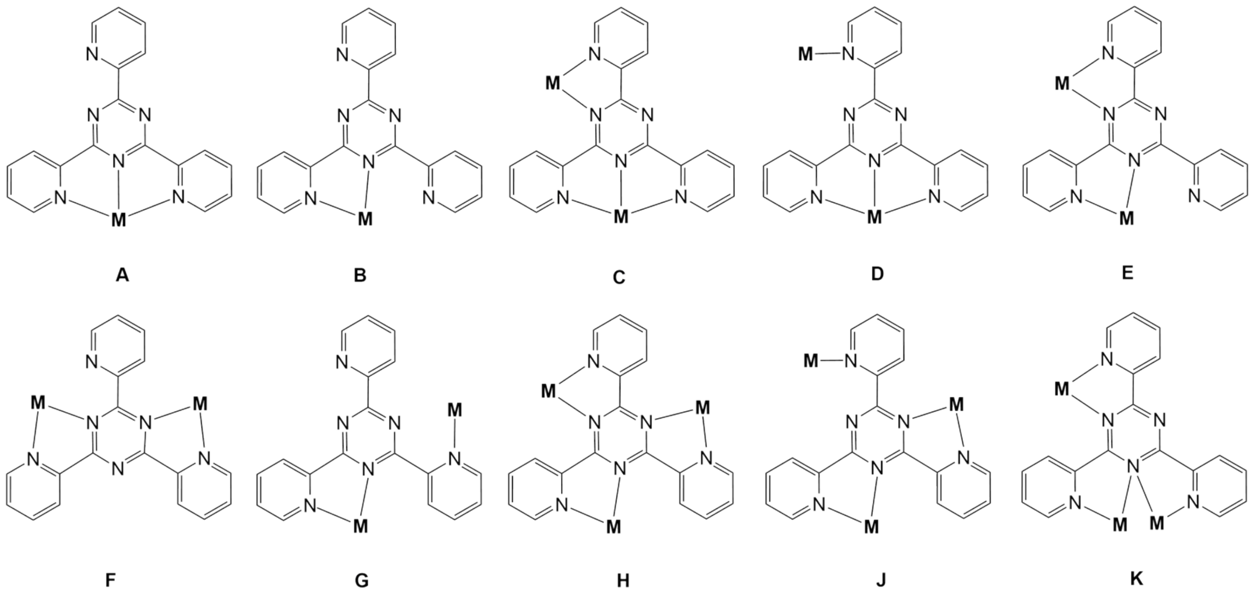

Table S1. Coordination modes displayed by the tpt ligand in its metal complexes.

N	CSD code	Compound	Coord-ination mode	References	Metal ion
1	ABEZUD	$[Ru(tpt)(PPh_3)_2(Cl)]BF_4{\cdot}H_2O$	**A**	S. Sharma, M. Chandra, D.S. Pandey, *Eur. J. Inorg. Chem.*, 2004, 3555, DOI: 10.1002/ejic.200400069	Ru(II)
2	ABIBAP	$[Ru(tpt)(AsPh_3)_2(Cl)]BF_4{\cdot}H_2O$	**A**		Ru(II)
3	ABIBET	$[Ru(tpt)(PPh_3)(dtc)]Cl{\cdot}H_2O$	**A**		Ru(II)
4	ACOKIN	$[Mn(tpt)(N_3)_2]_n$	**A**	A. Das, G.M. Rosair, M.S. El Fallah, J. Ribas, S. Mitra, *Inorg. Chem.*, 2006, **45**, 3301, DOI: 10.1021/ic052088t	Mn(II)
5	ACUGIP	$[La(tpt)(NO_3)_3(MeOH)_2]$	**A**	S.A. Cotton, V. Franckevicius, M.F. Mahon, Li Ling Ooi, P.R. Raithby, S.J. Teat, *Polyhedron*, 2006, **25**, 1057, DOI: 10.1016/j.poly.2005.12.012	La(III)
6	ACUGOV	$[La(tpt)(NO_3)_3(H_2O)]{\cdot}$acetone	**A**		La(III)
7	ACUGUB	$[Y(tpt)(NO_3)_3(H_2O)]{\cdot}EtOH$	**A**		Y(III)
8	ACUHAI	$[La(tpt)(NO_3)_3(H_2O)]{\cdot}EtOH$	**A**		La(III)
9	ACUHEM	$[Ce(tpt)(NO_3)_3(H_2O)]{\cdot}EtOH$	**A**		Ce(III)
10	ACUHIQ	$[Pr(tpt)(NO_3)_3(H_2O)]{\cdot}EtOH$	**A**		Pr(III)
11	ACUHOW	$[Nd(tpt)(NO_3)_3(H_2O)]{\cdot}EtOH$	**A**		Nd(III)
12	ACUHUC	$[Sm(tpt)(NO_3)_3(H_2O)]{\cdot}EtOH$	**A**		Sm(III)
13	ACUJAK	$[Eu(tpt)(NO_3)_3(H_2O)]{\cdot}EtOH$	**A**		Eu(III)
14	ACUJEO	$[Gd(tpt)(NO_3)_3(H_2O)]{\cdot}EtOH$	**A**		Gd(III)
15	ACUJIS	$[Tb(tpt)(NO_3)_3(H_2O)]{\cdot}EtOH$	**A**		Tb(III)
16	ACUJOY	$[Dy(tpt)(NO_3)_3(H_2O)]{\cdot}EtOH$	**A**		Dy(III)
17	ACUJUE	$[Ho(tpt)(NO_3)_3(H_2O)]{\cdot}EtOH$	**A**		Ho(III)
18	ACUKAL	$[Er(tpt)(NO_3)_3(H_2O)]{\cdot}EtOH$	**A**		Er(III)
19	ACUKEP	$[Tm(tpt)(NO_3)_3(H_2O)]{\cdot}EtOH$	**A**		Tm(III)

20	ACUKIT	$[Yb(tpt)(NO_3)_3(H_2O)]\cdot EtOH$	**A**		Yb(III)
21	ACUKOZ	$[Yb(tpt)(NO_3)_3(EtOH)]\cdot EtOH$	**A**		Yb(III)
22	ACUKUF	$[Lu(tpt)(NO_3)_3(EtOH)]\cdot EtOH$	**A**		Lu(III)
23	ACULAM	$[Lu(tpt)(NO_3)_3(H_2O)]\cdot MeCN$	**A**		Lu(III)
24	ACULEQ	$[Lu(tpt)(NO_3)_2(H_2O)_2]NO_3\cdot MeOH$	**A**		Lu(III)
25	AFATEG	$[Ni(tpt)(H_2O)_3](NO_3)_2\cdot 3H_2O$	**A**	E. Freire, S. Baggio, J.C. Munoz, R. Baggio, *Acta Cryst. C*, 2002, **58**, m221, DOI: 10.1107/S0108270102002834	Ni(II)
26	AHIJEI	$[(UO_2)_2(tpt)_2(BrC_8H_3O_4)_2]\cdot 2H_2O$	**A**	S.G. Thangavelu, S.J.A. Pope, Ch.L. Cahill, *CrystEngComm*, 2015, **17**, 6236, DOI: 10.1039/C5CE00984G	U(VI)
27	AHIJIM	$[(UO_2)_2(tpt)_2(ClC_8H_3O_4)_2]\cdot 4H_2O$	**A**		U(VI)
28	AHIJOS	$[(UO_2)_2(tpt)_2(C_8H_3IO_4)_2]\cdot 2PrOH$	**A**		U(VI)
29	AHIJUY	$[(UO_2)_2(tpt)_2(C_9H_6O_4)_2]\cdot 2H_2O$	**A**		U(VI)
30	AHIKAF	$[(UO_2)_2(tpt)_2(C_6H_2O_4S)_2]\cdot 4H_2O$	**A**		U(VI)
31	AHUJOF	$[Ru(tpt)(MeCN)(Cl)_2]\cdot MeCN\cdot 0.68H_2O$	**A**	M. Daryanavard, H. Hadadzadeh, M. Weil, H. Farrokhpour, *J. CO₂ Util.*, 2017, **17**, 80, DOI: 10.1016/j.jcou.2016.11.009	Ru(II)
32	AQELUE	$[Mn(tpt)(Br)_2(H_2O)]\cdot H_2O$	**A**	K. Ha, *Z. Kristallogr. NCS*, 2011, 226, 57, DOI: 10.1524/ncrs.2011.0028	Mn(II)
33	ASAKEK	$[Bi(tpt)(C_6F_5S)_3]$	**A**	J.P.H. Charmant, A.H.M.M. Jahan, N.C. Norman, A.G. Orpen, T.J. Podesta, *CrystEngComm*, 2004, **6**, 29, DOI: 10.1039/b315176j	Bi(III)
34	AYOMAD	$[Mn(tpt)(MeCO_2)_2(H_2O)]\cdot H_2O$	**A**	K. Ha, *Acta Cryst. E*, 2011, **67**, m1238, DOI: 10.1107/S1600536811032016	Mn(II)
35	AZIZUF	$[Pb_2(tpt)_2(MeCO_2)_2(N_3)_2]$	**A**	M. Dayani, A. Ghaemi, S.W. Ng, E.R.T. Tiekink, *Acta Cryst. E*, 2011, **67**, m1419, DOI: 10.1107/S1600536811038116	Pb(II)
36	BALYIX	$[Pb(tpt)_2(ClO_4)(H_2O)]ClO_4\cdot 2H_2O$	**A**	J.M. Harrowfield, H. Miyamae, B.W. Skelton, A.A. Soudi, A.H. White, *Aust. J. Chem.*, 2002, **55**, 661, DOI: 10.1071/CH02083	Pb(II)
37	BEJFUR	$[Hg_4(tpt)_2(CF_3CO_2)_8]$	**C**	J. Halfpenny, R.W.H. Small, *Acta Cryst. B*, 1982, **38**, 939, DOI: 10.1107/S0567740882004506	Hg(II)
38	BEMGUW	$[Cu_2(tpt)(MeOH)(Cl)_4]$	**C**	T. Glaser, T. Lugger, R. Fröhlich, *Eur. J. Inorg. Chem.*, 2004, 394, DOI: 10.1002/ejic.200300443	Cu(II)
39	BENHAD	$[Cu(tpt)(Medpt)](BF_4)_2\cdot 2MeOH$	**A**		Cu(II)
40	BIWWUA	$[Ni(tpt)(Hsalagluc)]ClO_4\cdot MeOH$	**A**	A. Burkhardt, W. Plass, *Inorg. Chem. Commun.*, 2008, **11**, 303, DOI: 10.1016/j.inoche.2007.12.006	Ni(II)
41	BOPKEX	$[Tb_{0.1}Gd_{0.9}(tpt)(H_2O)_6]Cl_3\cdot 3H_2O$	**A**	Y.-F. Zhao, Y.-L. Zhao, F. Bai, Y. Wang, *J. Fluoresc.*, 2009, **19**, 179, DOI: 10.1007/s10895-008-0401-7	Gd(III) Tb(III)
42	BOZNIO	[Ni(tpt)(*i*-PrOpdt)$_2$]	**A**	M.C. Aragoni, M. Arca, M. Crespo, F.A. Devillanova, M.B. Hursthouse, S.L. Huth, F. Isaia, V. Lippolis, G. Verani, *Dalton Trans.*, 2009, 2510, DOI:10.1039/b819326f	Ni(II)
43	BOZNOU	$[Ni(tpt)(EtOpdt)_2]$	**A**		Ni(II)
44	BOZNUA	$[Ni(tpt)(PrOpdt)_2]$	**A**		Ni(II)
45	BOZPAI	$[Ni(tpt)(BuOpdt)_2]$	**A**		Ni(II)
46	BOZPEM	$[Ni(tpt)((EtO)_2(PS_2))_2]$	**A**		Ni(II)
47	BOZPIQ	$[Ni(tpt)(EtOpdt)(H_2O)]NO_3$	**A**		Ni(II)
48	BUDNOF	$[Mn_2(tpt)_2(N_3)_2(NO_3)_2(H_2O)]$	**A**	P. Wang, L. Kong, D. Zhang, *J. Chem. Res.*, 2014, **38**, 477, DOI:10.3184/174751914X14052744149037	Mn(II)
49	BUFRUQ	$[Ni_2(tpt)_2(SO_4)_2(H_2O)_2]\cdot 6H_2O$	**A**	M.C. Aragoni, M. Arca, M. Crespo, F.A.	Ni(II)

				Devillanova, M.B. Hursthouse, S.L. Huth, F. Isaia, V. Lippolis, G. Verani, *Dalton Trans.*, 2009, 2510, DOI:10.1039/b819326f	
50	CICXIW	$[Cd(tpt)Cl_2]\cdot 3H_2O$	**A**	H.-Zh. Xie, W.-J. Pan, *Acta Cryst. C*, 2007, **63**, m204, DOI: 10.1107/S0108270107015703	Cd(II)
51	COMNAV	$[Cu(tpt)(Ph_3P)_2]NO_3\cdot H_2O$	**B**	A. Báez-Castro, J. Baldenebro-López, A. Cruz-Enríquez, H. Höpfl, D. Glossman-Mitnik, M.-S. Valentín, M. Parra-Hake, J.J. Campos-Gaxiola, *RSC Advances*, 2014, **4**, 42624, DOI: 10.1039/C4RA06512C	Cu(I)
52	CUZLUG	$\{Na_2[(UO_2)_2(adc)_2(pca)_2](tpt)_2\}_n$	**A**	S.G. Thangavelu, Ch.L. Cahill, *Cryst. Growth Des.*, 2016, **16**, 42, DOI: 10.1021/acs.cgd.5b00778	UO_2, Na(I)
53	DAHTIR	$[Ru(tpt)(P\text{-}PPh_2Py)_2Cl]BF_4\cdot H_2O$	**A**	P. Kumar, A.K. Singh, R. Pandey, D.S. Pandey, *J. Organomet. Chem.*, 2011, **696**, 3454, DOI: 10.1016/j.jorganchem.2011.06.031	Ru(II)
54	DEBTEK	$[Ru(tpt)(PPh_3)_2Cl]PF_6$	**A**	K.S. Singh, Yu.A. Mozharivskyj, M.R. Kollipara, *Z. Anorg. Allg. Chem.*, 2006, **632**, 172, DOI: 10.1002/zaac.200500301	Ru(II)
55	DEJGIJ	$[Cu_2(tpt)(CN)_2]_n$	**E**	X.-P. Zhou, D. Li, T. Wu, X. Zhang, *Dalton Trans.*, 2006, 2435, DOI: 10.1039/b517969f	Cu(I)
56	DEJGOP	$[Cu_2(tpt)(CN)(SCN)]_n$	**E**		Cu(I)
57	DEJGUV	$[Cu_2(tpt)(SCN)_2]_n$	**A**		Cu(I)
58	DEMLUD	$[Cu_2(tpt)(CN)_2]_n$	**F**		Cu(I)
59	DIDVOC	$[Cu(tpt)(2\text{-}pa)]N(CN)_2\cdot 7H_2O$	**A**	Q.-H. Zhao, M.-S. Zhang, R.-B. Fang, *J. Struct. Chem.*, 2006, **47**, 764, DOI: 10.1007/s10947-006-0367-8	Cu(II)
60	DIYLAZ	$[Ru(tpt)(PPh_3)Cl_2]$	**A**	S. Sharma, S.K. Singh, D.S. Pandey, *Inorg. Chem.*, 2008, **47**, 1179, DOI: 10.1021/ic701518e	Ru(II)
61	DIYLED	$[Ru(tpt)(dppm)Cl]BF_4$	**A**		Ru(II)
62	DIYLIH	$[Ru(tpt)(PPh_3)(pa)]Cl\cdot CH_2Cl_2\cdot H_2O$	**A**		Ru(II)
63	DIYLON	$[Ru_2(tpt)(PPh_3)(cym)Cl_3]PF_6\cdot H_2O$	**C**		Ru(II)
64	DIYLUT	$[RuRh(tpt)(PPh_3)(Cp)Cl_3]BF_4\cdot H_2O$	**C**		Ru(II), Rh(II)
65	ECAKUO	$[Re(tpt)(CO)_3Cl]$	**B**	X. Chen, F.J. Femia, J.W. Babich, J.A. Zubieta, *Inorg. Chem.*, 2001, **40**, 2769, DOI: 10.1021/ic000446g	Re(I)
66	ECALAV	$[Re(tpt)(CO)_3Br]$	**B**		Re(I)
67	ECALEZ	$[Re(tpt)(CO)_3Cl]_2\cdot$acetone	**F**		Re(I)
68	ECALID	$[Re(tpt)(CO)_3Br]_2\cdot$acetone	**F**		Re(I)
69	ECALOJ	$[Re(tpt)(CO)_3Br]_2\cdot CH_2Cl_2\cdot 0.5H_2O$	**F**		Re(I)
70	ELUWIT	$[Ru(tpt)(dmbpy)Cl]PF_6\cdot dmf\cdot 2H_2O$	**A**	H. Hadadzadeh, H. Farrokhpour, J. Simpson, J. Shakeri, M. Daryanavard, M. Shokrollahi, *New J. Chem.*, 2016, **40**, 6347, DOI: 10.1039/C5NJ03600C	Ru(II)
71	EMELIS	$[Mn(tpt)(MeCO_2)(H_2O)_2]NO_3\cdot H_2O$	**A**	M.M. Najafpour, D.M. Boghaei, V. McKee, *Polyhedron*, 2010, **29**, 3246, DOI: 10.1016/j.poly.2010.09.001	Mn(II)
72	EREVED	$[Nd(tpt)(NO_3)_3(H_2O)]\cdot 2H_2O$	**A**	J. Zhou, G.-X. Lu, Y.-G. Zhang, D.-Y. Wei, *Acta Cryst. E*, 2011, **67**, m699, DOI: 10.1107/S1600536811014589	Nd(III)
73	EREWEF	$\{[Ni(tpt)(H_2O)_3][Ni(tpt)(Cl)(H_2O)_2]\}Cl_3\cdot 5H_2O$	**A**	A. Boshala, I. Warad, U. Flörke, *CSD Communication*, 2016.	Ni(II)
74	ETIHOG	$[Cu_4(tpt)_2(MeCN)_2(C_2H_4)_2](PF_6)_4\cdot$	**K**	M. Maekawa, K. Sugimoto, T. Okubo, T.	Cu(I)

		MeEtCO		Kuroda-Sowa, M. Munakata, *ChemistrySelect*, 2016, **1**, 3812, DOI: 10.1002/slct.201600791	
75	EYIMUU	$[Zn(tpt)_2]S_2O_8\cdot 2H_2O$	**A**	M.A. Harvey, S. Baggio, A. Ibanez, R. Baggio, *Acta Cryst. C*, 2004, **60**, m375, DOI: 10.1107/S0108270104014337	Zn(II)
76	FEGNOW	$\{[Pr(tpt)(fa)_3]\cdot H_2O\}_n$	**A**	N. Lopez, H. Zhao, D. Zhao, H.-C. Zhou, J.P. Riebenspies, K.R. Dunbar, *Dalton Trans.*, 2013, **42**, 54, DOI: 10.1039/c2dt31842c	Pr(III)
77	FEGNUC	$\{[Sm(tpt)(fa)_3]\cdot H_2O\}_n$	**A**		Sm(III)
78	FIGGAE	$[Mn(tpt)(MeCO_2)(H_2O)_2]ClO_4$	**A**	A. Majumder, C.R. Choudhury, S. Mitra, C. Marschner, J. Baumgartner, *Z. Naturforsch. B*, 2005, **60**, 99, DOI: 10.1515/znb-2005-0115	Mn(II)
79	FIGGEI	$[Co(tpt)(SO_4)(H_2O)_2]\cdot H_2O$	**A**		Co(II)
80	FOLXAG	$[Ag_2(tpt)(dppm)_2(dmf)](BF_4)_2\cdot dmf$	**B**	L. Zhang, X.-Q. Lü, Q. Zhang, Ch.-L. Chen, B.-Sh. Kang, *Trans. Met. Chem.*, 2005, **30**, 76, DOI: 10.1007/s11243-004-3000-8	Ag(I)
81	FOLXEK	$\{[Ag_2(tpt)_2(dppe)_2](BF_4)_2\cdot MeOH\cdot 4H_2O\}_n$	**B**		Ag(I)
82	FOLXIO	$[Ag_2(tpt)_2(dppp)_2](BF_4)_2$	**B**		Ag(I)
83	FOLXOU	$[Ag_2(tpt)_2(dppb)_2](BF_4)_2$	**A**		Ag(I)
84	GADLON	$[Cd_2(tpt)_2(SO_4)_2(H_2O)_2]\cdot 4H_2O$	**A**	M. Harvey, S. Baggio, S. Russi, R. Baggio, *Acta Cryst. C*, 2003, **59**, m171, DOI: 10.1107/S0108270103006462	Cd(II)
85	GIHQAQ	$[Mn(tpt)(MeOH)(Cl)_2]\cdot H_2O$	**A**	H. Zhao, M. Shatruk, A.V. Prosvirin, K.R. Dunbar, *Chem. Eur. J.*, 2007, **13**, 6573, DOI: 10.1002/chem.200700298	Mn(II)
86	GIHQEU	$[Mn(tpt)(NO_3)(H_2O)_2]NO_3\cdot 1.5H_2O$	**A**		Mn(II)
87	GIHQIY	$[Mn_2(tpt)_2(MeCO_2)_2(H_2O)_4]$ $[Mn_2W_2(tpt)_2(CN)_{16}(MeOH)_{3.16}$ $(H_2O)_{0.84}]\cdot 5MeOH\cdot 9.85H_2O$	**A**		Mn(II), W(V)
88	GIHQOE	$\{[Mn_2W(tpt)_2(CN)_8(MeOH)_2]\cdot 2MeOH\}_n$	**A**		Mn(II), W(IV)
89	GIHQUK	$\{[Mn_2W(tpt)_2(CN)_8(MeCO_2)(MeOH)_3]$ $\cdot 3.5MeOH\cdot 0.25H_2O\}_n$	**A**		Mn(II), W(IV)
90	GIHRAR	$[Mn_6W_4(tpt)_6(CN)_{32}(MeOH)_4(dmf)_2]\cdot 2.3MeOH\cdot 8.2H_2O$	**A**		Mn(II), W(V)
91	GIHREV	$\{[Mn_2W(tpt)_2(CN)_8(MeOH)_3]$ $[MnW(tpt)(CN)_8(MeOH)]\cdot MeOH\cdot 2H_2O\}_n$	**A**		Mn(II), W(V)
92	GIHRIZ	$[Mn_4W_2(tpt)_4(CN)_{16}(MeOH)_4(NO_3)_2$ $(dmf)_2]\cdot 6MeOH$	**A**		Mn(II), W(V)
93	GOLPUS	$[Sn(tpt)(Me)_2(Cl)_2][Sn(Me)_2(Cl)_2$ $(H_2O)]$	**A**	K.M. Lo, V.G.K. Das, S.W. Ng, *Acta Cryst. C*, 1999, **55**, 1058, DOI: 10.1107/S0108270199004928	Sn(II)
94	GULPAF	$[(AgCN)_3(tpt)]_n$	**D**	J.-D. Lin, M.-Zh. Lin, C.-C. Jia, Zh.-H. Li, Sh.-W. Du, *Inorg. Chem. Commun.*, 2009, **12**, 487, DOI: 10.1016/j.inoche.2009.04.002	Ag(I)
95	GUTHOV	$[Ni_3(tpt)_3(saltag^{Br})]NO_3$	**A**	M. Böhme, A.E. Ion, B. Kintzel, A. Buchholz, H. Görls, W. Plass, *Z. Anorg. Allg. Chem.*, 2020, **646**, 999, DOI: 10.1002/zaac.202000054	Ni(II)
96	GUTHUB	$[Ni_5(tpt)_4(saltag^{Br})_2]$	**A**		Ni(II)
97	HAZBAN	$[Ag_4(tpt)_2(F_3CCO_2)_4(H_2O)]_n$	**C**	G. Meyer, M. Sehabi, I. Pantenburg, *Design and Construction of Coordination Polymers*, Wiley, 2009, DOI: 10.1002/9780470467336	Ag(I)
98	HOLDOB	$[Eu(tpt)(Cl)_3(MeOH)_2]\cdot MeOH$	**A**	R. Wietzke, M. Mazzanti, J.-M. Latour,	Eu(III)

99	HOLDUH	$[Pr(tpt)(O_2CMe)_3]_2 \cdot 2MeOH$	**A**	J. Pecaut, *Inorg. Chem.*, 1999, **38**, 3581, DOI: 10.1021/ic990122w	Pr(III)
100	HUJKOM	$[Fe(tpt)(Cl)_3] \cdot MeCN \cdot 0.5H_2O$	**A**	S.A. Cotton, V. Franckevicius, J. Fawcett, *Polyhedron*, 2002, **21**, 2055, DOI: 10.1016/S0277-5387(02)01137-3	Fe(III)
101	IDAPUA	$[Mn(tpt)(Br)_2]$	**A**	K. Ha, *Acta Cryst. E*, 2011, **67**, m1655, DOI: 10.1107/S1600536811045211	Mn(II)
102	IGALAD	$[RuH(CO)(PPh_3)_2(tpt)]BF_4$	**B**	M. Chandra, A.N. Sahay, D.S. Pandey, M.C. Puerta, P. Valerga, *J. Organomet. Chem.*, 2002, **648**, 39, DOI: 10.1016/S0022-328X(01)01470-X	Ru(II)
103	IGAWOC	$[Rh(tpt)(Cl)_3] \cdot dmso$	**A**	F.P. Pruchnik, P. Jakimowicz, Z. Ciunik, J. Zakrzewska-Czerwinska, A. Opolski, J. Wietrzyk, E. Wojdat, *Inorg. Chim. Acta*, 2002, **334**, 59, DOI: 10.1016/S0020-1693(02)00776-4	Rh(III)
104	IQESAY	$[Eu(tpt)(dbm)_3] \cdot Me_2CO$	**A**	C.R. De Silva, J. Wang, M.D. Carducci, S.A. Rajapakshe, Z. Zheng, *Inorg. Chim. Acta*, 2004, **357**, 630, DOI: 10.1016/j.ica.2003.08.006	Eu(III)
105	IZOGIO	$[Mn(tpt)(tda)(H_2O)] \cdot 2H_2O$	**A**	A. Grirrane, A. Pastor, A. Galindo, E. Alvarez, C. Mealli, A. Ienco, A. Orlandini, P. Rosa, A. Caneschi, A.-L. Barra, J.F. Sanz, *Chem. Eur. J.*, 2011, **17**, 10600, DOI: 10.1002/chem.201100988	Mn(II)
106	IZOGOU	$[Mn(tpt)(tda)(H_2O)]_2 \cdot 2H_2O$	**A**		Mn
107	JATJEU	$[Os(tpt)(PPh_3)_2(Cl)]BF_4 \cdot H_2O$	**A**	S.K. Singh, S. Sharma, M. Chandra, D.S. Pandey, *J. Organomet. Chem.*, 2005, **690**, 3105, DOI:10.1016/j.jorganchem.2005.03.051	Os(III)
108	JATRUR	$[Cu(tpt)(pca)_2]CF_3SO_3$	**A**	J. Faus, M. Julve, J.M. Amigo, T. Debaerdemaeker, *J. Chem. Soc., Dalton Trans.*, 1989, 1681, DOI: 10.1039/dt9890001681	Cu(II)
109	JEBCAX	$[Ni(tpt)(Cl)_2(H_2O)] \cdot H_2O$	**A**	N.K. Yagci, K. Guven, G.D. Yildiz, *Z. Kristallogr. NCS*, 2017, **232**, 485, DOI: 10.1515/ncrs-2016-0332	Ni(II)
110	JEQTUV	$[Rh(tpt)(Cl)(Cp^*)]BF_4 \cdot dcm$	**B**	S.K. Singh, M. Chandra, S.K. Dubey, D.S. Pandey, *Eur. J. Inorg. Chem.*, 2006, 3954, DOI: 10.1002/ejic.200600355	Rh(III)
111	JUTJUG	$\{[Cd(tpt)(pa)(H_2O)] \cdot 2dmf\}_n$	**A**	J.-F. Chu, Sh.-Y. Wang, J.-C. Liu, H.-B. Hu, Q.-X. Xu, *Z. Anorg. Allg. Chem.*, 2020, **646**, 420, DOI: 10.1002/zaac.202000112	Cd(II)
112	JUXPEX	$[AuRu_2(tpt)_2(terpy)_2](ClO_4)_5 \cdot H_2O$	**C**	N. Gupta, N. Grover, A. Neyhart, P. Singh, H.H. Thorp, *Inorg. Chem.*, 1993, **32**, 310, DOI: 10.1021/ic00055a014	Ru(II), Ag(I)
113	KANNOE	$[Cu_2(tpt)_2(dpaa)_2](ClO_4)_2 \cdot 3H_2O$	**B**	H.-W. Xu, L.-x. Zhang, Y.-h. Li, H.-f. Wang, *Synthesis and Reactivity in Inorganic, Metal-Organic, and Nano-Metal Chemistry*, 2011, **41**, 743, DOI: 10.1080/15533174.2011.591297	Cu(II)
114	KEWCEW	$[Sm(tpt)(acacF_3)_2(NO_3)]$	**A**	L. Panayiotidou, M. Stylianou, N. Arabatzis, C. Drouza, P. Lianos, E. Stathatos, A.D. Keramidas, *Polyhedron*,	Sm(III)
115	KEWCOG	$[Eu(tpt)(acacF_3)_2(MeOH)_2]Cl$	**A**		Eu(III)

				2013, **52**, 856, DOI: 10.1016/j.poly.2012.07.029	
116	KEZHIH	$\{[Ag(tpt)]ClO_4\}_n$	**H**	X.-P. Zhou, X. Zhang, Sh.-H. Lin, D. Li, *Cryst. Growth Des.*, 2007, **7**, 485, DOI: 10.1021/cg0608256	Ag(I)
117	KEZHON	$\{[Ag(tpt)]BF_4\}_n$	**H**		Ag(I)
118	KEZHUT	$\{[Ag(tpt)]PF_6\}_n$	**H**		Ag(I)
119	KEZJAB	$\{[Ag_2(tpt)(CF_3CO_2)_2(H_2O)][Ag_2(tpt)(CF_3CO_2)_2]\}\cdot0.5H_2O$	**C**		Ag(I)
120	KIBJEL	$[Tb(tpt)(dbm)_3]$	**A**	C.R. De Silva, J.R. Maeyer, A. Dawson, Z. Zheng, *Polyhedron*, 2007, **26**, 1229, DOI: 10.1016/j.poly.2006.10.049	Tb(III)
121	KIBJOV	$[Er(tpt)(dbm)_3]\cdot Et_2O$	**A**		Er(III)
122	KIBJUB	$[Er(tpt)(tta)_3]\cdot EtOH$	**A**		Eu(III)
123	KIBKAI	$[Er(tpt)(ba)_3]$	**A**		Eu(III)
124	KIBKEM	$[Er(tpt)(btfa)_3]\cdot EtOH$	**A**		Eu(III)
125	KIBLAJ	$[Pb(tpt)(btfa)_2]\cdot H_2O$	**A**	F. Marandi, N. Asghari, M. Gorbanloo, A.A. Soudi, P. Mayer, *Z. Anorg. Allg. Chem.*, 2007, **633**, 536, DOI: 10.1002/zaac.200600341	Pb(II)
126	KUHXER	$[Co(tpt)(dca)]_2(ClO_4)_2$	**A**	A. Das, C. Marschner, J. Cano, J. Baumgartner, J. Ribas, M.S. El Fallah, S. Mitra, *Polyhedron*, 2009, **28**, 2436, DOI: 10.1016/j.poly.2009.04.024	Co(II)
127	KUJXET	$\{[UO_2(tpt)(py)]O\}(I_3)_2$	**A**	J.-C. Berthet, P. Thuery, M.R.S. Foreman, M. Ephritikhine, *Radiochim. Acta*, 2008, **96**, 189, DOI: 10.1524/ract.2008.1478	U(VI)
128	LAFHAE	$[Cu_2(tpt)(pop)_2](PF_6)_2\cdot 2dcm$	**F**	S. Keller, A. Prescimone, E.C. Constable, C.E. Housecroft, *Polyhedron*, 2016, **116**, 3, DOI: 10.1016/j.poly.2016.01.033	Cu(I)
129	LAMXUU	$[Zn(tpt)(hmdc)]\cdot 1.5diox$	**A**	H.D. Arman, P. Poplaukhin, E.R.T. Tiekink, *Acta Cryst. E*, 2012, **68**, m319, DOI: 10.1107/S160053681200671X	Zn(II)
130	LAQWOS	$[Eu(tpt)(tdf)_3]$	**A**	P.G. Jones, S. Schaumburg, W. Kowalsky, H.-H. Johannes, *CSD Communication*, 2017.	Eu(III)
131	LIBWUP	$[Mn(tpt)(SCN)_2(H_2O)]\cdot dmf$	**A**	X.-P. Sun, W. Gu, X. Liu, *Acta Cryst. E*, 2007, **63**, m1027, DOI: 10.1107/S1600536807010768	Mn(II)
132	LOFNUS	$[Y(tpt)(SCN)_3(H_2O)_2]_2\cdot tpt\cdot 3.5H_2O$	**A**	S.P. Petrosyants, A.B. Ilyukhin, A.V. Gavrikov, N.N. Efimov, *Russ. J. Coord. Chem. (Koordinatsionnaia khimiia)*, 2018, **44**, 745, DOI: 10.1134/S1070328418120060	Y(III)
133	LOFPAA	$[Y(tpt)(SCN)_2(H_2O)_3](SCN)\cdot tpt\cdot 1.25MeOH\cdot 1.5H_2O$	**A**		Y(III)
134	LOFPEE	$[Y(tpt)(SCN)_2(H_2O)_3]_5[Y(tpt)(SCN)_3(H_2O)_2]_5[Y(tpt)(SCN)_4(H_2O)]_2(SCN)_3\cdot 37H_2O$	**A**		Y(III)
135	LOFPII	$[Y(tpt)_2(SCN)_3]\cdot MeCN$	**A**		Y(III)
136	LOSDAZ	$[Mn(tpt)(CF_3CO_2)(H_2O)_2]CF_3CO_2$	**A**	K.M. Lo, S.W. Ng, *Acta Cryst. E*, 2009, **65**, m591, DOI: 10.1107/S1600536809015098	Mn(II)
137	METJUR	$[Eu(tpt)(hfac)_2(EtOH)(H_2O)]CF_3CO_2\cdot EtOH\cdot H_2O$	**A**	C.R. De Silva, R. Wang, Zh. Zheng, *Polyhedron*, 2006, **25**, 3449, DOI: 10.1016/j.poly.2006.06.032	Eu(III)
138	METKAY	$[Eu(tpt)(hfac)]\cdot EtOH$	**A**		Eu(III)
139	METKOM	$[Mn_2(tpt)_2(dca)_2(H_2O)_2](ClO_4)_2$	**A**	G.-Y. Hsu, P. Misra, Sh.-Ch. Cheng, H.-H. Wei, S. Mohanta, *Polyhedron*, 2006, **25**, 3393, DOI: 10.1016/j.poly.2006.06.019	Mn(II)

140	MOFJEY	$\{[Cd_2(tpt)(pdc)(Cl)_2]\cdot 2H_2O\}_n$	**A**	X. Jing, L. Ya, *Chinese J. Struct. Chem.*, 2014, **33**, 345	Cd(II)
141	MUZZAL	$[NpO_2(tpt)(fa)(H_2O)]\cdot 3H_2O$	**A**	G. Andreev, N. Budantseva, *ChemistrySelect*, 2020, **5**, 14217, DOI: 10.1002/slct.202004025	Np(V)
142	NAVDOD	$[Ru(tpt)_2](PF_6)_2\cdot H_2O$	**A**	P. Paul, B. Tyagi, M.M. Bhadbhade, E. Suresh, *J. Chem. Soc., Dalton Trans.*, 1997, 2273, DOI: 10.1039/a608433h	Ru(II)
143	NAXLIJ	$[Ni(tpt)(Cl)_2(MeOH)]\cdot 0.5Et_2O$	**A**	H. Hadadzadeh, M. Maghami, J. Simpson, A.D. Khalaji, K. Abdi, *J. Chem. Crystallogr.*, 2012, **42**, 656, DOI: 10.1007/s10870-012-0296-7	Ni(II)
144	NAXLOP	$[Cu(tpt)_2](PF_6)_2\cdot MeCN$	**A**	K. Abdi, H. Hadadzadeh, M. Salimi, J. Simpson, A.D. Khalaji, *Polyhedron*, 2012, **44**, 101, DOI: 10.1016/j.poly.2012.06.089	Cu(II)
145	NEXPOY	$\{[Zn(tpt)(fum)]\cdot dmf\}_n$	**A**	P. Abdolaliana, A. Morsali, G. Bruno, *Ultrason. Sonochem.*, 2017, **37**, 654, DOI: 10.1016/j.ultsonch.2017.02.023	Zn(II)
146	NILNEC	$[Ag_2(tpt)(dppm)_2(MeCN)](SbF_6)_2\cdot 2MeCN\cdot 2H_2O$	**B**	H.-W. Xu, J.-x. Li, P. Pin, Zh.-N. Chen, J.-g. Wu, *Transition Met. Chem.*, 2007, **32**, 839, DOI: 10.1007/s11243-007-0270-y	Ag(I)
147	NILNIG	$[Ag_2(tpt)_2(dppm)_2](SbF_6)_2\cdot 1.75H_2O$	**B**		Ag(I)
148	NILNOM	$[Ag_2(tpt)_2(dppm)](SbF_6)_2\cdot 2MeCN$	**A**		Ag(I)
149	NIZMAN	$[Ni(tpt)(NCS)_2(MeOH)]\cdot MeOH$	**A**	K. Ha, IUCrData, 2019, 4, x190169, DOI: 10.1107/S241431461900169X	Ni(II)
150	NUDGUQ	$[Tb(tpt)(NO_3)_2(EtO)(Cl)]\cdot EtOH$	**A**	Zh. Dan, *CSD Communication*, 2015.	Tb(III)
151	NUDHAX	$\{[Gd(tpt)(ta)(Cl)]\cdot 0.5H_2ta\}_n$	**A**		Gd(III)
152	NUDHEB	$\{[Zn(tpt)(ta)(Cl)]\cdot 3H_2O\}_n$	**A**		Zn(II)
153	OCEVEY	$[Ru(tpt)(acac)(ee)]ClO_4\cdot 2H_2O$	**A**	S. Ghumaan, S. Kar, S.M. Mobin, B. Harish, V.G. Puranik, G.K. Lahiri, *Inorg. Chem.*, 2006, **45**, 2413, DOI: 10.1021/ic0514288	Ru(II)
154	OCEVIC	$[Ru(tpt)(acac)(ta)]ClO_4\cdot 2H_2O$	**A**		Ru(II)
155	OCEVOI	$[Ru(tpt)(acac)(MeCN)]ClO_4\cdot 2H_2O$	**A**		Ru(II)
156	OFONEZ	$\{[Ni(tpt)(Hbtb)]\cdot 0.7dmf\}_n$	**A**	D. Sensharma, P. Wix, A.Ch. Kathalikkattil, W. Schmitt, *CrystEngComm*, 2018, **20**, 5127, DOI: 10.1039/C8CE01211C	Ni(II)
157	OFOHID	$\{[Cd(tpt)(Hbtb)]\cdot dmf\}_n$	**A**		Cd(II)
158	OFOMEE	$\{[Zn(tpt)(Hbtb)]\cdot dmf\}_n$	**A**		Zn(II)
159	OFOMII	$\{[Mn(tpt)(Hbtb)]\cdot 1.25dmf\}_n$	**A**		Mn(II)
160	OGAZEE	$[Mn(tpt)(NO_3)(MeOH)_2]NO_3$	**A**	K.N. Lazarou, I. Stamatopoulos, V. Psycharis, C. Duboc, C.P. Raptopoulou, Y. Sanakis, *Polyhedron*, 2018, **155**, 291, DOI: 10.1016/j.poly.2018.08.014	Mn(II)
161	OGAZII	$[Mn(tpt)(NO_3)_2(MeOH)]$	**A**		Mn(II)
162	OGEBAG	$[Mn(tpt)(MeCN)(H_2O)_2](ClO_4)_2$	**A**		Mn(II)
163	OGUCEA	$[Tb(tpt)(Br\text{-}ba)_3(H_2O)]\cdot H_2O$	**A**	C. Wang, J. Kang, X. Zhang, Y. Zhao, H. Chu, *J. Lumin.*, 2019, **215**, 116638, DOI: 10.1016/j.jlumin.2019.116638	Tb(III)
164	OHACIK OHACIK01	$[Ag(tpt)(NO_3)]_n$	**D**	Ch. Yan, L. Chen, R. Feng, F. Jiang, M. Hong, *CrystEngComm*, 2009, **11**, 2529, DOI: 10.1039/b909549g G. Meyer, M. Sehabi, I. Pantenburg, *Design and Construction of Coordination Polymers*, Wiley, 2009, DOI: 10.1002/9780470467336	Ag(I)
165	OHACOQ	$\{[Ag_2(tpt)(Ph_3P)_3(NO_3)(H_2O)](NO_3)\cdot 2H_2O\}_n$	**G**	Ch. Yan, L. Chen, R. Feng, F. Jiang, M. Hong, *CrystEngComm*, 2009, **11**, 2529, DOI: 10.1039/b909549g	Ag(I)
166	OHACUW	$[Ag_4(tpt)_2(CN)(NO_3)_2]NO_3$	**D**		Ag(I)
167	OMUVIC	$[Zn(tpt)(NO_3)(H_2O)_2]NO_3$	**A**	Ch. Yan, Q. Chen, L. Chen, R. Feng, X.	Zn(II)

168	OMUVOI	$[Zn_2(tpt)_2(4,4'\text{-bpy})(H_2O)_4](NO_3)_4 \cdot 4H_2O$	**A**	Shan, F. Jiang, M. Hong, *Aust. J. Chem.*, 2011, **64**, 104, DOI: 10.1071/CH10175	Zn(II)
169	OMUVUO	$[Zn(tpt)(MeCO_2)_2]\cdot 5H_2O$	**A**		Zn(II)
170	ORESIO	$[Cd(tpt)(sal)_2(H_2O)]\cdot H_2O$	**A**	G. Wu, X.-F. Wang, L. Guo, H.-H. Li, *J. Chem. Crystallogr.*, 2011, **41**, 1071, DOI: 10.1007/s10870-011-0048-0	Cd(II)
171	ORESOU	$[Zn(tpt)(sal)_2]\cdot H_2O$	**A**		Zn(II)
172	PANTEY	$[Zn(tpt)(SO_4)(H_2O)_2]\cdot 2H_2O$	**A**	M.A. Harvey, S. Baggio, R. Baggio, *Acta Cryst. C*, 2004, **60**, m498, DOI: 10.1107/S0108270104019821	Zn(II)
173	PIDKUJ	$[Co(tpt)(SCN)_2(H_2O)]$	**A**	X.-P. Sun, W. Gu, X. Liu, *Acta Cryst. E*, 2007, **63**, m1339, DOI: 10.1107/S1600536807013335	Co(II)
174	PIPXIX	$[Eu_2(tpt)_2(poa)_6]\cdot 2MeOH$	**A**	A. Wang, X. Wei, H. Zhang, B. Yue, Y. Qu, J. Kang, Zh. Wang, H. Chu, Y. Zhao, *Dalton Trans.*, 2014, **43**, 2620, DOI: 10.1039/C3DT53068J	Eu(III)
175	PIPXOD	$[EuGd(tpt)_2(poa)_6]\cdot 2MeOH$	**A**		Eu(III), Gd(III)
176	PUDKEG	$[Mn_3(tpt)_2(MeCO_2)_6]$	**A**	Y.-Zh. Zhang, H.-H. Zhao, E. Funck, K.R. Dunbar, *Angew. Chem., Int. Ed.*, 2015, **54**, 5583, DOI: 10.1002/anie.201410664	Mn(II)
177	PUXZIS	$[Ag_2(tpt)(NO_3)_2]_n$	**C**	M.M. Najafpour, M. Holynska, M. Amini, S.H. Kazemi, T. Lis, M. Bagherzadeh, *Polyhedron*, 2010, **29**, 2837, DOI: 10.1016/j.poly.2010.07.005	Ag(I)
178	PUXZOY	$[Ag_5(tpt)](NO_3)_5\cdot 7H_2O$	**J**		Ag(I)
179	PYPRTZ10	$[Ni(Htpt)(H_2O)_3]Br_3\cdot H_2O$	**A**	G.A. Barclay, R.S. Vagg, E.C. Watton, *Acta Cryst. B*, 1977, **33**, 3487, DOI: 10.1107/S0567740877011261	Ni(II)
180	QEFNIA	$[Ce(tpt)(I)_3(MeCN)_2]\cdot 1.5MeCN$	**A**	J.-C. Berthet, J.-M. Onno, F. Gupta, C. Riviere, P. Thuery, M. Nierlich, C. Madic, M. Ephritikhine, *Polyhedron*, 2012, **45**, 107, DOI: 10.1016/j.poly.2012.07.040	Ce(III)
181	QEFNOG	$[Ce(tpt)_2(CF_3SO_3)_3]\cdot MeCN\cdot Et_2O$	**A**		Ce(III)
182	QEFNUM	$[Nd(tpt)_2(I)_2(Py)]I\cdot 3.5Py$	**A**		Nd(III)
183	QEFPAU	$[Ce(tpt)_2(I)_2(H_2O)]I\cdot 2.5Py$	**A**		Ce(III)
184	QEFPEY	$[Ce(tpt)_2(I)_3]\cdot 0.7(MeCN)$	**A**		Ce(III)
185	QEFPIC	$[Ce_2(OH)_2(tpt)_4(I)_2]I(I_3)\cdot 2MeCN$	**A**		Ce(III)
186	QEFPOI	$[Ce(tpt)_3(I)]I_2\cdot 2MeCN$	**A**		Ce(III)
187	QEFPUO	$[U(tpt)_2(CF_3SO_3)_3]\cdot 2Py$	**A**		U(III)
188	QEFQAV	$[U_2(tpt)_4(CF_3SO_3)_6]\cdot 2Py$	**A**		U(III)
189	QEFQEZ	$[U_3O_3(tpt)_3(CF_3SO_3)_6(Py)_2]\cdot 3Py\cdot 0.5Et_2O$	**A**		U(III)
190	QEFQID	$[Ce(tpt)_2(CF_3SO_3)_3]\cdot 2Py$	**A**		Ce(III)
191	QEZHIM	$[Fe_2O(tpt)_2(dca)_2(NO_3)_2]$	**A**	A. Majumder, G. Pilet, M.S. El Fallah, J. Ribas, S. Mitra, *Inorg. Chim. Acta*, 2007, **360**, 2307, DOI: 10.1016/j.ica.2006.11.015	Fe(III)
192	QIXSAU	$[Hg(tpt)(I)_2]$	**A**	Z. Yaghobi, Z.R. Ranjbar, S. Gharbi, *Polyhedron*, 2019, **164**, 176, DOI: 10.1016/j.poly.2019.02.039	Hg(II)
193	QIXSEY	$[Cd(tpt)(Cl)_2]$	**A**		Cd(II)
194	QOMQOZ	$[Fe(tpt)(NO_3)(MeOH)_2]NO_3$	**A**	C.P. Raptopoulou, Y. Sanakis, A.K. Boudalis, *Eur. J. Inorg. Chem.*, 2008, 5632, DOI: 10.1002/ejic.200800560	Fe(II)
195	QOMQUF	$[Fe(Htpt)_2](ClO_4)_4$	**A**		Fe(II)
196	QUQMAS	$[Eu(tpt)(tpip)_3]$	**A**	M. Pietraszkiewicz, O. Pietraszkiewicz, J. Karpiuk, A. Majka, G. Dutkiewicz, T. Borowiak, A.M. Kaczmarek, R. Van Deun, *J. Lumin.*, 2016, **170**, 411, DOI: 10.1016/j.jlumin.2015.10.033	Eu(III)

197	RADVIE	$\{Na[UO_2(nda)_2](Htpt)\cdot H_2O\}_n$	**A**	S.G. Thangavelu, Ch.L. Cahill, *Cryst. Growth Des.*, 2016, **16**, 42, DOI: 10.1021/acs.cgd.5b00778	Na(I), U(IV)
198	RAHSOK	$[Mn(tpt)_2](I_3)_2$	**A**	K. Ha, *Z. Kristallogr. NCS*, 2011, **226**, 483, DOI: 10.1524/ncrs.2011.0215	Mn(II)
199	RAQQUV	$\{[Pb(tpt)(NO_3)_2]\cdot 2.4H_2O\}_n$	**A**	J.M. Harrowfield, D.L. Kepert, H. Miyamae, B.W. Skelton, A.A. Soudi, A.H. White, *Aust. J. Chem.*, 1996, **49**, 1147, DOI: 10.1071/CH9961147	Pb(II)
200	RAQRAC	$[Pb(tpt)_2(NO_3)_2]\cdot MeOH$	**A**		Pb(II)
201	RAQREC	$[Pb(tpt)_2(NO_3)_2]\cdot 6H_2O$	**A**		Pb(II)
202	RAQRIK	$\{[Pb(tpt)(Cl)_2]\cdot MeOH\}_n$	**A**	J.M. Harrowfield, H. Miyamae, B.W. Skelton, A.A. Soudi, A.H. White, *Aust. J. Chem.*, 1996, **49**, 1157, DOI: 10.1071/CH9961157	Pb(II)
203	RAQROQ	$\{[Pb(tpt)(Br)_2]\cdot MeOH\}_n$	**A**		Pb(II)
204	RAQRUW	$\{[Pb(tpt)(I)_2]\cdot MeOH\}_n$	**A**		Pb(II)
205	RAQSAD	$[Pb(tpt)(SCN)_2]_n$	**A**		Pb(II)
206	RAQZAM	$[Mn(tpt)(H_2O)_3](CF_3SO_3)_2\cdot MeOH$	**A**	M.M. Najafpour, M. Holynska, A.N. Shamkhali, M. Amini, S.H. Kazemi, S. Zaynalpoor, R. Mohamadi, M. Bagherzadeh, T. Lis, *Polyhedron*, 2012, **34**, 202, DOI: 10.1016/j.poly.2011.12.027	Mn(II)
207	RAQZEQ	$[Mn(tpt)(MeCO_2)(H_2O)_2](CF_3SO_3)\cdot 3H_2O$	**A**		Mn(II)
208	REHKUL	$[Ni(tpt)(SO_4)(H_2O)_2]\cdot 2H_2O$	**A**	M.E.D. de Vivar, S. Baggio, R. Baggio, *Acta Cryst. E*, 2006, **62**, m986, DOI: 10.1107/S1600536806011640	Ni(II)
209	REHMEX	$[Fe_2O(tpt)_2(Cl)_4]\cdot 2H_2O$	**A**	R. Zibaseresht, W.T. Robinson, R.M. Hartshorn, *Acta Cryst. E*, 2006, **62**, m1150, DOI: 10.1107/S1600536806014437	Fe(III)
210	REYQAQ	$\{[Pr(tpt)(H_2O)_4Fe(CN)_6]\cdot 8H_2O\}_n$	**A**	H. Zhao, N. Lopez, A. Prosvirin, H.T. Chifotides, K.R. Dunbar, *Dalton Trans.*, 2007, 878, DOI: 10.1039/b616016f	Pr(III), Fe(III)
211	REYQES	$\{[Nd(tpt)(H_2O)_4Fe(CN)_6]\cdot 8H_2O\}_n$	**A**		Nd(III), Fe(III)
212	REYQIW	$\{[Sm(tpt)(H_2O)_4Fe(CN)_6]\cdot 8H_2O\}_n$	**A**		Sm(III), Fe(III)
213	REYQOC	$\{[Eu(tpt)(H_2O)_4Fe(CN)_6]\cdot 6H_2O\}_n$	**A**		Eu(III), Fe(III)
214	REYQUI	$\{[Gd(tpt)(H_2O)_4Fe(CN)_6]\cdot 6H_2O\}_n$	**A**		Gd(III), Fe(III)
215	REYRAP	$\{[Tb(tpt)(H_2O)_4Fe(CN)_6]\cdot 8H_2O\}_n$	**A**		Tb(III), Fe(III)
216	REYRET	$\{[Sm(tpt)(H_2O)_4Co(CN)_6]\cdot 8H_2O\}_n$	**A**		Sm(III), Co(III)
217	REYRIX	$\{[La(tpt)(dmf)(H_2O)_3Fe(CN)_6]\cdot 5H_2O\}_n$	**A**		La(III), Fe(III)
218	RUBMEH	$[Mn_2(tpt)_2(Cl)_4]\cdot 2MeCN$	**A**	P. Tyagi, U.P. Singh, *J. Coord. Chem.*, 2009, **62**, 1613, DOI: 10.1080/00958970802680682	Mn(II)
219	RUBMIL	$[Mn(tpt)(MeCO_2)(N_3)(H_2O)]\cdot H_2O$	**A**		Mn(II)
220	RUKNOD	$[Cu(tpt)(Cl)_2]\cdot 2H_2O$	**A**	K. Abdi, H. Hadadzadeh, M. Weil, H.A. Rudbari, *Inorg. Chim. Acta*, 2014, **416**, 109, DOI: 10.1016/j.ica.2014.03.021	Cu(II)
221	RUSNID RUSNID01	$[Mn(tpt)(Cl)_2]$	**A**	K. Ha, *Acta Cryst. E*, 2010, **66**, m262, DOI: 10.1107/S1600536810004204 K. Ha, *Acta Cryst. E*, 2011, **67**, m1306, DOI: 10.1107/S1600536811034118	Mn(II)
222	SOBWEO	$\{[Fe^{II}(tpt)]_2[Fe^{III}(Tp^*)(CN)_3]_4\}\cdot H_2O$	**A**	J.-H. Wang, K.R. Vignesh, J. Zhao, Zh.-Y. Li, K.R. Dunbar, *Inorg. Chem. Front.*, 2019, **6**, 493,	Fe(III), Fe(II)
223	SOCDOG	$\{[Co^{II}(tpt)]_2[Fe^{III}(Tp^*)(CN)_3]_4\}\cdot H_2O$	**A**		Co(II),

				DOI: 10.1039/C8QI01245H	Fe(III)
224	SOCDUM	$\{[Ni^{II}(tpt)]_2[Fe^{III}(Tp^*)(CN)_3]_4\}\cdot 2MeOH\cdot 4H_2O$	**A**		Ni(II), Fe(III)
225	SOZHIA	$\{[(tpt)Mn^{II}(H_2O)Mn^{III}(CN)_6]_2Mn^{II}(H_2O)_2\cdot 4MeOH\cdot 2H_2O\}_n$	**A**	Y.-Zh. Zhang, H.-H. Zhao, E. Funck, K.R. Dunbar, *Angew. Chem., Int. Ed.*, 2015, **54**, 5583, DOI: 10.1002/anie.201410664	Mn(II), Mn(III)
226	TABDOP	$[Co(tpt)_2]I_2\cdot 2H_2O$	**A**	B.N. Figgis, E.S. Kucharski, S. Mitra, B.W. Skelton, A.H. White, *Aust. J. Chem.*, 1990, **43**, 1269, DOI: 10.1071/CH9901269	Co(II)
227	TABDUV	$[Co(tpt)_2]I_2\cdot 3.75H_2O$	**A**		Co(II)
228	TANXIQ	$[Ni(tpt)(H_2O)_3]Cl_2\cdot 3H_2O$	**A**	R. Zibaseresht, R.M. Hartshorn, *Aust. J. Chem.*, 2005, **58**, 345, DOI: 10.1071/CH04280	Ni(II)
229	TANXOW	$[Ni(tpt)(Cl)(H_2O)_2][Ni(tpt)(Cl)_2(H_2O)]Cl\cdot 4H_2O$	**A**		Ni(II)
230	TANXUC	$[Ni(Htpt)(Cl)(H_2O)_2]Cl_2\cdot 2H_2O$	**A**		Ni(II)
231	TANYAJ	$[Ni(tpt)(H_2O)_3](NO_3)_2$	**A**		Ni(II)
232	TANYEN	$[Ni(tpt)_2](ClO_4)_2$	**A**		Ni(II)
233	TANYIR	$[Ni_2(tpt)(NO_3)_3(EtOH)_2(H_2O)]NO_3$	**C**		Ni(II)
234	TCAZCO	$\{[Co_2(tpt)(Cl)_4(H_2O)]\cdot H_2O\}_n$	**D**	G.A. Barclay, R.S. Vagg, E.C. Watton, *Acta Cryst. B*, 1978, **34**, 1833, DOI: 10.1107/S0567740878006780	Co(II)
235	TEPLUV	$[Ni(Htpt)(H_2O)_3](NO_3)_3\cdot H_2O$	**A**	P. Byers, G.Y.S. Chan, M.G.B. Drew, M.J. Hudson, C. Madic, *Polyhedron*, 1996, **15**, 2845, DOI: 10.1016/0277-5387(95)00588-9	Ni(II)
236	TEQKUW	$[Cu(tpt)(ox)(H_2O)]\cdot 4H_2O$	**A**	Y.-Q. Zheng, W. Xu, F. Lin, G.-S. Fang, *J. Coord. Chem.*, 2006, **59**, 1825, DOI: 10.1080/00958970600571760	Cu(II)
237	TEXJAK	$[Zn(tpt)(Cl)_2]$	**A**	G.B. Güven, *CSD Communication*, 2018.	Zn(II)
238	TOGLIM	$[Nd_2(tpt)_2(bpdc)_3(H_2O)]\cdot 3dma\cdot 7H_2O$	**A**	J.-H. Liao, W.-Sh. Hwang, G.-Y. Chen, *Z. Anorg. Allg. Chem.*, 2014, **640**, 1793, DOI: 10.1002/zaac.201300619	Nd(III)
239	TOGLOS	$[Sm_2(tpt)_2(bpdc)_3(H_2O)]\cdot 3dma\cdot 7H_2O$	**A**		Sm(III)
240	TOGLUY	$[Eu_2(tpt)_2(bpdc)_3(H_2O)]\cdot 3dma\cdot 7H_2O$	**A**		Eu(III)
241	TOGMAF	$[Gd_2(tpt)_2(bpdc)_3(H_2O)]\cdot 3dma\cdot 7H_2O$	**A**		Gd(III)
242	TOGMEJ	$[Tb_2(tpt)_2(bpdc)_3(H_2O)]\cdot 3dma\cdot 7H_2O$	**A**		Tb(III)
243	TOGMIN	$[Dy_2(tpt)_2(bpdc)_3(H_2O)]\cdot 3dma\cdot 7H_2O$	**A**		Dy(III)
244	TOLKEN	$[Ni(tpt)(Py)(Cl)_2]$	**A**	K. Ha, *Z. Kristallogr. NCS*, 2019, **234**, 775, DOI: 10.1515/ncrs-2019-0098	Ni(II)
245	UJIFUQ	$[Eu_2(tpt)_2(PhCO_2)_6(H_2O)_2]\cdot MeOH\cdot 7H_2O$	**A**	N. Goel, *J. Coord. Chem.*, 2015, **68**, 529, DOI: 10.1080/00958972.2014.992339	Eu(III)
246	UJIGAX	$[Eu(tpt)(SCN)_3(MeOH)_2(H_2O)]\cdot MeOH$	**A**		Eu(III)
247	UJIGEV	$[Tb(tpt)(PhCO_2)_3]_2[Tb(tpt)(PhCO_2)_3(MeOH)]_2\cdot 2MeOH\cdot 4H_2O$	**A**		Tb(III)
248	UJIGIF	$[Gd(tpt)(SCN)_3(MeOH)_2(H_2O)]\cdot MeOH$	**A**		Gd(III)
249	UJIGOL	$[Gd_2(tpt)_2(PhCO_2)_6(H_2O)_2]\cdot 2H_2O$	**A**		Gd(III)
250	UJIGUR	$[Tb(tpt)(SCN)_3(H_2O)_3]$	**A**		Tb(III)
251	UNIYOG	$[Ni(tpt)(pla)(H_2O)_2]\cdot 3H_2O$	**A**	Ch.-H. Jin, *Acta Cryst. E*, 2011, **67**, m393, DOI: 10.1107/S1600536811006842	Ni(II)
252	VARROV	$[Rh(tpt)(Cl)_3]\cdot 2H_2O$	**A**	P. Paul, B. Tyagi, A.K. Bilakhiya, M.M. Bhadbhade, E. Suresh, G. Ramachandraiah, *Inorg. Chem.*, 1998, **37**, 5733, DOI: 10.1021/ic9709739	Rh(III)

253	VEVLEO	$[Co(Htpt)(Cl)_3]\cdot H_2O$	**A**	J.D. Holbrey, K.B. Vigour, W.M. Reichert, R.D. Rogers, *J. Chem. Crystallogr.*, 2006, **36**, 799, DOI: 10.1007/s10870-006-9157-6	Co(II)
254	VIMZUO	$\{[Fe(tpt)W(CN)_8]\cdot 2MeOH\}_n$	**A**	H. Zhao, A.J. Brown, A.V. Prosvirin, K.R. Dunbar, *Polyhedron*, 2013, **64**, 321, DOI: 10.1016/j.poly.2013.06.006	Fe(III), W(V)
255	VINBAX	$\{(H_3O)[Cu(tpt)Mo(CN)_8]\cdot MeOH\}_n$	**A**		Cu(II), Mo(V)
256	VINBEB	$\{[Co_3(tpt)_2W(CN)_{16}(H_2O)_6]\cdot 2H_2O\}_n$	**A**		Co(II), W(V)
257	VINFAB	$[Cu(tpt)(CF_3SO_3)_2(MeOH)]\cdot MeOH$	**A**		Cu(II)
258	VIYTAZ	$[Ni(tpt)(Hsal^{NO}{}_2\text{-}Glc)]ClO_4\cdot 0.38MeCN\cdot 0.75H_2O$	**A**	A. Burkhardt, H. Gorls, W. Plass, *Carbohydr. Res.*, 2008, **343**, 1266, DOI: 10.1016/j.carres.2008.01.039	Ni(II)
259	VIYTED	$[Ni(tpt)(Hsal^{H}\text{-}Man)]ClO_4\cdot 1.88MeOH\cdot 1.19H_2O$	**A**		Ni(II)
260	VOGZUP	$[Pr(tpt)(NO_3)_3(MeCN)]$	**A**	Z. Yue, H. Lu, Z. Li, Sh. Guo, J. Song, Y. Ren, Y.-Y. Huang, J. Lin, J.-Q. Wang, *CrystEngComm*, 2019, **21**, 5059, DOI: 10.1039/C9CE00867E	Pr(III)
261	VOHBAY	$[Nd(tpt)(NO_3)_3(MeCN)]$	**A**		Nd(III)
262	VOHBEC	$[Pr(tpt)(NO_3)_3(H_2O)]\cdot MeCN$	**A**		Pr(III)
263	VOHBIG	$[Nd(tpt)(NO_3)_3(H_2O)]\cdot MeCN$	**A**		Nd(III)
264	VOHBOM	$[Sm(tpt)(NO_3)_3(H_2O)]\cdot MeCN$	**A**		Sm(III)
265	VOHBUS	$[Eu(tpt)(NO_3)_3(H_2O)]\cdot MeCN$	**A**		Eu(III)
266	VOHCAZ	$[Gd(tpt)(NO_3)_3(H_2O)]\cdot MeCN$	**A**		Gd(III)
267	VOHCED	$[Tb(tpt)(NO_3)_3(H_2O)]\cdot MeCN$	**A**		Tb(III)
268	VOHCIH	$[Dy(tpt)(NO_3)_3(H_2O)]\cdot MeCN$	**A**		Dy(III)
269	VOHCON	$[Ho(tpt)(NO_3)_3(H_2O)]\cdot MeCN$	**A**		Ho(III)
270	VOHCUT	$[Er(tpt)(NO_3)_3(H_2O)]\cdot MeCN$	**A**		Er(III)
271	VOHDAA	$[Tm(tpt)(NO_3)_3(H_2O)]\cdot 2MeCN$	**A**		Tm(III)
272	VOHDEE	$[Yb(tpt)(NO_3)_3(H_2O)]\cdot 2MeCN$	**A**		Yb(III)
273	VOHDII	$[Lu(tpt)(NO_3)_3(H_2O)]\cdot 2MeCN$	**A**		Lu(III)
274	VOHDOO	$[UO_2(tpt)(NO_3)_2]$	**A**		U(VI)
275	VUGHIP	$[Ru(tpt)(PPh_3)(val)]BF_4$	**A**	P. Kumar, A.K. Singh, J.K. Saxena, D.S. Pandey, *J. Organomet. Chem.*, 2009, **694**, 3570, DOI: 10.1016/j.jorganchem.2009.07.014	Ru(II)
276	VUGLUH	$[Sm(tpt)(dbm)_3]\cdot MeCN$	**A**	N. Hasan, K. Iftikhar, *J. Lumin.*, 2020, **223**, 117135, DOI: 10.1016/j.jlumin.2020.117135	Sm(III)
277	VULPUP	$[Eu_2(tpt)_2(Brba)_6]$	**A**	C. Wang, J. Kang, X. Zhang, Y. Zhao, H. Chu, *J. Lumin.*, 2019, **215**, 116638, DOI: 10.1016/j.jlumin.2019.116638	Eu(III)
278	WAZDOT	$[Cu(tpt)(PPh_3)_2]PF_6\cdot 2.5HCl_3$	**B**	A. Báez-Castro, J. Baldenebro-López, A. Cruz-Enríquez, H. Höpfl, D. Glossman-Mitnik, V. Miranda-Soto, M. Parra-Hake, E. Reynoso-Soto, J.J. Campos-Gaxiola, *Inorg. Chim. Acta*, 2017, **466**, 486, DOI: 10.1016/j.ica.2017.07.007	Cu(I)
279	WEHTOT	$[Zn(tpt)(S_2O_3)(H_2O)]\cdot 0.5H_2O$	**A**	M.E.D. de Vivar, S.Baggio, R.Baggio, *Acta Cryst. C*, 2006, **62**, m192, DOI: 10.1107/S0108270106010560	Zn(II)
280	WEHTUZ	$[Cd_2(tpt)_2(SO_3)_2]\cdot 8H_2O$	**A**	M.E.D. de Vivar, S. Baggio, M.T. Garland, R. Baggio, *Acta Cryst. C*, 2006, **62**, m195, DOI: 10.1107/S0108270106012078	Cd(II)

281	WEPLOT	$[Co(tpt)(ox)(H_2O)]\cdot 4H_2O$	**A**	D.-Y. Cheng, W. Xu, Y.-Q. Zheng, *Acta Cryst. E*, 2006, **62**, m2561, DOI: 10.1107/S1600536806036361	Co(II)
282	WIBBUG	$[Eu(tpt)(PhCO_2)_3(H_2O)]_2\cdot EtOH\cdot 1.25H_2O$	**A**	Y.-F. Zhao, H.-B. Chu, F. Bai, D.-Q. Gao, H.-X. Zhang, Y.-Sh. Zhou, X.-Y. Wei, M.-N. Shan, H.-Y. Li, Y.-L. Zhao, *J. Organomet. Chem.*, 2012, **716**, 167, DOI: 10.1016/j.jorganchem.2012.06.031	Eu(III)
283	WIGLEE	$[Ni(tpt)(MeOpdt)_2]\cdot MeOH$	**A**	M.C. Aragoni, M. Arca, F.A. Devillanova, M.B. Hursthouse, S.L. Huth, F. Isaia, V. Lippolis, A. Mancini, S. Soddu, G. Verani, *Dalton Trans.*, 2007, 2127, DOI: 10.1039/b701458a	Ni(II)
284	WIGLII	$[Ni(tpt)_2](MeOpdt)_2\cdot 4H_2O$	**A**		Ni(II)
285	WIGLOO	$[Ni(tpt)_2](I_3)_2$	**A**		Ni(II)
286	WIGLUU	$[Ni_2(tpt)_2(Br)_4]$	**A**		Ni(II)
287	WOQFOA	$[Co(tpt)(Cl)_2]\cdot 2H_2O$	**A**	Z. Azarkamanzad, F. Farzaneh, M. Maghami, J. Simpson, *New J. Chem.*, 2019, **43**, 12020, DOI: 10.1039/C9NJ02055A	Co(II)
288	WOSDOA	$[Mn(tpt)(Cl)_2(EtOH)]\cdot (NH_2)_2S$	**A**	A.A. Hassoon, R.G. Harrison, N. Nawar, S.J. Smith, M.M. Mostafa, *J. Mol. Struct.*, 2020, **1203**, 127240, DOI: 10.1016/j.molstruc.2019.127240	Mn(II)
289	WOSDUG	$[Mn(tpt)(MeCO_2)(Cl)(H_2O)]\cdot 0.4H_2O$	**A**		Mn(II)
290	XABNUL XUBNUL 01	$[Mn(tpt)(Cl)_2(H_2O)]\cdot H_2O$	**A**	M.M. Najafpour, M. Amini, M. Bagherzadeh, D.M. Boghaei, V. McKee, *Trans. Met. Chem.*, 2010, **35**, 297, DOI: 10.1007/s11243-010-9327-4 W.H. Al-Assy, A. Moneum H. El-Askalany, M.M. Mostafa, *Spectrochim. Acta A*, 2013, **116**, 401, DOI: 10.1016/j.saa.2013.07.086	Mn(II)
291	XAHMID	$[Ir(H)_2(tpt)(PPh_3)_2]PF_6$	**B**	M. Maekawa, T. Minematsu, H. Konaka, K. Sugimoto, T. Kuroda-Sowa, Y. Suenaga, M. Munakata, *Inorg. Chim. Acta*, 2004, **357**, 3456, DOI: 10.1016/j.ica.2004.03.052	Ir(III)
292	XAHMOJ	$[Ir_2(H)_4(tpt)(PPh_3)_4](PF_6)_2\cdot 2H_2O$	**F**		Ir(III)
293	XAZKUF	$[Mn_2(tpt)_2(SO_4)_2(H_2O)_2]\cdot 4H_2O$	**A**	M.E.D.de Vivar, S. Baggio, M.T. Garland, R. Baggio, *Acta Cryst. E*, 2006, **62**, m141, DOI: 10.1107/S1600536805041528	Mn(II)
294	XEPLEL	$[Co(tpt)(dca)_2(H_2O)]_n$	**A**	J. Luo, L. Qiu, B. Liu, X. Zhang, F. Yang, L. Cui, *Chin. J. Chem.*, 2012, **30**, 522, DOI: 10.1002/cjoc.201100553	Co(II)
295	XESTAR	$[Co(tpt)(H_2btca)(H_2O)_2]_n$	**A**	A. Majumder, V. Gramlich, G.M. Rosair, S.R. Batten, J.D. Masuda, M.S.El Fallah, J. Ribas, J.-P. Sutter, C. Desplanches, S. Mitra, *Cryst. Growth Des.*, 2006, **6**, 2355, DOI: 10.1021/cg060337y	Co(II)
296	XIBYOX	$[Zn(tpt)(ox)(H_2O)]\cdot 4H_2O$	**A**	H.-Zh. Xie, W.-J. Pan, *Acta Cryst. E*, 2007, **63**, m1231, DOI: 10.1107/S1600536807013517	Zn
297	XIGDUO	$[U(tpt)_2(CF_3SO_3)_3(H_2O)]\cdot 2.5Py$	**A**	J. C. Berthet, P. Thuery, M. Ephritikhine, *CSD Communication*, 2013.	U(III)
298	XIGFAW	$[Sm(tpt)_2(CF_3SO_3)_2(H_2O)]CF_3SO_3\cdot CF_3SO_3H\cdot 0.5tpt$	**A**		Sm(III)
299	XIGFEA	$[Ce(tpt)_2(CF_3SO_3)_3]\cdot 2tpt$	**A**		Ce(III)
300	XIHSIR	$[Mn(tpt)(NO_3)(Cl)(H_2O)]\cdot 0.5H_2O$	**A**	A. Das, G. Pilet, S. Mitra, *Indian J. Chem. A*, 2006, **45**, 1988	Mn(II)

301	XIHSOX	[Mn(tpt)$(SCN)_2$$(H_2O)$]	**A**		Mn(II)
302	XORKUN	[Co(tpt)$(Cl)_2$$(H_2O)$]·$H_2O$	**A**	A.L. Rheingold, *CSD Communication*, 2019.	Co(II)
303	XOXRIO	{K(H_2tpt)0.5[Cu_2(tpt)(H_8L)]·3.6H_2O}$_n$	**A**	D. Quiñone, S. Martinez, F. Bozoglian, C. Bazzicalupi, J. Torres, N. Veiga, C. Kremer, A. Bianchi, *ChemPlusChem*, 2019, **84**, 540, DOI: 10.1002/cplu.201900141	Cu(II), K(I)
304	XOZDIB	[Tb(tpt)$(NO_3)_3$$(H_2O)$]·MeOH·EtOH	**A**	Zh. Dan, *CSD Communication*, 2014.	Tb(III)
305	XUDZIG	[Ru(tpt)$(tbbpy)_2$]$(PF_6)_2$·0.5EtOH·0.5Et_2O	**B**	M. Schwalbe, M. Karnahl, H. Gorls, D. Chartrand, F. Laverdiere, G.S. Hanan, S. Tschierlei, B. Dietzek, M. Schmitt, J. Popp, J.G. Vos, S. Rau, *Dalton Trans.*, 2009, 4012, DOI: 10.1039/b822550h	Ru(II)
306	YEHYOB	{[Zn(tpt)(cppa)]·3H_2O}$_n$	**A**	J.-Ch. Zhu, Sh.-J. Liu, *Z. Kristallogr. NCS*, 2012, **227**, 353, DOI: 10.1524/ncrs.2012.0168	Zn(II)
307	YENSAM YENSAM 01	[Mn(tpt)$(MeCO_2)$(dca)(H_2O)]·2H_2O	**A**	A. Majumder, G. Pilet, M.T.G. Rodriguez, S. Mitra, *Polyhedron*, 2006, **25**, 2550, DOI: 10.1016/j.poly.2006.03.021 M. Zhang, R. Fang, Q. Zhao, *J. Chem. Crystallogr.*, 2008, **38**, 601, DOI: 10.1007/s10870-008-9352-8	Mn(II)
308	YENSEQ	[Zn(tpt)$(dca)_2$]·2H_2O	**A**	A. Majumder, G. Pilet, M.T.G. Rodriguez, S. Mitra, *Polyhedron*, 2006, **25**, 2550, DOI: 10.1016/j.poly.2006.03.021	Zn(II)
309	YENSIU	[$Cd_2$$(tpt)_2$$(dca)_2$]$(ClO_4)_2$	**A**		Cd(II)
310	YEQQAN	[Cu_2(tpt)$(I)_2$]$_n$	**E**	X.-P. Zhou, D. Li, Sh.-L. Zheng, X. Zhang, T. Wu, *Inorg. Chem.*, 2006, **45**, 7119, DOI: 10.1021/ic060564p	Cu(I)
311	YEQQER	[Cu_3(tpt)$(I)_3$]$_n$	**J**		Cu(I)
312	YEQQIV	[$Cu_4$$(tpt)_2$($(I)_4$$(Cl)_2$]$_n$	**C**		Cu(I), Cu(II)
313	YEQRIY	[CrMn(tpt)$(NO_3)$$(CN)_4$(phen)$(H_2O)$]·2$H_2O$	**A**	M.-G. Alexandru, D. Visinescu, B. Braun-Cula, F. Lloret, M. Julve, *Eur. J. Inorg. Chem.*, 2018, 349, DOI: 10.1002/ejic.201700313	Mn(II), Cr(III)
314	YEQRUK	[CrMn(tpt)$(NO_3)$$(CN)_4$(ampy)$(H_2O)$]·MeCN	**A**		Mn(II), Cr(III)
315	YIVYOT	[$Sm_2$$(tpt)_2$$(Clba)_4$$(NO_3)_2$$(H_2O)_2$]	**A**	B. Yue, Y.-N. Chen, H.-B. Chu, Y.-R. Qu, A.-L. Wang, Y.-L. Zhao, *Inorg. Chim. Acta*, 2014, **414**, 39, DOI: 10.1016/j.ica.2014.01.024	Sm(III)
316	YIVYUZ	[$Tb_2$$(tpt)_2$$(Clba)_3$$(NO_3)_2$$(H_2O)_3$]Clba·EtOH·2$H_2O$	**A**		Tb(III)
317	YIVZAG	[$Tb_2$$(tpt)_2$$(Brba)_4$$(NO_3)_2$$(H_2O)_2$]	**A**		Tb(III)
318	YODSUH	{[Co_2(tpt)$(Cl)_4$$(H_2O)$]·0.25$H_2O$}$_n$	**D**	M. Maghami, F. Farzaneh, J. Simpson, A. Moazeni, *Polyhedron*, 2014, **73**, 22, DOI: 10.1016/j.poly.2014.02.012	Co(II)
319	ZENCEA	[Li(tpt)$(EtOH)_2$]BPh_4	**A**	H. Schödel, T.T.H. Van, H. Bock, *Acta Cryst. C*, 1995, **51**, 2001, DOI: 10.1107/S0108270195004641	Li(I)
320	ZETFEM	[TbGd$(tpt)_2$$(poa)_6$]·2MeOH	**A**	Zh.-X. Wang, A.-L. Wang, X.-Y. Wei, Y.-R. Qu, B. Yue, J. Kang, H.-B. Chu, Y.-L. Zhao, *Luminescence*, 2015, **30**, 835, DOI: 10.1002/bio.2829	Tb(III), Gd(III)
321	ZIXLUP	[$U_2O$$(tpt)_2$$(MeCN)_2$$(I)_2$$(Cp^*)_2$]$(I)_2$·4MeCN	**A**	J. Maynadie, J. C. Berthet, P. Thuery, M. Ephritikhine, *CSD Communication*, 2013	U(III)
322	ZOLXUW	[Nd(tpt)$(tta)_3$]·EtOH	**A**	Q. Liu, P. Cai, X. Wan, Sh. Zhang, K.	Nd(III)

323	ZOLYAD	[Nd(tpt)(btfa)$_3$]·EtOH	**A**	Du, Q. Yin, *J. Mol. Struct.*, 2019, **1193**, 151, DOI: 10.1016/j.molstruc.2019.05.008	Nd(III)
324	ZUGQAV	[Co(tpt)(Cl)$_2$(MeOH)]·MeOH·0.5H$_2$O	**A**	M. Maghami, F. Farzaneh, J. Simpson, M. Ghiasi, M. Azarkish, *J. Mol. Struct.*, 2015, **1093**, 24, DOI: 10.1016/j.molstruc.2015.03.037	Co(II)

dtc = diethyldithiocarbamate; Medpt = N,N-bis(3-aminopropyl)methylamine; H$_2$salagluc = benzyl-2-deoxy-2-salicylideneamino-α-D-glucopyranoside; ROpdt = (RO)(4-MeOC$_6$H$_4$)PS$_2^-$ R = Et, Pr, *i*-Pr, Bu; H$_2$adc = anthracene-9,10-dicarboxylic acid; Hpca = pyridine-2-carboxylic acid; 2-pa = bis(2-pyridylcarbonyl)amido; dppm = bis(diphenylphosphino)methane; dppe = bis(diphenylphosphino)ethane; dppp = bis(diphenylphosphino)propane; dppb = bis(diphenylphosphino)butane; pa = phenylalanine; cym = *p*-cymene; Cp* = pentamethylcyclopentadiene; dmbpy = 4,4′-dimethyl-2,2′-bipyridine; Hfa = formic acid; H$_5$saltag^{Br} = 1,2,3-tris[(5-bromosalicylidene)amino]guanidine); dbm = dibenzoylmethane; H$_2$tda = thiodiacetic acid; pca = bis(2-pyridylcarbonyl)amide; H$_2$pa = pamoic acid; tta = 2-thienoyltrifluoroacetone; ba = 1-benzoylacetone; Hbtfa = 4,4,4-trifluoro-1-phenyl-1,3-butanedione; Htta = 4,4,4-trifluoro-1-(2-thienyl)-1,3-butanedione; dca = dicyanamide; pop = bis(2-(diphenylphosphino)phenyl)ether; hmdc = N-(hydroxyethyl)-N-methyldithiocarbamate; diox = 1,4-dioxane; tdf = 1,1,1,2,2,3,3,7,7,8,8,9,9,9-tetradecafluorononane-4,6-ditionate; hfac = 1,1,1,5,5,5-hexafluoropentane-2,4-dionate; H$_2$pdc = pyridine-2,4-dicarboxylic acid; H$_2$fum = fumaric acid; H$_2$ta = terephthalic acid; ee = 1-ethoxyethylamino; ta = *p*-toluidine; H$_3$btb = 1,3,5-tris(4-carboxyphenyl)benzene; 4,4′-bpy = 4,4′-bipyridine; Hsal = salicylic acid; Hpoa = phenoxylacetic acid; tpip = tetraphenylimidodiphosphinate; Hnda = 1,4- naphthalene dicarboxylic acid; Tp* = tris(3,5-dimethylpyrazol-1-yl)borohydride; H$_2$bpdc = 4,4′-biphenyldicarboxylic acid; dma = N,N-dimethylacetamide; H$_2$pla = pimelic acid; H$_2$sal$^{NO}{}_2$-Glc = 2-deoxy-2-(5-nitrosalicylideneamino)-α-D-glucopyranoside; H$_2$sal^H-Man = 2-deoxy-2-salicylideneamino-α-D-mannopyranoside; Hval = valine; HBrba = 4-bromobenzoic acid; HClba = 4-chlorobenzoic acid; H$_2$ox = oxalic acid; MeOpdt = O-methyl-(4-methoxyphenyl)phosphonoditioate; H$_4$btca = 1,2,4,5-benzenetetracarboxylic acid; H$_{12}$L = phytate; tbbpy = 4,4′-di-tert-butyl-2,2′-bipyridine); H$_2$cppa = 3-(4-carboxyphenyl)-propionic acid; phen = 1,10-phenanthroline; ampy = 2-aminomethylpyridine

Table S2. Fragments observed in positive/negative ion mode ESI mass spectrometry of **2–7**.

Ion	Molecular formula	Calculated[1] *m/z*	Observed *m/z*	Relative abundance
2, ESI+				
{tpt+H}$^+$	$C_{18}H_{13}N_6^{+1}$	313.11962	313.11890	17
[Fe^{III}(tpt)(MeO)$_2$]$^+$	$C_{20}H_{18}FeN_6O_2^{+1}$	430.08406	430.08249	75
[Fe^{III}(tpt)(Cl)(MeO)]$^+$	**$C_{19}H_{15}ClFeN_6O^{+1}$**	**434.03397**	**434.03281**	**100**
{[Fe^{III}(piv)(Cl)$_2$(acetone)(MeOH)$_6$]+Na}$^+$	$C_{14}H_{39}Cl_2FeNaO_9^{+1}$	500.12182	500.12396	26
3, ESI+				
{tpt+H}$^+$	$C_{18}H_{13}N_6^{+1}$	313.11962	313.11914	43
{tpt+Na}$^+$	**$C_{18}H_{12}N_6Na^{+1}$**	**335.10157**	**335.10098**	**100**
[Fe^{III}(tpt)(MeO)$_2$]$^+$	$C_{20}H_{18}FeN_6O_2^{+1}$	430.08406	430.08298	75
[Fe^{III}(tpt)(Cl)(MeO)]$^+$	$C_{19}H_{15}ClFeN_6O^{+1}$	434.03397	434.03299	71
[Fe^{III}_2O(tpt)$_2$(Cl)$_3$)]$^+$	$C_{39}H_{24}Cl_3Fe_2N_{12}O^{+1}$	856.99549	856.99463	2
3a, ESI+				
{tpt+H}$^+$	$C_{18}H_{13}N_6^{+1}$	313.11962	313.11896	21
[Fe^{II}(tpt)$_2$]$^{2+}$	$C_{36}H_{24}FeN_{12}^{+2}$	340.07926	340.07849	89
[Fe^{II}(tpt)(MeCO$_2$)(MeOH)$_2$]$^+$	$C_{22}H_{23}FeN_6O_4^{+1}$	491.11247	491.35931	53
[Fe^{II}(tpt)(Cl)(thf)$_2$(MeOH)$_2$(H$_2$O)$_2$]$^+$	**$C_{28}H_{40}ClFeN_6O_6^{+1}$**	**647.20417**	**647.21265**	**100**
4a, ESI+				
[Fe^{III}_3O(piv)$_6$]$^+$	$C_{30}H_{54}Fe_3O_{13}^{+1}$	790.16070	790.16245	40
[Fe^{III}_3O(piv)$_6$(thf)]$^+$	$C_{34}H_{62}Fe_3O_{14}^{+1}$	862.21822	862.21887	90
[Fe^{III}_3O(OH)$_2$(piv)$_4$(tpt)]$^+$	$C_{38}H_{50}Fe_3N_6O_{11}^{+1}$	934.15857	934.27383	50
[Fe^{III}_3O(piv)$_4$(tpt-O)(MeO)(MeOH)$_2$]$^+$	$C_{41}H_{59}Fe_3N_6O_{13}^{+1}$	1011.21827	1011.22138	5
[Fe^{III}_6O$_4$(piv)$_4$(tpt-O)(MeO)$_4$(MeOH)$_3$(MeCN)$_3$(H$_2$O)$_6$]$^+$	$C_{51}H_{93}Fe_6N_9O_{26}^{+1}$	1583.23224	1583.23120	3
[Fe^{III}_7O$_4$(piv)$_7$(tpt-O)(MeO)$_4$(MeOH)(MeCN)$_2$(H$_2$O)]$^+$	$C_{62}H_{99}Fe_7N_8O_{25}^{+1}$	1747.22201	1747.21614	34
[Fe^{III}_7O$_4$(piv)$_8$(tpt-O)(MeO)$_3$(MeOH)(MeCN)$_3$]$^+$	$C_{68}H_{106}Fe_7N_9O_{25}^{+1}$	1840.27399	1840.27698	10
[Fe^{III}_7O$_4$(piv)$_9$(tpt-O)(MeO)$_2$(MeOH)(MeCN)$_3$]$^+$	**$C_{72}H_{112}Fe_7N_9O_{26}^{+1}$**	**1910.31586**	**1910.31726**	**100**
{[Fe^{III}_7O$_5$(piv)$_{10}$(tpt-O)(MeOH)(MeCN)(H$_2$O)$_9$]+H}$^+$	$C_{71}H_{128}Fe_7N_7O_{36}^{+1}$	2046.38405	2046.31628	11
4a, ESI–				
[Fe^{III}_7O$_5$(piv)$_{11}$(MeO)]$^-$	**$C_{56}H_{102}Fe_7O_{28}^{-1}$**	**1614.20087**	**1614.18713**	**100**

$[Fe^{III}_7O_4(piv)_{12}(MeO)_2]^-$	$C_{62}H_{114}Fe_7O_{30}^{-1}$	1730.28460	1730.26984	12
$[Fe^{III}_7O_5(piv)_9(tpt\text{-}O)(MeO)_3(MeCN)_3]^-$	$C_{72}H_{112}Fe_7N_9O_{27}^{-1}$	1926.31187	1926.29722	20
4b,[2] ESI+				
$\{[Fe^{III}_7O_4(piv)_4(tpt\text{-}O)(MeO)_8(H_2O)_5]+H\}^+$	$C_{46}H_{83}Fe_7N_6O_{26}^{+1}$	1527.07971	1527.20312	28
$\{[Fe^{III}_7O_4(piv)_5(tpt\text{-}O)(MeO)_7(H_2O)_5]+H\}^+$	**$C_{50}H_{89}Fe_7N_6O_{27}^{+1}$**	**1597.12157**	**1597.24479**	**100**
$\{[Fe^{III}_7O_4(piv)_6(tpt\text{-}O)(MeO)_6(H_2O)_5]+H\}^+$	$C_{54}H_{95}Fe_7N_6O_{28}^{+1}$	1667.16344	1667.28601	48
$[Fe^{III}_7O_4(piv)_7(tpt)(MeO)_5]^+$	$C_{58}H_{90}Fe_7N_6O_{23}^{+1}$	1630.14974	1630.15123	3
$[Fe^{III}_7O_4(piv)_8(tpt)(MeO)_4]^+$	$C_{62}H_{96}Fe_7N_6O_{24}^{+1}$	1700.19160	1700.19223	9
$[Fe^{III}_7O_4(piv)_9(tpt)(MeO)_3]^+$	$C_{66}H_{102}Fe_7N_6O_{25}^{+1}$	1770.23347	1770.23466	55
$[Fe^{III}_7O_4(piv)_{10}(tpt)(MeO)_2]^+$	$C_{70}H_{108}Fe_7N_6O_{26}^{+1}$	1840.27533	1840.27616	77
$[Fe^{III}_7O_4(piv)_{11}(tpt)(MeO)]^+$	$C_{74}H_{114}Fe_7N_6O_{27}^{+1}$	1910.31720	1910.31748	45
4b, ESI–				
$[Fe^{III}_2O(piv)_3(MeO)_2]^-$	$C_{21}H_{39}Fe_2O_{10}^{-1}$	493.08288	493.08048	35
$[Fe^{III}_2O(piv)_4(MeO)]^-$	**$C_{21}H_{39}Fe_2O_{10}^{-1}$**	**563.12474**	**563.12226**	**100**
$[Fe^{III}_2O(piv)_5]^-$	$C_{25}H_{45}Fe_2O_{11}^{-1}$	633.16661	633.16381	47
$[Fe^{III}_5O_3(piv)_6(MeO)_4]^-$	$C_{34}H_{66}Fe_5O_{19}^{-1}$	1058.09506	1058.09141	26
$[Fe^{III}_5O_3(piv)_7(MeO)_3]^-$	$C_{38}H_{72}Fe_5O_{20}^{-1}$	1128.13692	1128.13342	46
$[Fe^{III}_5O_3(piv)_8(MeO)_2]^-$	$C_{42}H_{78}Fe_5O_{21}^{-1}$	1198.17879	1198.17470	21
$[Fe^{III}_7O_5(piv)_2(tpt\text{-}O)(OH)(MeO)_6(MeOH)_4)]^-$	$C_{38}H_{65}Fe_6N_6O_{21}^{-1}$	1277.03044	1277.12255	5
$[Fe^{III}_7O_5(piv)_3(tpt\text{-}O)(OH)(MeO)_5(MeOH)_4)]^-$	$C_{42}H_{71}Fe_6N_6O_{22}^{-1}$	1347.07231	1347.16500	27
$[Fe^{III}_7O_5(piv)_4(tpt\text{-}O)(OH)(MeO)_4(MeOH)_4)]^-$	$C_{46}H_{77}Fe_6N_6O_{23}^{-1}$	1417.11417	1417.20691	38
$[Fe^{III}_7O_5(piv)_5(tpt\text{-}O)(OH)(MeO)_3(MeOH)_4)]^-$	$C_{50}H_{83}Fe_6N_6O_{24}^{-1}$	1487.15604	1487.24853	5
$\{[Fe^{III}_7O_5(piv)_5(tpt\text{-}O)(OH)_5(MeO)_2(dioxane)(H_2O)]+H\}^-$	$C_{49}H_{79}Fe_7N_6O_{26}^{-1}$	1559.04950	1559.17844	19
$\{[Fe^{III}_7O_5(piv)_6(tpt\text{-}O)(OH)_5(MeO)(dioxane)(H_2O)]+H\}^-$	$C_{53}H_{85}Fe_7N_6O_{27}^{-1}$	1629.09137	1629.21974	64
$\{[Fe^{III}_7O_5(piv)_7(tpt\text{-}O)(OH)_5(dioxane)(H_2O)]+H\}^-$	$C_{57}H_{91}Fe_7N_6O_{28}^{-1}$	1699.13269	1699.26106	5
5, ESI+				
$\{[Fe^{III}_7O_4(piv)_4(tpt\text{-}O)(MeO)_8(H_2O)_5]+H\}^+$	$C_{46}H_{83}Fe_7N_6O_{26}^{+1}$	1527.07971	1527.20178	3
$\{[Fe^{III}_7O_4(piv)_5(tpt\text{-}O)(MeO)_7(H_2O)_5]+H\}^+$	$C_{50}H_{89}Fe_7N_6O_{27}^{+1}$	1597.12157	1597.24390	52
$\{[Fe^{III}_7O_4(piv)_6(tpt\text{-}O)(MeO)_6(H_2O)_5]+H\}^+$	$C_{54}H_{95}Fe_7N_6O_{28}^{+1}$	1667.16344	1667.28577	34

$[Fe^{III}_7O_4(piv)_9(tpt)(MeO)_3]^+$	$C_{66}H_{102}Fe_7N_6O_{25}^{+1}$	1770.23347	1770.23352	21
$[Fe^{III}_7O_4(piv)_{10}(tpt)(MeO)_2]^+$	**$C_{70}H_{108}Fe_7N_6O_{26}^{+1}$**	**1840.27533**	**1840.27454**	**100**
$[Fe^{III}_7O_4(piv)_{11}(tpt)(MeO)]^+$	$C_{74}H_{114}Fe_7N_6O_{27}^{+1}$	1910.31720	1913.31604	43
$[Fe^{III}_7O_5(piv)_8(tpt\text{-}O)(MeO)(i\text{-}PrOH)(thf)_3]^+$	$C_{77}H_{127}Fe_7N_6O_{28}^{+1}$	1975.41384	1975.27930	9
$[Fe^{III}_7O_5(piv)_9(tpt\text{-}O)(i\text{-}PrOH)(thf)_3]^+$	$C_{81}H_{133}Fe_7N_6O_{29}^{+1}$	2045.45470	2045.32104	24
5, ESI–				
$[Fe^{III}_7O_5(piv)_5(tpt\text{-}O)(i\text{-}PrO)(MeO)_5]^-$	$C_{55}H_{85}Fe_7N_6O_{23}^{-1}$	1519.06985	1519.16357	1
$[Fe^{III}_7O_5(piv)_6(tpt\text{-}O)(i\text{-}PrO)(MeO)_4]^-$	$C_{55}H_{85}Fe_7N_6O_{23}^{-1}$	1589.11171	1589.20393	6
$[Fe^{III}_7O_5(piv)_7(tpt\text{-}O)(i\text{-}PrO)(MeO)_3]^-$	$C_{59}H_{91}Fe_7N_6O_{24}^{-1}$	1659.15358	1659.28613	21
$[Fe^{III}_7O_5(piv)_8(tpt\text{-}O)(i\text{-}PrO)(MeO)_2]^-$	$C_{63}H_{97}Fe_7N_6O_{25}^{-1}$	1729.19544	1729.32385	9
$[Fe^{III}_7O_5(piv)_9(tpt\text{-}O)(i\text{-}PrO)(MeO)]^-$	$C_{67}H_{103}Fe_7N_6O_{26}^{-1}$	1799.23731	1799.36267	6
$[Fe^{III}_7O_4(piv)_{10}(tpt)(MeO)_4]^-$	$C_{72}H_{114}Fe_7N_6O_{28}^{-1}$	1902.31321	1902.31140	14
$[Fe^{III}_7O_4(piv)_{11}(tpt)(MeO)_3]^-$	$C_{76}H_{120}Fe_7N_6O_{29}^{-1}$	1972.35507	1972.35181	82
$[Fe^{III}_7O_4(piv)_{12}(tpt)(MeO)_2]^-$	**$C_{80}H_{126}Fe_7N_6O_{30}^{-1}$**	**2042.39694**	**2042.39221**	**100**
7, ESI+				
$[Mn^{II}(ib)(tpt)]^+$	**$C_{22}H_{19}MnN_6O_2^{+1}$**	**454.09444**	**454.09826**	**100**
$[Mn^{II}_2(OH)_2(ib)(tpt)(MeOH)(H_2O)_6]^+$	$C_{23}H_{37}Mn_2N_6O_{11}^{+1}$	683.12757	683.12778	13
$[Mn^{II}_2(OH)_2(ib)(tpt)(MeOH)_2(H_2O)_5]^+$	$C_{24}H_{39}Mn_2N_6O_{11}^{+1}$	697.14377	697.14358	1
$[Mn^{II}(ib)(tpt)_2]^+$	$C_{40}H_{31}MnN_{12}O_2^{+1}$	766.20679	766.21393	4

[1] L. Patiny, A. Borel, *J. Chem. Inf. Model.*, 2013, **53**, 1223.

[2] in MeOH

Table S3. Crystal data and details of structural determinations for **1–7**

	1 [Fe(tpt)(tptH)][$FeCl_4$]$_4$·2(thf)·0.23(H_2O)	**2** [Fe(piv)(tpt)($Cl)_2$]	**3** [$Fe_2O(tpt)_2Cl_4$]	**3a** [Fe(tpt)Cl_2]·2(H_2O)	**4a** [$Fe_7O_4(piv)_{12}$(tpt-O)]·MeCN
Empirical formula	$C_{44}H_{41.46}Cl_{16}Fe_5N_{12}O_{2.23}$	$C_{23}H_{21}Cl_2FeN_6O_2$	$C_{36}H_{24}Cl_4Fe_2N_{12}O$	$C_{18}H_{16}Cl_2FeN_6O_2$	$C_{80}H_{123}Fe_7N_7O_{29}$
M_r / g mol^{-1}	1620.49	540.21	894.17	475.12	2037.80
T / K	100(2)	100(2)	173(2)	100(2)	100(2)
Wavelength / Å	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Triclinic	Triclinic	Monoclinic
Space group	$P2_1/m$	$P2_1/c$	P-1	P-1	$P2_1/n$
Unit cell dimensions					
a / Å	11.9688(17)	9.2814(9)	8.410(4)	8.7197(17)	24.887(18)
b / Å	40.521(6)	15.3813(15)	9.221(5)	9.1076(18)	12.069(9)
c / Å	15.230(2)	15.9903(1)	11.896(6)	13.374(3)	35.14(2)
α / °	90	90	81.328(7)	106.09(3)	90
β /°	111.591(4)	93.392(3)	80.254(7)	99.73(3)	108.01(2)
γ /°	90	90	83.965(8)	100.60(3)	90
V / Å^3	6867.9(17)	2278.8(4)	895.8(8)	975.5(4)	10036(12)
Z, ρ / Mg m^{-3}	2, 1.427	4, 1.575	1, 1.658	2, 1.618	4, 1.349
μ / mm^{-1}	1.687	0.931	1.160	1.075	1.056
F(000)	2915	1108	452	484	4264
Crystal size / mm^3	0.22 × 0.20 × 0.06	0.16 × 0.16 × 0.11	0.34 × 0.16 × 0.08	0.44 × 0.28 × 0.12	0.22 × 0.22 × 0.06
θ range for data collection	1.005° to 24.998°	2.198° – 25.026°	1.75° – 23.21°	2.400° – 24.999°	1.219° – 23.817°
Index ranges	$-14 \leq h \leq 14$, $-48 \leq k \leq 48$, $-18 \leq l \leq 18$	$-11 \leq h \leq 11$, $-18 \leq k \leq 18$, $-19 \leq l \leq 19$	$-9 \leq h \leq 3$, $-10 \leq k \leq 9$, $-13 \leq l \leq 11$	$-10 \leq h \leq 8$, $-10 \leq k \leq 10$, $-15 \leq l \leq 15$	$-28 \leq h \leq 28$, $-13 \leq k \leq 13$, $-39 \leq l \leq 37$
Reflections collected	75500	24615	2890	12311	71446
Independent reflections	12286 [R_{int} = 0.2133]	4019 [R_{int} = 0.1771]	7123 [R_{int} = 0.0370]	3438 [R_{int} = 0.0554]	15422 [R_{int} = 0.2388]
Data / restraints / parameters	12286 / 27 / 657	4019 / 0 / 304	7123 / 137 / 550	3438 / 0 / 262	15422 / 108 / 1196
Goodness-of-fit on F^2	1.003	0.908	1.090	1.084	1.003
Final R indices [$I > 2\sigma(I)$]: R_1, wR_2	0.0946, 0.2070	0.0440, 0.0937	0.0413, 0.0949	0.0819, 0.2299	0.0832, 0.1766
R indices (all data): R_1, wR_2	0.1646, 0.2252	0.0694, 0.1005	0.0486, 0.1001	0.0870, 0.2377	0.1590, 0.2189
Largest diff. peak, hole / e Å^{-3}	0.927 and -0.724	0.631, –0.589	3.776, –1.588	0.682, –1.157	0.739, –1.053

	4b [$Fe_7O_4(piv)_{12}$(tpt-O)] 4(diox)	**5** [$Fe_7O_4(piv)_{11}$(tpt-O) (*i*-PrO)(*i*-PrOH)] ·0.75(*i*-PrOH)	**6** [Mn(NO_3)(tpt) $(H_2O)_2$](NO_3)	**7** [Mn(ib)(Cl)(tpt) (MeOH)]·MeOH	
Empirical formula	$C_{94}H_{152}Fe_7N_6O_{37}$	$C_{81.25}H_{132}Fe_7N_6O_{29.75}$	$C_{18}H_{16}MnN_8O8$	$C_{24}H_{27}ClMnN_6O_4$	
M_r / g mol^{-1}	2349.17	2059.87	527.33	553.90	
T / K	100(2)	100(2)	293(2)	293(2)	
Wavelength / Å	0.71073	0.71073	0.71073	0.71073	
Crystal system	Triclinic	Triclinic	Monoclinic	Triclinic	
Space group	*P*-1	*P*-1	*C*2/*c*	*P*-1	
Unit cell dimensions					
a / Å	12.6917(11)	16.277(6)	20.4359(8)	8.8127(6)	
b / Å	18.5226(17)	22.189(8)	13.3612(4)	10.9546(5)	
c / Å	24.683(2)	31.533(11)	16.7266(6)	15.1293(6)	
α	93.070(2)	70.195(9)	90	71.115(4)	
β	93.369(2)	79.277(12)	107.782(4)	81.894(4)	
γ	97.272(2)	72.259(11)	90	68.777(5)	
V / Å^3	5735.1(9)	10162(6)	4348.9(3)	1287.75(12)	
Z, ρ / Mg m^{-3}	2, 1.360	4,1.346	8, 1.611	2, 1.429	
μ / mm^{-1}	0.939	1.044	0.672	0.658	
F(000)	2472	4326	2152	574	
Crystal size / mm^3	0.25 × 0.21 × 0.16	0.25 × 0.14 × 0.09	0.4 x 0.2 x 0.12	0.53 × 0.20 × 0.08	
θ range for data collection	1.94° – 24.41°	1.011° – 25.000°	3.307° to 25.495°	2.992° – 25.541°	
Index ranges	$-14 \leq h \leq 14$, $-21 \leq k \leq 21$, $-28 \leq l \leq 28$	$-19 \leq h \leq 19$, $-26 \leq k \leq 26$, $-37 \leq l \leq 37$	$-24 \leq h \leq 15$, $-16 \leq k \leq 10$, $-14 \leq l \leq 20$	$-10 \leq h \leq 10$, $-12 \leq k \leq 13$, $-13 \leq l \leq 18$	
Reflections collected	58376	84896	7918	7205	
Independent reflections	18881 [R_{int} = 0.0628]	35797 [R_{int} = 0.1783]	4029 [R_{int} = 0.0291]	4782 [R_{int} = 0.0275]	
Data / restraints / parameters	18881 / 70 / 1375	35797 / 217 / 2340	4029 / 1 / 318	4782 / 0 / 330	
Goodness-of-fit on F^2	1.049	0.989	1.079	1.006	
Final R indices [$I > 2\sigma(I)$]: R_1, wR_2	0.0501, 0.1151	0.0773, 0.1265	0.0540, 0.1350	0.0490, 0.1186	
R indices (all data):R_1, wR_2	0.0729, 0.1295	0.1926, 0.1666	0.0803, 0.1491	0.0687, 0.1351	
Largest diff. peak, hole / e Å^{-3}	0.844, –0.835	0.904, –0.998	1.002, –0.583	0.523, –0.450	

Table S4. Selected bond distances (Å) for **1–7**

1

Fe1–N8	1.844(8)	Fe3–Cl5	2.207(3)
Fe1–N2	1.873(7)	Fe4–Cl9	2.176(5)
Fe1–N3	1.984(8)	Fe4–Cl11	2.186(3)
Fe1–N1	1.995(7)	Fe4–Cl11[#1]	2.186(3)
Fe1–N9	1.999(8)	Fe4–Cl10	2.204(5)
Fe1–N7	2.015(7)	Fe5–Cl14	2.163(14)
Fe2–Cl3	2.163(4)	Fe5–Cl13	2.183(4)
Fe2–Cl2	2.169(3)	Fe5–Cl15	2.183(5)
Fe2–Cl4	2.189(3)	Fe5–Cl12	2.195(3)
Fe2–Cl1	2.194(4)	Fe6–Cl17	2.117(7)
Fe3–Cl6	2.173(3)	Fe6–Cl16[#1]	2.173(4)
Fe3–Cl7	2.176(3)	Fe6–Cl16	2.173(4)
Fe3–Cl8	2.201(3)	Fe6–Cl18	2.191(8)

Symmetry transformations used to generate equivalent atoms: #1 *x*, −*y*+1/2, *z*

2

Fe1–O1	2.110(2)
Fe1–O2	2.151(2)
Fe1–N2	2.170(3)
Fe1–N3	2.290(3)
Fe1–N1	2.293(3)
Fe1–Cl1	2.3000(2)
Fe1–Cl2	2.3416(2)

3

Fe1–O1	1.805(2)
Fe1–N2	2.136(9)
Fe1–N1	2.198(8)
Fe1–N5	2.218(8)
Fe1–Cl2	2.332(3)
Fe1–Cl1	2.398(4)

3a

Fe1–N2	2.102(4)
Fe1–N1	2.211(4)
Fe1–N3	2.220(4)
Fe1–Cl2	2.2930(17)
Fe1–Cl1	2.3278(14)

4a

Fe1–O2	1.958(5)	Fe4–O18	2.023(6)
Fe1–O1	1.992(5)	Fe4–O5	2.118(5)
Fe1–O6	2.011(6)	Fe4–N6	2.175(7)
Fe1–O8	2.023(6)	Fe5–O3	1.951(6)
Fe1–O12	2.040(6)	Fe5–O4	1.995(5)
Fe1–O10	2.049(6)	Fe5–O19	2.012(6)
Fe2–O2	1.900(5)	Fe5–O28	2.015(6)
Fe2–O1	1.929(6)	Fe5–O5	2.016(5)
Fe2–O14	2.005(6)	Fe5–O20	2.016(6)
Fe2–O13	2.082(6)	Fe6–O3	1.884(5)
Fe2–N2	2.106(7)	Fe6–O24	1.970(6)
Fe2–N1	2.156(7)	Fe6–O21	2.035(6)
Fe3–O1	1.843(6)	Fe6–O26	2.042(6)
Fe3–O7	2.013(6)	Fe6–O23	2.098(6)
Fe3–O9	2.014(6)	Fe6–O22	2.126(6)
Fe3–O15	2.057(6)	Fe7–O3	1.887(5)
Fe3–O16	2.067(6)	Fe7–O29	2.019(6)
Fe3–O17	2.167(6)	Fe7–O27	2.021(6)
Fe4–O2	1.847(5)	Fe7–O25	2.043(6)
Fe4–O4	2.013(5)	Fe7–N3	2.113(7)
Fe4–O11	2.020(5)	Fe7–N5	2.166(7)

4b

Fe1–O2	1.953(3)	Fe5–O17	2.010(3)
Fe1–O1	1.967(3)	Fe5–O18	2.018(3)
Fe1–O28	1.995(3)	Fe5–O5	2.022(3)
Fe1–O14	2.028(3)	Fe6–O3	1.874(3)
Fe1–O8	2.028(3)	Fe6–O23	1.998(3)
Fe1–O6	2.046(3)	Fe6–O21	2.020(3)
Fe2–O2	1.894(3)	Fe6–O25	2.036(3)
Fe2–O1	1.939(3)	Fe6–O26	2.099(3)
Fe2–O13	2.006(3)	Fe6–O27	2.127(3)
Fe2–O15	2.049(3)	Fe7–O3	1.868(3)
Fe2–N2	2.137(3)	Fe7–O19	2.002(3)
Fe2–N1	2.174(3)	Fe7–O24	2.014(3)
Fe3–O1	1.835(3)	Fe7–O22	2.053(3)
Fe3–O7	1.987(3)	Fe7–N3	2.122(3)
Fe3–O12	2.040(3)	Fe7–N5	2.150(3)
Fe3–O9	2.047(3)		

5

Fe1–O1	1.854(5)	Fe5–O18	2.014(5)	Fe10–O40	1.998(5)
Fe1–O8	2.010(5)	Fe5–O5	2.078(5)	Fe10–O45	1.999(6)
Fe1–O10	2.024(5)	Fe6–O4	1.819(5)	Fe10–O43	2.034(5)
Fe1–O6	2.026(5)	Fe6–O22	2.016(5)	Fe10–O38	2.034(6)
Fe1–O12	2.026(5)	Fe6–O24	2.017(5)	Fe11–O31	1.841(5)
Fe1–O28	2.114(5)	Fe6–O19	2.032(5)	Fe11–O46	2.000(6)
Fe2–O1	1.954(5)	Fe6–O20	2.082(5)	Fe11–O32	2.020(5)
Fe2–O2	1.954(5)	Fe6–O21	2.127(5)	Fe11–O47	2.050(6)
Fe2–O14	2.006(5)	Fe7–O4	1.880(5)	Fe11–O34	2.093(5)
Fe2–O9	2.024(5)	Fe7–O29	1.968(5)	Fe11–N11	2.195(7)
Fe2–O7	2.032(5)	Fe7–O23	2.019(5)	Fe12–O33	1.949(5)
Fe2–O26	2.034(5)	Fe7–O25	2.061(5)	Fe12–O48	1.974(6)
Fe3–O2	1.898(5)	Fe7–N4	2.108(6)	Fe12–O32	1.977(5)
Fe3–O1	1.929(5)	Fe7–N5	2.114(6)	Fe12–O51	1.988(5)
Fe3–O11	2.024(5)	Fe8–O30	1.855(5)	Fe12–O58	2.003(6)
Fe3–O27	2.065(5)	Fe8–O41	2.010(5)	Fe12–O34	2.068(5)

6

Mn1-O2W	2.138(3)
Mn1-O1W	2.192(2)
Mn1-N2	2.232(3)
Mn1-O3	2.269(2)
Mn1-N3	2.351(3)
Mn1-N1	2.378(3)
Mn1-O2	2.411(2)

7

Mn1-O2	2.226(2)
Mn1-O1	2.294(2)
Mn1-N2	2.295(2)
Mn1-O3	2.307(2)
Mn1-N1	2.399(2)
Mn1-N3	2.412(2)
Mn1-Cl1	2.486(1)

Fe3–O11	2.059(3)			Fe3–N2	2.161(6)	Fe8–O37	2.028(6)	Fe13–O33	1.830(5)				
Fe3–O10	2.162(3)			Fe3–N1	2.177(6)	Fe8–O39	2.052(6)	Fe13–O53	1.998(5)				
Fe4–O2	1.845(3)			Fe4–O2	1.856(5)	Fe8–O35	2.060(6)	Fe13–O55	2.010(5)				
Fe4–O16	1.994(3)			Fe4–O15	2.000(6)	Fe8–O57	2.099(6)	Fe13–O52	2.016(5)				
Fe4–O29	2.013(3)			Fe4–O16	2.018(5)	Fe9–O31	1.888(5)	Fe13–O49	2.109(5)				
Fe4–O4	2.023(3)			Fe4–O3	2.036(5)	Fe9–O30	1.939(5)	Fe13–O50	2.121(6)				
Fe4–O5	2.138(3)			Fe4–O5	2.084(5)	Fe9–O36	2.008(5)	Fe14–O33	1.878(5)				
Fe4–N6	2.172(3)			Fe4–N3	2.176(6)	Fe9–O44	2.057(5)	Fe14–O58	2.018(5)				
Fe5–O3	1.975(3)			Fe5–O4	1.949(5)	Fe9–N12	2.151(6)	Fe14–O54	2.021(6)				
Fe5–O4	1.986(3)			Fe5–O3	1.964(5)	Fe9–N10	2.164(6)	Fe14–O56	2.067(6)				
Fe5–O20	2.004(3)			Fe5–O17	1.982(5)	Fe10–O30	1.955(5)	Fe14–N8	2.109(6)				
				Fe5–O29	2.000(5)	Fe10–O31	1.960(5)	Fe14–N7	2.127(6)				

Table S5. Continuous shape measures (CShM) of the coordination geometries of compounds **1–7** using SHAPE v2.0 [1],*

CN 4	Seesaw (C_{2v})	Tetra-hedron (T_d)	Square (D_{4h})
1: Fe	8.712	0.078	31.199

CN 5	Johnson J12 (D_{3h})	Square pyramid (C_{4v})	Trigonal bipyramid (D_{3h})	Vacant octahedron (C_{4v})	Pentagon (D_{5h})
3a: Fe	9.310	2.017	5.950	3.750	30.789

CN 6	Johnson J2 (C_{5v})	Trigonal prism (D_{3h})	Octahedron (O_h)	Pentagonal pyramid (C_{5v})	Hexagon (D_{6h})
1: Fe	26.247	10.422	2.491	22.186	33.564
3: Fe	28.341	13.835	2.862	24.373	34.355
4a: Fe1	27.474	11.789	0.877	23.743	32.793
4a: Fe2	28.845	13.552	0.836	25.613	29.898
4a: Fe3	28.772	13.567	1.661	24.649	31.814
4a: Fe4	27.959	13.660	0.984	24.054	29.551
4a: Fe5	31.011	14.865	0.369	27.707	31.025
4a: Fe6	28.891	14.756	1.552	24.918	29.856

4a: Fe7	30.569	14.993	0.548	26.921	31.946
4b: Fe1	29.301	13.052	0.582	25.605	32.757
4b: Fe2	29.245	13.669	0.800	26.037	29.428
4b: Fe3	29.151	13.208	1.649	25.068	31.763
4b: Fe4	28.803	13.468	0.873	24.703	30.581
4b: Fe5	30.729	14.204	0.379	27.154	31.089
4b: Fe6	26.853	13.247	1.915	22.918	30.156
4b: Fe7	30.131	14.695	0.637	26.475	32.115
5: Fe1	30.977	14.798	0.352	27.192	31.218
5: Fe2	30.798	14.427	0.454	27.329	31.063
5: Fe3	28.622	13.524	0.901	25.276	29.705
5: Fe4	29.690	12.892	0.787	25.647	31.483
5: Fe5	30.238	14.080	0.539	26.717	30.860
5: Fe6	24.932	11.957	2.195	21.285	30.979
5: Fe7	28.554	12.031	0.957	24.993	29.811

CN 7	Johnson J7 (C_{3v})	Johnson J13 (D_{5h})	Capped trigonal prism (C_{2v})	Capped octahedron (C_{3v})	Pentagonal bipyramid (D_{5h})	Hexagonal pyramid (C_{6v})	Heptagon (D_{7h})
2: Fe	23.974	5.088	5.823	7.466	0.569	24.909	34.425
6: Mn	22.838	3.511	6.325	8.212	1.034	24.265	32.018
7: Mn	23.690	5.103	6.615	8.454	0.991	24.726	33.044

∗A value of zero corresponds to an exact match of the corresponding center to the ideal geometry. Listed Johnson solids are: pentagonal pyramid (J2), elongated triangular pyramid (J7), trigonal bipyramid (J12) and pentagonal bipyramid (J13).

[1] (a) M. Llunell, D. Casanova, J. Cirera, P. Alemany, S. Alvarez, *SHAPE 2.0*, Universitat de Barcelona, Barcelona, **2010**; (b) S. Alvarez , P. Alemany, D. Casanova, J. Cirera, M. Llunell, D. Avnir, *Coord. Chem. Rev.* **2005**, *249*, 1693–1708.

Table S6. Bond valence sum (BVS) calculations for metal atoms in **1–7**

Compound	Atom	BVS value
1		
	Fe1	2.974
	Fe2	3.15
	Fe3	3.06
	Fe4	3.07
	Fe5	3.13
	Fe6	3.29
2		
	Fe1	2.94
3		
	Fe1	2.95
3a		
	Fe1	2.02
6		
	Mn1	1.98
7		
	Mn1	1.94

Compound	Atom	BVS value	Compound	Atom	BVS value
4a			**4b**		
	Fe1	3.05		Fe1	3.12
	Fe2	3.09		Fe2	3.08
	Fe3	3.02		Fe3	3.06
	Fe4	3.03		Fe4	3.06
	Fe5	3.13		Fe5	3.11
	Fe6	2.99		Fe6	2.99
	Fe7	2.99		Fe7	3.06

Compound	Atom	BVS value	Atom	BVS value	
5					
	Fe1	3.12	Fe8	3.06	
	Fe2	3.13	Fe9	3.08	
	Fe3	3.01	Fe10	3.17	
	Fe4	3.05	Fe11	3.04	
	Fe5	3.18	Fe12	3.20	
	Fe6	3.11	Fe13	3.12	
	Fe7	3.14	Fe14	3.03	

Table S7. The effect of compounds **6** and **7** on the proteolytic activity of fungal strain *Fusarium gibbosum* CNMN FD 12

Compound	Concentration, %	Neutral proteases (pH 7.4)				Alkaline proteases (pH 9.0)			
		5th day		6th day		5th day		6th day	
		u/mL	%, related to the control	u/mL	%, related to the control	u/mL	%, related to the control	u/mL	%, related to the control
6	0.0005	25.52	141.6	25.52	77.3	19.45	100.0	37.47	172.1
	0.0010	67.47	374.4 / 204.4**	33.01	100.0	79.41	408.3 / 364.8**	38.89	178.6
	0.0015	56.51	313.6 / 171.3**	36.04	109.2	59,96	308.3 / 275.4**	33.01	151.6
7	0.0005	22.48	124.8	49.25	149.2	70.48	362.4 / 323.7**	40.51	186.1
	0.0010	23.91	132.7	63.41	192.1	88.57	455.4 / 406.8**	53.88	247.5
	0.0015	21.05	116.8	56.51	171.2	85.47	439.4 / 392.6**	41.93	192.6
Control*	-	18.02	100.0	33.01	100.0	19.45	100.0	21.77	100.0

* cultivated in the absence of coordination compounds

**374.4 / 204.4 - %, related to the control of d day / %, related to the maximal value of control (6th day)

Table S8. The effect of compound**s** **6** and **7** on the proteolytic activity of fungal strain *Trichoderma koningii* Oudemans CNMN FD 15

Compound	Concentration, %	Neutral proteases (pH 7.4)				Alkaline proteases (pH 9.0)			
		9th day		10th day		9th day		10th day	
		u/mL	%, related to the control	u/mL	%, related to the control	u/mL	%, related to the control	u/mL	%, related to the control
6	0.0005	71.91	140.9	51.03	366.6	10.52	44.7	16.42	184.0
	0.0010	55.49	108.7	49.43	355.1	10.52	44.7	16.42	184.0
	0.0015	44.96	88.1	49.43	355.1	13.56	57.6	23.91	268.0
7	0.0005	94.39	185.0	61.38	440.9	10.52	44.7	13.56	152.0
	0.0010	79.41	155.6	61.38	440.9	10.52	44.7	16.42	184.0
	0.0015	62.98	123.4	53.88	387.1	13.56	57.6	25.52	286.0
Control*	-	51.03	100.0	13.92	100,0	23.55	100	8.92	100.0

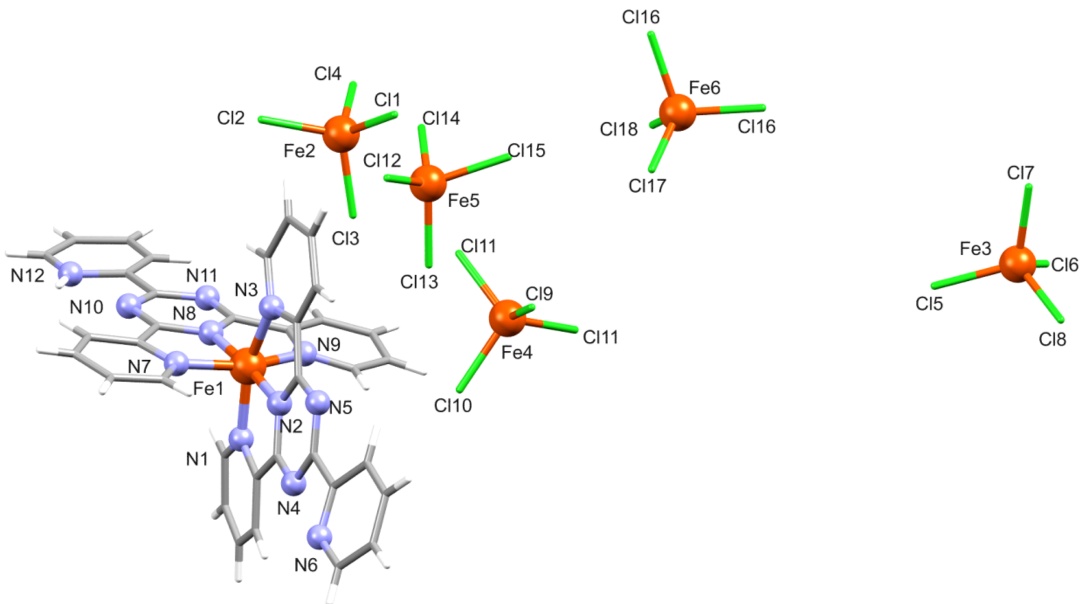

Figure S1. Asymmetric unit in the solid-state structure of [Fe(tpt)(tptH)][$FeCl_4$]$_4$ (**1**) with a partial atom numbering. Tetrahydrofuran and water molecules are omitted.

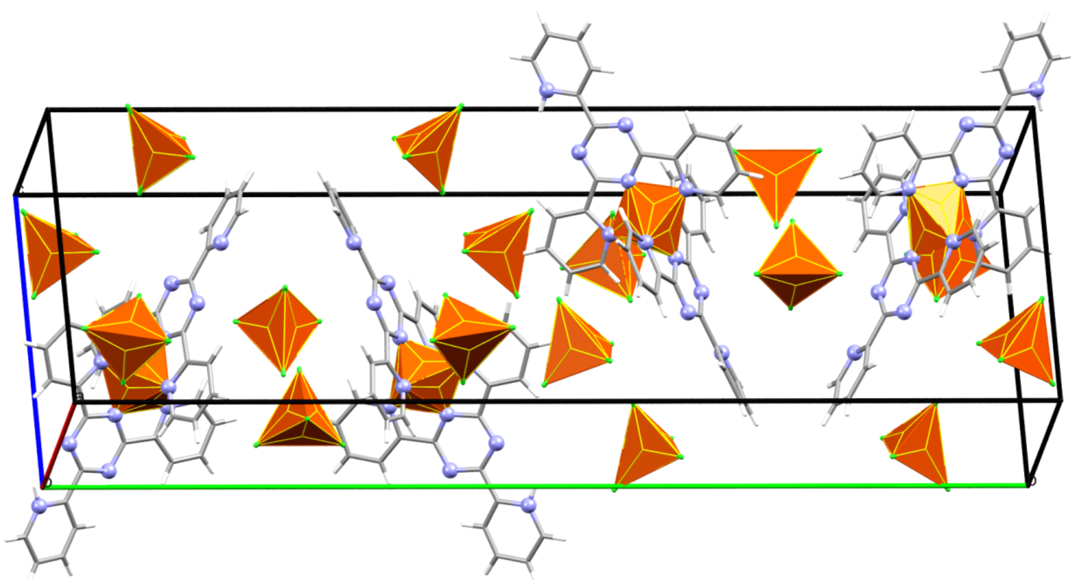

Figure S2. Packing diagram for **1**. [$FeCl_4$]: brown polyhedra. Tetrahydrofuran and water molecules are omitted.

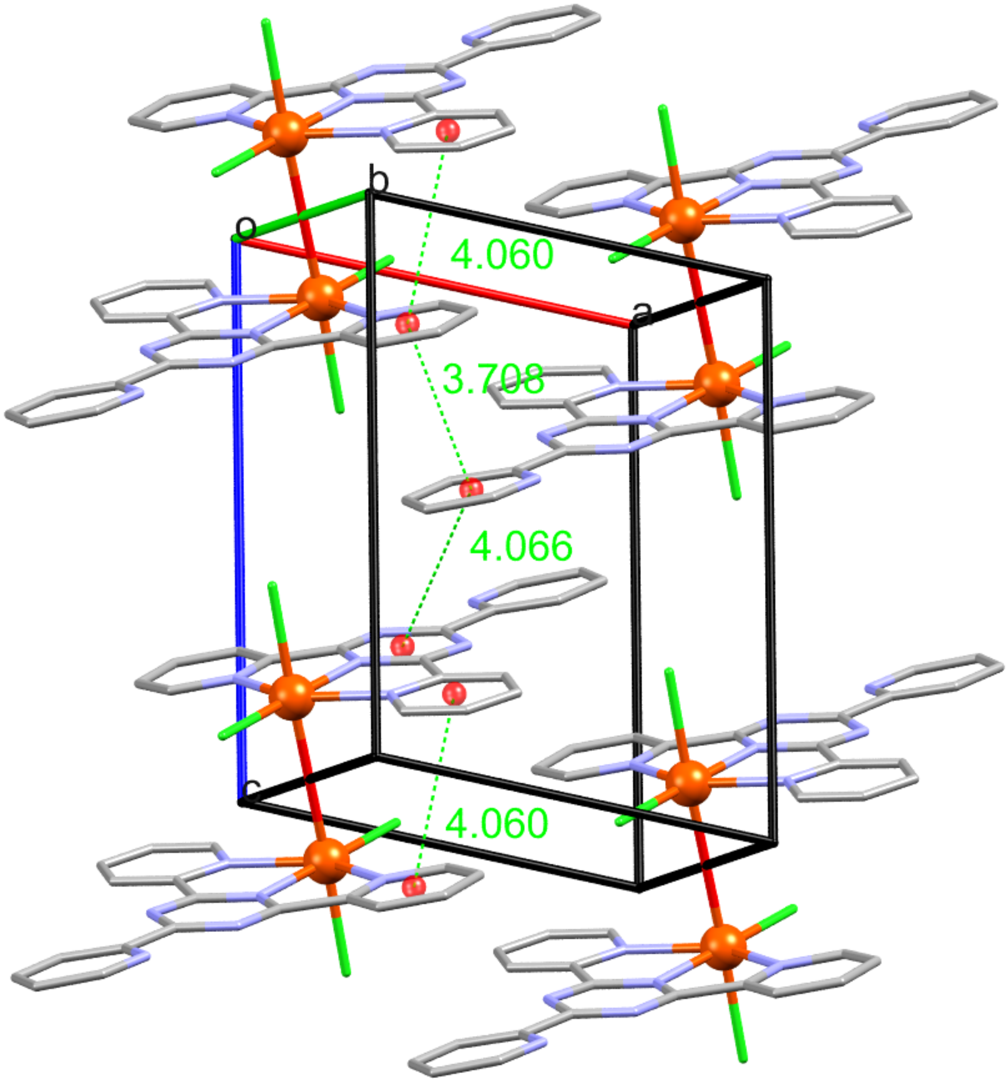

Figure S3. Packing diagram showing the π-π interactions in $[Fe_2O(tpt)_2Cl_4]$ (**3**).

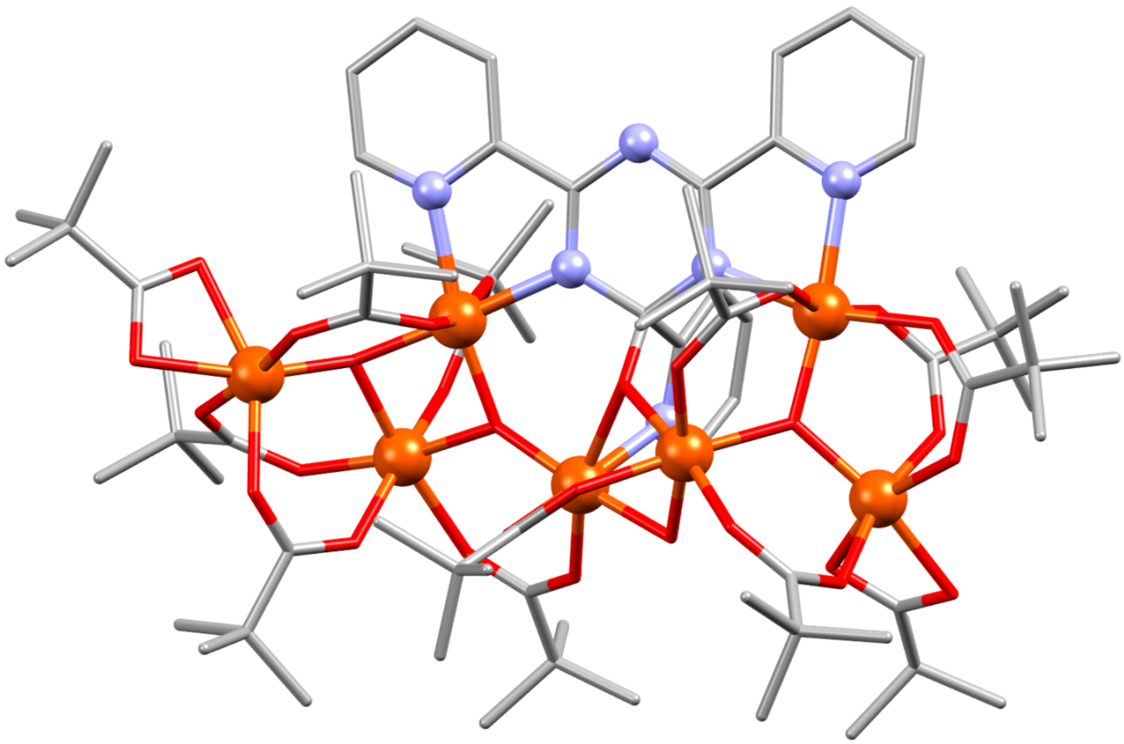

Figure S4. Structure of [$Fe_7O_4(piv)_{12}$(tpt-O)] in **4a** and **4b**. Hydrogen atoms and solvent molecules are omitted for clarity.

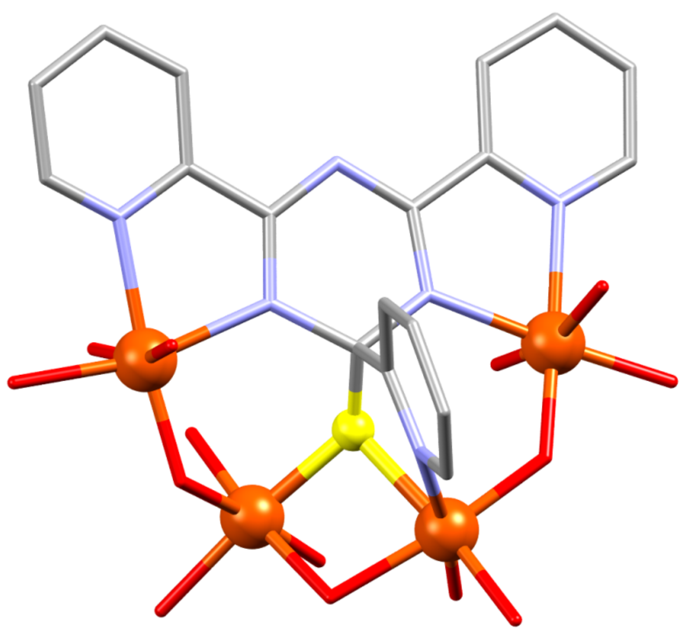

Figure S5. Coordination geometry of tpt-O in **4a, 4b** and **5**.

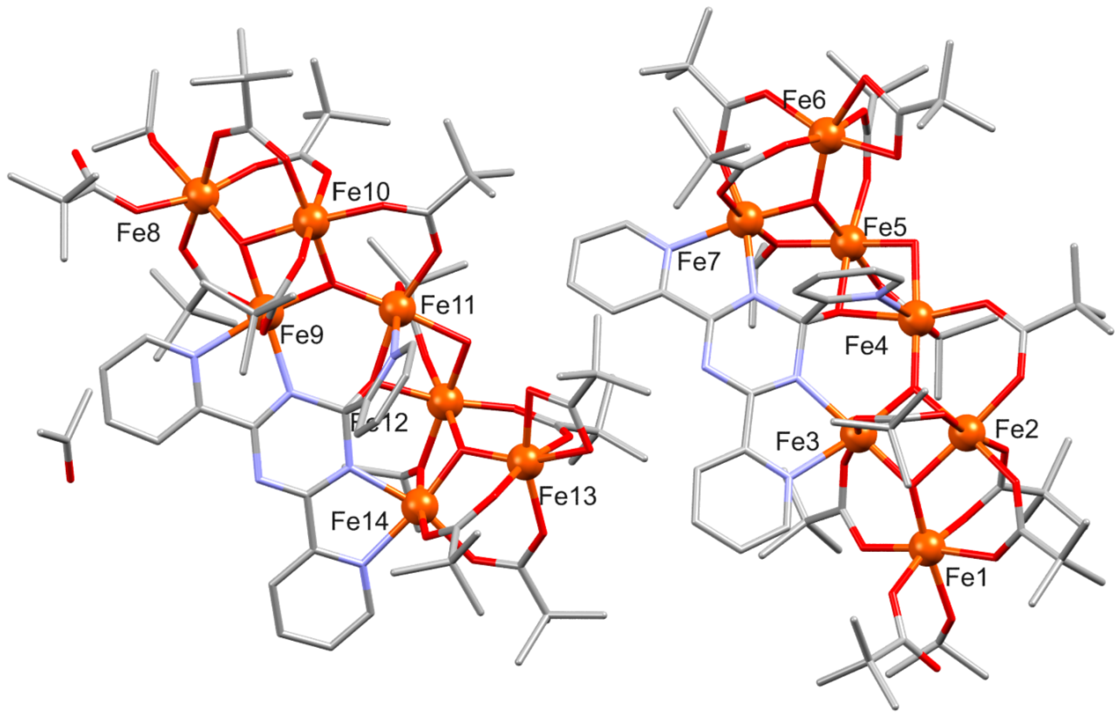

Figure S6. Asymmetric unit in the solid-state structure of $[Fe_7O_4(piv)_{11}$(tpt-O)(*i*-PrO)(*i*-PrOH)]·0.75(*i*-PrOH) (**5**) with a partial atom numbering. Hydrogen atoms are omitted for clarity.

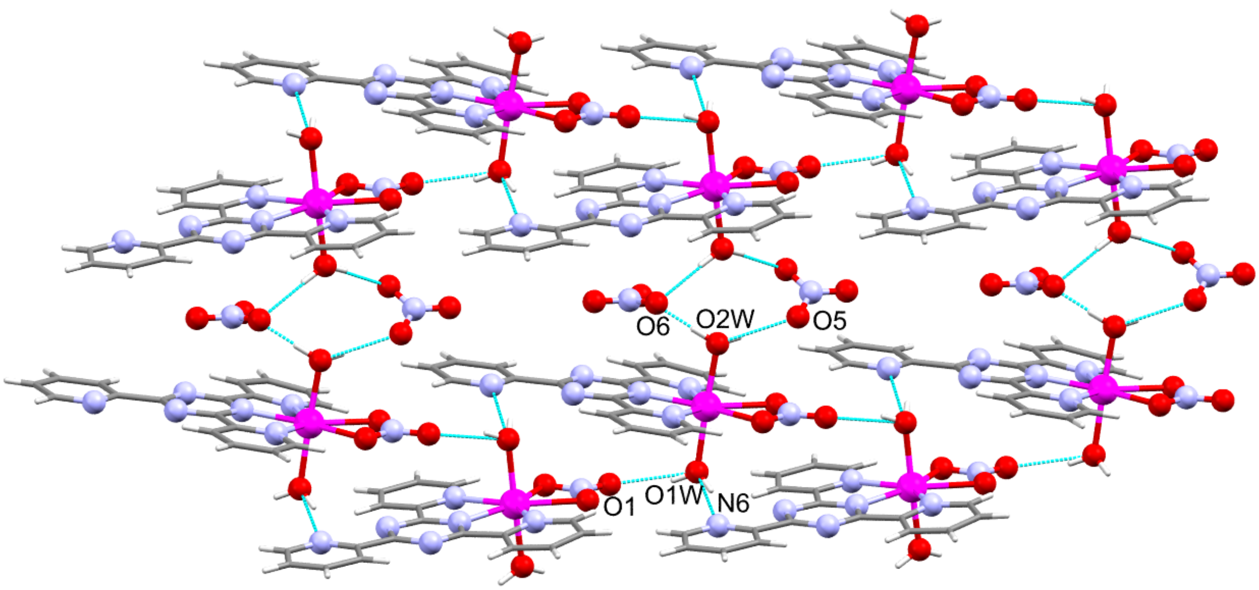

Figure S7. A supramolecular 2D network in $[Mn(NO_3)(tpt)(H_2O)_2](NO_3)$ (**6**).

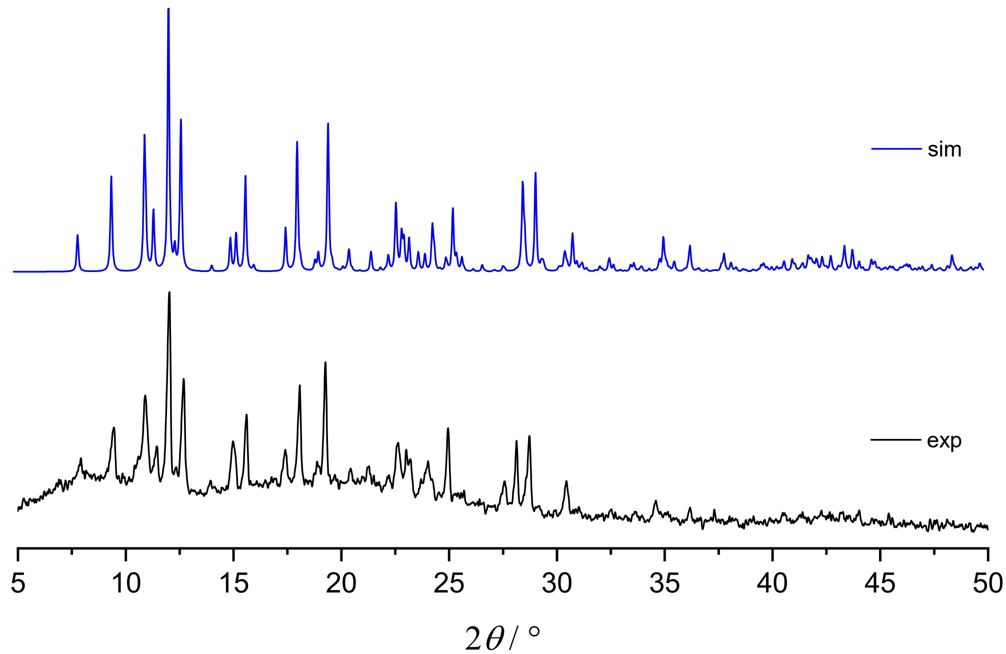

Figure S8. PXRD pattern of [Fe(piv)(tpt)(Cl)$_2$] (**2**).

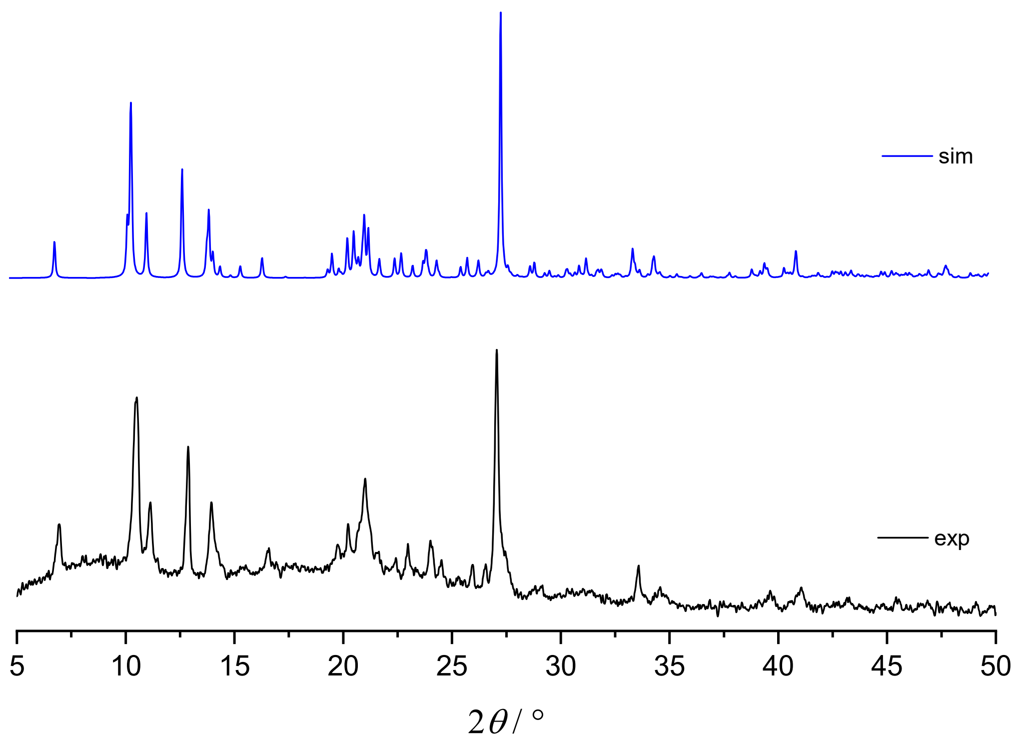

Figure S9. PXRD pattern of [Fe(tpt)Cl$_2$]·2(H_2O) (**3a**).

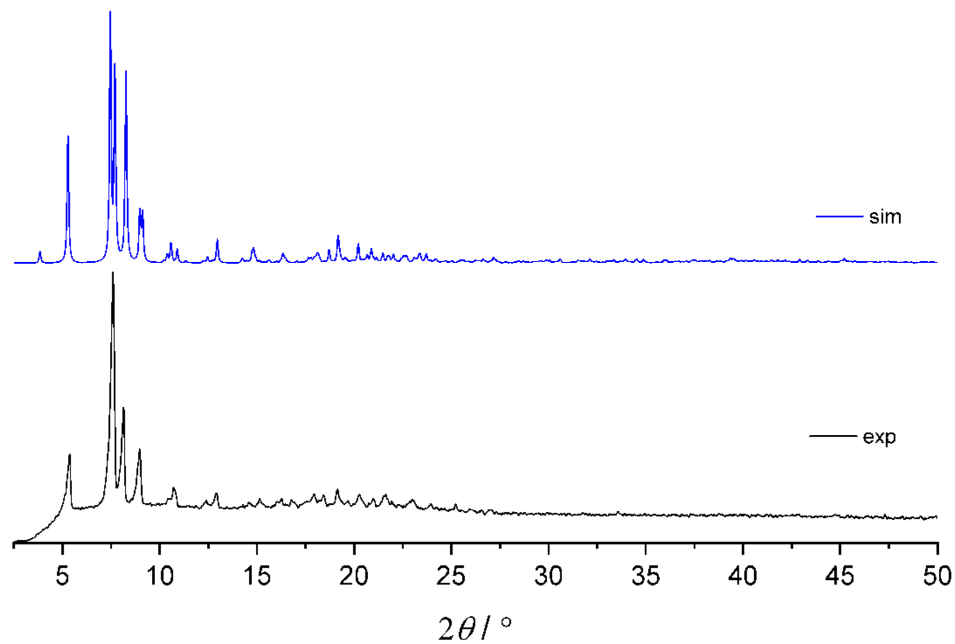

Figure S10. PXRD pattern of $[Fe_7O_4(piv)_{12}(tpt\text{-}O)]\cdot MeCN$ (**4a**).

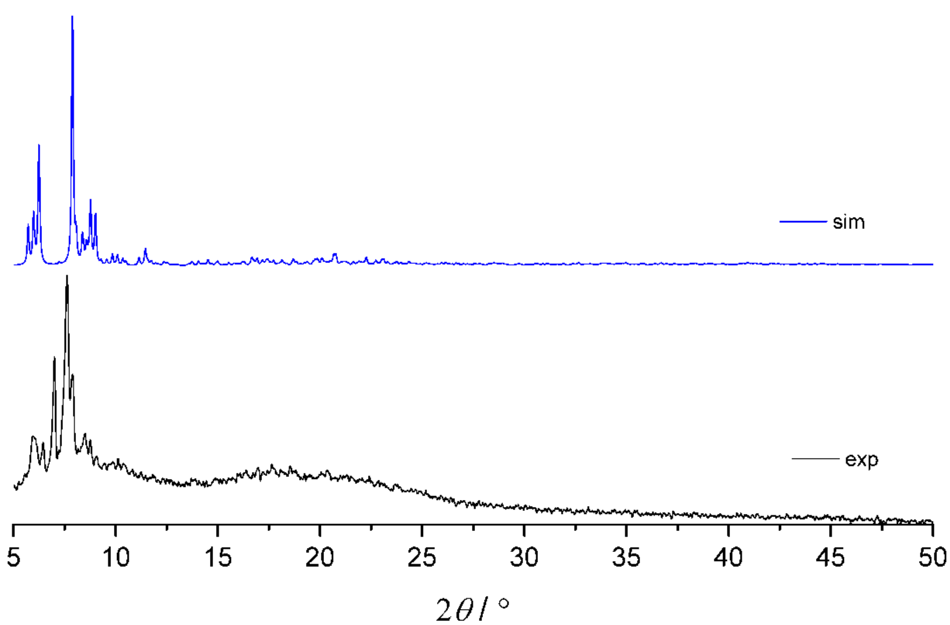

Figure S11. PXRD pattern of $[Fe_7O_4(piv)_{11}(tpt\text{-}O)(i\text{-}PrO)(i\text{-}PrOH)]\cdot 0.75(i\text{-}PrOH)$ (**5**).