

Electronic Supplementary Information (ESI) for Publication

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The list of calculation results of the magnitude of the ligand field splitting (Δ_0) octahedral hexacoordinated metal complex ML_6 used for the one-electron calculation (DV- $X\alpha$ molecular orbital method).

- ※ The label 'C' denotes the number of the valence electrons.
- ※ The central metal in each metal complex is shown with the atomic number 'Z' and the symbol of an element 'M'.
- ※ The metal-ligand coordination distance M-L is the average among 6 M-L distances.

ML ₆								Ser.	Z	M	C	CSD	Δ _o	M-L	Chiral
Ligand = I ⁻ ①								11	42	Mo	3	DEBLEB	2.41	2.45	
Ser.	Z	M	C	CSD	Δ _o	M-L	Chiral	11	42	Mo	3	PEPCOC	2.48	2.44	
	40	Zr	4	RIQPEN	2.27	2.86			42	Mo	4	FIPDEO	2.93	2.35	
17	78	Pt	4	PYPHI	2.89	2.67			42	Mo	4	ZICWOX	2.82	2.38	
17	78	Pt	4	KIBMIS	2.87	2.67			42	Mo	4	FUTPIT	2.80	2.38	
17	78	Pt	4	KIBMOY	2.91	2.66			42	Mo	5	JAWRUU	3.18	2.31	
Ligand = Br ⁻ ②									43	Tc	4	CIMFEJ	2.74	2.36	
7	24	Cr	3	YIBWOV	1.48	2.64			43	Tc	4	JEPQOL	2.77	2.35	
	29	Cu	2	TIVJEN	0.96	2.52			43	Tc	4	KAXQUW	2.76	2.35	
	40	Zr	3	SENPOQ	2.68	2.62			43	Tc	4	LALHAH	2.74	2.36	
	42	Mo	4	FUYGUB	2.73	2.53			44	Ru	2	WUGCOQ	2.26	2.37	
11	42	Mo	3	DOMTII	2.36	2.59		13	44	Ru	3	ENIDAG	2.42	2.38	
	43	Tc	5	PSBRNB	3.14	2.50		13	44	Ru	3	HEVCOA	2.43	2.37	
12	45	Rh	3	HUQMEL	2.43	2.50		13	44	Ru	3	HOCXUS	2.42	2.38	
12	45	Rh	3	ZOKHEM	2.51	2.53		13	44	Ru	3	TAVTUF	2.43	2.37	
	73	Ta	5	BDASTA	3.50	2.49		13	44	Ru	3	YOJBUU	2.44	2.37	
16	75	Re	4	AYOMAC	3.13	2.49			44	Ru	4	GAZNOK	2.74	2.32	
17	78	Pt	4	AZELEW	3.00	2.47			44	Ru	4	YARREP	2.72	2.33	
Ligand = S ²⁻ ③								12	45	Rh	3	FEWGET	2.44	2.35	
Ligand = SCN ⁻ ④								12	45	Rh	3	RIXHIP	2.45	2.34	
12	45	Rh	3	YURKIF	2.34	2.37		12	45	Rh	3	TIBWIK	2.43	2.35	
15	77	Ir	3	PORQAO	2.87	2.38		12	45	Rh	3	XISFEL	2.46	2.35	
17	78	Pt	4	BULVAF	2.39	2.68		14	46	Pd	4	JIZLOT	2.55	2.31	
17	78	Pt	4	EMUVOX	2.87	2.39		14	46	Pd	4	LAHFUV	2.10	2.42	
17	78	Pt	4	XECZAG	2.24	2.38			72	Hf	4	BARWIB	3.11	2.45	
Ligand = Cl ⁻ ⑤									72	Hf	4	FEBHIE	3.13	2.44	
	22	Ti	4	BARMAJ	2.08	2.34			72	Hf	4	JESFOC	3.09	2.45	
	22	Ti	4	FEPHOX	2.08	2.34			73	Ta	5	EMUCOE	3.51	2.34	
	23	V	4	SAHJER	2.03	2.31			73	Ta	5	FIKGAH	3.59	2.33	
8	23	V	3	YUDFUY	1.65	2.39			74	W	3	LEXSIR	2.20	2.58	
7	24	Cr	3	FAMVUK10	1.61	2.36			74	W	4	EGUKIB	3.31	2.34	
1	25	Mn	2	DEFWOB	0.86	2.57			74	W	4	HUYDIO	3.24	2.36	
1	25	Mn	2	LIDQUL	0.83	2.58			74	W	4	JAKBEC	3.10	2.38	
4	26	Fe	2	MAFECL	1.15	2.39			74	W	5	BUCBAC	3.48	2.30	
6	26	Fe	3	DALLIL	1.38	2.38			74	W	5	JATFIT	3.50	2.30	
6	26	Fe	3	KAPLOD	1.35	2.40		16	75	Re	4	AYOLUV	3.10	2.36	
6	26	Fe	3	PIMXIS	1.38	2.39		16	75	Re	4	AYOMEG	3.10	2.36	
6	26	Fe	3	TOQDAE	1.35	2.40		16	75	Re	4	HIDGIK	3.12	2.35	
3	27	Co	2	HOCQUL	0.94	2.47		16	75	Re	4	IWOZID	3.06	2.36	
2	28	Ni	2	ZALNIJ	0.98	2.45			76	Os	4	CEXRIG	3.10	2.33	
	29	Cu	2	FOWCUP	0.93	2.51			76	Os	4	ENIDUA	3.06	2.34	
	29	Cu	2	GOKWUY	0.93	2.50			76	Os	4	GEBLUU	3.09	2.33	
	29	Cu	2	POCJAS	0.99	2.47			76	Os	5	CEXREC	3.37	2.28	
	39	Y	3	WAPJUT	2.44	2.62			77	Ir	4	GALQAL	3.01	2.66	
	40	Zr	4	TUCNIO	2.86	2.47			77	Ir	4	MIRKEE	3.01	2.33	
	40	Zr	4	FOHREZ	2.86	2.47			77	Ir	4	NAYQOU	3.05	2.32	
	40	Zr	4	JAVKEW	2.88	2.46			77	Ir	4	RIHFAP	3.03	2.32	
	41	Nb	4	KEWHOJ	2.88	2.41			77	Ir	4	TEVFIJ	3.02	2.33	
	41	Nb	5	FIRMOJ	3.25	2.34		17	78	Pt	4	AKCLPT	2.91	2.32	
	41	Nb	5	NUYFOC	3.26	2.34		17	78	Pt	4	BIBRIN	2.85	2.33	
	41	Nb	5	GOLJEW	3.24	2.34		17	78	Pt	4	MIMDPT	2.90	2.32	
								17	78	Pt	4	MINLAW	2.88	2.32	

Ser.	Z	M	C	CSD	Δ_0	M-L	Chiral	Ligand = N_3^- ⑥							
	22	Ti	4	BEYNUP	1.54	2.02		Ser.	Z	M	C	CSD	Δ_0	M-L	Chiral
Ligand = F^- ⑦								Ligand = H_2O ⑩							
	21	Sc	3	DEONAC	2.15	2.03		13	44	Ru	3	OLABAE	3.49	2.03	Δ
	21	Sc	3	HEYRUZ	2.20	2.05		12	45	Rh	3	CAZCIP	3.49	2.02	Δ
	22	Ti	4	AHUNEW	3.08	1.84		12	45	Rh	3	LIKRIH	3.36	2.01	Δ
	22	Ti	4	KOYXOL	3.06	1.86		12	45	Rh	3	SOZFIW	3.38	2.01	Δ
	22	Ti	4	LORCEA	3.16	1.84			21	Sc	3	CEMXXAU	1.99	2.09	
	22	Ti	4	SIXXAY	3.82	1.76			22	Ti	3	LIMPUS	2.23	2.03	
8	23	V	3	LIDYUT	2.00	1.97		5	23	V	2	VEPSUE	1.64	2.12	
8	23	V	3	WOHDIG	2.49	1.90		5	23	V	2	YEGSAF	2.52	1.96	
7	24	Cr	3	ADOSOC	2.13	1.90		8	23	V	3	COLNUM	2.18	2.00	
7	24	Cr	3	GAWBUC	2.17	1.90		8	23	V	3	FEMHOV	2.24	1.99	
6	26	Fe	3	FULHOJ	1.79	1.90			24	Cr	2	GIMZIM	1.66	2.04	
	40	Zr	4	TIZXAC	4.11	2.01		7	24	Cr	3	UCOME	2.17	1.97	
	40	Zr	4	KOJVAG	4.28	2.01		7	24	Cr	3	IWOJOT	2.27	1.97	
	40	Zr	4	QOFCOE	4.18	2.01		7	24	Cr	3	MEWZET01	2.11	1.96	
	41	Nb	4	ROZLOI	4.44	1.93		7	24	Cr	3	TAPBUH	2.15	1.96	
	42	Mo	4	ROZLIC	4.38	1.92		1	25	Mn	2	ASOVEJ	1.08	2.16	
	72	Hf	4	RENPAB	4.71	1.99		1	25	Mn	2	COLWUV	1.06	2.19	
	73	Ta	4	CEYCEO	5.93	1.86		1	25	Mn	2	HEHSIW	1.08	2.17	
	73	Ta	5	ECANAY	5.72	1.87		1	25	Mn	2	LEFYAX	1.09	2.17	
	73	Ta	5	GUCCEN	5.43	1.89		1	25	Mn	2	VIDGIZ	1.22	2.17	
	74	W	4	ZIYWAF	6.86	1.78			25	Mn	3	GUKGAV	1.33	2.16	
	74	W	5	ZOLKEQ	6.56	1.78		4	26	Fe	2	AMITAR	1.43	2.05	
	76	Os	4	UFEPEA	4.19	1.93		4	26	Fe	2	DIJRUK	1.19	2.10	
	77	Ir	4	TMAPTF01	3.72	1.92		4	26	Fe	2	EJATEO	1.22	2.10	
Ligand = $S_2O_3^{2-}$ ⑧								4	26	Fe	2	FEACIT	1.04	2.12	
Ligand = $OCOR^-$ ⑨								4	26	Fe	2	NATGEV	1.15	2.11	
Ligand = OCO_2^{2-} ⑩								4	26	Fe	2	QEDCOR	1.12	2.10	
Ligand = OH^- ⑪								4	26	Fe	2	ZILZID	1.32	2.12	
Ligand = $OCHO^-$ ⑫								6	26	Fe	3	MEWZAP	1.71	2.00	
7	24	Cr	3	GICNEL	2.35	1.98		6	26	Fe	3	XIGSEL	1.71	1.99	
11	42	Mo	3	GICNAH	3.59	2.11		3	27	Co	2	ASUDIB	1.18	2.10	
Ligand = OSO_3^{2-} ⑬								3	27	Co	2	BAVYOM	1.36	2.08	
Ligand = ONO_2^- ⑭								3	27	Co	2	NESFIB	1.17	2.09	
Ligand = ox^{2-} ⑮								3	27	Co	2	SUVBUG	1.16	2.07	
8	23	V	3	KOXLTV01	2.30	2.01	Δ	3	27	Co	2	WABLIU10	1.12	2.07	
7	24	Cr	3	CROXKH	2.52	1.97	Δ	9	27	Co	3	ASAWOH	1.97	1.98	
7	24	Cr	3	DITFER	2.60	1.96	Δ	2	28	Ni	2	JERNID	1.19	2.04	
7	24	Cr	3	FEPPOS	2.52	1.97	Δ	2	28	Ni	2	LUMVAQ	1.26	2.05	
7	24	Cr	3	GUKGID	2.58	1.97	Δ	2	28	Ni	2	MAPHER	1.25	2.05	
7	24	Cr	3	RUPGEP	2.44	1.97	Δ	2	28	Ni	2	SIYZEF	1.11	2.06	
	25	Mn	3	ZZZCCG10	2.05	2.00	Δ	2	28	Ni	2	VELQJ	1.21	2.07	
4	26	Fe	2	LIPXIS	1.83	2.00	Δ		29	Cu	2	DILCIL	1.20	2.10	
6	26	Fe	3	BEMPEO	1.91	2.00	Δ		29	Cu	2	DODDOP	1.26	2.12	
6	26	Fe	3	ARABEA	1.78	2.00	Δ		29	Cu	2	KAGNEM	1.26	2.11	
6	26	Fe	3	GEXQOP	1.82	2.01	Δ		29	Cu	2	SIYZIJ	1.16	2.11	
9	27	Co	3	PNIOCO	2.26	1.92	Δ		30	Zn	2	BENBIG	1.96	2.07	
9	27	Co	3	DAZVUV	2.48	1.90	Δ		30	Zn	2	CITDAK	2.84	2.07	
9	27	Co	3	GUKGEZ	2.42	1.89	Δ		30	Zn	2	FOGWUU	1.58	2.09	
	43	Tc	4	FOPBAN	4.00	1.99	Δ		30	Zn	2	KAMPEU	2.62	2.09	
13	44	Ru	3	DUKNOM	3.58	2.03	Δ		44	Ru	2	BONPEZ	2.39	2.12	
13	44	Ru	3	IDECOK	3.43	2.04	Δ		44	Ru	2	OLUXAU	2.86	2.09	
								13	44	Ru	3	BONPID	3.08	2.03	

Ser.	Z	M	C	CSD	Δ_o	M-L	Chiral	Ser.	Z	M	C	CSD	Δ_o	M-L	Chiral
Ligand = NCS ⁻ ⑰								3	27	Co	2	CAFWEM	2.51	1.87	
	21	Sc	3	BUQMOP	2.95	2.18		3	27	Co	2	OKOCAS	2.57	1.96	
	21	Sc	3	XAJMOK	2.90	2.16		3	27	Co	2	RAJNIZ	1.48	2.17	
7	24	Cr	3	GETMUO	2.20	2.00		9	27	Co	3	CANYAS	2.88	1.97	
7	24	Cr	3	LUHWAM	2.71	1.99		9	27	Co	3	EYAQEA	2.95	1.96	
7	24	Cr	3	KADXAP	2.68	2.01		9	27	Co	3	XEDNAV	3.13	1.97	
7	24	Cr	3	NICHOC10	2.43	2.00		2	28	Ni	2	BICSIQ	1.68	2.14	
1	25	Mn	2	GEGBOK	1.19	2.23		2	28	Ni	2	NUHJUV	1.69	2.14	
1	25	Mn	2	XILJIM	1.38	2.24		12	45	Rh	3	XEDNEZ	4.60	2.08	
	25	Mn	4	MUPSOF	1.20	2.22		15	77	Ir	3	XEDNID	5.12	2.09	
6	26	Fe	3	MIJMUN	1.54	2.09		Ligand = en ⑳							
6	26	Fe	3	NEPSAC	1.75	2.06		5	23	V	2	HIDMEM	2.10	2.20	Δ
6	26	Fe	3	TMFETC	1.82	2.05		7	24	Cr	3	CRENTC	2.75	2.08	Δ
3	27	Co	2	BUQMIJ01	1.43	2.09		7	24	Cr	3	ENDACR	2.82	2.08	Δ
3	27	Co	2	KIPYUD	1.36	2.12		7	24	Cr	3	ETDHCO	2.95	2.08	Δ
2	28	Ni	2	TIGGEW	1.25	2.09		7	24	Cr	3	GOZCIH	2.87	2.08	Δ
2	28	Ni	2	BEZXIN	1.40	2.10		1	25	Mn	2	ASEBEF	1.32	2.29	Δ
2	28	Ni	2	TOWCAJ	1.37	2.09		1	25	Mn	2	KIBFUX	1.48	2.27	Δ
	39	Y	3	KAKQES	3.22	2.33		1	25	Mn	2	QIBZOR	1.44	2.27	Δ
11	42	Mo	3	KMOITC	4.15	2.08		1	25	Mn	2	RAGTOI	1.38	2.28	Δ
	43	Tc	4	FEKWEX	4.39	2.00		4	26	Fe	2	FEBMAB	1.50	2.20	Δ
16	75	Re	4	OGAKIR	5.10	2.05		4	26	Fe	2	LIWKOR01	1.59	2.21	Δ
16	75	Re	4	XUCBON	4.76	1.98		4	26	Fe	2	RITKUA	1.51	2.22	Δ
	76	Os	3	QIJJEY	4.36	2.02		3	27	Co	2	HIQYUC	1.25	2.28	Δ
	76	Os	4	QIJJAU	4.40	2.01		3	27	Co	2	HOSPOV	1.57	2.18	Δ
Ligand = ONO ⁻ ㉑								3	27	Co	2	ICETEQ	1.65	2.18	Δ
Ligand = CH ₃ CN ㉒								3	27	Co	2	JEQNEZ	1.64	2.17	Δ
5	23	V	2	BEQQIX	2.10	2.11		3	27	Co	2	KIBGAE	1.64	2.17	Δ
7	24	Cr	3	ACALEW	2.00	2.00		9	27	Co	3	ABIXIT	3.08	1.97	Δ
1	25	Mn	2	ZOTYAI	2.17	2.21		9	27	Co	3	FIRQIH	3.06	1.97	Δ
4	26	Fe	2	ACEYOW	2.15	2.15		9	27	Co	3	PERHIE	3.11	1.97	Δ
4	26	Fe	2	HIRTIL	2.17	2.16		9	27	Co	3	TENCON	3.22	1.97	Δ
4	26	Fe	2	HMCIFE15	2.16	2.16		9	27	Co	3	WOQFAK	3.09	1.97	Δ
3	27	Co	2	OCELIS	2.11	2.11		2	28	Ni	2	BINYAY	1.81	2.13	Δ
3	27	Co	2	JOYPUI	2.10	2.11		2	28	Ni	2	DASSUL	1.72	2.15	Δ
3	27	Co	2	OFINAT	2.10	2.11		2	28	Ni	2	EFATOV	1.84	2.13	Δ
2	28	Ni	2	FUJVAH	2.08	2.08		2	28	Ni	2	ENIACH	1.81	2.13	Δ
2	28	Ni	2	XUGBIK	2.07	2.07		2	28	Ni	2	XAPNOS	1.85	2.13	Δ
2	28	Ni	2	OCELAK	2.06	2.07			44	Ru	2	BABRAX	3.84	2.13	Δ
	43	Tc	2	TEQNAE	4.62	2.06		12	45	Rh	3	AGUJIW	4.49	2.09	Δ
	44	Ru	2	ACEYAI	4.54	2.09		12	45	Rh	3	CRHENC	4.68	2.06	Δ
	44	Ru	2	PUHSOB	4.56	2.03		12	45	Rh	3	DARGUY	4.66	2.07	Δ
	44	Ru	2	FEWRII	4.87	2.01		12	45	Rh	3	TENRHC	4.65	2.06	Δ
12	45	Rh	3	VENYAO	4.44	1.99			76	Os	3	FISFAO	5.25	2.11	Δ
Ligand = py ㉓								15	77	Ir	3	UBEFEM	5.12	2.10	Δ
4	26	Fe	2	PYFEFE	1.46	2.26		15	77	Ir	3	DARHAF	5.36	2.20	Δ
	44	Ru	2	HPYRUB	4.31	2.13		Ligand = bpy ㉔							
Ligand = NH ₃ ㉕									24	Cr	2	ACAYUZ	3.00	2.08	Δ
1	25	Mn	2	PUHJIL	1.33	2.29		7	24	Cr	3	FERYEG	3.14	2.04	Δ

Ser.	Z	M	C	CSD	Δ_0	M-L	Chiral	Ser.	Z	M	C	CSD	Δ_0	M-L	Chiral
1	25	Mn	2	GUXJOY	1.73	2.24	Δ								
4	26	Fe	2	LIPXIS	3.11	1.98	Δ	6	26	Fe	3	KAHKIN	4.22	2.02	
3	27	Co	2	CAMHED	1.91	2.13	Δ	6	26	Fe	3	BIWYOW	4.56	1.93	
3	27	Co	2	CIBDOH	2.04	2.12	Δ	4	26	Fe	2	FETGIV	4.66	1.94	
3	27	Co	2	IXODII	3.33	1.93	Δ	4	26	Fe	2	CEJYEV	4.87	1.95	
9	27	Co	3	DUPPAG	3.25	1.93	Δ	4	26	Fe	2	EYIQUY	5.05	1.91	
9	27	Co	3	FIXKUT	3.26	1.93	Δ	4	26	Fe	2	FAWNOH	4.87	1.93	
2	28	Ni	2	AGADAO	2.19	2.09	Δ	4	26	Fe	2	GIJVEA	5.04	1.90	
	28	Ni	3	CUHVUW	2.94	1.98	Δ	9	27	Co	3	AENCOC	5.02	1.88	
	44	Ru	2	AXAFIO	4.89	2.05	Δ	9	27	Co	3	DIENCO	4.93	1.89	
12	45	Rh	3	DIWGIZ	4.64	2.04	Δ	9	27	Co	3	HIGZAY	4.86	1.90	
12	45	Rh	3	FERYIK	4.74	2.04	Δ	9	27	Co	3	PEHACO	4.77	1.90	
	76	Os	2	HIRDOB	5.20	2.06	Δ		42	Mo	4	HITPOQ	6.80	2.90	
15	77	Ir	3	CEZMAV	5.46	2.02	Δ		44	Ru	2	QEZYAV	6.76	2.03	
Ligand = phen ²⁴									44	Ru	2	WUGSEW	6.99	2.03	
8	23	V	3	CEHBEX	3.92	1.99	Δ	13	44	Ru	3	KAGLAG	6.60	2.05	
7	24	Cr	3	LIYWUL	3.15	2.05	Δ		76	Os	3	OCIJIU	7.06	2.06	
1	25	Mn	2	GUHGOF	1.87	2.23	Δ	17	78	Pt	4	YASNUC	6.76	2.02	
1	25	Mn	2	LUHKAA	1.50	2.25	Δ	17	78	Pt	4	COZVAO	6.81	1.99	
4	26	Fe	2	ADETIM	3.13	1.97	Δ	Ligand = CO ²⁹							
4	26	Fe	2	AFIRAJ	3.11	1.98	Δ	4	26	Fe	2	CEHHON	4.94	1.91	
4	26	Fe	2	MIKJEW	3.10	1.98	Δ	4	26	Fe	2	HOLMIE	4.93	1.91	
6	26	Fe	3	BIPGEN	3.09	1.98	Δ	4	26	Fe	2	HOLMOK	4.95	1.91	
6	26	Fe	3	FUTDOO	3.09	1.97	Δ		44	Ru	2	LARPAW	6.82	2.02	
6	26	Fe	3	SOGXOC	3.19	1.97	Δ		44	Ru	2	LARPIE	6.59	2.04	
3	27	Co	2	AGOYIF	1.94	2.13	Δ		76	Os	2	CEHHIH	8.25	2.00	
3	27	Co	2	BUYLIR	3.17	1.94	Δ		76	Os	2	LARPEA	7.96	2.02	
3	27	Co	2	HOCFIP	3.19	1.94	Δ		76	Os	2	LARPOK	7.89	2.03	
3	27	Co	2	SALVEH	1.93	2.13	Δ	15	77	Ir	3	XOLYIG	7.26	2.03	
9	27	Co	3	KIWRIS	3.08	1.94	Δ	Ligand = glycine							
9	27	Co	3	KULRAL	3.06	1.94	Δ	8	23	V	3	AGASIL	2.62	2.05	Δ
9	27	Co	3	MOHFAR	2.99	1.94	Δ	7	24	Cr	3	TGLYCR	2.51	2.02	Δ
2	28	Ni	2	FUHWEL	2.09	2.09	Δ	9	27	Co	3	AVUWET	2.60	1.93	Δ
2	28	Ni	2	MODCAK	2.07	2.09	Δ	9	27	Co	3	SEZMEQ	2.73	1.92	Δ
2	28	Ni	2	IYULIX	2.07	2.09	Δ	Ligand = urea							
Ligand = SO ₃ ²⁻ ²⁵									22	Ti	3	TIUREA01	2.80	2.01	
Ligand = NO ₂ ⁻ ²⁶								7	24	Cr	3	DAPFEF	2.13	1.97	
9	27	Co	3	WERKIN10	3.58	1.96		7	24	Cr	3	COLHIU	2.24	1.97	
12	45	Rh	3	TEDDOV	5.83	2.03		7	24	Cr	3	HOHPOJ	2.14	1.97	
Ligand = PPh ₃ ²⁷								7	24	Cr	3	HOHPUP	2.02	1.97	
Ligand = CN ⁻ ²⁸								1	25	Mn	2	WITQAR	1.05	2.18	
	22	Ti	3	NAYWOZ	3.85	2.18			25	Mn	3	BOPWEI	1.93	1.99	
8	23	V	3	JEHBAA	3.72	2.14		4	26	Fe	2	WITQEV	1.56	1.99	
7	24	Cr	3	BIJZOK	3.86	2.07		6	26	Fe	3	MANJIU	1.77	1.99	
7	24	Cr	3	AFOVIA	3.99	2.08		3	27	Co	2	COLLAQ01	1.21	2.11	
7	24	Cr	3	COLHIU	4.03	2.08		3	27	Co	2	RUBLEG	1.24	2.10	
7	24	Cr	3	ELONUO	4.00	2.08		3	27	Co	2	WITLIU	1.19	2.09	
	25	Mn	3	BIFZOG	4.33	2.01		2	28	Ni	2	ADUFEK	1.33	2.06	

Ligand = I ⁻ ①					
Ser.	Z	M	C	CSD	GS
17	78	Pt	4	KIBMIS	low
Ligand = Br ⁻ ②					
7	24	Cr	3	YIBWVOV	high
11	42	Mo	3	DOMTII	low
12	45	Rh	3	HUQMEL	low
16	75	Re	4	AYOMAC	low
17	78	Pt	4	AZELEW	low
Ligand = SCN ⁻ ④					
12	45	Rh	3	YURKIF	low
15	77	Ir	3	PORQAO	low
17	78	Pt	4	BULVAF	low
Ligand = Cl ⁻ ⑤					
8	23	V	3	YUDFUY	low
7	24	Cr	3	FAMVUK10	high
1	25	Mn	2	DEFWOB	high
4	26	Fe	2	MAFECL	low
6	26	Fe	3	DALLIL	low
6	26	Fe	3	KAPLOD	low
3	27	Co	2	HOCQUL	low
2	28	Ni	2	ZALNIJ	high
11	42	Mo	3	DEBLEB	low
13	44	Ru	3	TAVTUF	low
12	45	Rh	3	FEWGET	low
14	46	Pd	4	JIZLOT	low
14	46	Pd	4	LAHFUV	low
16	75	Re	4	AYOLUV	low
17	78	Pt	4	MIMDPT	low
Ligand = F ⁻ ⑦					
8	23	V	3	LIDYUT	low
8	23	V	3	WOHDIG	low
7	24	Cr	3	ADOSOC	high
6	26	Fe	3	FULHOJ	low
Ligand = OCHO ⁻ ⑩					
7	24	Cr	3	GICNEL	low
11	42	Mo	3	GICNAH	low
Ligand = ox ²⁻ ⑮					
8	23	V	3	KOXLTV01	low
7	24	Cr	3	FEPDOS	high
4	26	Fe	2	LIPXIS	low
6	26	Fe	3	GEXQOP	low
9	27	Co	3	DAZVUV	low
13	44	Ru	3	DUKNOM	low
12	45	Rh	3	CAZCIP	low
Ligand = H ₂ O ⑯					
5	23	V	2	VEPSUE	high
8	23	V	3	FEMHOV	low
7	24	Cr	3	MEWZET01	high
1	25	Mn	2	ASOVEJ	high
4	26	Fe	2	FEACIT	high
6	26	Fe	3	MEWZAP	high
3	27	Co	2	SUVBUG	high
9	27	Co	3	ASAWOH	high

Ser.	Z	M	C	CSD	GS
2	28	Ni	2	JERNID	high
13	44	Ru	3	BONPID	high
Ligand = NCS ⁻ ⑰					
7	24	Cr	3	LUHWAM	low
1	25	Mn	2	XILJIM	low
6	26	Fe	3	NEPSAC	low
3	27	Co	2	KIPYUD	low
2	28	Ni	2	TOWCAJ	low
11	42	Mo	3	KMOITC	low
16	75	Re	4	OGAKIR	low
Ligand = CH ₃ CN ⑱					
5	23	V	2	BEQQIX	low
7	24	Cr	3	ACALEW	low
1	25	Mn	2	ZOTYAI	low
4	26	Fe	2	HMCIFE15	low
3	27	Co	2	OCELIS	low
2	28	Ni	2	FUJVAH	low
12	45	Rh	3	VENYAO	low
Ligand = py ⑳					
4	26	Fe	2	PYFEFE	low
Ligand = NH ₃ ㉑					
7	24	Cr	3	LEBRUF	high
1	25	Mn	2	PUHJIL	high
3	27	Co	2	CAFWEM	high
3	27	Co	2	RAJNIZ	high
9	27	Co	3	EYAQEA	low
2	28	Ni	2	BICSIQ	low
12	45	Rh	3	XEDNEZ	low
15	77	Ir	3	XEDNID	low
Ligand = en ㉒					
5	23	V	2	HIDMEM	high
7	24	Cr	3	ENDACR	high
1	25	Mn	2	ASEBEF	low
1	25	Mn	2	RAGTOI	low
4	26	Fe	2	FEBMAB	low
3	27	Co	2	HIQYUC	low
9	27	Co	3	PERHIE	low
2	28	Ni	2	EFATOV	low
12	45	Rh	3	CRHENC	low
15	77	Ir	3	UBEFEM	low
Ligand = bpy ㉓					
7	24	Cr	3	FERYEG	low
1	25	Mn	2	GUXJOY	low
4	26	Fe	2	LIPXIS	low
3	27	Co	2	CIBDOH	low
3	27	Co	2	IXODII	low
9	27	Co	3	DUPPAG	low
2	28	Ni	2	AGADAO	low
12	45	Rh	3	FERYIK	low
15	77	Ir	3	CEZMAV	low
Ligand = phen ㉔					
8	23	V	3	CEHBEX	low
7	24	Cr	3	LIYWUL	low

	Z	M	C	CSD	GS
1	25	Mn	2	LUHKAA	low
4	26	Fe	2	ADETIM	low
6	26	Fe	3	BIPGEN	low
3	27	Co	2	AGOYIF	low
9	27	Co	3	MOHFAR	low
2	28	Ni	2	FUHWEL	low
Ligand = NO ₂ ⁻ ⑳					
12	45	Rh	3	TEDDOV	low
Ligand = CN ⁻ ㉘					
8	23	V	3	JEHBAA	low
7	24	Cr	3	COLHIU	low
6	26	Fe	3	BIWYOW	low
4	26	Fe	2	CEJYEV	low
9	27	Co	3	DIENCO	low
13	44	Ru	3	KAGLAG	low
17	78	Pt	4	YASNUC	low
Ligand = CO ㉙					
4	26	Fe	2	HOLMIE	low
15	77	Ir	3	XOLYIG	low

Metal Series No.	Metal	Valence	Metal Atomic No.	Ligand Series No.	Ligand	Ligand Field Splitting Δ (eV)	Metal Ligand Distance M-L (Å)	Chirality (bidentate ligand)	CSD Reference Code
1	Mn	2+	25	5	Cl ⁻	0.86	2.57		DEFWOB
1	Mn	2+	25	5	Cl ⁻	0.83	2.58		LIDQUL
1	Mn	2+	25	16	H ₂ O	1.08	2.16		ASOVEJ
1	Mn	2+	25	16	H ₂ O	1.06	2.19		COLWUV
1	Mn	2+	25	16	H ₂ O	1.08	2.17		HEHSIW
1	Mn	2+	25	16	H ₂ O	1.09	2.17		LEFYAX
1	Mn	2+	25	16	H ₂ O	1.22	2.17		VIDGIZ
1	Mn	2+	25	17	NCS ⁻	1.19	2.23		GEGBOK
1	Mn	2+	25	17	NCS ⁻	1.38	2.24		XILJIM
1	Mn	2+	25	19	CH ₃ CN	2.21	2.22		ZOTYAI
1	Mn	2+	25	19	CH ₃ CN	2.12	2.19		ZOTYAI2
1	Mn	2+	25	21	NH ₃	1.33	2.29		PUHJIL
1	Mn	2+	25	22	en	1.32	2.29	Δ	ASEBEF
1	Mn	2+	25	22	en	1.48	2.27	Δ	KIBFUX
1	Mn	2+	25	22	en	1.44	2.27	Δ	QIBZOR
1	Mn	2+	25	22	en	1.38	2.28	Δ	RAGTOI
1	Mn	2+	25	23	bpy	1.73	2.24	Δ	GUXJOY
1	Mn	2+	25	24	phen	1.87	2.23	Δ	GUHGOF
1	Mn	2+	25	24	phen	1.50	2.25	Δ	LUHKAA
1	Mn	2+	25		urea	1.05	2.18		WITQAR
2	Ni	2+	28	5	Cl ⁻	0.98	2.45		ZALNIJ
2	Ni	2+	28	16	H ₂ O	1.19	2.04		JERNID
2	Ni	2+	28	16	H ₂ O	1.26	2.05		LUMVAQ
2	Ni	2+	28	16	H ₂ O	1.25	2.05		MAPHER
2	Ni	2+	28	16	H ₂ O	1.11	2.06		SIYZEF
2	Ni	2+	28	16	H ₂ O	1.21	2.07		VELQEJ
2	Ni	2+	28	17	NCS ⁻	1.25	2.09		TIGGEW
2	Ni	2+	28	17	NCS ⁻	1.40	2.10		BEZXIN
2	Ni	2+	28	17	NCS ⁻	1.37	2.09		TOWCAJ
2	Ni	2+	28	19	CH ₃ CN	2.08	2.08		FUJVAH
2	Ni	2+	28	19	CH ₃ CN	2.07	2.07		XUGBIK
2	Ni	2+	28	19	CH ₃ CN	2.06	2.07		OCELAK
2	Ni	2+	28	21	NH ₃	1.68	2.14		BICSIQ
2	Ni	2+	28	21	NH ₃	1.69	2.14		NUHJUV
2	Ni	2+	28	22	en	1.81	2.13	Δ	BINYAY
2	Ni	2+	28	22	en	1.72	2.15	Δ	DASSUL
2	Ni	2+	28	22	en	1.84	2.13	Δ	EFATOV
2	Ni	2+	28	22	en	1.81	2.13	Δ	ENIACH
2	Ni	2+	28	22	en	1.85	2.13	Δ	XAPNOS
2	Ni	2+	28	23	bpy	2.12	2.09	Δ	AGADAO
2	Ni	2+	28	23	bpy	2.26	2.08	Δ	AGADAO2
2	Ni	2+	28	24	phen	2.09	2.09	Δ	FUHWEL
2	Ni	2+	28	24	phen	2.07	2.09	Δ	MODCAK
2	Ni	2+	28	24	phen	2.07	2.09	Δ	IYULIX
2	Ni	2+	28		urea	1.33	2.06		ADUFEK
3	Co	2+	27	5	Cl ⁻	0.94	2.47		HOCQUL
3	Co	2+	27	16	H ₂ O	1.18	2.10		ASUDIB
3	Co	2+	27	16	H ₂ O	1.36	2.08		BAVYOM
3	Co	2+	27	16	H ₂ O	1.17	2.09		NESFIB
3	Co	2+	27	16	H ₂ O	1.16	2.07		SUVBUG
3	Co	2+	27	16	H ₂ O	1.12	2.07		WABLIU10
3	Co	2+	27	17	NCS ⁻	1.43	2.09		BUQMIJ01
3	Co	2+	27	17	NCS ⁻	1.36	2.12		KIPYUD
3	Co	2+	27	19	CH ₃ CN	2.11	2.11		OCELIS

3	Co	2+	27	19	CH3CN	2.10	2.11		JOYPUI
3	Co	2+	27	19	CH3CN	2.10	2.11		OFINAT
3	Co	2+	27	21	NH3	2.51	1.87		CAFWEM
3	Co	2+	27	21	NH3	2.57	1.96		OKOCAS
3	Co	2+	27	21	NH3	1.48	2.17		RAJNIZ
3	Co	2+	27	22	en	1.25	2.28	Δ	HIQYUC
3	Co	2+	27	22	en	1.57	2.18	Λ	HOSPOV
3	Co	2+	27	22	en	1.65	2.18	Λ	ICETEQ
3	Co	2+	27	22	en	1.64	2.17	Λ	JEQNEZ
3	Co	2+	27	22	en	1.64	2.17	Λ	KIBGAE
3	Co	2+	27	23	bpy	1.91	2.13	Δ	CAMHED
3	Co	2+	27	23	bpy	2.04	2.12	Λ	CIBDOH
3	Co	2+	27	23	bpy	3.28	1.93	Λ	IXODII
3	Co	2+	27	23	bpy	3.38	1.93	Δ	IXODII2
3	Co	2+	27	24	phen	1.94	2.13	Λ	AGOYIF
3	Co	2+	27	24	phen	3.17	1.94	Δ	BUYLIR
3	Co	2+	27	24	phen	3.19	1.94	Λ	HOCFIP
3	Co	2+	27	24	phen	1.93	2.13	Δ	SALVEH
3	Co	2+	27		urea	1.21	2.11		COLLAQ01
3	Co	2+	27		urea	1.24	2.10		RUBLEG
3	Co	2+	27		urea	1.19	2.09		WITLIU
4	Fe	2+	26	5	Cl-	1.15	2.39		MAFECL
4	Fe	2+	26	15	ox2-	1.83	2.00	Δ	LIPXIS
4	Fe	2+	26	16	H2O	1.43	2.05		AMITAR
4	Fe	2+	26	16	H2O	1.19	2.10		DIJRUK
4	Fe	2+	26	16	H2O	1.22	2.10		EJATEO
4	Fe	2+	26	16	H2O	1.04	2.12		FEACIT
4	Fe	2+	26	16	H2O	1.15	2.11		NATGEV
4	Fe	2+	26	16	H2O	1.12	2.10		QEDCOR
4	Fe	2+	26	16	H2O	1.32	2.12		ZILZID
4	Fe	2+	26	19	CH3CN	2.15	2.15		ACEYOW
4	Fe	2+	26	19	CH3CN	2.17	2.16		HIRTIL
4	Fe	2+	26	19	CH3CN	2.16	2.16		HMCIFE15
4	Fe	2+	26	20	py	1.46	2.26		PYFEFE
4	Fe	2+	26	22	en	1.50	2.20	Λ	FEBMAB
4	Fe	2+	26	22	en	1.59	2.21	Δ	LIWKOR01
4	Fe	2+	26	22	en	1.51	2.22	Λ	RITKUA
4	Fe	2+	26	23	bpy	3.10	1.98	Δ	LIPXIS
4	Fe	2+	26	23	bpy	3.12	1.98	Δ	LIPXIS2
4	Fe	2+	26	24	phen	3.13	1.97	Λ	ADETIM
4	Fe	2+	26	24	phen	3.11	1.98	Λ	AFIRAJ
4	Fe	2+	26	24	phen	3.10	1.98	Λ	MIKJEW
4	Fe	2+	26	28	CN-	4.87	1.95		CEJYEV
4	Fe	2+	26	28	CN-	5.05	1.91		EYIQUY
4	Fe	2+	26	28	CN-	4.87	1.93		FAWNOH
4	Fe	2+	26	28	CN-	5.04	1.90		GIJVEA
4	Fe	2+	26	29	CO	4.94	1.91		CEHHON
4	Fe	2+	26	29	CO	4.93	1.91		HOLMIE
4	Fe	2+	26	29	CO	4.95	1.91		HOLMOK
4	Fe	2+	26		urea	1.56	1.99		WITQEV
5	V	2+	23	16	H2O	1.64	2.12		VEPSUE
5	V	2+	23	16	H2O	2.52	1.96		YEGSAF
5	V	2+	23	19	CH3CN	2.10	2.11		BEQQIX
5	V	2+	23	22	en	2.10	2.20	Δ	HIDMEM
6	Fe	3+	26	5	Cl-	1.38	2.38		DALLIL
6	Fe	3+	26	5	Cl-	1.35	2.40		KAPLOD
6	Fe	3+	26	5	Cl-	1.38	2.39		PIMXIS
6	Fe	3+	26	5	Cl-	1.35	2.40		TOQDAE
6	Fe	3+	26	7	F-	1.79	1.90		FULHOJ

6	Fe	3+	26	15	ox2-	1.91	2.00	Δ	BEMPEO
6	Fe	3+	26	15	ox2-	1.78	2.00	Δ	ARABEA
6	Fe	3+	26	15	ox2-	1.82	2.01	Λ	GEXQOP
6	Fe	3+	26	16	H2O	1.71	2.00		MEWZAP
6	Fe	3+	26	16	H2O	1.71	1.99		XIGSEL
6	Fe	3+	26	17	NCS-	1.54	2.09		MIJMUN
6	Fe	3+	26	17	NCS-	1.75	2.06		NEPSAC
6	Fe	3+	26	17	NCS-	1.85	2.05		TMFETC
6	Fe	3+	26	17	NCS-	1.79	2.05		TMFETC2
6	Fe	3+	26	24	phen	3.09	1.98	Δ	BIPGEN
6	Fe	3+	26	24	phen	3.09	1.97	Λ	FUTDOO
6	Fe	3+	26	24	phen	3.19	1.97	Λ	SOGXOC
6	Fe	3+	26	28	CN-	4.56	1.93		BIWYOW
6	Fe	3+	26	28	CN-	4.66	1.94		FETGIV
6	Fe	3+	26		urea	1.77	1.99		MANJIU
7	Cr	3+	24	2	Br-	1.48	2.64		YIBWOV
7	Cr	3+	24	5	Cl-	1.61	2.36		FAMVUK10
7	Cr	3+	24	7	F-	2.13	1.90		ADOSOC
7	Cr	3+	24	7	F-	2.17	1.90		GAWBUC
7	Cr	3+	24	12	OCHO-	2.35	1.98		GICNEL
7	Cr	3+	24	15	ox2-	2.52	1.97	Λ	CROXKH
7	Cr	3+	24	15	ox2-	2.60	1.96	Λ	DITFER
7	Cr	3+	24	15	ox2-	2.52	1.97	Δ	FEPCOS
7	Cr	3+	24	15	ox2-	2.58	1.97	Λ	GUKGID
7	Cr	3+	24	15	ox2-	2.44	1.97	Δ	RUPGEP
7	Cr	3+	24	16	H2O	2.17	1.97		UCOMEE
7	Cr	3+	24	16	H2O	2.27	1.97		IWOJOT
7	Cr	3+	24	16	H2O	2.11	1.96		MEWZET01
7	Cr	3+	24	16	H2O	2.15	1.96		TAPBUH
7	Cr	3+	24	17	NCS-	2.20	2.00		GETMUO
7	Cr	3+	24	17	NCS-	2.71	1.99		LUHWAM
7	Cr	3+	24	17	NCS-	2.68	2.01		KADXAP
7	Cr	3+	24	17	NCS-	2.43	2.00		NICHOC10
7	Cr	3+	24	19	CH3CN	2.00	2.00		ACALEW
7	Cr	3+	24	21	NH3	2.81	2.08		LEBRUF
7	Cr	3+	24	22	en	2.75	2.08	Λ	CRENTC
7	Cr	3+	24	22	en	2.82	2.08	Δ	ENDACR
7	Cr	3+	24	22	en	2.95	2.08	Λ	ETDHCO
7	Cr	3+	24	22	en	2.87	2.08	Δ	GOZCIH
7	Cr	3+	24	23	bpy	3.14	2.04	Δ	FERYEG
7	Cr	3+	24	23	bpy	3.18	2.05	Λ	FERYEG2
7	Cr	3+	24	24	phen	3.15	2.05	Λ	LIYWUL
7	Cr	3+	24	28	CN-	3.86	2.07		BIJZOK
7	Cr	3+	24	28	CN-	3.99	2.08		AFOVIA
7	Cr	3+	24	28	CN-	4.03	2.08		COLHIU
7	Cr	3+	24	28	CN-	4.00	2.08		ELONUO
7	Cr	3+	24		glycine	2.51	2.02	Λ	TGLYCR
7	Cr	3+	24		urea	2.13	1.97		DAPFEF
7	Cr	3+	24		urea	2.24	1.97		COLHIU
7	Cr	3+	24		urea	2.14	1.97		HOHPOJ
7	Cr	3+	24		urea	2.02	1.97		HOHPUP
8	V	3+	23	5	Cl-	1.66	2.39		YUDFUY
8	V	3+	23	5	Cl-	1.64	2.39		YUDFUY2
8	V	3+	23	7	F-	2.00	1.97		LIDYUT
8	V	3+	23	7	F-	2.49	1.90		WOHDIG
8	V	3+	23	15	ox2-	2.30	2.01	Δ	KOXLTV01
8	V	3+	23	16	H2O	2.18	2.00		COLNUM
8	V	3+	23	16	H2O	2.24	1.99		FEMHOV

8	V	3+	23	24	phen	3.92	1.99	Λ	CEHBEX
8	V	3+	23	28	CN-	3.72	2.14		JEHBAA
8	V	3+	23		glycine	2.62	2.05	Δ	AGASIL
9	Co	3+	27	15	ox2-	2.26	1.92	Λ	PNIOCO
9	Co	3+	27	15	ox2-	2.48	1.90	Δ	DAZVUV
9	Co	3+	27	15	ox2-	2.42	1.89	Λ	GUKGEZ
9	Co	3+	27	16	H2O	1.97	1.98		ASAWOH
9	Co	3+	27	21	NH3	2.88	1.97		CANYAS
9	Co	3+	27	21	NH3	2.95	1.96		EYAQEA
9	Co	3+	27	21	NH3	3.13	1.97		XEDNAV
9	Co	3+	27	22	en	3.08	1.97	Λ	ABIXIT
9	Co	3+	27	22	en	3.06	1.97	Λ	FIRQIH
9	Co	3+	27	22	en	3.11	1.97	Δ	PERHIE
9	Co	3+	27	22	en	3.22	1.97	Λ	TENCON
9	Co	3+	27	22	en	3.09	1.97	Λ	WOQFAK
9	Co	3+	27	23	bpy	3.25	1.93	Δ	DUPPAG
9	Co	3+	27	23	bpy	3.26	1.93	Λ	FIXKUT
9	Co	3+	27	24	phen	3.08	1.94	Δ	KIWRIS
9	Co	3+	27	24	phen	3.06	1.94	Λ	KULRAL
9	Co	3+	27	24	phen	2.99	1.94	Δ	MOHFAR
9	Co	3+	27	26	NO2-	3.62	1.96		WERKIN2
9	Co	3+	27	26	NO2-	3.58	1.96		WERKIN10
9	Co	3+	27	28	CN-	5.02	1.88		AENCOC
9	Co	3+	27	28	CN-	4.93	1.89		DIENCO
9	Co	3+	27	28	CN-	4.86	1.90		HIGZAY
9	Co	3+	27	28	CN-	4.77	1.90		PEHACO
9	Co	3+	27		glycine	2.60	1.93	Λ	AVUWET
9	Co	3+	27		glycine	2.73	1.92	Δ	SEZMEQ
11	Mo	3+	42	2	Br-	2.36	2.59		DOMTII
11	Mo	3+	42	5	Cl-	2.41	2.45		DEBLEB
11	Mo	3+	42	5	Cl-	2.48	2.44		PEPCOC
11	Mo	3+	42	12	OCHO-	3.59	2.11		GICNAH
11	Mo	3+	42	17	NCS-	4.15	2.08		KMOITC
12	Rh	3+	45	2	Br-	2.43	2.50		HUQMEL
12	Rh	3+	45	2	Br-	2.51	2.53		ZOKHEM
12	Rh	3+	45	4	SCN-	2.34	2.37		YURKIF
12	Rh	3+	45	5	Cl-	2.44	2.35		FEWGET
12	Rh	3+	45	5	Cl-	2.45	2.34		RIXHIP
12	Rh	3+	45	5	Cl-	2.43	2.35		TIBWIK
12	Rh	3+	45	5	Cl-	2.46	2.35		XISFEL
12	Rh	3+	45	15	ox2-	3.49	2.02	Λ	CAZCIP
12	Rh	3+	45	15	ox2-	3.36	2.01	Δ	LIKRIH
12	Rh	3+	45	15	ox2-	3.38	2.01	Λ	SOZFIW
12	Rh	3+	45	19	CH3CN	4.44	1.99		VENYAO
12	Rh	3+	45	21	NH3	4.62	2.08		XEDNEZ
12	Rh	3+	45	21	NH3	4.57	2.07		XEDNEZ2
12	Rh	3+	45	22	en	4.49	2.09	Λ	AGUJIW
12	Rh	3+	45	22	en	4.68	2.06	Δ	CRHENC
12	Rh	3+	45	22	en	4.66	2.07	Λ	DARGUY
12	Rh	3+	45	22	en	4.65	2.06	Λ	TENRHC
12	Rh	3+	45	23	bpy	4.64	2.04	Λ	DIWGIZ
12	Rh	3+	45	23	bpy	4.76	2.02	Λ	FERYIK
12	Rh	3+	45	23	bpy	4.72	2.06	Δ	FERTIK2
12	Rh	3+	45	26	NO2-	5.83	2.03		TEDDOV
12	Rh	3+	45	26	NO2-	6.04	2.08		TEDDOV2
13	Ru	3+	44	5	Cl-	2.42	2.38		ENIDAG
13	Ru	3+	44	5	Cl-	2.43	2.37		HEVCOA
13	Ru	3+	44	5	Cl-	2.42	2.38		HOCXUS
13	Ru	3+	44	5	Cl-	2.43	2.37		TAVTUF

13	Ru	3+	44	5	Cl-	2.44	2.37		YOJBUE
13	Ru	3+	44	15	ox2-	3.58	2.03	Λ	DUKNOM
13	Ru	3+	44	15	ox2-	3.43	2.04	Λ	IDECOK
13	Ru	3+	44	15	ox2-	3.49	2.03	Λ	OLABAE
13	Ru	3+	44	16	H2O	3.08	2.03		BONPID
13	Ru	3+	44	28	CN-	6.60	2.05		KAGLAG
14	Pd	4+	46	5	Cl-	2.55	2.31		JIZLOT
14	Pd	4+	46	5	Cl-	2.10	2.42		LAHFUV
15	Ir	3+	77	4	SCN-	2.87	2.38		PORQAO
15	Ir	3+	77	21	NH3	4.99	2.10		XEDNID
15	Ir	3+	77	21	NH3	5.24	2.08		XEDNID2
15	Ir	3+	77	22	en	5.12	2.10	Δ	UBEFEM
15	Ir	3+	77	22	en	5.36	2.20	Λ	DARHAF
15	Ir	3+	77	23	bpy	5.46	2.02	Δ	CEZMAV
15	Ir	3+	77	29	CO	7.26	2.03		XOLYIG
16	Re	4+	75	2	Br-	3.13	2.49		AYOMAC
16	Re	4+	75	5	Cl-	3.10	2.36		AYOLUV
16	Re	4+	75	5	Cl-	3.10	2.36		AYOMEG
16	Re	4+	75	5	Cl-	3.12	2.35		HIDGIK
16	Re	4+	75	5	Cl-	3.06	2.36		IWOZID
16	Re	4+	75	17	NCS-	5.08	2.02		OGAKIR
16	Re	4+	75	17	NCS-	5.11	2.07		OGAKIR2
16	Re	4+	75	17	NCS-	4.76	1.98		XUCBON
17	Pt	4+	78	1	I-	2.89	2.67		PYPTHI
17	Pt	4+	78	1	I-	2.87	2.67		KIBMIS
17	Pt	4+	78	1	I-	2.91	2.66		KIBMOY
17	Pt	4+	78	2	Br-	3.00	2.47		AZELEW
17	Pt	4+	78	2	Br-	2.99	2.47		AZELEW2
17	Pt	4+	78	4	SCN-	2.39	2.68		BULVAF
17	Pt	4+	78	4	SCN-	2.87	2.39		EMUVOX
17	Pt	4+	78	4	SCN-	2.24	2.38		XECZAG
17	Pt	4+	78	5	Cl-	2.91	2.32		AKCLPT
17	Pt	4+	78	5	Cl-	2.85	2.33		BIBRIN
17	Pt	4+	78	5	Cl-	2.90	2.32		MIMDPT
17	Pt	4+	78	5	Cl-	2.88	2.32		MINLAW
17	Pt	4+	78	28	CN-	6.76	2.02		YASNUC
17	Pt	4+	78	28	CN-	6.81	1.99		COZVAO
	Sc	3+	21	7	F-	2.15	2.03		DEDNAC
	Sc	3+	21	7	F-	2.20	2.05		HEYRUZ
	Sc	3+	21	16	H2O	1.99	2.09		CEMXXAU
	Sc	3+	21	17	NCS-	2.95	2.18		BUQMOP
	Sc	3+	21	17	NCS-	2.90	2.16		XAJMOK
	Ti	3+	22	16	H2O	2.23	2.03		LIMPUS
	Ti	3+	22	28	CN-	3.85	2.18		NAYWOZ
	Ti	3+	22		urea	2.80	2.01		TIUREA01
	Ti	4+	22	5	Cl-	2.08	2.34		BARMAJ
	Ti	4+	22	5	Cl-	2.08	2.34		FEPHOX
	Ti	4+	22	6	N3-	1.54	2.02		BEYNUP
	Ti	4+	22	7	F-	3.08	1.84		AHUNEW
	Ti	4+	22	7	F-	3.06	1.86		KOYXOL
	Ti	4+	22	7	F-	3.16	1.84		LORCEA
	Ti	4+	22	7	F-	3.82	1.76		SIXXAY
	V	4+	23	5	Cl-	2.03	2.31		SAHJER
	Cr	2+	24	16	H2O	1.66	2.04		GIMZIM
	Cr	2+	24	23	bpy	3.00	2.08	Λ	ACAYUZ

	Mn	3+	25	15	ox2-	2.05	2.00	Δ	ZZZCCG10
	Mn	3+	25	16	H2O	1.33	2.16		GUKGAV
	Mn	3+	25	28	CN-	4.33	2.01		BIFZOG
	Mn	3+	25	28	CN-	4.22	2.02		KAHKIN
	Mn	3+	25		urea	1.93	1.99		BOPWEI
	Mn	4+	25	17	NCS-	1.22	2.22		MUPSOF1
	Mn	4+	25	17	NCS-	1.17	2.23		MUPSOF2
	Ni	3+	28	23	bpy	2.94	1.98	Δ	CUHVUW
	Cu	2+	29	2	Br-	0.96	2.52		TIVJEN
	Cu	2+	29	5	Cl-	0.93	2.51		FOWCUP
	Cu	2+	29	5	Cl-	0.93	2.50		GOKWUY
	Cu	2+	29	5	Cl-	0.99	2.47		POCJAS
	Cu	2+	29	16	H2O	1.20	2.10		DILCIL
	Cu	2+	29	16	H2O	1.26	2.12		DODDOP
	Cu	2+	29	16	H2O	1.26	2.11		KAGNEM
	Cu	2+	29	16	H2O	1.16	2.11		SIYZIJ
	Zn	2+	30	16	H2O	1.96	2.07		BENBIG
	Zn	2+	30	16	H2O	2.84	2.07		CITDAK
	Zn	2+	30	16	H2O	1.58	2.09		FOGWUU
	Zn	2+	30	16	H2O	2.62	2.09		KAMPEU
	Y	3+	39	5	Cl-	2.44	2.62		WAPJUT
	Y	3+	39	17	NCS-	3.22	2.33		KAKQES
	Zr	3+	40	2	Br-	2.68	2.62		SENPOQ
	Zr	4+	40	1	I-	2.27	2.86		RIQPEN
	Zr	4+	40	5	Cl-	2.86	2.47		TUCNIO
	Zr	4+	40	5	Cl-	2.86	2.47		FOHREZ
	Zr	4+	40	5	Cl-	2.88	2.46		JAVKEW
	Zr	4+	40	7	F-	4.11	2.01		TIZXAC
	Zr	4+	40	7	F-	4.28	2.01		KOJVAG
	Zr	4+	40	7	F-	4.18	2.01		QOFCOE
	Nb	4+	41	5	Cl-	2.88	2.41		KEWHOJ
	Nb	4+	41	7	F-	4.44	1.93		ROZLOI
	Nb	5+	41	5	Cl-	3.25	2.34		FIRMOJ
	Nb	5+	41	5	Cl-	3.26	2.34		NUYFOC
	Nb	5+	41	5	Cl-	3.24	2.34		GOLJEW
	Mo	4+	42	2	Br-	2.73	2.53		FUYGUB
	Mo	4+	42	5	Cl-	2.93	2.35		FIPDEO
	Mo	4+	42	5	Cl-	2.82	2.38		ZICWOX
	Mo	4+	42	5	Cl-	2.80	2.38		FUTPIT
	Mo	4+	42	7	F-	4.38	1.92		ROZLIC
	Mo	4+	42	28	CN-	6.80	2.90		HITPOQ
	Mo	5+	42	5	Cl-	3.18	2.31		JAWRUU
	Tc	2+	43	19	CH3CN	4.62	2.06		TEQNAE
	Tc	4+	43	5	Cl-	2.74	2.36		CIMFEJ
	Tc	4+	43	5	Cl-	2.77	2.35		JEPQOL
	Tc	4+	43	5	Cl-	2.76	2.35		KAXQUW
	Tc	4+	43	5	Cl-	2.74	2.36		LALHAH
	Tc	4+	43	15	ox2-	4.00	1.99	Λ	FOPBAN
	Tc	4+	43	17	NCS-	4.39	2.00		FEKWEX
	Tc	5+	43	2	Br-	3.14	2.50		PSBRNB
	Ru	2+	44	5	Cl-	2.26	2.37		WUGCOQ
	Ru	2+	44	16	H2O	2.39	2.12		BONPEZ
	Ru	2+	44	16	H2O	2.86	2.09		OLUXAU

	Ru	2+	44	19	CH3CN	4.54	2.09		ACEYAI
	Ru	2+	44	19	CH3CN	4.56	2.03		PUHSOB
	Ru	2+	44	19	CH3CN	4.87	2.01		FEWRII
	Ru	2+	44	20	py	4.31	2.13		HPYRUB
	Ru	2+	44	22	en	3.84	2.13	Δ	BABRAX
	Ru	2+	44	23	bpy	4.89	2.05	Λ	AXAFIO
	Ru	2+	44	28	CN-	6.76	2.03		QEZYAV
	Ru	2+	44	28	CN-	6.99	2.03		WUGSEW
	Ru	2+	44	29	CO	6.82	2.02		LARPAW
	Ru	2+	44	29	CO	6.59	2.04		LARPIE
	Ru	4+	44	5	Cl-	2.74	2.32		GAZNOK
	Ru	4+	44	5	Cl-	2.72	2.33		YARREP
	Hf	4+	72	5	Cl-	3.11	2.45		BARWIB
	Hf	4+	72	5	Cl-	3.13	2.44		FEBHIE
	Hf	4+	72	5	Cl-	3.09	2.45		JESFOC
	Hf	4+	72	7	F-	4.71	1.99		RENPAB
	Ta	4+	73	7	F-	5.93	1.86		CEYCEO
	Ta	5+	73	2	Br-	3.50	2.49		BDASTA
	Ta	5+	73	5	Cl-	3.51	2.34		EMUCOE
	Ta	5+	73	5	Cl-	3.59	2.33		FIKGAH
	Ta	5+	73	7	F-	5.72	1.87		ECANAY
	Ta	5+	73	7	F-	5.43	1.89		GUCCEN
	W	3+	74	5	Cl-	2.20	2.58		LEXSIR
	W	4+	74	5	Cl-	3.31	2.34		EGUKIB
	W	4+	74	5	Cl-	3.24	2.36		HUYDIO
	W	4+	74	5	Cl-	3.10	2.38		JAKBEC
	W	4+	74	7	F-	6.86	1.78		ZIYWAF
	W	5+	74	5	Cl-	3.48	2.30		BUCBAC
	W	5+	74	5	Cl-	3.50	2.30		JATFIT
	W	5+	74	7	F-	6.56	1.78		ZOLKEQ
	Os	2+	76	23	bpy	5.14	2.04	Λ	HIRDOB
	Os	2+	76	23	bpy	5.25	2.08	Λ	HIRDOB2
	Os	2+	76	29	CO	8.25	2.00		CEHHIH
	Os	2+	76	29	CO	7.96	2.02		LARPEA
	Os	2+	76	29	CO	7.89	2.03		LARPOK
	Os	3+	76	17	NCS-	4.36	2.02		QIJJEY
	Os	3+	76	22	en	5.25	2.11	Δ	FISFAO
	Os	3+	76	28	CN-	7.07	2.05		OCIJIU
	Os	3+	76	28	CN-	7.04	2.07		OCIJIU2
	Os	4+	76	5	Cl-	3.10	2.33		CEXRIG
	Os	4+	76	5	Cl-	3.06	2.34		ENIDUA
	Os	4+	76	5	Cl-	3.09	2.33		GEBLUU
	Os	4+	76	7	F-	4.19	1.93		UFPEEA
	Os	4+	76	17	NCS-	4.40	2.01		QIJJAU
	Os	4+	76	17	NCS-	4.40	2.01		QIJJAU2
	Os	5+	76	5	Cl-	3.37	2.28		CEXREC
	Ir	4+	77	5	Cl-	3.01	2.66		GALQAL
	Ir	4+	77	5	Cl-	3.01	2.33		MIRKEE
	Ir	4+	77	5	Cl-	3.05	2.32		NAYQOU
	Ir	4+	77	5	Cl-	3.03	2.32		RIHFAP
	Ir	4+	77	5	Cl-	3.02	2.33		TEVFIJ
	Ir	4+	77	7	F-	3.72	1.92		TMAPTF01
				3	S2-				

				8	S2O32-				
				9	OCOR-				
				10	OCO22-				
				11	OH-				
				13	OSO32-				
				14	ONO2-				
				18	ONO-				
				25	SO32-				
				27	PPh3				

Ligand Series No.	Ligand	Metal	Valence	Metal Atomic No.	Metal Series No.	Ligand Field Splitting Δ (eV)	Metal Ligand Distance M-L (Å)	Chirality (bidentate ligand)	CSD Reference Code
1	I-	Zr	4+	40		2.27	2.86		RIQPEN
1	I-	Pt	4+	78	17	2.89	2.67		PYPTHI
1	I-	Pt	4+	78	17	2.87	2.67		KIBMIS
1	I-	Pt	4+	78	17	2.91	2.66		KIBMOY
2	Br-	Cr	3+	24	7	1.48	2.64		YIBWOV
2	Br-	Cu	2+	29		0.96	2.52		TIVJEN
2	Br-	Zr	3+	40		2.68	2.62		SENPOQ
2	Br-	Mo	4+	42		2.73	2.53		FUYGUB
2	Br-	Mo	3+	42	11	2.36	2.59		DOMTII
2	Br-	Tc	5+	43		3.14	2.50		PSBRNB
2	Br-	Rh	3+	45	12	2.43	2.50		HUQMEL
2	Br-	Rh	3+	45	12	2.51	2.53		ZOKHEM
2	Br-	Ta	5+	73		3.50	2.49		BDASTA
2	Br-	Re	4+	75	16	3.13	2.49		AYOMAC
2	Br-	Pt	4+	78	17	3.00	2.47		AZELEW
2	Br-	Pt	4+	78	17	2.99	2.47		AZELEW2
3	S2-								
4	SCN-	Rh	3+	45	12	2.34	2.37		YURKIF
4	SCN-	Ir	3+	77	15	2.87	2.38		PORQAO
4	SCN-	Pt	4+	78	17	2.39	2.68		BULVAF
4	SCN-	Pt	4+	78	17	2.87	2.39		EMUVOX
4	SCN-	Pt	4+	78	17	2.24	2.38		XECZAG
5	Cl-	Ti	4+	22		2.08	2.34		BARMAJ
5	Cl-	Ti	4+	22		2.08	2.34		FEPHOX
5	Cl-	V	4+	23		2.03	2.31		SAHJER
5	Cl-	V	3+	23	8	1.66	2.39		YUDFUY
5	Cl-	V	3+	23	8	1.64	2.39		YUDFUY2
5	Cl-	Cr	3+	24	7	1.61	2.36		FAMVUK10
5	Cl-	Mn	2+	25	1	0.86	2.57		DEFWOB
5	Cl-	Mn	2+	25	1	0.83	2.58		LIDQUL
5	Cl-	Fe	2+	26	4	1.15	2.39		MAFECL
5	Cl-	Fe	3+	26	6	1.38	2.38		DALLIL
5	Cl-	Fe	3+	26	6	1.35	2.40		KAPLOD
5	Cl-	Fe	3+	26	6	1.38	2.39		PIMXIS
5	Cl-	Fe	3+	26	6	1.35	2.40		TOQDAE
5	Cl-	Co	2+	27	3	0.94	2.47		HOCQUL
5	Cl-	Ni	2+	28	2	0.98	2.45		ZALNIJ
5	Cl-	Cu	2+	29		0.93	2.51		FOWCUP
5	Cl-	Cu	2+	29		0.93	2.50		GOKWUY
5	Cl-	Cu	2+	29		0.99	2.47		POCJAS
5	Cl-	Y	3+	39		2.44	2.62		WAPJUT
5	Cl-	Zr	4+	40		2.86	2.47		TUCNIO
5	Cl-	Zr	4+	40		2.86	2.47		FOHREZ
5	Cl-	Zr	4+	40		2.88	2.46		JAVKEW
5	Cl-	Nb	4+	41		2.88	2.41		KEWHOJ
5	Cl-	Nb	5+	41		3.25	2.34		FIRMOJ
5	Cl-	Nb	5+	41		3.26	2.34		NUYFOC
5	Cl-	Nb	5+	41		3.24	2.34		GOLJEW
5	Cl-	Mo	3+	42	11	2.41	2.45		DEBLEB
5	Cl-	Mo	3+	42	11	2.48	2.44		PEPCOC

5	Cl-	Mo	4+	42		2.93	2.35		FIPDEO
5	Cl-	Mo	4+	42		2.82	2.38		ZICWOX
5	Cl-	Mo	4+	42		2.80	2.38		FUTPIT
5	Cl-	Mo	5+	42		3.18	2.31		JAWRUU
5	Cl-	Tc	4+	43		2.74	2.36		CIMFEJ
5	Cl-	Tc	4+	43		2.77	2.35		JEPQOL
5	Cl-	Tc	4+	43		2.76	2.35		KAXQUW
5	Cl-	Tc	4+	43		2.74	2.36		LALHAH
5	Cl-	Ru	2+	44		2.26	2.37		WUGCOQ
5	Cl-	Ru	3+	44	13	2.42	2.38		ENIDAG
5	Cl-	Ru	3+	44	13	2.43	2.37		HEVCOA
5	Cl-	Ru	3+	44	13	2.42	2.38		HOCXUS
5	Cl-	Ru	3+	44	13	2.43	2.37		TAVTUF
5	Cl-	Ru	3+	44	13	2.44	2.37		YOJBUU
5	Cl-	Ru	4+	44		2.74	2.32		GAZNOK
5	Cl-	Ru	4+	44		2.72	2.33		YARREP
5	Cl-	Rh	3+	45	12	2.44	2.35		FEWGET
5	Cl-	Rh	3+	45	12	2.45	2.34		RIXHIP
5	Cl-	Rh	3+	45	12	2.43	2.35		TIBWIK
5	Cl-	Rh	3+	45	12	2.46	2.35		XISFEL
5	Cl-	Pd	4+	46	14	2.55	2.31		JIZLOT
5	Cl-	Pd	4+	46	14	2.10	2.42		LAHFUV
5	Cl-	Hf	4+	72		3.11	2.45		BARWIB
5	Cl-	Hf	4+	72		3.13	2.44		FEBHIE
5	Cl-	Hf	4+	72		3.09	2.45		JESFOC
5	Cl-	Ta	5+	73		3.51	2.34		EMUCOE
5	Cl-	Ta	5+	73		3.59	2.33		FIKGAH
5	Cl-	W	3+	74		2.20	2.58		LEXSIR
5	Cl-	W	4+	74		3.31	2.34		EGUKIB
5	Cl-	W	4+	74		3.24	2.36		HUYDIO
5	Cl-	W	4+	74		3.10	2.38		JAKBEC
5	Cl-	W	5+	74		3.48	2.30		BUCBAC
5	Cl-	W	5+	74		3.50	2.30		JATFIT
5	Cl-	Re	4+	75	16	3.10	2.36		AYOLUV
5	Cl-	Re	4+	75	16	3.10	2.36		AYOMEG
5	Cl-	Re	4+	75	16	3.12	2.35		HIDGIK
5	Cl-	Re	4+	75	16	3.06	2.36		IWOZID
5	Cl-	Os	4+	76		3.10	2.33		CEXRIG
5	Cl-	Os	4+	76		3.06	2.34		ENIDUA
5	Cl-	Os	4+	76		3.09	2.33		GEBLUU
5	Cl-	Os	5+	76		3.37	2.28		CEXREC
5	Cl-	Ir	4+	77		3.01	2.66		GALQAL
5	Cl-	Ir	4+	77		3.01	2.33		MIRKEE
5	Cl-	Ir	4+	77		3.05	2.32		NAYQOU
5	Cl-	Ir	4+	77		3.03	2.32		RIHFAP
5	Cl-	Ir	4+	77		3.02	2.33		TEVFIJ
5	Cl-	Pt	4+	78	17	2.91	2.32		AKCLPT
5	Cl-	Pt	4+	78	17	2.85	2.33		BIBRIN
5	Cl-	Pt	4+	78	17	2.90	2.32		MIMDPT
5	Cl-	Pt	4+	78	17	2.88	2.32		MINLAW
6	N3-	Ti	4+	22		1.54	2.02		BEYNUP
7	F-	Sc	3+	21		2.15	2.03		DEDNAC
7	F-	Sc	3+	21		2.20	2.05		HEYRUZ

7	F-	Ti	4+	22		3.08	1.84		AHUNEW
7	F-	Ti	4+	22		3.06	1.86		KOYXOL
7	F-	Ti	4+	22		3.16	1.84		LORCEA
7	F-	Ti	4+	22		3.82	1.76		SIXXAY
7	F-	V	3+	23	8	2.00	1.97		LIDYUT
7	F-	V	3+	23	8	2.49	1.90		WOHDIG
7	F-	Cr	3+	24	7	2.13	1.90		ADOSOC
7	F-	Cr	3+	24	7	2.17	1.90		GAWBUC
7	F-	Fe	3+	26	6	1.79	1.90		FULHOJ
7	F-	Zr	4+	40		4.11	2.01		TIZXAC
7	F-	Zr	4+	40		4.28	2.01		KOJVAG
7	F-	Zr	4+	40		4.18	2.01		QOFCOE
7	F-	Nb	4+	41		4.44	1.93		ROZLOI
7	F-	Mo	4+	42		4.38	1.92		ROZLIC
7	F-	Hf	4+	72		4.71	1.99		RENPAB
7	F-	Ta	4+	73		5.93	1.86		CEYCEO
7	F-	Ta	5+	73		5.72	1.87		ECANAY
7	F-	Ta	5+	73		5.43	1.89		GUCCEN
7	F-	W	4+	74		6.86	1.78		ZIYWAF
7	F-	W	5+	74		6.56	1.78		ZOLKEQ
7	F-	Os	4+	76		4.19	1.93		UFEPEA
7	F-	Ir	4+	77		3.72	1.92		TMAPTF01
8	S2O32-								
9	OCOR-								
10	OCO22-								
11	OH-								
12	OCHO-	Cr	3+	24	7	2.35	1.98		GICNEL
12	OCHO-	Mo	3+	42	11	3.59	2.11		GICNAH
13	OSO32-								
14	ONO2-								
15	ox2-	V	3+	23	8	2.30	2.01	Δ	KOXLTV01
15	ox2-	Cr	3+	24	7	2.52	1.97	Λ	CROXKH
15	ox2-	Cr	3+	24	7	2.60	1.96	Λ	DITFER
15	ox2-	Cr	3+	24	7	2.52	1.97	Δ	FPCOS
15	ox2-	Cr	3+	24	7	2.58	1.97	Λ	GUKGID
15	ox2-	Cr	3+	24	7	2.44	1.97	Δ	RUPGEP
15	ox2-	Mn	3+	25		2.05	2.00	Δ	ZZZCCG10
15	ox2-	Fe	2+	26	4	1.83	2.00	Δ	LIPXIS
15	ox2-	Fe	3+	26	6	1.91	2.00	Δ	BEMPEO
15	ox2-	Fe	3+	26	6	1.78	2.00	Δ	ARABEA
15	ox2-	Fe	3+	26	6	1.82	2.01	Λ	GEXQOP
15	ox2-	Co	3+	27	9	2.26	1.92	Λ	PNIOCO
15	ox2-	Co	3+	27	9	2.48	1.90	Δ	DAZVUV
15	ox2-	Co	3+	27	9	2.42	1.89	Λ	GUKGEZ
15	ox2-	Tc	4+	43		4.00	1.99	Λ	FOPBAN
15	ox2-	Ru	3+	44	13	3.58	2.03	Λ	DUKNOM
15	ox2-	Ru	3+	44	13	3.43	2.04	Λ	IDECOK
15	ox2-	Ru	3+	44	13	3.49	2.03	Λ	OLABAE
15	ox2-	Rh	3+	45	12	3.49	2.02	Λ	CAZCIP
15	ox2-	Rh	3+	45	12	3.36	2.01	Δ	LIKRIH
15	ox2-	Rh	3+	45	12	3.38	2.01	Λ	SOZFIW
16	H2O	Sc	3+	21		1.99	2.09		CEMXXU
16	H2O	Ti	3+	22		2.23	2.03		LIMPUS
16	H2O	V	2+	23	5	1.64	2.12		VEPSUE
16	H2O	V	2+	23	5	2.52	1.96		YEGSAF
16	H2O	V	3+	23	8	2.18	2.00		COLNUM
16	H2O	V	3+	23	8	2.24	1.99		FEMHOV
16	H2O	Cr	2+	24		1.66	2.04		GIMZIM

16	H2O	Cr	3+	24	7	2.17	1.97		UCOME
16	H2O	Cr	3+	24	7	2.27	1.97		IWOJOT
16	H2O	Cr	3+	24	7	2.11	1.96		MEWZET01
16	H2O	Cr	3+	24	7	2.15	1.96		TAPBUH
16	H2O	Mn	2+	25	1	1.08	2.16		ASOVEJ
16	H2O	Mn	2+	25	1	1.06	2.19		COLWUV
16	H2O	Mn	2+	25	1	1.08	2.17		HEHSIW
16	H2O	Mn	2+	25	1	1.09	2.17		LEFYAX
16	H2O	Mn	2+	25	1	1.22	2.17		VIDGIZ
16	H2O	Mn	3+	25		1.33	2.16		GUKGAV
16	H2O	Fe	2+	26	4	1.43	2.05		AMITAR
16	H2O	Fe	2+	26	4	1.19	2.10		DIJUK
16	H2O	Fe	2+	26	4	1.22	2.10		EJATEO
16	H2O	Fe	2+	26	4	1.04	2.12		FEACIT
16	H2O	Fe	2+	26	4	1.15	2.11		NATGEV
16	H2O	Fe	2+	26	4	1.12	2.10		QEDCOR
16	H2O	Fe	2+	26	4	1.32	2.12		ZILZID
16	H2O	Fe	3+	26	6	1.71	2.00		MEWZAP
16	H2O	Fe	3+	26	6	1.71	1.99		XIGSEL
16	H2O	Co	2+	27	3	1.18	2.10		ASUDIB
16	H2O	Co	2+	27	3	1.36	2.08		BAVYOM
16	H2O	Co	2+	27	3	1.17	2.09		NEFIB
16	H2O	Co	2+	27	3	1.16	2.07		SUBUG
16	H2O	Co	2+	27	3	1.12	2.07		WABLIU10
16	H2O	Co	3+	27	9	1.97	1.98		ASAWOH
16	H2O	Ni	2+	28	2	1.19	2.04		JERNID
16	H2O	Ni	2+	28	2	1.26	2.05		LUMVAQ
16	H2O	Ni	2+	28	2	1.25	2.05		MAPHER
16	H2O	Ni	2+	28	2	1.11	2.06		SIYZEF
16	H2O	Ni	2+	28	2	1.21	2.07		VELQEJ
16	H2O	Cu	2+	29		1.20	2.10		DILCIL
16	H2O	Cu	2+	29		1.26	2.12		DODDOP
16	H2O	Cu	2+	29		1.26	2.11		KAGNEM
16	H2O	Cu	2+	29		1.16	2.11		SIYZIJ
16	H2O	Zn	2+	30		1.96	2.07		BENBIG
16	H2O	Zn	2+	30		2.84	2.07		CITDAK
16	H2O	Zn	2+	30		1.58	2.09		FOGWUU
16	H2O	Zn	2+	30		2.62	2.09		KAMPEU
16	H2O	Ru	2+	44		2.39	2.12		BONPEZ
16	H2O	Ru	2+	44		2.86	2.09		OLUXAU
16	H2O	Ru	3+	44	13	3.08	2.03		BONPID
17	NCS-	Sc	3+	21		2.95	2.18		BUQMOP
17	NCS-	Sc	3+	21		2.90	2.16		XAJMOK
17	NCS-	Cr	3+	24	7	2.20	2.00		GETMUO
17	NCS-	Cr	3+	24	7	2.71	1.99		LUHWAM
17	NCS-	Cr	3+	24	7	2.68	2.01		KADXAP
17	NCS-	Cr	3+	24	7	2.43	2.00		NICHOC10
17	NCS-	Mn	2+	25	1	1.19	2.23		GEGBOK
17	NCS-	Mn	2+	25	1	1.38	2.24		XILJIM
17	NCS-	Mn	4+	25		1.22	2.22		MUPSO1
17	NCS-	Mn	4+	25		1.17	2.23		MUPSO2
17	NCS-	Fe	3+	26	6	1.54	2.09		MIJMUN
17	NCS-	Fe	3+	26	6	1.75	2.06		NEPSAC

17	NCS-	Fe	3+	26	6	1.85	2.05		TMFETC
17	NCS-	Fe	3+	26	6	1.79	2.05		TMFETC2
17	NCS-	Co	2+	27	3	1.43	2.09		BUQMIJ01
17	NCS-	Co	2+	27	3	1.36	2.12		KIPYUD
17	NCS-	Ni	2+	28	2	1.25	2.09		TIGGEW
17	NCS-	Ni	2+	28	2	1.40	2.10		BEZXIN
17	NCS-	Ni	2+	28	2	1.37	2.09		TOWCAJ
17	NCS-	Y	3+	39		3.22	2.33		KAKQES
17	NCS-	Mo	3+	42	11	4.15	2.08		KMOITC
17	NCS-	Tc	4+	43		4.39	2.00		FEKWEX
17	NCS-	Re	4+	75	16	5.08	2.02		OGAKIR
17	NCS-	Re	4+	75	16	5.11	2.07		OGAKIR2
17	NCS-	Re	4+	75	16	4.76	1.98		XUCBON
17	NCS-	Os	3+	76		4.36	2.02		QIJJEY
17	NCS-	Os	4+	76		4.40	2.01		QIJJAU
17	NCS-	Os	4+	76		4.40	2.01		QIJJAU2
18	ONO-								
19	CH3CN	V	2+	23	5	2.10	2.11		BEQQIX
19	CH3CN	Cr	3+	24	7	2.00	2.00		ACALEW
19	CH3CN	Mn	2+	25	1	2.21	2.22		ZOTYAI
19	CH3CN	Mn	2+	25	1	2.12	2.19		ZOTYAI2
19	CH3CN	Fe	2+	26	4	2.15	2.15		ACEYOW
19	CH3CN	Fe	2+	26	4	2.17	2.16		HIRTIL
19	CH3CN	Fe	2+	26	4	2.16	2.16		HMCIFE15
19	CH3CN	Co	2+	27	3	2.11	2.11		OCELIS
19	CH3CN	Co	2+	27	3	2.10	2.11		JOYPUI
19	CH3CN	Co	2+	27	3	2.10	2.11		OFINAT
19	CH3CN	Ni	2+	28	2	2.08	2.08		FUJVAH
19	CH3CN	Ni	2+	28	2	2.07	2.07		XUGBIK
19	CH3CN	Ni	2+	28	2	2.06	2.07		OCELAK
19	CH3CN	Tc	2+	43		4.62	2.06		TEQNAE
19	CH3CN	Ru	2+	44		4.54	2.09		ACEYAI
19	CH3CN	Ru	2+	44		4.56	2.03		PUHSOB
19	CH3CN	Ru	2+	44		4.87	2.01		FEWRII
19	CH3CN	Rh	3+	45	12	4.44	1.99		VENYAO
20	py	Fe	2+	26	4	1.46	2.26		PYFEFE
20	py	Ru	2+	44		4.31	2.13		HPYRUB
21	NH3	Cr	3+	24	7	2.81	2.08		LEBRUF
21	NH3	Mn	2+	25	1	1.33	2.29		PUHJIL
21	NH3	Co	2+	27	3	2.51	1.87		CAFWEM
21	NH3	Co	2+	27	3	2.57	1.96		OKOCAS
21	NH3	Co	2+	27	3	1.48	2.17		RAJNIZ
21	NH3	Co	3+	27	9	2.88	1.97		CANYAS
21	NH3	Co	3+	27	9	2.95	1.96		EYAQEA
21	NH3	Co	3+	27	9	3.13	1.97		XEDNAV
21	NH3	Ni	2+	28	2	1.68	2.14		BICSIQ
21	NH3	Ni	2+	28	2	1.69	2.14		NUHJUV
21	NH3	Rh	3+	45	12	4.62	2.08		XEDNEZ
21	NH3	Rh	3+	45	12	4.57	2.07		XEDNEZ2
21	NH3	Ir	3+	77	15	4.99	2.10		XEDNID
21	NH3	Ir	3+	77	15	5.24	2.08		XEDNID2
22	en	V	2+	23	5	2.10	2.20	Δ	HIDMEM
22	en	Cr	3+	24	7	2.75	2.08	Λ	CRENTC
22	en	Cr	3+	24	7	2.82	2.08	Δ	ENDACR

22	en	Cr	3+	24	7	2.95	2.08	△	ETDHCO
22	en	Cr	3+	24	7	2.87	2.08	△	GOZCIH
22	en	Mn	2+	25	1	1.32	2.29	△	ASEBEF
22	en	Mn	2+	25	1	1.48	2.27	△	KIBFUX
22	en	Mn	2+	25	1	1.44	2.27	△	QIBZOR
22	en	Mn	2+	25	1	1.38	2.28	△	RAGTOI
22	en	Fe	2+	26	4	1.50	2.20	△	FEBMAB
22	en	Fe	2+	26	4	1.59	2.21	△	LIWKOR01
22	en	Fe	2+	26	4	1.51	2.22	△	RITKUA
22	en	Co	2+	27	3	1.25	2.28	△	HIQYUC
22	en	Co	2+	27	3	1.57	2.18	△	HOSPOV
22	en	Co	2+	27	3	1.65	2.18	△	ICETEIQ
22	en	Co	2+	27	3	1.64	2.17	△	JEQNEZ
22	en	Co	2+	27	3	1.64	2.17	△	KIBGAE
22	en	Co	3+	27	9	3.08	1.97	△	ABIXIT
22	en	Co	3+	27	9	3.06	1.97	△	FIRQIH
22	en	Co	3+	27	9	3.11	1.97	△	PERHIE
22	en	Co	3+	27	9	3.22	1.97	△	TENCON
22	en	Co	3+	27	9	3.09	1.97	△	WOQFAK
22	en	Ni	2+	28	2	1.81	2.13	△	BINYAY
22	en	Ni	2+	28	2	1.72	2.15	△	DASSUL
22	en	Ni	2+	28	2	1.84	2.13	△	EFATOV
22	en	Ni	2+	28	2	1.81	2.13	△	ENIACH
22	en	Ni	2+	28	2	1.85	2.13	△	XAPNOS
22	en	Ru	2+	44		3.84	2.13	△	BABRAX
22	en	Rh	3+	45	12	4.49	2.09	△	AGUJIW
22	en	Rh	3+	45	12	4.68	2.06	△	CRHENC
22	en	Rh	3+	45	12	4.66	2.07	△	DARGUY
22	en	Rh	3+	45	12	4.65	2.06	△	TENRHC
22	en	Os	3+	76		5.25	2.11	△	FISFAO
22	en	Ir	3+	77	15	5.12	2.10	△	UBEFEM
22	en	Ir	3+	77	15	5.36	2.20	△	DARHAF
23	bpy	Cr	2+	24		3.00	2.08	△	ACAYUZ
23	bpy	Cr	3+	24	7	3.14	2.04	△	FERYEG
23	bpy	Cr	3+	24	7	3.18	2.05	△	FERYEG2
23	bpy	Mn	2+	25	1	1.73	2.24	△	GUXJOY
23	bpy	Fe	2+	26	4	3.10	1.98	△	LIPXIS
23	bpy	Fe	2+	26	4	3.12	1.98	△	LIPXIS2
23	bpy	Co	2+	27	3	1.91	2.13	△	CAMHED
23	bpy	Co	2+	27	3	2.04	2.12	△	CIBDOH
23	bpy	Co	2+	27	3	3.28	1.93	△	IXODII
23	bpy	Co	2+	27	3	3.38	1.93	△	IXODII2
23	bpy	Co	3+	27	9	3.25	1.93	△	DUPPAG
23	bpy	Co	3+	27	9	3.26	1.93	△	FIXKUT
23	bpy	Ni	2+	28	2	2.12	2.09	△	AGADAO
23	bpy	Ni	2+	28	2	2.26	2.08	△	AGADAO2
23	bpy	Ni	3+	28		2.94	1.98	△	CUHVUW
23	bpy	Ru	2+	44		4.89	2.05	△	AXAFIO
23	bpy	Rh	3+	45	12	4.64	2.04	△	DIWGIZ
23	bpy	Rh	3+	45	12	4.76	2.02	△	FERYIK
23	bpy	Rh	3+	45	12	4.72	2.06	△	FERTIK2
23	bpy	Os	2+	76		5.14	2.04	△	HIRDOB
23	bpy	Os	2+	76		5.25	2.08	△	HIRDOB2
23	bpy	Ir	3+	77	15	5.46	2.02	△	CEZMAV
24	phen	V	3+	23	8	3.92	1.99	△	CEHBEX
24	phen	Cr	3+	24	7	3.15	2.05	△	LIYWUL
24	phen	Mn	2+	25	1	1.87	2.23	△	GUHGOF
24	phen	Mn	2+	25	1	1.50	2.25	△	LUHCAA
24	phen	Fe	2+	26	4	3.13	1.97	△	ADETIM
24	phen	Fe	2+	26	4	3.11	1.98	△	AFIRAJ
24	phen	Fe	2+	26	4	3.10	1.98	△	MIKJEW
24	phen	Fe	3+	26	6	3.09	1.98	△	BIPGEN
24	phen	Fe	3+	26	6	3.09	1.97	△	FUTDOO
24	phen	Fe	3+	26	6	3.19	1.97	△	SOGXOC
24	phen	Co	2+	27	3	1.94	2.13	△	AGOYIF
24	phen	Co	2+	27	3	3.17	1.94	△	BUYLIR
24	phen	Co	2+	27	3	3.19	1.94	△	HOCHFIP

24	phen	Co	2+	27	3	1.93	2.13	Δ	SALVEH
24	phen	Co	3+	27	9	3.08	1.94	Δ	KIWRIS
24	phen	Co	3+	27	9	3.06	1.94	Λ	KULRAL
24	phen	Co	3+	27	9	2.99	1.94	Δ	MOHFAR
24	phen	Ni	2+	28	2	2.09	2.09	Λ	FUHWEL
24	phen	Ni	2+	28	2	2.07	2.09	Δ	MODCAK
24	phen	Ni	2+	28	2	2.07	2.09	Λ	IYULIX
25	SO32-								
26	NO2-	Co	3+	27	9	3.62	1.96		WERKIN2
26	NO2-	Co	3+	27	9	3.58	1.96		WERKIN10
26	NO2-	Rh	3+	45	12	5.83	2.03		TEDDOV
26	NO2-	Rh	3+	45	12	6.04	2.08		TEDDOV2
27	PPh3								
28	CN-	Ti	3+	22		3.85	2.18		NAYWOZ
28	CN-	V	3+	23	8	3.72	2.14		JEHBAA
28	CN-	Cr	3+	24	7	3.86	2.07		BIJZOK
28	CN-	Cr	3+	24	7	3.99	2.08		AFOVIA
28	CN-	Cr	3+	24	7	4.03	2.08		COLHIU
28	CN-	Cr	3+	24	7	4.00	2.08		ELONUO
28	CN-	Mn	3+	25		4.33	2.01		BIFZOG
28	CN-	Mn	3+	25		4.22	2.02		KAHKIN
28	CN-	Fe	3+	26	6	4.56	1.93		BIWYOW
28	CN-	Fe	3+	26	6	4.66	1.94		FETGIV
28	CN-	Fe	2+	26	4	4.87	1.95		CEJYEV
28	CN-	Fe	2+	26	4	5.05	1.91		EYIQUY
28	CN-	Fe	2+	26	4	4.87	1.93		FAWNOH
28	CN-	Fe	2+	26	4	5.04	1.90		GIJVEA
28	CN-	Co	3+	27	9	5.02	1.88		AENCOC
28	CN-	Co	3+	27	9	4.93	1.89		DIENCO
28	CN-	Co	3+	27	9	4.86	1.90		HIGZAY
28	CN-	Co	3+	27	9	4.77	1.90		PEHACO
28	CN-	Mo	4+	42		6.80	2.90		HITPOQ
28	CN-	Ru	2+	44		6.76	2.03		QEZYAV
28	CN-	Ru	2+	44		6.99	2.03		WUGSEW
28	CN-	Ru	3+	44	13	6.60	2.05		KAGLAG
28	CN-	Os	3+	76		7.07	2.05		OCIJIU
28	CN-	Os	3+	76		7.04	2.07		OCIJIU2
28	CN-	Pt	4+	78	17	6.76	2.02		YASNUC
28	CN-	Pt	4+	78	17	6.81	1.99		COZVAO
29	CO	Fe	2+	26	4	4.94	1.91		CEHHON
29	CO	Fe	2+	26	4	4.93	1.91		HOLMIE
29	CO	Fe	2+	26	4	4.95	1.91		HOLMOK
29	CO	Ru	2+	44		6.82	2.02		LARPAW
29	CO	Ru	2+	44		6.59	2.04		LARPIE
29	CO	Os	2+	76		8.25	2.00		CEHHIH
29	CO	Os	2+	76		7.96	2.02		LARPEA
29	CO	Os	2+	76		7.89	2.03		LARPOK
29	CO	Ir	3+	77	15	7.26	2.03		XOLYIG
	glycine	V	3+	23	8	2.62	2.05	Δ	AGASIL
	glycine	Cr	3+	24	7	2.51	2.02	Λ	TGLYCR
	glycine	Co	3+	27	9	2.60	1.93	Λ	AVUWET
	glycine	Co	3+	27	9	2.73	1.92	Δ	SEZMEQ
	urea	Ti	3+	22		2.80	2.01		TIUREA01
	urea	Cr	3+	24	7	2.13	1.97		DAPFEF
	urea	Cr	3+	24	7	2.24	1.97		COLHIU

	urea	Cr	3+	24	7	2.14	1.97		HOHPOJ
	urea	Cr	3+	24	7	2.02	1.97		HOHPUP
	urea	Mn	2+	25	1	1.05	2.18		WITQAR
	urea	Mn	3+	25		1.93	1.99		BOPWEI
	urea	Fe	2+	26	4	1.56	1.99		WITQEV
	urea	Fe	3+	26	6	1.77	1.99		MANJIU
	urea	Co	2+	27	3	1.21	2.11		COLLAQ01
	urea	Co	2+	27	3	1.24	2.10		RUBLEG
	urea	Co	2+	27	3	1.19	2.09		WITLIU
	urea	Ni	2+	28	2	1.33	2.06		ADUFEK

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