Supplementary Material

Coordination preferences of NNO and NNS Schiff base ligands with Co(III) complexes: Synthesis, characterization and DFT calculation

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Table S1. Selected bond lengths (Å) and angles (°) of complexes **1** and **2.**

	1		**2**
Co1–N2	1.909(2)	Co1–N2	1.8516(15)
Co1–N6	1.907(2)	Co1–N1	1.9189(16)
Co1–N1	1.964(2)	Co1–O1	1.9272(13)
Co1–N5	1.953(2)	Co1–N11	1.9615(17)
Co1–S4	2.2257(8)	Co1–N8	1.9632(16)
Co1–S2	2.2230(8)	Co1–N5	1.9704(18)
S2–C6	1.738(3)	O1–C8	1.289(2)

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S4–C12	1.743(3)	N3–C8	1.313(2)
N7–C12	1.315(4)	N2–C6	1.291(2)
N3–C6	1.326(4)	N2–N3	1.386(2)
N6–N7	1.380(3)	N5–N6	1.206(2)
N2–N3	1.372(3)	N6–N7	1.155(2)
N6–C10	1.296(4)	N8–N9	1.205(2)
N2–C4	1.303(3)	N9–N10	1.149(3)
		N11–N12	1.211(2)
		N12–N13	1.152(3)

N2–Co1–N6	177.20(10)	N2–Co1–N1	82.77(7)
N2–Co1–N1	82.42(9)	N2–Co1–O1	82.67(6)
N6–Co1–N1	97.94(9)	N1–Co1–O1	165.12(6)
N2–Co1–N5	100.58(10)	N2–Co1–N11	91.46(7)
N6–Co1–N5	82.22(10)	N1–Co1–N11	88.11(7)
N1–Co1–N5	88.49(9)	O1–Co1–N11	89.19(6)
N2–Co1–S4	91.75(7)	N2–Co1–N8	179.26(7)
N6–Co1–S4	85.46(7)	N1–Co1–N8	97.82(7)
N1–Co1–S4	92.00(7)	O1–Co1–N8	96.75(6)
N5–Co1–S4	167.61(7)	N11–Co1–N8	88.99(7)
N2–Co1–S2	85.79(7)	N2–Co1–N5	87.89(7)
N6–Co1–S2	94.04(7)	N1–Co1–N5	89.77(7)
N1–Co1–S2	167.55(7)	O1–Co1–N5	92.77(6)
N5–Co1–S2	89.78(7)	N11–Co1–N5	177.84(7)
S4–Co1–S2	92.32(3)	N8–Co1–N5	91.68(7)

Table S2. Comparison of Co-$N_{thiazole}$, Co-N_{imine} and Co-$S_{thiolate}$ bond lengths (Å) in octahedral Co(III)-N_4S_2 complexes with thiosemicarbazone based ligands.

Complexes	Co-$N_{thiazole}$	mean values	Co-N_{imine}	mean values	Co-$S_{thiolate}$	mean values	References
$[Co(L^1)_2]BF_4 \cdot H_2O$ (1)	**1.964(2)**	**1.9585**	**1.909(2)**	**1.908**	**2.2230(8)**	**2.2243**	**this work**
	1.953(2)		**1.907(2)**		**2.2257(8)**		
$[Co(L^1)_2]_2[Co(NCS)_4] \cdot 2H_2O$	1.958(5)	1.960	1.903(5)	1.907	2.225(2)	2.222	[1]
CCDC 1854180	1.962(6)		1.911(5)		2.220(2)		
$[Co(L^3)_2]BF_4 \cdot H_2O$	1.945(2)	1.955	1.907(3)	1.905	2.228(1)	2.226	[2]
CCDC 1498846	1.964(3)		1.902(3)		2.225(1)		
$[Co(L^4)_2]BF_4 \cdot Et_2O$	1.978(3)	1.986	1.890(3)	1.890	2.2108(9)	2.2163	[2]
CCDC 1498852	1.994(3)		1.890(3)		2.2218(9)		
	Co-$N_{thiazoline}$						
$[Co(L^5)_2]_2[CoCl_4] \cdot 2H_2O$	1.933(2)	1.936	1.903(2)	1.9015	2.225(1)	2.229	[3]
CCDC 759081	1.939(2)		1.900(2)		2.234(1)		
$[Co(L^5)_2]NO_3 \cdot H_2O$	1.936(3)	1.933	1.897(3)	1.900	2.216(1)	2.223	[3]
CCDC 759082	1.930(3)		1.903(3)		2.229(1)		

HL^1 = (*E*)-2-(1-(thiazol-2-yl)ethylidene)hydrazine-1-carbothioamide;
HL^3 = condensation product of 2-thiazolecarboxaldehyde and 4-phenylthiosemicarbazide; HL^4 = condensation product of 4-methyl-2-thiazolecarboxaldehyde and 4-phenylthiosemicarbazide; HL^5 = 2-acetyl-2-thiazoline thiosemicarbazone.

References: [1] B. Čobeljić, I. Turel, A. Pevec, Z. Jagličić, D. Radanović, K. Anđelković, M. R. Milenković, *Polyhedron* 155 (2018) 425–432. [2] R. J. Laverick, A. B. Carter, H. A. Klein, A. J. Fitzpatrick, T. D. Keene, G. G. Morgan, J. A. Kitchen, *Inorg. Chim. Acta* 463 (2017) 126-133. [3] E.Vinuelas-Zahinos, F. Luna-Giles, P.Torres-Garcia, M.C. Fernandez-Calderon, *Eur. J. Med. Chem.* 46 (2011) 150–159.

Table S3. Comparison of Co-N_{py}, Co-N_{imine}, Co-N_{azide} and Co-$O_{enolate}$ bond lengths (Å) in octahedral Co(III)N_4O_2–Co(III)$N_2O(N_3)_3$ complexes with hydrazone and azide ligands.

Complexes	Co-N_{py}	Co-N_{imine}	Co-N_{azide}	Co-$O_{enolate}$	References
$[Co(L^2)(N_3)_3]$ (2)	**1.9189(16)**	**1.8516(15)**	**1.9704(18)** **1.9632(16)** **1.9615(17)** **mean value:** **1.9650**	**1.9272(13)**	**this work**
$[Co(L^6)_2]^+[Co(L^6)(N_3)_3]^-\cdot CH_3OH$ CCDC 828862	1.9240(14) 1.9170(13) 1.9162(14) mean value: 1.9190	1.8606(12) 1.8644(13) 1.8482(14) mean value: 1.8577	1.9573(15) 1.9633(14) 1.9685(14) mean value: 1.9630	1.9235(13) 1.9060(12) 1.9110(12) mean value: 1.9135	[1]
$[Co(L^7)_2]$ $[Co(L^7)(N_3)_3]$ CCDC 894063	1.916(3) 1.909(3) 1.917(3) mean value: 1.914	1.860(3) 1.861(3) 1.862(3) mean value: 1.861	1.971(3) 1.949(3) 1.956(3) mean value: 1.959	1.922(2) 1.896(2) 1.944(3) mean value: 1.921	[2]

HL^2 = naziv liganda;

HL^6 = *N′*-[(1*E*)-1-pyridin-2-ylethylidene]-2-furohydrazide; HL^7= methyl 2-pyridyl ketone semicarbazone.

References: [1] R. Bikas, H. H. Monfared, T. Lis, M. Siczek, *Inorg. Chem. Commun*. 15 (2012) 151-155; [2] B. Shaabani, A. A. Khandar, F. Mahmoudi, S. S. Balula, L. Cunha-Silva, *J. Mol. Struct*. 1045 (2013) 55-61;

Table S4. Hydrogen-bond parameters for complex **1**.

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)	Symm. operation on A
N4–H4NA···N7	0.86	2.59	3.446(4)	172	-1/2+*x*, *y*, 3/2-*z*
N8–H8NA···N3	0.86	2.28	3.109(4)	162	1/2+*x*, *y*, 3/2-*z*
N4–H4NB···S4	0.86	2.81	3.611(3)	155	1-*x*,1/2+*y*,3/2-*z*
O1W–H2W···F1	1.01(7)	1.74(8)	2.728(7)	167(8)	
O1W-H1W···N3	1.02(7)	2.01(8)	2.962(7)	155(9)	

Table S5. Intermolecular π···π interaction parameters for complex **1**.

Cg(*I*)[a]	Cg(*J*)[a]	Cg(*I*)···Cg(*J*)[b] (Å)	α[c] (°)	β[d] (°)	γ[e] (°)	Slippage[f] (Å)	Sym. code on (*J*)
Cg(1)	Cg(1)	4.0189(16)	0.00(14)	25.9	25.9	1.755	1-*x*, 1-*y*, 2-*z*
Cg(2)	Cg(2)	3.8200(16)	0.00(14)	23.9	23.9	1.550	1-*x*, 2-*y*, 2-*z*

[a] Labels of aromatic rings: (1) = S(1),C(2),C(1),N(1),C(3); (2) = S(3),C(8),C(7),N(5),C(9).

[b]Cg(*I*)···Cg(*J*) = Distance between ring centroids (Ang.).

[c]α = Dihedral angle between planes (*I*) and (*J*) (Deg).

[d]β = Angle between Cg(*I*)–Cg(*J*) vector and normal to plane (*I*) (Deg).

[e]γ = Angle between Cg(*I*) –Cg(*J*) vector and normal to plane (*J*) (Deg).

Slippage = Distance between Cg(*I*) and perpendicular projection of Cg(*J*) on ring (*I*) (Ang).

Table S6. Intermolecular π···π interaction parameters for complex **2**.

Cg(*I*)[a]	Cg(*J*)[a]	Cg(*I*)···Cg(*J*)[b] (Å)	α[c] (°)	β[d] (°)	γ[e] (°)	Slippage[f] (Å)	Sym. code on (*J*)
Cg(1)	Cg(1)	3.4540(13)	0.03(11)	24.3	24.3	1.419	1-x, 1-y, 1-z
Cg(2)	Cg(2)	3.9788(14)	0.00	28.5	28.5	1.901	-x, 1-y, -z

[a] Labels of aromatic rings: (1) = N(1),C(1),C(2),C(3),C(4),C(5); (2) = N(4),C(10),C(11),C(12),C(13),C(14).

[b]Cg(*I*)···Cg(*J*) = Distance between ring centroids (Ang.).

[c]α = Dihedral angle between planes (*I*) and (*J*) (Deg).

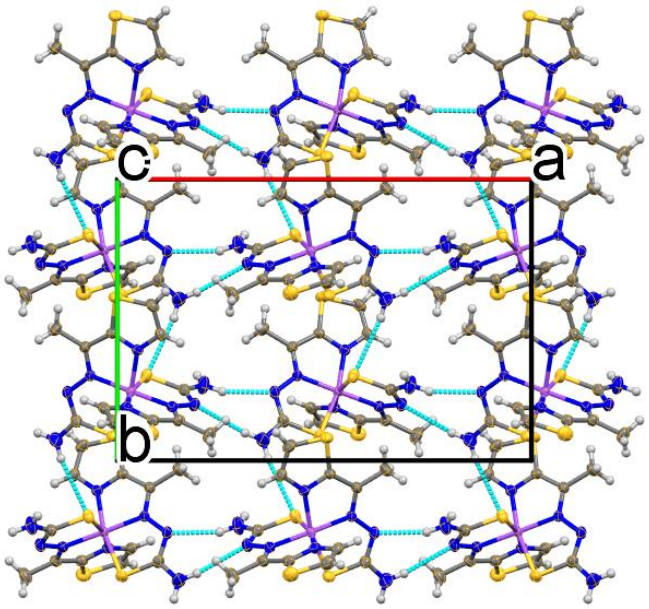
[d]β = Angle between Cg(*I*)–Cg(*J*) vector and normal to plane (*I*) (Deg).

[e]γ = Angle between Cg(*I*) –Cg(*J*) vector and normal to plane (*J*) (Deg).

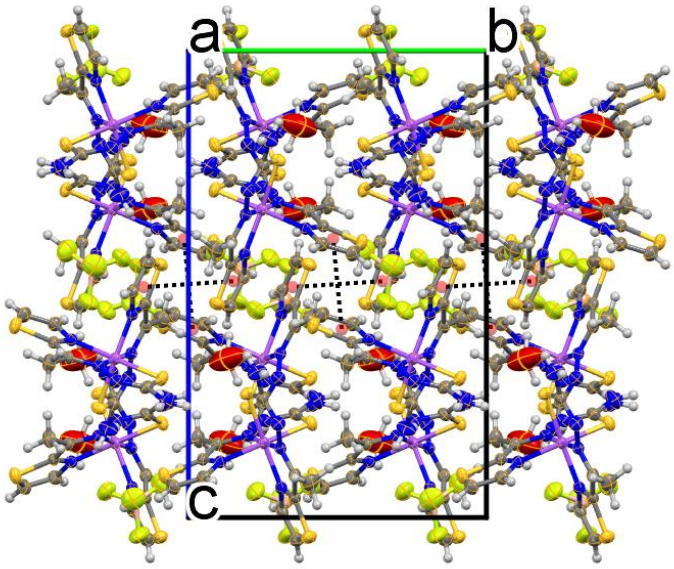
Slippage = Distance between Cg(*I*) and perpendicular projection of Cg(*J*) on ring (*I*) (Ang).

Table S7. Hydrogen-bond parameters for complex **2**.

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)	Symm. operation on A
C1–H1···N7	0.95	2.53	3.341(3)	143	1+x, y, z
C7–H7B···N11	0.98	2.48	3.445(3)	167	1-x, -y, 1-z
C9–H9A···N10	0.99	2.54	3.379(3)	142	x, -1+y, z
C10–H10···N10	0.95	2.51	3.339(3)	145	x, -1+y, z
C12–H12···O1	0.95	2.52	3.272(3)	136	-x, 1-y, -z
C14–H14···N8	0.95	2.30	3.230(3)	167	-1+x, y, z
Intra C7–H7C···N3	0.98	2.56	2.935(2)	103	



(a)



(b)

Fig. S1. (a) Crystal packing of **1** showing self-assembled complex cations within a layer parallel with the (001) lattice plane by means of intermolecular N–H···N and N–H···S hydrogen bonds and (b) Intermolecular π···π interactions between thiazole rings.

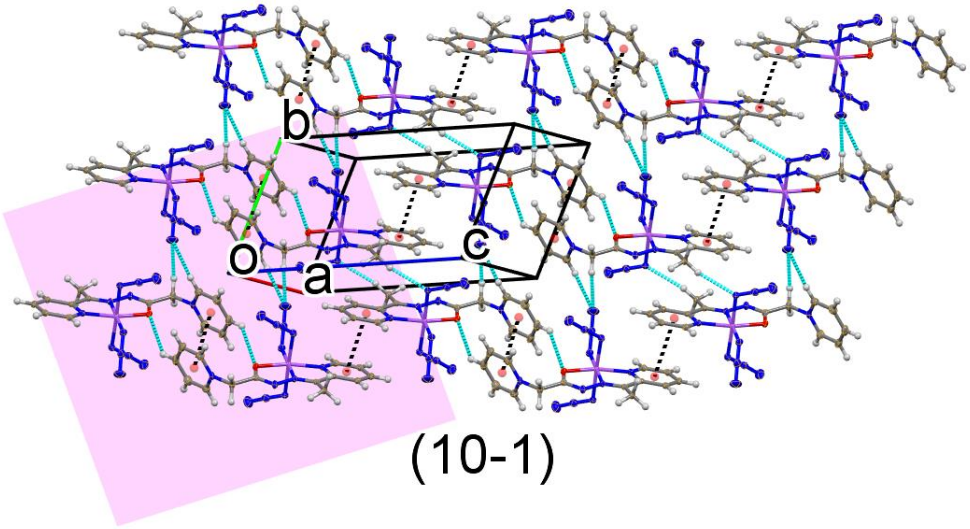


Fig. S2. Crystal packing of **2** showing 2D assembly parallel with the (10-1) lattice plane generated by intermolecular π···π interactions and C–H···N hydrogen bonds.

Cartesian coordinates of all optimized structures

All structures from Table 2 in the main text, optimized at BP86-D3BJ/Def2-TZVP-PCM(H2O) level of theory:

39
$[Co(\mathbf{L^1})_2]^+$

27	0.602833	9.074593	6.401248
16	1.300909	7.244271	10.273337
16	1.319338	9.758729	4.392051
16	0.041220	13.142922	7.802657
16	-0.188263	7.168252	5.530595
7	0.341658	8.380562	8.195433
7	2.375174	8.423800	6.653640
7	3.347693	8.525118	5.732125
7	3.837305	9.295216	3.631930
1	4.785028	8.953561	3.757405
1	3.590588	9.754891	2.763841
7	0.929578	10.841893	7.135445
7	-1.168572	9.741239	6.186293
7	-2.178624	9.026392	5.662849
7	-2.745626	6.990307	4.781607
1	-3.692475	7.336465	4.662053
1	-2.527891	6.043298	4.496094
6	-0.694941	8.317625	9.083564
1	-1.671952	8.708896	8.812356
6	-0.357781	7.728736	10.275903
1	-0.985569	7.552029	11.143208
6	1.480305	7.851796	8.670649
6	2.638310	7.859013	7.824425
6	3.974611	7.313082	8.189121
1	4.267558	6.518934	7.486302
1	3.968580	6.902513	9.205966
1	4.740365	8.100375	8.126745
6	2.937257	9.145641	4.619170
6	2.002817	11.504931	7.660603
1	2.974235	11.020118	7.710539
6	1.707263	12.777474	8.079456
1	2.369126	13.512080	8.526510
6	-0.196884	11.571976	7.135280
6	-1.390579	10.980180	6.604324
6	-2.719678	11.646373	6.524230
1	-3.060855	11.693668	5.479377
1	-2.675449	12.664332	6.929662
1	-3.471178	11.071367	7.085313
6	-1.805896	7.787519	5.318665

29
$[Co(\mathbf{L^1})(N_3)_3]^-$

27	0.779421	9.373172	6.622885
16	-2.974220	10.585490	4.789072

16	1.935748	8.435462	8.286732
7	0.658983	7.652928	5.653706
7	-0.530811	10.107836	5.377547
7	-0.764719	8.986442	7.660136
7	-0.727185	8.391921	8.866902
7	0.668404	7.508843	10.452854
1	-0.151898	7.270853	11.001020
1	1.582769	7.231055	10.787199
7	0.849748	11.170115	7.495993
7	2.334426	9.876009	5.527425
7	-0.187493	5.672568	6.648018
6	-0.497788	10.713327	4.156265
1	0.460592	10.884057	3.671700
6	-1.737711	11.048275	3.670192
1	-1.991408	11.534409	2.733687
6	-1.770427	9.961349	5.861492
6	-1.933150	9.334999	7.142887
6	-3.239368	9.102300	7.822870
1	-3.383774	8.029957	8.022077
1	-4.073220	9.462778	7.207791
1	-3.267465	9.618856	8.794049
6	0.522168	8.097565	9.249094
7	1.928216	11.622163	7.785212
7	2.944945	12.108809	8.088896
7	3.080773	9.042997	5.078886
7	3.841582	8.290644	4.612362
7	0.221893	6.665724	6.190550

67

$[Co(\mathbf{L}^2)_2]^{3+}$

27	0.000052	-0.000140	-0.164585
8	-1.388377	0.078672	-1.506015
7	1.365820	0.409450	1.118862
7	-0.182083	1.853745	-0.230113
7	-1.198504	2.345208	-1.007177
7	-4.139758	0.889089	-1.623933
8	1.388629	-0.078965	-1.505795
7	0.182119	-1.854040	-0.230208
7	1.198728	-2.345504	-1.007062
7	-1.365892	-0.409731	1.118674
6	2.144773	-0.453289	1.783655
1	1.918567	-1.511893	1.668674
6	3.203572	-0.015060	2.581291
1	3.815992	-0.749321	3.101817
6	3.451782	1.351847	2.686935
1	4.277826	1.719296	3.295188
6	2.629351	2.250941	2.005001
1	2.796764	3.325001	2.068843
6	1.584883	1.761374	1.222044
6	0.655972	2.590128	0.453210
6	0.663961	4.075518	0.457987

1	1.602738	4.451652	0.022768
1	0.600685	4.456634	1.487701
1	-0.178226	4.458956	-0.126618
6	-1.771196	1.313546	-1.606519
6	-3.047797	1.550576	-2.384932
1	-3.267660	2.617801	-2.468764
1	-2.993763	1.096807	-3.381110
6	-4.857470	1.613073	-0.727866
1	-4.660183	2.682287	-0.700822
6	-5.771721	0.985968	0.100035
1	-6.336574	1.584925	0.811461
6	-5.939255	-0.398302	0.012055
1	-6.645132	-0.908506	0.666690
6	-5.196128	-1.121049	-0.923215
1	-5.302670	-2.198906	-1.027021
6	-4.296338	-0.454400	-1.737143
1	-3.676143	-0.952264	-2.477642
6	1.771495	-1.313836	-1.606286
6	3.048128	-1.550805	-2.384642
7	4.139974	-0.888804	-1.623910
1	3.268212	-2.618017	-2.468062
1	2.993988	-1.097443	-3.381003
6	4.858190	-1.612439	-0.727964
6	5.772238	-0.984877	0.099817
6	5.939086	0.399472	0.011803
6	5.195521	1.121843	-0.923399
6	4.295901	0.454754	-1.737171
1	4.661473	-2.681755	-0.700911
1	6.337485	-1.583555	0.811165
1	5.301560	2.199743	-1.027272
1	3.675359	0.952316	-2.477581
1	6.644803	0.910013	0.666346
6	-1.585075	-1.761651	1.221687
6	-0.656025	-2.590414	0.453000
6	-0.664000	-4.075806	0.457861
1	-1.602692	-4.451984	0.022497
1	-0.600897	-4.456841	1.487614
1	0.178289	-4.459273	-0.126578
6	-2.629747	-2.251228	2.004354
6	-3.452246	-1.352147	2.686230
6	-3.203870	0.014747	2.580837
6	-2.144886	0.452990	1.783448
1	-2.797265	-3.325280	2.068042
1	-4.278469	-1.719596	3.294240
1	-3.816314	0.748992	3.101358
1	-1.918588	1.511593	1.668641

43

[Co(**L**^{2})(N_3)$_3$]

27	4.281731	2.987055	4.264904
8	2.991925	2.288381	2.988342

7	5.229580	3.532769	5.827523
7	3.009488	2.429180	5.489626
7	1.865210	1.872374	4.985133
7	0.542547	2.101968	1.701382
7	3.467075	4.795333	4.143559
7	2.297593	4.879927	3.860471
7	1.171576	5.025941	3.588860
7	5.649060	3.536463	2.955605
7	5.267380	4.057121	1.936204
7	4.958382	4.567024	0.933878
7	5.145780	1.202248	4.396048
7	5.375614	0.655310	3.344138
7	5.623092	0.075820	2.363791
6	6.426274	4.125746	5.882462
1	6.902925	4.309477	4.919032
6	7.010880	4.479081	7.101429
1	7.987369	4.961658	7.107840
6	6.326299	4.203417	8.285424
1	6.758717	4.469117	9.250330
6	5.077364	3.581933	8.225230
1	4.519177	3.354442	9.132585
6	4.540025	3.250839	6.979129
6	3.247220	2.605703	6.764847
6	2.323745	2.208014	7.863389
1	2.050201	3.082140	8.473843
1	2.808214	1.478993	8.531130
1	1.414108	1.762211	7.447837
6	1.983732	1.850296	3.662996
6	0.831924	1.254286	2.877580
1	1.099344	0.251606	2.518892
1	-0.065282	1.184538	3.498435
6	1.335388	1.997441	0.605204
1	2.099551	1.225385	0.634878
6	1.148018	2.845115	-0.472817
1	1.792530	2.742135	-1.343515
6	0.137218	3.807945	-0.418994
1	-0.026170	4.481007	-1.260319
6	-0.662064	3.899731	0.721480
1	-1.457195	4.637941	0.804155
6	-0.432931	3.039099	1.781426
1	-1.004259	3.064264	2.705822

19

L^{1-}

16	1.455267	7.224364	10.162788
16	1.613013	9.890264	3.813833
7	0.048292	8.422417	8.347430
7	2.187598	8.550522	6.465986
7	3.257513	8.572756	5.644138
7	4.144786	9.094663	3.627534
1	5.033995	8.859958	4.064385

1	4.158640	9.705667	2.818655
6	-0.763184	8.218357	9.430490
1	-1.799880	8.554974	9.392749
6	-0.192934	7.587967	10.511333
1	-0.642569	7.326487	11.464791
6	1.272616	7.954624	8.558274
6	2.398840	7.993617	7.638203
6	3.729007	7.414782	8.046791
1	4.048003	6.644246	7.328750
1	3.702620	6.967111	9.048846
1	4.507643	8.192912	8.034692
6	3.039612	9.151253	4.443713

33

L^2

8	2.815679	3.058801	2.464160
7	5.913406	3.428634	6.039915
7	3.376577	2.908015	5.134622
7	2.106351	2.633208	4.693008
7	0.109914	3.146685	1.803645
6	7.136098	3.699313	6.508876
1	7.892186	3.948770	5.756135
6	7.484048	3.678872	7.865004
1	8.501967	3.909148	8.181338
6	6.484754	3.354475	8.783285
1	6.697574	3.323182	9.853512
6	5.203324	3.069275	8.315003
1	4.413767	2.816206	9.021056
6	4.935485	3.112390	6.928927
6	3.575608	2.811599	6.422736
6	2.509561	2.416921	7.415023
1	2.314291	3.225811	8.137478
1	2.812327	1.532352	7.997361
1	1.582259	2.191842	6.878206
6	1.997844	2.730992	3.354929
6	0.571882	2.296001	2.908969
1	0.609076	1.259862	2.545399
1	-0.140933	2.366893	3.734527
6	0.701379	3.006643	0.590572
1	1.409992	2.189773	0.496491
6	0.373234	3.863778	-0.450817
1	0.850036	3.723707	-1.419291
6	-0.559729	4.877300	-0.237371
1	-0.832293	5.555807	-1.045513
6	-1.148634	5.009813	1.024936
1	-1.882727	5.786013	1.232894
6	-0.791977	4.134135	2.034252
1	-1.202215	4.182274	3.040621

3

N_3^-

7	5.635663	3.540727	2.947877
7	5.291462	4.053523	1.941923
7	4.947695	4.566350	0.935879

39

$[Co(\mathbf{L}^{\mathbf{1}(S\rightarrow O)})_2]^+$

27	0.604617	9.103971	6.470470
16	1.200701	7.176073	10.273564
8	1.339151	9.606642	4.752383
16	0.140287	13.188636	7.749370
8	-0.195187	7.533332	5.672069
7	0.312128	8.408021	8.222688
7	2.324838	8.384983	6.699064
7	3.197914	8.520973	5.696012
7	3.278567	9.441022	3.576377
1	4.228551	9.099527	3.490572
1	2.841696	9.912694	2.793599
7	0.960738	10.841706	7.173045
7	-1.117009	9.799997	6.187778
7	-2.030633	9.000730	5.628015
7	-2.187120	6.839222	4.822246
1	-3.146189	7.032526	4.559054
1	-1.776351	5.940588	4.599091
6	-0.730691	8.386635	9.108038
1	-1.680382	8.842743	8.841677
6	-0.431082	7.752895	10.285056
1	-1.069022	7.591648	11.147687
6	1.424530	7.804908	8.687589
6	2.587079	7.774064	7.841650
6	3.900363	7.152579	8.168855
1	4.113001	6.317727	7.483743
1	3.913055	6.773276	9.197754
1	4.710372	7.887465	8.051608
6	2.569320	9.193618	4.690495
6	2.040858	11.473566	7.726093
1	2.986274	10.947437	7.827455
6	1.781472	12.765642	8.100289
1	2.453575	13.485900	8.554829
6	-0.141223	11.615752	7.110896
6	-1.340164	11.050766	6.552857
6	-2.649217	11.742258	6.390865
1	-2.908159	11.832235	5.324841
1	-2.623295	12.746366	6.831041
1	-3.449433	11.163247	6.874954
6	-1.434378	7.798780	5.386271

29

$[Co(\mathbf{L}^{\mathbf{1}(S\rightarrow O)})(N_3)_3]^-$

27	0.700267	9.320353	6.693903
16	-2.927694	10.618882	4.757248
8	1.537339	8.469283	8.234853

7	0.565592	7.582004	5.754486
7	-0.521915	10.067692	5.427567
7	-0.847463	8.988802	7.682195
7	-0.718730	8.405813	8.880680
7	0.959176	7.630771	10.273789
1	0.235434	7.254064	10.875296
1	1.910196	7.302361	10.395915
7	0.831159	11.098902	7.578895
7	2.342501	9.733438	5.679141
7	0.138542	5.580006	6.954281
6	-0.428689	10.659257	4.200336
1	0.550259	10.790569	3.746217
6	-1.639116	11.029658	3.672960
1	-1.847151	11.513636	2.724395
6	-1.786278	9.965752	5.875853
6	-2.004201	9.356823	7.159227
6	-3.320696	9.166741	7.832941
1	-3.484870	8.104359	8.067675
1	-4.142835	9.516245	7.196212
1	-3.354068	9.720771	8.783558
6	0.609171	8.176533	9.086982
7	1.899337	11.364845	8.072217
7	2.907543	11.679650	8.567633
7	3.161124	8.864502	5.514666
7	3.990901	8.066183	5.320417
7	0.346275	6.583336	6.394853

67

$[Co(\mathbf{L}^{2(O\rightarrow S)})_2]^{3+}$

27	-0.000005	0.000014	-0.256629
16	1.487259	0.559449	-1.831016
7	-1.148523	-0.836436	1.078064
7	0.838885	-1.694688	-0.239043
7	1.970463	-1.951911	-0.963978
7	4.708599	-0.555787	-1.434626
16	-1.487290	-0.559518	-1.830954
7	-0.838908	1.694710	-0.239124
7	-1.970501	1.951887	-0.964049
7	1.148525	0.836547	1.077996
6	-2.193538	-0.289376	1.710678
1	-2.396544	0.761173	1.511453
6	-2.992212	-1.029888	2.583865
1	-3.836427	-0.546007	3.072248
6	-2.688351	-2.371745	2.806769
1	-3.297336	-2.974452	3.480060
6	-1.590239	-2.938300	2.157597
1	-1.324081	-3.982678	2.312361
6	-0.830906	-2.150329	1.290536
6	0.331932	-2.620705	0.548486
6	0.880987	-3.994844	0.685203
1	0.137270	-4.732878	0.346416

1	1.103414	-4.213607	1.740184
1	1.790939	-4.103334	0.088643
6	2.332727	-0.929406	-1.701325
6	3.676287	-1.049491	-2.387434
1	3.899816	-2.094212	-2.625977
1	3.728769	-0.442694	-3.296613
6	5.253884	-1.424043	-0.546569
1	4.968142	-2.467809	-0.653911
6	6.109488	-0.964546	0.439493
1	6.537386	-1.677873	1.141094
6	6.399747	0.399988	0.513486
1	7.065136	0.778854	1.288711
6	5.830829	1.273883	-0.415305
1	6.036556	2.342191	-0.394849
6	4.979940	0.772283	-1.385347
1	4.492864	1.394317	-2.132802
6	-2.332766	0.929337	-1.701331
6	-3.676354	1.049364	-2.387389
7	-4.708608	0.555656	-1.434516
1	-3.899924	2.094073	-2.625945
1	-3.728857	0.442546	-3.296552
6	-5.253863	1.423917	-0.546447
6	-6.109412	0.964424	0.439666
6	-6.399630	-0.400115	0.513708
6	-5.830732	-1.274018	-0.415089
6	-4.979908	-0.772420	-1.385189
1	-4.968162	2.467690	-0.653838
1	-6.537298	1.677759	1.141267
1	-6.036430	-2.342331	-0.394597
1	-4.492857	-1.394458	-2.132656
1	-7.064965	-0.778978	1.288979
6	0.830886	2.150442	1.290420
6	-0.331972	2.620765	0.548369
6	-0.881062	3.994893	0.685045
1	-0.137360	4.732938	0.346251
1	-1.103509	4.213675	1.740018
1	-1.791010	4.103345	0.088472
6	1.590226	2.938465	2.157427
6	2.688369	2.371961	2.806592
6	2.992256	1.030103	2.583732
6	2.193570	0.289535	1.710602
1	1.324051	3.982845	2.312154
1	3.297359	2.974710	3.479841
1	3.836499	0.546263	3.072108
1	2.396592	-0.761017	1.511415

43

$[Co(\mathbf{L}^{2(O\rightarrow S)})(N_3)_3]$

27	4.499091	3.131708	4.219438
16	3.262239	2.474583	2.485564
7	5.310024	3.568575	5.934709

7	3.112434	2.478959	5.313110
7	1.957632	1.956995	4.796818
7	0.352628	2.054501	1.610630
7	3.687783	4.940957	4.159489
7	2.490218	5.070243	4.148871
7	1.337359	5.258233	4.134373
7	6.014773	3.786165	3.153628
7	5.846889	4.606578	2.284617
7	5.755360	5.397787	1.433714
7	5.379558	1.345223	4.345619
7	5.938462	0.915881	3.366597
7	6.491555	0.446649	2.453733
6	6.492940	4.151169	6.142112
1	7.050455	4.411988	5.241335
6	6.971198	4.399089	7.432229
1	7.941592	4.876445	7.563355
6	6.190267	4.025169	8.526204
1	6.538206	4.204912	9.543639
6	4.953624	3.414912	8.305735
1	4.322103	3.109986	9.139140
6	4.530481	3.195355	6.991411
6	3.264378	2.576420	6.616425
6	2.262550	2.119015	7.618578
1	1.961035	2.955977	8.266790
1	2.697087	1.342824	8.267383
1	1.379137	1.715013	7.115766
6	1.972835	1.924788	3.483142
6	0.733170	1.333781	2.848943
1	0.902844	0.283629	2.580315
1	-0.104703	1.385463	3.555081
6	0.286149	1.390915	0.431976
1	0.514415	0.327974	0.461030
6	-0.054933	2.063189	-0.730383
1	-0.101828	1.509496	-1.666034
6	-0.325916	3.431676	-0.673829
1	-0.594737	3.977017	-1.578244
6	-0.243466	4.095874	0.552691
1	-0.439210	5.163081	0.637853
6	0.103905	3.386830	1.688852
1	0.219438	3.852896	2.669397

19

L$^{1(S\rightarrow O)-}$

16	1.450489	7.234769	10.170263
8	1.953302	9.711683	4.044640
7	0.056951	8.417401	8.329548
7	2.221096	8.535630	6.463285
7	3.285337	8.548179	5.645458
7	4.106099	9.073059	3.573703
1	4.999849	8.884048	4.021079
1	4.130784	9.767560	2.832452

6	-0.763026	8.220790	9.408786
1	-1.800095	8.555913	9.358217
6	-0.205725	7.600933	10.500835
1	-0.665292	7.347274	11.451594
6	1.283070	7.953612	8.551909
6	2.414433	7.983688	7.647168
6	3.740314	7.403762	8.066356
1	4.054475	6.613176	7.366912
1	3.713007	6.979080	9.078851
1	4.527250	8.173836	8.034880
6	3.007161	9.161657	4.434575

33

L$^{2(O\rightarrow S)}$

16	3.513764	3.413695	2.156709
7	5.894525	2.116288	6.600360
7	3.739461	2.079828	4.894807
7	2.607134	1.813342	4.191401
7	0.421183	2.806263	1.773887
6	7.007725	2.298477	7.321115
1	7.813753	1.577930	7.147912
6	7.176995	3.326859	8.255778
1	8.109876	3.420231	8.812694
6	6.118507	4.214661	8.448591
1	6.199597	5.035401	9.163192
6	4.948902	4.037981	7.709946
1	4.112813	4.724719	7.838435
6	4.866848	2.978755	6.786398
6	3.637633	2.792521	5.974708
6	2.358176	3.458805	6.407380
1	2.329194	4.511895	6.083692
1	2.242984	3.443829	7.499682
1	1.507138	2.947583	5.938910
6	2.509535	2.277883	2.973008
6	1.301606	1.710437	2.227185
1	1.619817	1.154907	1.335959
1	0.722240	1.054369	2.885964
6	0.716315	3.431277	0.606987
1	1.501618	2.981146	0.007790
6	0.001390	4.559115	0.219941
1	0.239939	5.034610	-0.729690
6	-0.999882	5.053283	1.052077
1	-1.570950	5.935499	0.763159
6	-1.271292	4.402306	2.263129
1	-2.045025	4.757950	2.940792
6	-0.538834	3.281201	2.605622
1	-0.680726	2.732405	3.534501