

Electronic supporting information

Magnetically bistable cobalt-dioxolene complexes with tetradentate N-donor base

Maxim G. Chegerev, Denis V. Korchagin, Gennady V. Shilov, Nikolay N. Efimov,
Andrey G. Starikov, Alexandr V. Piskunov, Anatoly V. Chernyshev, Aleksei N.
Bulgakov, Vladimir I. Minkin, Andrei V. Palii, Sergey M. Aldoshin

Table S1. Crystallographic data for **1a**, **1b**, **2** and **3**.

Parameter	1a	1b	2		3
Temperature/K	100	100	85	292	240
CCDC Number	2204050	2204051	2204052	2204053	2204054
Empirical formula	C ₃₄ H ₄₂ Co N ₄ O ₂	C _{34.51} H _{41.03} Co N ₄ O _{2.17}	C _{34.53} H ₄₂ Co F ₆ N ₄ O _{2.53} P		C ₆₁ H ₇₀ B Co N ₄ O ₅
Formula weight	597.64	605.57	757.46		1008.95
Crystal system	Monoclinic	Triclinic	Triclinic		Orthorhombic
Space group	P2 ₁ /n	P-1	P-1		Pbca
a/Å	13.4993(4)	10.9948(3)	8.7477(2)	8.8404(2)	15.2084(7)
b/Å	15.0232(4)	11.5726(4)	10.1501(3)	10.3033(3)	19.1822(7)
c/Å	15.4663(5)	14.2748(4)	19.8757(6)	20.5273(8)	37.2725(14)
α/°	90	93.787(3)	90.741(3)	90.874(3)	90
β/°	90.154(2)	90.104(3)	95.833(2)	97.072(3)	90
γ/°	90	111.805(3)	101.638(3)	100.999(2)	90
Volume/Å ³	3136.6(2)	1681.99(9)	1718.53(9)	1819.97(10)	10873.5(8)
Z	4	2	2		8
ρ _{calc} /g/cm ³	1.266	1.196	1.464	1.382	1.233
μ/mm ⁻¹	0.583	0.545	0.618	0.584	0.368
F(000)	1268	641	787		4288
Crystal size/mm ³	0.50 x 0.22 x 0.20	0.50 x 0.40 x 0.30	0.30 x 0.18 x 0.10		0.35 x 0.20 x 0.10
2θ range for data collection/°	2.96 - 29.33	3.23 - 29.07	2.81 - 29.33	2.783 - 29.330	2.882 - 26.320
Index ranges	-18<=h<=18, -20<=k<=20, -20<=l<=21	-15<=h<=14, -15<=k<=13, -16<=l<=19	11<=h<=12, -13<=k<=13, -21<=l<=27	-12<=h<=12, -14<=k<=14, -27<=l<=28	-18<=h<=12, -16<=k<=23, -36<=l<=46
Reflections collected	42644	14878	17694	19389	47859
Independent reflections, [R(int)]	8607 [0.0561]	8991 [0.0280]	9409 [0.0281]	9978 [0.0236]	11043 [0.0747]
Data/restraints/parameters	8607 / 0 / 370	8991 / 0 / 407	9409 / 0 / 439	9978 / 0 / 434	11043 / 84 / 604
Goodness-of-fit on F ²	1.123	1.040	1.065	1.305	1.082
Final R indexes [I>=2σ (I)], (R ₁ , wR ₂)	0.0616, 0.1376	0.0548, 0.1395	0.0685, 0.1696	0.0771, 0.2214	0.1062, 0.2889
Final R indexes [all data], (R ₁ , wR ₂)	0.0825, 0.1472	0.0734, 0.1539	0.0891, 0.1842	0.1099, 0.2391	0.1861, 0.3434
Largest diff. peak/hole / e Å ⁻³	0.975 / -0.482	0.716 / -0.553	1.159 / -1.024	0.790 / -2.546	1.161 / -0.520

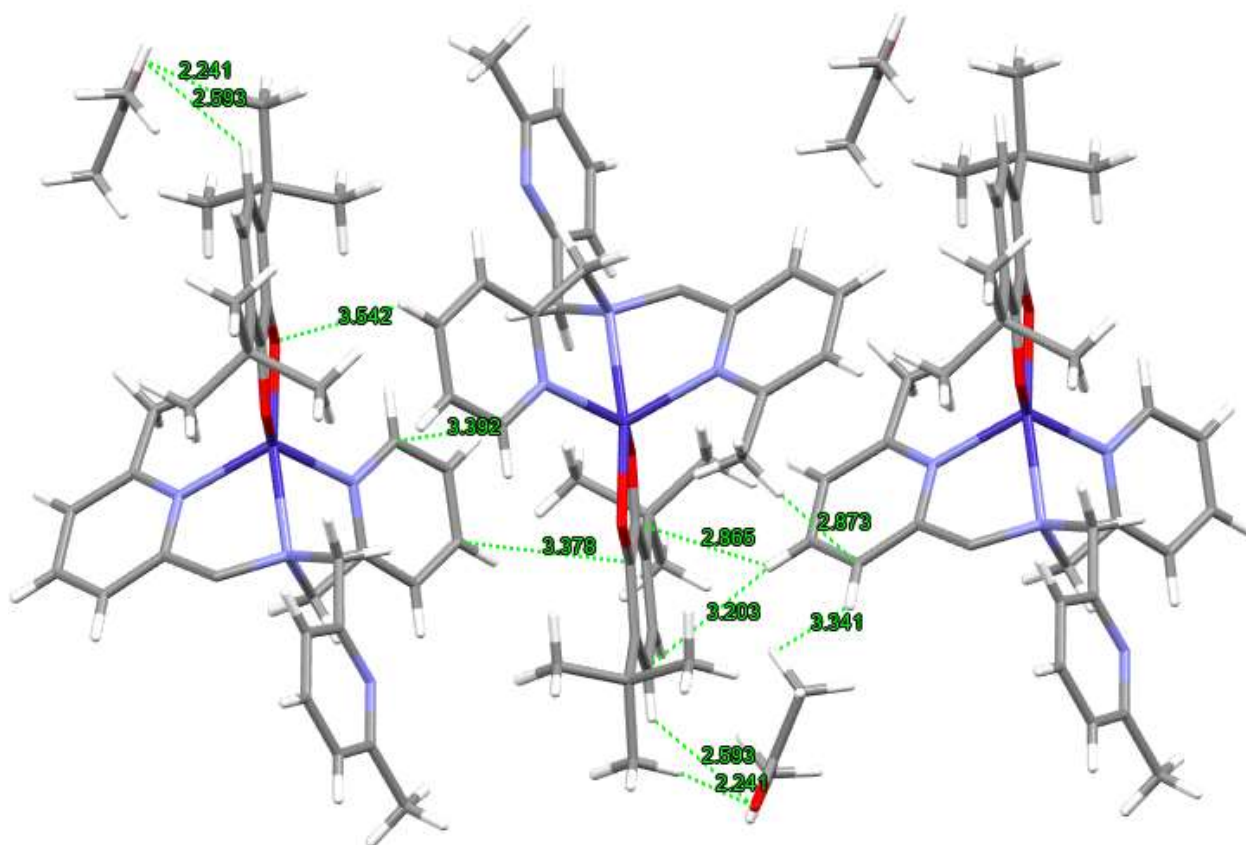


Fig. S1 Fragment of crystal packing and intermolecular interactions of complex **1b**.

Table S2. *SHAPE* analysis for Co ion in **1a**, **1b**, **2**, and **3**

	<i>SHAPE</i> index			
	OC-6	TPR-6	SPY-5	TBPY-5
1a	2.023	13.391	-	-
1b	-	-	2.948	2.641
2 (85 K)	0.953	13.659	-	-
2 (292 K)	1.695	13.098	-	-
3 (240 K)	3.483	8.987	-	-

OC-6 Octahedron (O_h), **TPR-6** Trigonal prism (D_{3h}), **SPY-5** Square pyramid (C_{4v}), **TBPY-5** Trigonal bipyramid (D_{3h})

Table S3. The SA-CASSCF/NEVPT2 calculated spin-free state (δ_E) and spin-orbit state (Δ_E) energies (cm^{-1}) for complexes under study.

Complex	Energy Levels, cm^{-1}		
	Spin	Spin-free States (δ_E)	Spin-orbit States (Δ_E)
1a	3/2	0.0	0.0
			135.6
	3/2	750.7	730.4
			1016.2
1b	3/2	1032.4	1385.6
			1544.5
	3/2	0.0	0.0
			43.6
3	3/2	2558.8	2600.9
			2714.9
	3/2	4888.7	4846.7
			4990.8
3	3/2	0.0	0.0
			55.1
	3/2	2336.0	2344.6
			2497.2
3	3/2	3088.8	3169.7
			3286.7

DFT calculations

Previously it was shown that UTPSSh/6-311++G(d,p) approximation provides a good reproduction of the energies and magnetic properties of magnetically bistable transition metal compounds.¹⁻³ However, geometry optimization of the isomer **1a** using the UTPSSh/6-311++G(d,p) approach led to a structure, in which one of the coordination Co-N bonds is significantly elongated up to 3.26 Å. This finding is inconsistent with the structural data obtained from XRD. We supposed that revealed discrepancy between the theoretical and experimental data is caused, most likely, by the fact that chosen UTPSSh functional does not take into account for non-covalent interactions. Therefore, we carried out the corresponding calculations using B3LYP functional with inclusion of the Grimme dispersion corrections D3BJ⁴, which allowed us to reproduce well the XRD data. Thus, on the basis of the data obtained one can conclude that dispersion interactions play an important role in stabilization of the isomer **1a** comprising the hexacoordinated cobalt ion. In this connection, the study of the mechanism of interconversion between **1a** and **1b** isomers was carried out using the B3LYP/6-311++G(d,p)+D3BJ approximation (Fig. S2).

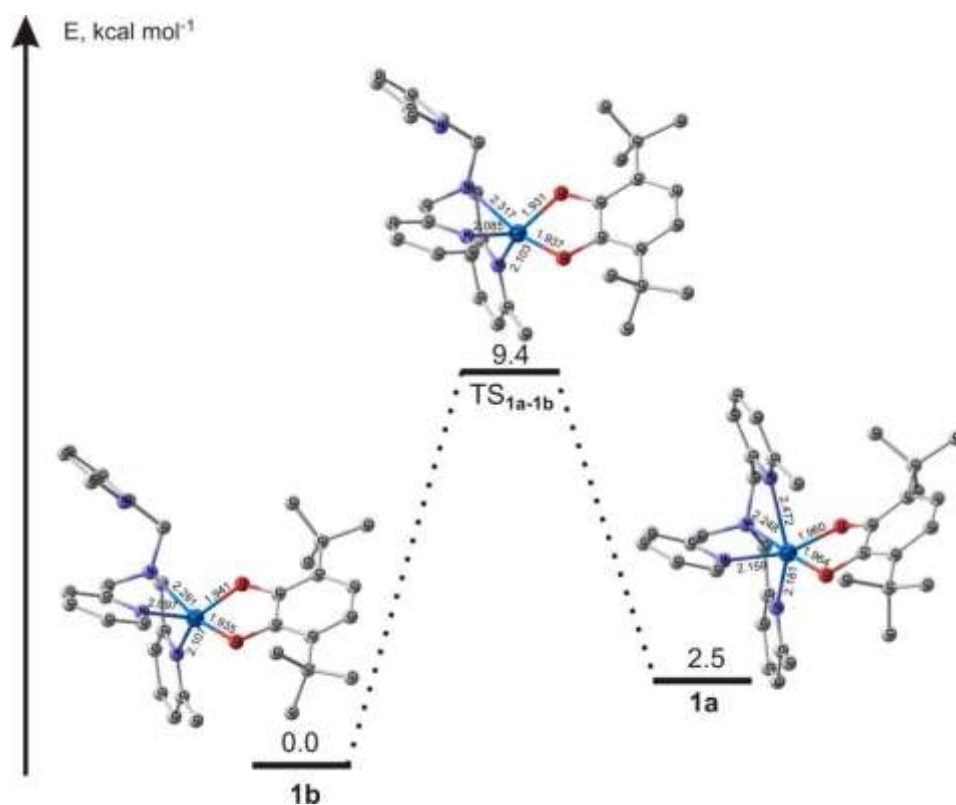


Fig. S2 Spatial structures and probable mechanism of interconversion between **1a** and **1b** isomers according to the DFT calculations (B3LYP/6-311++G(d,p) + D3BJ). Bond lengths are given in Å.

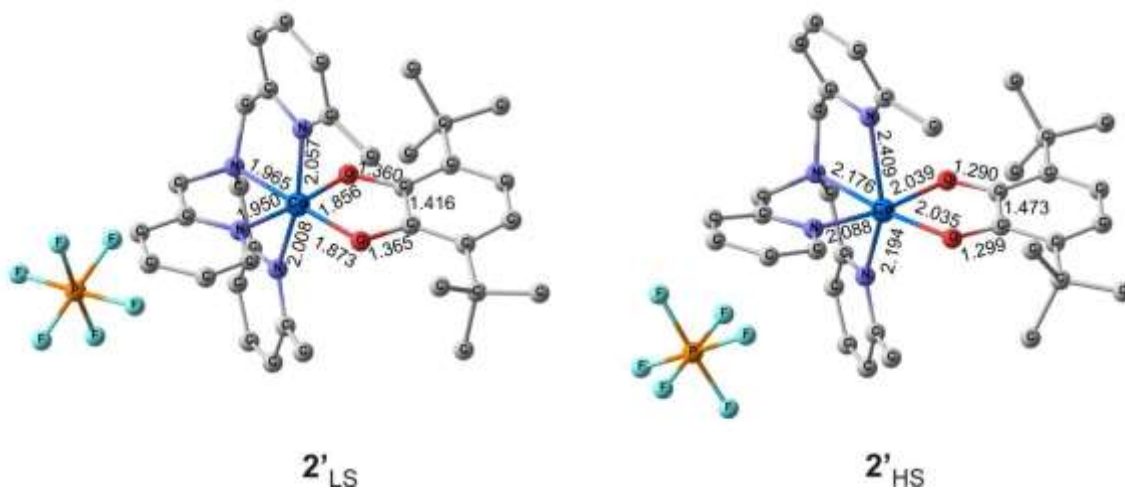


Fig. S3 Optimized geometries of isomers of the model compound **2'** according to the DFT (UTPSSh/6-311++G(d,p)) calculations. Bond lengths are given in Å.

Variable temperature UV-Vis spectra

At 300 K (green-brown solution) the spectrum demonstrates two-band absorption observed at 410 and 595 nm, which is characteristic for the hs-Co^{II} -SQ charge distribution. According to literature data, the band at 595 nm (with shoulders in the range of 500-630 nm) arises from the metal-to-ligand charge transfers (MLCT). At the same time, the band at 410 nm and broad absorptions in the range of 650-850 nm are ligand-based transitions in the semiquinone moiety ($\pi \rightarrow \pi^*$). Upon cooling, the corresponding broad MLCT bands gradually decrease in intensity and the color of the solution becomes light-brown at 188 K, which is a characteristic feature of the $\text{ls-Co}^{\text{III}}$ -Cat charge distribution. Comparison of the low temperature spectrum with those observed for the compounds of similar structure allows us to assign bands at 395 and 845 nm to ligand-to-metal charge transfers (LMCT), while a broad band at 523 nm can be attributed to the d-d transitions ($^1\text{A}_1 \rightarrow ^1\text{T}_1$), which are often seen for the Co^{III} complexes in octahedral geometry. Color change was reproduced on multiple heating and cooling cycles, which is consistent with a reversible thermally induced VT transition. There are some points, which could be tentatively assigned as isosbestic points (~ 380 nm, ~ 420 nm, and ~ 850 nm), but we observed their slight displacement upon cooling/heating. We suppose that this displacement can be most likely explained by additional equilibrium in the system caused by the possible coordination-decoordination of the pyridine fragment in **2**

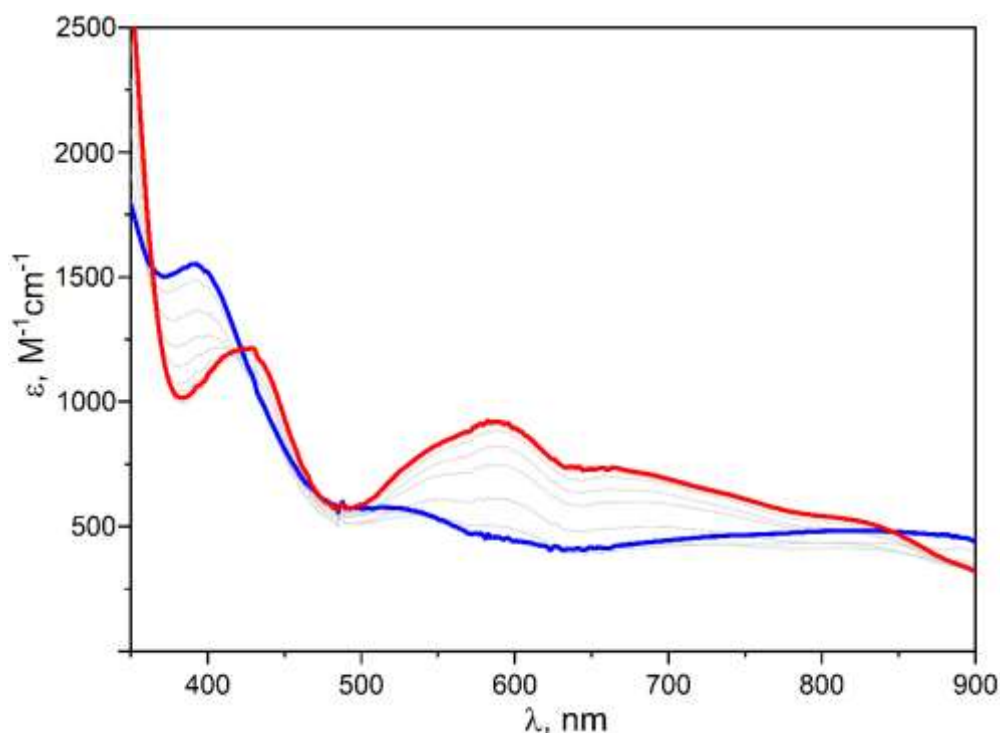


Fig. S4. Temperature dependence of the UV-Vis absorption spectra of **2** in acetone solution from 300 K (red) to 188 K (blue).

References:

1. A. V. Piskunov, K. I. Pashanova, I. V. Ershova, A. S. Bogomyakov, I. V. Smolyaninov, A. G. Starikov, S. P. Kubrin, G. K. Fukin, *J. Mol. Struct.*, 2018, **1165**, 51.
2. T. Tezgerevska, E. Rousset, R. W. Gable, G. N. L. Jameson, E. Carolina Sañudo, A. Starikova, C. Boskovic, *Dalton Trans.*, 2019, **48**, 11674.
3. G. K. Gransbury, B. N. Livesay, J. T. Janetzki, M. A. Hay, R. W. Gable, M. P. Shores, A. Starikova, C. Boskovic, *J. Am. Chem. Soc.*, 2020, **142**, 10692.
4. S. Grimme, S. Ehrlich, L. Goerigk, *J. Comp. Chem.*, 2011, **32**, 1456;

Cartesian coordinates:

TS_{1a-1b}

27	0.121461000	0.072107000	-0.743977000
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1a

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1b

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6	1.455109000	-3.897710000	-0.054231000
6	0.528306000	1.596355000	3.175213000
6	2.194553000	-5.241808000	-0.158464000
1	2.608833000	-5.399223000	-1.157707000
1	1.496030000	-6.058888000	0.046746000
1	3.011186000	-5.310506000	0.564772000
6	-1.813897000	0.317906000	3.869586000
1	-2.741356000	-0.189931000	4.103241000
6	-6.025066000	-2.213969000	-0.974683000
1	-7.027586000	-2.624158000	-0.967044000
6	4.110795000	-0.449794000	-0.780602000
6	0.151109000	1.531371000	4.517660000
1	0.783084000	1.983507000	5.271285000
6	-2.178701000	-0.427191000	-1.026132000
6	4.499213000	1.577556000	-2.219718000
1	3.477282000	1.901171000	-2.025984000
1	4.504152000	0.974509000	-3.132175000
1	5.128025000	2.459329000	-2.387976000
6	-6.989902000	0.107448000	-1.308812000
1	-6.901283000	0.645744000	-2.255888000
1	-6.987868000	0.854294000	-0.510122000
1	-7.946285000	-0.417131000	-1.292269000
6	5.088161000	1.645459000	0.231045000
1	4.095307000	2.021068000	0.473105000
1	5.759617000	2.495944000	0.066338000
1	5.464600000	1.074448000	1.084940000
6	5.032669000	0.752904000	-1.027925000
6	-1.029547000	0.888944000	4.867214000
1	-1.336965000	0.834093000	5.905023000
6	-3.646363000	-2.470507000	-0.846438000
1	-2.755181000	-3.075876000	-0.735491000

6	1.775155000	2.296134000	2.724915000
1	2.440600000	2.495337000	3.565167000
1	1.520840000	3.253391000	2.257199000
1	2.298765000	1.705433000	1.968779000
6	3.732361000	-2.859468000	-0.641149000
1	4.158377000	-3.850978000	-0.716318000
6	4.568953000	-1.769544000	-0.868335000
1	5.603535000	-1.967300000	-1.114146000
6	-4.915312000	-3.038280000	-0.827431000
1	-5.037711000	-4.107914000	-0.700455000
6	6.471872000	0.326778000	-1.361295000
1	6.514034000	-0.286823000	-2.264892000
1	6.926788000	-0.237646000	-0.542979000
1	7.083447000	1.217709000	-1.533326000
1	-2.080421000	0.205196000	-1.910639000
1	-1.383247000	-1.170367000	-1.055265000

2_{LS} (Is-Co^{III}-Cat)

27	-0.537801000	-0.368591000	0.308195000
8	-1.265805000	1.314284000	0.010038000
8	-2.298835000	-1.031546000	0.076543000
6	-3.158781000	-0.030465000	-0.282007000
6	-2.584146000	1.258086000	-0.313547000
6	-3.325194000	2.407575000	-0.654051000
6	-4.672943000	2.188274000	-0.963034000
1	-5.304194000	3.026955000	-1.231441000
6	-5.242782000	0.918042000	-0.944763000
1	-6.290522000	0.832028000	-1.203861000
6	-4.517354000	-0.236010000	-0.611744000
6	-5.187173000	-1.621434000	-0.633721000
6	-5.067666000	-2.312898000	0.741202000
1	-5.584309000	-3.279790000	0.722574000
1	-5.522396000	-1.696739000	1.523081000
1	-4.023161000	-2.485938000	1.001011000
6	-6.688095000	-1.533036000	-0.971369000
1	-7.114568000	-2.541590000	-0.962451000
1	-6.859934000	-1.107487000	-1.964701000
1	-7.234330000	-0.932028000	-0.238007000
6	-4.530118000	-2.513030000	-1.710617000
1	-5.022514000	-3.491993000	-1.746217000
1	-3.473370000	-2.676308000	-1.490801000
1	-4.617256000	-2.050387000	-2.698954000

6	-2.698083000	3.808429000	-0.671765000
6	-1.514449000	3.848550000	-1.664898000
1	-1.861199000	3.633749000	-2.680725000
1	-0.758892000	3.107357000	-1.398007000
1	-1.051810000	4.842352000	-1.664282000
6	-2.207624000	4.178914000	0.746507000
1	-1.498613000	3.438071000	1.120421000
1	-3.051760000	4.222198000	1.442163000
1	-1.721039000	5.161366000	0.736196000
6	-3.706170000	4.886781000	-1.108863000
1	-4.083932000	4.702670000	-2.119462000
1	-3.209985000	5.862957000	-1.109551000
1	-4.559265000	4.946238000	-0.425805000
7	-0.600689000	0.085713000	2.283554000
6	0.176579000	1.173317000	2.533452000
6	0.200304000	1.805700000	3.767851000
1	0.848457000	2.660859000	3.920035000
6	-0.616350000	1.318717000	4.785208000
1	-0.637377000	1.802105000	5.755921000
6	-1.380073000	0.187860000	4.540636000
1	-2.006657000	-0.240474000	5.314163000
6	-1.343755000	-0.435114000	3.286950000
6	-2.083070000	-1.714878000	3.052803000
1	-2.435226000	-1.757564000	2.022587000
1	-2.922234000	-1.804196000	3.744796000
1	-1.407948000	-2.560392000	3.230439000
6	1.021852000	1.651446000	1.384738000
1	1.994364000	2.027247000	1.719658000
1	0.490335000	2.435598000	0.846135000
6	1.638598000	0.960832000	-0.906689000
1	2.724946000	0.924673000	-0.997994000
1	1.315179000	1.998567000	-1.022252000
6	0.960631000	0.141295000	-1.962089000
6	1.414298000	0.081225000	-3.277130000
1	2.343239000	0.572642000	-3.541465000
6	-0.520113000	-1.237439000	-3.817047000
1	-1.141180000	-1.779187000	-4.520039000
6	-0.902472000	-1.163341000	-2.484308000
1	-1.802594000	-1.621824000	-2.098345000
7	-0.166875000	-0.495910000	-1.579333000
6	0.662205000	-0.616795000	-4.216904000
1	0.995522000	-0.675806000	-5.247273000

7	0.524846000	-2.138156000	0.513747000
6	1.847342000	-1.858219000	0.658308000
6	2.858505000	-2.799853000	0.514231000
1	3.890574000	-2.478794000	0.601715000
6	2.497990000	-4.114160000	0.240283000
1	3.254077000	-4.880502000	0.107835000
6	1.149190000	-4.421090000	0.135269000
1	0.824666000	-5.435951000	-0.065814000
6	0.171322000	-3.428565000	0.270067000
6	-1.272594000	-3.821553000	0.176812000
1	-1.908300000	-2.967934000	-0.049410000
1	-1.597951000	-4.239226000	1.137183000
1	-1.400283000	-4.603827000	-0.575080000
6	2.176636000	-0.458307000	1.062832000
1	2.059400000	-0.387668000	2.149775000
1	3.202681000	-0.185425000	0.820641000
7	1.209770000	0.505032000	0.455672000
15	5.705507000	0.628038000	-0.353432000
9	4.548781000	-0.020269000	-1.370225000
9	6.845989000	-0.282373000	-1.055621000
9	5.367244000	-0.602648000	0.713332000
9	5.939576000	1.839771000	-1.407381000
9	4.475406000	1.504990000	0.370914000
9	6.768167000	1.256414000	0.692545000
2_{HS} (hs-Co^{II}-SQ)			
27	0.645063000	-0.293137000	-0.470148000
8	1.718609000	1.330730000	0.243150000
8	2.474461000	-1.115404000	-0.134332000
6	3.363492000	-0.323028000	0.386130000
6	2.921911000	1.061803000	0.613521000
6	3.805258000	2.030821000	1.203378000
6	5.069885000	1.576744000	1.514865000
1	5.790073000	2.253571000	1.959669000
6	5.497466000	0.241936000	1.282880000
1	6.514367000	-0.002220000	1.566848000
6	4.691560000	-0.735353000	0.727887000
6	5.181326000	-2.171396000	0.496849000
6	5.083034000	-2.532457000	-1.002707000
1	5.447431000	-3.553247000	-1.164062000
1	5.696880000	-1.853543000	-1.603528000
1	4.051495000	-2.472976000	-1.351571000
6	6.648514000	-2.349332000	0.927256000

1	6.952859000	-3.383801000	0.739273000
1	6.787671000	-2.150902000	1.994793000
1	7.320976000	-1.696438000	0.361462000
6	4.326564000	-3.158976000	1.324064000
1	4.685144000	-4.182821000	1.169651000
1	3.278023000	-3.112557000	1.026258000
1	4.399893000	-2.930289000	2.392252000
6	3.351618000	3.472283000	1.455227000
6	2.132363000	3.482254000	2.406499000
1	2.393953000	3.039937000	3.373057000
1	1.300349000	2.919029000	1.982236000
1	1.806076000	4.513467000	2.580850000
6	2.973345000	4.145397000	0.114751000
1	2.172054000	3.600433000	-0.386134000
1	3.838977000	4.182575000	-0.554685000
1	2.640035000	5.173099000	0.297278000
6	4.463198000	4.313530000	2.107294000
1	4.762265000	3.908525000	3.079537000
1	4.093157000	5.330511000	2.270396000
1	5.351113000	4.381498000	1.470197000
7	0.671287000	0.784819000	-2.388394000
6	-0.135482000	1.866525000	-2.372637000
6	-0.225040000	2.743430000	-3.450172000
1	-0.898431000	3.591712000	-3.401167000
6	0.558513000	2.502601000	-4.574791000
1	0.517109000	3.170567000	-5.428593000
6	1.383763000	1.384121000	-4.592050000
1	1.998562000	1.158685000	-5.455961000
6	1.413691000	0.529156000	-3.486820000
6	2.244713000	-0.721941000	-3.490625000
1	2.692743000	-0.893300000	-2.510403000
1	3.031011000	-0.665904000	-4.245722000
1	1.612224000	-1.585959000	-3.724148000
6	-0.921126000	2.099320000	-1.102182000
1	-0.304333000	2.691369000	-0.420423000
1	-1.840858000	2.658423000	-1.315355000
6	-1.621575000	1.012003000	0.978853000
1	-2.692989000	1.211877000	1.046331000
1	-1.079133000	1.887588000	1.350692000
6	-1.232715000	-0.158699000	1.847932000
6	-1.992899000	-0.526670000	2.957703000
1	-2.942503000	-0.038720000	3.140779000

6	-0.312994000	-2.164979000	3.474214000
1	0.088929000	-2.959250000	4.092516000
6	0.372205000	-1.757373000	2.335849000
1	1.308834000	-2.215309000	2.038098000
7	-0.077578000	-0.777657000	1.535160000
6	-1.522989000	-1.543859000	3.782487000
1	-2.098534000	-1.853950000	4.648078000
7	-0.731571000	-1.900739000	-1.083736000
6	-2.009656000	-1.452652000	-1.105401000
6	-3.110832000	-2.303527000	-1.108887000
1	-4.108492000	-1.880777000	-1.081435000
6	-2.884097000	-3.676288000	-1.121649000
1	-3.718152000	-4.370035000	-1.113352000
6	-1.574934000	-4.142327000	-1.137929000
1	-1.361280000	-5.205452000	-1.156393000
6	-0.511275000	-3.235472000	-1.114919000
6	0.908135000	-3.729821000	-1.163463000
1	1.593545000	-3.033851000	-0.680790000
1	1.227309000	-3.843565000	-2.206528000
1	0.989766000	-4.711107000	-0.690087000
6	-2.210824000	0.037194000	-1.212041000
1	-2.079021000	0.305048000	-2.266404000
1	-3.225485000	0.313574000	-0.923221000
7	-1.203404000	0.810819000	-0.435553000
15	-5.777006000	0.601940000	0.589853000
9	-4.502298000	-0.311908000	1.164232000
9	-6.809044000	-0.579242000	1.006133000
9	-5.544619000	-0.109083000	-0.889606000
9	-5.916069000	1.300348000	2.054590000
9	-4.661814000	1.761661000	0.153363000
9	-6.972338000	1.511221000	-0.013732000

2'_{LS} (ls-Co^{III}-Cat)

27	0.447747000	-0.384424000	0.189076000
8	1.522798000	0.895813000	0.994148000
8	1.773762000	-0.531449000	-1.125146000
7	1.197716000	-1.792845000	1.487894000
7	-0.612116000	1.034503000	-0.757982000
6	2.732193000	0.985578000	0.378100000
7	-0.751623000	-1.757620000	-0.503832000
6	0.565801000	-1.697128000	2.685386000
7	-0.907281000	-0.092604000	1.582525000

6	3.448208000	0.568732000	-4.001223000
1	2.386764000	0.631119000	-3.757346000
1	3.859830000	1.582306000	-3.984208000
1	3.547406000	0.171600000	-5.018949000
6	3.333836000	1.688550000	3.359498000
1	2.439083000	1.091222000	3.174945000
1	4.173864000	1.006077000	3.525102000
1	3.186061000	2.277685000	4.272531000
6	-2.072122000	3.272100000	-1.576575000
1	-2.641310000	4.135003000	-1.902201000
6	3.773861000	1.790603000	0.876865000
6	-0.285017000	-0.478611000	2.870013000
1	-1.041248000	-0.624402000	3.648553000
1	0.373375000	0.342364000	3.164283000
6	5.676874000	-0.393271000	-3.438269000
1	6.112290000	0.601372000	-3.566812000
1	6.290366000	-0.949776000	-2.722468000
1	5.736513000	-0.903110000	-4.405791000
6	-1.451719000	2.441660000	-2.495723000
1	-1.530502000	2.633578000	-3.559320000
6	4.043968000	0.284727000	-1.589859000
6	4.199667000	-0.333358000	-2.994097000
6	-0.755160000	1.302595000	-2.080755000
6	3.622597000	2.619472000	2.160360000
6	-2.005185000	2.932704000	-0.231793000
1	-2.548117000	3.487432000	0.522478000
6	4.953987000	1.795543000	0.121218000
1	5.802036000	2.382113000	0.453845000
6	-1.186749000	1.375909000	1.561945000
1	-0.344963000	1.868940000	2.050073000
1	-2.118453000	1.600056000	2.089234000
6	4.899240000	3.414554000	2.489179000
1	4.738476000	3.989276000	3.407565000
1	5.757394000	2.755031000	2.653077000
1	5.152633000	4.120851000	1.692588000
6	2.863483000	0.228983000	-0.812042000
6	-0.263734000	0.335881000	-3.114308000
1	-0.081792000	0.857191000	-4.055941000
1	0.640640000	-0.167711000	-2.779471000
1	-1.047828000	-0.408471000	-3.295905000
6	-1.271077000	1.816816000	0.134028000
6	5.077911000	1.078403000	-1.063608000

1	6.015972000	1.150790000	-1.599370000
6	0.744759000	-2.605574000	3.719961000
1	0.196636000	-2.477469000	4.646083000
6	-0.492847000	-2.579071000	-1.540000000
6	-1.927506000	-1.853033000	0.145922000
6	-2.640811000	-3.613054000	-1.315131000
1	-3.390053000	-4.324618000	-1.644007000
6	-1.409279000	-3.525783000	-1.968111000
1	-1.166801000	-4.166535000	-2.807346000
6	3.654027000	-1.771672000	-3.102440000
1	2.599779000	-1.817547000	-2.828575000
1	3.766147000	-2.126172000	-4.133386000
1	4.214310000	-2.451657000	-2.452838000
6	-2.905255000	-2.767512000	-0.245707000
1	-3.862313000	-2.769810000	0.261130000
6	2.087007000	-2.803365000	1.311124000
6	2.470268000	3.636262000	1.995039000
1	1.535191000	3.129889000	1.749471000
1	2.333600000	4.208660000	2.920311000
1	2.697175000	4.340001000	1.188096000
6	2.310507000	-3.739830000	2.330515000
1	3.025273000	-4.533609000	2.148904000
6	-2.146387000	-0.888480000	1.276750000
1	-2.947607000	-0.200642000	1.003086000
1	-2.474046000	-1.418285000	2.175670000
6	1.636240000	-3.656560000	3.537494000
1	1.802190000	-4.389485000	4.319515000
15	-5.376211000	0.685074000	-0.114553000
9	-3.985364000	0.326067000	-0.954815000
9	-6.266173000	0.007986000	-1.288557000
9	-5.430668000	2.141914000	-0.840822000
9	-4.408561000	1.333084000	1.086807000
9	-6.693297000	1.022879000	0.764748000
9	-5.232881000	-0.785807000	0.644255000
6	2.875497000	-2.920777000	0.046790000
1	2.237334000	-2.887017000	-0.832617000
1	3.568808000	-2.079340000	-0.044495000
1	3.443502000	-3.852726000	0.056209000
1	0.467039000	-2.432839000	-2.018521000

2'_{HS} (hs-Co^{II}-SQ)

27	0.422818000	0.384913000	-0.111883000
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8	1.973130000	-0.393902000	-1.183611000
8	1.759870000	0.000198000	1.372586000
7	1.062785000	2.619833000	-0.742973000
7	-0.692809000	-1.480710000	-0.407227000
6	3.000892000	-0.729696000	-0.479729000
7	-1.127777000	1.431552000	0.815759000
6	0.354862000	2.984516000	-1.830075000
7	-0.806036000	0.788582000	-1.861882000
6	2.649939000	-1.620930000	3.908934000
1	1.705489000	-1.269713000	3.493085000
1	2.777723000	-2.675516000	3.645207000
1	2.596677000	-1.546415000	5.000783000
6	4.188789000	-0.105292000	-3.292049000
1	4.280825000	-0.250270000	-4.374370000
1	3.218197000	0.344512000	-3.078707000
1	4.971952000	0.591219000	-2.975066000
6	-1.903056000	-3.845377000	-1.236439000
1	-2.380811000	-4.765482000	-1.553971000
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1	5.309266000	-2.322234000	3.888692000
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6	3.832364000	-0.776178000	3.383857000
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6	-1.672513000	-2.817985000	-2.145141000
1	-1.985265000	-2.899583000	-3.179705000
6	5.199341000	-1.594283000	-0.158327000
1	6.133519000	-2.008170000	-0.520128000
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6	-1.132671000	1.852218000	2.093705000
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6	-3.193040000	3.018804000	1.772436000
1	-4.009837000	3.626867000	2.145308000
6	-2.146632000	2.642101000	2.614151000
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9	-4.158023000	-1.389698000	-1.028052000
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6	2.504838000	3.148099000	1.154176000
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1	3.479951000	2.794492000	0.801339000
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