Supporting information for the manuscript:

Macrocycle- and metal-centered reduction of cobalt trithiadodecaazahexaphyrin (Hhp). Metal-to-ligand charge transfer in $\{(Co^{I}_2Co^{II}O)(Hhp^{\bullet 4-})\}^{2-}$.

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Table S1. IR-spectra (cm^{-1} in KBr) of starting compounds and compound **1**.

Components	Crypt	$Co_3O(Hhp)^+$ as salt with acetate anion	**1**
Crypt(K^+)	476w 735m 922m 948w 982m 1038w 1071m 1100s 1127s 1213w 1295m 1329m 1377w 1446m 1462m 1490w 2790w 2877w 2943w		- - - 933w 949w - 1030w* 1080m 1102m* 1126m* 1165m - 1302m* - 1357m 1440w 1456m* 1501m 2811w 2880w 2958w
Hhp			502w 579w 596w - 660w 667w - 754w* 783w 816w 831w 848w 1030w* 1103s* 1126m* 1195w 1210w - 1261m 1274m 1302w* 1364m - 1470m 1524s 1600w - 3061w
$C_6H_4Cl_2$			655w* 754w* 1030w 1126m* 1456m *

*****bands coincided, w - weak, m - middle, s – strong, vs - very strong intensity, split- band is split into two bands.

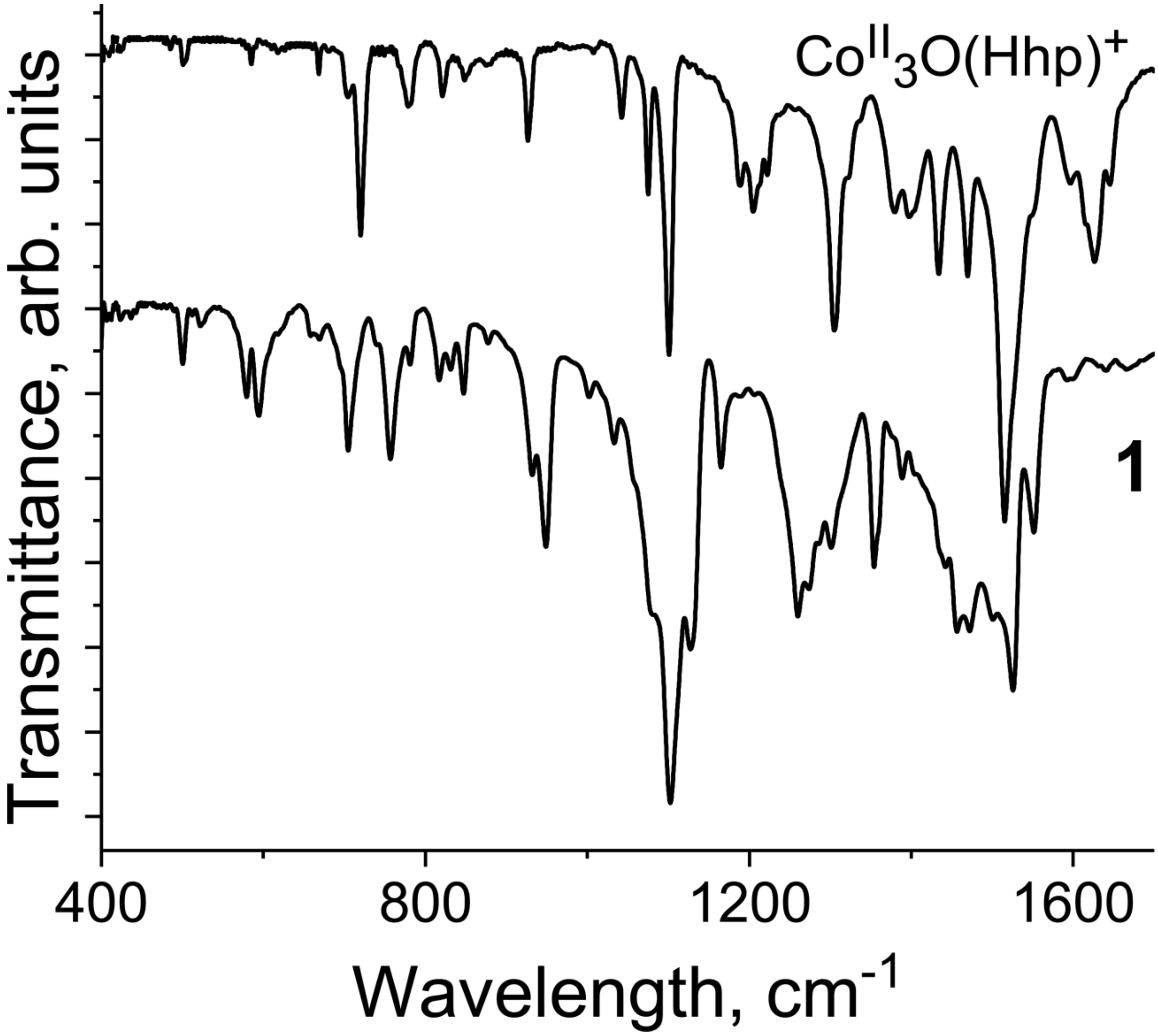

Fig. S1. IR-spectra of starting H_3Hhp and salt {Crypt(K^+)}$_2$ {($Co^{II}Co^{I}_2O$)$^{2+}$(Hhp$^{\bullet 4-}$)}$^{2-}$·$2C_6H_4Cl_2$ (**1**) in KBr pellets. Pellet for **1** was prepared in anaerobic conditions.

Crystal structure of 1.

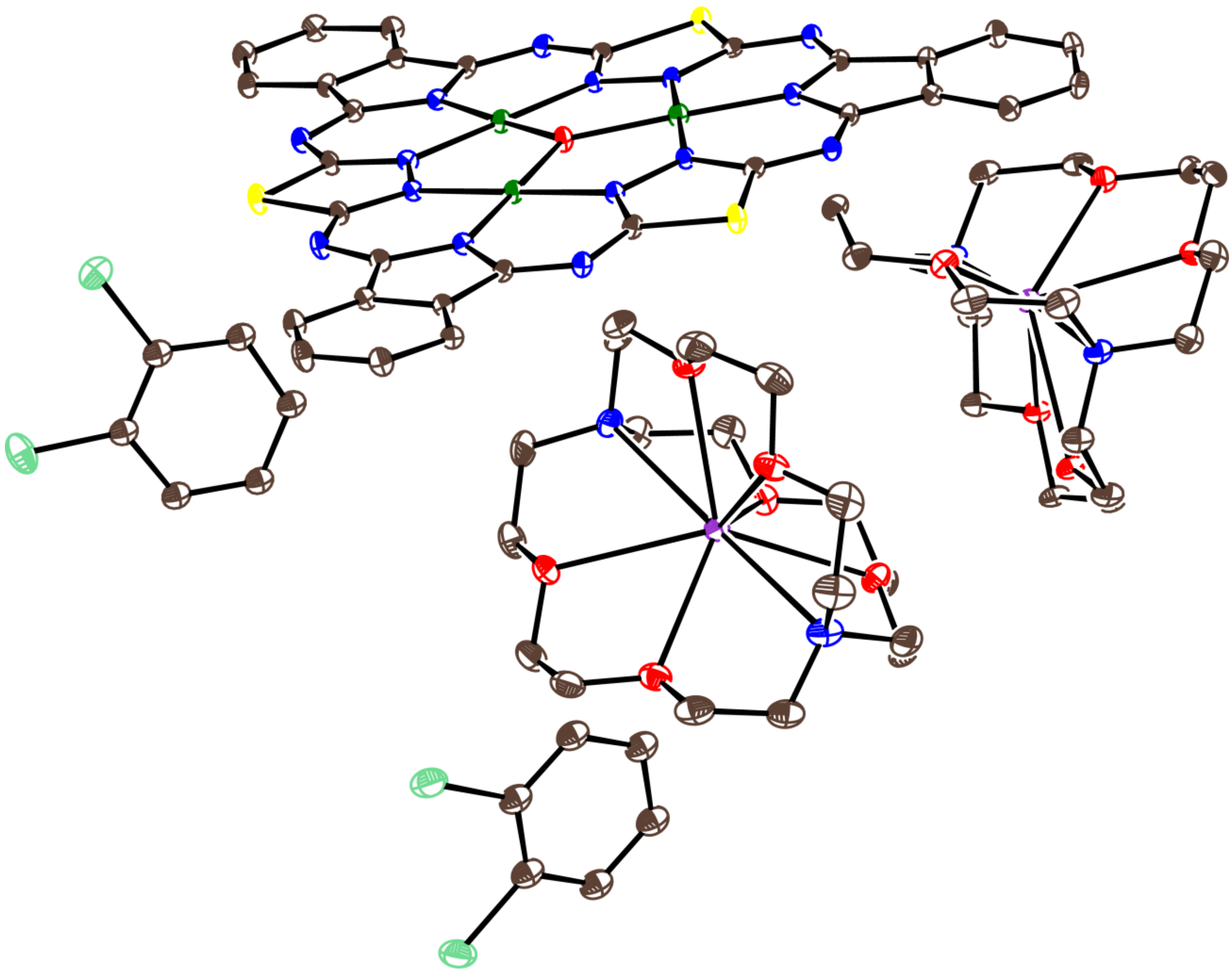

Fig. S2. Crystallographically independent units in the structures of $\{Crypt(K^+)\}_2$ $\{(Co_3O)Hhp\}^{2-}\cdot 2C_6H_4Cl_2$ (**1**). One $\{(Co_3O)Hhp\}^{2-}$ dianion, two $\{Crypt(K^+)\}$ cations, one whole and two halves of solvent $C_6H_4Cl_2$ molecules are independent. One disordered $C_6H_4Cl_2$ molecule with full occupancy is not shown for clarity. Color code: carbon, brown; oxygen, red; nitrogen, blue; chlorine, aquamarine; cobalt, green; potassium, violet. Ellipsoid probability is 25%.

Magnetic data for the $\{(Co^{II}_3O)(Hhp)\}^+$ compound as acetate salt.

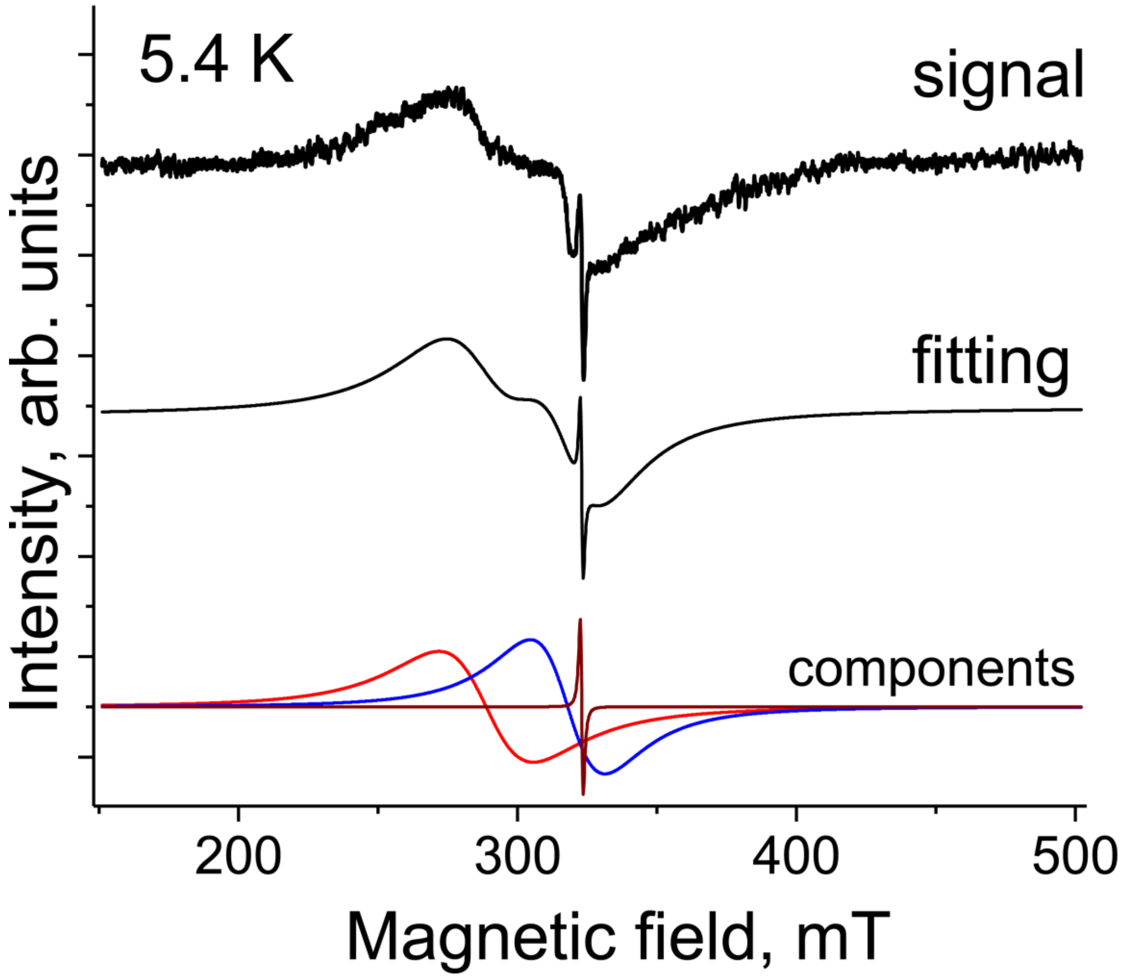

Fig. S3. EPR spectrum of polycrystalline compound containing the $\{(Co^{II}_3O)(Hhp)\}^+$ cations with acetate counter anions measured at 5.4 K. Fitting of the signal by three Lorentzian lines is shown below.

Magnetic data for complex 1

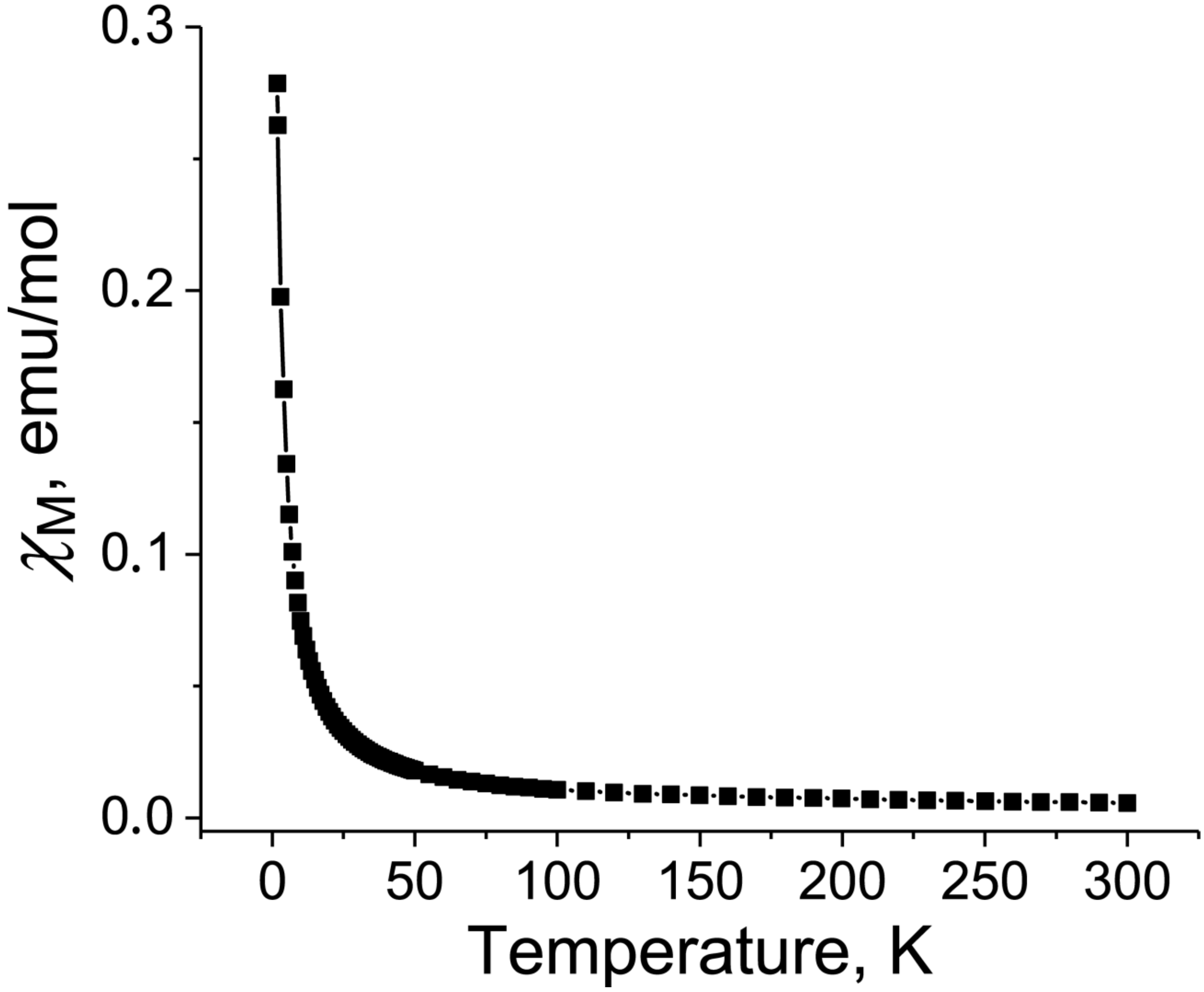

Fig. S4. Temperature dependence of molar magnetic susceptibility of polycrystalline $\{Crypt(K^+)\}_2\{(Co^{II}Co^{I}_2O)^{2+}(Hhp^{\bullet 4-})\}^{2-}\cdot 2C_6H_4Cl_2$ (**1**) measured in the 1.9-300 K range in the anaerobic conditions after the subtraction of temperature-independent contribution.

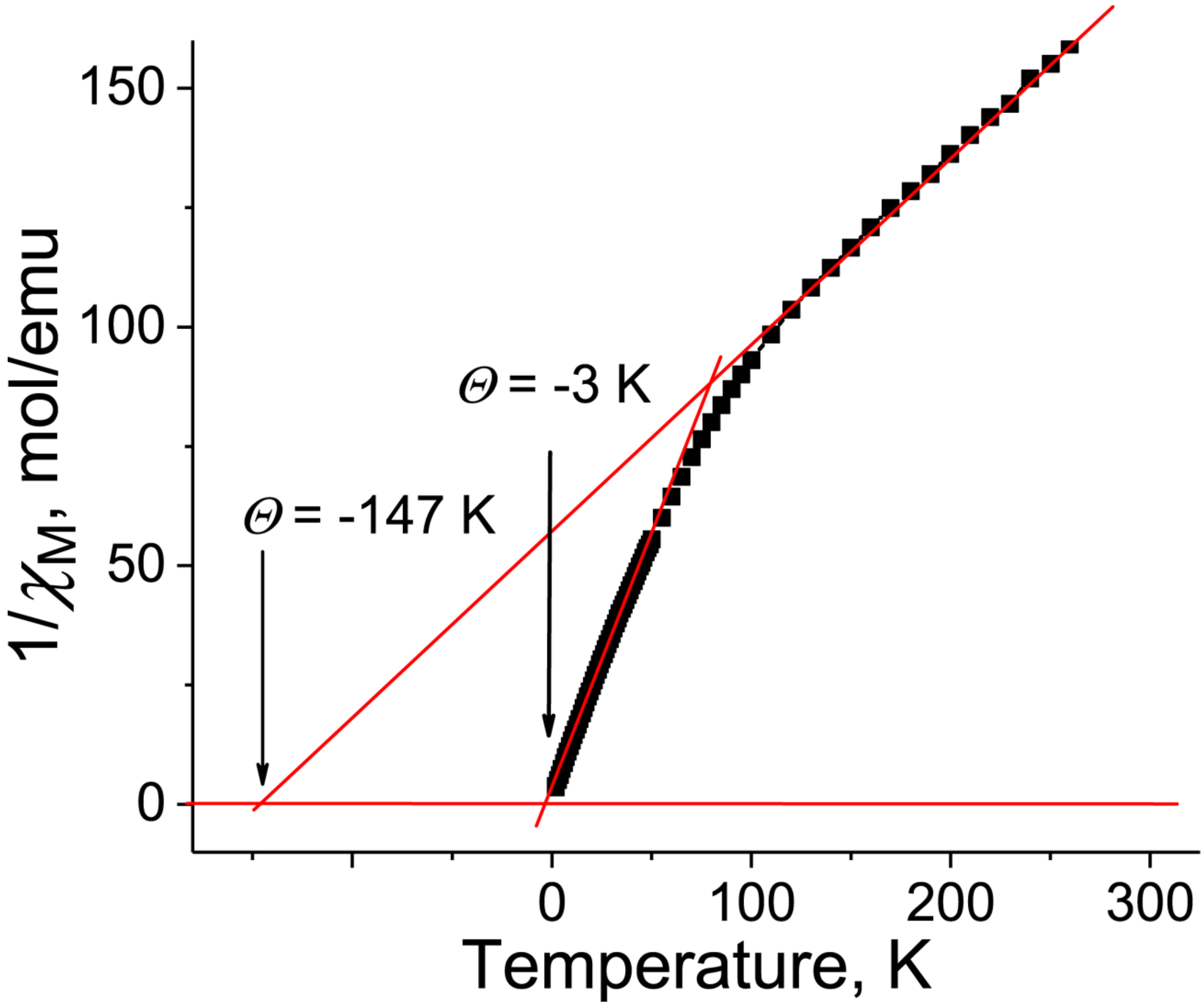

Fig. S5. Temperature dependence of the reciprocal molar magnetic susceptibility of polycrystalline **1** measured in the 1.9-300 K range. Red line shows the determination of Weiss temperatures in the 2-70 and 120-300 K ranges.

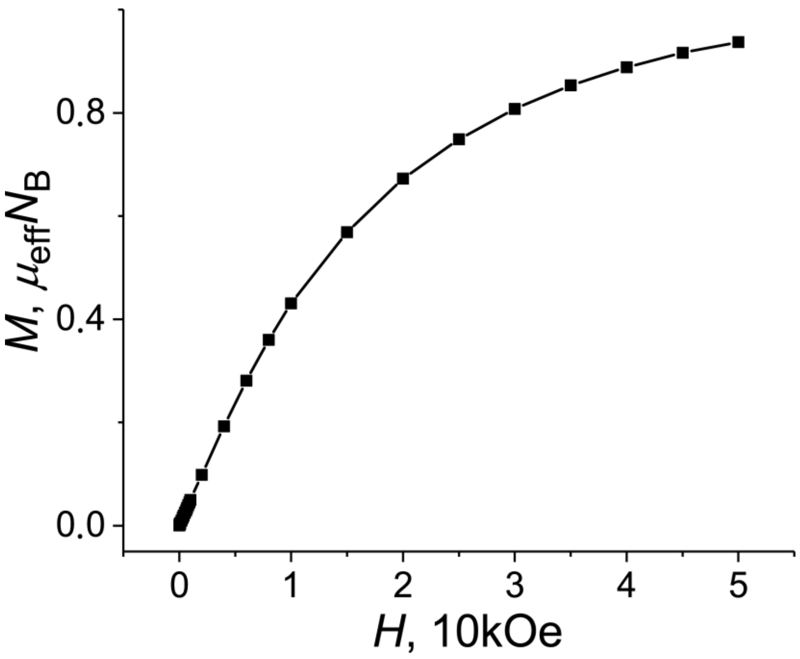

Fig. S6. Dependence of magnetization *vs* magnetic field up to 50 kOe (black line is a guide to the eye) for polycrystalline **1** at 2 K.

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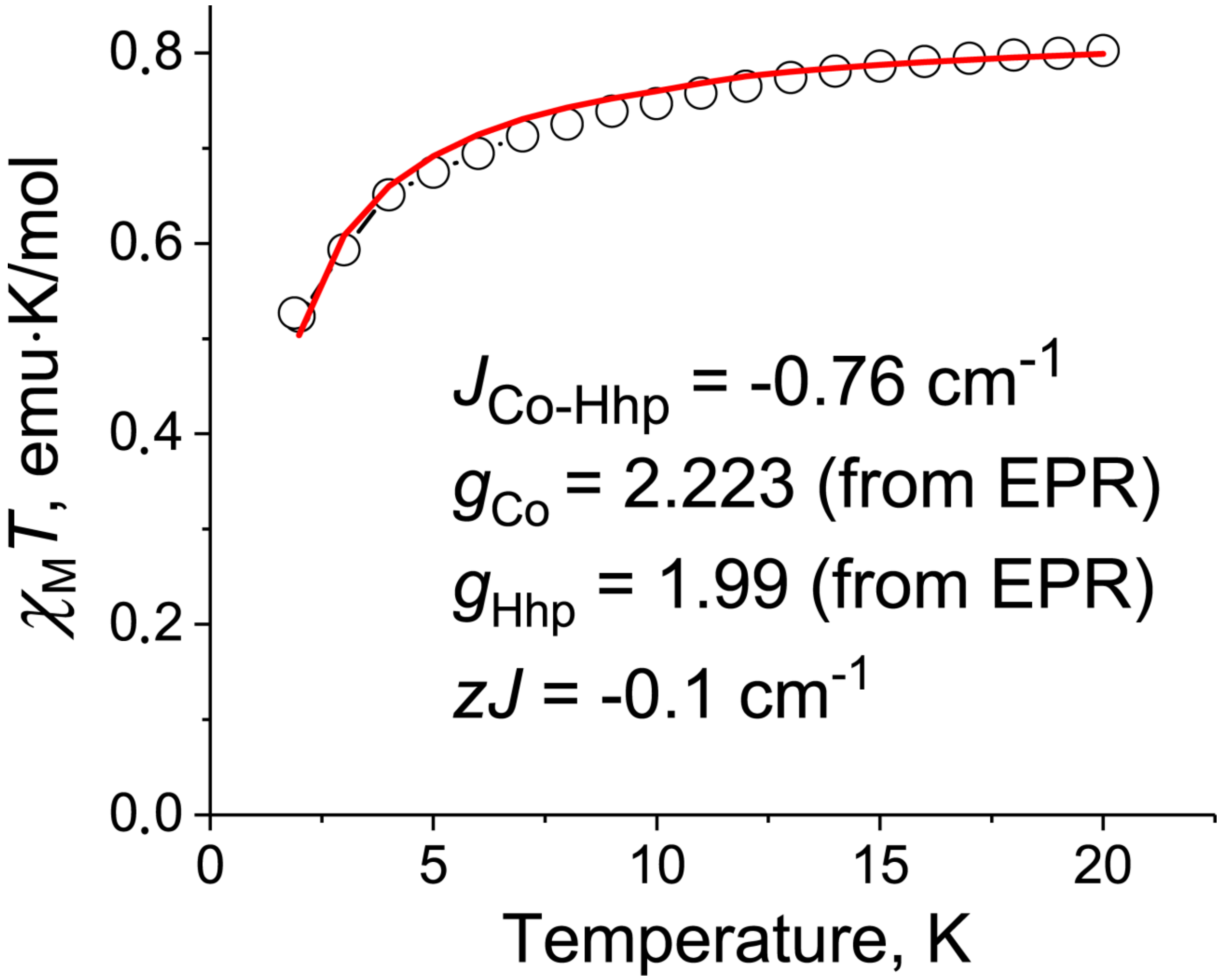

Fig. S7. Temperature dependence of the $\chi_M T$ values below 20 K and fitting of the data by PHI program. Parameters of fitting are given below. The g-factor values for Co^{II} and the $Hhp^{\bullet 4-}$ radical tetraanion were taken from measured EPR spectra.

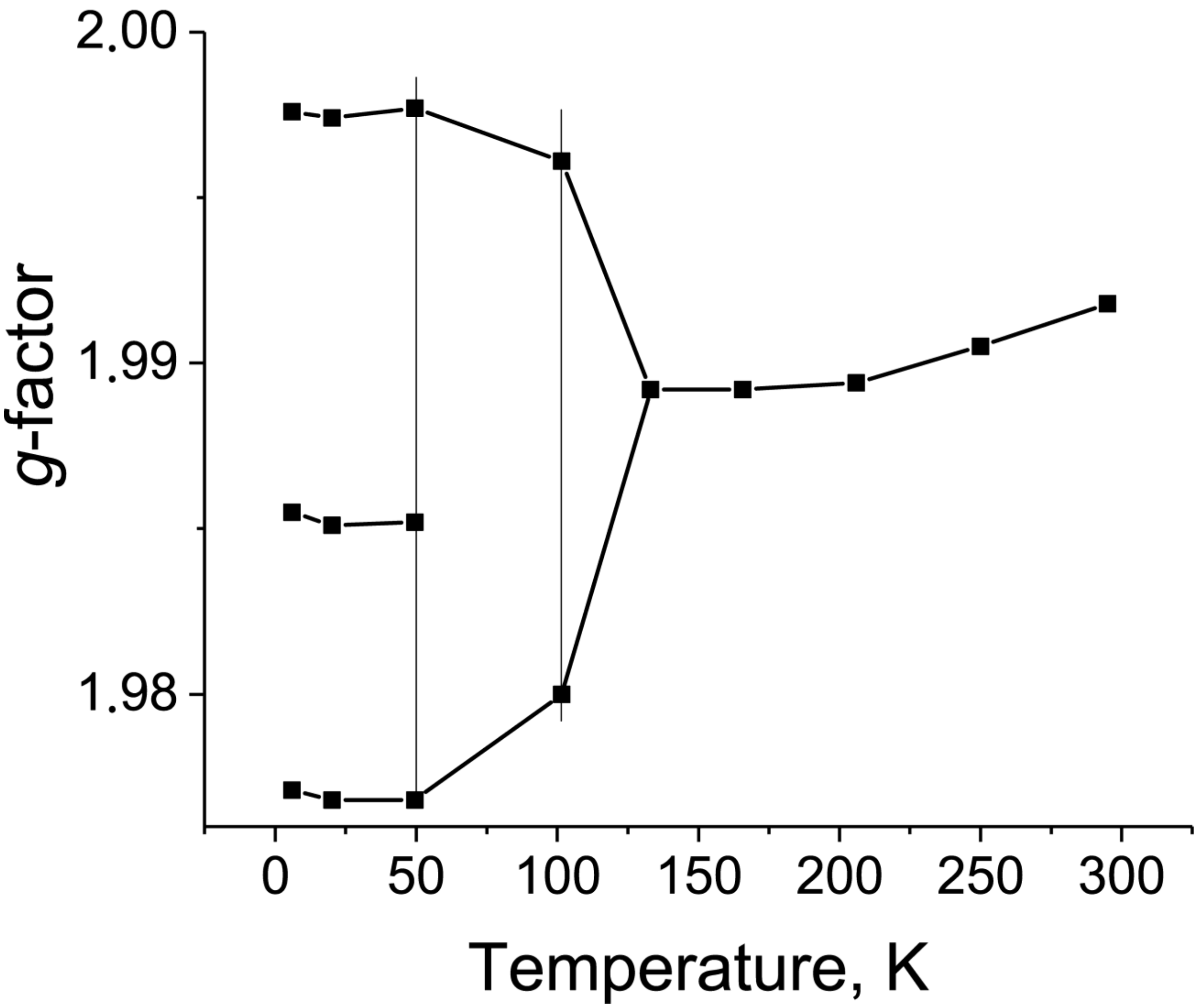

Fig. S8. G-factors of the components of the EPR signal attributed to the radical-tetraanion $Hhp^{\bullet 4-}$ species in **1**. Signal split into two and three lines at the temperature decrease below 100 and 50 K, respectively.

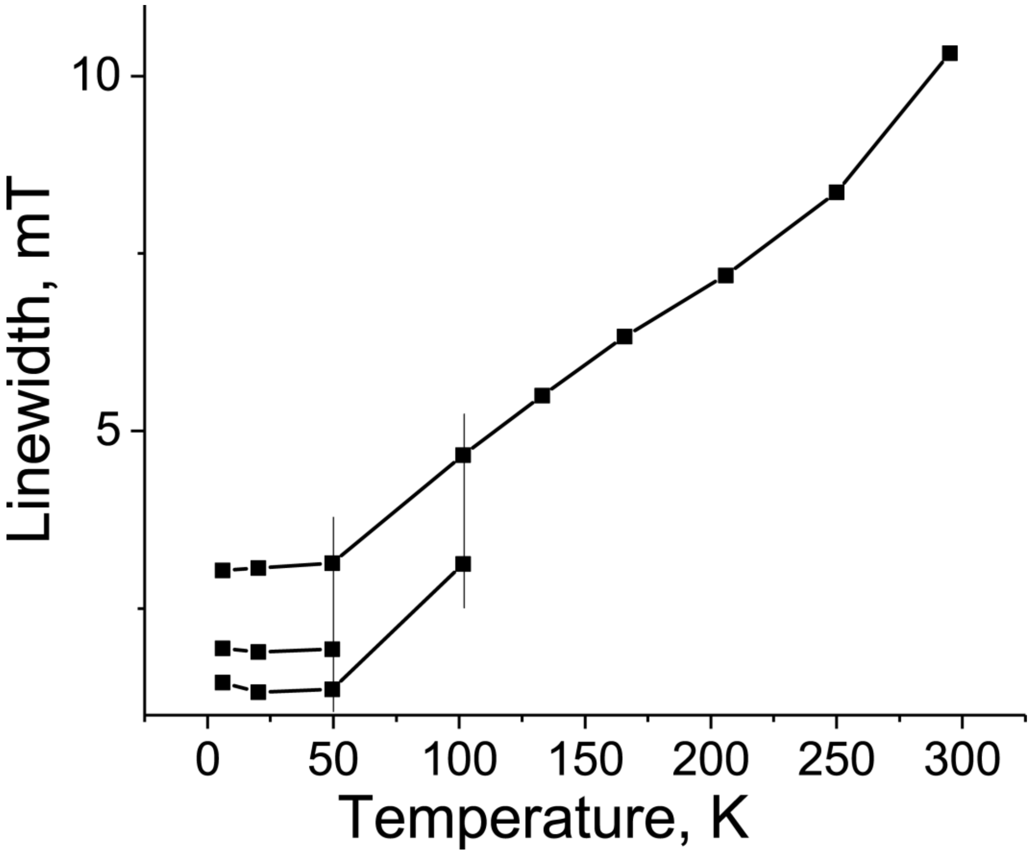

Fig. S9. Linewidth of the components of the EPR signal attributed to the radical-tetraanion Hhp$^{\bullet 4-}$ species in **1**. Signal split into two and three lines at the temperature decrease below 100 and 50 K, respectively.

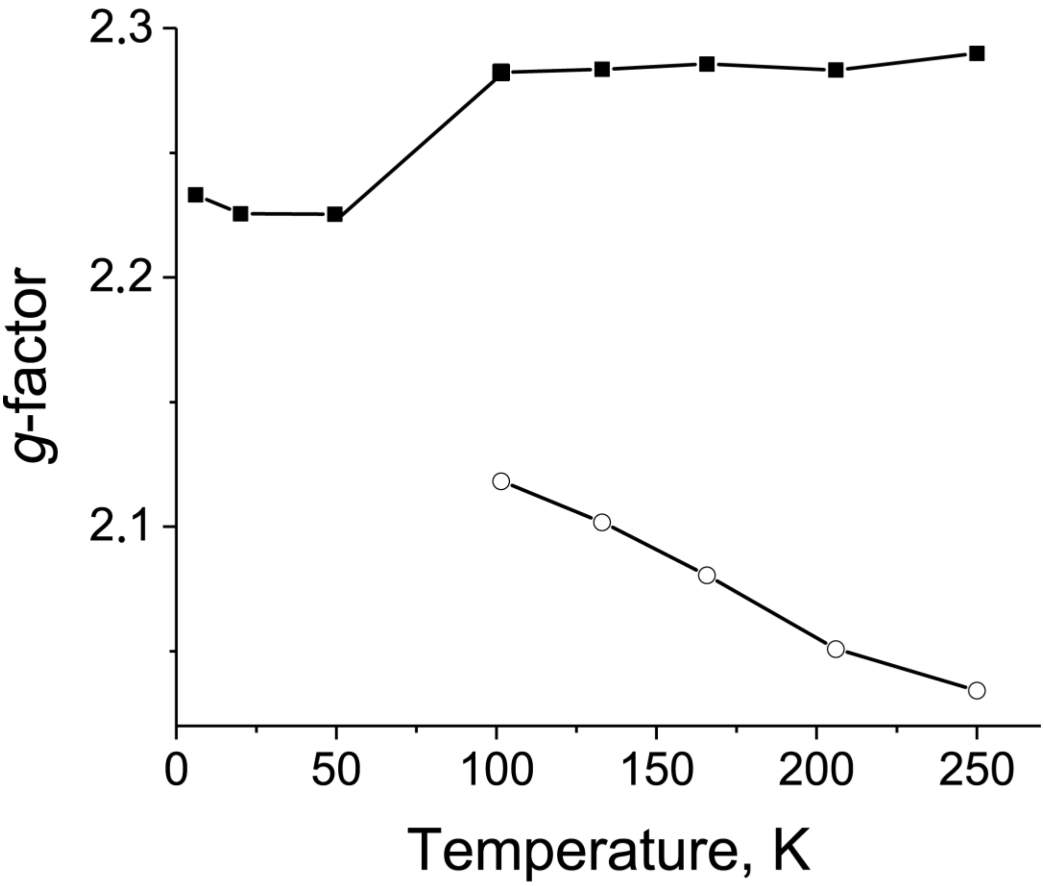

Fig. 10. *G*-factors of the components of the EPR signal attributed to the low-spin Co^{II} (S = 1/2) species (solid black squares) and the temperature-activated EPR signal appeared above 100 K attributed to the excited state (contributions from two Co^{II} (S = 1/2) and triplet Hhp^{5-} (S = 1) species (open circles)).

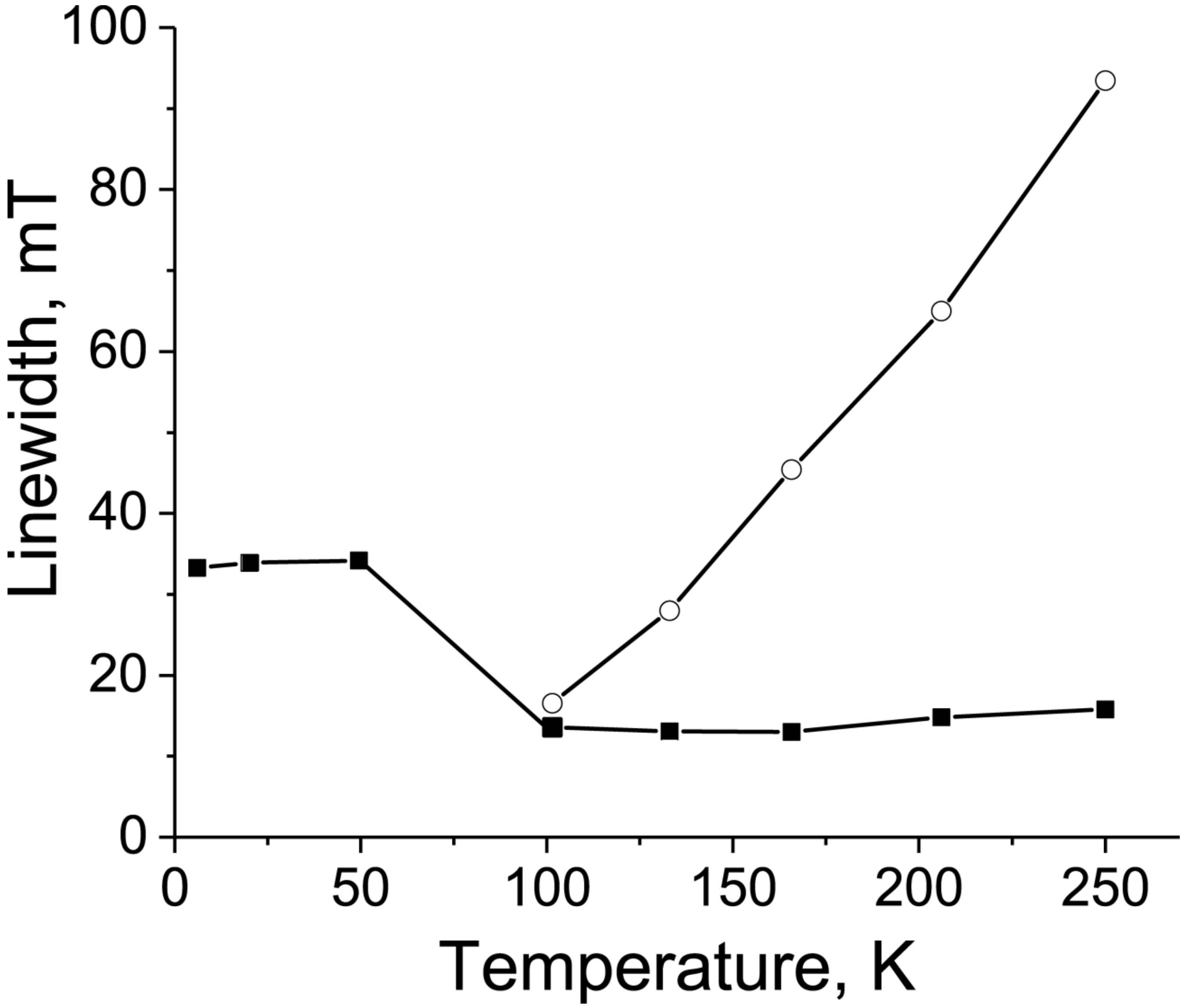

Fig. S11. Linewidth of the components of the EPR signal attributed to the low-spin Co^{II} (S = 1/2) species (solid black squares) and the temperature-activated EPR signal attributed to the the excited state (contributions from two Co^{II} (S = 1/2) and triplet Hhp^{5-} (S = 1) species (open circles)).

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Theoretical calculations

DFT calculations were performed using the PBE density functional theory[2] with the extended basis set: Co [9s9p8d/5s5p4d], C N,O, S [5s5p2d/3s3p2d], H [5s1p/3s1p], for the valence electrons and the SBK pseudopotential[3]. Calculations in the all-electron basis Co[23s18p13d8f4g/8s7p5d3f1g]. S[18s13p5d2f/5s4p2d1f]. C,N,O [12s8p4d2f/4s3p2d1f], H [8s4p2d/3s2p1d]][4]. give almost the same results for relative energies and optimized geometries of molecular systems. The Hirschfeld method was applied to determine the charge on the atoms.[5] All calculations were carried out using the PRIRODA program[6] at Joint Supercomputer Center of Russian Academy of Sciences.

The H_3Hhp macrocycle has planar D_{3h} symmetry. Its LUMO is doubly degenerate. Therefore, its radical anion reduces C_{2v} symmetry due to the Jahn-Teller effect. Accordingly, the dianion has a triplet ground state and D_{3h} symmetry is restored. The trianion has a doublet ground state and the energy of a quartet state (S = 3/2) in the symmetric H_3Hhp^{3-} trianion is higher by 0.403 eV. Electron affinity of the macrocycle is 2.462, 0.131, and -2.357 eV for the 1st, 2nd, and 3rd electron, respectively. In symmetrical structures of diamagnetic H_3Hhp and H_3Hhp^{3-} trianion in the quartet state, the bond lengths in the C-N-C-N-N fragment of the inner ring are 1.305 (bond **1**), 1.359 (bond **2**), 1.377 (bond **5**), 1.343 (bond **3**) (the **2** - **1** bond difference is 0.054) and 1.336 (bond **1**), 1.346 (bond **2**), 1.337 (bond **5**), 1.357 (bond **3**) Å (the **2** - **1** bond difference is 0.010), respectively (number of bonds are given according to Scheme 1). Obviously, the bond lengths only slightly change under reduction. The replacement of H atoms by the Co3O cluster (Fig 12a) weakly affects the geometry of the macrocycle.

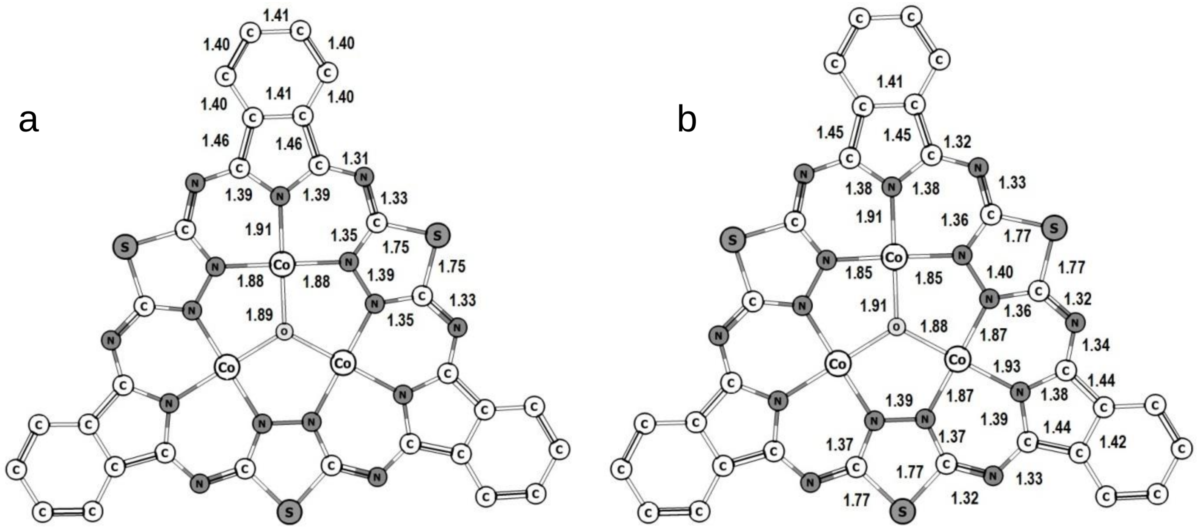


Fig. S12. Structure of complexes $\{Co_3O(Hhp)\}^+$ in the quartet state (a) and $\{Co_3O(Hhp)\}^{2-}$ in the excited triplet state (b). Hydrogen atoms are omitted. The lengths of bonds are shown in Å.

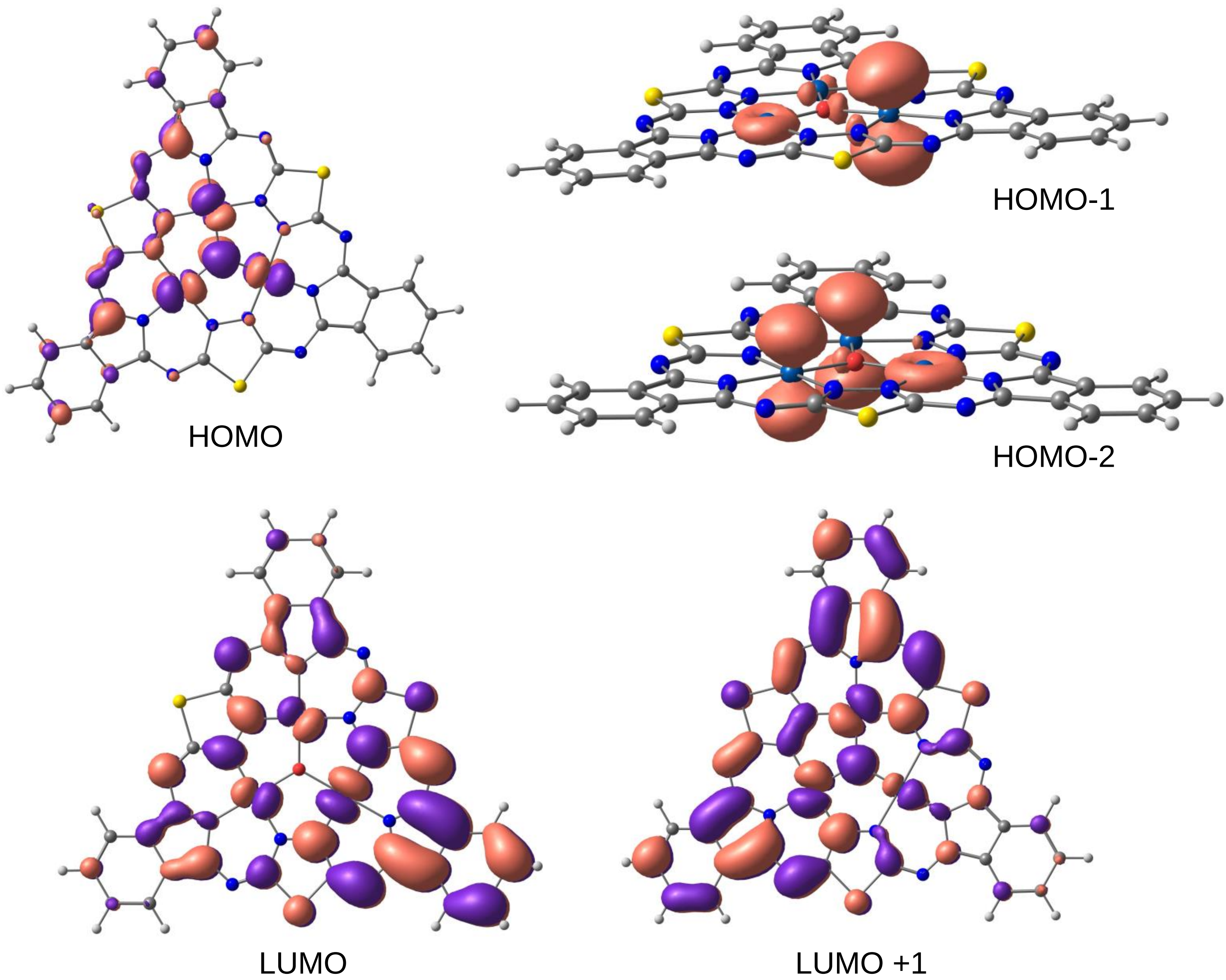


Fig. S13. Frontiers molecular orbitals for the $\{Co^{I}_{3}O(Hhp^{3-})\}^{2-}$ dianion in singlet state.

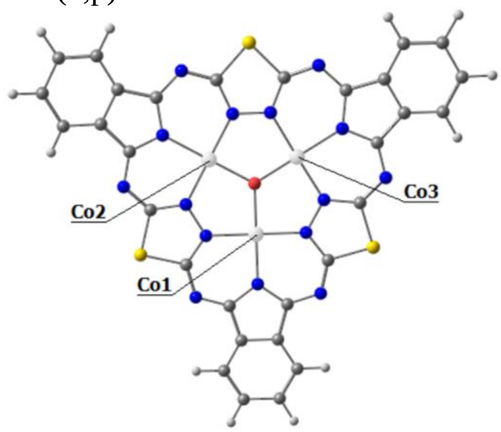
Aromaticity of the macrocyclic systems.

Computational details

Geometry optimizations of all paramagnetic complexes having charge 2^+ with various multiplicity were carried out using GAUSSIAN16 software[7] at the DFT level of theory using the long range corrected UCAM-B3LYP hybrid functional[8] and the basis sets 6-31G(d,p) without geometry constrains. Second derivatives calculations shown no imaginary frequencies. Criteria NICS were calculated by GIAO procedure. ACID (Anisotropy of the Induced Current Density) calculations were carried out using the ACID-3.0.4 software package.[9]

In order to estimate aromatic character of triple-reduced forms of Co_3OHhps, GIAO DFT/UB3LYP/6-31(d,p) method with respect of spin-orbital approach was used. At the first stage full geometry optimization was carried out with the following initial atomic charges (q_i) and multiplicities (M_i) (Table **S2**). No imaginary frequencies were found for optimized structures.

Table S2. Charge (q, a.u.), multiplicity (M) on atoms or fragments, relative energy (ΔE, a.u., kcal/mol) by DFT/UB3LYP/6-31(d,p).



	Total*		Co1		Co2		Co3		Hhp		ΔE, a.u.	ΔE, kcal/mol
	q_{tot}	M_{tot}	q_1	M_1	q_2	M_2	q_3	M_3	q_L	M_L		
E1	**2-**	**3**	**2**	**2**	**1**	**1**	**1**	**1**	**4-**	**2**	**0,0000**	**0,00**
E2	**2-**	**3**	**1**	**1**	**2**	**2**	**2**	**2**	**5-**	**1**	**0,0021**	**1,32**
E2a	**2-**	**3**	**1**	**1**	**2**	**2**	**2**	**-2**	**5-**	**3**	**0,0021**	**1,32**
E3	**2-**	**5**	**1**	**1**	**2**	**2**	**2**	**2**	**5-**	**3**	**0,0152**	**9,55**
E5	**2-**	**1**	**1**	**1**	**2**	**2**	**2**	**-2**	**5-**	**1**	**0,0546**	**34,24**

* including O (q=-2, M=1)

Following the results, shown in Table **S2**, the most stable structure is that which corresponds to triplet dianion $\{(Co^{I}Co^{I}Co^{II}O)(Hhp)\}^{2-}$. It is in good agreement with experimental and calculated by "PRIRODA" data. An electron transfer from one Co^{I} to macrocyclic ligand Hhp^{4-} can led to two triplet dianions **E2** and **E2a**. In **E2**, two electrons located on Hhp^{5-} are antiferromagnetically and two electrons of two Co^{II} atoms are ferromagnetically coupled. Inverse spin distribution was applied to calculate **E2a**. But after optimization, both structures have the same energy. Structure **E3** has 4 unpaired electrons with parallel spins. It worthy to note that energy difference between ground state **E1** and products of intramolecular electron transfer **E2** and **E2a** is very small and corresponds to 1,32 kcal/mol or 660 K (0,057 eV) which is in row with experimental value (estimated gap is 497 K). The transition from the ground triplet to the quintet state (**E1**=>**E3**) is more energetically demanding, requiring 9.55 kcal/mol.

Model complexes with optimized geometries were used, which correspond to the triplet ground state **(E1)** and the quintet excited state **(E3)**, in order to estimate the aromatic character of the complexes. NICS criteria were calculated for the centers of the various cycles formed within them. Since the centers of the **E1** and **E3** complexes are occupied by oxygen (O) atoms, criteria for evaluating global aromaticity have been calculated for the $(N\text{-}C)_{thiadiazol}\text{-}N_{ex}\text{-}(C\text{-}N)_{pyrr}$ (NCNCN) fragments. The results presented in Table **S3** demonstrate that the macrocyclic conjugated systems, which form the backbone of the organic ligands, are aromatic, in agreement with the data previously obtained for the reduced nickel and copper trithiadodecaazahexaphyrins.[10]

As result of the complexation, nine new metal-containing cycles are formed: six six-membered rings, including $Co\text{-}(N\text{-}C)_{thiadiazol}\text{-}N_{ex}\text{-}(C\text{-}N)_{pyrr}$ and three of five-membered rings containing oxygen, two Co-atoms and N-N fragment from thiadiazol ring. The values of the NICS criteria for the various centers are presented in Table **S3**. Figs. **S14** and **S15** show the GIAO isotropic shielding tensors (in ppm) and the corresponding centers.

Table S3. NICS criteria (in ppm) of selected centers of the **E1** and **E3** complexes and metal free $H_3Hhp(OCH_3)_6$.[11]

Ring	**E1**	**E3**	**$H_3Hhp(OCH_3)_6$** [11]
Thiadiazol	-3.719 -3.780 -10.154	-0.676 -0.689 +3.827	–14.69
Pyrrole	-6.837 -2.257 -2.352	-4.079 -7.140 -7.132	–1.46
Benzene	-7.291 -8.681 -8.644	-9.100 -7.791 -7.790	–9.63
NCNCN	-5.173 -5.172 -6.064 -8.134 -8.326 -5.851	-10.331 -10.337 -8.448 -7.320 -7.316 8.440	
CoNCNCN	-2.339 -2.402 -3.844 -5.971 -6.327 -3.449	-7.642 -7.652 -5.215 -4.183 -4.185 -5.212	
CoNNCoO	+0.873 +1.174 -3.905	-6.146 -6.140 -1.623	

The NICS criterion for global aromaticity calculated at the center of the $H_3Hhp(OCH_3)_6$ molecule using the GIAO/DFT/B3LYP/6-311G(d,p) method, was found to be a positive value of +0.85 ppm, indicating a non-aromatic character of the macrocycle.[11]

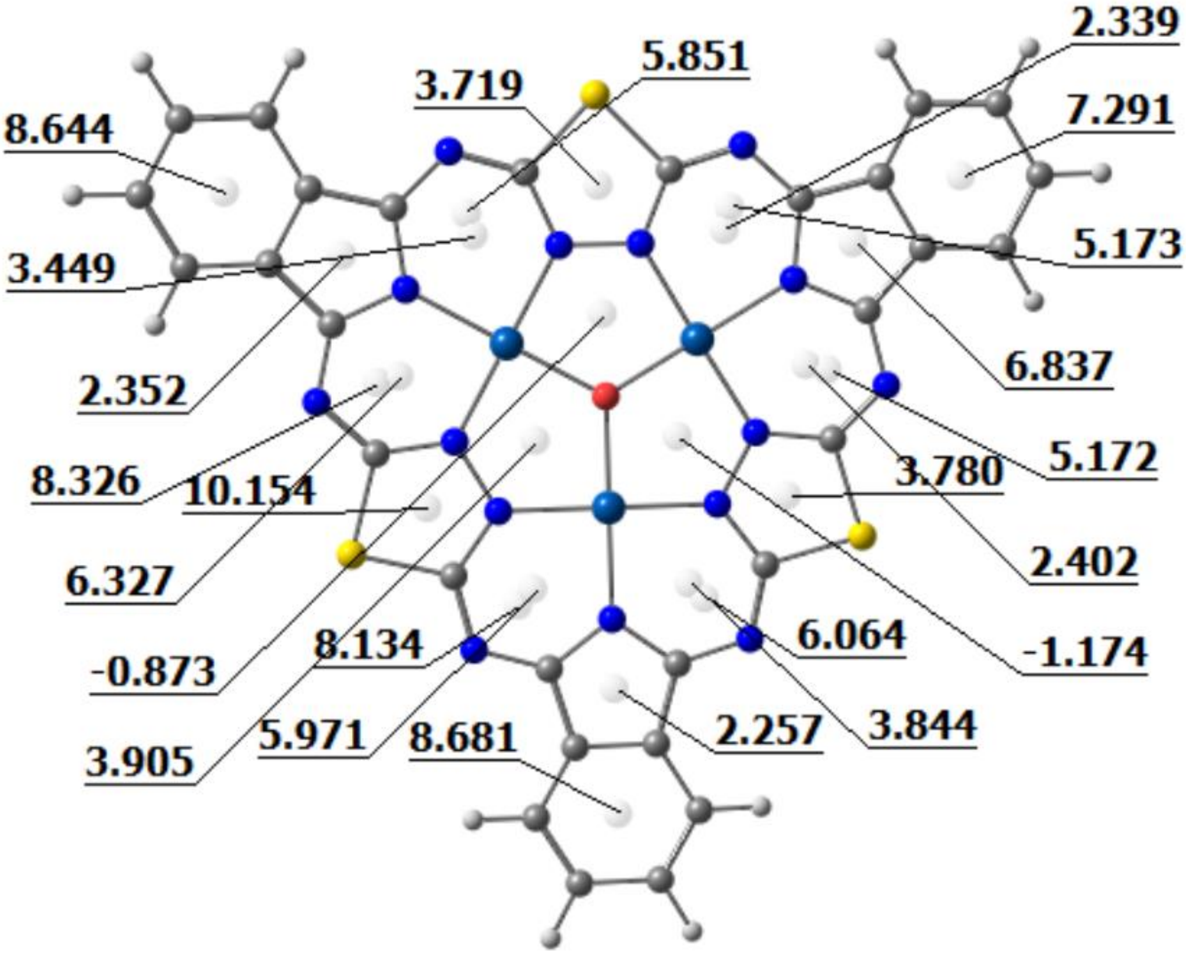


Fig. S14. View of complex **E1** and values of the isotropic shielding tensor GIAO (ppm) calculated for the centers of the conjugation contours.

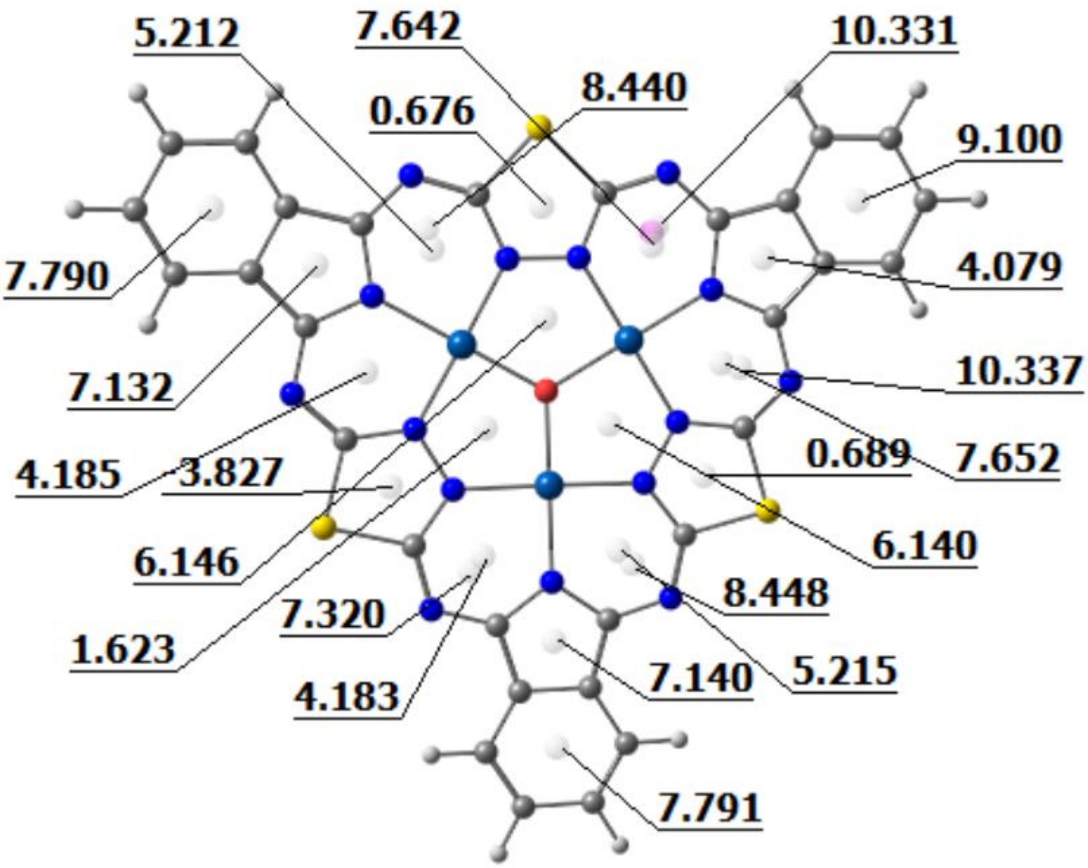


Fig. S15. View of complex **E3** and values of the isotropic shielding tensor GIAO (ppm) calculated for the centers of the conjugation contours.

To investigate diatropic and paratropic ring currents within various conjugation contours of **H_3Hhp** and **E3**, ACID (Anisotropy of the Induced Current Density) calculations were carried out using the ACID-3.0.4 software package.[9] The results are shown in Figure **S15**.

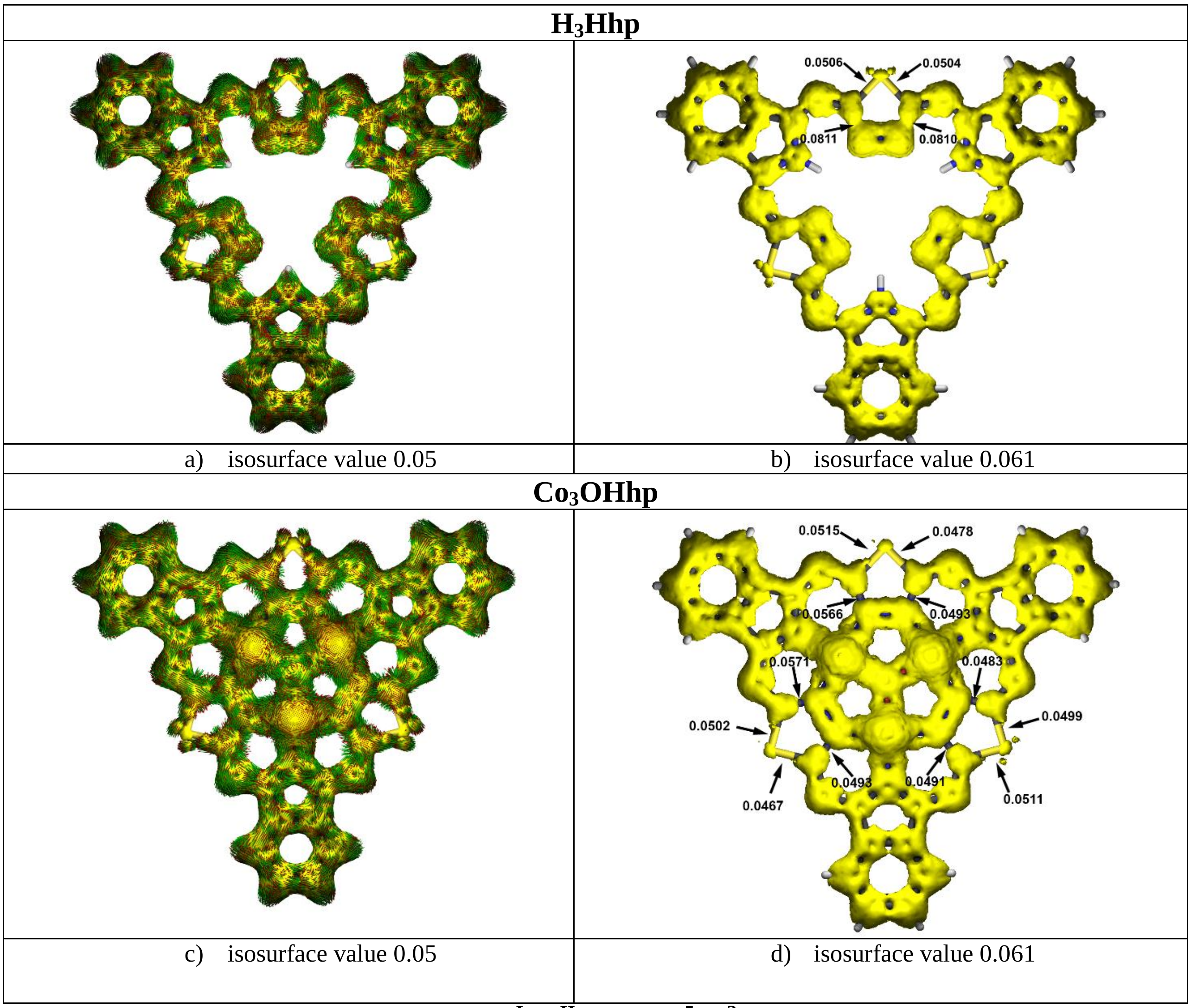


Fig. S16. ACID plots of **H$_3$Hhp** and **{(Co^{I}Co$^{II}{}_2$O)(Hhp^{5-})}$^{2-}$** (**E3**) at standard isosurface values of 0.05 (**a, c**) and at 0.061 (**b, d**). CIVs representing the strength of delocalization are given for selected bonds.

At the standard isosurface value of 0.05 the delocalized systems include all bonds a part sulfur atoms of the thiadiazol rings (Figure **S16a,c**). Upon increasing the isosurface value to 0.061 these atoms (S) are isolated. Ongoing from initial **H$_3$Hhp** to **E3** a formation of new nine-membered cycle containing three Co atoms and three -NN- fragments of thiadiazol subunits takes place. The work in this area is in progress.

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Cartesian coordinates of the molecular structures optimized using the PBE density functional theory

H_3Hhp

1	-0.88373466	0.35821116	-2.70443234
1	2.79361350	0.16016070	0.62979542
1	-1.91254696	-0.49598563	2.07826610
16	3.46152381	0.88242019	-3.76404228
16	-5.06045592	-0.23434127	-1.13047467
16	1.59960547	-0.66550288	4.89164804
7	0.18666883	-0.40639872	2.72282434
7	-3.60301634	0.23156692	-3.36009697
7	-1.19980760	0.48079133	-3.67582845
7	3.79622530	0.21246028	0.85471996
7	-2.59788133	-0.67991542	2.82326329
7	1.28593375	0.50659102	-2.38820128
7	1.45897768	-0.22499877	2.33168007
7	-1.09178410	-0.87003789	4.72923156
6	4.79770674	0.45163006	-0.08269591
7	-2.46999618	-0.01866001	-1.23212699
7	2.27989347	0.45709547	-1.48585504
6	-3.55078573	0.02377403	-2.01789044
7	-2.74829927	-0.24959349	0.06163413
6	-3.59165648	0.70325973	-6.44405772
6	7.37979623	0.64413580	0.21855901
7	3.69902902	-0.18545243	3.25647488
6	-2.26637593	-0.87645882	4.16133159
7	4.69385661	0.64168729	-1.36928398
7	0.95107295	0.82676676	-4.76731312
6	8.39696323	0.58691219	1.17995858
7	-4.65108180	-0.63805617	1.51185196
6	-4.57282839	-1.03674163	3.93077048
6	6.06697672	0.45262989	0.65458887
6	1.70304274	0.72256771	-3.63989587
6	-5.90499606	-1.21616153	4.30949714
6	2.34835923	-0.32077793	3.32522409
6	-2.53202351	0.43115511	-4.07799750
6	8.10529301	0.34445472	2.53618053
6	-4.05290247	-0.39285509	0.31623775
6	3.49623965	0.63341362	-2.01188817
6	-6.16592478	-1.46772841	5.66257033
6	6.78778808	0.15199805	2.97131557
6	4.32075953	0.05511059	2.13495973
6	0.05296526	-0.64839126	4.03082543
6	-0.88150614	1.05491722	-7.28171236
6	-1.93707785	1.10655799	-8.20110747
6	-2.53781825	0.65216996	-5.52911296
6	5.77519039	0.21005356	2.01132841
6	-5.12231205	-1.53695449	6.60558969
6	-3.27231531	0.93329159	-7.78840958

6	-3.52884593	-1.10611914	4.87411514
6	-0.34880805	0.71574388	-4.75266055
6	-3.97271199	-0.76451923	2.61913104
6	-1.20209811	0.82538641	-5.94199970
6	-3.78674683	-1.35669477	6.22355633
1	-4.62212727	0.56762831	-6.11439379
1	-4.07088596	0.97928143	-8.53049235
1	-1.72297793	1.28395056	-9.25619530
1	0.15561558	1.18764865	-7.59106209
1	7.59509926	0.83125202	-0.83385712
1	9.43427615	0.73265598	0.87458222
1	8.92140024	0.30632539	3.25938949
1	6.55145589	-0.03632845	4.01899447
1	-2.97153799	-1.40847604	6.94583910
1	-5.36027626	-1.73470718	7.65190843
1	-7.19537608	-1.61298124	5.99369500
1	-6.70580875	-1.16081769	3.57154584

$H_3Hhp^{\bullet-}$, S = 1/2

1	-0.89762200	0.34391931	-2.71531319
1	2.81747030	0.15125570	0.63367139
1	-1.92857930	-0.51130588	2.07733677
16	3.47816923	0.94281671	-3.78331645
16	-5.06726576	-0.31611703	-1.14656995
16	1.60262474	-0.61347482	4.93555579
7	0.20192863	-0.42667914	2.74270072
7	-3.61846316	0.18849040	-3.37483176
7	-1.21119501	0.47179911	-3.68665468
7	3.81866907	0.20881927	0.85909054
7	-2.61190643	-0.69063701	2.82505498
7	1.30909320	0.49172619	-2.40589057
7	1.46593287	-0.25111265	2.35086469
7	-1.09624066	-0.84194605	4.74130222
6	4.81793084	0.45051758	-0.08089737
7	-2.48222966	-0.03201776	-1.24308087
7	2.29559327	0.43721985	-1.50810375
6	-3.55616547	-0.01897509	-2.03294312
7	-2.76281912	-0.26499318	0.06144836
6	-3.59587186	0.69402702	-6.45259176
6	7.39469118	0.63524306	0.22058489
7	3.70231481	-0.17991955	3.27694923
6	-2.27668785	-0.86505738	4.17285336
7	4.70449480	0.65199430	-1.38360560
7	0.94995657	0.85541924	-4.77034464
6	8.41032016	0.57453904	1.17667177
7	-4.66781913	-0.68287281	1.50383453
6	-4.57878238	-1.04470078	3.92973275
6	6.07227612	0.44760914	0.64884044
6	1.71162569	0.74430898	-3.65988292
6	-5.91150447	-1.22797459	4.31182004
6	2.37026280	-0.31278502	3.35093221

6	-2.53904309	0.40936681	-4.08885069
6	8.11716351	0.33123785	2.54012522
6	-4.06064553	-0.43797145	0.31264905
6	3.52581485	0.64628862	-2.02248200
6	-6.17923897	-1.45896124	5.66561237
6	6.80295691	0.14413882	2.97272817
6	4.34007071	0.05393436	2.14154870
6	0.05116341	-0.63312004	4.05910475
6	-0.89320987	1.09089661	-7.28575252
6	-1.94701601	1.13978114	-8.20352844
6	-2.54310120	0.64484600	-5.53336800
6	5.77812386	0.20346989	2.01690556
6	-5.13479037	-1.50532977	6.61465033
6	-3.28387109	0.94387607	-7.79349603
6	-3.53194802	-1.09069318	4.87957372
6	-0.35438078	0.72978508	-4.76308133
6	-3.98179025	-0.78820128	2.61829403
6	-1.20376185	0.84117149	-5.94300909
6	-3.80172686	-1.32233212	6.23431808
1	-4.62390309	0.54081095	-6.12126849
1	-4.08365252	0.98844077	-8.53519249
1	-1.73450250	1.33284727	-9.25707066
1	0.14258366	1.24102976	-7.59308387
1	7.60962738	0.82218771	-0.83261869
1	9.44889073	0.71660625	0.87074605
1	8.93452603	0.28971494	3.26303393
1	6.56606890	-0.04392636	4.02101186
1	-2.98822519	-1.35635313	6.96021075
1	-5.37474933	-1.68752986	7.66422680
1	-7.20951969	-1.60573902	5.99535097
1	-6.70811576	-1.18940912	3.56749389

H_3Hhp^{2-}, $S = 0$

1	-0.89330666	0.34928725	-2.74042471
1	2.82911999	0.15177474	0.63643725
1	-1.93484461	-0.51497221	2.10235316
16	3.46757348	0.93879824	-3.76731075
16	-5.06846437	-0.31981597	-1.14752708
16	1.59933642	-0.60876063	4.91683237
7	0.18008033	-0.42673393	2.74014296
7	-3.63060670	0.18579988	-3.38090244
7	-1.21013661	0.47652546	-3.71184332
7	3.83203974	0.20988939	0.86226692
7	-2.62123347	-0.69468095	2.84853095
7	1.28838849	0.49104319	-2.41234200
7	1.47920136	-0.24825020	2.33983174
7	-1.09047527	-0.84046942	4.76909345
6	4.83130024	0.45158751	-0.08288424
7	-2.48200056	-0.02908965	-1.25102567
7	2.30339128	0.43370596	-1.49244119
6	-3.55223797	-0.01857832	-2.04025205
7	-2.76593841	-0.26506710	0.06931281

6	-3.59810921	0.69535292	-6.47315427
6	7.40800154	0.63421547	0.22417577
7	3.71477889	-0.17983625	3.28849719
6	-2.28417625	-0.86662443	4.19284066
7	4.72066977	0.65305298	-1.38865253
7	0.96619544	0.86516957	-4.79115190
6	8.42759437	0.57411382	1.17756034
7	-4.68112932	-0.68707660	1.50312257
6	-4.58895649	-1.04749049	3.93367697
6	6.08388608	0.44810971	0.64754113
6	1.69686501	0.74329204	-3.65241243
6	-5.92166810	-1.23451210	4.32871601
6	2.36325377	-0.30975082	3.33135442
6	-2.54693364	0.41126219	-4.11059456
6	8.13343295	0.33062670	2.54596343
6	-4.06003184	-0.44050375	0.32057746
6	3.51174193	0.64110963	-2.00772181
6	-6.19050523	-1.46460219	5.68034541
6	6.81671050	0.14476182	2.97475424
6	4.35137722	0.05429257	2.14929306
6	0.04051209	-0.62904375	4.04703579
6	-0.89510766	1.09633222	-7.30236055
6	-1.94333590	1.14512190	-8.22486208
6	-2.55073771	0.64511909	-5.54170772
6	5.78819036	0.20333271	2.02300001
6	-5.14015769	-1.50863986	6.63591276
6	-3.28803149	0.94551476	-7.81235244
6	-3.53321228	-1.09189978	4.89413889
6	-0.35318982	0.73567083	-4.78369421
6	-3.99770585	-0.79359106	2.63426244
6	-1.19911741	0.84560920	-5.95634282
6	-3.81033423	-1.32328669	6.24940731
1	-4.62754636	0.54058365	-6.14394899
1	-4.08884798	0.98899505	-8.55465761
1	-1.72870567	1.33915269	-9.27867001
1	0.14224936	1.24799332	-7.60725886
1	7.62146124	0.82068919	-0.83022037
1	9.46637374	0.71589983	0.86925248
1	8.95010647	0.28857512	3.27087161
1	6.57812007	-0.04301726	4.02351679
1	-2.99454807	-1.35494832	6.97436730
1	-5.37840992	-1.69021505	7.68685711
1	-7.22189986	-1.61275831	6.00974600
1	-6.72030951	-1.19814553	3.58512786

H_3Hhp^{2-}, S = 1

1	-0.89307252	0.34813520	-2.74145696
1	2.82941921	0.15440994	0.63660184
1	-1.93521839	-0.51606899	2.10290436
16	3.49293785	0.95351728	-3.79435416
16	-5.10530407	-0.32748960	-1.15675252
16	1.61113903	-0.61092488	4.95383967

7	0.20117734	-0.42435564	2.76177660
7	-3.62822871	0.18121338	-3.38122364
7	-1.20951114	0.47523359	-3.71125656
7	3.83079703	0.21119035	0.86201903
7	-2.62052973	-0.69501498	2.84796516
7	1.31615229	0.49988605	-2.42186578
7	1.47362173	-0.24926536	2.36967217
7	-1.09117095	-0.83902907	4.76785252
6	4.83075770	0.45310128	-0.08217949
7	-2.50972529	-0.03962656	-1.24424129
7	2.31031969	0.44402910	-1.52071865
6	-3.58100966	-0.02547827	-2.05292733
7	-2.78796023	-0.27023213	0.04917501
6	-3.59715006	0.69223247	-6.47308965
6	7.40725257	0.63320848	0.22445259
7	3.71421292	-0.17860740	3.28686516
6	-2.28464169	-0.86597581	4.19253921
7	4.71936304	0.65657035	-1.38688812
7	0.96483692	0.86802811	-4.78989002
6	8.42540817	0.57120234	1.17790611
7	-4.67899914	-0.68972311	1.50327802
6	-4.58671639	-1.04758800	3.93308041
6	6.08156581	0.44772905	0.64814731
6	1.71375223	0.75492044	-3.67832266
6	-5.92085427	-1.23477137	4.32856814
6	2.37755860	-0.31019961	3.36013119
6	-2.54575854	0.40829676	-4.11113834
6	8.13160658	0.32719039	2.54412331
6	-4.09102525	-0.44816193	0.31785142
6	3.53612274	0.65211679	-2.02659274
6	-6.18851565	-1.46334025	5.67974481
6	6.81602839	0.14212834	2.97373518
6	4.35107373	0.05461645	2.14839067
6	0.04515374	-0.63066943	4.07893002
6	-0.89557071	1.09791008	-7.30142932
6	-1.94388132	1.14562147	-8.22247372
6	-2.54874549	0.64266922	-5.54047863
6	5.78630686	0.20244291	2.02115541
6	-5.13985179	-1.50604525	6.63413921
6	-3.28636685	0.94388337	-7.81086664
6	-3.53282391	-1.09061080	4.89220785
6	-0.35375879	0.73624976	-4.78340413
6	-3.99690550	-0.79489107	2.63453786
6	-1.19956730	0.84532317	-5.95415085
6	-3.81054158	-1.32099625	6.24910332
1	-4.62624572	0.53568847	-6.14399722
1	-4.08685883	0.98691375	-8.55373820
1	-1.73008457	1.34095591	-9.27633983
1	0.14152579	1.25153410	-7.60585997
1	7.62061588	0.82033316	-0.82973569
1	9.46458693	0.71218335	0.87012765
1	8.94881688	0.28379373	3.26854010

1	6.57721906	-0.04634364	4.02221105
1	-2.99486781	-1.35159063	6.97407670
1	-5.37887421	-1.68661208	7.68521610
1	-7.21983354	-1.61152442	6.00977956
1	-6.71915913	-1.19932207	3.58472740

$H_3Hhp^{\bullet 3-}$, S = 1/2

1	-0.87333061	0.35984593	-2.76783152
1	2.85463051	0.16295257	0.61442840
1	-1.95853598	-0.51694295	2.12892148
16	3.51277134	0.92701514	-3.81810373
16	-5.14144952	-0.28514522	-1.16146665
16	1.62820210	-0.64206750	4.98031748
7	0.20507011	-0.42377329	2.78647431
7	-3.63036615	0.20605944	-3.38382303
7	-1.19991596	0.48357874	-3.73430514
7	3.85339097	0.21684739	0.85026953
7	-2.64330349	-0.69772773	2.87315986
7	1.32885471	0.50971080	-2.44549920
7	1.47105205	-0.24607845	2.39523244
7	-1.08752006	-0.85948315	4.78761191
6	4.85455676	0.45760317	-0.09170578
7	-2.53464557	-0.03467696	-1.23896216
7	2.33269815	0.45663294	-1.53470102
6	-3.59836480	-0.00129158	-2.06065444
7	-2.81294483	-0.26460878	0.04830243
6	-3.60084402	0.70226132	-6.48796922
6	7.42765406	0.64107407	0.22953647
7	3.72098108	-0.18204483	3.28551773
6	-2.30161755	-0.87981547	4.21686041
7	4.74706839	0.65629165	-1.40487213
7	0.98124191	0.85548702	-4.82154291
6	8.44852922	0.58279934	1.18234844
7	-4.70348347	-0.66899801	1.50691536
6	-4.60481643	-1.04653871	3.94139229
6	6.09891726	0.45420211	0.64395974
6	1.72234458	0.74499864	-3.70056607
6	-5.94017096	-1.23339629	4.34981026
6	2.39102026	-0.31731556	3.37318195
6	-2.54721947	0.42309775	-4.12722204
6	8.14793499	0.33792788	2.55204375
6	-4.12461676	-0.42946677	0.33177780
6	3.55606401	0.64802226	-2.03683381
6	-6.21006940	-1.47190764	5.69688648
6	6.83170628	0.15062456	2.97633230
6	4.36894043	0.05780070	2.14728021
6	0.03893043	-0.64890333	4.10924942
6	-0.89975717	1.08183365	-7.32497861
6	-1.94744855	1.13308233	-8.24863517
6	-2.55329588	0.64844048	-5.54815812
6	5.79464210	0.20715980	2.02511950
6	-5.15418545	-1.52750099	6.65490114

6	-3.29404532	0.94329633	-7.82787356
6	-3.53804695	-1.10271414	4.90927401
6	-0.34543594	0.73248414	-4.80939274
6	-4.02170955	-0.78920572	2.65623430
6	-1.19553886	0.83998826	-5.97359330
6	-3.82745406	-1.34464174	6.26670298
1	-4.63142332	0.55544034	-6.15606585
1	-4.09900438	0.98753357	-8.56811551
1	-1.73384023	1.32055125	-9.30512414
1	0.13927083	1.22538523	-7.63149163
1	7.64140050	0.82809531	-0.82567500
1	9.48890656	0.72626086	0.87579419
1	8.96296458	0.29638981	3.28134237
1	6.59173984	-0.03783402	4.02547962
1	-3.01082037	-1.38514315	6.99193868
1	-5.39191275	-1.71614759	7.70645581
1	-7.24330504	-1.61867591	6.02666273
1	-6.74104515	-1.18872931	3.60744669

$H_3Hhp^{\bullet 3-}$, S = 3/2

1	-0.90113543	0.35684659	-2.76407738
1	2.85346965	0.15763477	0.64218959
1	-1.95240647	-0.51542945	2.12175768
16	3.50356816	0.92567267	-3.80798081
16	-5.12094614	-0.28536361	-1.15259503
16	1.61725419	-0.64047778	4.96058402
7	0.19785804	-0.42392888	2.77624061
7	-3.64818352	0.20514270	-3.38783517
7	-1.21754520	0.48183284	-3.73452459
7	3.85518886	0.21437620	0.86771046
7	-2.63772273	-0.69647332	2.86678848
7	1.31890404	0.50640662	-2.43524910
7	1.48374366	-0.24362271	2.38034956
7	-1.08955898	-0.86014192	4.78542974
6	4.85445689	0.45615846	-0.08163310
7	-2.52136595	-0.03021468	-1.25254339
7	2.32351398	0.45337817	-1.52382550
6	-3.58791841	-0.00049771	-2.05869762
7	-2.80264414	-0.26360000	0.05480989
6	-3.60447612	0.70290678	-6.49301770
6	7.42831701	0.64156629	0.23069745
7	3.72664172	-0.18493889	3.30260334
6	-2.29589802	-0.87913738	4.21142508
7	4.73766840	0.65468549	-1.39770827
7	0.97497023	0.85335963	-4.81136820
6	8.44886364	0.58364678	1.18125998
7	-4.70165174	-0.66893137	1.50879591
6	-4.60218395	-1.04584465	3.94069845
6	6.09745784	0.45407581	0.64598850
6	1.71327262	0.74269244	-3.69102065
6	-5.93627977	-1.23170754	4.34621784
6	2.38815104	-0.31670269	3.36270520

6	-2.55861597	0.42273934	-4.12986757
6	8.15346945	0.33838407	2.55471102
6	-4.10147082	-0.42660749	0.32829132
6	3.54749246	0.64591384	-2.02692186
6	-6.20719216	-1.47058045	5.69454770
6	6.83712259	0.15071625	2.97950875
6	4.37269267	0.05618514	2.15822121
6	0.04036899	-0.64596484	4.08551545
6	-0.90078005	1.08134791	-7.32560179
6	-1.94617973	1.13293380	-8.24913712
6	-2.55995472	0.64859255	-5.55236371
6	5.79949454	0.20667694	2.03135131
6	-5.15169244	-1.52670309	6.65191817
6	-3.29709384	0.94384868	-7.83313172
6	-3.53753052	-1.10254345	4.90636087
6	-0.35549313	0.73095429	-4.80832987
6	-4.01723137	-0.78740440	2.65014157
6	-1.19731641	0.83925254	-5.97198900
6	-3.82381795	-1.34399600	6.26229048
1	-4.63559121	0.55643452	-6.16192821
1	-4.09990885	0.98867305	-8.57537599
1	-1.72968500	1.32051792	-9.30525691
1	0.13837145	1.22466731	-7.63203487
1	7.64192462	0.82874462	-0.82458082
1	9.48858820	0.72767026	0.87194474
1	8.97030931	0.29736266	3.28171628
1	6.59806980	-0.03799445	4.02903937
1	-3.00632983	-1.38468248	6.98640120
1	-5.38857750	-1.71524425	7.70348134
1	-7.24047785	-1.61690186	6.02372565
1	-6.73634810	-1.18636257	3.60317776

$\{Co_3O(Hhp)\}^+$, S = 1/2

27	-0.57871982	0.22846649	-1.77795912
27	1.83195624	0.11145539	0.41401033
27	-1.25481042	-0.33286303	1.36489246
16	3.37229754	0.97326569	-3.66084391
16	-4.92219376	-0.43792860	-1.13707074
16	1.55275599	-0.53899247	4.79793700
8	0.01366904	-0.00761906	0.00157718
7	0.12789980	-0.36577854	2.63056158
7	-3.54537353	0.10111268	-3.33676868
7	-1.16676143	0.46040044	-3.57876981
7	3.69396245	0.21204414	0.83253247
7	-2.52752567	-0.66922346	2.74677227
7	1.19264844	0.51870209	-2.31913540
7	1.44347563	-0.19646521	2.22186481
7	-1.08697184	-0.75447087	4.68830050
6	4.73669944	0.44115205	-0.06343838
7	-2.34799044	-0.08290952	-1.24021921
7	2.22012910	0.44894432	-1.38862352

6	-3.44826830	-0.10420110	-2.02195766
7	-2.63544066	-0.32140018	0.09597213
6	-3.57266644	0.64512075	-6.39634208
6	7.32863084	0.59236283	0.19392329
7	3.64935138	-0.16297211	3.22100443
6	-2.25947217	-0.80792036	4.10910319
7	4.63291261	0.65479874	-1.35145350
7	0.93087690	0.92144718	-4.69201966
6	8.34512351	0.51150340	1.15494074
7	-4.57983912	-0.75701229	1.47172135
6	-4.53276740	-1.05061329	3.88922455
6	6.01593376	0.42060665	0.63977752
6	1.63407483	0.78922143	-3.56472236
6	-5.86456109	-1.25619507	4.25702055
6	2.31948918	-0.26732184	3.24691494
6	-2.47684098	0.36880676	-4.04486153
6	8.05321958	0.26874632	2.51200150
6	-3.95171964	-0.52184275	0.31826300
6	3.43498718	0.65993607	-1.93885012
6	-6.12763406	-1.45254551	5.61923970
6	6.73476627	0.09849274	2.95477351
6	4.27337709	0.05589587	2.09048690
6	0.01515575	-0.55575091	3.96124951
6	-0.87217470	1.15720504	-7.21129961
6	-1.92820917	1.18229064	-8.13183598
6	-2.51669699	0.62227185	-5.48221976
6	5.72487357	0.17857158	1.99292089
6	-5.09206206	-1.44334279	6.57497937
6	-3.25555468	0.93036487	-7.73106128
6	-3.50012524	-1.04159514	4.84194039
6	-0.36823023	0.76233679	-4.68250618
6	-3.90466344	-0.81599334	2.59220360
6	-1.19322016	0.87321997	-5.88164721
6	-3.75749098	-1.23776187	6.20097504
1	-4.59761122	0.44914899	-6.08127520
1	-4.05060964	0.95856368	-8.47724577
1	-1.72154082	1.40076499	-9.18025065
1	0.15655137	1.35069382	-7.51543056
1	7.54868433	0.78067682	-0.85694723
1	9.38431107	0.63888576	0.84910675
1	8.87211379	0.21291770	3.23030946
1	6.50321135	-0.08873958	4.00336329
1	-2.95219489	-1.23015739	6.93558521
1	-5.33708188	-1.59980000	7.62621860
1	-7.15425949	-1.61616138	5.94934321
1	-6.66185567	-1.26281687	3.51374387

$\{Co_3O(Hhp)\}^0$, $S = 1$

27	-0.57608281	0.21792703	-1.76488422
27	1.83947412	0.12573478	0.41771922
27	-1.24649948	-0.33755656	1.35078288
16	3.33413373	1.21825549	-3.60790022

16	-4.80973683	-0.98545868	-1.21057901
16	1.51806283	-0.25808849	4.82034095
8	0.03882889	-0.07491488	-0.00548809
7	0.11352021	-0.22915602	2.62638688
7	-3.47727213	-0.22893822	-3.38147114
7	-1.16970476	0.46308483	-3.56946623
7	3.70175442	0.22042977	0.83557329
7	-2.52628298	-0.66335567	2.73807704
7	1.17011520	0.63682121	-2.27906083
7	1.43915352	-0.11179998	2.21504420
7	-1.12605587	-0.44721287	4.69615712
6	4.73746225	0.42181240	-0.06268910
7	-2.29475473	-0.30601690	-1.26907998
7	2.20917209	0.51584296	-1.35929065
6	-3.37105584	-0.46060330	-2.07414444
7	-2.58146778	-0.54780160	0.06747397
6	-3.54786245	0.51165215	-6.41089643
6	7.34054265	0.45062899	0.17496168
7	3.63860952	-0.10609250	3.22874255
6	-2.28468594	-0.62819495	4.10473934
7	4.62459039	0.69164922	-1.34716149
7	0.87982096	1.20047092	-4.61701386
6	8.36123196	0.31861182	1.12541459
7	-4.50838844	-1.10033166	1.42690913
6	-4.51756633	-1.11106560	3.86951846
6	6.02252544	0.33362572	0.62523115
6	1.59436977	1.01014352	-3.50534951
6	-5.83396481	-1.40642821	4.23414711
6	2.30967411	-0.14123126	3.25367612
6	-2.44470773	0.22558048	-4.05851948
6	8.06856957	0.08245404	2.48371680
6	-3.87453725	-0.88752632	0.27499846
6	3.42256817	0.76225663	-1.91106475
6	-6.12600402	-1.46317089	5.60318440
6	6.74629566	-0.02893393	2.93290719
6	4.27462875	0.04777750	2.08545484
6	-0.01566254	-0.30697916	3.96819683
6	-0.93902514	1.43680037	-7.13845680
6	-1.97910758	1.38594922	-8.07574312
6	-2.50915538	0.56802629	-5.47758237
6	5.73032240	0.09777998	1.98141338
6	-5.12981167	-1.23430786	6.57328896
6	-3.26342675	0.92979079	-7.71739706
6	-3.52348268	-0.88303610	4.83773894
6	-0.40444724	0.92609470	-4.63131857
6	-3.86799353	-0.96663804	2.56857236
6	-1.22752135	1.02296331	-5.83542016
6	-3.81010559	-0.94285268	6.20397263
1	-4.53852238	0.15553664	-6.12681309
1	-4.04942136	0.90238056	-8.47381442
1	-1.79373772	1.70420255	-9.10286228
1	0.05830740	1.78531321	-7.40830504

1	7.55912461	0.63691205	-0.87697952
1	9.40296561	0.40045308	0.81097525
1	8.88891386	-0.01432181	3.19677611
1	6.51199069	-0.20812243	3.98269639
1	-3.03275763	-0.76754593	6.94824924
1	-5.39355254	-1.28617614	7.63081956
1	-7.14329758	-1.68890334	5.92701752
1	-6.59906995	-1.58420022	3.47787733

{Co_3O(Hhp)}, S = 2

27	-0.58194627	0.24111660	-1.78597390
27	1.83853989	0.08494495	0.40839646
27	-1.26244367	-0.29412707	1.37372830
16	3.41523269	0.61709602	-3.72124378
16	-4.97374067	-0.03128053	-1.07101706
16	1.56006438	-0.59933836	4.79133830
8	0.00436081	-0.09093288	-0.01434262
7	0.12985928	-0.42645898	2.62426175
7	-3.57867204	0.41229873	-3.28649456
7	-1.17147515	0.47026068	-3.59377746
7	3.70688849	0.17982477	0.83470945
7	-2.53526903	-0.63342961	2.76634464
7	1.21302296	0.34588882	-2.34892019
7	1.44642827	-0.18039301	2.22527253
7	-1.06713359	-0.91140355	4.67426293
6	4.75058029	0.37207663	-0.06955172
7	-2.37182360	0.10513429	-1.20964011
7	2.23312883	0.30717997	-1.42050886
6	-3.48465893	0.20010150	-1.98654399
7	-2.65766592	-0.15139240	0.11572174
6	-3.58535327	0.82947052	-6.37912194
6	7.33461877	0.61603405	0.20499439
7	3.64345172	-0.07621971	3.24301001
6	-2.25352284	-0.89689523	4.10172210
7	4.64939200	0.47948899	-1.37469604
7	0.96269241	0.62958202	-4.74038561
6	8.34077083	0.63024737	1.17682826
7	-4.60313782	-0.51702238	1.51260021
6	-4.53671998	-1.03437047	3.89469568
6	6.01724813	0.44001400	0.64367156
6	1.65764492	0.51531247	-3.62342939
6	-5.87155699	-1.21886780	4.27362833
6	2.32110806	-0.23842735	3.25216494
6	-2.49203090	0.52258133	-4.03381319
6	8.03970798	0.47166623	2.54693419
6	-3.98345280	-0.25668566	0.36412307
6	3.46058506	0.44362868	-1.97224145
6	-6.12387480	-1.52806035	5.61423070
6	6.72251489	0.29317219	2.98352096
6	4.27281770	0.11592217	2.10211471
6	0.02186565	-0.66039656	3.94972587
6	-0.85988389	0.94819123	-7.25284688

6	-1.91689591	1.06478701	-8.15799072
6	-2.52551106	0.71066398	-5.46871024
6	5.71765704	0.27842091	2.01019345
6	-5.07323019	-1.64902574	6.54974016
6	-3.26309617	1.00685192	-7.72632405
6	-3.48912622	-1.15191116	4.82890366
6	-0.36057559	0.61899474	-4.71680520
6	-3.91978221	-0.70861239	2.61817912
6	-1.18121375	0.77343442	-5.89913840
6	-3.73980542	-1.46287668	6.16995209
1	-4.62068012	0.78236548	-6.03988758
1	-4.06222424	1.10145838	-8.46343502
1	-1.70446023	1.20487833	-9.21918017
1	0.17989007	0.99274194	-7.57855916
1	7.56041932	0.73820938	-0.85472379
1	9.37982317	0.76732201	0.87295241
1	8.85135158	0.48774602	3.27598160
1	6.48115647	0.16824572	4.03952594
1	-2.92239898	-1.55328247	6.88598003
1	-5.30913305	-1.89100961	7.58720292
1	-7.15205585	-1.68022887	5.94657529
1	-6.67827053	-1.12470559	3.54611533

$\{Co_3O(Hhp)\}^-$, S = 3/2

27	-0.56576703	0.20570206	-1.77058259
27	1.82503417	0.07993701	0.39835437
27	-1.26852489	-0.31416539	1.37970023
16	3.41314975	0.01319794	-3.76185286
16	-4.95379070	0.13412831	-1.03593880
16	1.50885267	-0.19849588	4.82798892
8	-0.00737882	-0.09369500	0.00243722
7	0.10363069	-0.29182757	2.62548505
7	-3.55882891	0.64819571	-3.23359663
7	-1.16142446	0.45489287	-3.57945156
7	3.69375990	0.19877830	0.82517828
7	-2.53833506	-0.66078047	2.75948249
7	1.21377606	0.13188772	-2.35519438
7	1.41711273	-0.02556062	2.22402212
7	-1.08186493	-0.76358902	4.68583197
6	4.74716908	0.20502571	-0.08372707
7	-2.34737287	0.17002306	-1.19126581
7	2.23198553	0.07747108	-1.43142397
6	-3.45860300	0.36187142	-1.94501614
7	-2.63609041	-0.15072825	0.13941719
6	-3.55124421	1.13400883	-6.32043287
6	7.33332172	0.41970149	0.18422784
7	3.59006945	0.27401619	3.25154010
6	-2.25766814	-0.87844661	4.09784092
7	4.65181682	0.10698882	-1.40373941
7	0.95743098	0.30647254	-4.75546212
6	8.32976502	0.57347159	1.15041896
7	-4.59724124	-0.58427418	1.49550533

6	-4.52456157	-1.16078020	3.87030626
6	6.00068406	0.35359666	0.62039259
6	1.65217888	0.15184340	-3.64421070
6	-5.84960417	-1.41933816	4.23704474
6	2.28311355	0.06352580	3.26413383
6	-2.46848480	0.67368460	-3.99270118
6	8.01034308	0.65749635	2.52766662
6	-3.96683048	-0.24439398	0.37412721
6	3.47216258	0.05366321	-1.99300320
6	-6.10359628	-1.73898476	5.57718867
6	6.68571476	0.58900507	2.96568466
6	4.24209164	0.31948392	2.09468163
6	-0.00816930	-0.44728760	3.96638078
6	-0.85809951	0.86205227	-7.24651713
6	-1.90438789	1.12468537	-8.13323700
6	-2.50230000	0.87468116	-5.42602729
6	5.68168513	0.43913204	1.99777654
6	-5.05993565	-1.79201447	6.52444221
6	-3.23804657	1.25960383	-7.67588345
6	-3.48136827	-1.21378249	4.81712348
6	-0.35794343	0.47841271	-4.71507519
6	-3.90738933	-0.79447393	2.60062785
6	-1.16853379	0.73825659	-5.88309444
6	-3.73429835	-1.52684411	6.15693674
1	-4.57577978	1.23312436	-5.95849260
1	-4.03155239	1.46441783	-8.39752984
1	-1.69407136	1.22831183	-9.19988996
1	0.17118002	0.75535020	-7.59231937
1	7.57259862	0.35271430	-0.87814353
1	9.37586410	0.63009563	0.84189353
1	8.81520776	0.77703162	3.25586733
1	6.42946043	0.64964629	4.02452947
1	-2.92118227	-1.56103193	6.88334916
1	-5.29189633	-2.04339852	7.56141902
1	-7.12620144	-1.95019154	5.89655300
1	-6.65079154	-1.37150103	3.49825280

$\{Co_3O(Hhp)\}^{-}$, $S = 1/2$

27	-0.58133509	0.23083878	-1.78275552
27	1.84057643	0.10189519	0.41413893
27	-1.25926688	-0.33231870	1.36868928
16	3.37826667	0.89180669	-3.67186124
16	-4.93782460	-0.27279162	-1.11095189
16	1.55944660	-0.61805068	4.78295438
8	-0.00000798	0.00013405	0.00005472
7	0.12071630	-0.40328121	2.60641420
7	-3.55836706	0.20382287	-3.31665776
7	-1.17127613	0.46500602	-3.59201175
7	3.70844463	0.20510498	0.83439165
7	-2.53719121	-0.66983444	2.75766971
7	1.17915945	0.47565659	-2.31386144
7	1.44586678	-0.21769218	2.19834568

7	-1.07372443	-0.84088581	4.67371521
6	4.74138402	0.44060729	-0.05588632
7	-2.33528439	-0.01661000	-1.23162524
7	2.21450451	0.42045717	-1.37471698
6	-3.44959840	0.00559583	-2.00884856
7	-2.62509126	-0.25742114	0.11559232
6	-3.57766514	0.69283365	-6.40195882
6	7.33614512	0.63484146	0.20712358
7	3.64744486	-0.17960519	3.21987092
6	-2.26338197	-0.85847234	4.10097466
7	4.63203746	0.63758002	-1.35699202
7	0.94335890	0.83434899	-4.70292724
6	8.35415948	0.57487694	1.16723604
7	-4.59085205	-0.65435109	1.48312160
6	-4.54013514	-1.03368404	3.89442525
6	6.01965217	0.44579651	0.64266345
6	1.62950393	0.71695750	-3.57292077
6	-5.87443527	-1.21609521	4.27515587
6	2.32588801	-0.30157903	3.23023316
6	-2.47801293	0.41801529	-4.04506926
6	8.06180763	0.33228512	2.52620784
6	-3.95546565	-0.41475131	0.34278324
6	3.43674234	0.62058836	-1.93360112
6	-6.13769093	-1.45554940	5.62982261
6	6.74376967	0.14326391	2.96073240
6	4.28065596	0.05819893	2.08579735
6	0.01277957	-0.62550024	3.94254106
6	-0.86927786	1.07227007	-7.23597014
6	-1.92404216	1.12255323	-8.15613855
6	-2.52280100	0.64280898	-5.48362049
6	5.72758218	0.20335327	2.00034782
6	-5.09339623	-1.51080557	6.57719821
6	-3.26069547	0.93530826	-7.74453194
6	-3.49681961	-1.08890086	4.84090895
6	-0.37150060	0.71317001	-4.69373802
6	-3.90916090	-0.77135373	2.60794908
6	-1.18741007	0.82994980	-5.89482946
6	-3.75843676	-1.32805117	6.19477394
1	-4.60791903	0.54682362	-6.07429842
1	-4.05966196	0.98072318	-8.48753043
1	-1.71119587	1.30970697	-9.21071271
1	0.16714679	1.21581972	-7.54471082
1	7.55238470	0.82190976	-0.84565810
1	9.39271512	0.71798592	0.86165690
1	8.87905962	0.29176559	3.24933574
1	6.50799026	-0.04481915	4.00912940
1	-2.94443398	-1.36896923	6.91991433
1	-5.33297642	-1.69939977	7.62576396
1	-7.16777351	-1.60232607	5.96124846
1	-6.67508122	-1.17156132	3.53550314

$\{Co_3O(Hhp)\}^{2-}$, $S = 0$

27	-0.58731401	0.23185807	-1.79438470
27	1.85259864	0.10178655	0.41899868
27	-1.27152834	-0.33500018	1.38185175
16	3.39143518	0.89000027	-3.68630009
16	-4.94209208	-0.26942423	-1.11221002
16	1.56030930	-0.61766464	4.78738768
8	0.01276805	0.00337479	-0.01420617
7	0.11744186	-0.40302815	2.60492589
7	-3.56549646	0.20616436	-3.31948043
7	-1.17228391	0.46592764	-3.60091107
7	3.71772713	0.20548977	0.83466507
7	-2.54401664	-0.67078513	2.76451863
7	1.19276743	0.47516600	-2.31640067
7	1.45299903	-0.21627322	2.19643284
7	-1.07222686	-0.84138587	4.67805626
6	4.75635818	0.43991333	-0.05148155
7	-2.33406817	-0.01400790	-1.23860051
7	2.21551173	0.42073307	-1.38846548
6	-3.44968979	0.00887906	-2.01399181
7	-2.62395675	-0.25645319	0.11887818
6	-3.58419360	0.69480367	-6.40676491
6	7.34979475	0.63364849	0.21627655
7	3.65086871	-0.17905148	3.22728886
6	-2.26947550	-0.85979962	4.10702079
7	4.63763636	0.63623279	-1.36378001
7	0.94990078	0.83232087	-4.70957467
6	8.36493372	0.57413835	1.17822954
7	-4.59641435	-0.65260057	1.48207672
6	-4.54534824	-1.03348120	3.89585040
6	6.02297275	0.44577740	0.64133543
6	1.63267397	0.71627471	-3.58933607
6	-5.88020417	-1.21685773	4.28228028
6	2.33107582	-0.30005535	3.23026954
6	-2.48233270	0.42008728	-4.05309376
6	8.07340981	0.33246531	2.54060875
6	-3.95734758	-0.41328366	0.34626938
6	3.45269671	0.61949429	-1.93811423
6	-6.14547361	-1.45740950	5.63788428
6	6.74975232	0.14464508	2.96706477
6	4.28941781	0.05911151	2.09029807
6	0.00956498	-0.62561709	3.94376370
6	-0.87957077	1.07112961	-7.24923364
6	-1.93622625	1.12181848	-8.16603345
6	-2.53040844	0.64354516	-5.48793330
6	5.73267100	0.20352413	2.00808970
6	-5.10012560	-1.51340847	6.58578348
6	-3.27619101	0.93628906	-7.75441496
6	-3.49779273	-1.08961307	4.84582030
6	-0.37664530	0.71314647	-4.70884652
6	-3.91541855	-0.77163705	2.61445128
6	-1.18599401	0.82932640	-5.89865112
6	-3.76443932	-1.33017425	6.20067993

1	-4.61369773	0.54951313	-6.07330771
1	-4.07811724	0.98193747	-8.49542501
1	-1.72348006	1.30851485	-9.22230409
1	0.15606830	1.21385549	-7.56316210
1	7.57084548	0.81997863	-0.83629271
1	9.40501933	0.71711644	0.87228009
1	8.88921196	0.29207499	3.26662618
1	6.50862856	-0.04286004	4.01534507
1	-2.94916295	-1.37150095	6.92519853
1	-5.33871551	-1.70274373	7.63554016
1	-7.17681153	-1.60428802	5.96885020
1	-6.68079988	-1.17165865	3.54180379

$\{(Co_3O)Hhp\}^{2-}$, $S = 1$

27	-0.57734968	0.24701042	-1.78240423
27	1.84075111	0.11831295	0.41125362
27	-1.26592137	-0.36597177	1.37424662
16	3.33248126	1.37261840	-3.59335840
16	-4.91661243	-0.51465827	-1.14287637
16	1.57522350	-0.86489216	4.74529608
8	0.00632669	0.00451071	-0.00637196
7	0.12293885	-0.48014917	2.59690397
7	-3.53788364	-0.03893921	-3.35006743
7	-1.17523815	0.47147526	-3.60002817
7	3.71741151	0.21099914	0.83792491
7	-2.54165841	-0.68448128	2.76168582
7	1.17288923	0.65518788	-2.28647891
7	1.45412574	-0.32557621	2.18145135
7	-1.07089190	-0.89625871	4.67094740
6	4.74114756	0.56866690	-0.03067048
7	-2.32540135	-0.12395535	-1.24727564
7	2.19850093	0.60057631	-1.35624829
6	-3.42832429	-0.19370271	-2.04632626
7	-2.62049691	-0.33277470	0.10885238
6	-3.54265905	0.46173724	-6.44335166
6	7.33164395	0.74979067	0.23498112
7	3.66427528	-0.42171645	3.18359705
6	-2.26851584	-0.85400556	4.10864191
7	4.60379679	0.92299500	-1.30826225
7	0.91400615	1.11964264	-4.65479549
6	8.35828206	0.57904722	1.16739415
7	-4.59226034	-0.70530789	1.47762813
6	-4.55055527	-0.96072930	3.90662891
6	6.01118256	0.49861243	0.64547049
6	1.59619993	1.02222744	-3.53355179
6	-5.88883560	-1.09427197	4.29953306
6	2.34966181	-0.50220029	3.19499545
6	-2.46167853	0.28189645	-4.07457441
6	8.07951661	0.16409486	2.49526310
6	-3.94649232	-0.52501778	0.33172328
6	3.41887737	0.92497532	-1.88059257
6	-6.15880555	-1.28268312	5.66191872

6	6.76841107	-0.08699302	2.90962791
6	4.30081962	-0.07808786	2.05955497
6	0.01671630	-0.73904152	3.92613875
6	-0.88984474	1.18710789	-7.22273062
6	-1.92454449	1.12615007	-8.15995830
6	-2.50646494	0.51900451	-5.49701161
6	5.73214462	0.08072799	1.97644517
6	-5.11344300	-1.33971688	6.61005127
6	-3.24155533	0.76655366	-7.77391503
6	-3.50370493	-1.01788656	4.85611278
6	-0.38894661	0.84138220	-4.68422225
6	-3.91608837	-0.76411044	2.61421900
6	-1.18626223	0.88133201	-5.88344639
6	-3.77426534	-1.20967613	6.21746790
1	-4.55326666	0.18532947	-6.13581772
1	-4.02963883	0.72828871	-8.53053868
1	-1.71942369	1.35901775	-9.20825658
1	0.12610951	1.46373277	-7.51174968
1	7.53791598	1.06945059	-0.78849163
1	9.39398647	0.76760035	0.87242908
1	8.90449605	0.03982288	3.20166197
1	6.54338725	-0.40541087	3.92957353
1	-2.95873528	-1.25482836	6.94149678
1	-5.35522505	-1.48794315	7.66559884
1	-7.19339439	-1.38762644	5.99839773
1	-6.68884127	-1.05126502	3.55825961

$\{Co_3O(Hhp)\}^{2-}$, $S = 0$, full electron basis calculation

27	-0.58641227	0.23239258	-1.79365546
27	1.85195069	0.10239199	0.41817400
27	-1.27030065	-0.33421378	1.38074904
16	3.39255248	0.89135704	-3.68761989
16	-4.94043610	-0.26896624	-1.10978275
16	1.55900893	-0.61696737	4.78546876
8	0.01461801	0.00434248	-0.01583929
7	0.12060483	-0.40295058	2.60933432
7	-3.56476597	0.20629394	-3.31712249
7	-1.17308580	0.46681383	-3.60387553
7	3.72048757	0.20611684	0.83511919
7	-2.54613811	-0.67105560	2.76747622
7	1.20123482	0.47707448	-2.31941250
7	1.45328131	-0.21668592	2.20237353
7	-1.07168121	-0.84062209	4.67611820
6	4.75426016	0.44057049	-0.05450182
7	-2.34000042	-0.01397909	-1.23838331
7	2.21798417	0.42298091	-1.39709704
6	-3.45107881	0.00986032	-2.01711790
7	-2.62802781	-0.25584508	0.11618977
6	-3.57835298	0.69382109	-6.40054240
6	7.34241045	0.63194529	0.21992180
7	3.64877701	-0.17872245	3.22613917
6	-2.26567559	-0.85894297	4.10581693

7	4.63600594	0.63661986	-1.36398572
7	0.94995718	0.83256801	-4.70772873
6	8.35510928	0.57239118	1.17844781
7	-4.59357380	-0.65182296	1.48166673
6	-4.54110765	-1.03251513	3.89229132
6	6.01696755	0.44533466	0.64008154
6	1.63289583	0.71792970	-3.59507701
6	-5.87186809	-1.21613261	4.27980002
6	2.33463459	-0.29935727	3.23089131
6	-2.48339666	0.41963087	-4.04901437
6	8.06332823	0.33096744	2.53902154
6	-3.95844215	-0.41326362	0.34924483
6	3.45845574	0.62088813	-1.93904366
6	-6.13836662	-1.45648795	5.63131974
6	6.74247071	0.14435844	2.96161593
6	4.28520106	0.05892807	2.09079057
6	0.00690477	-0.62574274	3.94594141
6	-0.88265039	1.06913219	-7.24130967
6	-1.93531494	1.11949240	-8.15631405
6	-2.52876248	0.64261142	-5.48198021
6	5.72648572	0.20307489	2.00645108
6	-5.09481382	-1.51240016	6.57785076
6	-3.27360359	0.93413115	-7.74495525
6	-3.49447249	-1.08859728	4.84161501
6	-0.37405301	0.71343277	-4.70650127
6	-3.91386611	-0.77065838	2.61084862
6	-1.18454056	0.82842828	-5.89257430
6	-3.76317478	-1.32910412	6.19245631
1	-4.60817372	0.54765543	-6.06173434
1	-4.07685964	0.97956059	-8.48720011
1	-1.72270678	1.30615878	-9.21450704
1	0.15605014	1.21168609	-7.55228920
1	7.56055430	0.81845447	-0.83532975
1	9.39721690	0.71521697	0.87278292
1	8.88024876	0.29018985	3.26647558
1	6.49561210	-0.04375764	4.01059580
1	-2.94346500	-1.36971040	6.91504041
1	-5.33415481	-1.70236043	7.62918235
1	-7.17134912	-1.60392994	5.96279218
1	-6.67059729	-1.17001111	3.53441032

$\{Co_3O(Hhp)\}^{2-}$, $S = 1$, full electron basis calculation

27	-0.57546603	0.23446378	-1.79001889
27	1.84746240	0.10517454	0.40770824
27	-1.26789965	-0.33196056	1.37817609
16	3.39671640	0.89369759	-3.69202445
16	-4.94479942	-0.26761066	-1.10447825
16	1.55428857	-0.61613078	4.79018807
8	0.00807180	0.00441115	-0.00871200
7	0.12093002	-0.40208413	2.61435140
7	-3.57142290	0.20658686	-3.31183704
7	-1.17707773	0.46848382	-3.60946210

7	3.72649657	0.20715896	0.83860116
7	-2.54558010	-0.66979411	2.76695150
7	1.20285108	0.47984214	-2.32653615
7	1.44722845	-0.21637537	2.20753525
7	-1.07615722	-0.84024576	4.67853981
6	4.75844535	0.44205711	-0.05801329
7	-2.34465821	-0.01347964	-1.23173864
7	2.22507040	0.42542704	-1.39925706
6	-3.45613496	0.01191948	-2.01991359
7	-2.63307218	-0.25450245	0.11636209
6	-3.57810277	0.69353493	-6.40227466
6	7.34336019	0.63059889	0.21831841
7	3.64422441	-0.17882647	3.23320342
6	-2.26601098	-0.85837825	4.10708846
7	4.64013945	0.63806983	-1.36692518
7	0.95262792	0.83409012	-4.71205143
6	8.35637963	0.57112980	1.17371534
7	-4.59554393	-0.65136440	1.48644179
6	-4.54207498	-1.03324029	3.89421611
6	6.01842982	0.44535273	0.63771875
6	1.63671310	0.72013318	-3.59996783
6	-5.87234744	-1.21782756	4.28096691
6	2.33799602	-0.29811318	3.23558326
6	-2.48462350	0.42111800	-4.05247777
6	8.05938532	0.32931565	2.53740896
6	-3.96046337	-0.41195180	0.35163981
6	3.46304798	0.62305808	-1.94318697
6	-6.13911091	-1.45919898	5.63204836
6	6.74411178	0.14402569	2.96119707
6	4.28881153	0.06005465	2.09170327
6	0.00481978	-0.62474609	3.94811379
6	-0.88117903	1.06759436	-7.24250131
6	-1.93072268	1.11784636	-8.15814538
6	-2.52788069	0.64177093	-5.47638316
6	5.72081499	0.20257411	2.00606511
6	-5.09556263	-1.51511668	6.57856487
6	-3.27167625	0.93202940	-7.74131430
6	-3.49631671	-1.08928209	4.84273779
6	-0.37087759	0.71499454	-4.71094093
6	-3.91507634	-0.77003975	2.61137282
6	-1.18229936	0.82836303	-5.89424362
6	-3.76432989	-1.33076172	6.19296272
1	-4.60881413	0.54815057	-6.06575290
1	-4.07501746	0.97716796	-8.48399610
1	-1.71997646	1.30347480	-9.21659481
1	0.15836995	1.20941069	-7.55214850
1	7.56006670	0.81655725	-0.83766832
1	9.39885238	0.71290307	0.86984726
1	8.87671127	0.28825831	3.26491099
1	6.49962522	-0.04354157	4.01085860
1	-2.94433071	-1.37129181	6.91524171
1	-5.33458707	-1.70588488	7.62976498

1	-7.17203524	-1.60743611	5.96317007
1	-6.67081995	-1.17161434	3.53529041

Energy = -7387.4826257366