

Heterometallic Co^{II}-Li^I carboxylate complexes with N-heterocyclic carbene, triphenylphosphine and pyridine: a comparative study of magnetic properties

**Dmitriy S. Yambulatonov, Stanislav A. Nikolaevskii, Maxim A. Shmelev,
Konstantin A. Babeshkin, Denis V. Korchagin, Nikolay N. Efimov,
Alexander S. Goloveshkin, Pavel A. Petrov, Mikhail A. Kiskin,
Maxim N. Sokolov and Igor L. Eremenko**

Table of contents

General remarks.....	S2
Synthesis of [Co ₂ Li ₂ (Piv) ₆ (IMes) ₂] (1).....	S2
Synthesis of [Co ₂ Li ₂ (Piv) ₆ (Ph ₃ P) ₂] (2)	S3
Synthesis of [Co ₂ Li ₂ (Fur) ₆ (py) ₂] (5).....	S3
Single crystal X-ray studies	S3
Powder X-ray diffraction studies.....	S5
Magnetic measurements	S7
Computational details	S11
References	S12

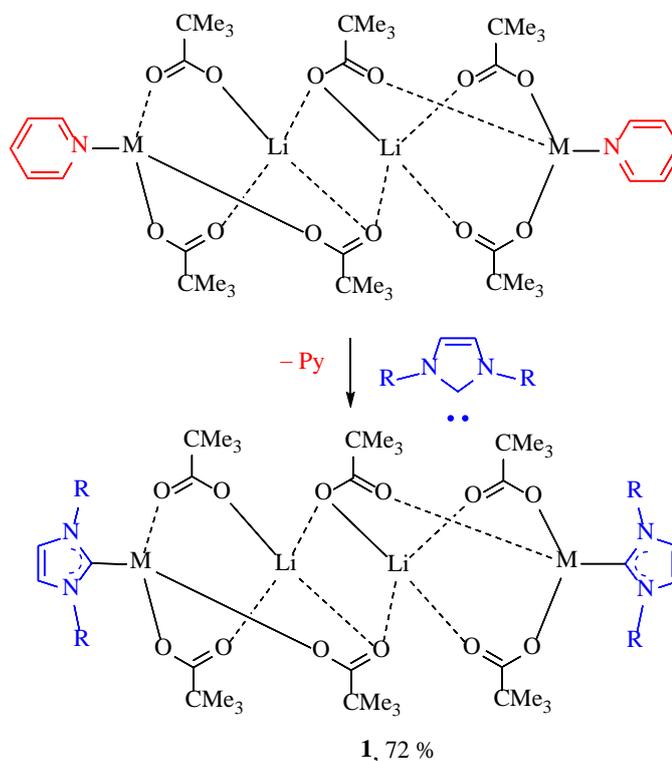
General remarks

All manipulations were carried out under an inert atmosphere using vacuumed evacuated glass ampoules or argon-filled glovebox. Solvents were dried with common methods (THF – reflux over Na with benzophenone, Hexane – over Na, Acetonitrile – over P₂O₅) and withdrawn by condensation just before the synthesis. Cobalt and lithium trimethylacetates and [Co₂Li₂(Piv)₆(Py)₂] were synthesized as reported^{S1-S3}. IMes (1,3-Bis(2,4,6-trimethylphenyl)imidazol-2-ylidene) was synthesized according to known procedure^{S4}. Triphenylphosphine (99 %, Alfa Aesar) and 2-furoic acid (FurH) were used as received.

IR spectra of the compounds were recorded on a Perkin Elmer Spectrum 65 spectrophotometer equipped with a Quest ATR Accessory (Specac) by the attenuated total reflectance (ATR) in the range of 400–4000 cm⁻¹.

Synthesis of [Co₂Li₂(Piv)₆(IMes)₂] (1)

In a glass ampoule were placed [Co₂Li₂(Piv)₆(Py)₂] (0.224 g, 0.250 mmol), IMes (0.152 g, 0.500 mmol) and THF (15 mL) was condensed into the ampoule, the latter was sealed and heated in an oil bath at 100°C in 10 h. Then all volatile products were evaporated and 1 ml of hexane was condensed to the residue. The glass ampoule was sealed, heated at 120 °C for 5 hours (until the reactants completely dissolved). The pink-colored reaction mixture was slowly cooled (10°C/h) to RT. In 24 h pink needle-like crystals were formed (0.242 g, 72%). Anal. calcd for C₇₂H₁₀₂Co₂Li₂N₄O₁₂ (1347.34) C, 64.18; H, 7.63; N, 4.16. Found: C, 64.14; H, 7.57; N, 4.13. IR, ν/cm⁻¹: 3182 w, 3161 w, 3134 w, 2954 m, 2920 m, 2864 m, 1613 s, 1579 s, 1558 s, 1480 s, 1455 m, 1420 m, 1401 vs, 1365 m, 1355 s, 1273 w, 1260 w, 1223 s, 1164 w, 1101 w, 1080 w, 1032 m, 1017 w, 963 w, 929 m, 892 m, 848 m, 791 m, 764 w, 734 m, 692 m, 640 w, 609 s, 573 m, 460 m, 445 m, 435 m, 418 m.



Scheme S1

Synthesis of $[\text{Co}_2\text{Li}_2(\text{Piv})_6(\text{Ph}_3\text{P})_2]$ (2)

Weighed portions of $[\text{Co}(\text{Piv})_2]_n$ (0.260 g, 1.000 mmol), $[\text{LiPiv}]_n$ (0.108 g, 1.000 mmol), Ph_3P (0.262 g, 1.000 mmol) were placed in a glass ampoule and degassed in a dynamic vacuum for 20 min, acetonitrile (20 ml) was condensed into the ampoule, the latter was fire-sealed and heated in an oil bath (120 °C) until the all reactants dissolved with formation of clear violet solution. The reaction mixture was slowly cooled (10°C/h) to 40 °C. Maintenance (1 h) at that temperature and further cooling to RT resulted the formation of rhombic violet crystals (0.587 g, 93%). Anal. calcd for $\text{C}_{66}\text{H}_{84}\text{Co}_2\text{Li}_2\text{O}_{12}\text{P}_2$ (1263.06) C, 62.76; H, 6.70. Found: C, 62.67; H, 6.64. IR, v/cm^{-1} : 3073 w, 3054 w, 2958 m, 2928 w, 2903 w, 2868 w, 1612 s, 1581 m, 1562 s, 1481 s, 1457 w, 1436 w, 1415 s, 1401 vs, 1354 s, 1222 s, 1185 w, 1099 m, 1028 m, 997 w, 937 w, 898 w, 791 m, 752 m, 744 m, 693 vs, 617 s, 576 m, 518 m, 496 s.

Synthesis of $[\text{Co}_2\text{Li}_2(\text{Fur})_6(\text{py})_2]$ (5)

In a glass ampoule were placed weighed portions of $[\text{Co}(\text{Piv})_2]_n$ (0.260 g, 1.000 mmol), $[\text{LiPiv}]_n$ (0.108 g, 1.000 mmol) and FurH (0.336 g, 3.000 mmol). Vial was degassed in dynamic vacuum for 20 min. To reactants was condensed acetonitrile (15 ml) and Pyridine (0.079 g, 1.000 mmol). Ampoule was fire-sealed and heated in an oil bath (100 °C) until the formation of clear solution. Reaction mixture color changed from violet to pink. Further cooling to RT lead to the formation of pink rectangle-shaped crystals (0.399 g, 84%). Anal. calcd for $\text{C}_{40}\text{H}_{28}\text{Co}_2\text{Li}_2\text{N}_2\text{O}_{18}$ (956.40) C, 50.23; H, 2.95; N, 2.93. Found: C, 50.14; H, 2.88; N, 2.84. IR, v/cm^{-1} : 3160 w, 3141 w, 3120 w, 1617 m, 1599 m, 1582 s, 1554 m, 1470 s, 1451 m, 1407 s, 1392 s, 1359 vs, 1245 w, 1228 w, 1218 w, 1199 s, 1138 w, 1075 w, 1045 w, 1022 w, 1007 m, 933 m, 883 m, 843 w, 799 m, 784 s, 753 vs, 696 s, 641 w, 614 w, 582 m, 496 s, 435 m, 420 w.

Single crystal X-ray studies

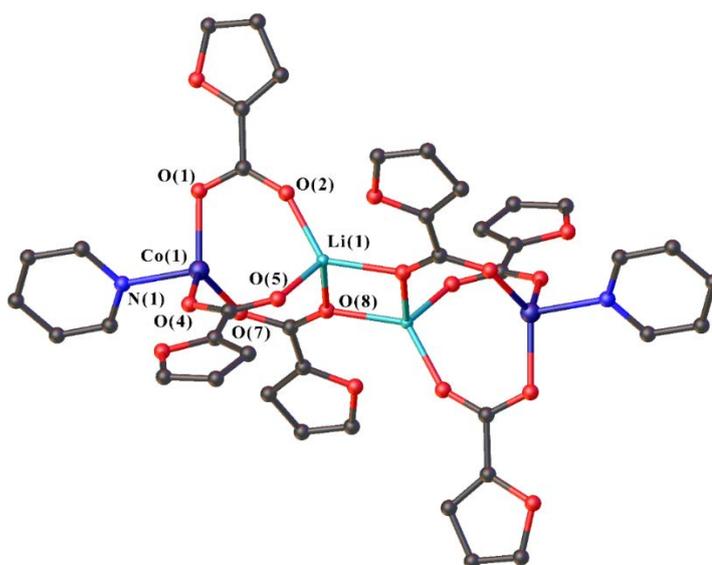


Figure S1. Molecular structure of $[\text{Co}_2\text{Li}_2(\text{Fur})_6(\text{py})_2]$ (5). Hydrogen atoms are omitted.

Table S1. Selected bond lengths (Å), angles (deg.) and distortion parameters in **1-5**.

Complex/ parameter	1	2	3	4	5
Ref.	This work	This work	Sapianik et al. ^{S3}	Dobrokhotova et al. ^{S5}	This work
Co-N/P/C	Co1A: 2.064 Co2A: 2.064 Co1B: 2.066 Co2B: 2.063	2.403(2)	2.103	2.080	2.040(5)
Co-O	Co1A: 1.952, 1.952, 1.968 Co2A: 1.949, 1.967, 1.982 Co1B: 1.933, 1.948, 1.987 Co2B: 1.952, 1.964, 1.980	1.926(6), 1.926(6), 1.933(7)	1.974, 1.974, 2.006	1.957, 1.979, 2.020, 2.394*	1.929(4), 1.955(5), 1.932(5), 2.591(5)*
O-Co-O	Co1A: 103.4, 117.0, 122.3 Co2A: 105.9, 110.5, 127.8 Co1B: 107.2, 115.4, 119.1 Co2B: 102.7, 109.5, 131.1	112.7(3), 114.7(3), 127.2(3)	104.9, 120.5, 129.4	104.8, 115.9, 133.3, 58.6*, 92.8*, 96.3*	113.5(2), 116.4(2), 123.2(2), 58.6(2)*, 92.8(2)*, 96.3(2)*
O-Co- N/P/C	Co1A: 99.5, 104.0, 109.8 Co2A: 100.4, 103.6, 106.5 Co1B: 99.9, 105.8, 108.1 Co2B: 98.6, 103.1, 111.1	92.43(17), 100.0(2), 101.11(17)	94.5, 96.9, 101.6	96.5, 97.5, 99.6, 155.9*	96.4(2), 99.9(2), 100.1(2), 155.9(2)*
Li-O	1.832-2.000	1.86(2)- 1.995(19)	1.887-2.022	1.815-1.979	1.888(11)- 2.029(12)
Li-Li-Co	112.5, 116.9, 117.5, 120.0	122.5(8)	123.4	123.3	117.1
Li...Co	3.243, 3.258, 3.271, 3.276	3.120(13)	3.114	3.157	3.182
Li...Li	2.73, 2.77	2.75(3)	2.752	2.69	2.884
Co...Co	7.916, 8.107	8.059	8.077	8.111	8.098
Co...Co _{min}	7.916	8.059	5.599	7.396	5.914
S _Q (P)	Co1: 0.805 (T-4) Co2: 0.831 (T-4) Co3: 0.421 (T-4) Co4: 1.355 (T-4)	1.154 (T- 4)	1.691 (T-4)	CoO ₃ N: 1.677 (T-4) CoO ₄ N*: 3.642 (TBPY-5)	1.002 (T- 4)

* the parameter for an O atom with an extended Co-O bond

Table S2. CH... π interactions in the crystal of compound **1**.

CH... π	Symmetry transformation	H..Cg, Å	H-Perp, Å	Gamma, °	XH..Cg, °	X..Cg, Å
C41 -H41F... π	Intramolecular	2.92	2.49	31.76	129	3.61(4)
C42 -H42F... π	Intramolecular	2.87	-2.43	31.86	118	3.43(5)
C49 -H49A... π	Intramolecular	2.94	-2.56	29.71	117	3.491(15)
C53 -H53... π	-1-X,1-Y,1-Z	2.57	-2.55	7.07	156	3.44(2)
C61B -H61G... π	Intramolecular	2.58	-2.13	34.23	129	3.27(2)
C70 -H70C... π	Intramolecular	2.76	2.33	32.21	110	3.22(3)
C70A -H70F... π		2.94	2.32	37.92	119	3.51(2)
C40B -H40C... π	Intramolecular	2.89	-2.57	27.45	120	3.48(4)

Powder X-ray diffraction studies

The powder patterns were measured with a step size of 0.020° using Bruker D8 Advance Vario ($\lambda(\text{Cu-K}\alpha 1) = 1.54060 \text{ \AA}$; Ge(111)-monochromator, transmission mode) diffractometer. The obtained patterns were Rietveld refined using TOPAS 5 software.

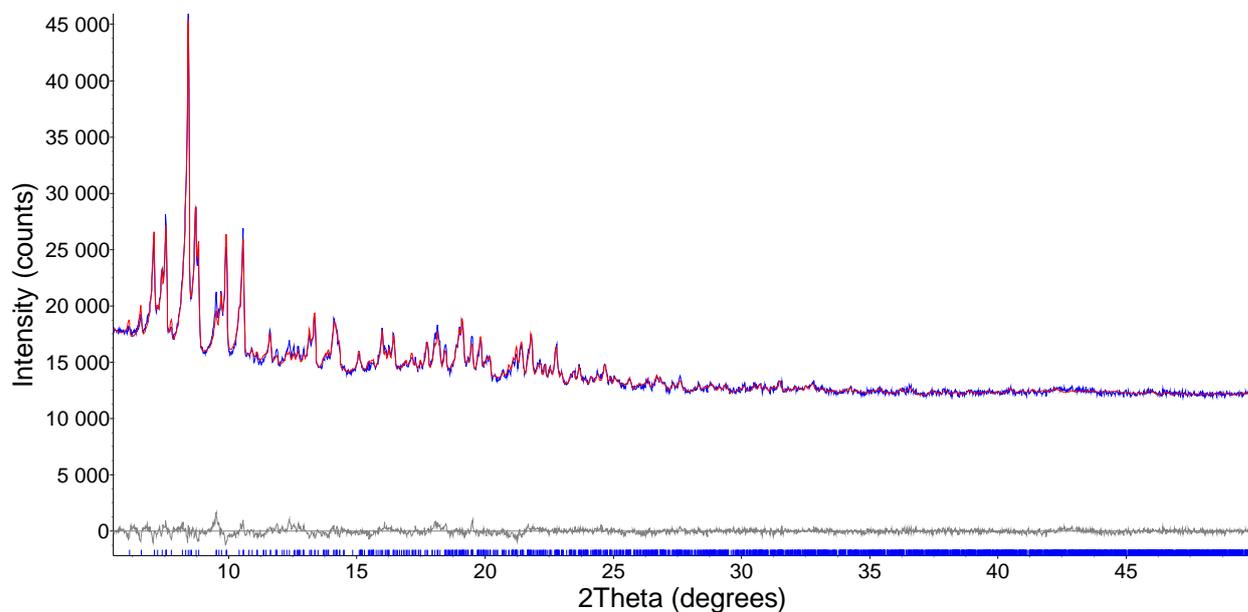


Figure S2. Theoretical (red line) and experimental (blue line) powder patterns of **1** and their difference (grey line).

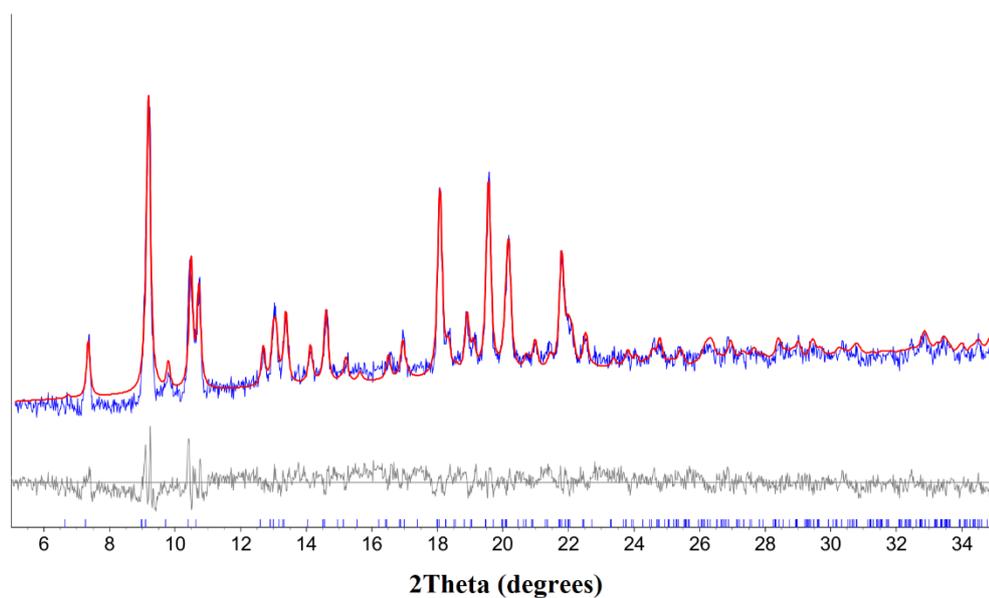


Figure S3. Theoretical (red line) and experimental (blue line) powder patterns of **2** and their difference (grey line).

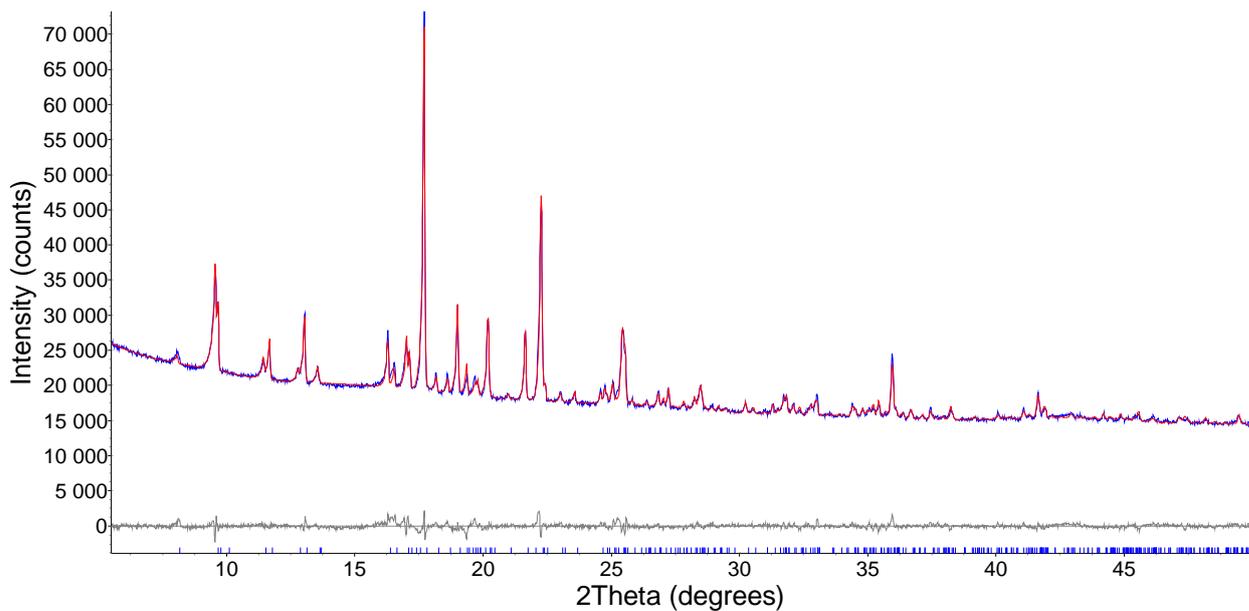


Figure S4. Theoretical (red line) and experimental (blue line) powder patterns of **5** and their difference (grey line).

Magnetic measurements

Magnetic susceptibility measurements were performed using a Quantum Design PPMS-9 susceptometer. All dc susceptibility measurements were carried out under magnetic field equal to 5000 Oe and in 2-300 K temperature range. For ac susceptibility measurements of all the samples, oscillating ac fields of 5 Oe, 3 Oe and 1 Oe within frequency ranges 10-100, 100-1000 and 1000-10000 Hz, respectively, have been applied. These settings allowed one both to avoid sample heating at low temperatures (which may occur when modulation amplitudes and frequency are high) and to obtain the best signal-to-noise ratio. All magnetic measurements were performed on polycrystalline samples sealed in polyethylene bags and covered with mineral oil in order to prevent field-induced orientation of crystallites. The paramagnetic components of the magnetic susceptibility χ were determined taking into account both the diamagnetic contribution evaluated from Pascal's constants and contributions of the sample holder and mineral oil.

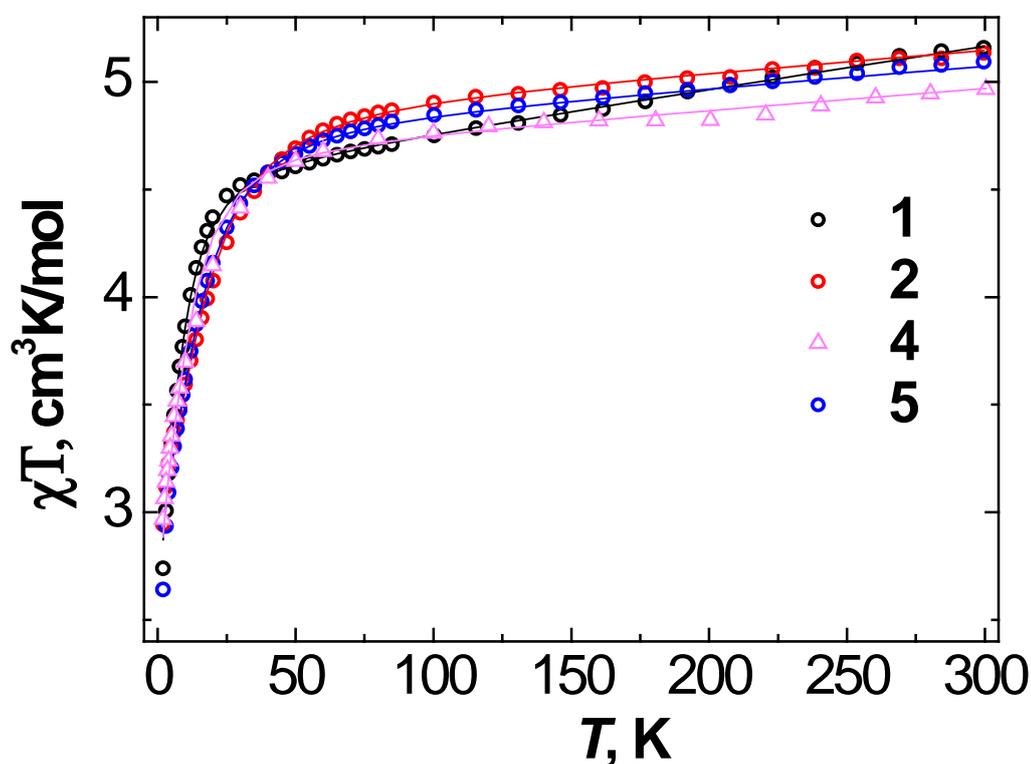


Figure S5. $\chi_m T$ vs. T dependencies for **1**, **2**, **4** and **5** under 5000 Oe dc-magnetic field. Theoretical curve (solid lines) are calculated using PHI^{S6}.

Table S3. Approximation parameters of the $\chi_M T(T)$ dependences for complexes **1**, **2**, **4** and **5** obtained by the PHI program and quantum chemical calculated (QCC) parameters of D and g tensors for **1–5**.

Fitting parameter	1		2		3	4		5	
	Value								
	PHI	QCC	PHI	QCC	QCC	PHI	QCC	PHI	QCC
g_x	-	2.297 (Co1) 2.301 (Co2) 2.294 (Co3) 2.325 (Co4)	-	2.344	2.431	-	2.415	-	2.320
g_y	-	2.228 (Co1) 2.239 (Co2) 2.234 (Co3) 2.228 (Co4)	-	2.255	2.274	-	2.246	-	2.270
g_z	-	2.133 (Co1) 2.130 (Co2) 2.134 (Co3) 2.137 (Co4)	-	2.044	2.082	-	2.108	-	2.090
g_{iso}	2.207 ± 0.001	2.219 (Co1) 2.223 (Co2) 2.221 (Co3) 2.230 (Co4)	2.274 ± 0.001	2.214	2.262	2.232	2.256	2.257 ± 0.002	2.227
D, cm^{-1}	10.4 ± 0.1	+14.58 (Co1) +15.79 (Co2) +14.66 (Co3) +15.06 (Co4)	20.5 ± 0.3	+28.82	+28.45	13.2	+23.85	18.0 ± 0.3	+22.69
E/D	-	0.201 (Co1) 0.189 (Co2) 0.179 (Co3) 0.302 (Co4)	-	0.138	0.248	-	0.332	-	0.097
TIP, cm^3/mol	0.002	-	0.001	-	-	0.001	-	0.001	-
Residual*	0.031		0.044					0.079	

* The residual values of the approximation parameters were calculated using the equation

$$Residual = \sum_{i=1}^n (\chi_{exp} - \chi_{calc})^2,$$

where n – number of the experimental points. In the case of complexes **1**, **2** and **5**, $n = 41$.

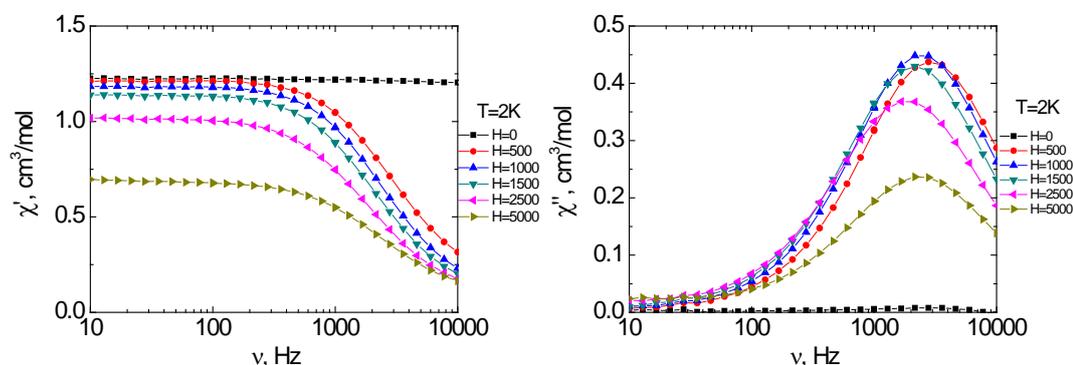


Figure S6. Frequency dependencies of the real, χ' (left) and imaginary, χ'' (right) components of dynamic magnetic susceptibility for complex **1** at $T = 2$ K under various dc magnetic fields (Oe). Solid lines are visual guides.

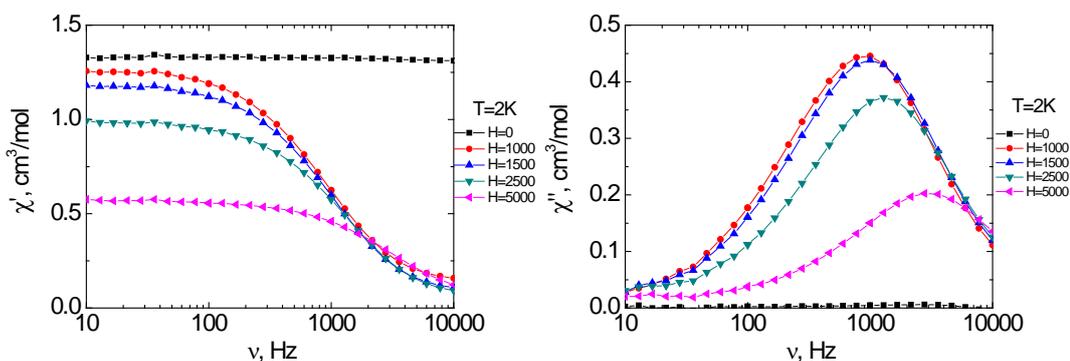


Figure S7. Frequency dependencies of the real, χ' (left) and imaginary, χ'' (right) components of dynamic magnetic susceptibility for complex **2** at $T = 2$ K under various dc magnetic fields (Oe). Solid lines are visual guides.

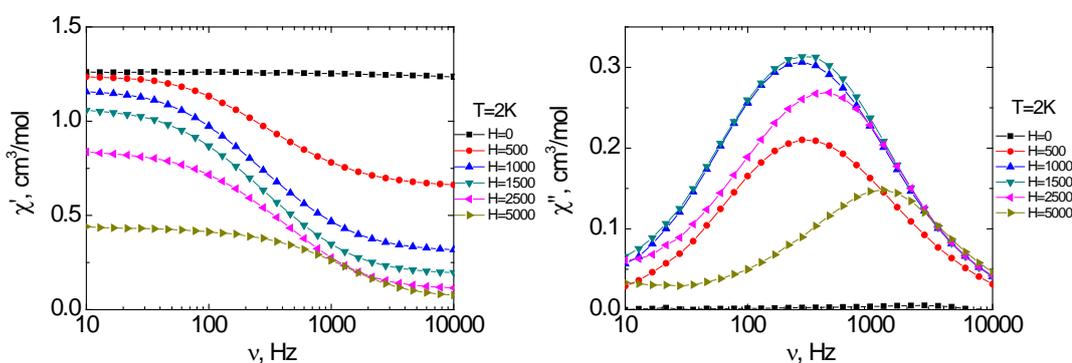


Figure S8. Frequency dependencies of the real, χ' (left) and imaginary, χ'' (right) components of dynamic magnetic susceptibility for complex **5** at $T = 2$ K under various dc magnetic fields (Oe). Solid lines are visual guides.

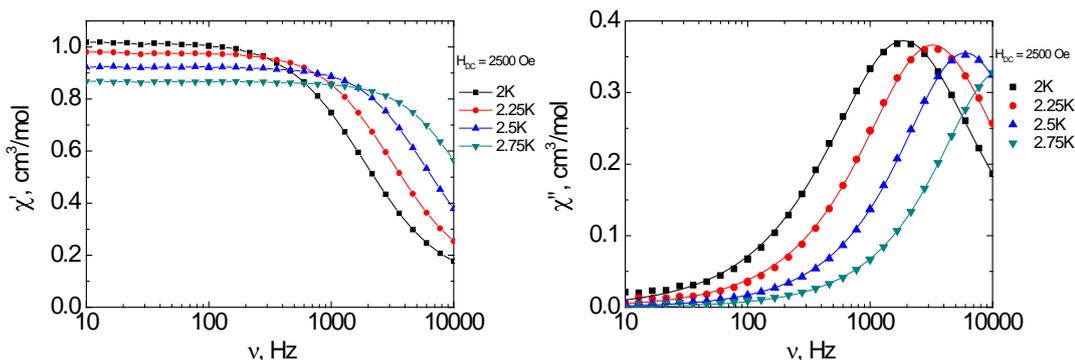


Figure S9. Frequency dependencies of the real (χ' , left) and imaginary (χ'' , right) parts of the ac susceptibility for complex **1** at 2500 Oe (2-2.75 K). Lines represent visual guides (left) and approximations of the experimental data by the generalized Debye model (right).

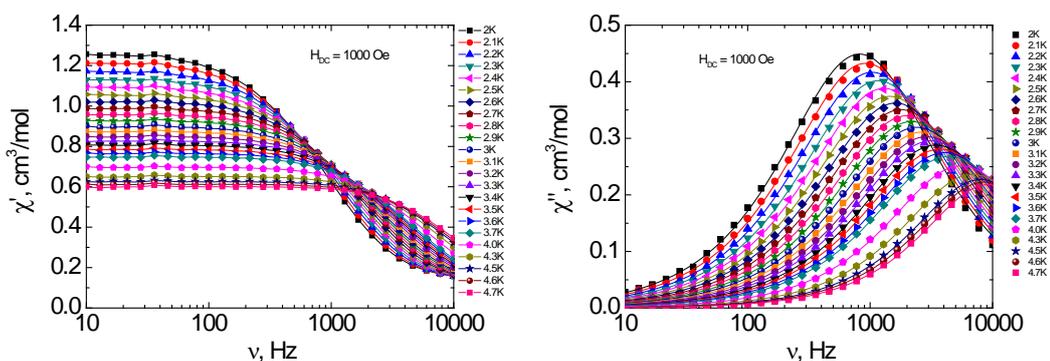


Figure S10. Frequency dependencies of the real (χ' , left) and imaginary (χ'' , right) parts of the ac susceptibility for complex **2** at 1000 Oe (2-4.7 K). Lines represent visual guides (left) and approximations of the experimental data by the generalized Debye model (right).

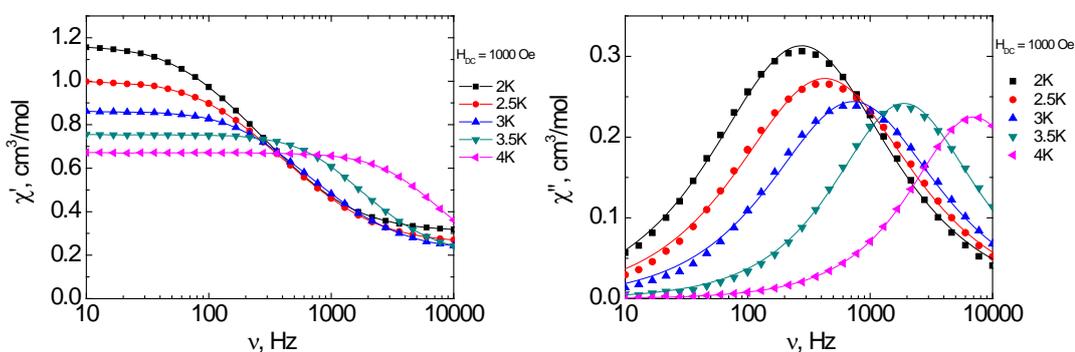


Figure S11. Frequency dependencies of the real (χ' , left) and imaginary (χ'' , right) parts of the ac susceptibility for complex **5** at 1000 Oe (2-4 K). Lines represent visual guides (left) and approximations of the experimental data by the generalized Debye model (right).

Computational details

Theoretical calculations of the electronic structure for fragments of complexes **1-5** were performed using a post-Hartree–Fock multi-reference wavefunction (WF) approach based on state-averaged complete active space self-consistent field calculations (SA-CASSCF) followed by N-electron valence second-order perturbation theory (NEVPT2)^{S7–S10}. Scalar relativistic effects were account for using a standard second-order Douglas–Kroll–Hess (DKH) procedure^{S11}. For calculations, a segmented all-electron relativistically contracted version^{S12} of Ahlrichs polarized triple-zeta basis set, def2-TZVP^{S13–S15}, was used for all atoms. To improve the calculation time, the resolution of the identity approximation with corresponding correlation fitting of the basis set^{S16} was employed. Spin–orbit effects were included using the quasi-degenerate perturbation theory (QDPT)^{S17}.

The CASSCF active space was constructed from 5 MOs with predominant contributions of 3d-AOs from the metal center and 7 electrons, corresponding to metal ion CAS(7, 5). Ten quartets and 40 doublet states were included in the WF expansion.

For all calculations, nuclei coordinates of non-hydrogen atoms were taken from x-ray diffraction experimental data, and positions of hydrogen atoms were optimized employing density functional theory with the BP86 functional and Ahlrichs polarized basis set def2-TZVP (optimized nuclei coordinates are listed in Table S4).

References

- [S1]. I. G. Fomina, G. G. Aleksandrov, Z. V Dobrokhotova, O. Y. Proshenkina, M. A. Kiskin, Y. A. Velikodnyi, V. N. Ikorskii, V. M. Novotortsev, I. L. Eremenko, *Russ. Chem. Bull.*, 2006, **55**, 1909–1919.
- [S2]. E. N. Zorina-Tikhonova, D. S. Yambulatov, M. A. Kiskin, E. S. Bazhina, S. A. Nikolaevskii, N. V. Gogoleva, I. A. Lutsenko, A. A. Sidorov, I. L. Eremenko, *Russ. J. Coord. Chem.*, 2020, **46**, 75–80.
- [S3]. A. A. Sapiyanik, M. A. Kiskin, K. A. Kovalenko, D. G. Samsonenko, D. N. Dybtsev, N. Audebrand, Y. Sun, V. P. Fedin, *Dalton Trans.*, 2019, **48**, 3676–3686.
- [S4]. A. J. Arduengo, H. V. R. Dias, R. L. Harlow, M. Kline, *J. Am. Chem. Soc.*, 1992, **114**, 5530–5534.
- [S5]. Z. Dobrokhotova, A. Emelina, A. Sidorov, G. Aleksandrov, M. Kiskin, P. Koroteev, M. Bykov, M. Fazyzbekov, A. Bogomyakov, V. Novotortsev, I. Eremenko, *Polyhedron*, 2011, **30**, 132–141.
- [S6]. N. F. Chilton, R. P. Anderson, L. D. Turner, A. Soncini, K. S. Murray, *J. Comput. Chem.*, 2013, **34**, 1164–1175.
- [S7]. C. Angeli, R. Cimiraglia, S. Evangelisti, T. Leininger, J.-P. Malrieu, *J. Chem. Phys.*, 2001, **114**, 10252–10264.
- [S8]. C. Angeli, R. Cimiraglia, J.-P. Malrieu, *Chem. Phys. Lett.*, **2001**, 350, 297–305.
- [S9]. C. Angeli, R. Cimiraglia, *Theor. Chem. Acc.*, 2002, **107**, 313–317.
- [S10]. C. Angeli, R. Cimiraglia, J.-P. Malrieu, *J. Chem. Phys.*, 2002, **117**, 9138–9153.
- [S11]. B. A. Hess, *Phys. Rev. A*, 1986, **33**, 3742–3748.
- [S12]. D. A. Pantazis, X.-Y. Chen, C. R. Landis, F. Neese, *J. Chem. Theory Comput.*, 2008, **4**, 908–919.
- [S13]. A. Schäfer, C. Huber, R. Ahlrichs, *J. Chem. Phys.*, 1994, **100**, 5829–5835.
- [S14]. A. Schäfer, H. Horn, R. Ahlrichs, *J. Chem. Phys.*, 1992, **97**, 2571–2577.
- [S15]. F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297–3305.
- [S16]. F. Neese, *J. Comput. Chem.*, 2003, **24**, 1740–1747.
- [S17]. D. Ganyushin, F. Neese, *J. Chem. Phys.*, 2006, **125**, 24103.

Table S4. Atomic coordinates of mononuclear Co^{II} based fragments of complexes **1-5** used for SA-CASSCF/NEVPT2 calculations (hydrogen atoms positions optimized at BP86/def2-TZVP level of theory while non-hydrogen atoms are fixed at positions obtained from single crystal X-ray diffraction)

1_Co1			
Co	-1.64013855563186	20.01985462700846	6.05606858230684
N	1.20880106461020	21.06536817958785	6.66442985709992
N	0.24741318078579	22.35879367649340	5.28340204425763
O	-2.29538976286958	20.63825961343269	7.78176905564529
O	-4.27514998877864	19.75724787463926	7.60387652255370
O	-2.79216808761378	20.32225429147064	4.50168400712782
O	-4.04989814502482	18.56635799837185	4.95891624436671
O	-0.98170257981838	18.20288800408724	5.77607688181471
O	-2.45827634221913	17.07091136142542	7.00766155409041
C	-3.36076563269769	20.36257819884470	8.23989023407988
C	-3.83233086488221	20.76751394560086	9.66363152588723
C	-3.48426964954318	22.22667145053702	9.87772907815013
H	-2.42109472442391	22.41016764456546	9.66678500928869
H	-4.07386023913906	22.87980322540451	9.21394653830692
H	-3.68396727895305	22.54663652804311	10.91739570198510
C	-2.99774273463774	19.90544295899405	10.58693768259527
H	-1.92205401107930	20.08211831958380	10.43944927444132
H	-3.22740487972781	20.10598320559507	11.65135732758737
H	-3.18528641842638	18.83714182988691	10.39663524718553
C	-5.29535695846864	20.47262970387665	9.90014144245921
H	-5.51018656414199	19.41190841633616	9.72833355005094
H	-5.56352533267941	20.73569624857770	10.94071737732501
H	-5.94011198493771	21.04435096295542	9.21825606989278
C	-3.71176950004095	19.45955148217610	4.20438431976738
C	-4.40992820412549	19.58822076273956	2.86748542974508
C	-4.76263659017340	18.23239881324085	2.33849239403620
H	-5.34403863711961	17.66657494965127	3.07719453654365
H	-5.34822173948876	18.31857541863414	1.40605707230907

H	-3.86231528438289	17.63840572510697	2.11056949054007
C	-3.60733405374203	20.35516723929768	1.89450560814930
H	-3.37841790797263	21.36034628015388	2.26838587073604
H	-2.64168995814745	19.86775715576031	1.68176055756961
H	-4.13954408449593	20.45920809470338	0.93047636973631
C	-5.71512784328108	20.33850435511374	3.11236178671914
H	-6.33877549607877	19.80592020517426	3.84473567615044
H	-5.52898243386540	21.35005181349247	3.50579471860285
H	-6.28511462527602	20.43963867792363	2.17242186738302
C	-1.56506103885295	17.13684277573288	6.14105699322495
C	-1.12959974919947	15.80303834073077	5.48225718265569
C	-0.20019601143883	16.10133554391123	4.31495753277367
H	-0.69278104989080	16.74606168638011	3.57351071800048
H	0.70718417145746	16.61728234894535	4.65408703757489
H	0.10996288327567	15.17057517443287	3.80448100462592
C	-2.38805179591723	15.04915586016507	5.00257223713428
H	-3.07030750717685	14.89376412765525	5.84797376086520
H	-2.93023817530490	15.63072565545521	4.24341349949307
H	-2.10709702109432	14.07367630005264	4.57006554523726
C	-0.41521767674637	14.94468668498693	6.54138922853452
H	-1.08017654383731	14.79096587418600	7.40211652960836
H	-0.13663050632870	13.96266505076337	6.12303900568099
H	0.50264769285403	15.43650632746921	6.90037340004540
C	0.04976429967274	21.17987418712858	5.92883271849486
C	2.08587596027237	22.14454400765789	6.48090013704721
H	3.04444564447631	22.19206705173426	6.98293255127067
C	1.48924846313253	22.96581776422309	5.61490299729868
H	1.79029152462349	23.91032796379489	5.17900691687269
C	1.57100764648731	19.86394749515339	7.42466714633345
C	2.16918563468601	18.81134551371398	6.74641338748975
C	2.47329587927325	17.72188083249554	7.48768571242377
H	2.93443698367728	16.86026905284660	6.99348595462634
C	2.26431664350929	17.66416026765915	8.86331539327010
C	1.65921175405014	18.73782486087622	9.47658158117230

H	1.46250476566752	18.69799135203003	10.55297756404248
C	1.32294502884512	19.90119973575323	8.78534168676063
C	2.40732508336174	18.86120881080329	5.26881829413548
H	2.89806379064937	19.79616370796061	4.96059307548717
H	3.03359547115159	18.01757097927221	4.94913413469740
H	1.44604968574924	18.79765698851256	4.73753223826357
C	2.59548877123223	16.36960450406324	9.71640589121438
H	3.43164616535300	15.81557746636418	9.26896447832789
H	2.85819824629895	16.65067301508727	10.74406041884239
H	1.71625351232648	15.70967013862232	9.74568297230019
C	0.68658978414150	21.10775496945391	9.46770557162466
H	0.57892261799192	20.91996240469908	10.54387149298521
H	1.29725077334313	22.01283979768757	9.33073906242757
H	-0.30998880933560	21.29771979142190	9.03942739392976
C	-0.63475643171180	22.93688641702136	4.29071752196842
C	-0.52924585756082	22.43042167953432	2.97932322774512
C	-1.32154731993228	23.05355479442787	2.04182095541567
H	-1.26005740034511	22.68306522753384	1.01099151060025
C	-2.18206228052269	24.05630765646215	2.31063073444985
C	-2.26653134804405	24.49877414114869	3.64198695395317
H	-2.97065289342565	25.29484043105346	3.90009814030672
C	-1.49838416590887	23.93154712671833	4.64151405100863
C	0.40259504965148	21.24683892151506	2.62642326411397
H	1.43297552000600	21.43408231681295	2.96007078186351
H	0.04168051724685	20.33657617863638	3.12633326116650
H	0.40170414802146	21.08219849312193	1.54121228511841
C	-3.08118102558280	24.70347459704799	1.23199575189254
H	-3.61649249320771	25.56790626943145	1.64450608915189
H	-2.48712242064983	25.03927240274242	0.36898059758163
H	-3.82373129043832	23.97924642258834	0.86472716366470
C	-1.60005243124683	24.37284847908510	6.10784371588009
H	-2.34319043804630	25.17434639446871	6.21327344085398
H	-1.90533834328949	23.52745737916693	6.74113709037404
H	-0.63560923896069	24.73952102311156	6.48742450961036

1_Co2

Co	-5.59531754401792	14.69996725327804	10.38525645383191
N	-7.71873663256637	14.96441799791767	12.60434099357768
N	-7.96655936386114	13.07555740852598	11.72314206318113
O	-5.12197469870313	16.73735346807323	7.76193318786715
O	-6.60926197800900	15.57571577838364	8.92967093352398
O	-3.57673148907573	14.04440312539704	8.24282279132332
O	-4.78079194923254	13.02485809233476	9.75915234501424
O	-2.91293695901167	16.26123825717982	10.05693766664062
O	-4.29522884129387	15.51254787008944	11.58103406927529
C	-6.27993965292807	16.28336170142298	7.93356548852486
C	-7.30907113944205	16.50695437775274	6.85170057190590
C	-8.69815926886067	16.44661419525348	7.45004765263611
H	-8.85835069007373	15.52210023219033	8.01516944400182
H	-8.87193663544859	17.29149431803533	8.13553612488455
H	-9.47123647765640	16.50567972265274	6.66115726731799
C	-7.09139506347143	15.32947957207450	5.93565733678517
H	-7.21699844770425	14.37691207408515	6.47119013785903
H	-7.80306830012884	15.33824892707487	5.08895456566425
H	-6.07076666668258	15.34336761321008	5.52714138993471
C	-7.12472070441075	17.78137947168288	6.12953951285337
H	-7.29364879211221	18.65062462470930	6.78647383229494
H	-6.09931879160009	17.86979453640702	5.74579417907342
H	-7.82931102401774	17.86128238674563	5.28300444210762
C	-3.89816990147100	13.05089624819583	8.89283235324060
C	-3.07374207339535	11.76563578279999	8.68189801850524
C	-3.98512156864561	10.57884078122960	8.85371491640428
H	-4.82129917138601	10.59568006639213	8.13758577327656
H	-3.42564352935899	9.63788719230042	8.69030167608904
H	-4.42476274452992	10.54124894059594	9.85892669625628
C	-2.05945025583044	11.68508695696436	9.61878968457709
H	-2.43184666908498	11.68906614879463	10.65822031753159
H	-1.45941723360537	10.75812619041749	9.51036050269259

H	-1.34155973401036	12.52331379739038	9.54798231459614
C	-2.59911171517422	11.69453653621711	7.32376697739281
H	-3.42067953840892	11.70601743617168	6.59063011546888
H	-1.95114965407637	12.54642427321714	7.06565063565847
H	-2.01669454900173	10.76881970439988	7.15347553037993
C	-3.17385490348444	15.95259102199729	11.19932670321364
C	-2.05089671063012	16.10909987067763	12.21251566838169
C	-1.88839591693784	14.89693185893775	12.98735772376293
H	-2.82831980549545	14.58868276854690	13.46783833274499
H	-1.56362908671442	14.04611310360228	12.36177219846701
H	-1.12984515494700	15.01041869108526	13.78502746867493
C	-2.43771669888598	17.25840579332324	13.21622787804810
H	-2.56244111406532	18.21239801488116	12.68328890738356
H	-3.37919801061935	17.03658174168199	13.73779646273593
H	-1.63990882890439	17.38001155016559	13.96796905232964
C	-0.80611550322153	16.57732873312856	11.60405246035600
H	-0.95500676153506	17.50860458816017	11.04233264077452
H	-0.03632028448380	16.75239166251331	12.37731416930386
H	-0.39481062644325	15.85365069812874	10.88062213253438
C	-7.14129254253538	14.17124599103437	11.64912714746102
C	-8.86639702301789	14.39227435278061	13.19294805377805
H	-9.43691971864388	14.91049893797814	13.95350484852574
C	-8.99234901132781	13.16939034158756	12.62723718471623
H	-9.70762333143210	12.36988906203320	12.77723455122317
C	-7.27944481536787	16.28763752201477	12.94868355155389
C	-7.74715037070536	17.42950876731928	12.31123663316945
C	-7.34699618276137	18.68565824343161	12.75647939452519
H	-7.72316137788127	19.57824181430151	12.25381888205903
C	-6.47912755735712	18.79593763468718	13.83616754544191
C	-6.00941474888821	17.65206914365591	14.47061751115633
H	-5.32389992795651	17.73604581533926	15.31612007053434
C	-6.41057620929526	16.39791771227535	14.02837360808001
C	-8.78890504630478	17.31211237052406	11.17421628304298
H	-8.36077272340700	16.76812538501565	10.31871762603464

H	-9.68028459998762	16.76334253778885	11.51306068473915
H	-9.09729068961898	18.30975162854896	10.84021851743507
C	-6.14209485979343	20.17803250494293	14.29233937117117
H	-5.37441818239180	20.17855938815792	15.08035420648776
H	-5.76427571746205	20.79257257535894	13.46104592107471
H	-7.02965880124512	20.69256070815694	14.69522899682042
C	-5.82785963433304	15.20413217772617	14.68201837671088
H	-6.58673497241723	14.46360674817043	14.97863357209181
H	-5.14188763330932	14.70085637668572	13.98109689885071
H	-5.25589838807011	15.48203979288835	15.57734870994605
C	-7.73127248790811	11.91101989465623	11.00713754446537
C	-8.32977090082216	11.72101781970241	9.76592851149609
C	-8.21156539335882	10.49736068058758	9.11767959668160
H	-8.68792217180978	10.35210225097301	8.14617765605338
C	-7.49285739564834	9.46570836827913	9.70764427118560
C	-6.89235171028397	9.65371319470315	10.94585633386338
H	-6.32828103085119	8.84487506394383	11.41435571900485
C	-7.01055831027300	10.87636995127721	11.59510486247979
C	-9.15953141198456	12.86358875757612	9.15679622083200
H	-9.58064011765341	12.55964436517193	8.19051558289205
H	-9.98540917765233	13.15852040886693	9.82078004387597
H	-8.52375488164354	13.74808193865802	9.00302464852835
C	-7.37449765670217	8.06805437359537	9.05132858251448
H	-7.95492656730517	8.01620462611752	8.12079926618346
H	-6.32498489283868	7.84128130554174	8.81376867209565
H	-7.74212718256065	7.28788012444681	9.73403192565669
C	-6.37935452913272	11.07233942087777	12.98937842094721
H	-5.64342540417292	11.88927200430101	12.96312343091358
H	-7.13757117982303	11.32967607335834	13.74321224584992
H	-5.87119467740816	10.15313868856710	13.30772855698965

1_Co3

Co	-4.71239479317748	2.39691513032422	5.82238589418196
N	-1.95257791219031	1.16730489974706	5.01184379695988

N	-2.83317584674496	-0.00089079367610	6.58798690408255
O	-3.99301594856427	4.21269278657387	5.77407883852860
O	-5.67636415456867	5.33885618711529	4.80799352511847
O	-5.55545318179728	1.79274944209642	4.19009995955333
O	-7.53113127633242	2.71706603563660	4.60060684697461
O	-5.67718015449827	2.19260474777519	7.54303706872142
O	-6.94515804430337	4.01927105781485	7.29084613759978
C	-4.56027979502905	5.27803222270030	5.39727966109528
C	-3.87705374737427	6.59396126056590	5.72735379966136
C	-2.59237075401825	6.41868678482328	6.51444938825241
H	-2.18797096252703	7.39936397485542	6.82131525792962
H	-2.76110083357442	5.81939000575477	7.41940903648332
H	-1.82195384171247	5.91071885303494	5.91902964115679
C	-3.61804732042145	7.37477845892013	4.43143899598996
H	-4.54889765858577	7.45618098705241	3.85480249117671
H	-3.23969062101855	8.38789644280190	4.65137415993692
H	-2.86952862054349	6.85926100927318	3.80963831632239
C	-4.88556309296254	7.36401941816382	6.63244126966364
H	-5.83971384655093	7.48855624598432	6.10620413833511
H	-5.08444899280727	6.79590560218374	7.55241161283396
H	-4.47923504798305	8.35212675478686	6.90834136110946
C	-6.72591765191259	2.13957582981599	3.81471431060236
C	-7.21335505262239	1.82944795696532	2.40867928745284
C	-6.91006924004959	0.34202235156112	2.12816585593073
H	-7.15644759019137	0.07220913623973	1.08581122827422
H	-5.84813220124081	0.13317474276821	2.30135610821285
H	-7.49933535997420	-0.31041622977746	2.79137275927100
C	-8.68655601284064	2.21466359284341	2.26274489562077
H	-9.02396592519198	2.03964865113833	1.22527555627373
H	-9.31506565817512	1.62549324478215	2.94390085198163
H	-8.82908508944674	3.27019932670252	2.52013854391304
C	-6.29098754476773	2.71718402412408	1.51065320284538
H	-6.53161522590204	2.58524892040856	0.44019262047171
H	-6.41713918300307	3.77833913397074	1.77074021315372

H	-5.23927361831042	2.45171391651983	1.67354450816803
C	-6.57378707943432	3.06359772472177	7.91088249823345
C	-7.15993471994727	2.78000568034701	9.27398942533785
C	-6.03786736324205	2.58746353579281	10.27835209330045
H	-5.38198906304966	1.76132707634554	9.98101182505361
H	-5.42081595266953	3.49692925433573	10.36581558614634
H	-6.44484002153346	2.36813903302047	11.28199372094085
C	-7.97086999260888	1.50992301437020	9.20208667361445
H	-7.35119239515455	0.66901256345253	8.86015980695333
H	-8.39373979566322	1.25289529172642	10.19008420835182
H	-8.80943213117322	1.61372842621992	8.49550130665387
C	-8.01901731468695	3.91116553120633	9.75360748685018
H	-7.44740881019692	4.84783372643452	9.82702887178106
H	-8.85099860939425	4.10548343473373	9.06254952793903
H	-8.43700668324078	3.68294572370077	10.74989502953314
C	-3.07116913618485	1.13604826680198	5.86062333295214
C	-1.08754679232969	0.09460828336375	5.22817950952576
H	-0.16571945271313	-0.03116532831296	4.67364237547591
C	-1.63518753781330	-0.61411714181358	6.23650083091434
H	-1.29844027062765	-1.51957086627235	6.72808031024295
C	-1.74976383522427	2.24520822301633	4.06682534766697
C	-2.21641524724461	2.09520950978161	2.77965408794229
C	-2.08057967050303	3.22600831925452	1.93270677125933
H	-2.47700627943666	3.15754580077337	0.91623025808621
C	-1.37185100300008	4.37403422284743	2.31484967811748
C	-0.89301293290312	4.45206582684152	3.60604841380028
H	-0.35326165551087	5.33987285460938	3.94209074457723
C	-1.09093687912682	3.39415034656086	4.51304617952383
C	-2.84588468735794	0.79733405187897	2.32348359439627
H	-3.07536551947759	0.83340197450293	1.25060141395665
H	-2.17867584569897	-0.05747071447128	2.50842059844019
H	-3.78488519967484	0.62888969530376	2.87439154943834
C	-1.22136424119146	5.59381848063849	1.38782157977786
H	-1.05047775036322	5.29013501538134	0.34492670041564

H	-2.13563264898725	6.20665155648341	1.41185468644808
H	-0.38219301606582	6.22442596934103	1.71116861995050
C	-0.56303132352226	3.51938097951862	5.92213738009876
H	0.11616736845336	4.37741631569038	6.00631154398833
H	-1.39981778566674	3.67494660315856	6.61975673662355
H	-0.02448570555860	2.61464230727824	6.24201559410756
C	-3.65717553492723	-0.52326348719476	7.66562194252159
C	-4.51791369459547	-1.57657651460662	7.42865679693233
C	-5.23999283386130	-2.07470156992972	8.49411592130614
H	-5.94401150029270	-2.89123311775244	8.30448173406023
C	-5.06214690831746	-1.62044276567087	9.75454393001391
C	-4.22245540887874	-0.55919338756587	9.97453699242137
H	-4.10099755670662	-0.15653843044593	10.98292646252060
C	-3.47751155743254	0.00800459290257	8.93299721562231
C	-4.70788107889699	-2.08597207799889	6.00328332009079
H	-3.76483923644510	-2.45247874639434	5.57199802267707
H	-5.43833507219975	-2.90594088779007	5.98251423686438
H	-5.07390334601241	-1.27758343733154	5.35265179107227
C	-5.86893030153660	-2.17071256554523	10.92517012862962
H	-5.26138046620858	-2.21507612655889	11.84030182974444
H	-6.73490946735071	-1.52400406176557	11.13301928754750
H	-6.24855074611712	-3.18006867231110	10.71348640081446
C	-2.60004750306725	1.17636564668716	9.17886155533705
H	-2.54261631637428	1.41015350718787	10.24993936911938
H	-1.57585747760365	1.01470166030937	8.80717525464483
H	-2.99485521253609	2.06168776083960	8.65573386580360

1_Co4

Co	-9.51357642965684	7.89361435339542	2.29282533947263
N	-11.81872196725558	7.52648041627198	0.30677606818519
N	-12.31682716772285	9.13871011466248	1.59531345723239
O	-7.17628335501849	8.48364372742131	4.00456609702388
O	-8.78925092873934	9.59786473383508	2.98368943767010
O	-6.79696982710983	6.35938863110954	2.00389631924226

O	-8.30551770458599	7.46886423382338	0.82363017066318
O	-8.44949978259601	5.76253111355783	4.74162181209083
O	-10.15795259917189	6.80245211882417	3.78516623082807
C	-7.71857199517851	9.55035672733811	3.64571180392552
C	-7.09616136770925	10.87994634247384	3.99226838002196
C	-5.81955801673465	10.81316531227232	4.61453293340339
H	-5.82642341645808	10.12540049012519	5.47091160382781
H	-5.02585004876327	10.43965794795467	3.94254952144493
H	-5.49551235071818	11.80725711470853	4.97006502332857
C	-7.30635721052205	11.81035736565421	2.99127535781434
H	-8.35551321385827	11.86893652931386	2.68357046735229
H	-6.99082070434909	12.83117145406186	3.28574491659428
H	-6.74415980445056	11.60581255428278	2.05267346309400
C	-7.98557578093850	11.47849849935225	5.00411832751292
H	-8.01567321070176	10.89898086392840	5.94658486927081
H	-7.64627977877375	12.49388959129487	5.27524807277091
H	-9.02559791471276	11.55305567894223	4.65578493410790
C	-7.18109374053172	6.93810711445967	0.94384927721208
C	-6.18277002401003	7.04585526635954	-0.19799926240624
C	-4.88330681187226	7.12302668495721	0.26205826850064
H	-4.65988812375435	6.32561458541531	0.98410023663356
H	-4.14066269659017	7.06407346306346	-0.55775707713504
H	-4.66752398505588	8.06687961594952	0.79998284348172
C	-6.26192075119345	5.70688134584096	-1.01859234258071
H	-7.27420782563114	5.53359238990770	-1.41047786676704
H	-5.55963868062033	5.75966852826755	-1.86600862366001
H	-5.98800570053462	4.85043334257406	-0.38346188287676
C	-6.56415840994423	8.03764303958067	-1.18940025046674
H	-7.57717851554285	7.86614276728663	-1.57567648810882
H	-6.55939448845504	9.06686174161461	-0.78435536148038
H	-5.87130007518617	8.03817167929201	-2.05149559116874
C	-9.65182344313524	6.10408753524704	4.72885378049531
C	-10.55613929025252	5.75370891665159	5.90055155123533
C	-11.31729067474712	8.18917777252791	1.33534783075087

C	-13.11094501110350	7.98238419166826	-0.09875242350329
H	-13.65675474181052	7.53771720134714	-0.91928423513710
C	-13.34057297187277	8.98421283528229	0.71728149802800
H	-14.21225784180159	9.63158390378758	0.76958241322289
C	-11.18405470611727	6.42328914496889	-0.33369367556560
C	-11.24417723599482	5.17155187812222	0.26857960181352
C	-10.63474058895907	4.09724075696855	-0.40481967344232
H	-10.65861717512255	3.10864108793945	0.05995567745372
C	-9.99497827820175	4.27259965825735	-1.62837818885600
C	-9.98476488484858	5.52417261905041	-2.20646365740017
H	-9.49433486067830	5.68170865708338	-3.16967740715057
C	-10.57034011571187	6.60955046543726	-1.55916343134688
C	-11.96844433586347	4.96896733679972	1.59747902192013
H	-11.98866735544198	3.90284858373836	1.85754733800645
H	-11.46167840479712	5.51911460751482	2.40776598177600
H	-13.00540502434857	5.33324589272511	1.54091411674154
C	-9.30302229337543	3.06159511076041	-2.29797351821577
H	-9.90926068153077	2.15205607214658	-2.18249299854860
H	-9.13903467047682	3.24181255160876	-3.36932006439298
H	-8.32438007744108	2.87692645664103	-1.83078400728468
C	-10.51285739944629	8.01025929279279	-2.18555110371323
H	-10.02277147685626	7.96976190741757	-3.16651020842611
H	-11.51420468349772	8.44547704456222	-2.31492733460966
H	-9.93783948547188	8.68558667573905	-1.53516684184235
C	-12.29836652963056	10.12467764070832	2.68443064346056
C	-12.94289396455088	9.86628507425868	3.88907609341409
C	-12.88342285365402	10.79335832588420	4.92308788233681
H	-13.39032053826249	10.58028654419803	5.86619095162500
C	-12.17842432174515	11.97882782590544	4.75245045628571
C	-11.53189691053085	12.23722776089205	3.54779748763632
H	-10.97344902010398	13.16415703973001	3.40843329600741
C	-11.59236800602815	11.31015082721228	2.51378946070617
C	-13.78263468730827	8.57629037326459	4.02630653376302
H	-13.23665629861716	7.71392616440149	3.62668838482308

H	-14.02114649779336	8.38398457624318	5.07971434240264
H	-14.72936322597768	8.66620101217269	3.47155808516882
C	-12.06470497594579	12.97721292703171	5.92220004777154
H	-12.96956656492333	12.96405247621380	6.54621297090270
H	-11.20841201849342	12.71541815286842	6.56336322196849
H	-11.90655065025822	14.00083701804046	5.55574896487796
C	-10.86743273970633	11.60574088503975	1.18781005777282
H	-11.52040392609578	11.42331540064125	0.32244150103838
H	-10.53158409202595	12.64980353380689	1.16367685830757
H	-9.98782359045854	10.95101719149767	1.10074494965217
C	-10.04892963018771	4.53316059102325	6.61966846879001
H	-9.00928086506801	4.67462833992825	6.94200837402679
H	-10.67388271326165	4.31229402247286	7.50277219012158
H	-10.06056524857550	3.64827192352917	5.96444893502695
C	-10.56893079106990	6.93844945097908	6.85161949909266
H	-10.92898715255445	7.84847581013571	6.34930028183649
H	-11.22578844533413	6.73893923243524	7.71600947648871
H	-9.55707314665555	7.14766029408401	7.22946002652351
C	-11.96705671112402	5.50210423628841	5.41505786109923
H	-12.35996849520789	6.36631603391244	4.87044657284946
H	-12.00855277695675	4.63257556870504	4.73835037535287
H	-12.64450049834052	5.29008811053544	6.26194522080598

2

Co	-1.03683946297864	6.33999451877317	10.09121970339092
P	-0.96144333610817	8.36159095259781	8.79311289425863
O	-1.87758071415835	5.24458430086043	13.10405882217075
O	-1.81520281951491	6.98221361307810	11.73282749014951
O	-1.62460325687794	3.77281881513671	10.42428370198014
O	-2.22523953409523	5.27844833344420	8.99521378875393
C	-0.38111076581540	8.02938499226799	7.10572665602402
O	0.94991037447106	4.73429572534696	11.79168477383774
O	0.88419921064968	6.22503193936289	10.17539223028235
C	-2.15473624301430	6.41469702726949	12.83370531492209

C	0.21277851056024	9.56433215656020	9.46118897989576
C	-0.95758787912591	8.58987756023496	5.97821513785359
H	-1.78200355655142	9.29976044257287	6.06181361477431
C	0.63585300955026	7.10650772092688	6.92489462979735
H	1.05884024540388	6.63750914048740	7.82099544064929
C	-4.84875520084175	10.70568501664176	8.25175210496923
H	-5.78643849596264	11.24975437903558	8.11113759253292
C	-2.47755394162001	9.33661248020838	8.61517003529993
C	-2.86637659900355	7.32922035279069	13.81541050693190
C	-2.29498682362399	4.13021078429566	9.50871728942944
C	1.93921417635567	11.31482828106265	10.71329270891590
H	2.62940119170264	12.01043542045555	11.19918846228702
C	2.95765350135345	5.92261293972946	11.27141779540445
C	-3.28120420633392	3.17146101802189	8.87567687829726
C	0.15733112558369	9.79969332621699	10.85431916551259
H	-0.57163562019426	9.24479007134097	11.45118957357826
C	-2.49271210563784	10.68473055097708	8.35579217562619
H	-1.53933121940900	11.21885785854227	8.29968897982567
C	0.99752483327498	10.69346699441352	11.42238884973088
H	0.92733564110168	10.86544876126242	12.50118817942514
C	1.18245721225963	10.21070556937883	8.72809305802830
H	1.27404433650503	10.03388240237314	7.65415034368923
C	-0.46108454356462	8.24447541660765	4.71285676910363
H	-0.91531635277388	8.69234731694778	3.82564059039293
C	1.49458892345004	5.58964310279864	11.07885580018413
C	-3.64880450478058	11.38075808761319	8.19557658476942
H	-3.62630721787873	12.45265780825905	7.98746113097971
C	1.12437544960679	6.76808331257427	5.70754268706931
H	1.93009921263333	6.03815231000649	5.61475561474617
C	-3.71248768241375	8.66251876458405	8.71336016045004
H	-3.71545066643521	7.59305740102134	8.93671050669759
C	-1.78917998075526	8.27199795254353	14.39540691945441
H	-1.00911833153804	7.70575619457400	14.92694403188993
H	-1.30683278342345	8.84602622394249	13.59367534125969

H	-2.24170887591934	8.98368077027196	15.10761050864628
C	0.55589862044127	7.35157483272026	4.58303847066415
H	0.92485140584807	7.08925226960166	3.58792807276757
C	2.04267636999581	11.10445125954417	9.35915457408684
H	2.81539027371131	11.61241588952831	8.77758532307846
C	-3.52190312565278	6.52669398188726	14.91030839943682
H	-4.30517074194253	5.86805571168743	14.50546989204623
H	-2.79122481752653	5.87873869851184	15.41205714291321
H	-3.98628482259693	7.19152458852889	15.65924103030631
C	-4.88157697962742	9.36254217795421	8.56115162467267
H	-5.83963452844690	8.84484558276585	8.64647288550823
C	-3.86570917574937	8.19351877900299	13.07620848539236
H	-3.38047746383999	8.77212822653789	12.28167733256115
H	-4.65376778754860	7.58378661869494	12.60470661720435
H	-4.36486453636002	8.89666883937279	13.76780748443781
C	3.49129119175225	7.07699274878510	10.48672991519177
H	3.50252372600488	6.88298843622497	9.40173880788048
H	2.87813295089585	7.97417019663835	10.64590447788135
H	4.52590336393618	7.30976684464053	10.79245819818830
C	3.74269878899553	4.62165108890269	11.25550657768144
H	3.21915876557469	3.88667975377317	11.87788777787754
H	3.83916146334343	4.19660192476979	10.24057265120115
H	4.76326871285453	4.77273934792946	11.64658585966396
C	2.97523382406663	6.29393952057861	12.74658066927076
H	2.37909205926711	7.19994551858821	12.94848811473387
H	2.55499040931369	5.48268815832738	13.35040885460439
H	4.00611185784909	6.50293705427090	13.08705580798720
C	-4.30360136408915	3.79184264028994	7.95237265176364
H	-4.84499077754993	4.60288064906735	8.45870659667465
H	-3.84514651368165	4.22363135677608	7.04847960770801
H	-5.04112583692276	3.03793514387686	7.62885665626525
C	-2.57138278201681	1.94174661556615	8.31182846494064
H	-1.97912324653314	2.18029295834187	7.41175194162721
H	-1.88819389705177	1.53017694169328	9.06631055379490

H	-3.30624944265480	1.16825704762852	8.03561984038272
C	-4.10668129603492	2.62886024610583	10.11876214416655
H	-3.42777732284802	2.19503959822935	10.86201451863588
H	-4.65794499747447	3.44852648958419	10.60352517243751
H	-4.83352656181375	1.86891415566121	9.78674328049624

3

Co	2.40349167968287	8.52890824644304	-13.96637476682712
O	0.52529934000646	9.23140198547295	-13.95071960575184
O	0.30565964399732	7.13911245251332	-13.34959489932586
O	3.04682457080193	8.75736847445466	-12.11407627058935
O	2.18091903425530	7.01670489438461	-10.98702795530231
O	3.22923859902375	7.18358390242819	-15.15362134197160
O	2.85325442073838	5.44195825332070	-13.78541303438364
N	3.45433322533035	10.14850818772171	-14.79940902537491
C	-0.17060443732414	8.27303013380156	-13.46531531094598
C	-1.59682644790617	8.55847913325359	-13.01967234914376
C	-2.25774324716938	7.42904787174833	-12.35532228097598
H	-2.23516561295811	6.52650152758191	-12.98005997792290
H	-1.77237523622351	7.15159320659154	-11.40483437913517
H	-3.30892597024558	7.67658725107721	-12.13300275747260
C	-1.68738259827578	9.79218813156906	-12.32422811174345
H	-1.25621673863105	10.62026473915640	-12.90485517664645
H	-2.73573303770607	10.05774469527711	-12.09356007537605
H	-1.15199547044716	9.78722503993516	-11.35699170645428
C	-2.42748068779673	8.75972636053258	-14.23986704275458
H	-2.45693664796569	7.86157074515371	-14.87956828185851
H	-3.46901351622385	8.99735251279273	-13.96369800937706
H	-2.05615672109093	9.58841268923232	-14.86617544217052
C	2.74562864330476	8.14486711623427	-11.01740991563114
C	3.05399479666195	8.90344277508808	-9.69801752510494
C	1.87966146423412	9.86603982940222	-9.46303212717536
H	1.76441958289128	10.56252486432063	-10.30661498081517
H	0.93904020243680	9.30581104289713	-9.35548949150068

H	2.03697024630128	10.45636257694368	-8.54392421986972
C	4.38481886818429	9.71984585067590	-9.82426851356857
H	5.23479955486466	9.04555862660382	-10.00414378556596
H	4.33135715150669	10.42738668563581	-10.66161057408166
H	4.57649856113555	10.28091256936239	-8.89372271932620
C	3.18486187608336	7.94502230693435	-8.51234260787296
H	4.05072494933713	7.27814071569746	-8.63696140767745
H	3.31389141513059	8.51138305133461	-7.57461382775516
H	2.29325973279616	7.30900462705492	-8.43179366933879
C	3.37045845990400	5.95149446937713	-14.82304824299934
C	4.19000302632581	5.04506824570816	-15.74912826206343
C	4.83217361620171	5.83868725380434	-16.91561349556714
H	4.06248153804407	6.34798032034651	-17.51096485330568
H	5.52531499463492	6.60548309330213	-16.53961327899651
H	5.39538808955028	5.15824916071234	-17.57770741684803
C	3.22847772121929	3.98203687219684	-16.33485121638834
H	2.44151849852731	4.44676795274242	-16.94948894177301
H	3.78503641972335	3.26996234452525	-16.96711654543440
H	2.74031801996837	3.43508981788247	-15.51732830747414
C	5.24393974677636	4.29704098196573	-14.94707053142406
H	6.00454317495891	4.98074536030392	-14.53623650917426
H	4.76991186993033	3.78198900268926	-14.10156443370347
H	5.76059503394209	3.55657751326209	-15.58133361610079
C	3.73179887422080	11.24629829248096	-14.05989655067443
H	3.38092260221203	11.20536193696586	-13.02759818837430
C	4.46767292990170	12.32968500063634	-14.55623978854192
H	4.69621811495199	13.17607237453830	-13.90880206325128
C	4.87211766944165	12.28329988813724	-15.87712542672121
H	5.44035004180724	13.11727036886872	-16.29867191141500
C	4.55666106049478	11.20451616315245	-16.65964303036404
H	4.85919229487020	11.14187081728335	-17.70509586952728
C	3.86375193244944	10.14710787287831	-16.07727574971856
H	3.63576308120249	9.23377182361194	-16.63125260337122

Co	1.08752785600016	-0.09533324636927	-3.91394968562220
O	0.86996959363334	0.88601113847416	-0.65412966454712
O	1.78367888607639	1.25828781354875	-2.64958234941563
O	2.26245375507343	-1.71408887203442	-3.63761952307291
C	1.05985517649724	-1.15651185343318	-6.89133514322420
H	0.04959305433103	-0.87160339591752	-6.55922299000112
H	1.40287286094505	-1.95044979245639	-6.20895937233494
H	1.02068322658910	-1.54972594902186	-7.91549456176142
N	2.04572022459821	0.64927734715327	-5.60465706571473
C	1.73075011097861	1.40233662237459	-1.38311107395719
C	1.74347741082167	-2.12896231351358	-2.55826203880611
C	2.86669993827672	2.22475708071048	-0.75807301621226
C	2.48169482138995	-2.71768896313983	-0.26145643711077
H	1.46480415512078	-2.48386277637315	0.07644477249205
H	3.08545171463421	-1.80644761535856	-0.14905606175368
H	2.91485602496375	-3.50077250495096	0.38382389142990
C	1.65909837987703	-4.48671062347164	-1.82846201178462
H	0.62538386790455	-4.32073345701156	-1.49551584124545
H	2.11165057151598	-5.27003548831435	-1.19749130547429
H	1.62935961761513	-4.86123282092894	-2.86424696986221
C	2.46436332880556	-3.18632818589479	-1.72949795245877
C	2.84414503006266	1.74065279171166	-5.50515595564454
H	2.85682492878807	2.19327213054111	-4.51097083057671
C	3.49950461867735	1.62439211989448	-7.78708326923702
C	4.28113491493277	2.13071761926793	-8.97689147399120
H	4.01324949771100	1.58517142448416	-9.89134801749059
H	5.36555189039946	2.01202166850008	-8.81781210126799
H	4.09782967889372	3.20266470185791	-9.14923833760286
C	2.68607776933308	0.50902379156198	-7.89460185657255
H	2.59521373564495	-0.01703201916582	-8.84774616318924
C	3.88829783548244	-3.41112098472608	-2.22359582800727
H	3.90049716600329	-3.73676204414536	-3.27357518351749

H	4.38951503320242	-4.18266512117013	-1.61467499450631
H	4.48072583536791	-2.48737614894802	-2.16041649308683
C	3.55612158146190	2.24461033582758	-6.55779368591916
H	4.17032104852567	3.13573177501514	-6.40713092667685
C	1.97920324901881	0.03295741044287	-6.79291260665804
C	3.52944141116652	3.14460503731111	-1.77863142911061
H	2.80363694532540	3.84685015449711	-2.21729140550802
H	3.98104946111501	2.57166586668863	-2.59897568226463
H	4.32781064452565	3.74020573166554	-1.30048405044548
C	3.89071076944324	1.20439585773172	-0.26698769521376
H	3.44041966604511	0.53937297960249	0.48445622928156
H	4.75917400547642	1.70744733900635	0.19425622335919
H	4.26106214486226	0.58409595702918	-1.09681236795589
C	2.35202362217778	3.03667938305046	0.41309241472367
H	1.80199663546285	2.38921293267695	1.10902827958887
H	1.65605834196108	3.82323520687508	0.08022670947981
H	3.18530467688742	3.52244068016061	0.94981151823891
O	0.65010901722358	-1.67268250239209	-2.16746376300189
O	-1.74993942667548	0.07017341853549	-2.45342992955046
C	-1.80213112958262	0.17997989724996	-3.69105368603576
C	-4.16290278115738	-0.60147330904261	-3.83291662177894
H	-3.90742535451393	-1.62717090906476	-4.14582284010145
H	-4.17728456377499	-0.58621272134684	-2.73453594540345
H	-5.17650783026884	-0.37920428133683	-4.20948878413199
C	-3.62198869744156	1.81717270165469	-3.93372046199427
H	-3.66257727822715	1.89038088762780	-2.83823500937670
H	-2.92081746163289	2.58193047133251	-4.30060934137226
H	-4.62032209005788	2.03841428266451	-4.34847031015962
O	-0.77604223665624	0.13253785729735	-4.46774592964522
C	-3.16496080769078	0.40047225226269	-4.35112594739957
C	-3.07976613352719	0.35405235450898	-5.88045555641175
H	-2.74074756489202	-0.63127142681774	-6.23372785774382
H	-4.06982355921382	0.55021900521141	-6.32928283974260
H	-2.37271881551306	1.10303330033954	-6.26080179594133

Co	0.57961426523080	4.92160386040244	3.37143872726027
O	2.55251003432424	3.74506059098108	1.03478892494960
O	1.50744116122741	3.28538707524422	2.94655416336734
O	2.63769367545119	6.76626027324246	1.95265020568170
O	1.69071838788544	6.43160568188864	3.92723196028586
O	0.04586425238916	5.79924824691869	0.64830592553339
O	-1.07413256101533	5.45157804268998	2.52492777498766
N	-0.13456715930149	4.31557027111910	5.18536104589036
O	-3.36867142324805	6.33960062175339	1.39301021052750
O	3.06526461118413	8.49014037396667	5.00424200209852
O	3.87485644595112	1.28644243635663	1.24597772842715
C	0.38986872637934	3.35420043662706	5.90960758426804
H	1.23889971047330	2.84061450328359	5.45110402094599
C	-2.20873805189625	6.36789051309482	0.72182077985847
C	2.31512239058259	2.99455725117512	2.01184616013863
C	2.46803889132050	7.04799961447776	3.14028828193201
C	2.99327860639737	1.73229535174335	2.16048343885877
C	-0.99503005332425	5.82787828354884	1.32040217624181
C	-0.06820830050860	3.00721805644308	7.15714221720089
H	0.42988186349617	2.19642224126281	7.69229556177214
C	3.23485023043028	8.12526994307198	3.72071744732429
C	4.18429577191108	8.88185631254865	3.16056011828013
H	4.50771041492754	8.77625234551047	2.12995082686182
C	2.97784271423532	0.89873050489274	3.20362550999422
H	2.37781724941419	1.00192769825756	4.09938836646942
C	-2.41359788878474	6.79938487084297	-0.48274348006735
H	-1.64746471008305	6.90665831853673	-1.24400545149338
C	-1.11269206408110	3.66464511949966	7.67837952372922
H	-1.49864391204311	3.41794405833103	8.67039056419858
C	-4.30340069633020	6.89309687252049	0.55637403365648

H	-5.30235352590260	6.97762776303123	0.97190682375357
C	3.98101359269902	9.54381690233263	5.22468378733091
H	3.97078468739861	9.95800837772954	6.22603860865011
C	4.66002106289937	9.76283828083896	4.11629554917631
H	5.43768364071891	10.51234211815671	3.98468967141127
C	-1.18906627991796	4.95298642508823	5.69362697716446
H	-1.63764440487487	5.72355171683999	5.06375584169980
C	4.39710937775998	0.09877359921639	1.75053358632175
H	5.12146708455031	-0.38948479720367	1.10876841792247
C	-3.75831601352617	7.22421655818070	-0.54715007100024
H	-4.25045286641891	7.67488524258568	-1.40613566934154
C	3.90910803156655	-0.11733463681313	2.89089314138064
H	4.14378533338105	-0.96996185645275	3.52845536184862
C	-1.67311231619860	4.65003133300002	6.94810481543393
H	-2.53144998672968	5.21236320323733	7.32241680906833