Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Flavonol dioxygenation catalysed by cobalt(II) complexes supported with 3N(COO) and 4N donor ligands: a comparative study to assess the carboxylate effects on quercetin 2,4-dioxygenase-like reactivity

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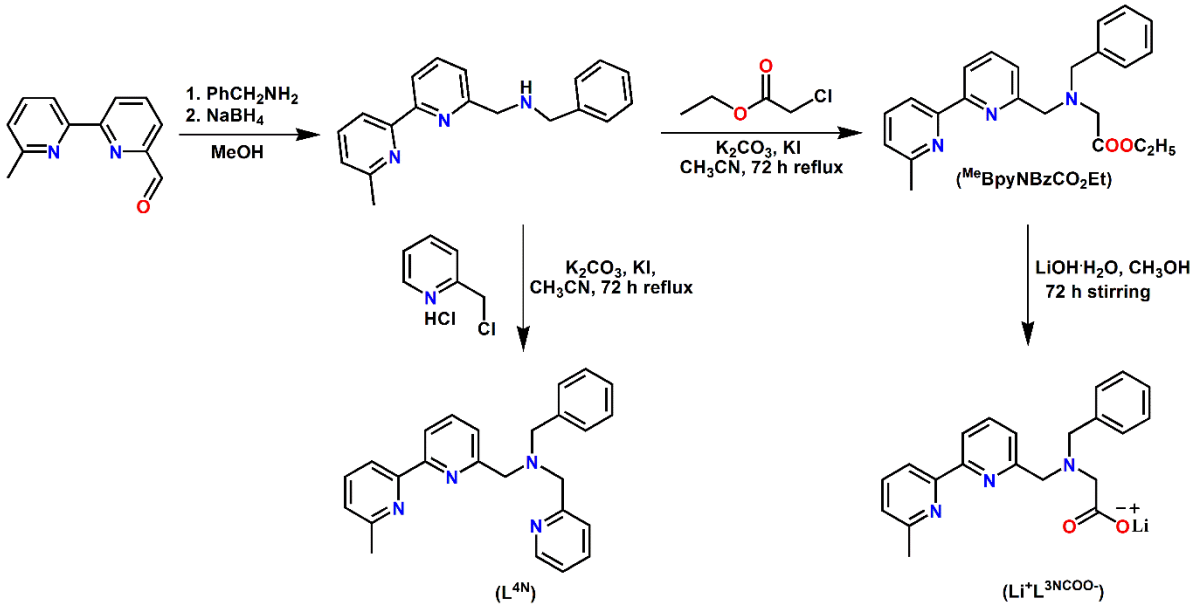
Table S1. Data collection and structure refinement parameters for $\mathbf{1^{OAc}\cdot 0.5H_2O}$, $\mathbf{2^{OAc}(PF_6)\cdot CH_2Cl_2}$ and $\mathbf{2^{fla}(ClO_4)\cdot 1.5H_2O}$			
	$\mathbf{1^{OAc}\cdot 0.5H_2O}$	$\mathbf{2^{OAc}(PF_6)\cdot CH_2Cl_2}$	$\mathbf{2^{fla}(ClO_4)\cdot 1.5H_2O}$
CCDC	2224092	2224093	2224094
Chemical formula	$2(C_{23}H_{23}CoN_3O_8)\cdot H_2O$	$C_{28}H_{29}Cl_2CoF_6N_4O_2P$	$2(C_{40}H_{33}CoN_4O_3)2(ClO_4)\cdot 3H_2O$
Formula weight	946.77	728.35	1606.16
Temperature (K)	296(2)	296(2)	296(2)
λ (Å)	*Mo-Kα* (0.71073)	*Mo-Kα* (0.71073)	*Mo-Kα* (0.71073)
Crystal system	Monoclinic	Triclinic	Triclinic
Space group	*C*2/c (no. 15)	$P\bar{1}$ (no. 2)	$P\bar{1}$ (no. 2)
a (Å)	30.46(3)	10.4596(6)	11.329(9)
b (Å)	10.531(7)	12.6026(7)	12.326(10)
c (Å)	15.734(14)	13.7868(9)	15.020(12)
α (°)	90	103.291(2)	93.25(2)
β (°)	116.17(4)	95.981(2)	104.03(2)
γ (°)	90	113.429(2)	105.307(18)
V/(Å^3)	4529(7)	1583.44(17)	1946(3)
Z	4	2	1
D_c (g cm^{-3})	1.385	1.528	1.365
μ (mm^{-1})	0.794	0.830	0.568
Reflections measured	11704	76149	30844
Unique reflections [R_{int}]	3334 [0.0924]	6953 [0.0384]	7959 [0.0477]
Number of reflections used [$I > 2\sigma(I)$]	2045	6036	5901
Number of parameters	286	397	493
Final R indices	[a]R_1 = 0.0779; [b]wR_2 = 0.1871	[a]R_1 = 0.0616; [b]wR_2 = 0.1885	[a]R_1 = 0.0536; [b]wR_2 = 0.1568
R indices (all data)	[a]R_1 = 0.1299; [b]wR_2 = 0.2331	[a]R_1 = 0.0696; [b]wR_2 = 0.1965	[a]R_1 = 0.0728; [b]wR_2 = 0.1729
Goodness-of-fit on F^2	1.013	1.035	1.030
Largest residual peak and hole (e.Å^{-3})	1.253 and -0.613	0.798 and -0.876	0.581 and -0.354
[a]$R_1 = \Sigma(\|F_o\| - \|F_c\|)/\Sigma\|F_o\|$. [b]$wR_2 = \{\Sigma[w(\|F_o\|^2 - \|F_c\|^2)^2]/\Sigma[w(\|F_o\|^2)^2]\}^{1/2}$.			



Scheme S1. Synthesis of ligands $Li^{+}L^{3NCOO-}$ and L^{4N}.

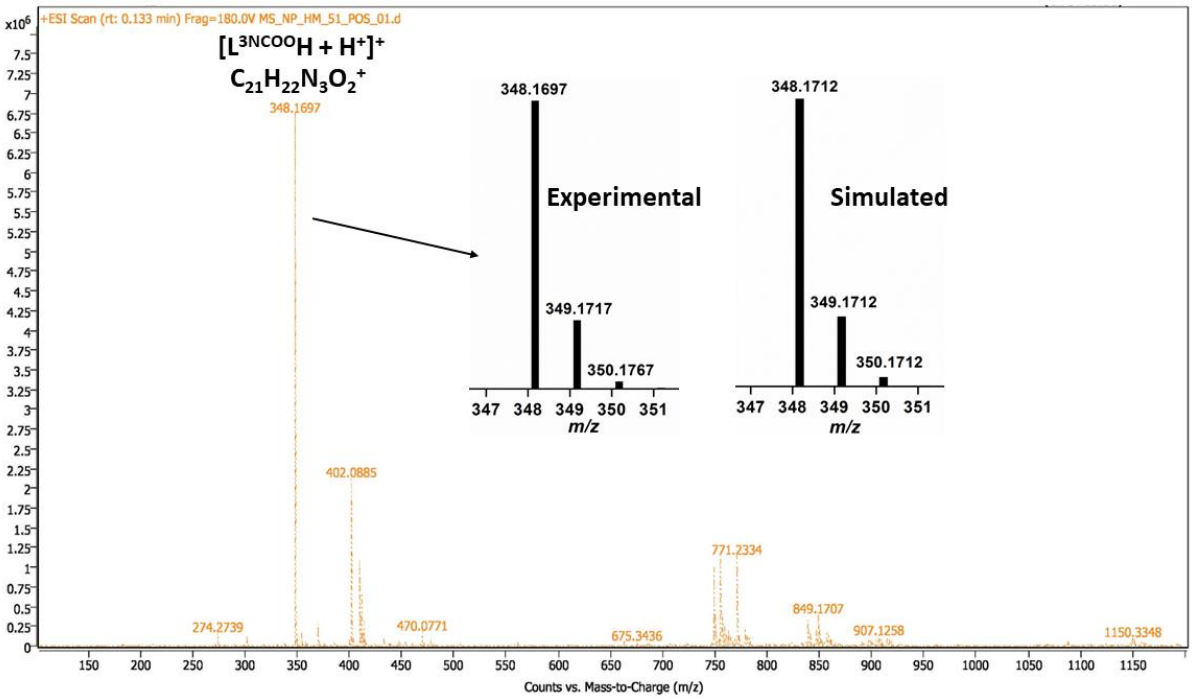


Figure S1. ESI(+)-MS of $Li^{+}L^{3NCOO-}$ in methanol with a trace quantity of HCOOH.

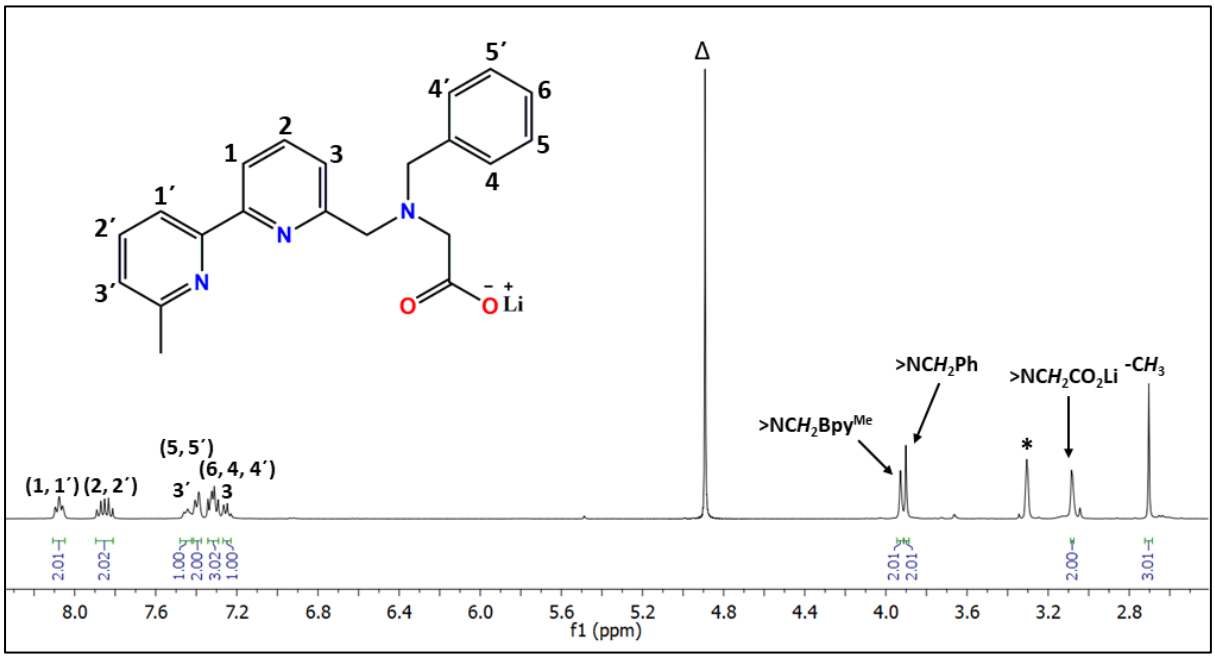


Figure S2. ^{1}H NMR (400 MHz, 300 K) spectrum of the ligand $Li^{+}L^{3NCOO-}$ in CD_3OD. Symbols (Δ) and (*) denote water and solvent residual peaks, respectively.

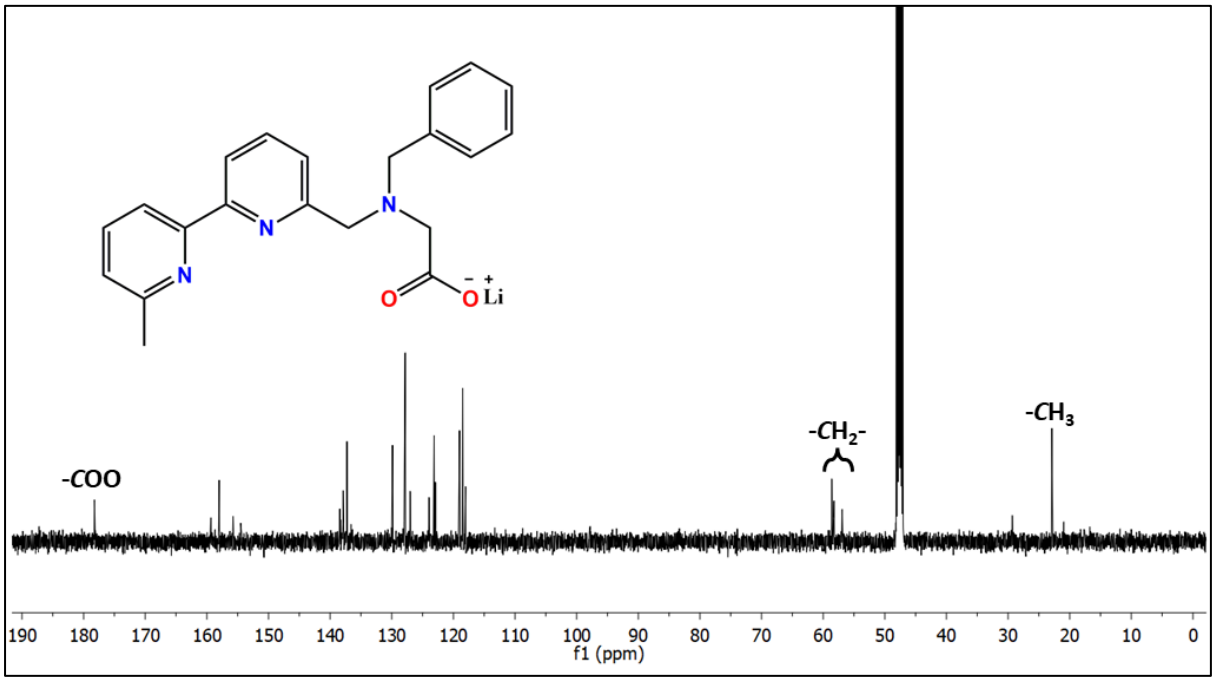


Figure S3. $^{13}C\{^{1}H\}$ NMR (125 MHz, 300 K) spectrum of the ligand $Li^{+}L^{3NCOO-}$ in CD_3OD.

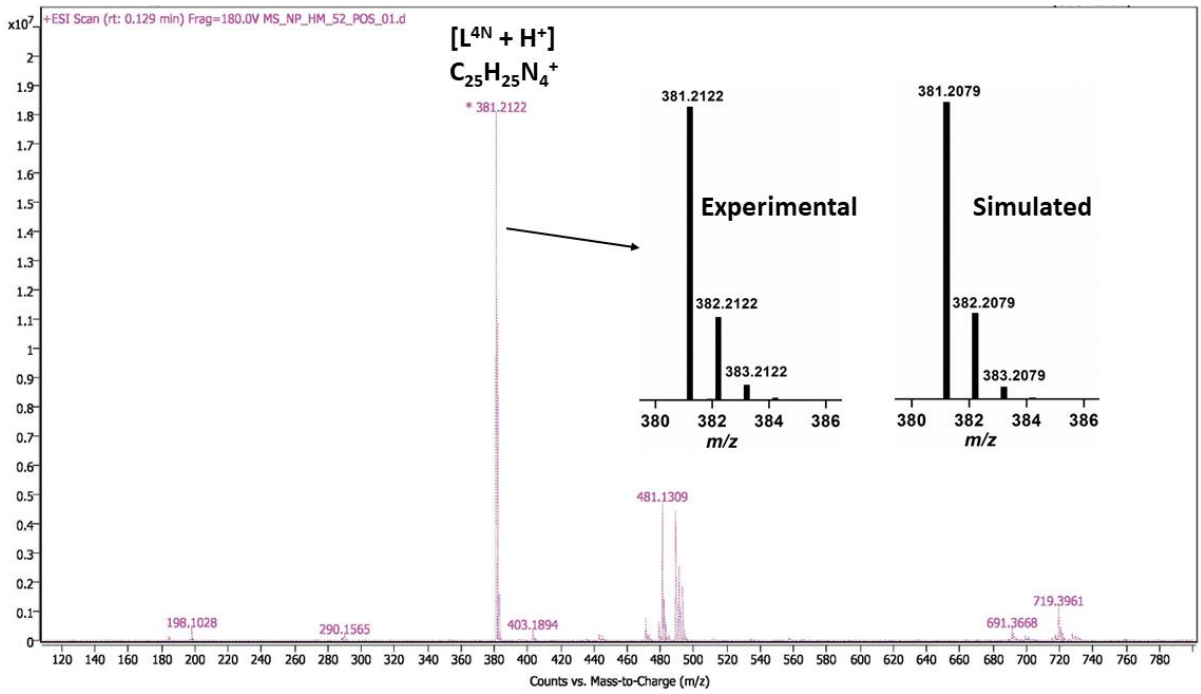


Figure S4. ESI(+)-MS of L^{4N} in methanol with a trace quantity of HCOOH.

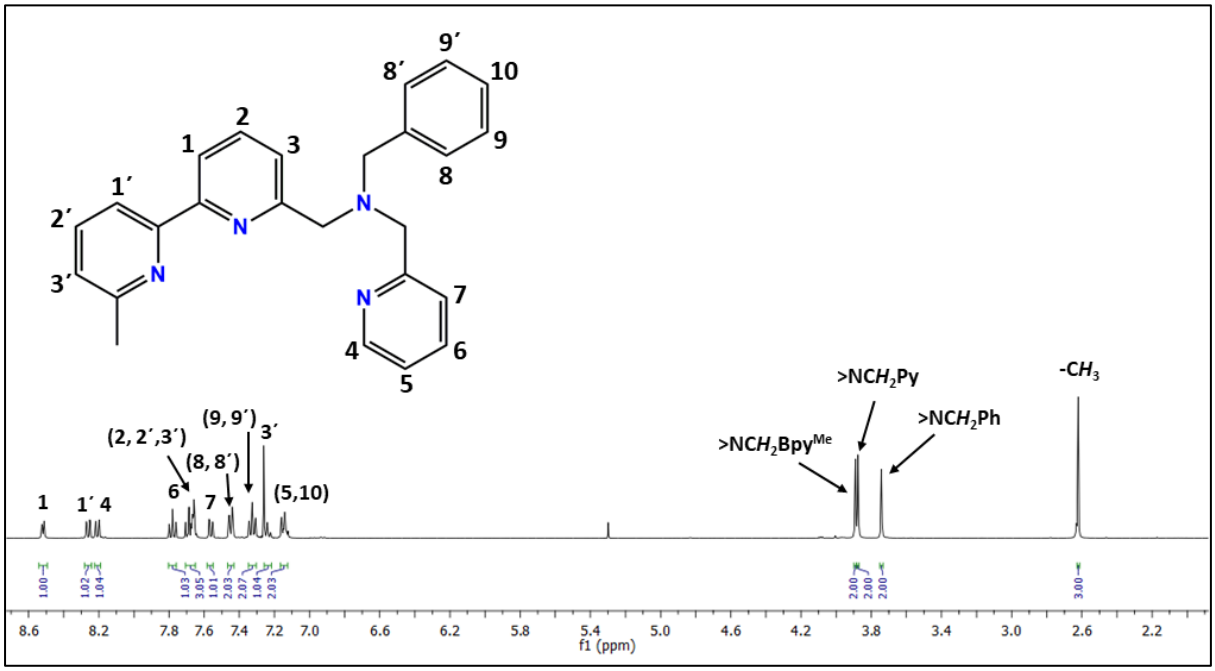


Figure S5. ^{1}H NMR (400 MHz, 300 K) spectrum of the ligand L^{4N} in $CDCl_3$.

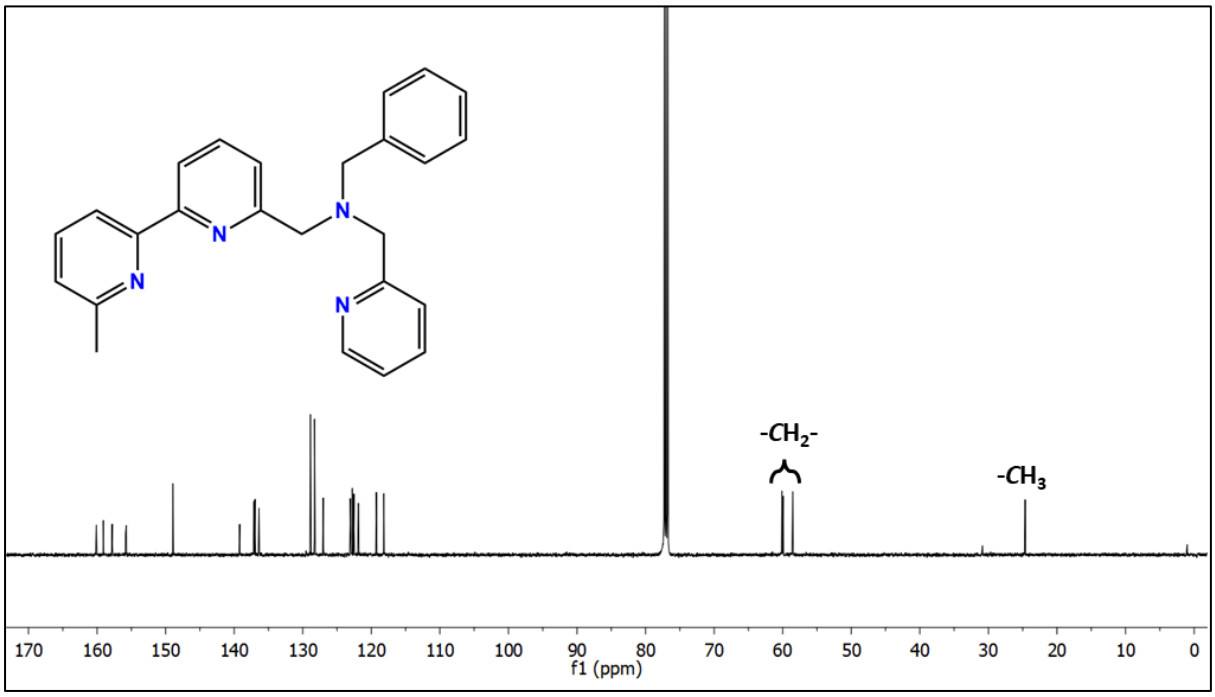


Figure S6. $^{13}C\{^{1}H\}$ NMR (125 MHz, 300 K) spectrum of the ligand L^{4N} in $CDCl_3$.

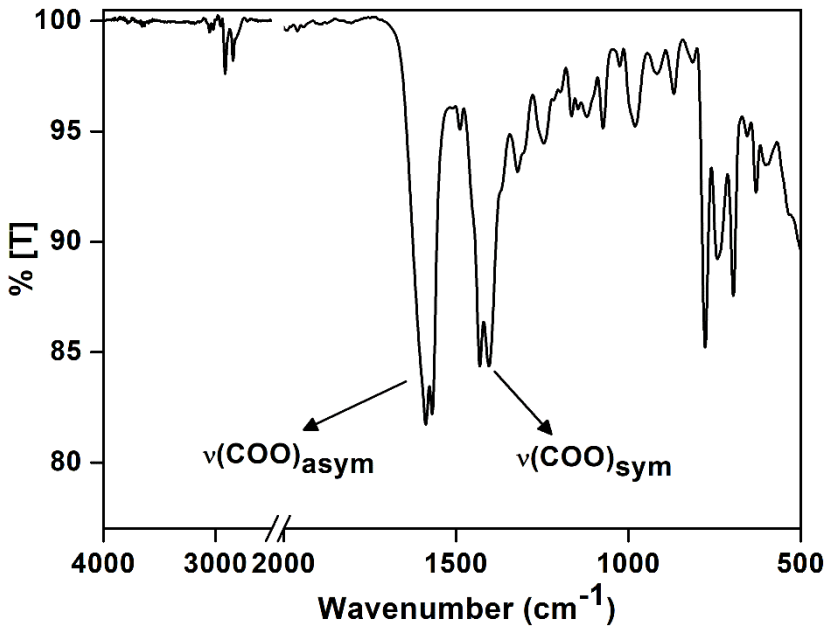


Figure S7. ATR-FTIR spectrum (solid sample) of ligand $Li^{+}L^{3NCOO-}$.

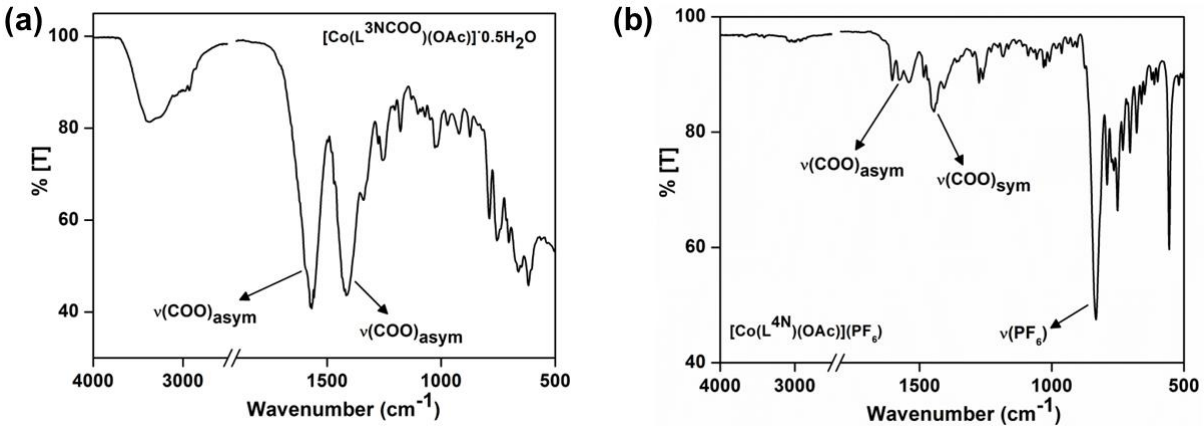


Figure S8. ATR-FTIR spectra (solid samples) of Co(II)-acetato complexes: (a) $[Co^{II}(L^{3NCOO})(OAc)]\cdot 0.5H_2O$ (**$1^{OAc}\cdot 0.5H_2O$**) and (b) $[Co^{II}(L^{4N})(OAc)](PF_6)$ (**$2^{OAc}(PF_6)$**).

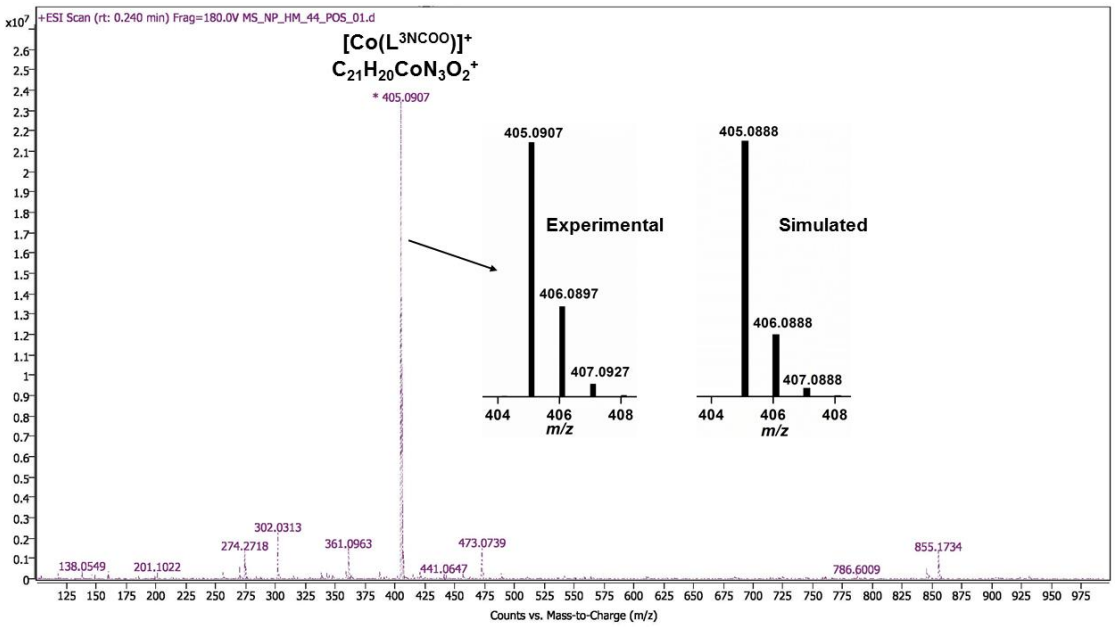


Figure S9. ESI(+)-MS of $[Co^{II}(L^{3NCOO})(OAc)]$ (**1^{OAc}**) in methanol with a trace quantity of HCOOH.

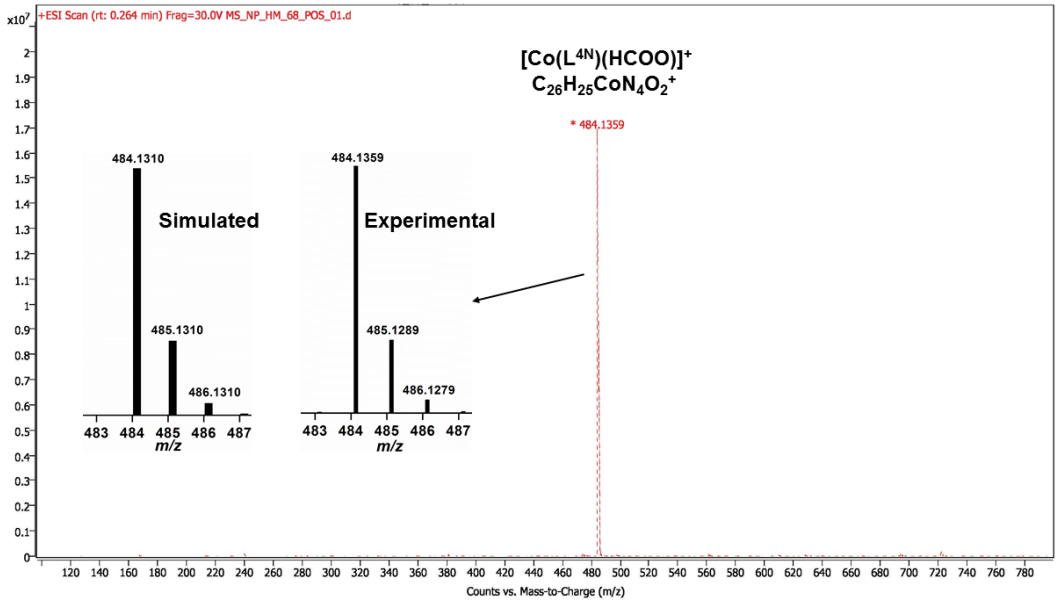


Figure S10. ESI(+)-MS of $[Co^{II}(L^{4N})(OAc)](PF_6)$ (**2^{OAc}(PF$_6$)**) in methanol with a trace quantity of HCOOH.

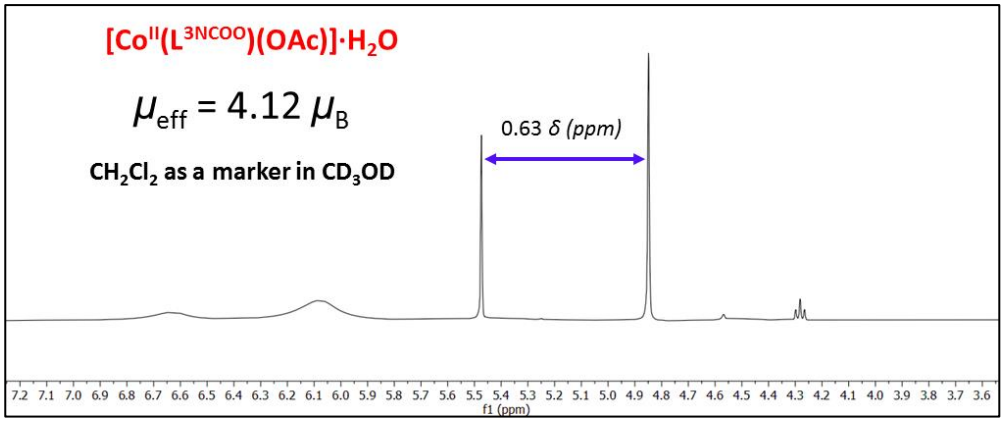


Figure S11. A representative ^{1}H NMR spectrum concerning the magnetic susceptibility measurement of complex **1^{OAc}·H$_2$O** at 300 K using the Evans method with CH_2Cl_2 as a marker and CD_3OD as a solvent.

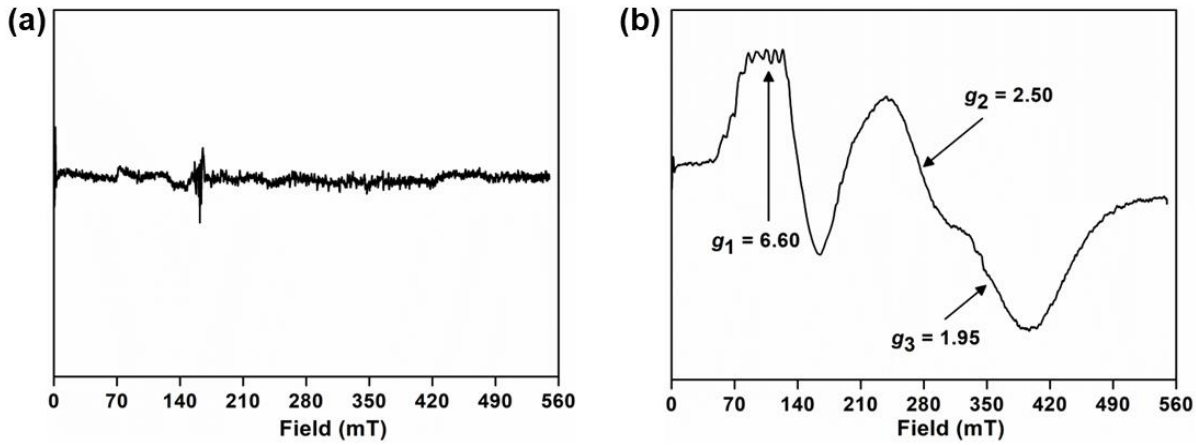


Figure S12. EPR spectra of complexes (a) $[Co^{II}(L^{3NCOO})(OAc)]\cdot 0.5H_2O$ (**$1^{OAc}\cdot 0.5H_2O$**) and (b) $[Co^{II}(L^{4N})(OAc)](PF_6)$ (**$2^{OAc}(PF_6)$**) recorded in DMF at 14 K (microwave frequency ~ 9.65 GHz).

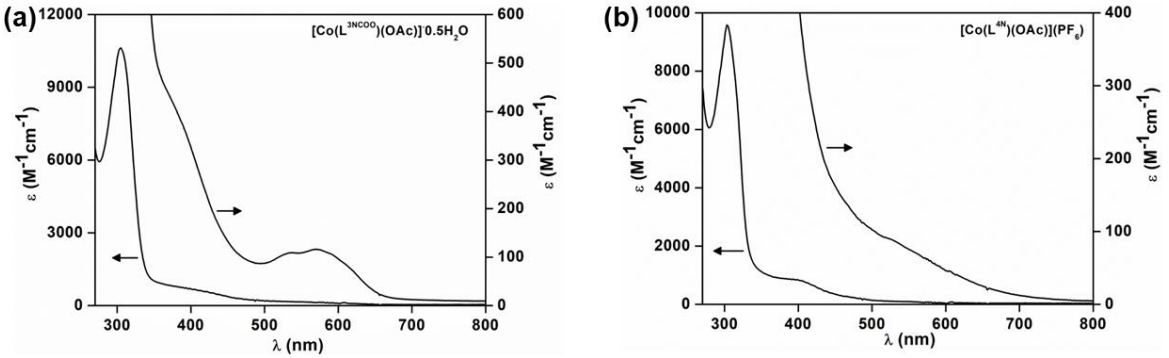


Figure S13. UV-vis spectra of complexes (a) $[Co^{II}(L^{3NCOO})(OAc)]\cdot 0.5H_2O$ (**$1^{OAc}\cdot 0.5H_2O$**) and (b) $[Co^{II}(L^{4N})(OAc)](PF_6)$ (**$2^{OAc}(PF_6)$**) in DMF.

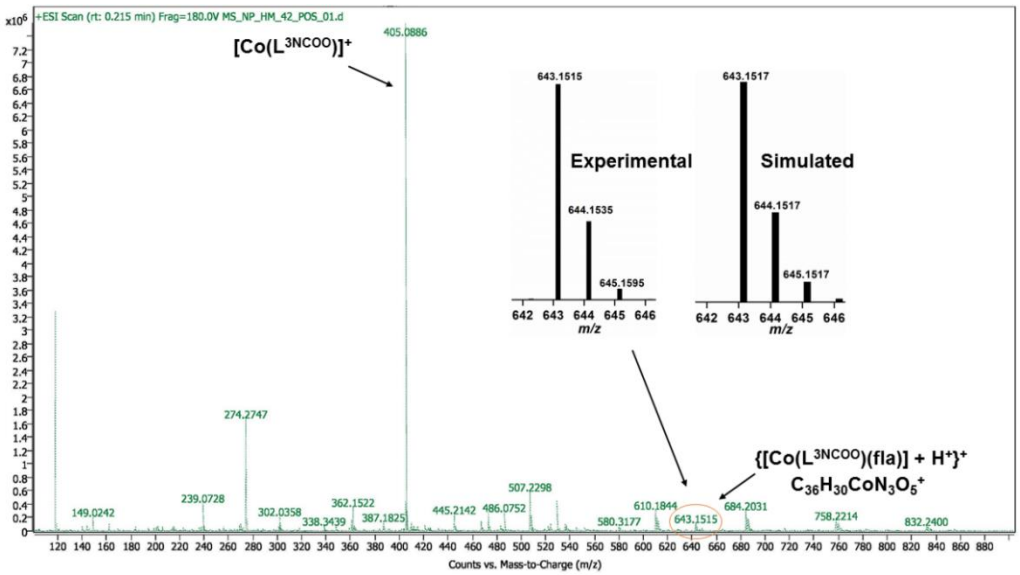


Figure S14. ESI(+)-MS of $[Co^{II}(L^{3NCOO})(fla)]$ (**1^{fla}**) in methanol with a trace quantity of HCOOH.

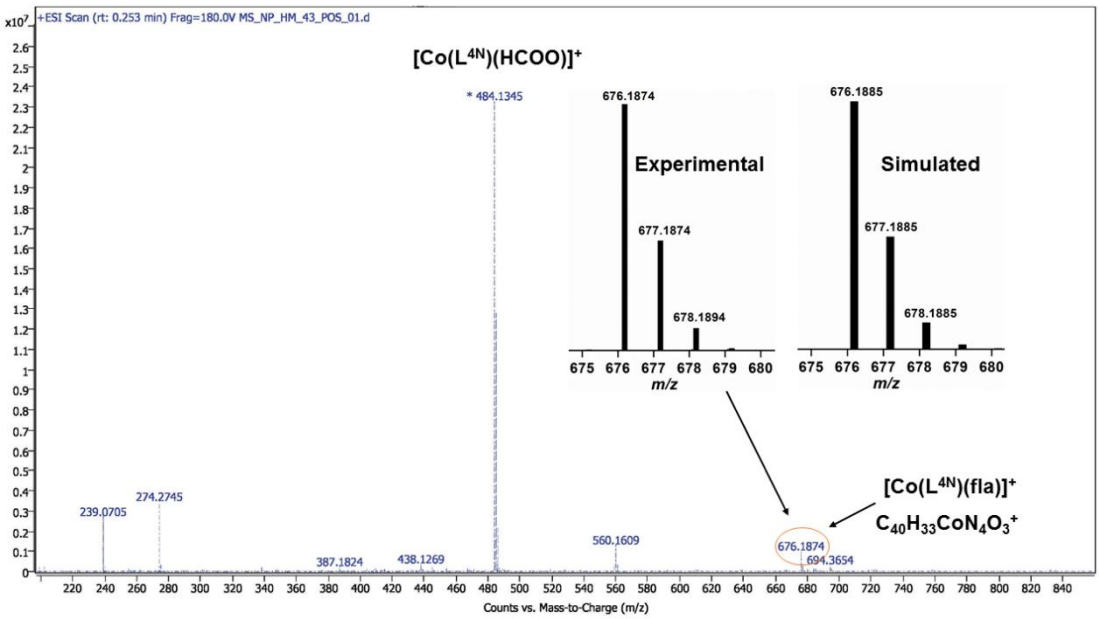


Figure S15. ESI(+)-MS of $[Co^{II}(L^{4N})(fla)](PF_6)$ (**$2^{fla}(PF_6)$**) in methanol with a trace quantity of HCOOH.

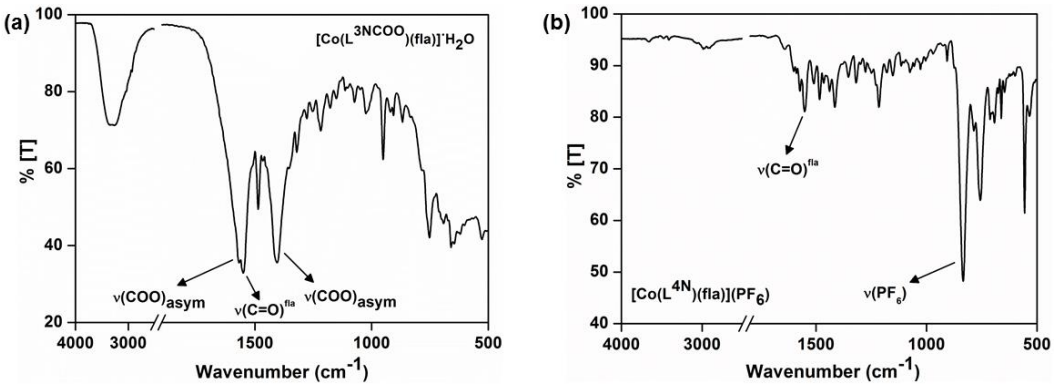


Figure S16. ATR-FTIR spectra (solid samples) of Co(II)-flavonolato complexes: (a) $[Co^{II}(L^{3NCOO})(fla)]\cdot H_2O$ (**$1^{fla}\cdot H_2O$**) and (b) $[Co^{II}(L^{4N})(fla)](PF_6)$ (**$2^{fla}(PF_6)$**).

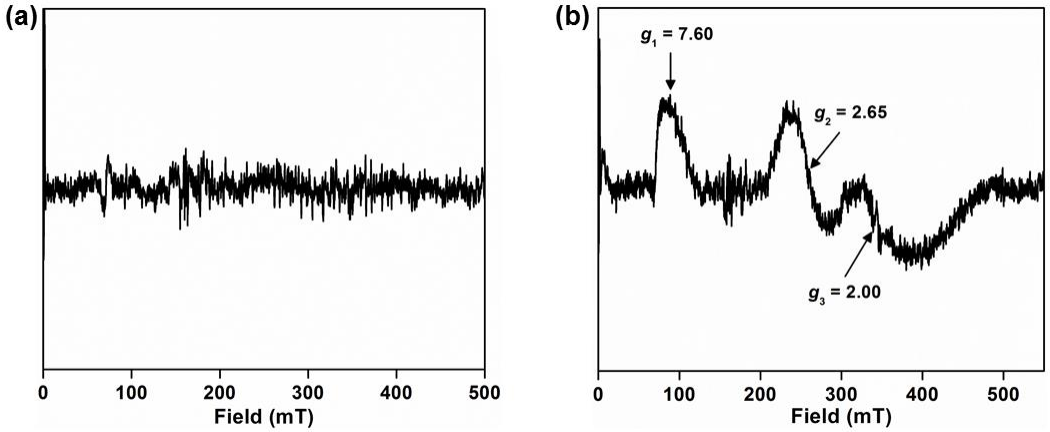


Figure S17. EPR spectra of complexes (a) $[Co^{II}(L^{3NCOO})(fla)]\cdot H_2O$ (**$1^{fla}\cdot H_2O$**) and (b) $[Co^{II}(L^{4N})(fla)](PF_6)$ (**$2^{fla}(PF_6)$**) recorded in DMF at 14 K (microwave frequency ~ 9.65 GHz).

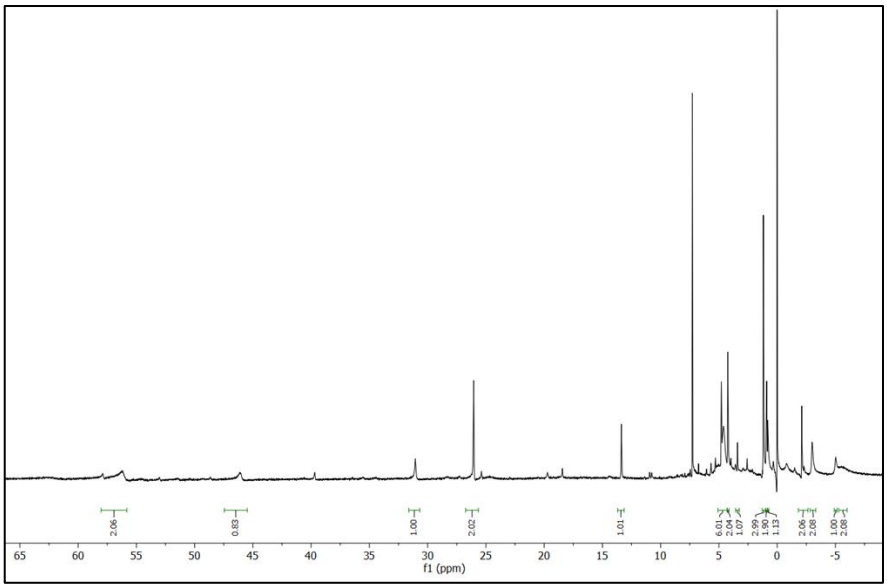


Figure S18. ^{1}H NMR (400 MHz, 300 K) spectrum of $[Co^{II}(L^{3NCOO})(fla)]\cdot H_2O$ (**$1^{fla}\cdot H_2O$**) in $CDCl_3$.

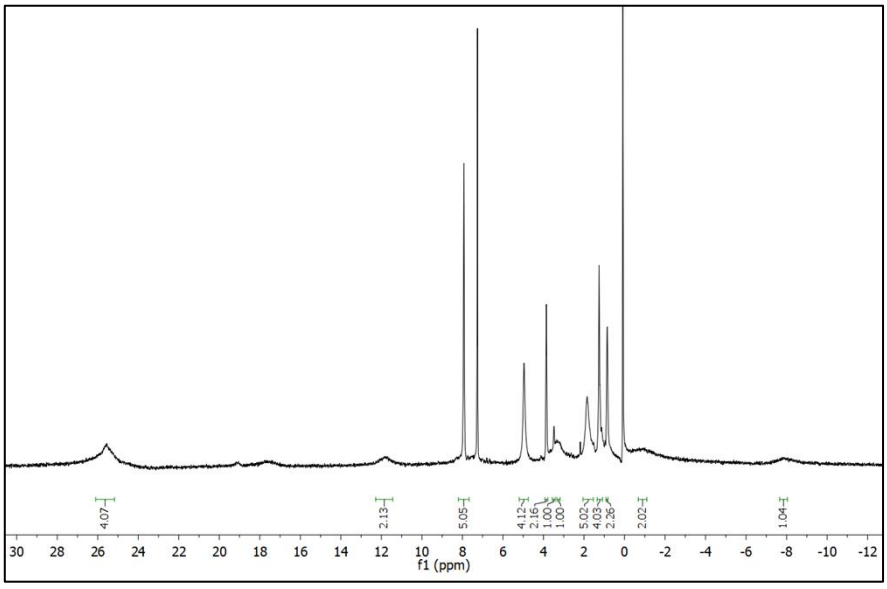


Figure S19. ^{1}H NMR (400 MHz, 300 K) spectrum of $[Co^{II}(L^{4N})(fla)](PF_6)$ (**$2^{fla}(PF_6)$**) in $CDCl_3$.

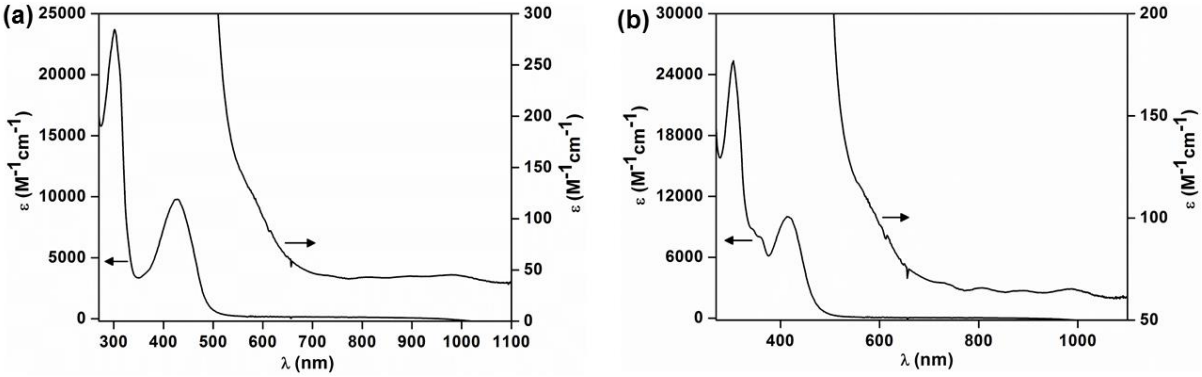


Figure S20. UV-vis spectra of complexes (a) $[Co^{II}(L^{3NCOO})(fla)]\cdot H_2O$ (**$1^{fla}\cdot H_2O$**) and (b) $[Co^{II}(L^{4N})(fla)](PF_6)$ (**$2^{fla}(PF_6)$**) in DMF.

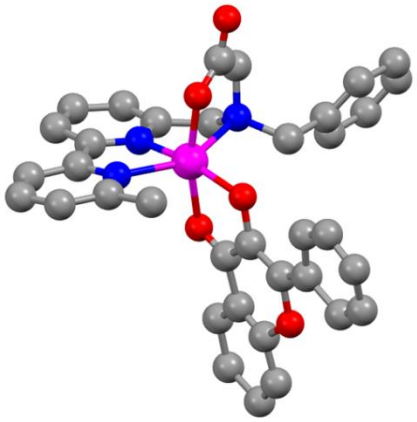


Figure S21. Ball and stick representation of the X-ray structure of the complex $[Co^{II}(L^{3NCOO})(fla)]$ (**1^{fla}**). Colour code: cobalt (magenta), oxygen (red), carbon (grey), nitrogen (blue). The hydrogen atoms are omitted for clarity.

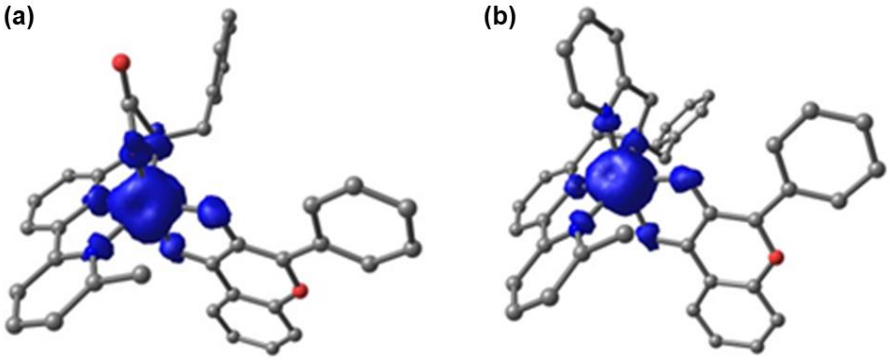


Figure 22. Mulliken spin-density plots for (a) **1^{fla}** and (b) **2^{fla+}** in their high-spin (quartet) states.

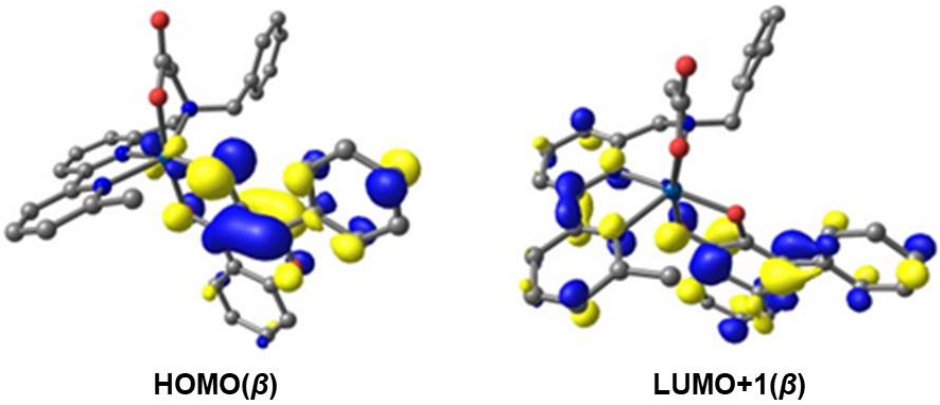


Figure 23. Beta molecular orbitals involved in the electronic transition for $\mathbf{1}^{\mathbf{fla}}$.

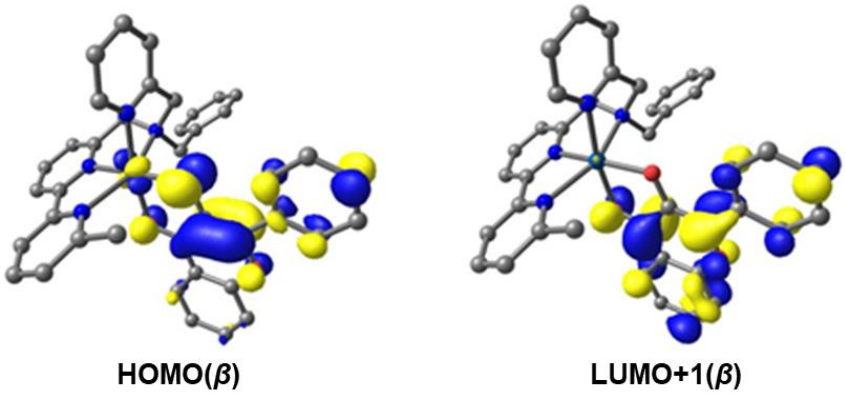


Figure S24. Beta molecular orbitals involved in the electronic transition for $\mathbf{2}^{\mathbf{fla+}}$.

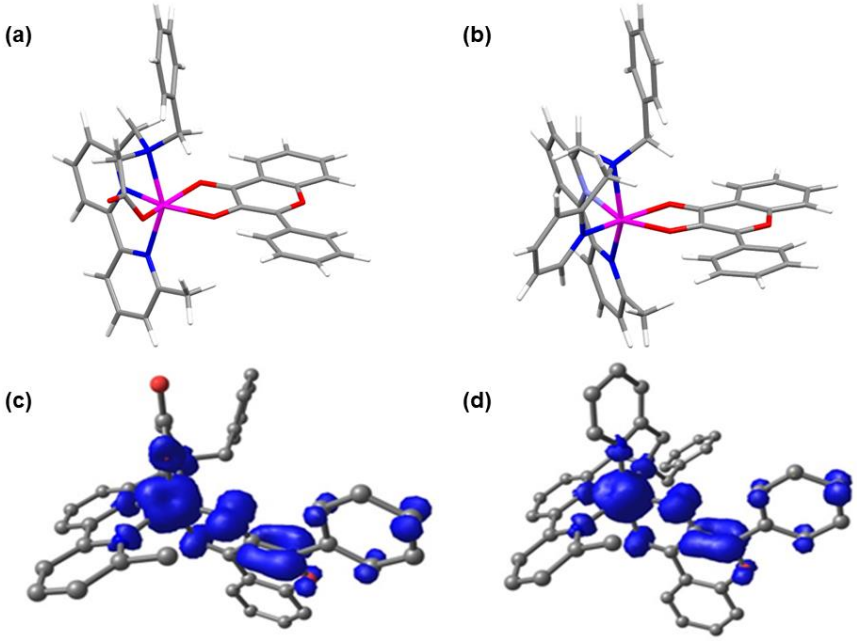


Figure 25. (Top) The optimised structures for (a) $\mathbf{1}^{\mathbf{fla\bullet+}}$ and (b) $\mathbf{2}^{\mathbf{fla\bullet2+}}$; (bottom) Mulliken spin-density plots for (c) $\mathbf{1}^{\mathbf{fla\bullet+}}$ and (d) $\mathbf{2}^{\mathbf{fla\bullet2+}}$ in their high-spin (S = 2) states.

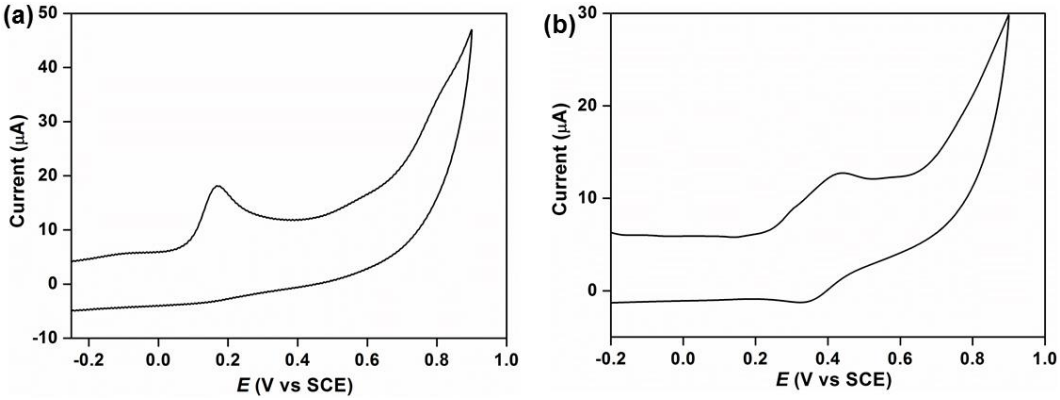


Figure S26. Cyclic voltammograms of the Co(II)-flavonolato complexes in DMF: (a) $[Co^{II}(L^{3NCOO})(fla)]\cdot H_2O$ (**$1^{fla}\cdot H_2O$**) and (b) $[Co^{II}(L^{4N})(fla)](PF_6)$ (**$2^{fla}(PF_6)$**) (scan rate: 100 $mV\cdot s^{-1}$; supporting electrolyte: TBAP).

Table S2. Kinetic data of complex $[Co^{II}(L^{3NCOO})(OAc)]\cdot 0.5H_2O$ (**$1^{OAc}\cdot 0.5H_2O$**)							
Exp No.	T (°C)	$[O_2]$ (10^{-3}M)	[flaH] (10^{-4} M)	[Complex] (10^{-6} M)	v_{in} (10^{-8} Ms^{-1})	k_3 ($10^5M^{-2}s^{-1}$)	k_3(av) ($10^5M^{-2}s^{-1}$)
1	70	1.07	1	1	6.34	5.93	6.00 ± 0.12
2	70	1.39	1	1	8.32	5.99	
3	70	1.71	1	1	10.08	5.89	
4	70	2.14	0.8	1	10.39	6.07	
5	70	2.14	1	1	12.75	5.96	
6	70	2.14	1.2	1	15.92	6.20	
7	70	2.14	1.4	0.5	8.62	5.75	
8	70	2.14	1.4	1	18.25	6.09	
9	70	2.14	1.4	1.5	27.26	6.07	
10	70	2.14	1.4	2	36.01	6.01	
11	65	2.14	1.4	2	32.21	5.38	
12	60	2.14	1.4	2	29.46	4.92	
13	55	2.14	1.4	2	26.51	4.42	

Table S3. Kinetic data of complex $[Co^{II}(L^{4N})(OAc)](PF_6)$ (**$2^{OAc}(PF_6)$**)							
Exp No.	T (°C)	$[O_2]$ (10^{-3}M)	[flaH] (10^{-4} M)	[Complex] (10^{-6} M)	v_{in} (10^{-8} Ms^{-1})	k_3 ($10^5M^{-2}s^{-1}$)	k_3 (av) ($10^5M^{-2}s^{-1}$)
1	70	1.07	1	1	5.05	4.72	4.85 ± 0.07
2	70	1.39	1	1	6.61	4.76	
3	70	1.71	1	1	8.37	4.89	
4	70	2.14	0.8	1	8.41	4.91	
5	70	2.14	1	1	10.6	4.95	
6	70	2.14	1.2	1	12.54	4.88	
7	70	2.14	1.4	0.5	7.25	4.84	
8	70	2.14	1.4	1	14.65	4.89	
9	70	2.14	1.4	1.5	21.64	4.82	
10	70	2.14	1.4	2.0	28.88	4.82	
11	65	2.14	1.4	2.0	23.99	4.00	
12	60	2.14	1.4	2.0	21.39	3.57	
13	55	2.14	1.4	2.0	17.41	2.91	

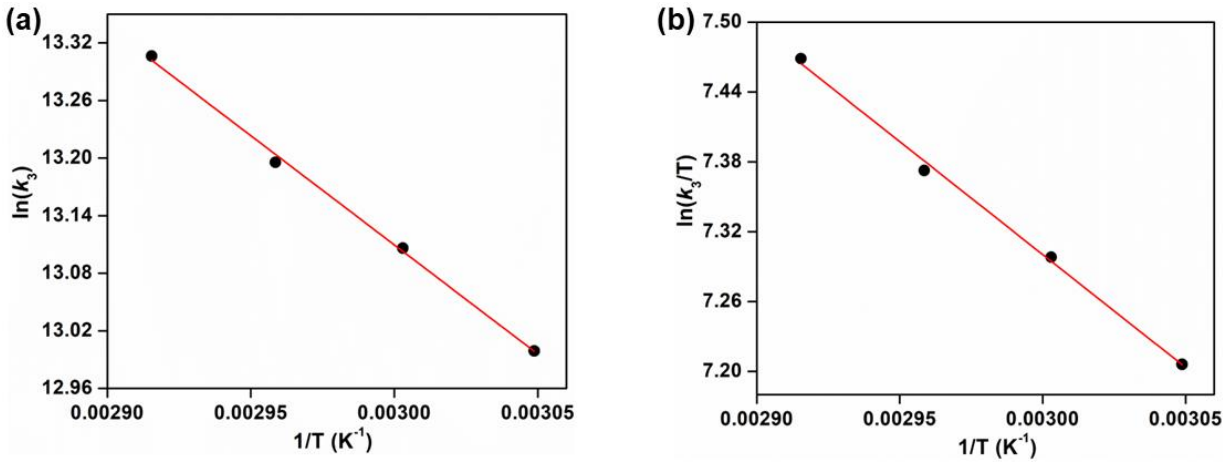


Figure S27. Determination of activation parameters: (a) Arrhenius plot and (b) Eyring plot for the oxygenative degradation of flavonol catalysed by $[Co^{II}(L^{3NCOO})(OAc)]\cdot 0.5H_2O$ (**$1^{OAc}\cdot 0.5H_2O$**).

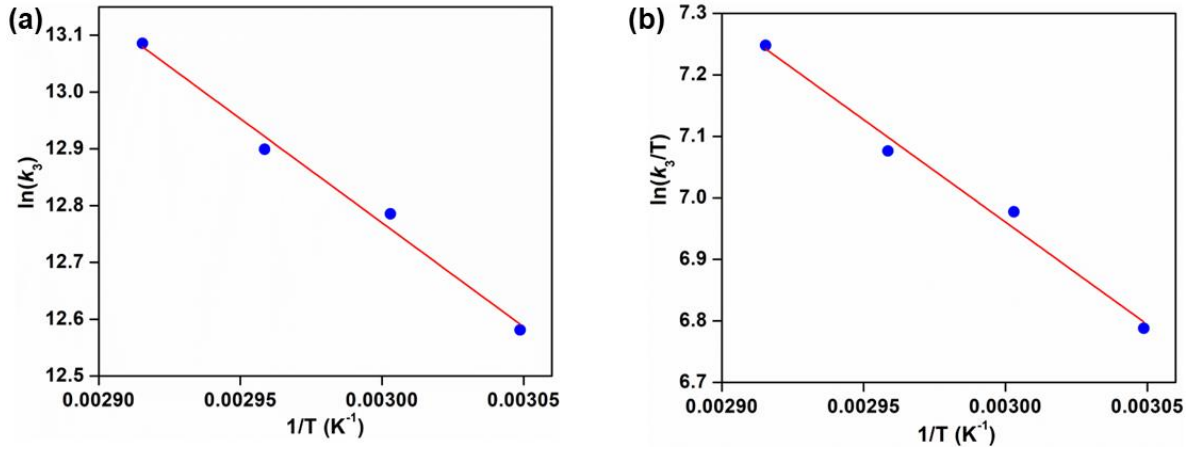


Figure S28. Determination of activation parameters: (a) Arrhenius plot and (b) Eyring plot for the oxygenative degradation of flavonol catalysed by $[Co^{II}(L^{4N})(OAc)](PF_6)$ (**$2^{OAc}(PF_6)$**).

Table S4. LC-MS analysis results for the dioxygenation of flavonol (10 mM) catalysed by Co^{II}-acetato complexes (1 mM) at 70 °C in DMF

Catalyst	**Yield (%)**					**Conv. (%)**	**TON**	**Conv. Rate (h^{-1})**
	o-benzoyl salicylic acid (RT: 24.40)	2-hydroxy benzoic acid (RT: 18.91)	Benzoic acid (RT: 17.75)	2-hydroxy-*N*,*N*-dimethyl benzamide (RT: 6.20)	*N*,*N*-dimethyl benzamide (RT:14.73)			
$1^{OAc}\cdot 0.5H_2O$	5	13	39	10	45	89	8.9	1.78
$2^{OAc}(PF_6)$	3	9	36	13	43	82	8.2	1.64

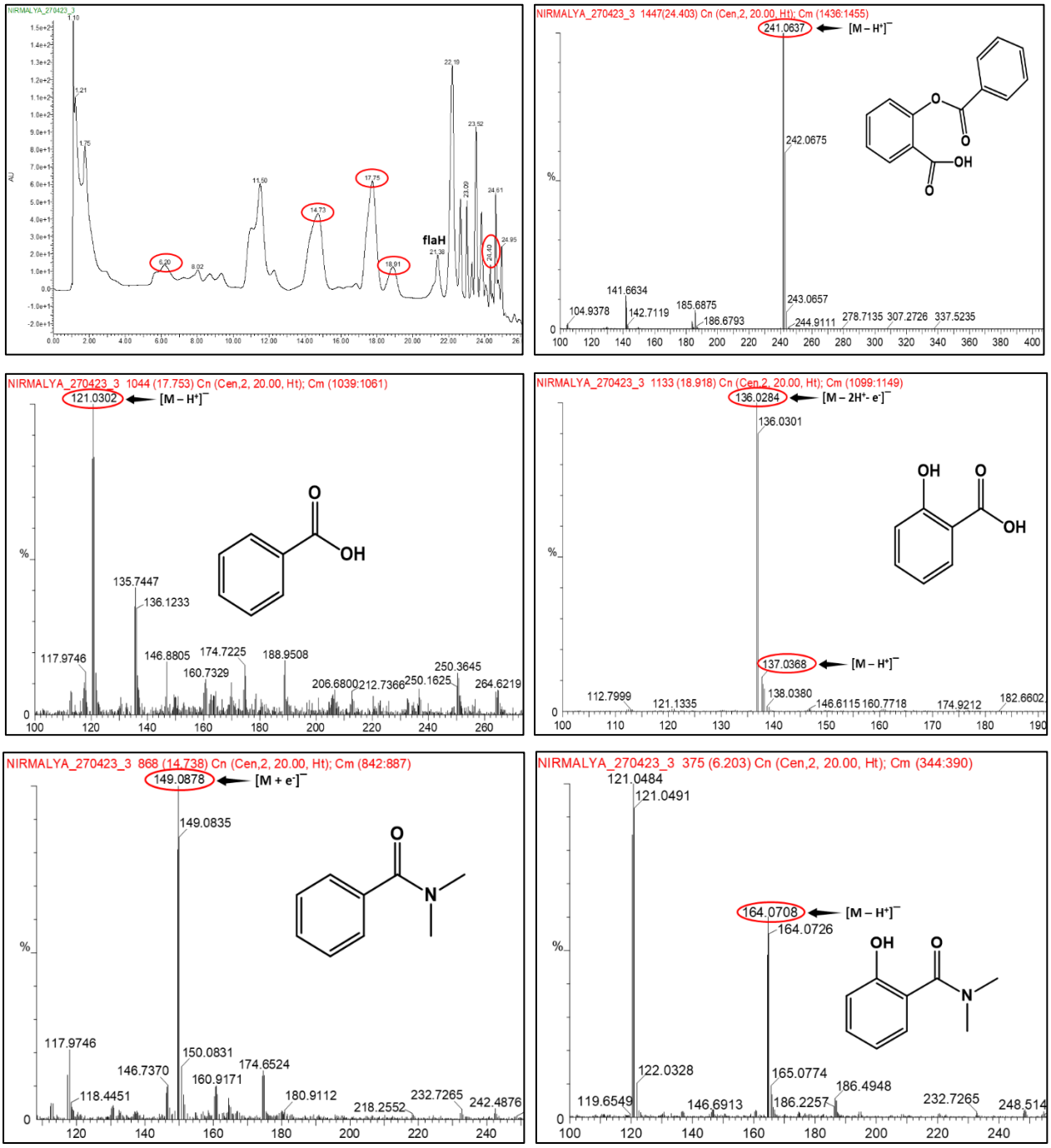


Figure S29. Representative liquid chromatogram and the mass spectrometry (negative ion mode) of the products obtained from the oxygenolysis of flavonol catalysed by $[Co^{II}(L^{3NCOO})(OAc)]\cdot 0.5H_2O$ (**$1^{OAc}\cdot 0.5H_2O$**).

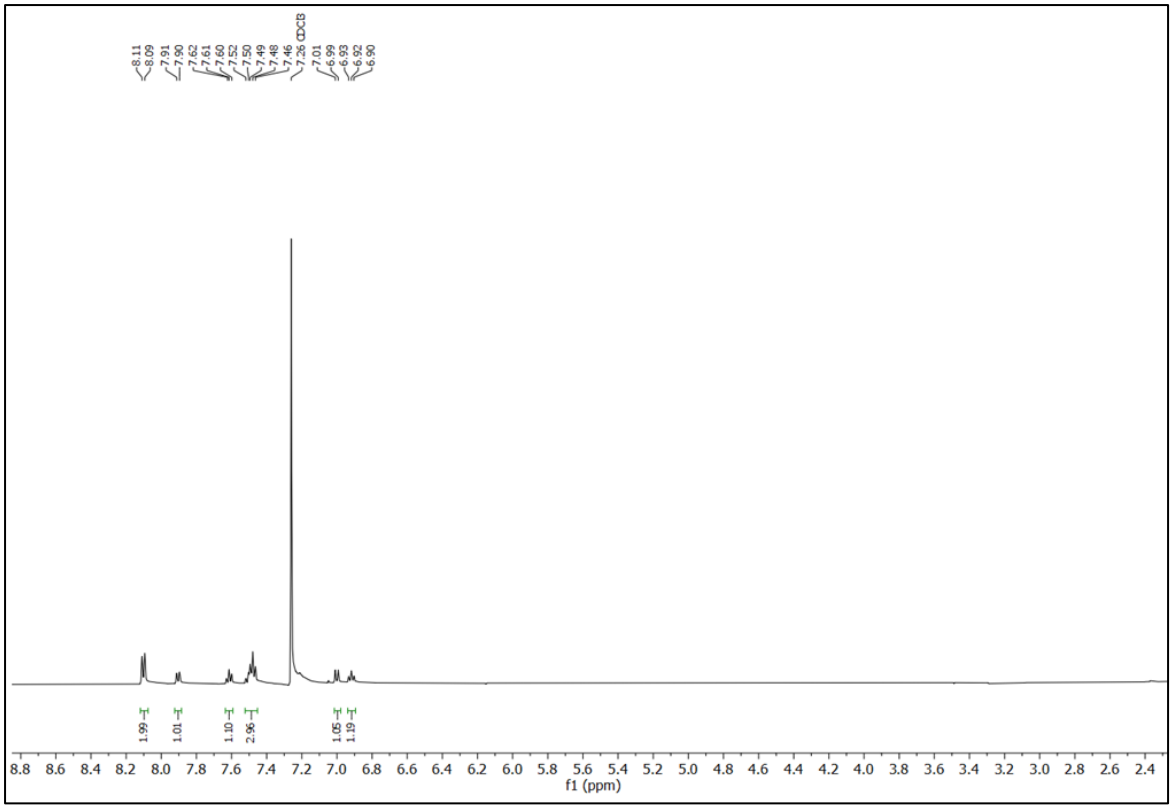


Figure S30. ^{1}H NMR spectrum (in $CDCl_3$) of the flavonol degraded products via dioxygenation catalysed by $[Co^{II}(L^{3NCOO})(OAc)]\cdot 0.5H_2O$ (**$1^{OAc}\cdot 0.5H_2O$**). Signals correspond to a mixture of benzoic acid [δ(ppm) = 8.10 (d, 2H), 7.61 (t, 1H), 7.51 (t, 2H))] and salicylic acid [δ(ppm) = 7.90 (d, 1H), 7.48 (t, 1H), 7.00 (d, 1H), 6.92 (t, 1H)] in ~50:50 ratio.

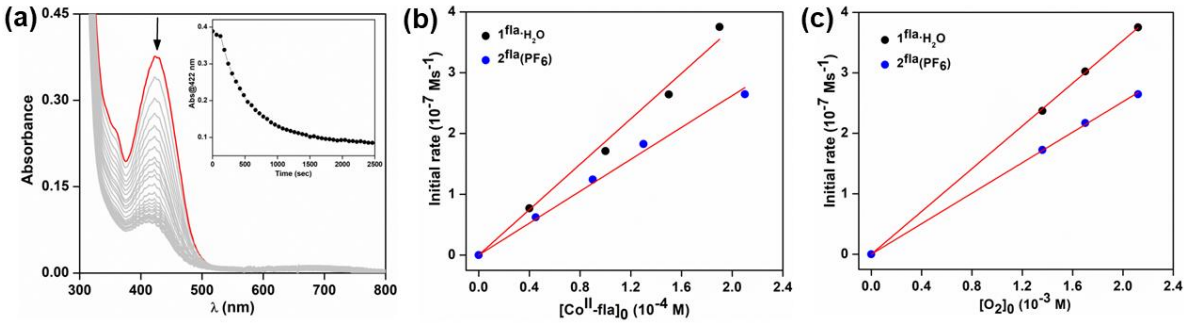


Figure S31. (a) UV-vis spectral changes observed during the dioxygenation reaction of **$1^{fla}\cdot H_2O$** in DMF (conditions: $[complex]_0 = 0.4 \times 10^{-4}$ M, $[O_2]_0 = 2.12 \times 10^{-3}$ M; T = 70° C). The inset shows a time trace of absorbance changes at 422 nm. Plots of initial rates *vs.* (b) $[Co^{II}\text{-fla}]_0$ and (c) $[O_2]_0$.

Table S5. Kinetic data of complex $[Co^{II}(L^{3NCOO})(fla)]\cdot H_2O$ ($\mathbf{1^{fla}\cdot H_2O}$)						
Exp No.	T (°C)	$[O_2]$ (10^{-3} M)	[Complex] (10^{-4} M)	v_{in} (10^{-8} Ms^{-1})	k_2 (10^{-2} $M^{-1}s^{-1}$)	k_2 (av) (10^{-2} $M^{-1}s^{-1}$)
1	70	1.36	1.90	23.71	91.76	88.82 ± 5.53
2	70	1.70	1.90	30.23	93.59	
3	70	2.12	1.90	37.52	93.15	
4	70	2.12	1.50	26.42	83.08	
5	70	2.12	1.00	17.10	80.66	
6	70	2.12	0.40	7.69	90.68	

Table S6. Kinetic data of complex $[Co^{II}(L^{4N})(fla)](PF_6)$ ($\mathbf{2^{fla}(PF_6)}$)						
Exp No.	T (°C)	$[O_2]$ (10^{-3} M)	$[Co(L^{4N})(fla)]$ (10^{-4} M)	v_{in} (10^{-8} Ms^{-1})	k_2 (10^{-2} $M^{-2}s^{-1}$)	k_2 (av) (10^{-2} $M^{-1}s^{-1}$)
1	70	1.36	2.10	17.25	60.40	62.85 ± 2.96
2	70	1.70	2.10	21.70	60.78	
3	70	2.12	2.10	26.46	59.43	
4	70	2.12	1.30	18.27	66.29	
5	70	2.12	0.90	12.42	65.09	
6	70	2.12	0.45	6.21	65.09	

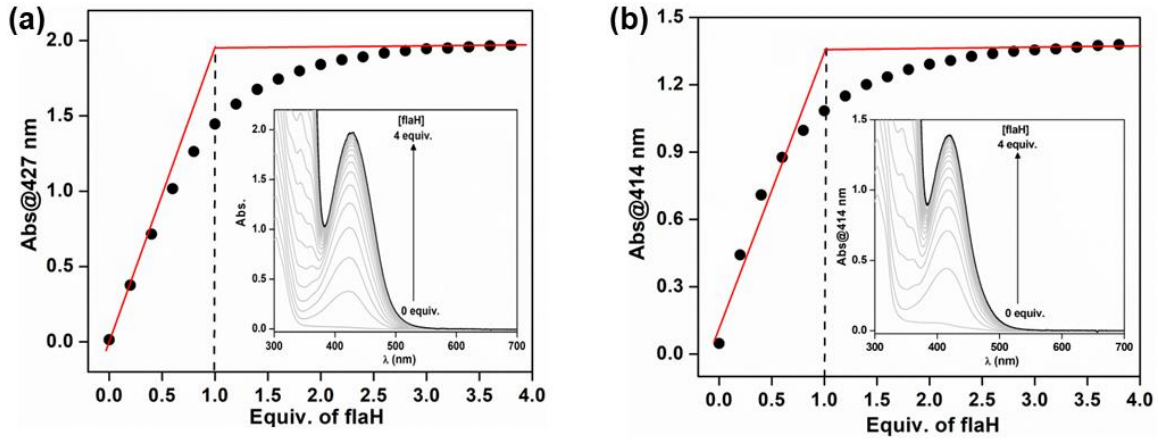


Figure S32. Spectrophotometric titration curves of the formation of Co(II)-flavonolato complexes upon the addition of flavonol into the DMF solution of complexes (a) $[Co^{II}(L^{3NCOO})(OAc)]$ ($\mathbf{1^{OAc}}$) and (b) $[Co^{II}(L^{4N})(OAc)](PF_6)$ ($\mathbf{2^{OAc}(PF_6)}$) at room temperature under N_2. The inset shows the growth of $\pi \rightarrow \pi^*$ band due to coordinated flavonolate.

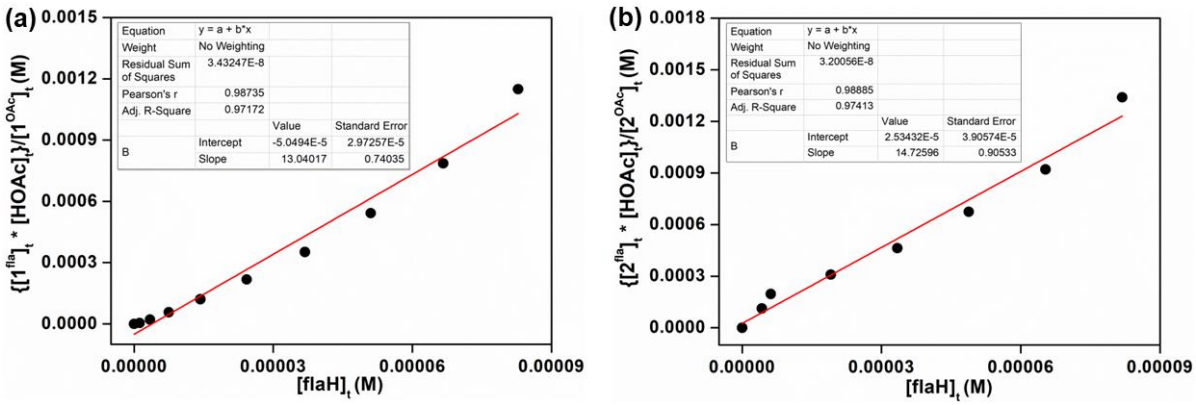


Figure S33. Plots to determine the formation constant (K_f) of species (a) $\mathbf{1^{fla}}$ and (b) $\mathbf{2^{fla+}}$. The slope of the linear fit represents the K_f values.

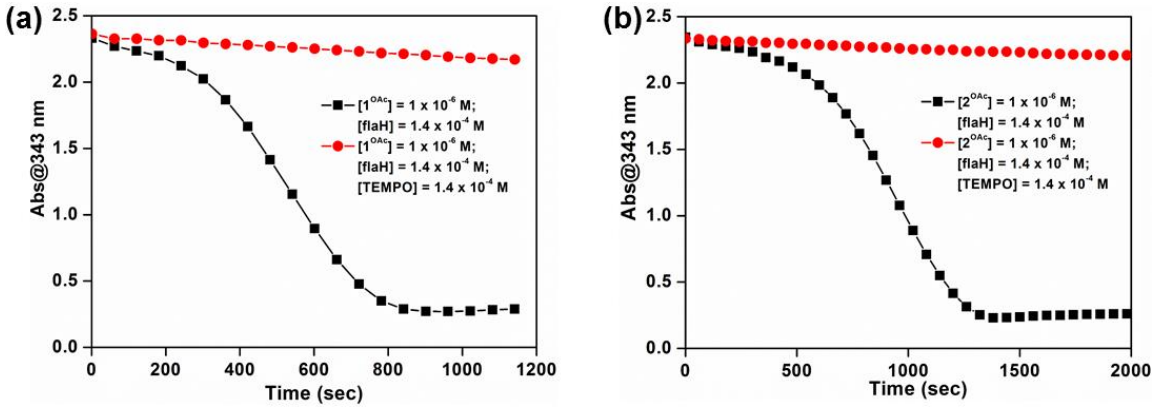


Figure S34. Time traces of the oxygenative degradation of flavonol catalysed by complexes (a) $[Co^{II}(L^{3NCOO})(OAc)]\cdot 0.5H_2O$ ($\mathbf{1^{OAc}\cdot 0.5H_2O}$) and (b) $[Co^{II}(L^{4N}(OAc)](PF_6)$ ($\mathbf{2^{OAc}(PF_6)}$) in DMF at 70 °C in the presence (red circle) and absence (black square) of TEMPO.

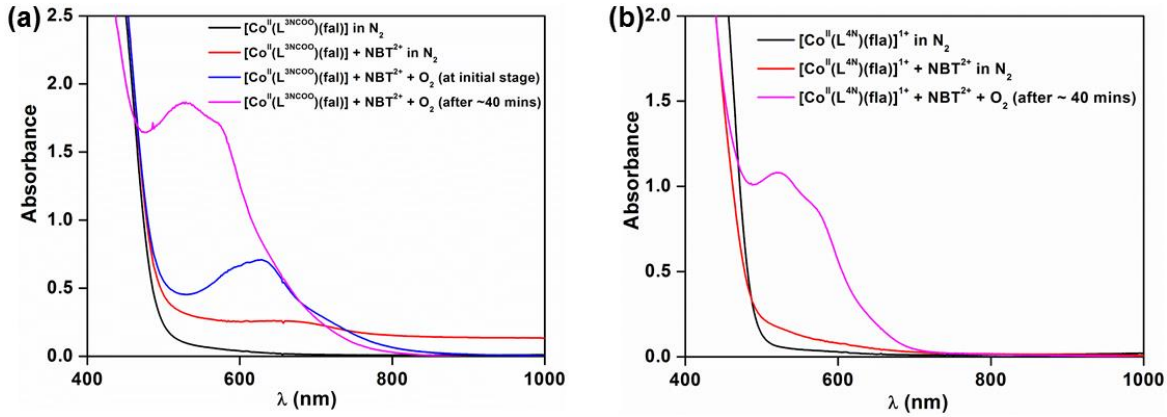


Figure S35. Spectral changes for the reaction of (a) $[Co^{II}(L^{3NCOO})(fla)]\cdot H_2O$ ($\mathbf{1^{fla}\cdot H_2O}$) and (b) $[Co^{II}(L^{4N})(fla)](PF_6)$ ($\mathbf{2^{fla}(PF_6)}$) with dioxygen in the presence of NBT^{2+} in DMF at 70 °C.

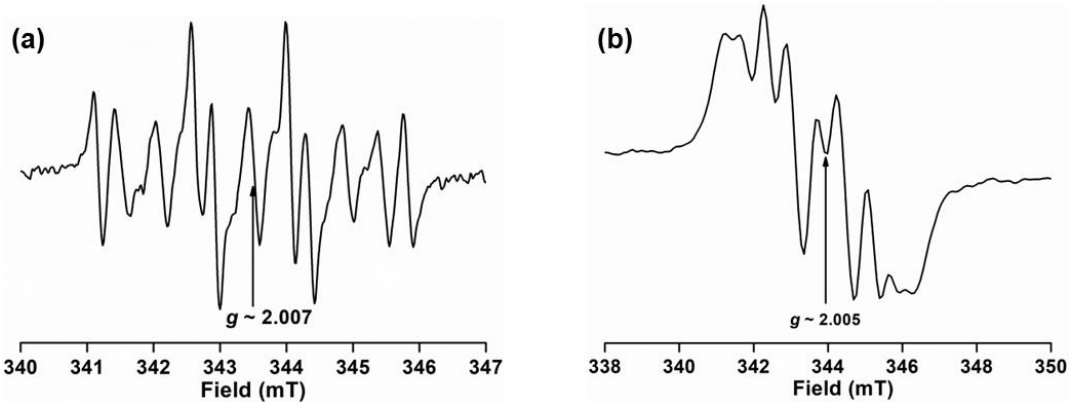


Figure S36. EPR spin-trapping experiment using DMPO under O_2 with complexes (a) $[Co^{II}(L^{3NCOO})(fla)]\cdot H_2O$ (**$1^{fla}\cdot H_2O$**) and (b) $[Co^{II}(L^{4N})(fla)](PF_6)$ (**$2^{fla}(PF_6)$**). The samples were prepared at 70 °C in DMF, and the spectra were recorded at 298 K (microwave frequency ~ 9.65 GHz). The signals correspond to a mixture of species DMPO-OOH and DMPO=O.

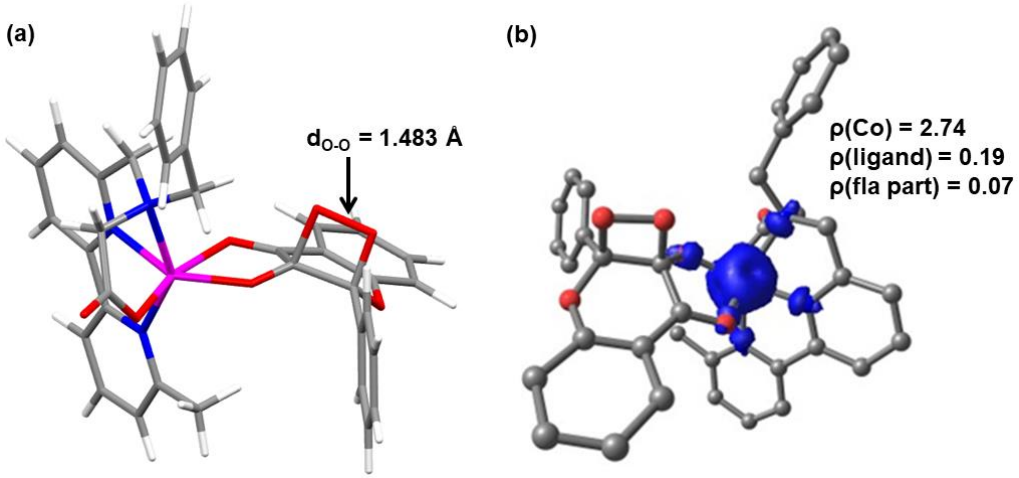


Figure S37. (a) The optimised structure and (b) Mulliken spin-density plot of intermediate **A** in its S = 3/2 state.

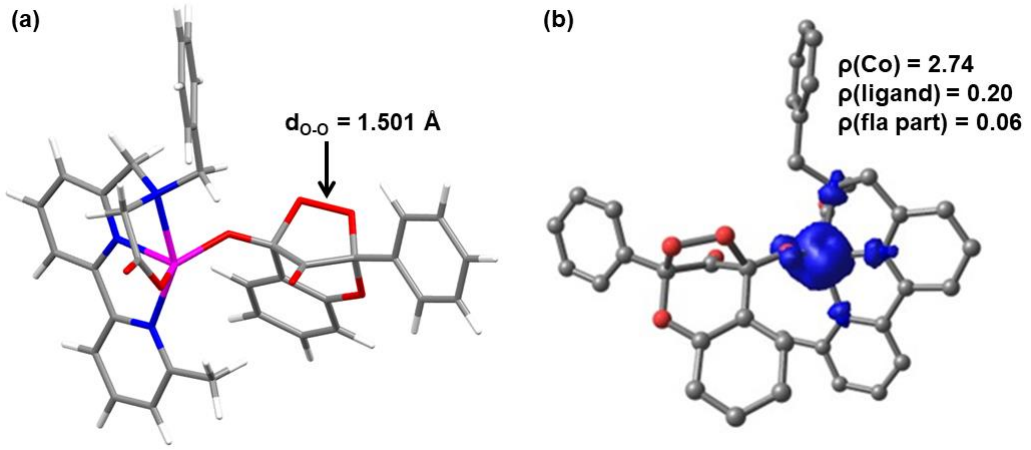


Figure S38. (a) The optimised structure and (b) Mulliken spin-density plot of intermediate **B** in its *S* = 3/2 state.

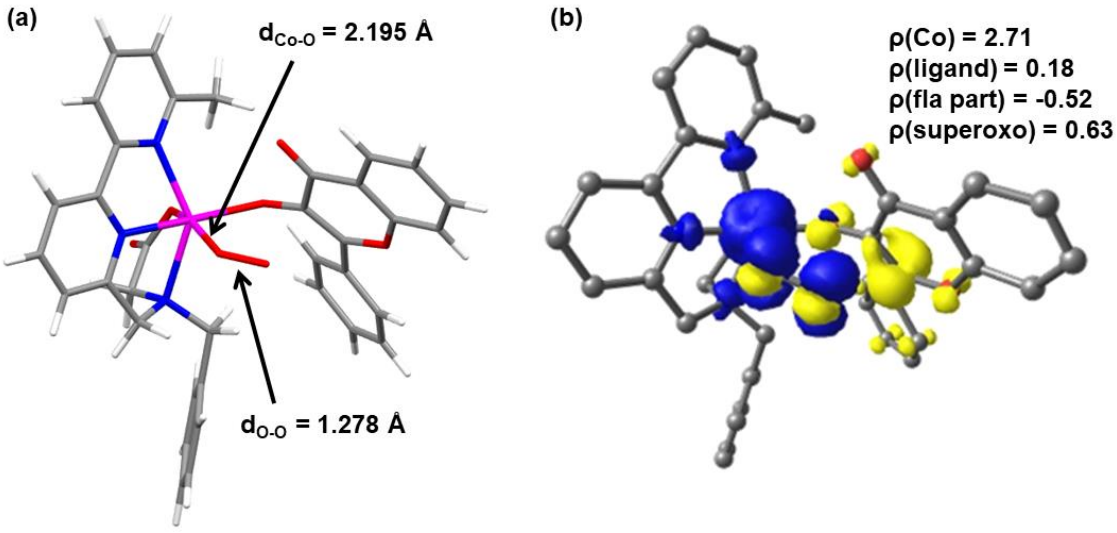


Figure S39. (a) The optimised structure and (b) Mulliken spin-density plot of species **C** in its *S* = 3/2 state.

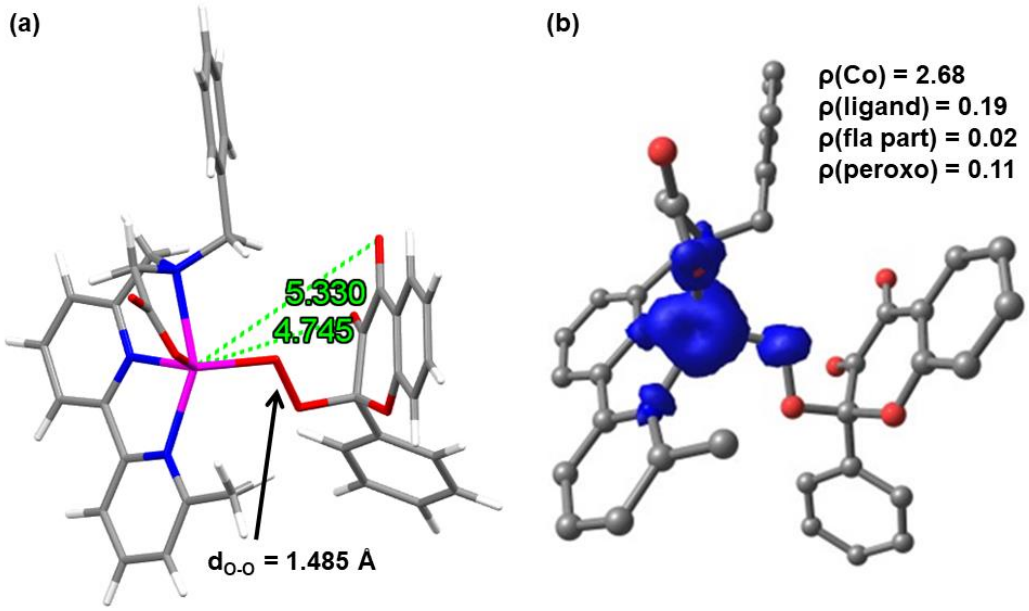


Figure S40. (a) The optimised structure and (b) Mulliken spin-density plot of species **D** in its *S* = 3/2 state.

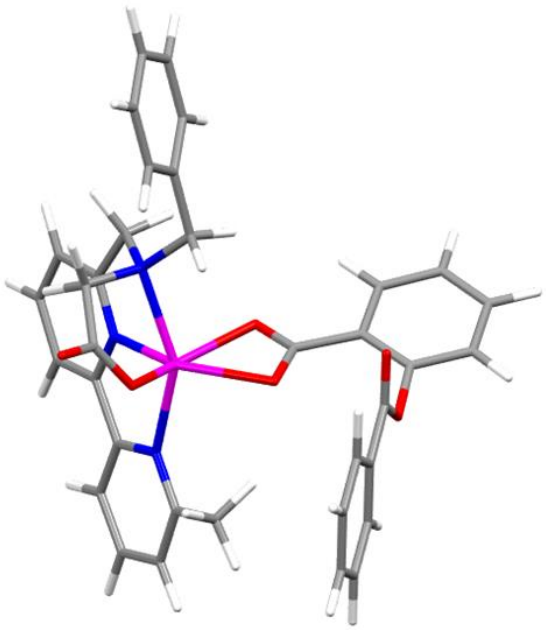


Figure S41. The optimised structure of the dioxygenated product [Co^{II}(L^{3NCOO})(Obs)] (**E**) in its *S* = 3/2 state.

***x, y, z* coordinates of the optimised structures:**

(1) [$Co^{II}(L^{3NCOO})$(fla)] (1^{fla}) in high-spin state (*S* = 3/2)

Co	1.181450000	0.610976000	9.586167000
O	0.133246000	1.799907000	8.214436000
N	1.463583000	-0.557204000	7.631958000
N	0.039903000	-1.149322000	9.835129000
N	-0.298753000	1.089087000	11.214323000
O	-0.689452000	1.935130000	6.131013000
C	-1.043134000	0.031158000	11.610222000
C	-0.862843000	-1.221799000	10.827225000
C	3.140290000	-0.863504000	5.714564000
O	2.627609000	-0.344756000	10.915113000
C	-0.427032000	2.272074000	11.841175000
O	2.785213000	1.884102000	9.502146000
C	-1.308704000	2.425322000	12.920057000
H	-1.394106000	3.388984000	13.409568000
C	-1.566968000	-2.407813000	11.059870000
H	-2.300121000	-2.481537000	11.852777000
C	-0.102693000	1.333471000	7.047633000
C	1.371695000	-1.982803000	8.003171000
H	2.330778000	-2.278766000	8.443541000
H	1.198358000	-2.634689000	7.137665000
O	5.905428000	2.010443000	11.348823000
C	-1.316587000	-3.507490000	10.239951000
H	-1.857404000	-4.434612000	10.399072000
C	-1.936911000	0.121549000	12.679647000
H	-2.524155000	-0.732329000	12.992217000
C	-2.064059000	1.338594000	13.344306000
H	-2.750492000	1.435751000	14.179186000
C	2.784048000	-0.195193000	7.031627000
H	3.542016000	-0.426872000	7.784823000
H	2.777357000	0.890574000	6.911469000
C	-0.380364000	-3.408092000	9.212445000
H	-0.174620000	-4.245308000	8.554538000
C	0.291664000	-2.196136000	9.045243000
C	0.322154000	-0.128356000	6.793518000
H	-0.546277000	-0.745500000	7.045795000
H	0.518815000	-0.283108000	5.728487000
C	0.393902000	3.426303000	11.336235000
H	0.185889000	4.331877000	11.909219000
H	1.462517000	3.203659000	11.400902000
H	0.171491000	3.611182000	10.281257000
C	3.662037000	0.364875000	11.075494000
C	2.872430000	-0.225723000	4.493449000
H	2.417385000	0.761567000	4.493841000
C	3.765949000	-2.119593000	5.688025000
H	4.014132000	-2.617567000	6.621675000
C	3.776579000	1.604172000	10.308190000
C	4.721877000	-1.166548000	12.767827000
H	3.869110000	-1.832207000	12.690830000
C	4.092569000	-2.731752000	4.476581000
H	4.578923000	-3.703000000	4.476891000
C	4.731348000	0.006662000	11.978090000

C	3.805391000	-2.092035000	3.268027000
H	4.062758000	-2.565869000	2.325240000
C	3.197929000	-0.834536000	3.279252000
H	2.983625000	-0.323738000	2.344953000
C	5.835001000	0.872417000	12.076208000
C	6.910440000	0.593471000	12.933493000
H	7.743815000	1.285971000	12.981940000
C	6.874391000	-0.562575000	13.694829000
H	7.700872000	-0.788279000	14.361372000
C	5.777514000	-1.447882000	13.613579000
H	5.767064000	-2.348946000	14.218167000
C	4.363492000	4.236786000	8.856992000
H	3.439533000	3.728041000	8.619453000
C	4.914827000	2.394124000	10.474491000
C	5.233249000	3.660273000	9.808969000
C	6.436712000	4.338570000	10.108358000
H	7.123041000	3.919661000	10.833945000
C	6.753378000	5.540140000	9.481754000
H	7.684349000	6.041860000	9.729719000
C	4.692118000	5.440289000	8.234889000
H	4.008071000	5.864464000	7.505215000
C	5.884231000	6.100087000	8.540432000
H	6.134363000	7.037758000	8.052929000

(2) [$Co^{II}(L^{3NCOO})$(fla)] (1^{fla}) in low-spin state (S = 1/2)

Co	1.158172000	0.511331000	9.685033000
O	-0.078754000	1.496582000	8.491597000
N	1.600796000	-0.598192000	7.679064000
N	-0.070373000	-1.012421000	9.830402000
N	-0.148694000	1.073786000	11.514089000
O	-0.948991000	1.731638000	6.446680000
C	-1.175201000	0.200353000	11.593468000
C	-1.073727000	-1.007734000	10.732251000
C	3.429479000	-1.075922000	5.951120000
O	2.578778000	-0.373615000	10.794192000
C	-0.156795000	2.176374000	12.281464000
O	2.509017000	1.927226000	9.540930000
C	-1.223386000	2.450971000	13.150209000
H	-1.205171000	3.351247000	13.754657000
C	-1.938523000	-2.102905000	10.832180000
H	-2.732187000	-2.117656000	11.567733000
C	-0.205124000	1.160737000	7.261979000
C	1.314724000	-1.982397000	8.084026000
H	2.183231000	-2.355231000	8.639290000
H	1.163255000	-2.654878000	7.228811000
O	5.813302000	2.062769000	11.039449000
C	-1.762902000	-3.187583000	9.977130000
H	-2.429744000	-4.041252000	10.038172000
C	-2.271580000	0.416970000	12.433944000
H	-3.099542000	-0.279512000	12.468138000
C	-2.291789000	1.565065000	13.220956000
H	-3.132022000	1.762955000	13.878727000
C	3.006595000	-0.386172000	7.238465000

H	3.643982000	-0.715345000	8.064294000
H	3.140039000	0.694289000	7.142852000
C	-0.727354000	-3.166704000	9.045807000
H	-0.567338000	-3.992999000	8.362202000
C	0.115579000	-2.056609000	9.007211000
C	0.595025000	-0.054044000	6.743249000
H	-0.138745000	-0.825171000	6.483040000
H	1.059717000	0.238331000	5.798654000
C	1.025614000	3.103102000	12.197777000
H	0.838867000	4.025001000	12.752363000
H	1.914523000	2.623437000	12.622487000
H	1.261618000	3.341896000	11.158640000
C	3.611223000	0.364162000	10.901313000
C	3.446820000	-0.372836000	4.736915000
H	3.180586000	0.681226000	4.724595000
C	3.822435000	-2.423892000	5.945991000
H	3.850927000	-2.980310000	6.878871000
C	3.601480000	1.640909000	10.210069000
C	4.879952000	-1.234137000	12.374293000
H	4.044830000	-1.925463000	12.345085000
C	4.196196000	-3.056782000	4.759305000
H	4.499058000	-4.099833000	4.776469000
C	4.771880000	-0.015266000	11.664505000
C	4.192028000	-2.348160000	3.554786000
H	4.486103000	-2.839175000	2.631710000
C	3.821374000	-1.001993000	3.547107000
H	3.829755000	-0.438997000	2.618217000
C	5.853971000	0.883508000	11.700853000
C	7.021790000	0.592723000	12.421950000
H	7.835153000	1.310101000	12.426675000
C	7.100305000	-0.607657000	13.107847000
H	7.999065000	-0.843344000	13.668947000
C	6.027668000	-1.525835000	13.085489000
H	6.108760000	-2.461138000	13.629579000
C	3.965152000	4.340436000	8.817789000
H	3.052486000	3.794621000	8.621959000
C	4.726349000	2.462877000	10.298927000
C	4.931726000	3.771211000	9.676325000
C	6.119459000	4.497472000	9.920366000
H	6.877282000	4.083785000	10.574314000
C	6.327548000	5.740507000	9.330876000
H	7.247733000	6.280439000	9.534670000
C	4.185927000	5.586026000	8.231957000
H	3.429810000	6.004676000	7.573888000
C	5.363077000	6.293940000	8.482815000
H	5.528954000	7.264370000	8.024425000

(3) $[Co^{II}(L^{4N})(fla)]^{+}$ (2^{fla+}) in high-spin state (S = 3/2)

Co	7.813386000	1.750933000	10.103510000
O	8.488616000	0.209038000	11.205639000
O	7.625980000	2.514235000	12.171193000
N	7.973946000	0.668442000	8.236689000
O	9.336031000	-0.145081000	14.716709000
N	5.723225000	0.795732000	9.845325000
N	6.650991000	3.349025000	9.412436000
C	8.647899000	0.431763000	12.491165000
C	8.897406000	0.866091000	7.283876000
H	9.614991000	1.658258000	7.471604000
N	9.272064000	3.439656000	9.878506000
C	8.150737000	1.712600000	12.991772000
C	9.231319000	-0.464315000	13.382994000
C	9.786039000	-1.790173000	13.092570000
C	7.037771000	-0.282668000	8.054065000
C	5.362193000	3.151017000	9.124023000
C	9.841367000	-2.300115000	11.776964000
H	9.464623000	-1.694419000	10.964636000
C	8.281356000	1.996449000	14.403871000
C	7.186238000	4.581267000	9.441908000
C	8.884294000	1.026381000	15.223164000
C	5.104903000	0.609611000	11.196023000
H	5.043914000	1.603173000	11.647927000
H	5.824240000	0.031460000	11.780485000
C	6.036047000	-0.480714000	9.173945000
H	5.140023000	-0.981865000	8.787468000
H	6.485794000	-1.137768000	9.925498000
C	7.009369000	-1.069118000	6.901765000
H	6.234776000	-1.818501000	6.779074000
C	3.742038000	-0.059480000	11.232504000
C	9.046959000	1.231219000	16.601470000
H	9.517828000	0.459818000	17.201062000
C	10.285414000	-2.595062000	14.141214000
H	10.255012000	-2.229200000	15.160037000
C	8.944321000	0.116126000	6.112637000
H	9.712324000	0.311687000	5.373124000
C	7.981061000	-0.873633000	5.921586000
H	7.978409000	-1.476725000	5.019394000
C	10.374461000	-3.564290000	11.529642000
H	10.407808000	-3.936018000	10.509438000
C	4.504307000	4.225559000	8.883236000
H	3.456971000	4.053254000	8.661474000
C	8.650120000	4.631908000	9.711112000
C	8.598407000	2.418142000	17.156752000
H	8.718521000	2.587166000	18.222236000
C	10.598982000	3.404517000	10.099161000
C	3.625609000	-1.458373000	11.247370000
H	4.521195000	-2.073776000	11.249788000
C	6.387529000	5.703043000	9.199877000
H	6.799207000	6.703721000	9.218717000
C	4.936880000	1.703869000	8.978990000
H	3.860660000	1.596132000	9.148002000
H	5.112446000	1.423268000	7.934791000

C	7.833033000	3.198363000	14.997734000
H	7.367720000	3.944720000	14.363107000
C	10.863111000	-4.349907000	12.575452000
H	11.276684000	-5.334184000	12.376637000
C	10.814995000	-3.855725000	13.882399000
H	11.191251000	-4.455631000	14.705976000
C	2.372052000	-2.071614000	11.278935000
H	2.302169000	-3.155409000	11.292666000
C	7.988684000	3.406843000	16.354985000
H	7.643355000	4.330230000	16.808361000
C	2.568463000	0.708937000	11.275377000
H	2.638155000	1.793641000	11.301082000
C	5.032124000	5.514515000	8.930419000
H	4.393411000	6.373015000	8.750825000
C	11.255822000	2.064733000	10.298428000
H	12.342584000	2.165377000	10.305170000
H	10.946568000	1.619895000	11.249301000
H	10.975922000	1.364138000	9.507338000
C	9.349648000	5.838661000	9.765288000
H	8.841485000	6.784939000	9.632365000
C	1.312247000	0.098729000	11.307233000
H	0.415778000	0.710874000	11.342078000
C	11.355228000	4.583675000	10.155460000
H	12.424011000	4.525587000	10.327618000
C	1.211321000	-1.293921000	11.304132000
H	0.235895000	-1.770610000	11.332231000
C	10.723268000	5.809639000	9.992074000
H	11.289898000	6.733954000	10.036111000

(4) $[Co^{II}(L^{4N})(fla)]^{+}$ (2^{fla+}) in low-spin state (S = 1/2)

Co	7.720801000	1.757809000	10.160827000
O	8.583136000	0.258799000	11.059956000
O	7.547996000	2.460855000	12.022903000
N	7.852926000	0.791051000	8.401882000
O	9.299876000	-0.136039000	14.597242000
N	5.620870000	0.783763000	10.003915000
N	6.729750000	3.278161000	9.430818000
C	8.672029000	0.447077000	12.360311000
C	8.776579000	1.046154000	7.461224000
H	9.440361000	1.878099000	7.665233000
N	9.379317000	3.339387000	9.860377000
C	8.090470000	1.674602000	12.865929000
C	9.270398000	-0.437512000	13.257939000
C	9.905766000	-1.723270000	12.964674000
C	6.975853000	-0.215287000	8.210790000
C	5.424806000	3.129545000	9.153669000
C	9.983350000	-2.226181000	11.647357000
H	9.565023000	-1.644183000	10.837895000
C	8.140975000	1.949811000	14.277803000
C	7.323044000	4.490721000	9.355152000
C	8.765959000	0.998927000	15.105621000
C	5.009474000	0.582792000	11.347547000
H	4.960883000	1.569004000	11.816938000

H	5.722896000	-0.013107000	11.923560000
C	5.965776000	-0.467148000	9.312169000
H	5.089891000	-0.982833000	8.896589000
H	6.422043000	-1.134199000	10.051328000
C	7.012172000	-1.000007000	7.057951000
H	6.285061000	-1.794202000	6.927456000
C	3.638877000	-0.072042000	11.376759000
C	8.861901000	1.187416000	16.492210000
H	9.351211000	0.432952000	17.098368000
C	10.458966000	-2.496715000	14.010067000
H	10.411991000	-2.134074000	15.029467000
C	8.880012000	0.299729000	6.292506000
H	9.643962000	0.542564000	5.562971000
C	7.981518000	-0.747087000	6.089648000
H	8.026451000	-1.349313000	5.188102000
C	10.591552000	-3.454895000	11.395015000
H	10.640657000	-3.823488000	10.374411000
C	4.631559000	4.223220000	8.804042000
H	3.576910000	4.082013000	8.595009000
C	8.780018000	4.532452000	9.652791000
C	8.325101000	2.337308000	17.046527000
H	8.392905000	2.494029000	18.118390000
C	10.699903000	3.291894000	10.102743000
C	3.503535000	-1.468298000	11.320744000
H	4.390686000	-2.094631000	11.281630000
C	6.580842000	5.618273000	8.992405000
H	7.049536000	6.590220000	8.915162000
C	4.865287000	1.719529000	9.147179000
H	3.803173000	1.741185000	9.411725000
H	4.903674000	1.364440000	8.111271000
C	7.601170000	3.114777000	14.871054000
H	7.119457000	3.846351000	14.231697000
C	11.134063000	-4.209537000	12.437049000
H	11.606328000	-5.166161000	12.234265000
C	11.063585000	-3.721528000	13.745601000
H	11.481614000	-4.298384000	14.565402000
C	2.242177000	-2.065851000	11.334502000
H	2.157566000	-3.147935000	11.293261000
C	7.692174000	3.305142000	16.236196000
H	7.277771000	4.199111000	16.690479000
C	2.476436000	0.708197000	11.472201000
H	2.561352000	1.789089000	11.554066000
C	5.221369000	5.480971000	8.724274000
H	4.630707000	6.349050000	8.451254000
C	11.332145000	1.946178000	10.338159000
H	12.415866000	2.001175000	10.214755000
H	11.123434000	1.597784000	11.355110000
H	10.929674000	1.196594000	9.654657000
C	9.490955000	5.735024000	9.700693000
H	8.998424000	6.686899000	9.549777000
C	1.212178000	0.113630000	11.486429000
H	0.324491000	0.734821000	11.562668000
C	11.473134000	4.461366000	10.149422000
H	12.538432000	4.393190000	10.340759000
C	1.092205000	-1.275416000	11.412342000
H	0.110732000	-1.740192000	11.426230000

C	10.859433000	5.692439000	9.954797000
H	11.436314000	6.610677000	9.995908000

(5) $[Co^{II}(L^{3NCOO})(fla^{\bullet})]^{+}$ ($1^{fla\bullet+}$) in high-spin state (S = 2)

Co	1.093298000	0.620458000	9.525902000
O	0.259412000	1.790549000	8.130724000
N	1.493692000	-0.622885000	7.670101000
N	-0.028978000	-1.089976000	9.847840000
N	-0.258927000	1.194118000	11.206808000
O	-0.520216000	1.896631000	6.033170000
C	-1.089087000	0.184924000	11.573562000
C	-0.925936000	-1.104949000	10.848729000
C	3.215186000	-1.046583000	5.813031000
O	2.686861000	-0.411349000	10.643564000
C	-0.380510000	2.401235000	11.790789000
O	2.673054000	1.997707000	9.662349000
C	-1.335044000	2.625844000	12.793424000
H	-1.408878000	3.607244000	13.247767000
C	-1.626330000	-2.277218000	11.145215000
H	-2.344175000	-2.316406000	11.954066000
C	0.021416000	1.292140000	6.962130000
C	1.334278000	-2.032579000	8.084930000
H	2.270406000	-2.354730000	8.554046000
H	1.151781000	-2.699078000	7.233687000
O	5.884690000	2.005501000	11.221157000
C	-1.382598000	-3.415288000	10.376115000
H	-1.922458000	-4.332647000	10.586044000
C	-2.058763000	0.352753000	12.561867000
H	-2.720554000	-0.458007000	12.837017000
C	-2.175513000	1.592903000	13.184861000
H	-2.921839000	1.748958000	13.956769000
C	2.848818000	-0.329926000	7.100677000
H	3.572753000	-0.576084000	7.881779000
H	2.888537000	0.751817000	6.946183000
C	-0.448569000	-3.373906000	9.342643000
H	-0.244165000	-4.246474000	8.732450000
C	0.230261000	-2.176809000	9.113900000
C	0.397938000	-0.188025000	6.770934000
H	-0.500880000	-0.765840000	7.008663000
H	0.630956000	-0.383577000	5.720846000
C	0.528768000	3.511414000	11.343375000
H	0.180209000	4.470835000	11.730095000
H	1.547500000	3.348032000	11.708193000
H	0.573943000	3.559445000	10.253371000
C	3.697355000	0.284684000	10.877047000
C	3.012099000	-0.427488000	4.569997000
H	2.602811000	0.578823000	4.531945000
C	3.785298000	-2.328761000	5.837331000
H	3.984318000	-2.813588000	6.789322000
C	3.719279000	1.643866000	10.291430000
C	4.909348000	-1.389217000	12.307412000
H	4.085189000	-2.084438000	12.193199000

C	4.119581000	-2.984510000	4.651205000
H	4.562039000	-3.975619000	4.689466000
C	4.825890000	-0.132281000	11.673168000
C	3.896132000	-2.363452000	3.419679000
H	4.159469000	-2.871952000	2.496917000
C	3.345638000	-1.080670000	3.381586000
H	3.182177000	-0.584767000	2.429323000
C	5.893441000	0.769890000	11.819811000
C	7.024710000	0.454549000	12.571462000
H	7.828877000	1.175907000	12.659679000
C	7.081391000	-0.790015000	13.188315000
H	7.954549000	-1.049704000	13.777601000
C	6.026864000	-1.712794000	13.058249000
H	6.092008000	-2.678219000	13.547809000
C	4.204423000	4.394931000	9.017341000
H	3.342750000	3.842688000	8.671103000
C	4.868296000	2.474667000	10.477836000
C	5.086133000	3.808215000	9.958001000
C	6.217898000	4.546317000	10.388472000
H	6.899656000	4.113231000	11.109466000
C	6.449264000	5.823522000	9.900233000
H	7.315129000	6.380718000	10.242370000
C	4.452445000	5.673926000	8.533914000
H	3.773090000	6.111467000	7.809802000
C	5.568855000	6.393135000	8.971484000
H	5.754496000	7.392660000	8.590862000

(6) $[Co^{II}(L^{3NCOO})(fla^{\bullet})]^{+}$ ($1^{fla^{\bullet+}}$) in broken symmetry state (S = 1)

Co	1.052797000	0.601684000	9.577274000
O	0.147019000	1.802491000	8.219669000
N	1.459706000	-0.561164000	7.655261000
N	-0.001560000	-1.163416000	9.836615000
N	-0.311341000	1.078431000	11.235370000
O	-0.588311000	1.983203000	6.110135000
C	-1.075525000	0.024110000	11.615785000
C	-0.901023000	-1.231215000	10.833604000
C	3.170546000	-0.872429000	5.764686000
O	2.604846000	-0.329568000	10.904290000
C	-0.437218000	2.261950000	11.861758000
O	2.783886000	1.906190000	9.533828000
C	-1.339759000	2.422811000	12.922446000
H	-1.425401000	3.387458000	13.409652000
C	-1.601824000	-2.417552000	11.066520000
H	-2.330979000	-2.495157000	11.862506000
C	-0.056121000	1.351764000	7.030559000
C	1.341642000	-1.992285000	8.009165000
H	2.292839000	-2.311877000	8.449768000
H	1.163237000	-2.626746000	7.132712000
O	5.887645000	2.018970000	11.286327000
C	-1.351789000	-3.515661000	10.242827000
H	-1.891386000	-4.443092000	10.403371000
C	-1.986007000	0.125140000	12.667356000

H	-2.591449000	-0.720954000	12.965442000
C	-2.113129000	1.344124000	13.330652000
H	-2.816281000	1.447993000	14.150426000
C	2.798627000	-0.212773000	7.081071000
H	3.540007000	-0.466695000	7.843543000
H	2.808829000	0.874365000	6.967370000
C	-0.417902000	-3.418338000	9.213012000
H	-0.213426000	-4.256779000	8.556647000
C	0.254314000	-2.207082000	9.043880000
C	0.342803000	-0.116606000	6.788009000
H	-0.542000000	-0.716281000	7.024777000
H	0.560998000	-0.277906000	5.728791000
C	0.422777000	3.404919000	11.397281000
H	0.014632000	4.358438000	11.738247000
H	1.436581000	3.312475000	11.802435000
H	0.496434000	3.416653000	10.307448000
C	3.637302000	0.344639000	11.066419000
C	2.931023000	-0.219606000	4.545695000
H	2.487048000	0.772658000	4.546731000
C	3.783920000	-2.134415000	5.738673000
H	4.011370000	-2.643376000	6.671594000
C	3.750968000	1.617356000	10.292330000
C	4.738119000	-1.185266000	12.725594000
H	3.888393000	-1.856085000	12.666113000
C	4.125476000	-2.738530000	4.527458000
H	4.601822000	-3.714595000	4.527227000
C	4.727867000	-0.012056000	11.943213000
C	3.866088000	-2.084589000	3.320291000
H	4.135208000	-2.552431000	2.377881000
C	3.271811000	-0.820867000	3.332119000
H	3.079766000	-0.299281000	2.399079000
C	5.827484000	0.858644000	12.019836000
C	6.919621000	0.593609000	12.843805000
H	7.749663000	1.289832000	12.876191000
C	6.905289000	-0.570329000	13.605344000
H	7.748397000	-0.790284000	14.251740000
C	5.817890000	-1.460648000	13.548160000
H	5.826767000	-2.362519000	14.150148000
C	4.343779000	4.251490000	8.827140000
H	3.421854000	3.747080000	8.578010000
C	4.928352000	2.431095000	10.443588000
C	5.223126000	3.681817000	9.782975000
C	6.430854000	4.362315000	10.091948000
H	7.113723000	3.942451000	10.819381000
C	6.739306000	5.561285000	9.469434000
H	7.664352000	6.072056000	9.715297000
C	4.668838000	5.452972000	8.210897000
H	3.989357000	5.878326000	7.479814000
C	5.861210000	6.112298000	8.526411000
H	6.107455000	7.051257000	8.040561000

(7) $[Co^{II}(L^{4N})(fla^{\bullet})]^{2+}$ ($2^{fla\bullet 2+}$) in high-spin state (S = 2)

Co	7.889190000	1.816241000	10.017443000
O	8.603105000	0.231748000	11.216571000
O	7.779696000	2.552023000	12.102619000
N	8.008791000	0.726183000	8.198059000
O	9.190215000	-0.209852000	14.707802000
N	5.827982000	0.793271000	9.892367000
N	6.677790000	3.373462000	9.412388000
C	8.675163000	0.428686000	12.469066000
C	8.894742000	0.952582000	7.213770000
H	9.585789000	1.773698000	7.370860000
N	9.308797000	3.518297000	9.803281000
C	8.199151000	1.749750000	12.958763000
C	9.171269000	-0.537696000	13.407925000
C	9.663207000	-1.867437000	13.127802000
C	7.101234000	-0.261134000	8.056240000
C	5.384333000	3.140031000	9.170684000
C	9.788655000	-2.358684000	11.803522000
H	9.516402000	-1.730571000	10.968231000
C	8.258696000	2.008359000	14.377389000
C	7.184968000	4.618231000	9.436127000
C	8.763731000	0.996177000	15.210303000
C	5.220838000	0.589287000	11.250466000
H	5.156591000	1.578690000	11.710645000
H	5.942345000	0.004187000	11.824924000
C	6.139430000	-0.479825000	9.206237000
H	5.237086000	-0.985975000	8.844339000
H	6.613951000	-1.141379000	9.939014000
C	7.065987000	-1.057324000	6.912266000
H	6.315753000	-1.834866000	6.819584000
C	3.863465000	-0.089088000	11.294689000
C	8.861331000	1.158510000	16.590879000
H	9.256816000	0.354227000	17.200279000
C	10.035866000	-2.709852000	14.208426000
H	9.944252000	-2.351659000	15.225765000
C	8.930565000	0.192077000	6.050599000
H	9.665624000	0.408517000	5.284335000
C	7.998904000	-0.834681000	5.900718000
H	7.989894000	-1.446053000	5.004389000
C	10.267427000	-3.643127000	11.580162000
H	10.361766000	-4.008075000	10.562846000
C	4.492426000	4.193116000	8.967912000
H	3.442820000	3.996205000	8.781858000
C	8.653865000	4.698394000	9.655166000
C	8.441221000	2.363494000	17.144086000
H	8.510071000	2.505687000	18.217391000
C	10.645900000	3.516294000	9.966002000
C	3.756945000	-1.488732000	11.287428000
H	4.655447000	-2.099344000	11.265445000
C	6.348409000	5.718809000	9.231951000
H	6.732942000	6.730114000	9.246864000
C	4.997265000	1.683006000	9.037407000
H	3.930479000	1.543217000	9.234057000
H	5.156824000	1.403406000	7.990792000

C	7.839707000	3.220657000	14.963187000
H	7.450224000	4.001954000	14.320227000
C	10.627652000	-4.462598000	12.654854000
H	10.999462000	-5.465824000	12.471679000
C	10.509760000	-3.989695000	13.968679000
H	10.788030000	-4.624772000	14.803036000
C	2.507601000	-2.109571000	11.329126000
H	2.444154000	-3.193687000	11.324826000
C	7.930796000	3.394308000	16.334346000
H	7.608740000	4.325718000	16.786650000
C	2.687308000	0.672445000	11.372466000
H	2.750830000	1.756783000	11.417324000
C	4.990087000	5.494716000	9.006801000
H	4.323404000	6.337272000	8.856588000
C	11.354994000	2.199454000	10.134179000
H	12.434585000	2.331439000	10.046059000
H	11.150813000	1.768861000	11.119774000
H	11.036281000	1.471982000	9.383130000
C	9.326661000	5.920098000	9.679955000
H	8.791046000	6.853061000	9.563012000
C	1.435785000	0.053802000	11.415092000
H	0.536656000	0.659612000	11.476940000
C	11.373883000	4.714154000	9.988963000
H	12.449895000	4.680682000	10.115178000
C	1.343368000	-1.339128000	11.387942000
H	0.371412000	-1.822123000	11.423915000
C	10.708211000	5.924600000	9.852403000
H	11.254133000	6.861907000	9.872735000

(8) $[Co^{II}(L^{4N})(fla^{\bullet})]^{2+}$ ($2^{fla\bullet 2+}$) in broken symmetry state (S = 1)

Co	7.870354000	1.810795000	10.007163000
O	8.522990000	0.207250000	11.242016000
O	7.741391000	2.550766000	12.140214000
N	8.013142000	0.685536000	8.213697000
O	9.247481000	-0.199428000	14.709264000
N	5.798928000	0.792397000	9.860925000
N	6.651710000	3.367099000	9.414611000
C	8.653235000	0.424275000	12.483162000
C	8.920929000	0.891452000	7.244894000
H	9.619689000	1.704840000	7.408306000
N	9.283475000	3.511564000	9.819569000
C	8.191590000	1.754621000	12.981353000
C	9.189216000	-0.533382000	13.412540000
C	9.687609000	-1.857138000	13.120741000
C	7.095262000	-0.290299000	8.059896000
C	5.363938000	3.135662000	9.143822000
C	9.795681000	-2.344575000	11.792995000
H	9.503138000	-1.717566000	10.963815000
C	8.294498000	2.014138000	14.398541000
C	7.158882000	4.611640000	9.449519000
C	8.826738000	1.006328000	15.219378000
C	5.180697000	0.607613000	11.215899000

H	5.118199000	1.602322000	11.665052000
H	5.894912000	0.025861000	11.802435000
C	6.108789000	-0.488906000	9.192193000
H	5.208971000	-0.990773000	8.817740000
H	6.563071000	-1.148242000	9.939557000
C	7.072348000	-1.095232000	6.921548000
H	6.313864000	-1.863688000	6.820294000
C	3.819631000	-0.064069000	11.257758000
C	8.962611000	1.172837000	16.595809000
H	9.378949000	0.372045000	17.195849000
C	10.089145000	-2.697576000	14.193204000
H	10.010788000	-2.342354000	15.212683000
C	8.969234000	0.122534000	6.087588000
H	9.721886000	0.324138000	5.334425000
C	8.027394000	-0.893018000	5.926628000
H	8.027674000	-1.510994000	5.034778000
C	10.284670000	-3.622956000	11.558769000
H	10.366427000	-3.984598000	10.539211000
C	4.476018000	4.189702000	8.928684000
H	3.430595000	3.993235000	8.719855000
C	8.625434000	4.692230000	9.686965000
C	8.552776000	2.377656000	17.158201000
H	8.651250000	2.522384000	18.228857000
C	10.618583000	3.510182000	9.998670000
C	3.707833000	-1.463256000	11.272318000
H	4.604337000	-2.077189000	11.269006000
C	6.326477000	5.713372000	9.234835000
H	6.711417000	6.724298000	9.258394000
C	4.983219000	1.678982000	8.992526000
H	3.912237000	1.534522000	9.162853000
H	5.169482000	1.405924000	7.948412000
C	7.887038000	3.225963000	14.993242000
H	7.476111000	4.003649000	14.359292000
C	10.672767000	-4.440318000	12.625515000
H	11.053077000	-5.438726000	12.433718000
C	10.572653000	-3.971402000	13.942482000
H	10.872359000	-4.605217000	14.770313000
C	2.455990000	-2.079196000	11.311863000
H	2.388789000	-3.163042000	11.324831000
C	8.015454000	3.404044000	16.361076000
H	7.701878000	4.335185000	16.819789000
C	2.645396000	0.702500000	11.310642000
H	2.712157000	1.787242000	11.337556000
C	4.972305000	5.491090000	8.984369000
H	4.308812000	6.334541000	8.825333000
C	11.329518000	2.193218000	10.158628000
H	12.408687000	2.326759000	10.067472000
H	11.130095000	1.760433000	11.144374000
H	11.009098000	1.467085000	9.407339000
C	9.294144000	5.914818000	9.741869000
H	8.756904000	6.848447000	9.638557000
C	1.391255000	0.088905000	11.350961000
H	0.493705000	0.698741000	11.393474000
C	11.342387000	4.709732000	10.050599000
H	12.416991000	4.677439000	10.188411000
C	1.293972000	-1.303963000	11.346376000

H	0.319969000	-1.782951000	11.380843000
C	10.674078000	5.920128000	9.928642000
H	11.216507000	6.858669000	9.972215000

(9) Intermediate A in *S* = 3/2 state

Co	1.329728000	0.610472000	9.481415000
O	0.318628000	1.896660000	8.249137000
N	1.425657000	-0.503403000	7.429553000
N	0.218643000	-1.140743000	9.751972000
N	0.096499000	1.054855000	11.250620000
O	-0.684929000	2.179350000	6.264537000
C	-0.635366000	0.000502000	11.679179000
C	-0.568600000	-1.227933000	10.839664000
C	2.828331000	-0.796640000	5.304399000
O	2.747459000	-0.454200000	11.120890000
C	0.065332000	2.218438000	11.923176000
O	3.145873000	1.500144000	9.326980000
C	-0.705451000	2.356711000	13.085312000
H	-0.716096000	3.304231000	13.611993000
C	-1.268933000	-2.406398000	11.111198000
H	-1.907091000	-2.494313000	11.980981000
C	-0.066066000	1.493802000	7.091450000
C	1.309719000	-1.937914000	7.748206000
H	2.299003000	-2.295139000	8.057473000
H	1.006134000	-2.541787000	6.883453000
O	5.804385000	2.168633000	11.622307000
C	-1.141458000	-3.480502000	10.230243000
H	-1.682604000	-4.401517000	10.420320000
C	-1.420438000	0.078023000	12.830796000
H	-2.002243000	-0.769494000	13.169358000
C	-1.448241000	1.274931000	13.543119000
H	-2.050582000	1.360459000	14.441636000
C	2.674998000	-0.171612000	6.680969000
H	3.510902000	-0.459914000	7.321925000
H	2.703056000	0.917855000	6.601370000
C	-0.329189000	-3.363498000	9.104661000
H	-0.222507000	-4.180005000	8.399098000
C	0.351163000	-2.161431000	8.900958000
C	0.214313000	0.015099000	6.758783000
H	-0.653331000	-0.547887000	7.118144000
H	0.254741000	-0.124176000	5.674248000
C	0.877686000	3.360779000	11.378587000
H	0.704940000	4.272025000	11.953982000
H	1.946620000	3.128138000	11.410044000
H	0.617081000	3.543930000	10.331927000
C	3.812564000	0.161011000	11.181272000
C	2.436100000	-0.099087000	4.151349000
H	2.028611000	0.904342000	4.245423000
C	3.389642000	-2.074122000	5.151596000
H	3.732270000	-2.619463000	6.027084000
C	4.172193000	1.079891000	9.999815000
C	4.667452000	-0.961076000	13.251459000

H	3.916918000	-1.732353000	13.113698000
C	3.532700000	-2.647967000	3.886940000
H	3.972010000	-3.636622000	3.789673000
C	4.747449000	0.071905000	12.297230000
C	3.122800000	-1.948001000	2.749271000
H	3.237129000	-2.391918000	1.764641000
C	2.577908000	-0.669204000	2.884133000
H	2.269551000	-0.112042000	2.004188000
C	5.714506000	1.083701000	12.460895000
C	6.576731000	1.067302000	13.558927000
H	7.305162000	1.862912000	13.669915000
C	6.483760000	0.032464000	14.485123000
H	7.160720000	0.018657000	15.333729000
C	5.532500000	-0.989013000	14.334366000
H	5.474334000	-1.791642000	15.061626000
C	5.750286000	3.550921000	8.302316000
H	6.080377000	2.691007000	7.730473000
C	5.409016000	2.018796000	10.270524000
C	5.385316000	3.389638000	9.644205000
C	4.958211000	4.501880000	10.382647000
H	4.676393000	4.382839000	11.423187000
C	4.904368000	5.761311000	9.784408000
H	4.575376000	6.618231000	10.364638000
C	5.697778000	4.812883000	7.708001000
H	5.988506000	4.929529000	6.668253000
C	5.275307000	5.920233000	8.446713000
H	5.235148000	6.901590000	7.983312000
O	6.284240000	1.095769000	9.599802000
O	5.165718000	0.214833000	9.184823000

(10) Intermediate B in *S* = 3/2 state

Co	1.093271000	0.383143000	9.577354000
O	-0.015832000	1.668583000	8.502985000
N	1.181601000	-0.570366000	7.468155000
N	0.249663000	-1.480377000	9.847024000
N	0.088415000	0.593730000	11.518131000
O	-1.190970000	2.000789000	6.624262000
C	-0.507707000	-0.553968000	11.925290000
C	-0.430791000	-1.708897000	10.985112000
C	2.525313000	-0.563972000	5.287621000
O	3.015674000	0.023805000	9.870202000
C	0.039182000	1.692002000	12.292769000
O	3.498044000	2.904856000	9.299721000
C	-0.613859000	1.669374000	13.532669000
H	-0.642670000	2.567192000	14.139602000
C	-1.017562000	-2.956417000	11.213138000
H	-1.569594000	-3.163344000	12.120835000
C	-0.465234000	1.309565000	7.346955000
C	1.221738000	-2.025426000	7.698808000
H	2.260087000	-2.300056000	7.914917000
H	0.911089000	-2.604263000	6.819659000
O	5.748948000	2.658848000	11.641359000
C	-0.890376000	-3.944182000	10.235803000

H	-1.345813000	-4.916667000	10.390820000
C	-1.166851000	-0.636571000	13.151989000
H	-1.637418000	-1.556793000	13.472856000
C	-1.215259000	0.494153000	13.965114000
H	-1.723418000	0.455019000	14.923035000
C	2.362271000	-0.058423000	6.710700000
H	3.240069000	-0.304954000	7.312117000
H	2.272859000	1.032074000	6.706219000
C	-0.190296000	-3.678720000	9.060415000
H	-0.089497000	-4.428673000	8.283828000
C	0.382137000	-2.415593000	8.901470000
C	-0.102153000	-0.119104000	6.897975000
H	-0.899577000	-0.770946000	7.270741000
H	-0.121020000	-0.185414000	5.805652000
C	0.718271000	2.936100000	11.790034000
H	0.416297000	3.808894000	12.371803000
H	1.805565000	2.832473000	11.872109000
H	0.479494000	3.106835000	10.736898000
C	4.028057000	0.718349000	10.343063000
C	1.997679000	0.156808000	4.204947000
H	1.481217000	1.095933000	4.386833000
C	3.222561000	-1.752433000	5.020822000
H	3.668142000	-2.310760000	5.839957000
C	4.261707000	2.154743000	9.845071000
C	3.560580000	-0.123793000	12.718496000
H	2.893585000	-0.858104000	12.279813000
C	3.369426000	-2.219159000	3.713219000
H	3.915513000	-3.139513000	3.527198000
C	4.214522000	0.768893000	11.867177000
C	2.825489000	-1.499031000	2.646584000
H	2.942240000	-1.859361000	1.628676000
C	2.142388000	-0.306570000	2.895333000
H	1.728070000	0.267045000	2.071247000
C	5.075576000	1.727856000	12.423800000
C	5.279843000	1.798618000	13.801062000
H	5.952050000	2.550565000	14.200850000
C	4.614999000	0.899116000	14.635466000
H	4.771118000	0.954203000	15.708526000
C	3.756558000	-0.064944000	14.098949000
H	3.241894000	-0.762937000	14.751465000
C	6.956890000	3.323034000	8.225778000
H	6.866846000	2.345393000	7.764833000
C	5.739867000	2.411832000	10.224618000
C	6.455746000	3.532983000	9.517665000
C	6.574407000	4.795808000	10.112051000
H	6.185159000	4.960814000	11.109677000
C	7.199156000	5.835074000	9.420957000
H	7.291452000	6.810352000	9.889242000
C	7.579368000	4.365982000	7.539796000
H	7.969361000	4.194260000	6.541161000
C	7.703283000	5.623384000	8.135887000
H	8.189892000	6.433805000	7.601432000
O	6.361415000	1.166936000	9.949754000
O	5.289005000	0.135242000	9.750358000

(11) Intermediate C in *S* = 3/2 state

Co	1.354738000	0.725109000	9.656999000
O	0.431031000	2.154917000	8.450804000
N	1.436887000	-0.246245000	7.557062000
N	0.064606000	-0.949060000	9.757880000
N	-0.137548000	1.194819000	11.284932000
O	-0.487564000	2.603758000	6.454269000
C	-0.898489000	0.137084000	11.652318000
C	-0.802567000	-1.059526000	10.778645000
C	2.956952000	-0.487710000	5.503814000
O	3.098849000	1.471336000	12.708394000
C	-0.243005000	2.353939000	11.962267000
O	2.862060000	2.031643000	10.016825000
C	-1.096263000	2.465611000	13.070880000
H	-1.161172000	3.411230000	13.597502000
C	-1.566625000	-2.219564000	10.941275000
H	-2.266741000	-2.320486000	11.760338000
C	0.069695000	1.843606000	7.262934000
C	1.226983000	-1.691521000	7.769957000
H	2.176993000	-2.127843000	8.095141000
H	0.928155000	-2.210718000	6.850916000
O	6.428580000	1.916548000	10.403236000
C	-1.426631000	-3.250471000	10.014134000
H	-2.016825000	-4.155104000	10.116940000
C	-1.756142000	0.185161000	12.752442000
H	-2.348582000	-0.674568000	13.037586000
C	-1.845142000	1.369892000	13.478187000
H	-2.502714000	1.437183000	14.338850000
C	2.750952000	0.055838000	6.907599000
H	3.524524000	-0.334064000	7.574983000
H	2.848722000	1.143511000	6.900566000
C	-0.541529000	-3.106004000	8.948165000
H	-0.427644000	-3.883154000	8.200509000
C	0.202351000	-1.928921000	8.858412000
C	0.298761000	0.377643000	6.845856000
H	-0.615467000	-0.163644000	7.109564000
H	0.408662000	0.305175000	5.760011000
C	0.568409000	3.532217000	11.507380000
H	0.198147000	4.451273000	11.967056000
H	1.614827000	3.387567000	11.787695000
H	0.531631000	3.621212000	10.420093000
C	4.111863000	1.561173000	12.013970000
C	2.678968000	0.308641000	4.382147000
H	2.326697000	1.327208000	4.522696000
C	3.451015000	-1.784901000	5.296710000
H	3.705132000	-2.407463000	6.150389000
C	4.016556000	1.884837000	10.552955000
C	5.693235000	0.986615000	13.885801000
H	4.834620000	0.853282000	14.535043000
C	3.638534000	-2.281520000	4.005511000
H	4.023995000	-3.287231000	3.865175000
C	5.464171000	1.357302000	12.546408000
C	3.341550000	-1.483581000	2.897672000
H	3.490152000	-1.868088000	1.892868000
C	2.865577000	-0.184611000	3.088927000

H	2.645644000	0.447438000	2.233461000
C	6.571750000	1.529078000	11.707075000
C	7.880739000	1.341407000	12.161880000
H	8.709590000	1.488962000	11.478341000
C	8.078341000	0.972263000	13.485892000
H	9.088973000	0.822209000	13.852123000
C	6.984309000	0.794369000	14.352118000
H	7.153512000	0.505463000	15.384192000
C	4.287655000	3.297485000	7.817677000
H	3.370183000	3.487939000	8.357358000
C	5.213979000	2.110330000	9.826397000
C	5.327640000	2.578373000	8.447252000
C	6.526347000	2.357519000	7.731442000
H	7.335283000	1.808670000	8.198826000
C	6.670260000	2.825120000	6.429743000
H	7.593843000	2.635769000	5.891315000
C	4.446841000	3.770096000	6.516957000
H	3.641946000	4.330733000	6.051449000
C	5.632384000	3.533715000	5.815618000
H	5.748702000	3.900692000	4.800374000
O	2.739449000	-0.841021000	10.326419000
O	3.999498000	-0.689715000	10.474825000

(12) Intermediate D in *S* = 3/2 state

Co	1.189442000	0.621038000	9.356966000
O	0.069310000	2.256374000	9.709240000
N	0.582494000	1.240970000	7.201856000
N	0.266240000	-1.067245000	8.598346000
N	0.879097000	-0.584927000	11.144315000
O	-1.513379000	3.621851000	8.902528000
C	0.299781000	-1.782537000	10.887377000
C	-0.060733000	-2.044861000	9.465349000
C	1.231996000	2.746852000	5.232758000
O	5.226538000	2.579483000	6.479934000
C	1.200083000	-0.246104000	12.405889000
O	5.517678000	0.048905000	7.499102000
C	0.962807000	-1.128594000	13.468614000
H	1.230855000	-0.835816000	14.477385000
C	-0.708888000	-3.196367000	9.013166000
H	-0.981274000	-3.993297000	9.692816000
C	-0.730779000	2.672491000	8.785560000
C	0.465180000	-0.008261000	6.428657000
H	1.464072000	-0.272114000	6.062906000
H	-0.180503000	0.096861000	5.547785000
O	5.493900000	1.940906000	10.546539000
C	-1.017960000	-3.302059000	7.656509000
H	-1.529407000	-4.185033000	7.287824000
C	0.043783000	-2.702545000	11.904233000
H	-0.412698000	-3.660398000	11.690761000
C	0.386558000	-2.366678000	13.212612000
H	0.198678000	-3.065148000	14.021442000
C	1.561344000	2.203653000	6.613081000
H	2.527001000	1.694203000	6.599177000
H	1.646049000	3.029573000	7.325049000

C	-0.679933000	-2.272270000	6.781014000
H	-0.919573000	-2.329758000	5.725134000
C	-0.019994000	-1.155162000	7.295342000
C	-0.729691000	1.862358000	7.473758000
H	-1.472665000	1.067326000	7.600310000
H	-1.072114000	2.491044000	6.645669000
C	1.816929000	1.105969000	12.628272000
H	1.980507000	1.290746000	13.691496000
H	2.775562000	1.171265000	12.104565000
H	1.167513000	1.890824000	12.228404000
C	5.260204000	2.421978000	7.691530000
C	0.540173000	3.959051000	5.085354000
H	0.252889000	4.522688000	5.969335000
C	1.628143000	2.059393000	4.074914000
H	2.194293000	1.135956000	4.163588000
C	5.351993000	0.981034000	8.246871000
C	5.080448000	4.840482000	8.273430000
H	5.008925000	5.049427000	7.211235000
C	1.321147000	2.555956000	2.806724000
H	1.638940000	2.010903000	1.922575000
C	5.215833000	3.495361000	8.676781000
C	0.617271000	3.755715000	2.675418000
H	0.380906000	4.144546000	1.689237000
C	0.231167000	4.459197000	3.818457000
H	-0.303943000	5.399798000	3.725346000
C	5.304228000	3.194867000	10.051402000
C	5.266284000	4.227132000	10.997458000
H	5.340725000	3.975949000	12.049793000
C	5.136040000	5.544484000	10.574517000
H	5.105680000	6.337569000	11.315569000
C	5.041364000	5.860714000	9.207987000
H	4.937395000	6.893084000	8.892000000
C	7.411444000	0.012638000	10.828329000
H	7.689863000	1.056149000	10.917900000
C	5.212244000	0.742970000	9.787066000
C	6.164270000	-0.332383000	10.292154000
C	5.812780000	-1.684052000	10.177143000
H	4.851513000	-1.955361000	9.757342000
C	6.694615000	-2.676537000	10.607211000
H	6.410128000	-3.720916000	10.520142000
C	8.292132000	-0.983782000	11.252436000
H	9.255990000	-0.705550000	11.668099000
C	7.935956000	-2.329796000	11.145372000
H	8.621571000	-3.103475000	11.478232000
O	3.033059000	1.178698000	9.195704000
O	3.912976000	0.315388000	10.023623000

(13) Dioxygenated product E in *S* = 3/2 state

Co	1.937515000	-0.396429000	9.734921000
O	0.755308000	0.894607000	8.729028000
N	2.183319000	-1.142727000	7.573561000
N	1.198335000	-2.334331000	9.800554000
N	0.820033000	-0.458080000	11.670093000
O	-0.417619000	1.254801000	6.853143000
C	0.287244000	-1.680419000	11.920545000
C	0.518141000	-2.732552000	10.889779000
C	3.596456000	-0.859794000	5.452937000
O	3.942938000	-0.947997000	10.182878000
C	0.609864000	0.551706000	12.535217000
C	-0.119893000	0.351885000	13.716112000
H	-0.265811000	1.180590000	14.399652000
C	0.074587000	-4.053898000	10.996234000
H	-0.468441000	-4.398794000	11.866451000
C	0.366214000	0.587966000	7.539152000
C	2.331178000	-2.605983000	7.678480000
H	3.377415000	-2.818191000	7.924811000
H	2.108906000	-3.121852000	6.735924000
O	5.545764000	2.811831000	11.280557000
C	0.341975000	-4.936493000	9.949574000
H	-0.002124000	-5.963702000	10.010031000
C	-0.452845000	-1.935083000	13.075567000
H	-0.874264000	-2.913705000	13.264688000
C	-0.650012000	-0.901867000	13.988948000
H	-1.218274000	-1.076574000	14.896727000
C	3.346564000	-0.485381000	6.904289000
H	4.224240000	-0.724388000	7.509829000
H	3.179046000	0.592367000	6.984301000
C	1.046873000	-4.498887000	8.830007000
H	1.263804000	-5.167125000	8.004110000
C	1.477110000	-3.171617000	8.797144000
C	0.888177000	-0.749865000	6.980097000
H	0.140129000	-1.505314000	7.242549000
H	0.928289000	-0.709962000	5.887278000
C	1.150307000	1.908956000	12.185073000
H	1.078034000	2.588149000	13.036573000
H	2.187813000	1.846630000	11.851342000
H	0.573842000	2.334382000	11.355890000
C	4.365826000	0.251348000	10.311929000
C	3.071742000	-0.080168000	4.410635000
H	2.493874000	0.810169000	4.645197000
C	4.373761000	-1.980808000	5.121990000
H	4.818177000	-2.581046000	5.911582000
C	6.688248000	-0.636632000	10.577889000
H	6.279420000	-1.590512000	10.265609000
C	4.600906000	-2.326452000	3.788648000
H	5.207520000	-3.196030000	3.552760000
C	5.812442000	0.459108000	10.661653000
C	4.059095000	-1.549958000	2.761210000
H	4.238322000	-1.816027000	1.723585000
C	3.297282000	-0.422473000	3.075345000
H	2.883883000	0.194795000	2.283023000
C	6.354712000	1.689655000	11.072573000

C	7.703936000	1.820635000	11.392179000
H	8.073027000	2.786474000	11.720613000
C	8.551814000	0.718166000	11.292742000
H	9.603707000	0.824594000	11.538772000
C	8.041545000	-0.515229000	10.881811000
H	8.693875000	-1.378984000	10.802700000
C	4.042372000	5.678054000	9.586675000
H	4.469387000	5.567304000	8.595879000
C	5.282956000	3.629102000	10.219506000
C	4.362935000	4.739334000	10.579378000
C	3.817146000	4.871541000	11.865948000
H	4.063927000	4.147961000	12.633608000
C	2.960142000	5.933508000	12.151516000
H	2.540185000	6.034190000	13.147460000
C	3.185372000	6.736863000	9.876992000
H	2.939879000	7.460533000	9.106001000
C	2.643470000	6.865763000	11.159474000
H	1.975574000	7.691732000	11.385269000
O	5.779825000	3.463117000	9.126178000
O	3.577735000	1.217401000	10.131902000
