ESI for:

Cobalt(II) acyl intermediates in carbon-carbon bond formation and oxygenation reactions

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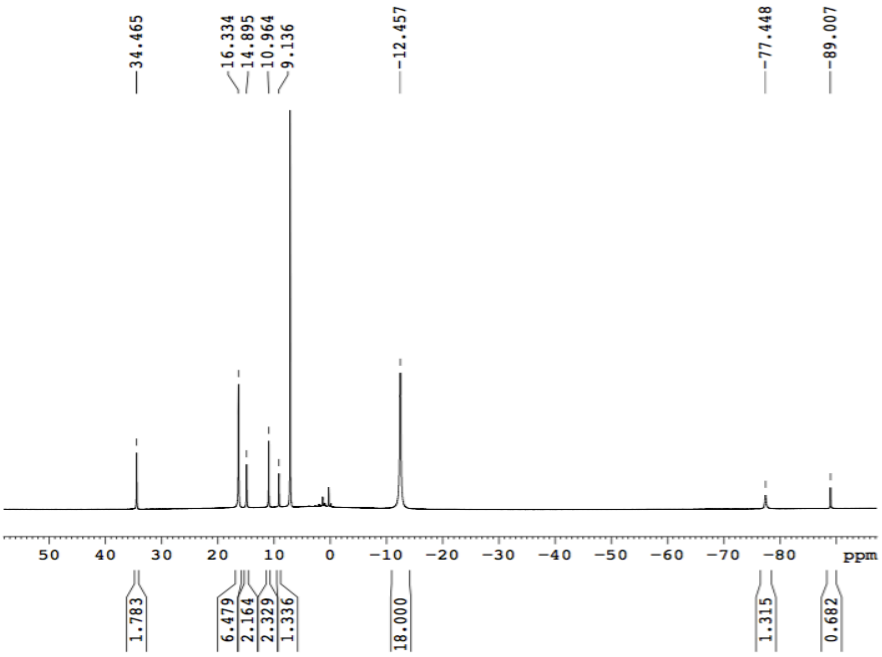


Figure S1. ^{1}H NMR spectrum of To^{M}CoBn (**1**) acquired in benzene-d_6 at room temperature.

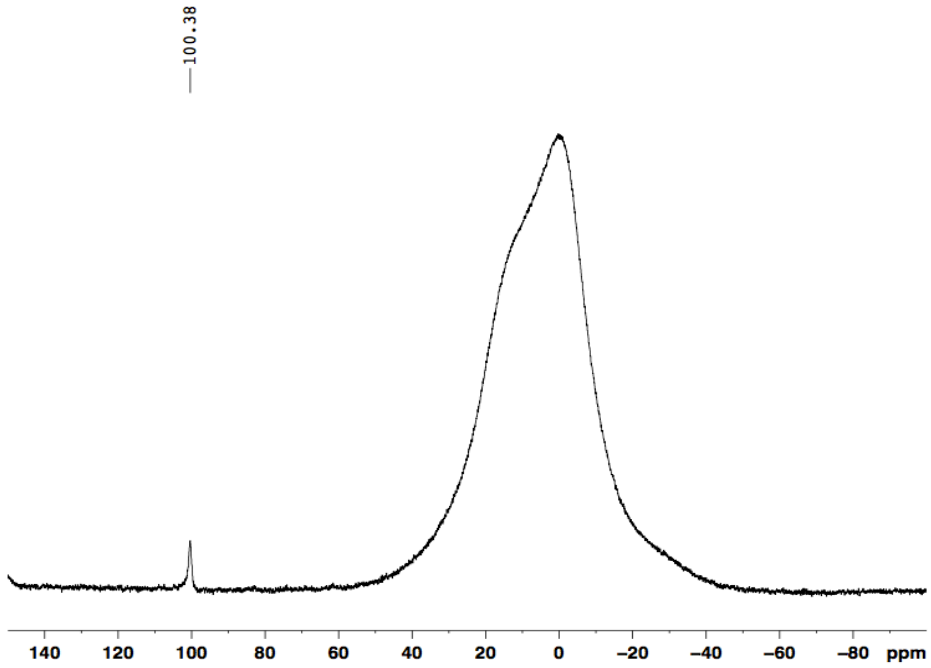


Figure S2. ^{11}B NMR spectrum of To^{M}CoBn (**1**) acquired in benzene-d_6 at room temperature.

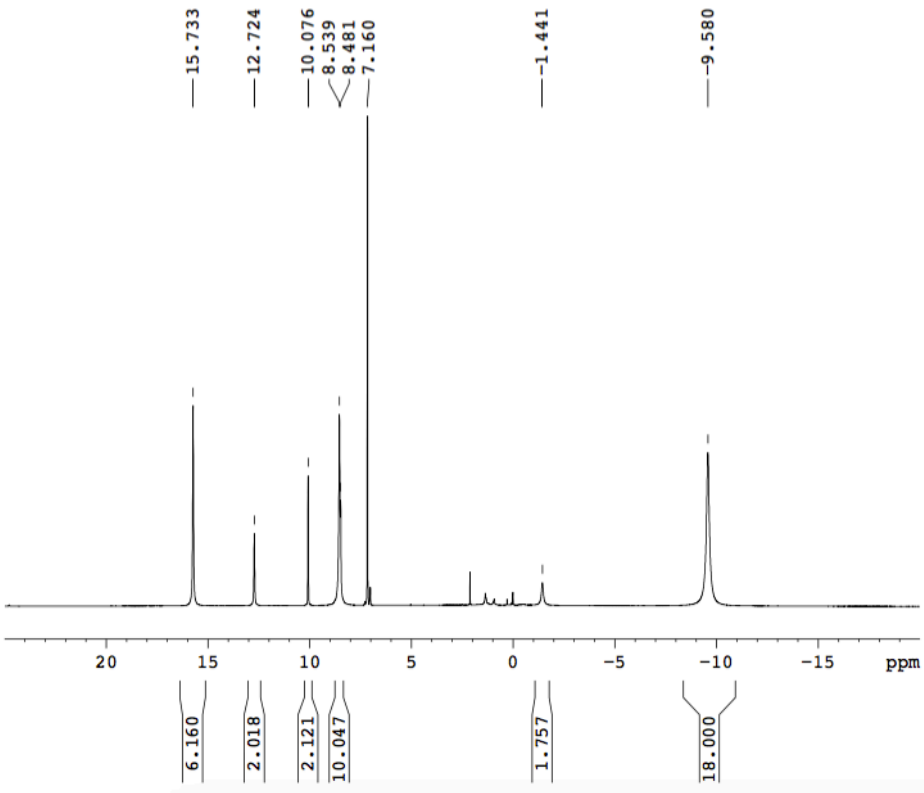


Figure S3. ^{1}H NMR spectrum of To^{iv}CoCH$_2$SiMe$_3$ (**2**) acquired in benzene-d_6 at room temperature.

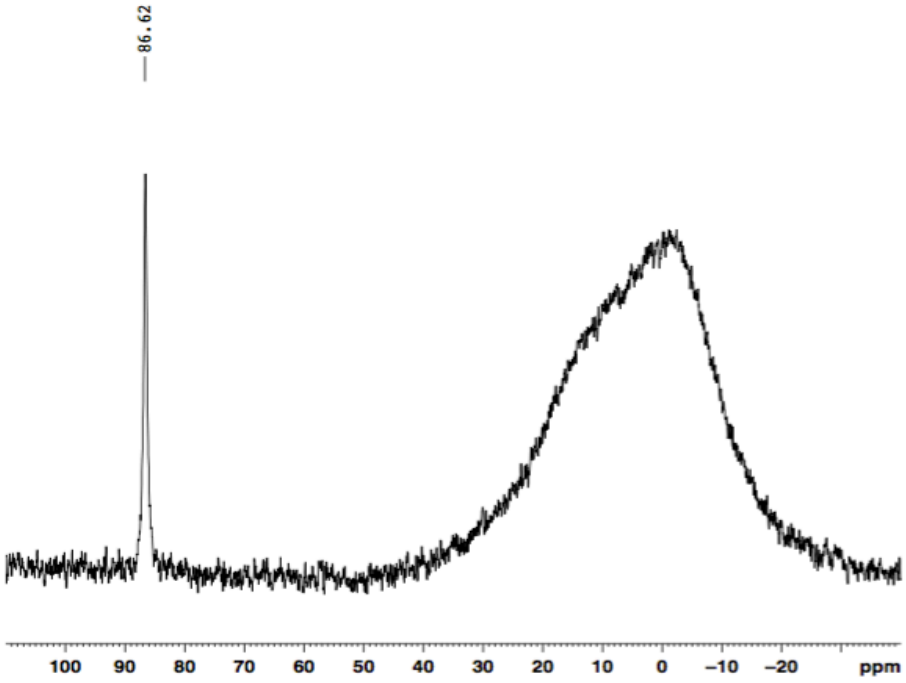


Figure S4. ^{11}B NMR spectrum of To^{M}CoCH$_2$SiMe$_3$ (**2**) acquired in benzene-d_6 at room temperature.

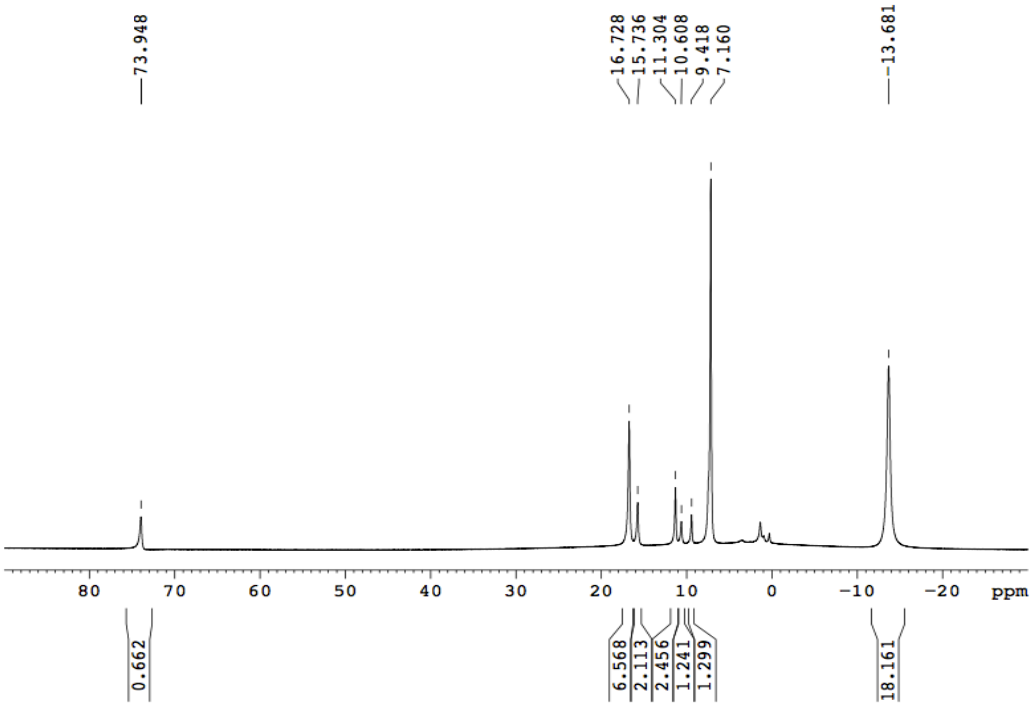


Figure S5. ^{1}H NMR spectrum of To^{M}CoPh (**3**) acquired in benzene-d_6 at room temperature.

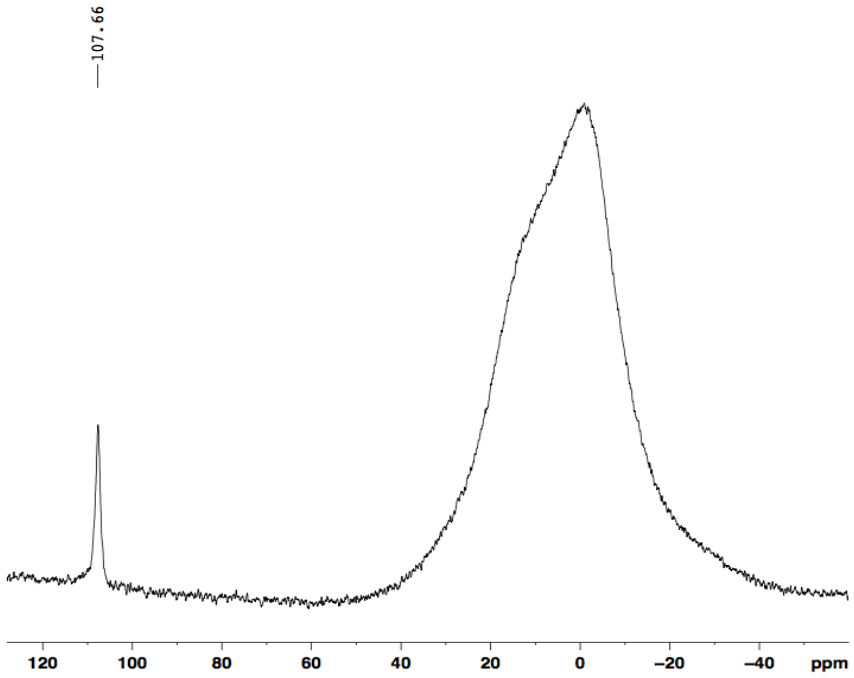


Figure S6. ^{11}B NMR spectrum of To^{M}CoPh (**3**) acquired in benzene-d_6 at room temperature.

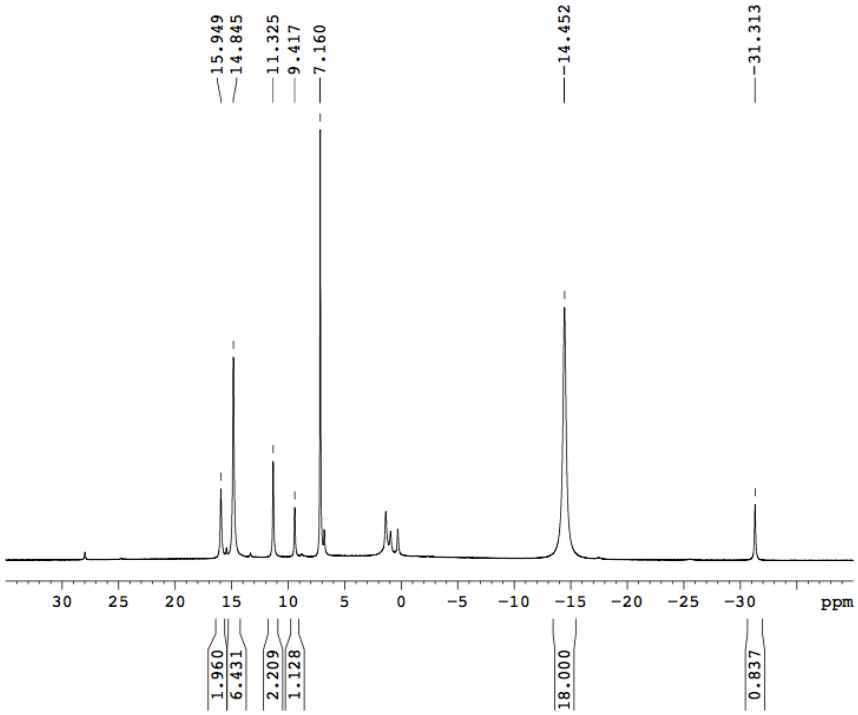
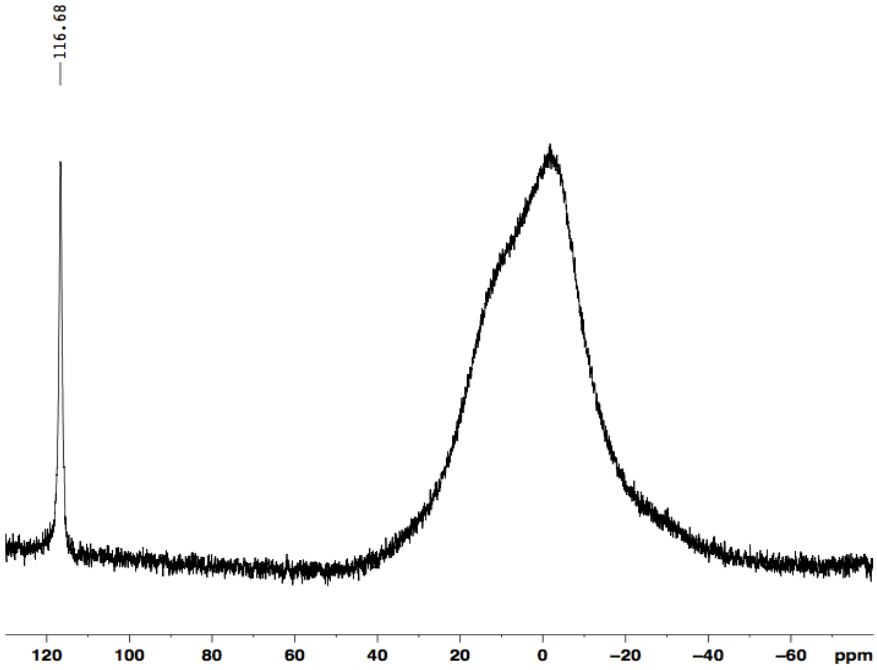


Figure S7. ^{1}H NMR spectrum of To^{M}CoEt (**4**) acquired in benzene-d_6 at room temperature.



F**igure S8.** ^{11}B NMR spectrum of To^{M}CoEt (**4**) acquired in benzene-d_6 at room temperature.

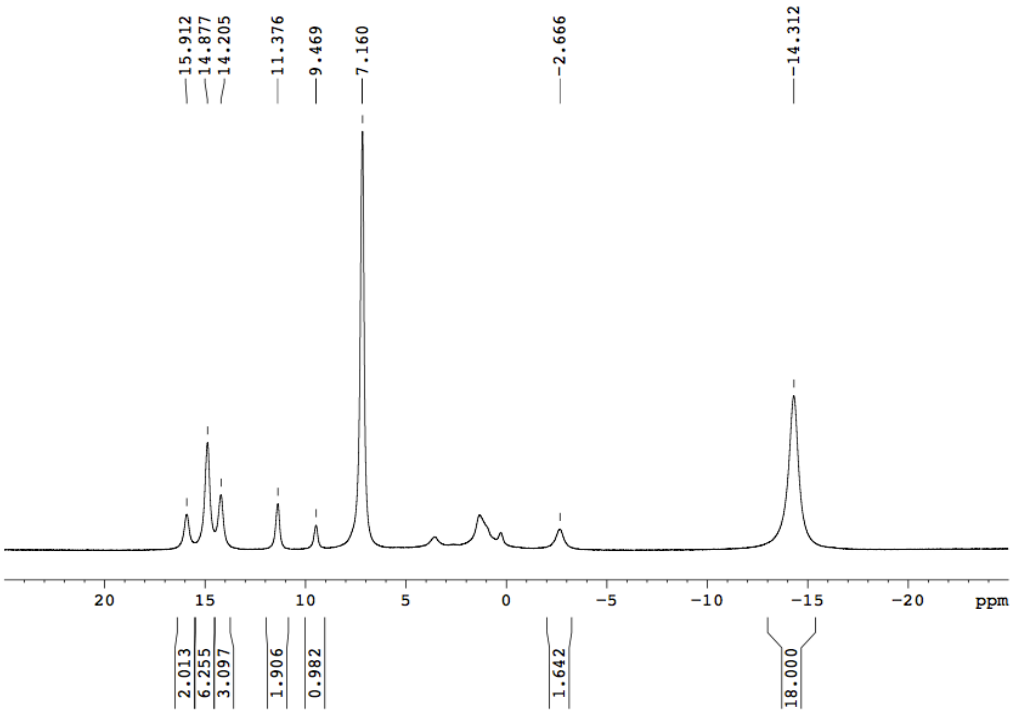


Figure S9. ^{1}H NMR spectrum of To^{M}Co^{n}Bu (**5**) acquired in benzene-d_6 at room temperature.

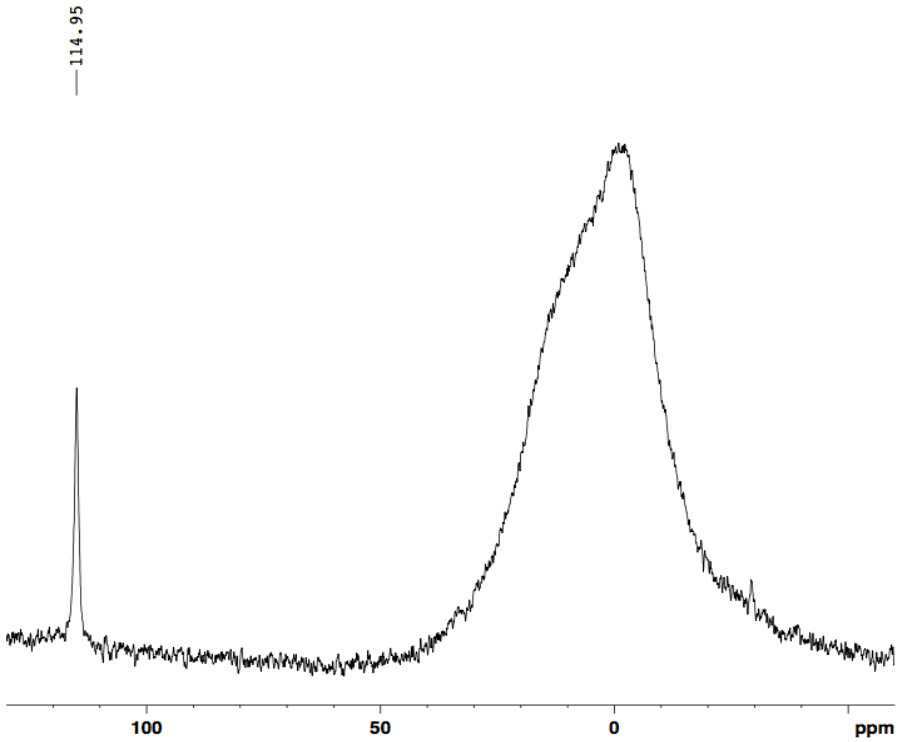


Figure S10. ^{11}B NMR spectrum of To^{M}Co^{n}Bu (**5**) acquired in benzene-d_6 at room temperature.

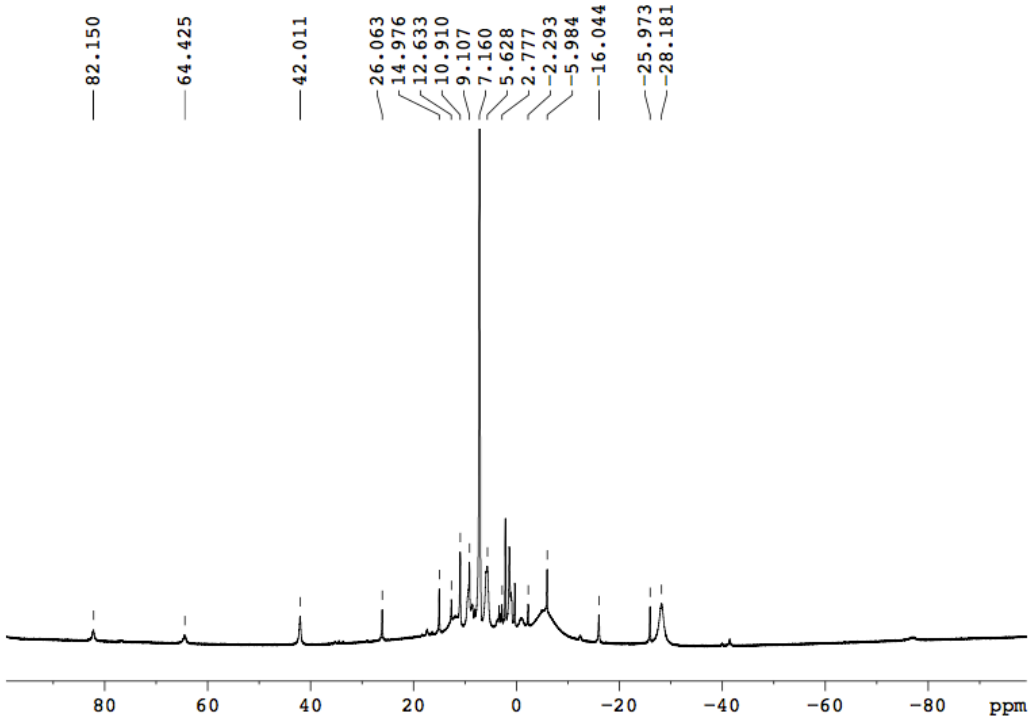


Figure S11. ^{1}H NMR spectrum of To^{M}Co{C(=O)Bn}CO (**7**) acquired in benzene-d_6 at room temperature.

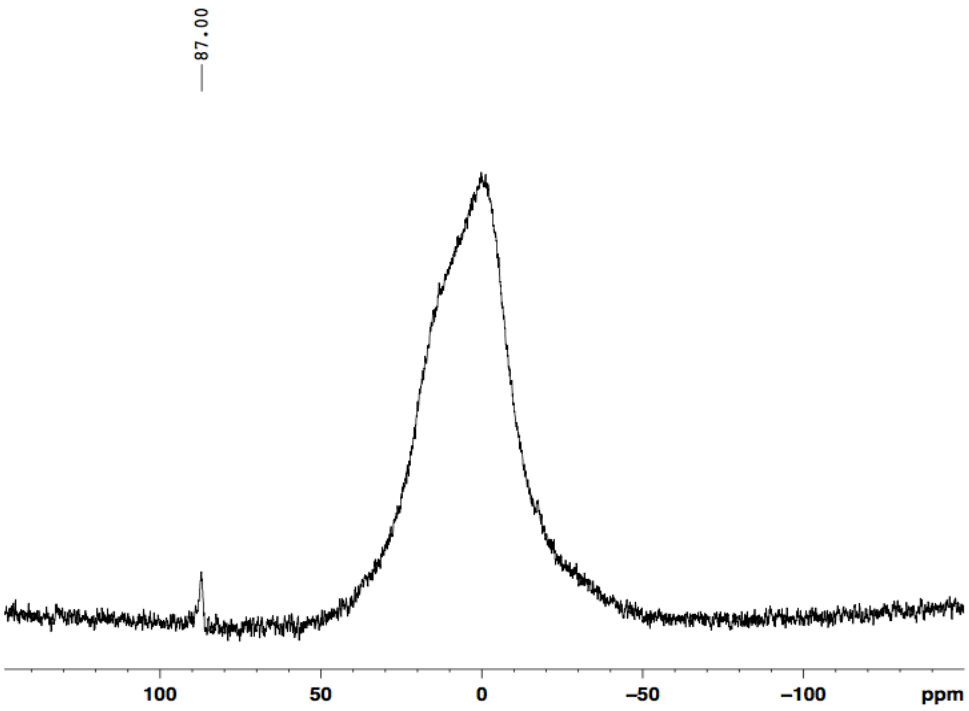


Figure S12. ^{11}B NMR spectrum of To^{M}Co{C(=O)Bn}CO (**7**) acquired in benzene-d_6 at room temperature.

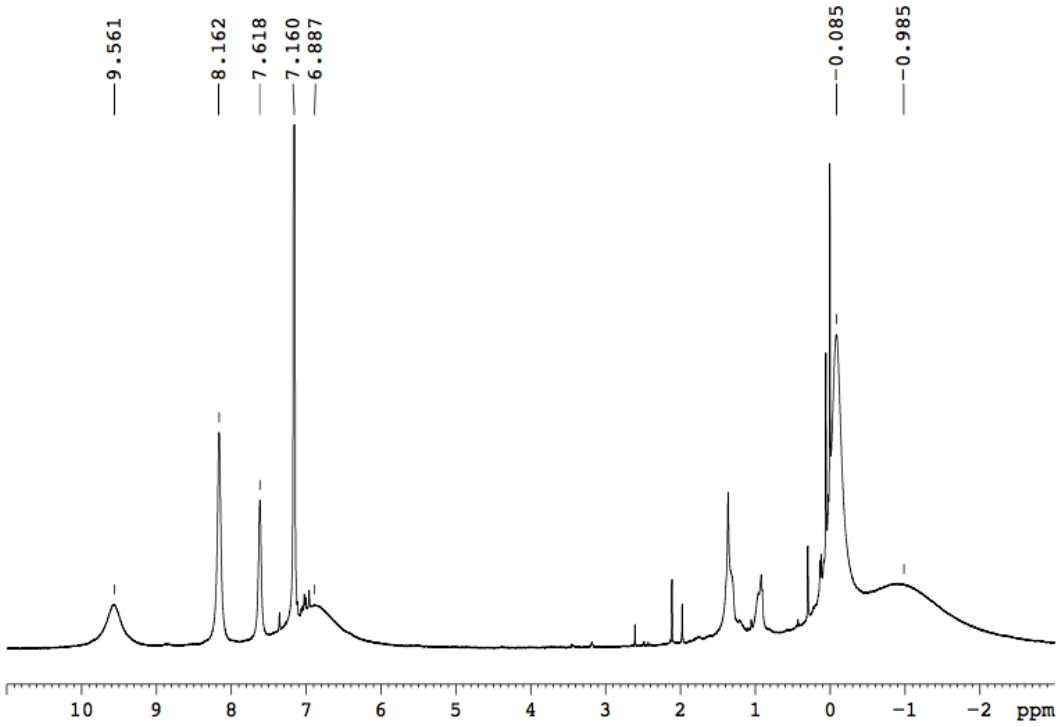


Figure S13. ^{1}H NMR spectrum of To^{M}Co{C(=O)CH$_2$SiMe$_3$}CO (**8**) acquired in benzene-d_6 at room temperature.

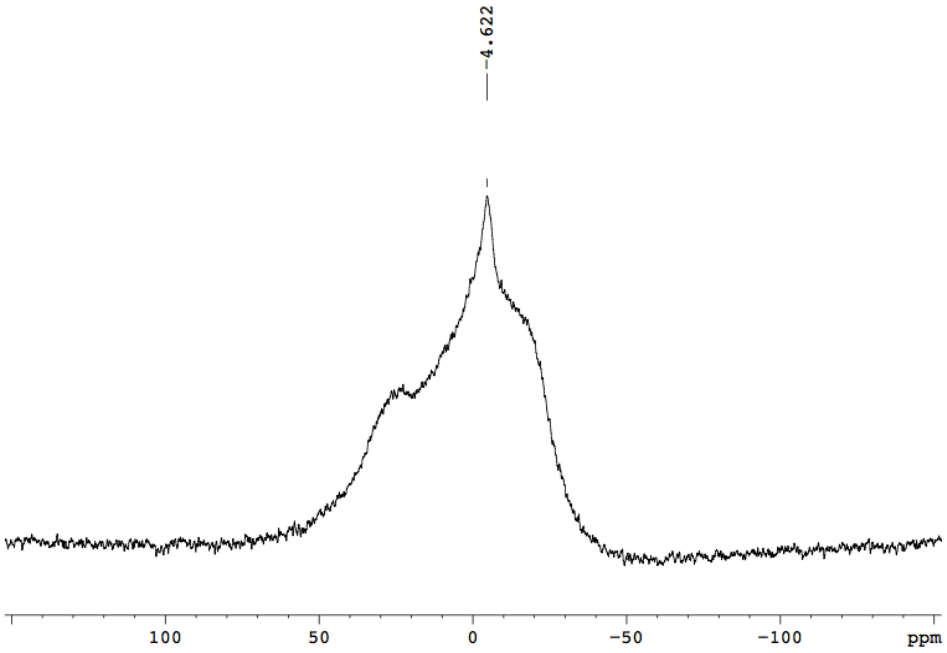


Figure S14. ^{11}B NMR spectrum of To^{M}Co{C(=O)CH$_2$SiMe$_3$}CO (**8**) acquired in benzene-d_6 at room temperature.

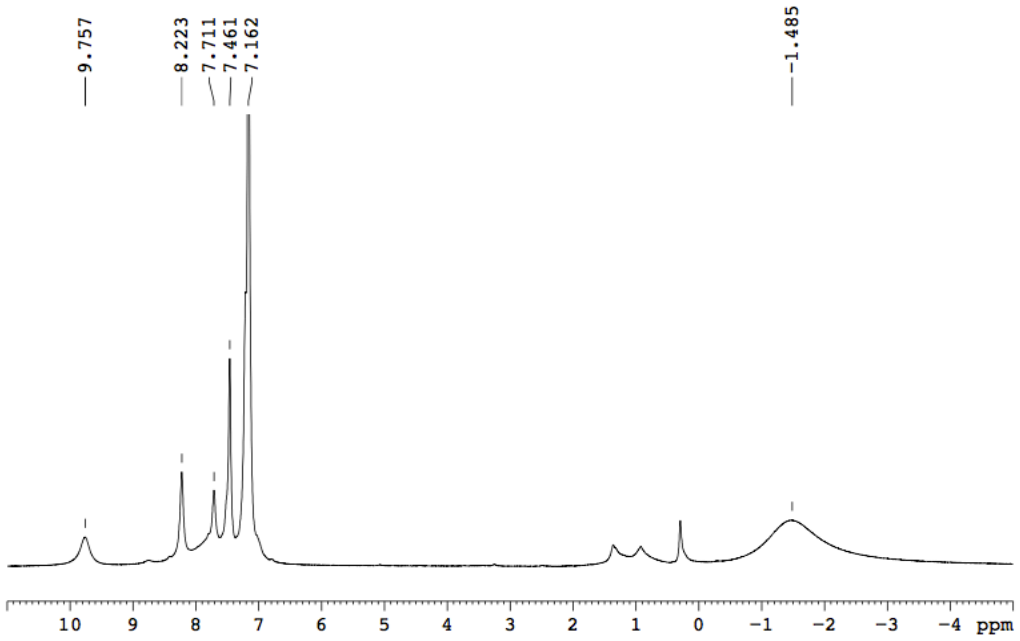


Figure S15. ^{1}H NMR spectrum of To^{M}Co{C(=O)Ph}CO (**9**) acquired in benzene-d_6 at room temperature.

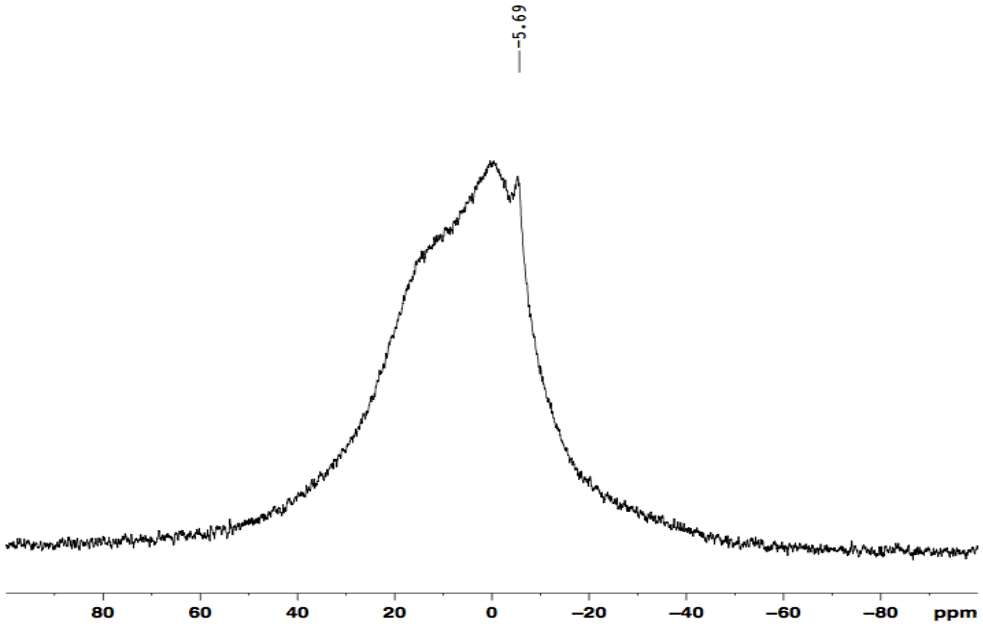


Figure S16. ^{11}B NMR spectrum of To^{M}Co{C(=O)Ph}CO (**9**) acquired in benzene-d_6 at room temperature.

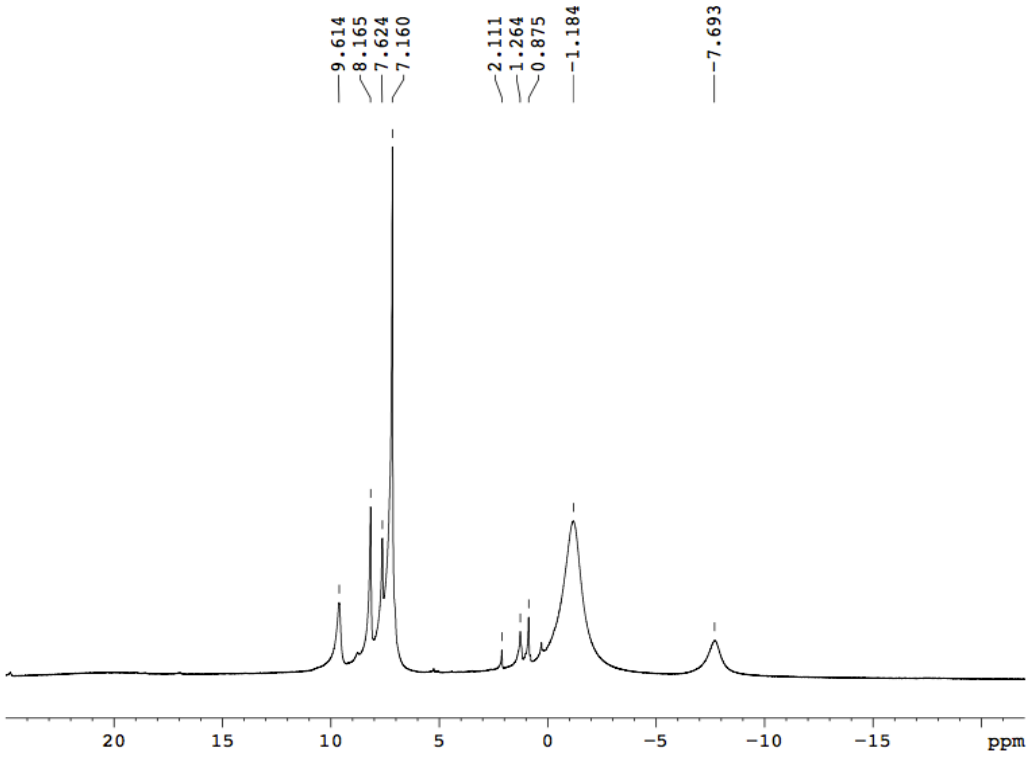


Figure S17. ^{1}H NMR spectrum of To^{M}Co{C(=O)Et}CO (**10**) acquired in benzene-d_6 at room temperature.

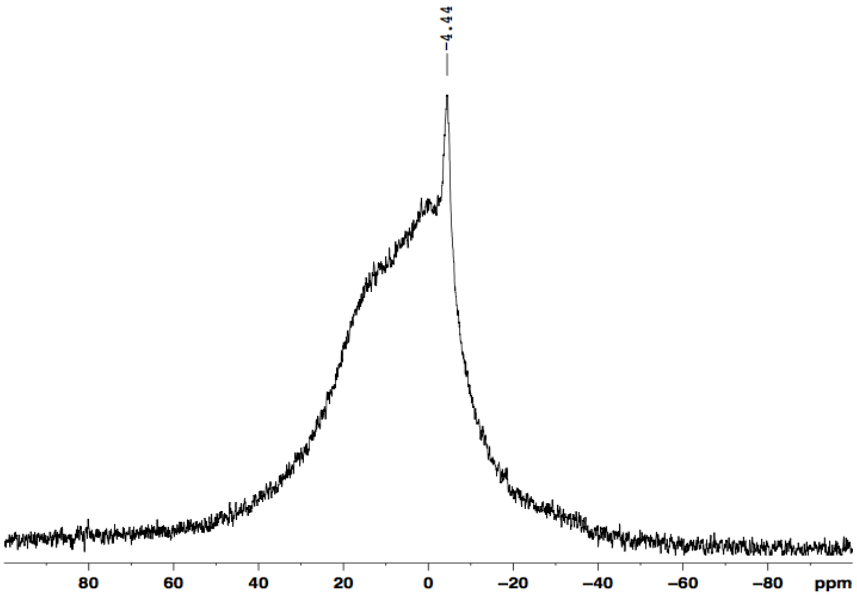


Figure S18. ^{11}B NMR spectrum of To^{M}Co{C(=O)Et}CO (**10**) acquired in benzene-d_6 at room temperature.

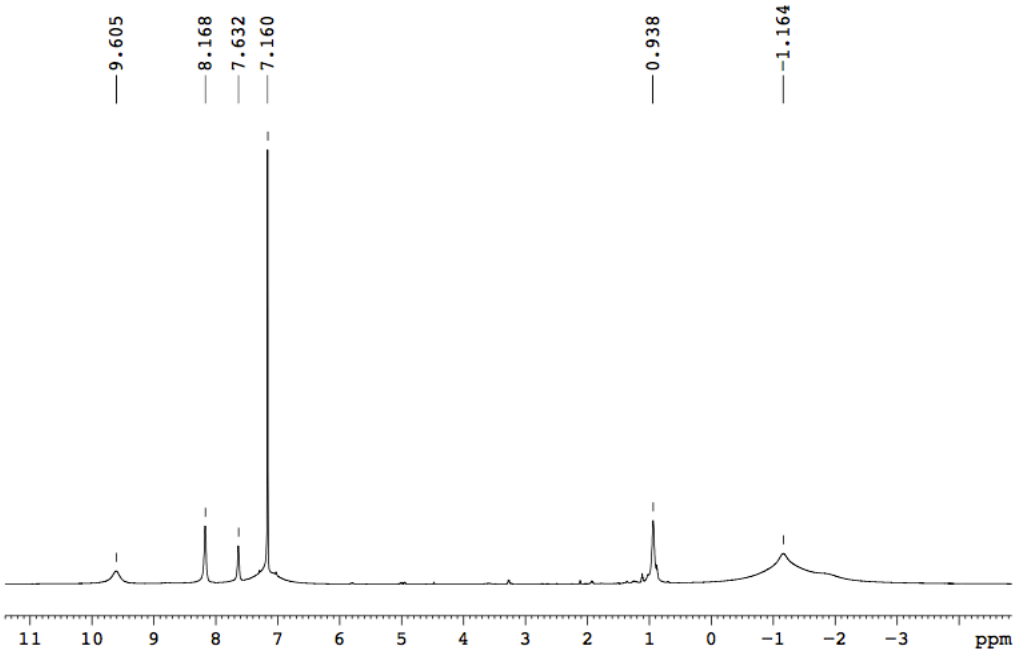


Figure S19. ^{1}H NMR spectrum of To^{M}Co{C(=O)^{n}Bu}CO (**11**) acquired in benzene-d_6 at room temperature.

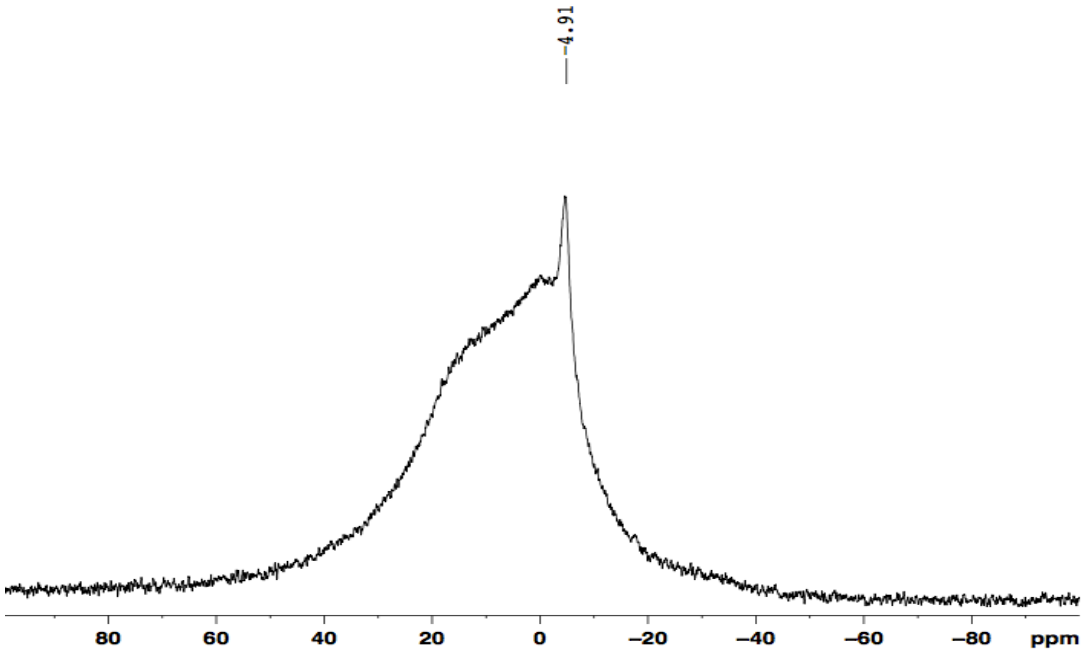


Figure S20. ^{11}B NMR spectrum of To^{M}Co{C(=O)^{n}Bu}CO (**11**) acquired in benzene-d_6 at room temperature.

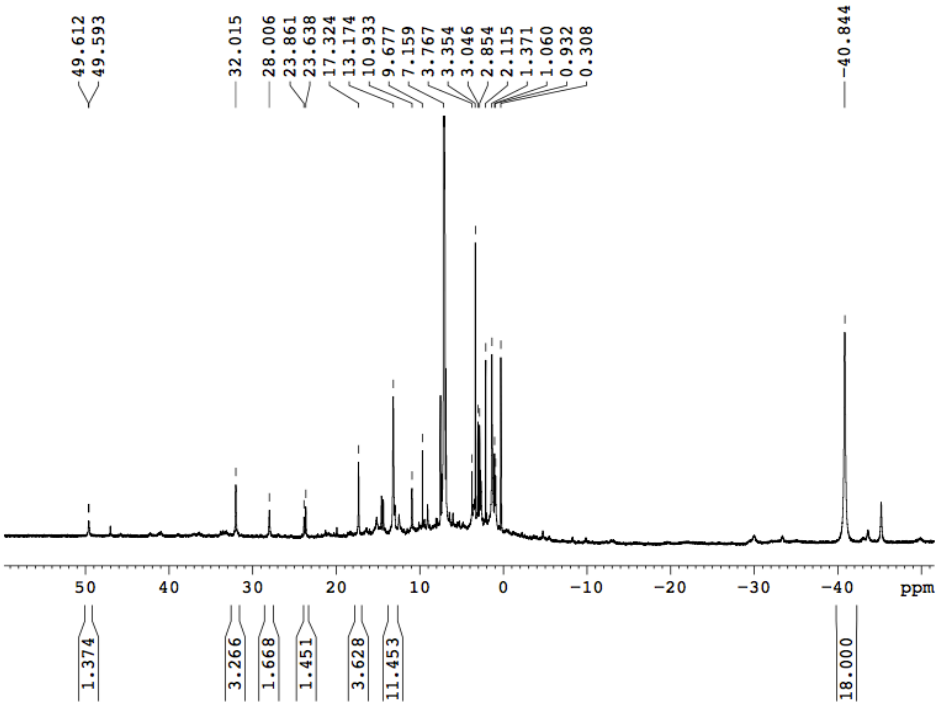


Figure S21. ^{1}H NMR spectrum of To^{M}CoO$_2$CBn (**13**) acquired in benzene-d_6 at room temperature.

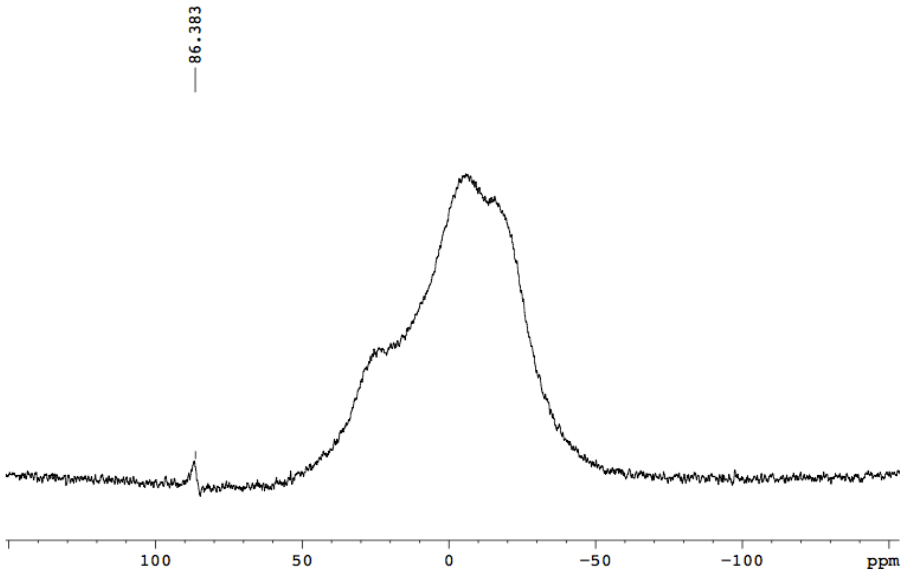


Figure S22. ^{11}B NMR spectrum of To^{M}CoO$_2$CBn (**13**) acquired in benzene-d_6 at room temperature.

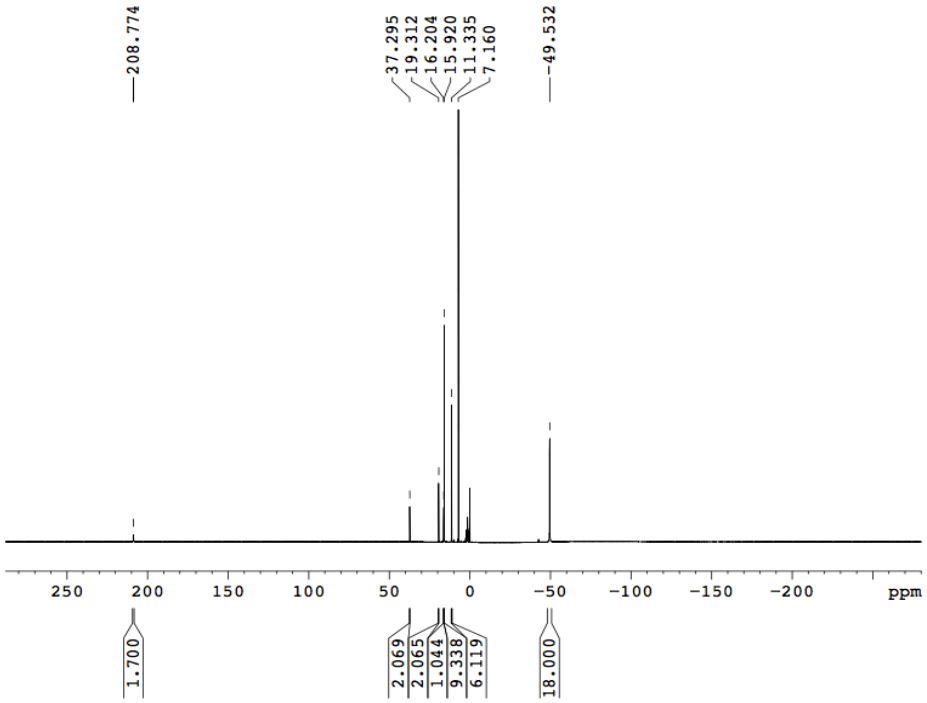


Figure S23. ^{1}H NMR spectrum of To^{M}CoO$_2$CCH$_2$SiMe$_3$ (**14**) acquired in benzene-d_6 at room temperature.

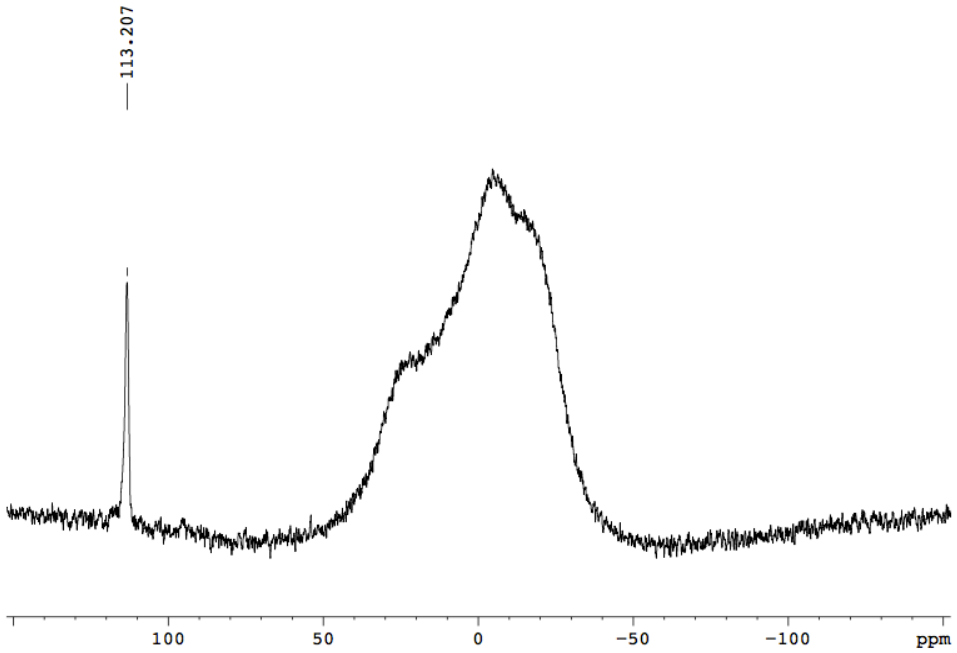


Figure S24. ^{11}B NMR spectrum of To^{M}CoO$_2$CCH$_2$SiMe$_3$ (**14**) acquired in benzene-d_6 at room temperature.

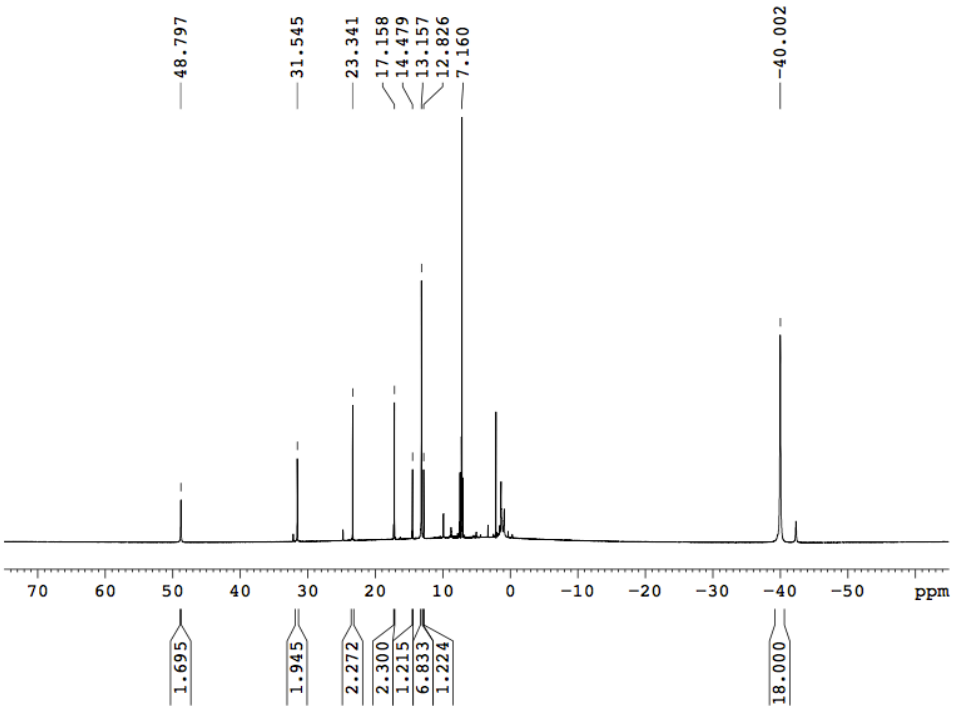
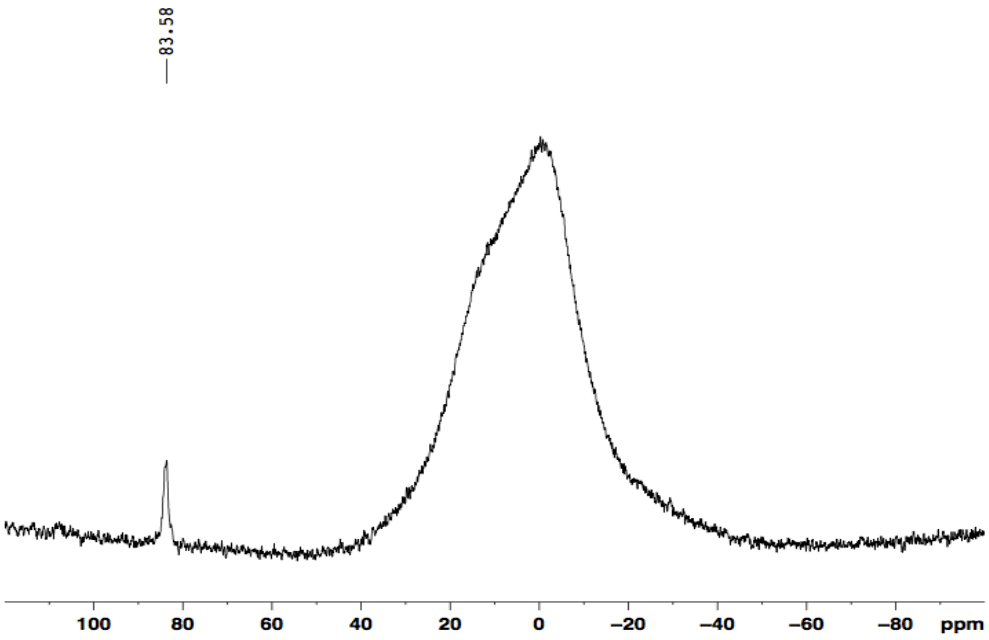
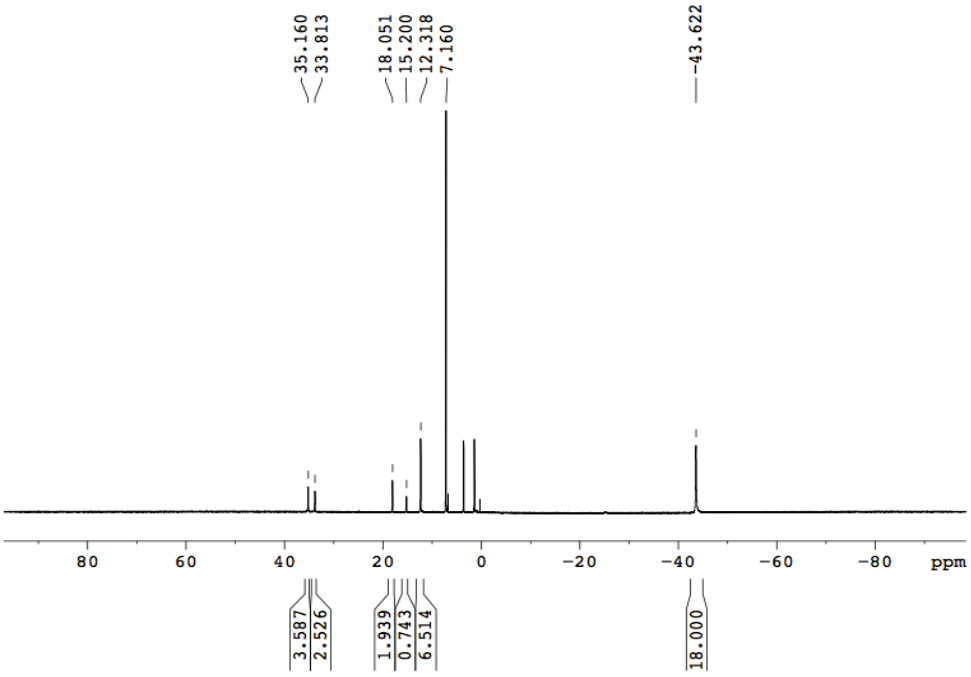


Figure S25. ^{1}H NMR spectrum of To^{M}CoO$_2$CPh (**15**) acquired in benzene-d_6 at room temperature.



F**igure S26.** ^{11}B NMR spectrum of To^{M}CoO$_2$CPh (**15**) acquired in benzene-d_6 at room temperature.



F**igure S27.** ^{1}H NMR spectrum of To^{M}CoO$_2$CEt (**16**) acquired in benzene-d_6 at room temperature.

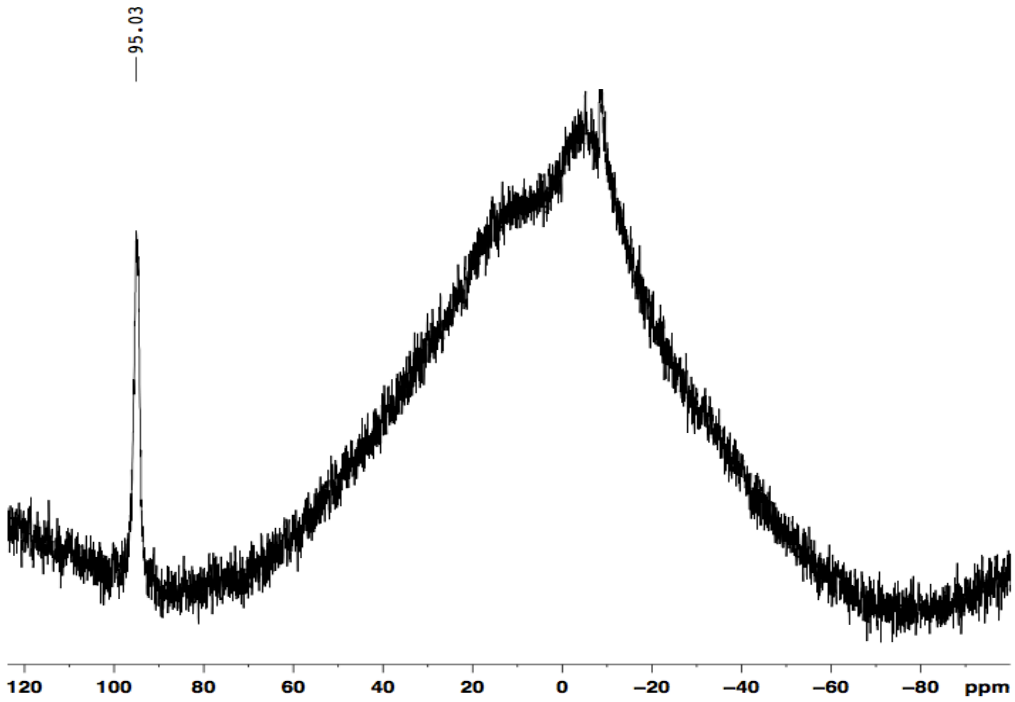


Figure S28. ^{11}B NMR spectrum of To^{M}CoO$_2$CEt (**16**) acquired in benzene-d_6 at room temperature.

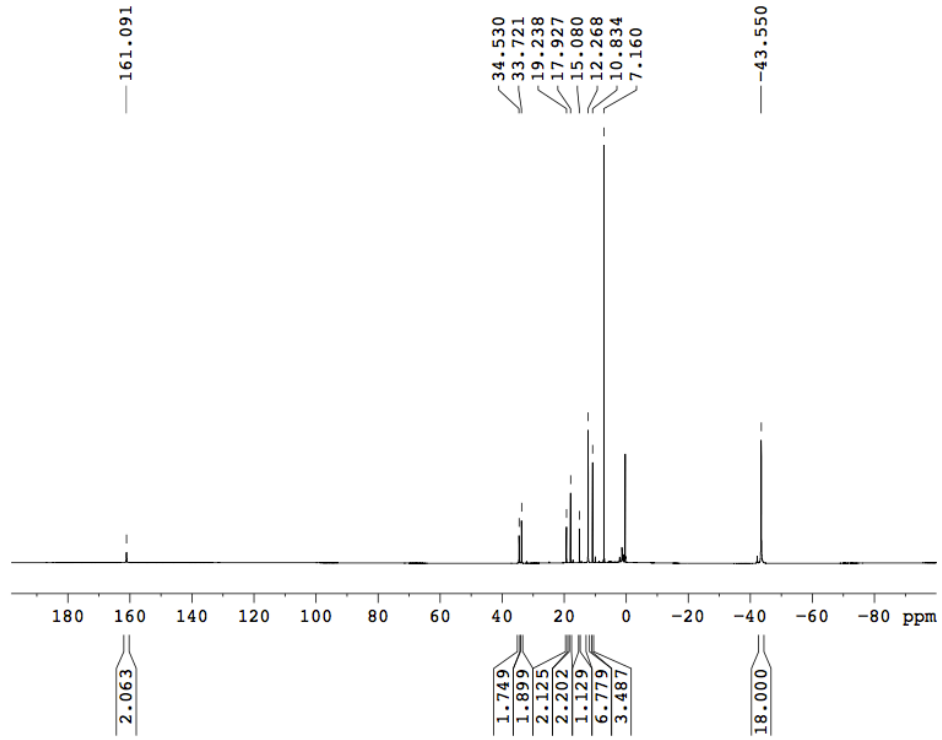
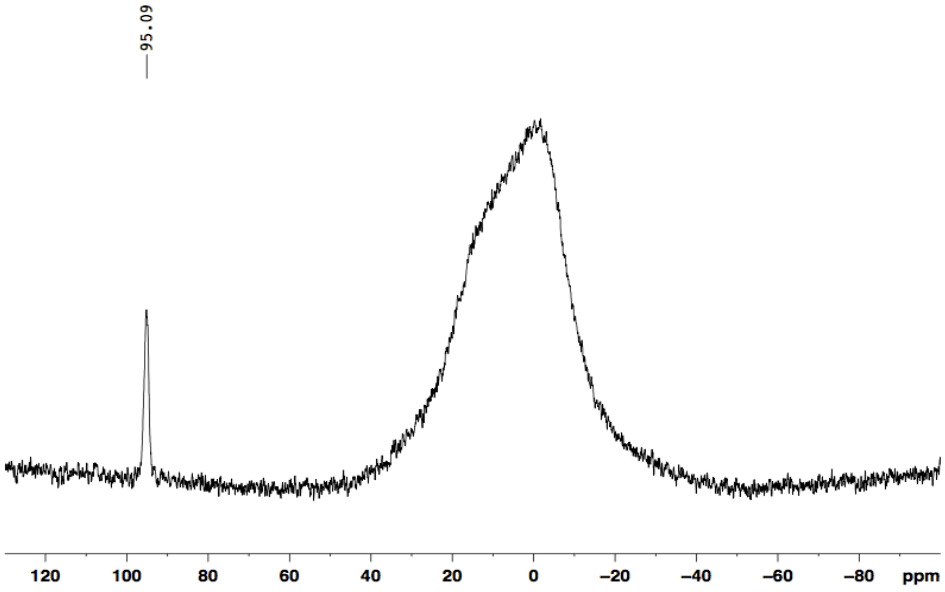


Figure S29. ^{1}H NMR spectrum of To^{M}CoO$_2$C^{n}Bu (**17**) acquired in benzene-d_6 at room temperature.



F**igure S30.** ^{11}B NMR spectrum of To^{M}CoO$_2$C^{n}Bu (**17**) acquired in benzene-d_6 at room temperature.

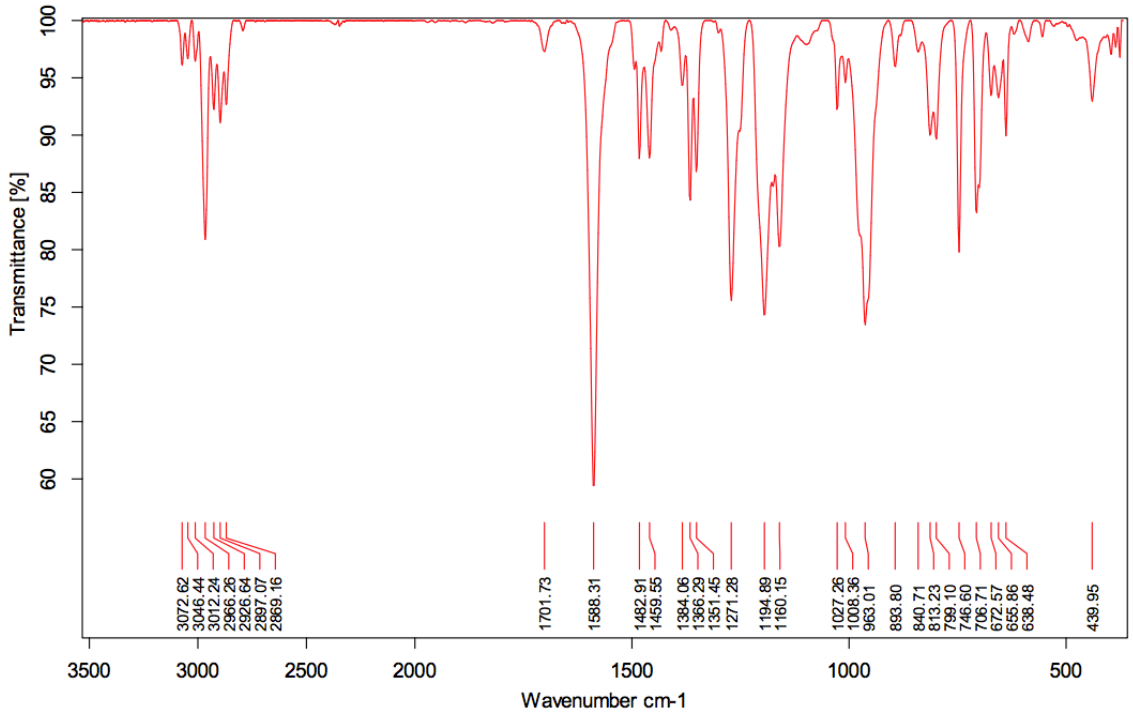


Figure S31. Infrared spectrum (KBr) of To^{M}CoBn (**1**).

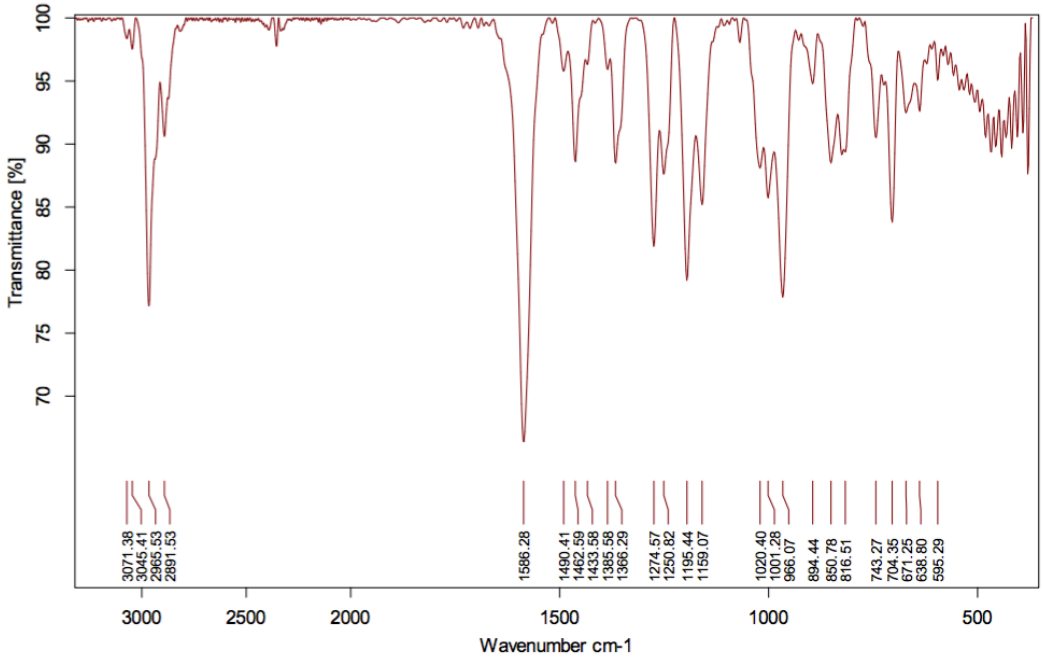


Figure S32. Infrared spectrum (KBr) of To^{M}CoCH$_2$SiMe$_3$ (**2**).

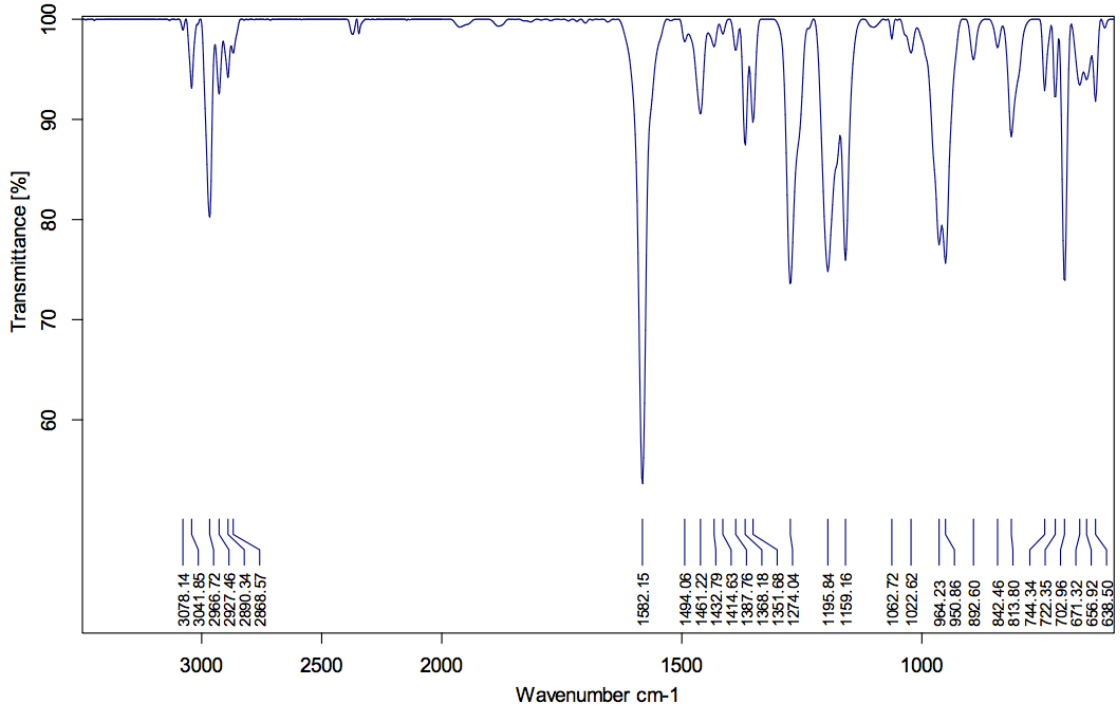


Figure S33. Infrared spectrum (KBr) of To^{M}CoPh (**3**).

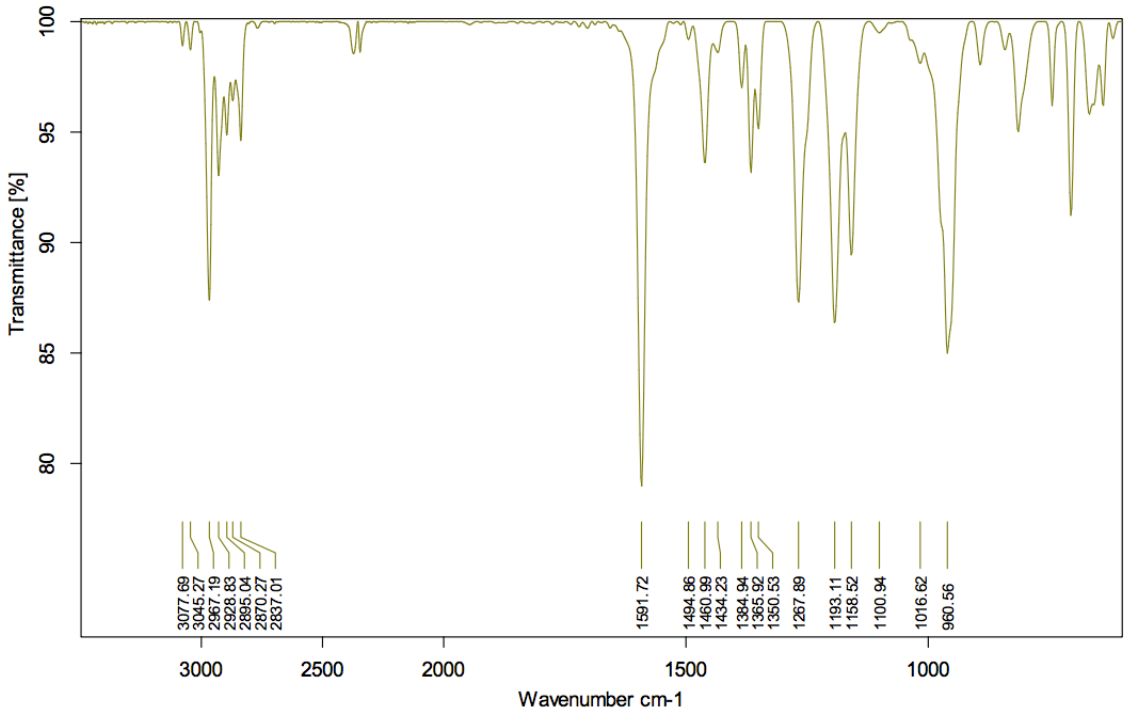


Figure S34. Infrared spectrum (KBr) of To^{M}CoEt (**4**).

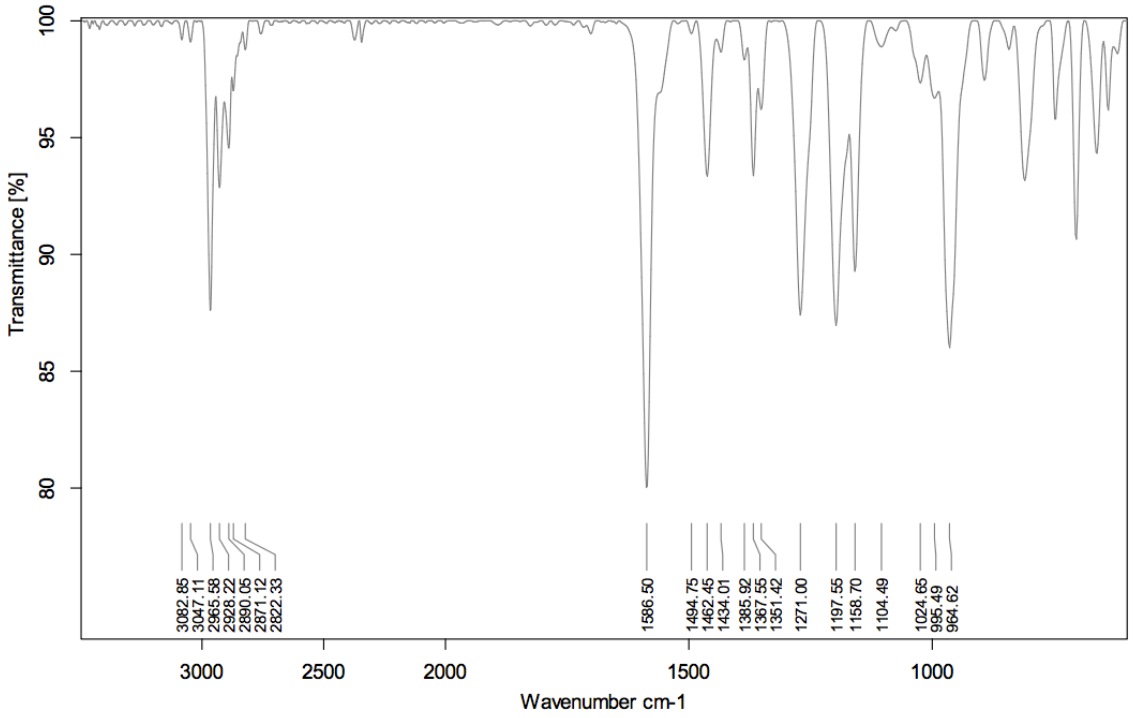


Figure S35. Infrared spectrum (KBr) of To^{M}Co^{n}Bu (**5**).

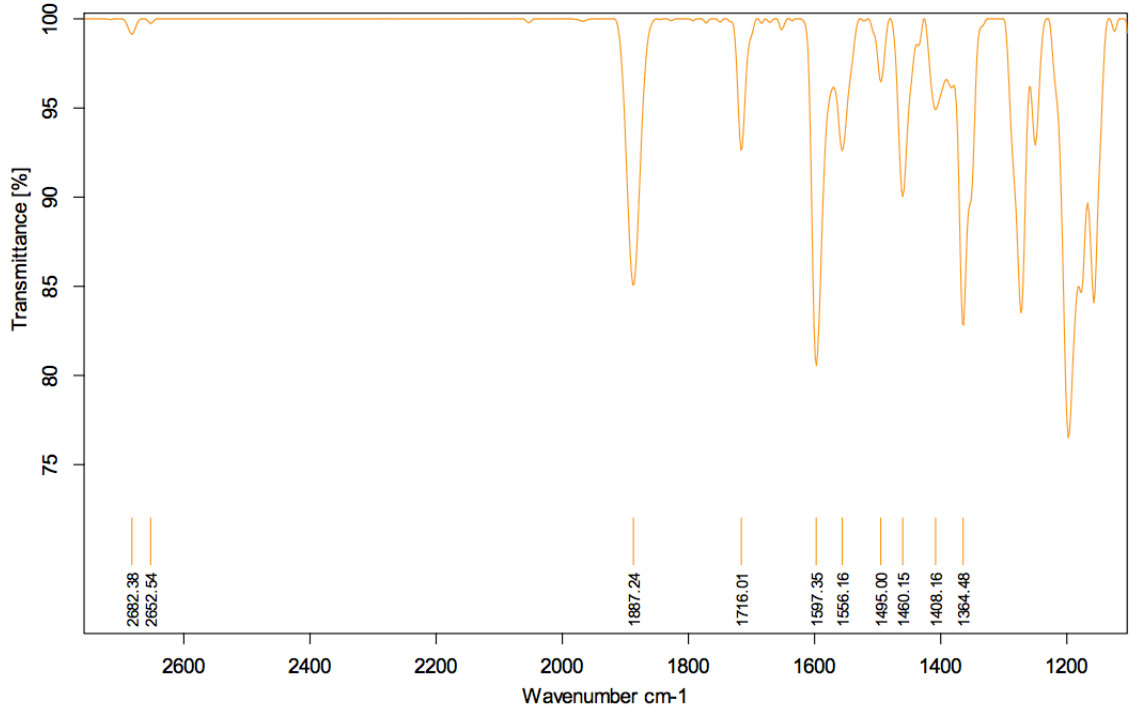


Figure S36. Infrared spectrum (ATR, ZnSe crystal) of To^{M}Co{C(=O)Bn}CO (**7**) in tetrahydrofuran.

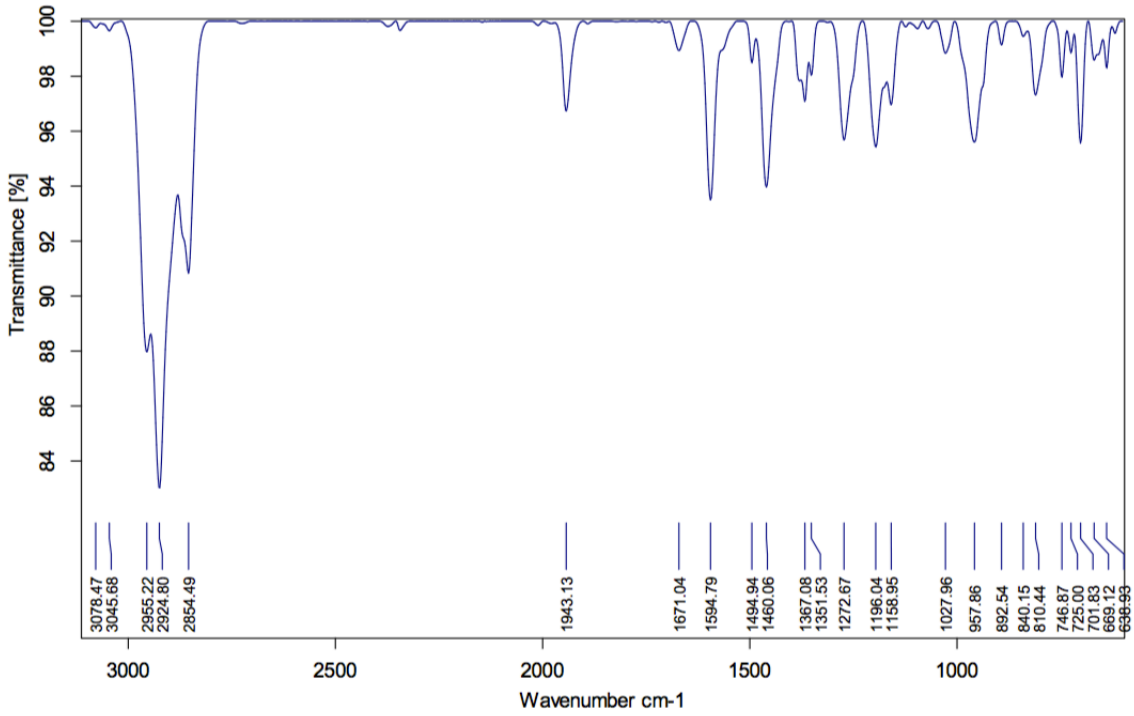


Figure S37. Infrared spectrum (KBr pellet) of crystals of **7**.

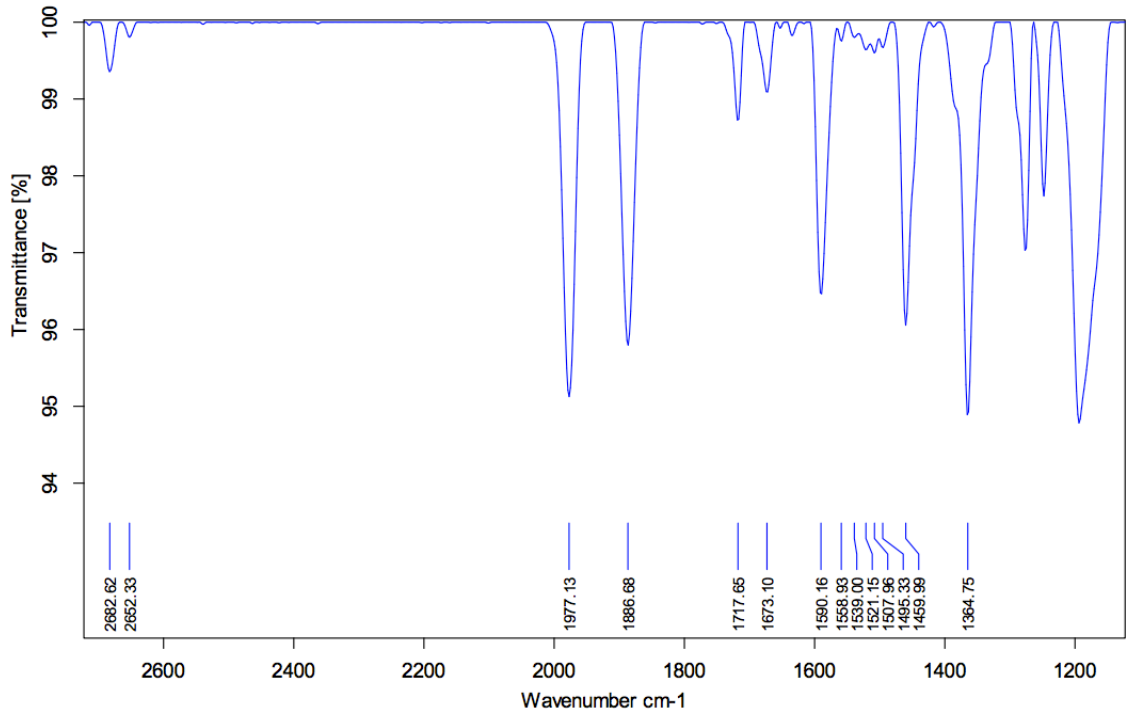


Figure S38. Infrared spectrum (ATR, ZnSe crystal) of To^{M}Co{C(=O)CH_2SiMe_3}CO (**8**) in tetrahydrofuran.

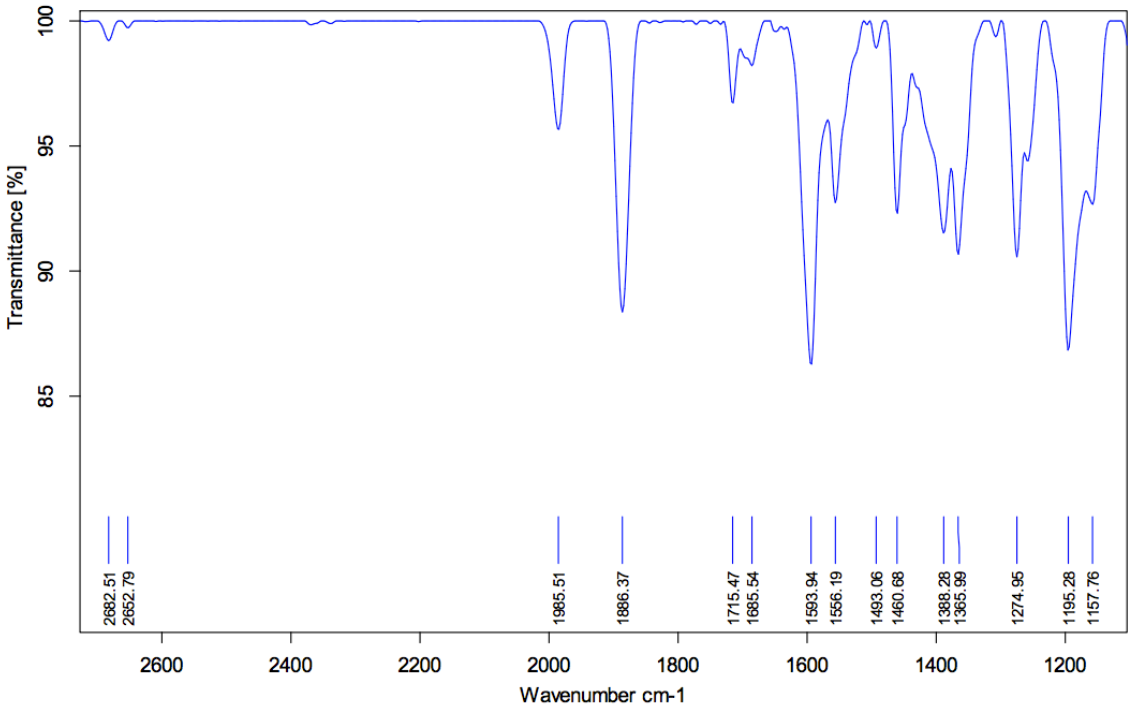


Figure S39. Infrared spectrum (ATR, ZnSe crystal) of To^{M}Co{C(=O)Ph}CO (**9**) in tetrahydrofuran.

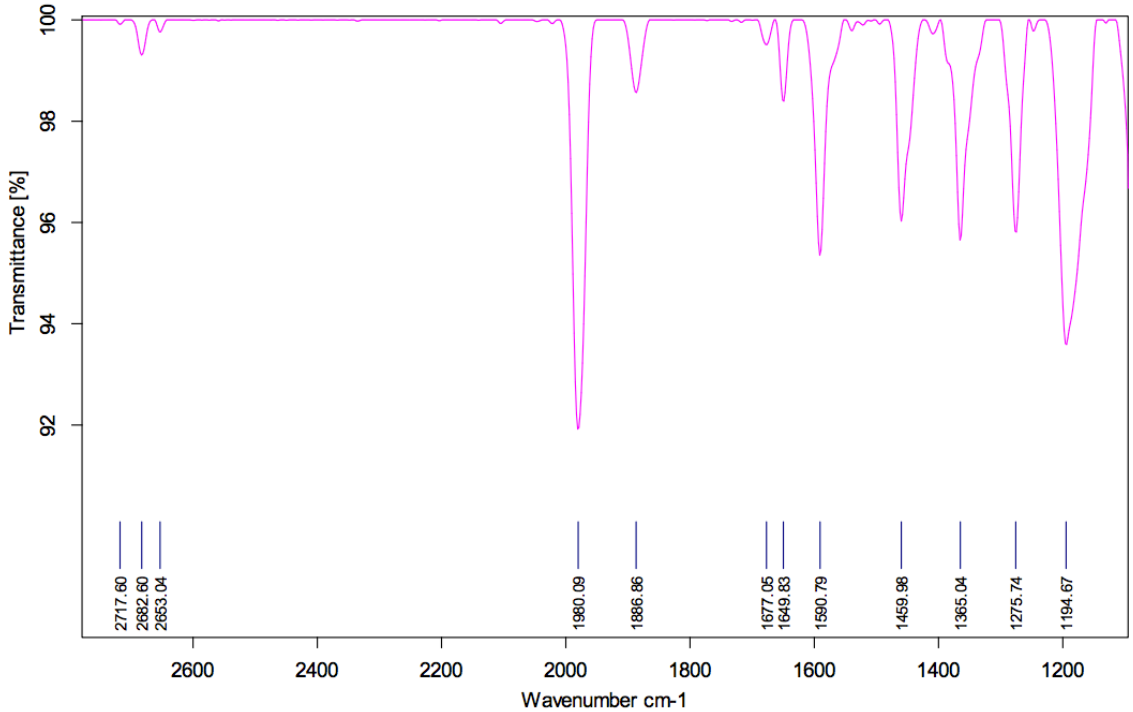


Figure S40. Infrared spectrum (ATR, ZnSe crystal) of To^{M}Co{C(=O)Et}CO (**10**) in tetrahydrofuran.

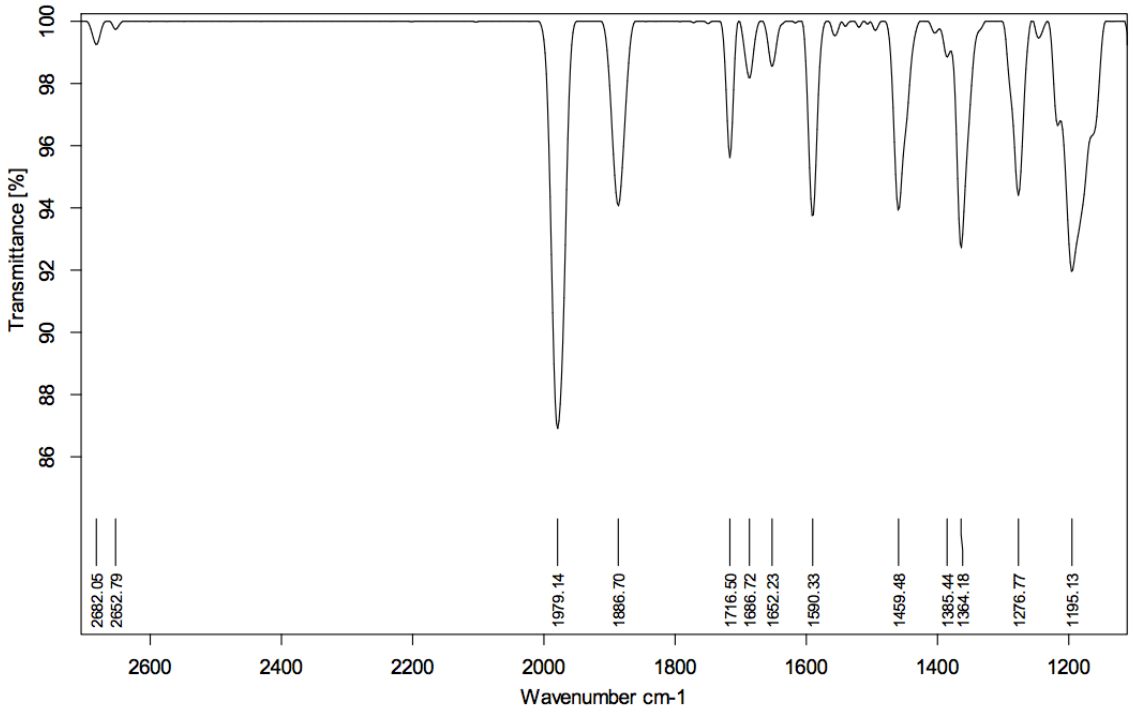


Figure S41. Infrared spectrum (ATR, ZnSe crystal) of To^{M}Co{C(=O)^{n}Bu}CO (**11**) in tetrahydrofuran.

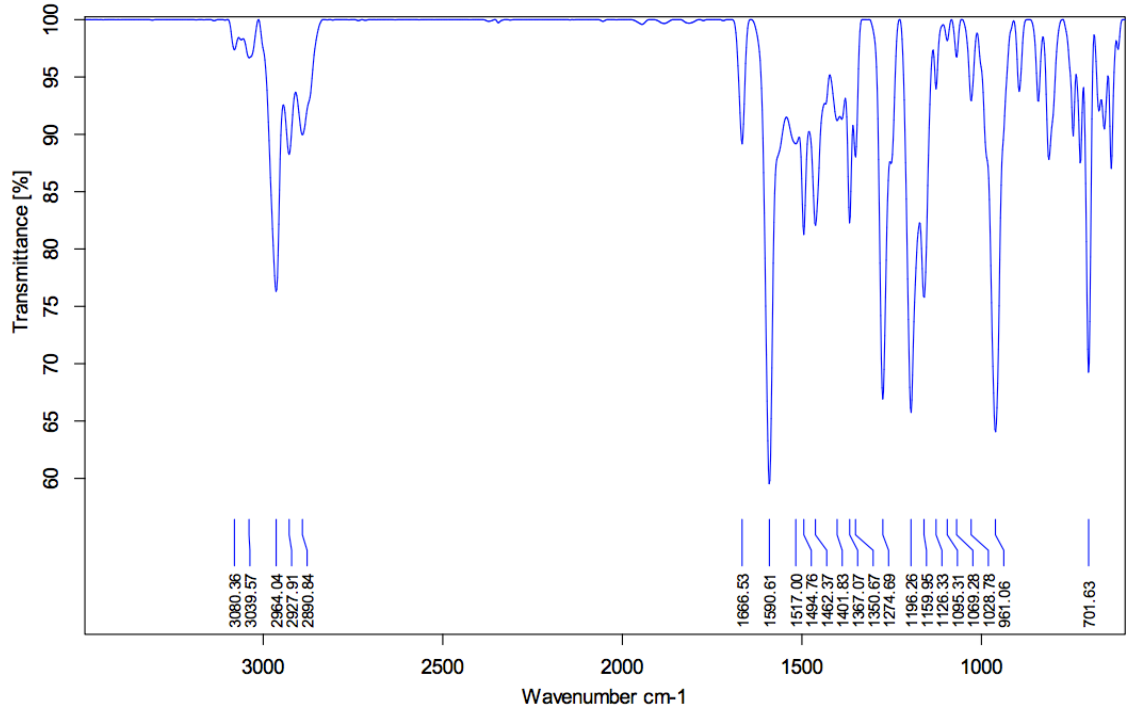


Figure S42. Infrared spectrum (KBr) of To^{M}CoO$_2$CBn (**13**).

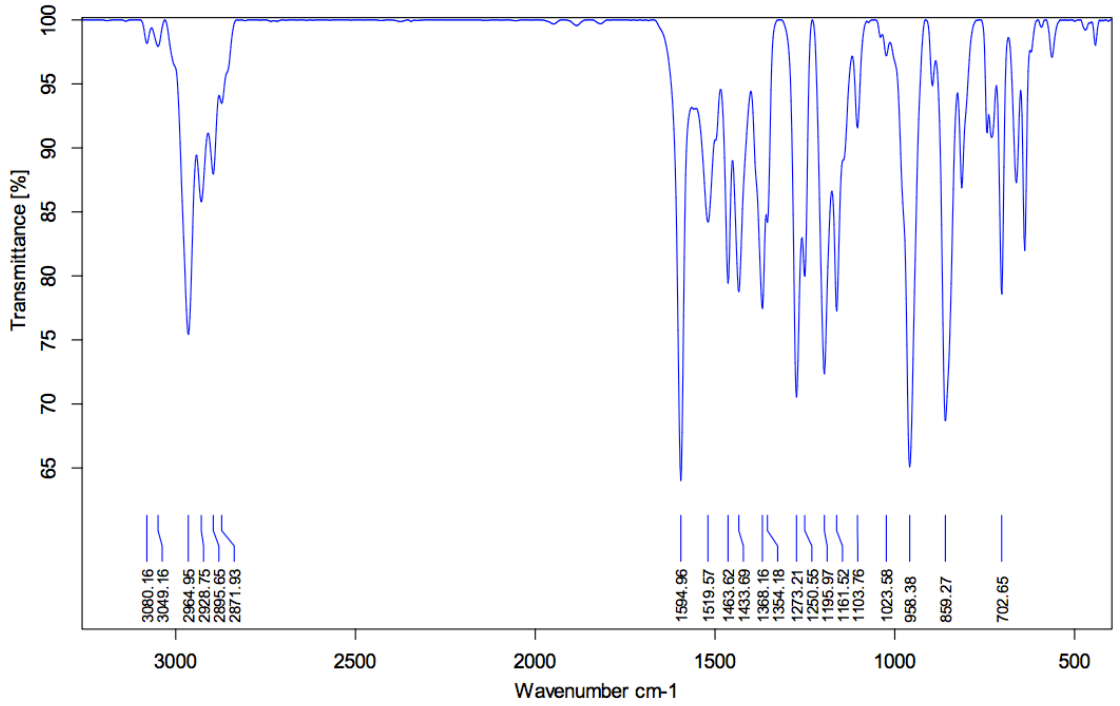


Figure S43. Infrared spectrum (KBr) of To^{M}CoO$_2$CCH$_2$SiMe$_3$ (**14**).

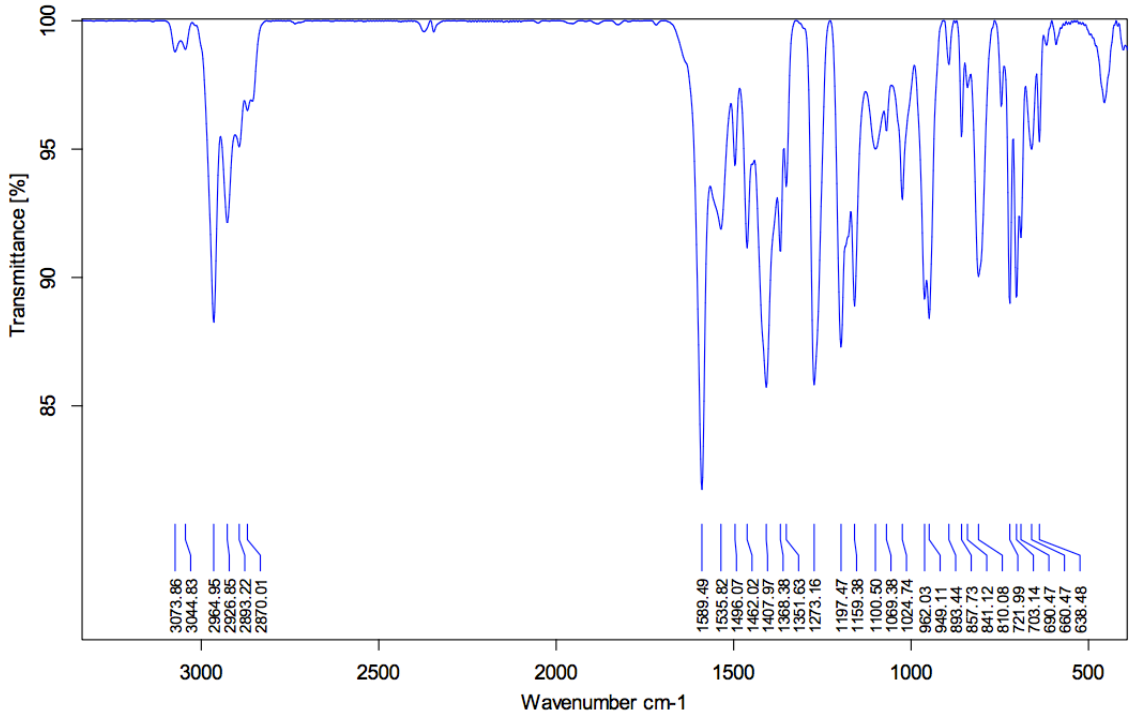


Figure S44. Infrared spectrum (KBr) of To^{M}CoO$_2$CPh (**15**).

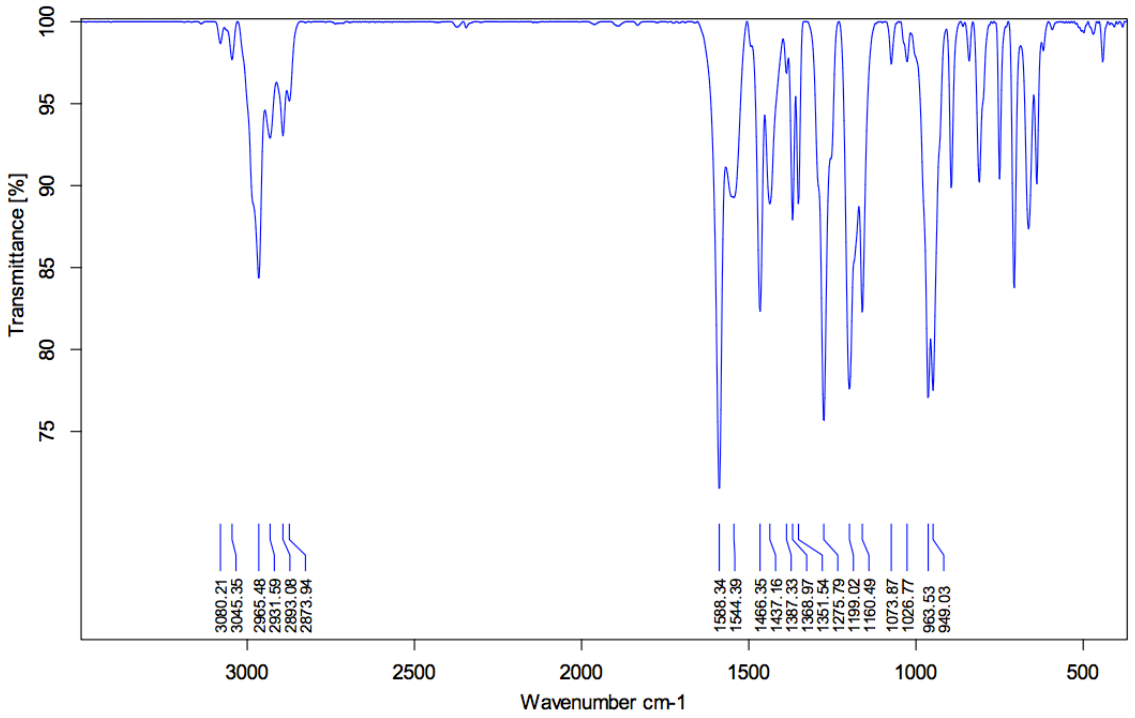


Figure S45. Infrared spectrum (KBr) of To^{M}CoO$_2$CEt (**16**).

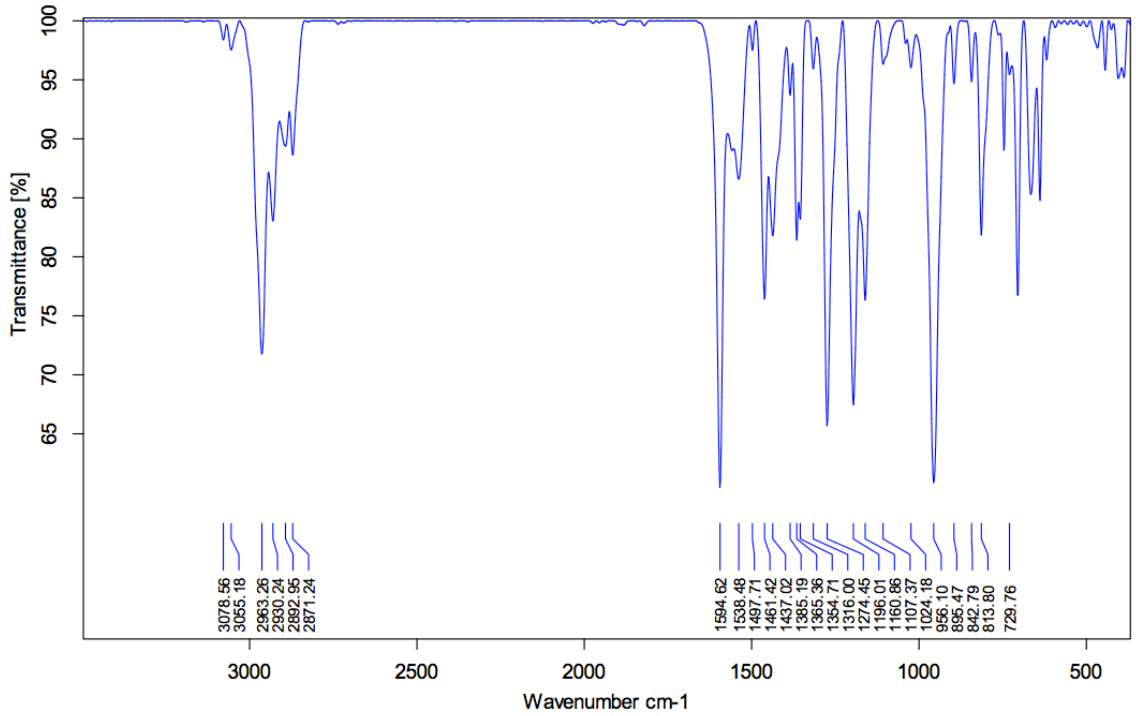


Figure S46. Infrared spectrum (KBr) of To^{M}CoO$_2$C^{n}Bu (**17**).

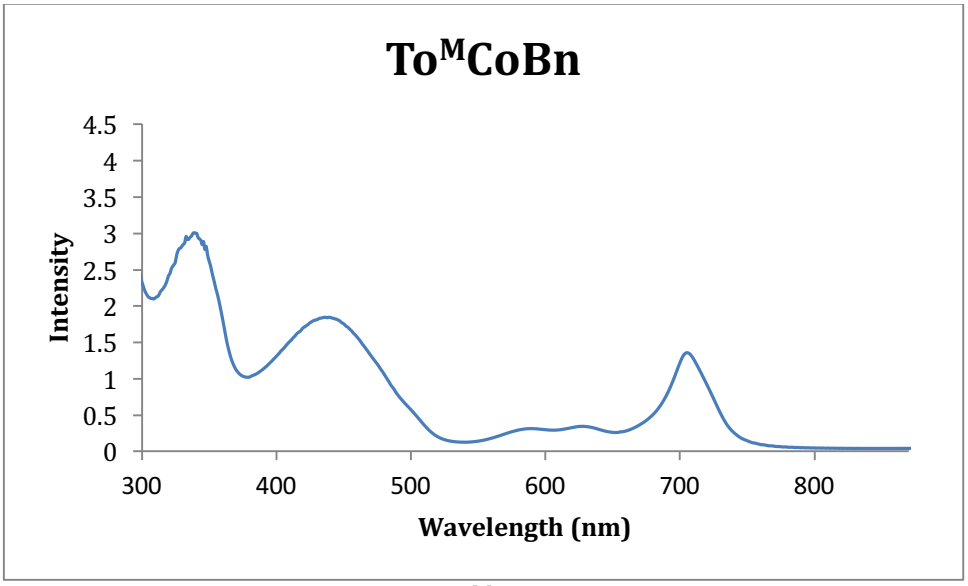


Figure S47. UV-Vis spectrum of To^{M}CoBn (**1**) in Et_2O.

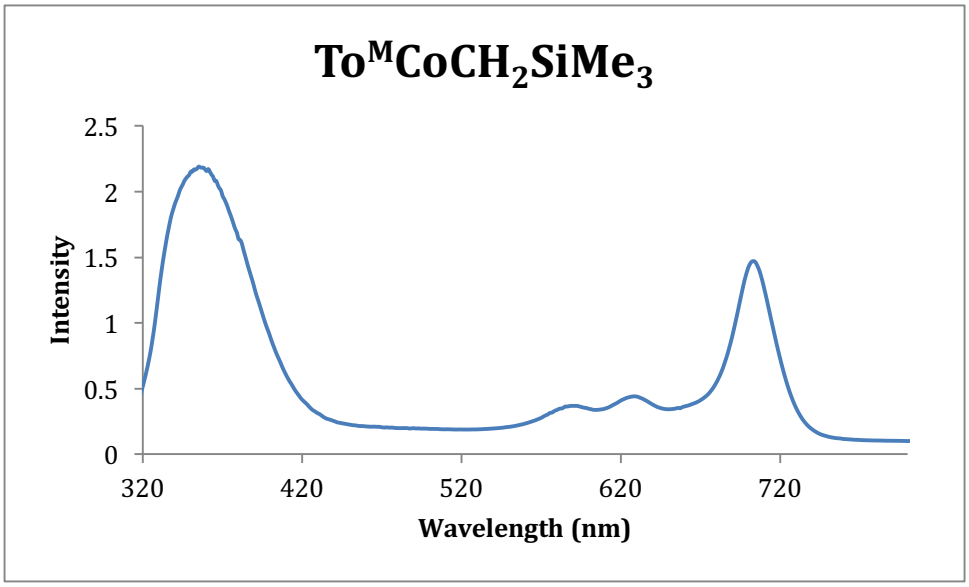


Figure S48. UV-Vis spectrum of To^{M}CoCH$_2$SiMe$_3$(**2**) in Et_2O.

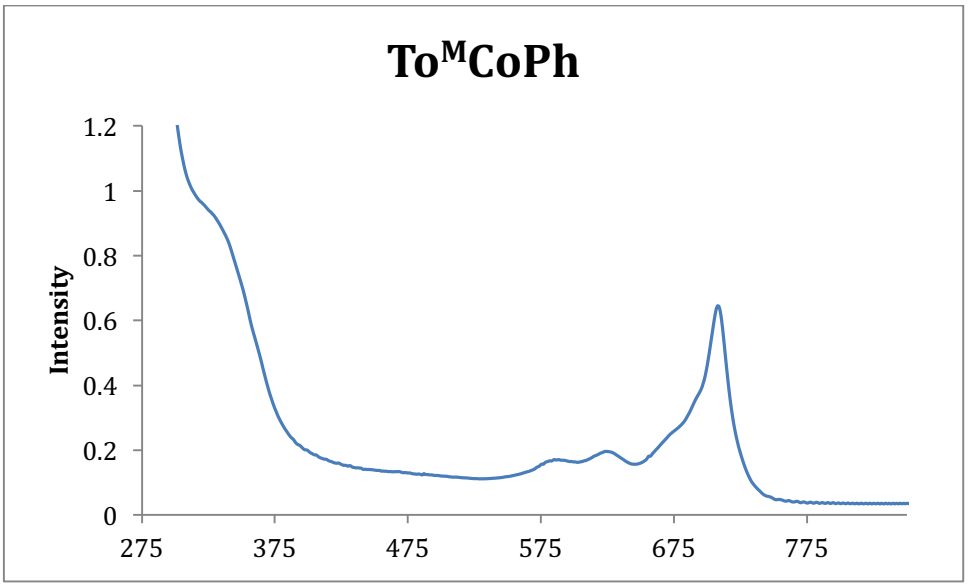


Figure S49. UV-Vis spectrum of To^{M}CoPh (**3**) in Et_2O.

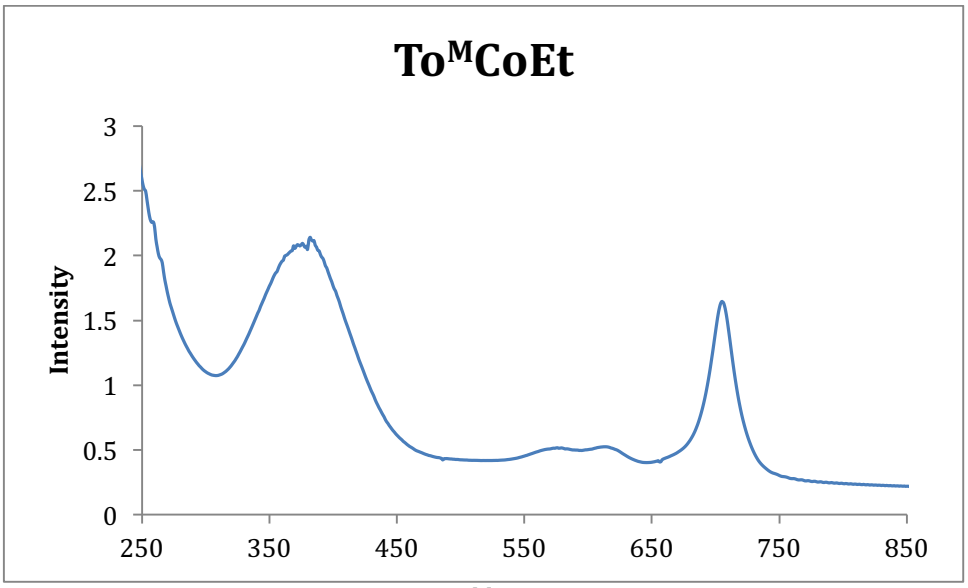


Figure S50. UV-Vis spectrum of To^{M}CoEt (**4**) in Et_2O.

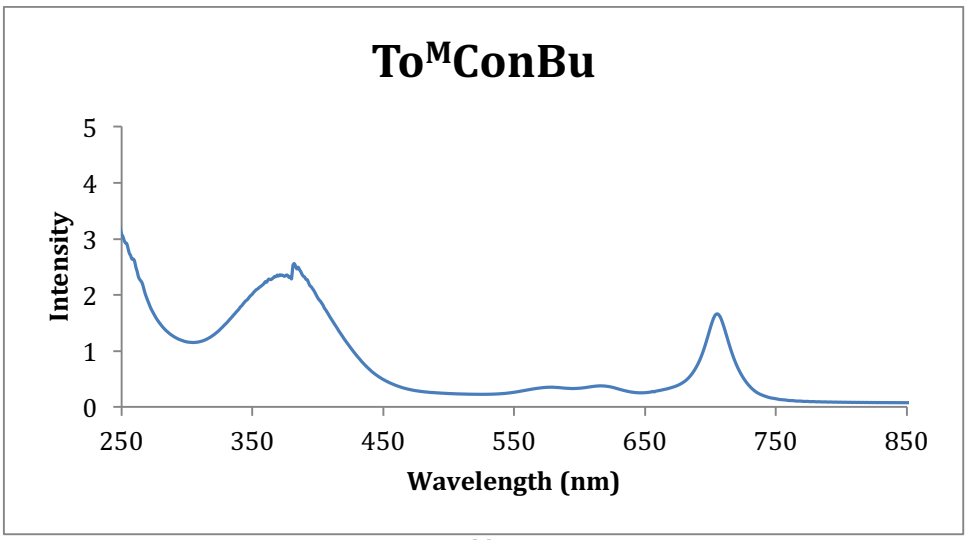


Figure S51. UV-Vis spectrum of To^{M}Co^{n}Bu (**5**) in Et_2O.

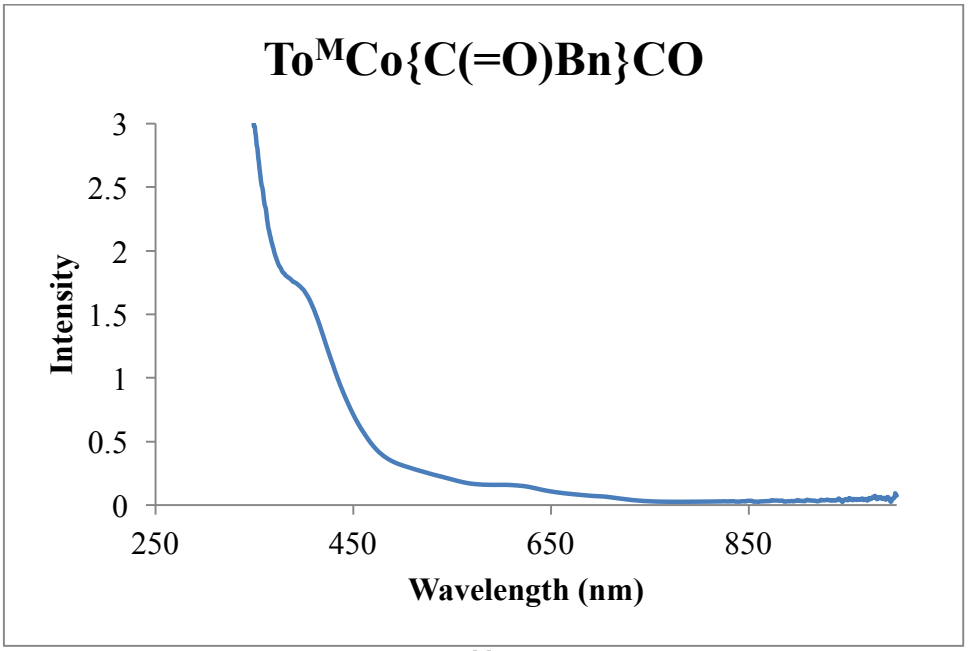


Figure S52. UV-Vis spectrum of To^{M}Co{C(=O)Bn}CO (**7**) in THF.

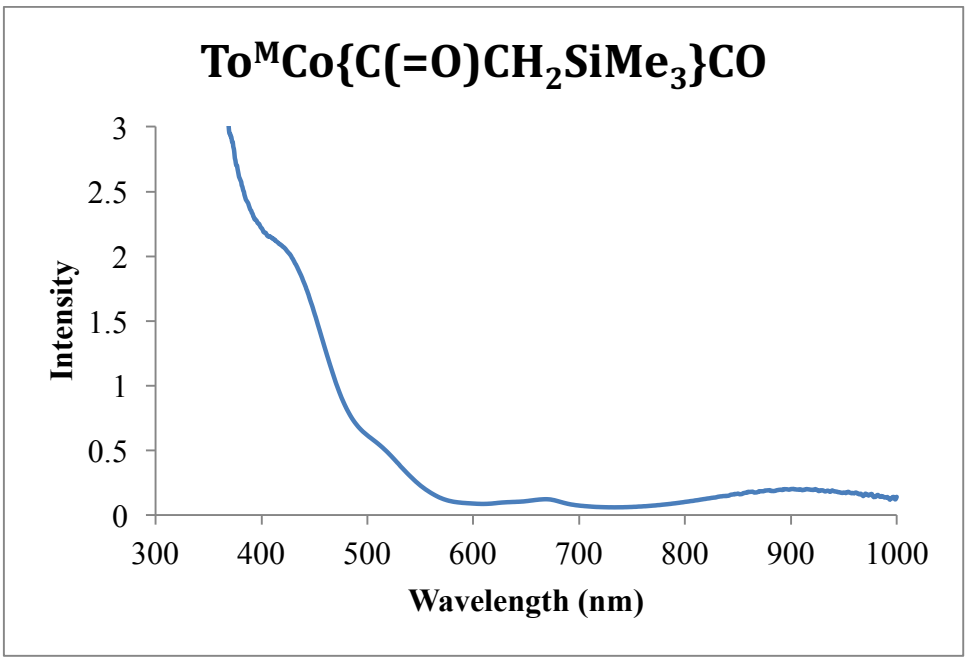


Figure S53. UV-Vis spectrum of To^{M}Co{C(=O)CH$_2$SiMe$_3$}CO (**8**) in THF.

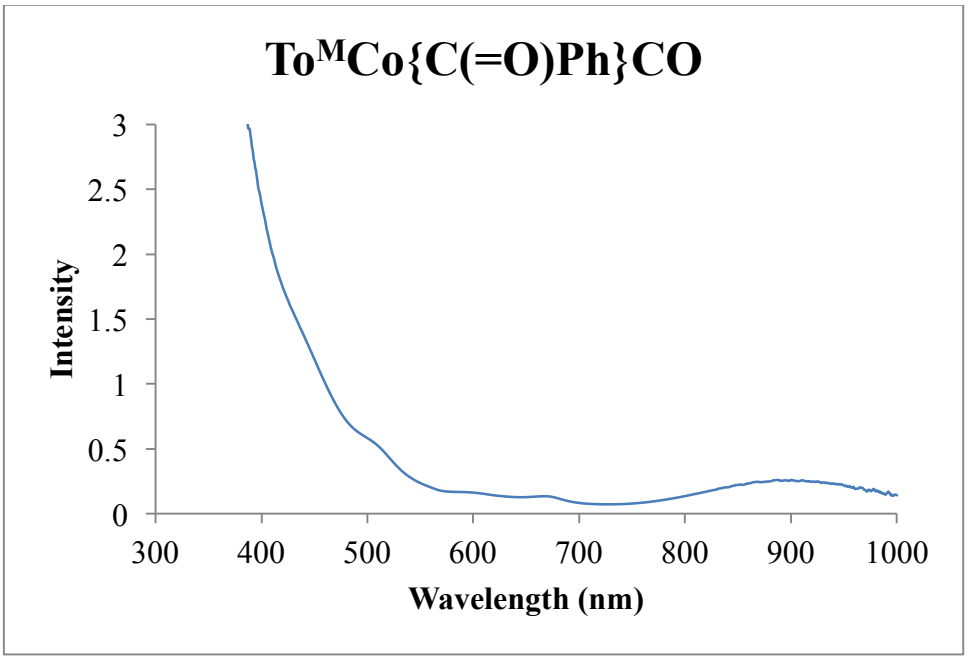


Figure S54. UV-Vis spectrum of To^{M}Co{C(=O)Ph}CO (**9**) in THF.

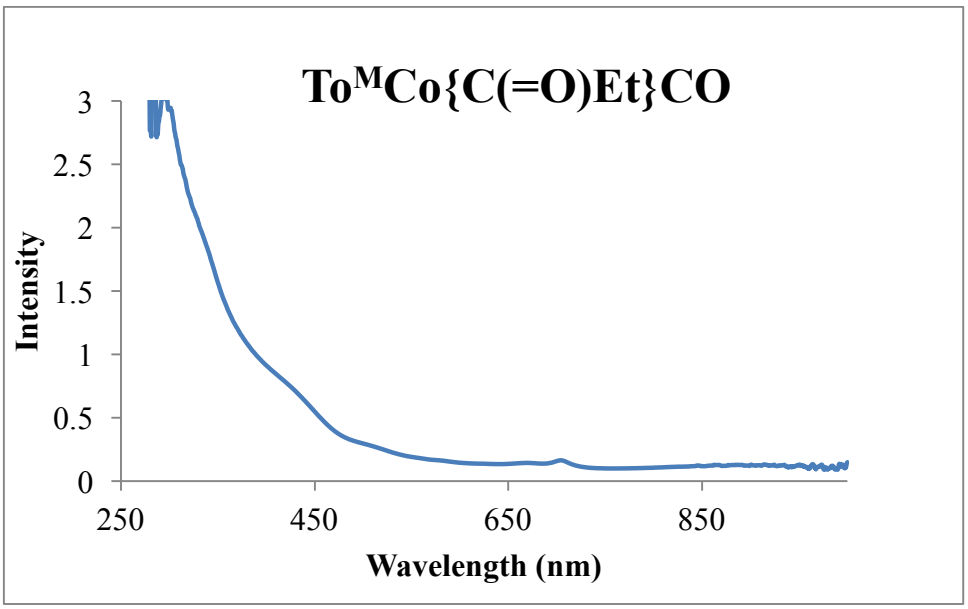


Figure S55. UV-Vis spectrum of To^{M}Co{C(=O)Et}CO (**10**) in THF.

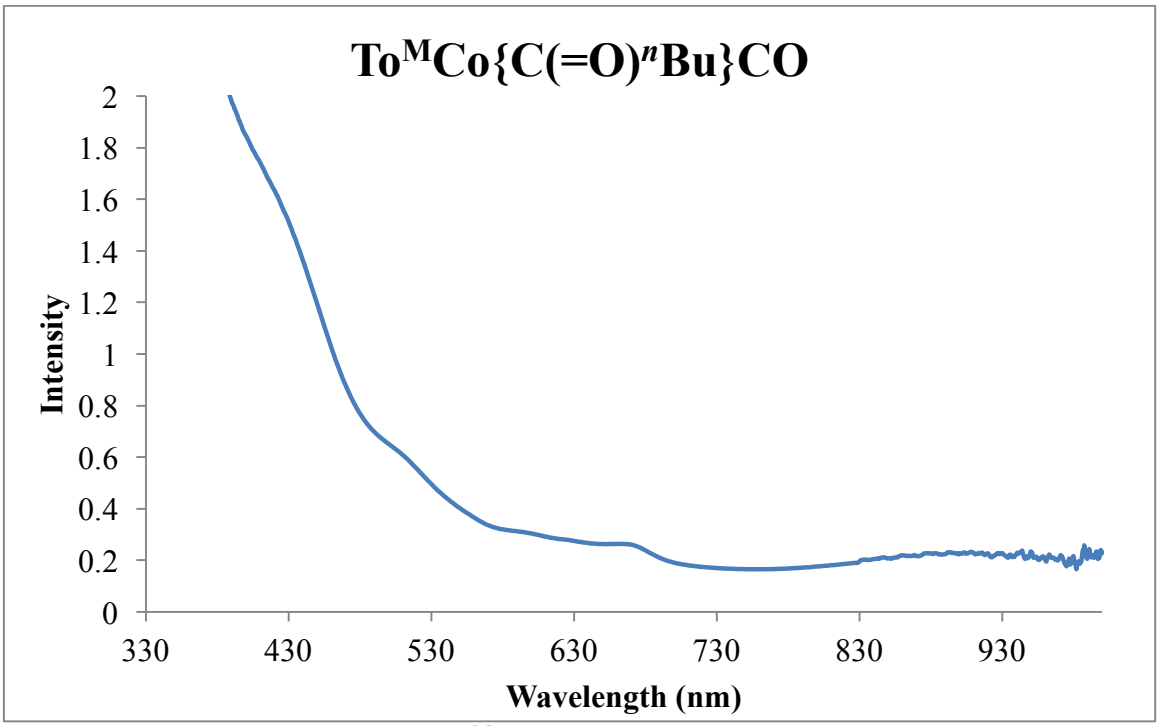


Figure S56. UV-Vis spectrum of To^{M}Co{C(=O)^{n}Bu}CO (**10**) in THF.

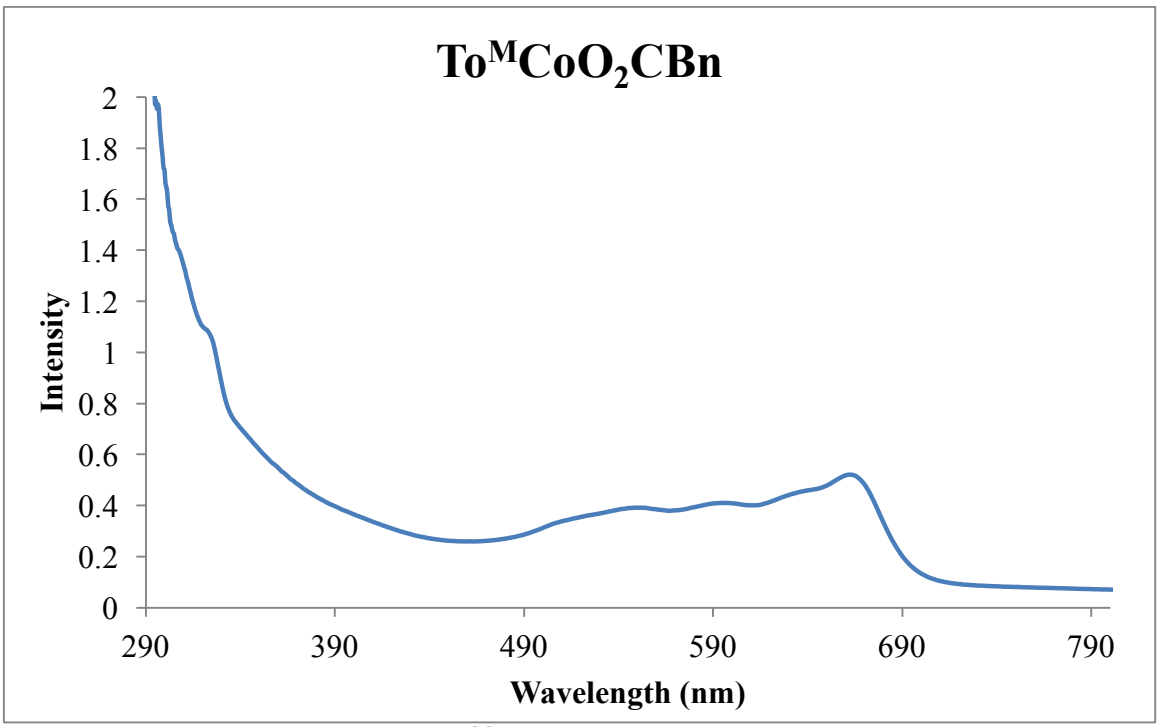


Figure S57. UV-Vis spectrum of To^{M}CoO$_2$CBn (**13**) in THF.

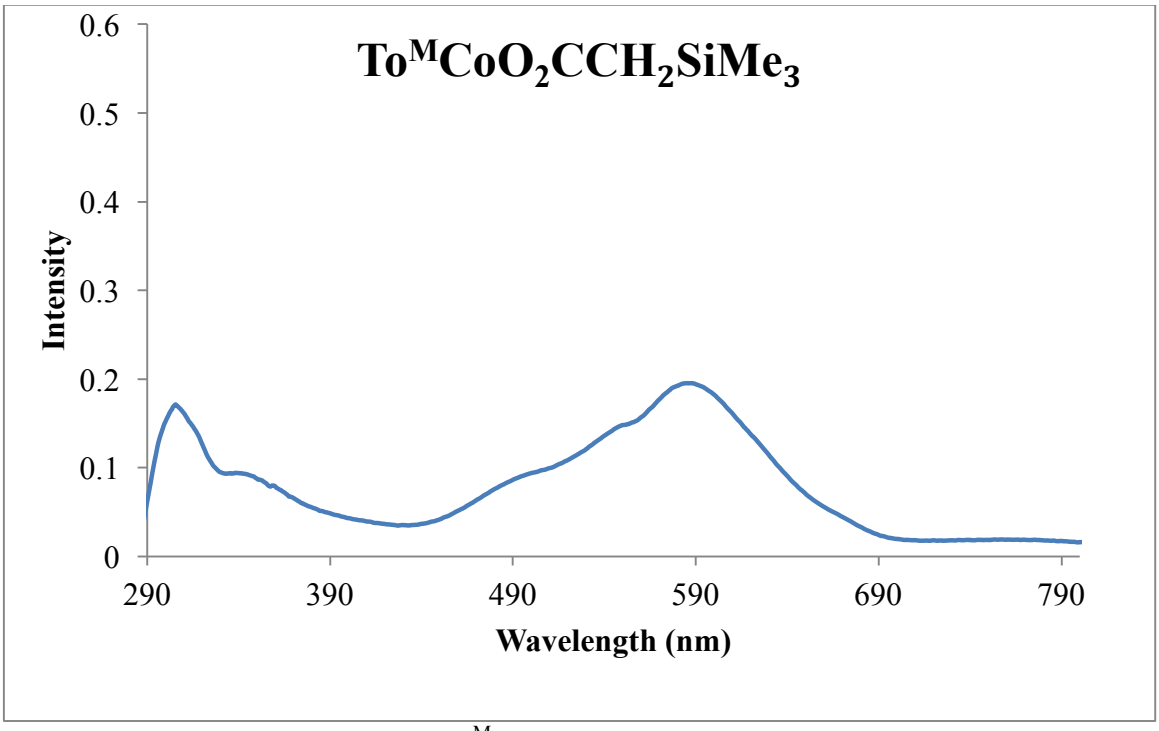


Figure S58. UV-Vis spectrum of To^{M}CoO$_2$CCH$_2$SiMe$_3$ (**14**) in THF.

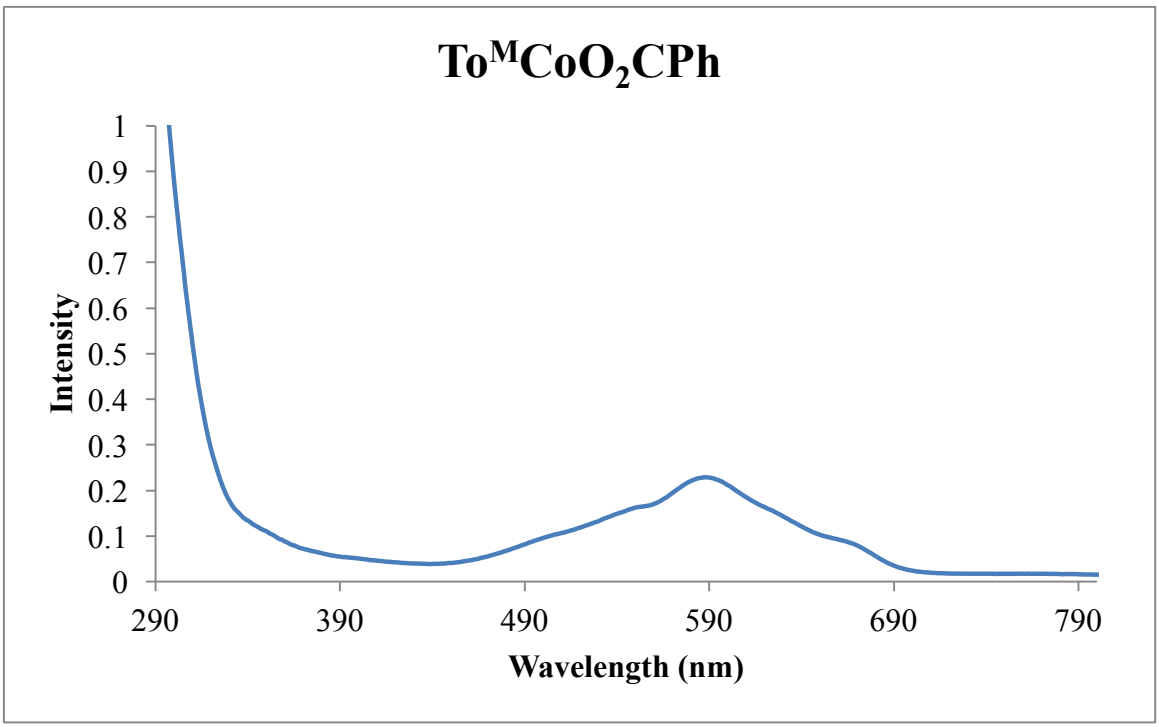


Figure S59. UV-Vis spectrum of To^{M}CoO$_2$CPh (**15**) in THF.

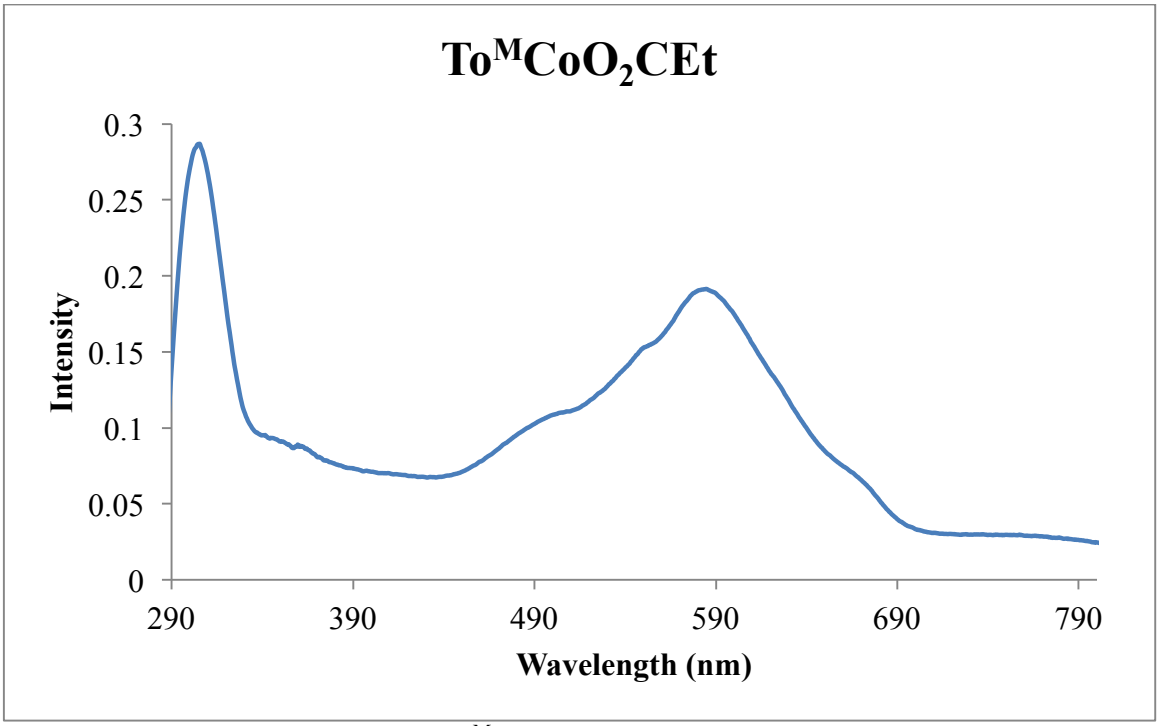


Figure S60. UV-Vis spectrum of To^{M}CoO$_2$CEt (**16**) in THF.

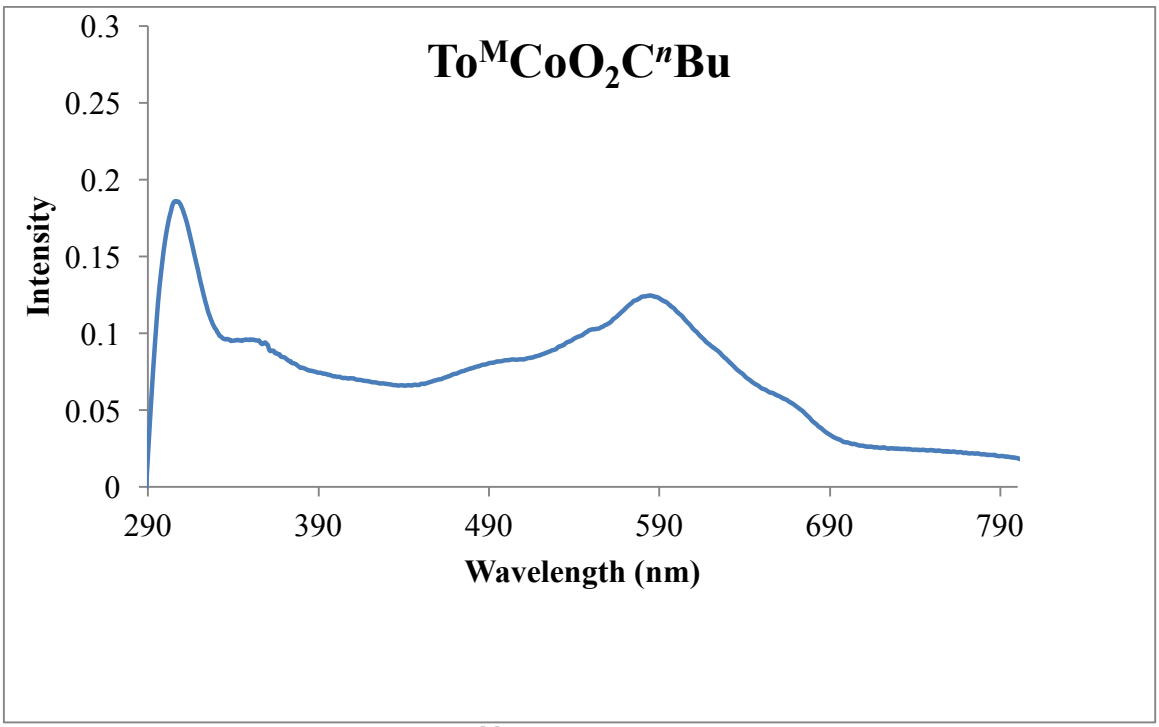


Figure S61. UV-Vis spectrum of $To^{M}CoO_2C^{n}Bu$ (**17**) in THF.

Table S1. UV-vis spectroscopic data and effective magnetic moment for compounds **1** – **6** and $To^{M}CoCl$.

Compound	**Bands, nm (ε, $M^{-1}cm^{-1}$)**				
$To^{M}CoBn$ (**1**)	339 (3205)	439 (1964)	704 (1444)	589 (332)	628 (365)
$To^{M}CoCH_2SiMe_3$ (**2**)	355 (2228)		703 (1495)	591 (374)	628 (448)
$To^{M}CoPh$ (**3**)	330 (1245)		708 (1333)	587 (176)	625 (252)
$To^{M}CoEt$ (**4**)	382 (1935)		705 (1255)	579 (268)	615 (286)
$To^{M}Co^{n}Bu$ (**5**)	382 (1679)		705 (1291)	576 (406)	613 (422)
$To^{M}CoMe$ (**6**)	346 (1412)		697 (1078)	581 (388)	617 (424)
$To^{M}CoCl$	n.a.			568 (362)	635 (641)

Table S2. Effective magnetic moment for compounds **1** – **6** and $To^{M}CoCl$. Parenthetical value is uncertainty.

Compound	**μ_{eff} (μ_B)**
$To^{M}CoBn$ (**1**)	4.2(7)
$To^{M}CoCH_2SiMe_3$ (**2**)	4.9(3)
$To^{M}CoPh$ (**3**)	4.0(1)
$To^{M}CoEt$ (**4**)	4.1(6)
$To^{M}Co^{n}Bu$ (**5**)	4.5(2)
$To^{M}CoMe$ (**6**)	4.2(2)
$To^{M}CoCl$	4.5(2)

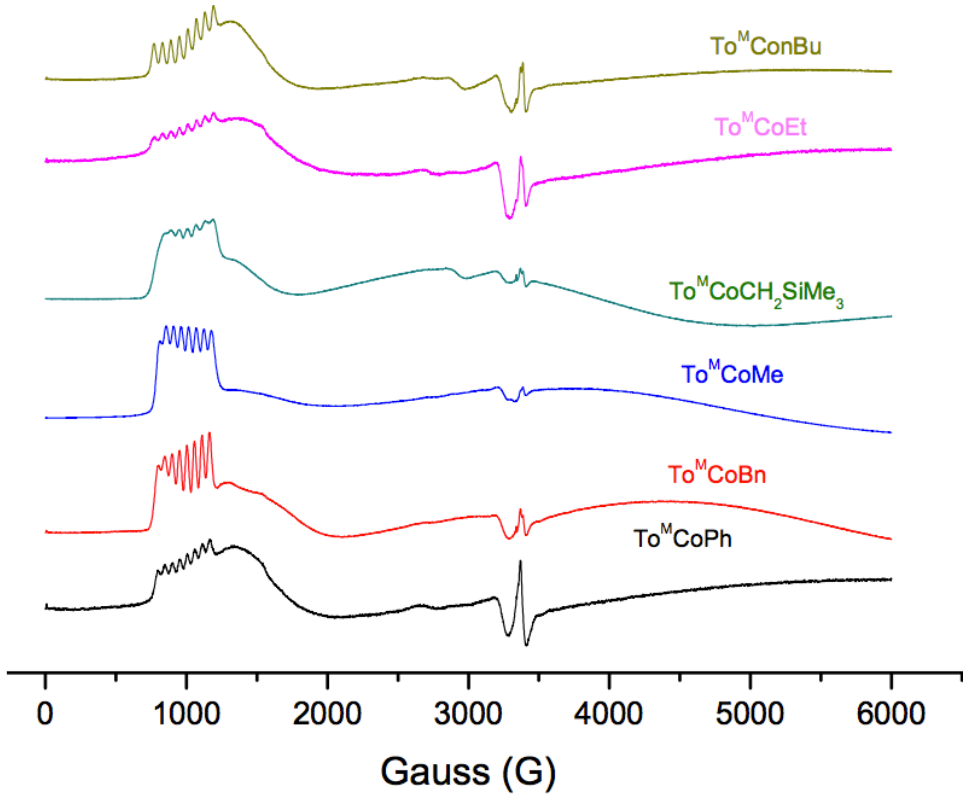


Figure S62. X-band EPR spectrum of **1 – 6** in toluene at 10 K.

Table S2. Selected interatomic distances (Å) and angles (°) for compounds **1 – 6**.

	1 (Bn)	**2 (CH_2SiMe_3)**	**3 (Ph)**	**4 (Et)**	**5 (^{n}Bu)**	**6 (Me)**
Co1-C22	2.023(2)	1.999(4)	1.996(2)	1.980(3)	2.010(3)	1.994(2)
Co1-N1	2.040(1)	2.044(3)	2.041(2)	2.046(2)	2.046(3)	2.0608(2)
Co1-N2	2.055(1)	2.062(3)	2.019(2)	2.045(2)	2.047(3)	2.0354(2)
Co1-N3	2.041(1)	2.059(3)	2.048(2)	2.046(2)	2.054(3)	2.0559(2)
N1-Co1-C22	122.94(6)	126.26(2)	121.41(9)	119.66(13)	121.34(2)	130.77(8)
N2-Co1-C22	131.33(6)	117.95(2)	121.50(9)	126.90(13)	124.37(2)	118.39(8)
N3-Co1-C22	116.37(6)	125.72(2)	128.00(1)	125.23(13)	126.29(2)	122.52(8)
N1-Co1-N2	91.68(5)	91.45(2)	92.29(9)	91.07(9)	91.23(1)	92.49(5)
N1-Co1-N3	94.00(4)	94.25(1)	91.37(9)	92.51(9)	91.52(1)	90.16(6)
N2-Co1-N3	91.00(5)	91.71(1)	92.95(9)	91.76(10)	92.39(1)	92.82(6)
B1-Co1-C22	171.3	173.8	175.6	175.4	176.9	172.8

Cartesian Coordinates and Vibrational Frequencies for Calculated Structures

Cartesian coordinates, chemical formulas, and single point energy values are provided for high spin and low spin configurations.

All energy calculations were performed using the 6-311+g* basis set and the M06-L functional using the NWChem Computational Chemistry suite. Cartesian coordinates are in units of angstroms.

Table S3. xyz-coordinates for To^{M}CoCl-calc. $CoBC_{21}ClH_{29}N_3O_3$. Calculated electronic energy for quartet (high spin) configuration is –1837.365306417430 Hartree (–1152964.383 kcal/mol); doublet (low spin) configuration is –1647.83399679521 Hartree (–1152925.089 kcal/mol). Quartet configuration is 39.29 kcal/mol lower than the doublet configuration. ZPE correction is 304.777 kcal/mol.

Atom	**x**	**y**	**z**
Co	0.11454547	1.75492296	-0.1605516
B	-0.0812329	-1.2895891	0.14367976
C	-1.6356918	1.56293704	-3.4985232
H	-1.235308	2.5434156	-3.2271296
H	-2.4136958	1.71151086	-4.2541318
H	-0.8294058	0.97638654	-3.9474485
C	-2.2013699	0.85996875	-2.2716726
C	-3.2932007	1.70304292	-1.620077
H	-3.703154	1.19923358	-0.7399397
H	-4.1126074	1.88555754	-2.3226406
H	-2.893286	2.67122111	-1.3063685
C	-2.671614	-0.5793927	-2.5739647
H	-3.7409006	-0.7328687	-2.4163951
H	-2.4059145	-0.9113264	-3.5814025
C	-1.0858449	-0.6447528	-0.9893847
C	-2.2060933	2.08670487	2.7083834
H	-2.0274807	2.97033784	2.08962707
H	-2.5931555	2.42228722	3.67580058
H	-2.9753693	1.47795328	2.22455808
C	-0.9161714	1.29290901	2.88995758
C	0.15280044	2.14635865	3.56057581
H	1.08845021	1.58996713	3.66470344

H	-0.1716094	2.46128161	4.55751233
H	0.35169455	3.0442529	2.96937507
C	-1.147736	-0.0481043	3.61758603
H	-0.4402578	-0.2197258	4.4330715
H	-2.1656728	-0.1720644	3.9923254
C	-0.4873918	-0.4593366	1.50700258
C	3.40025406	1.39027836	-1.9820693
H	2.9362858	0.84696622	-2.8098363
H	4.47323454	1.471155	-2.1832692
H	2.98280538	2.40050629	-1.9592479
C	3.15080669	0.67997113	-0.6582143
C	3.75739558	1.465076	0.5006501
H	3.31660336	2.46412787	0.55847301
H	4.83824118	1.57783811	0.36867784
H	3.57985283	0.95629388	1.45255836
C	3.61284037	-0.7935919	-0.6769315
H	3.9276045	-1.1287342	-1.6689624
H	4.403508	-1.0131071	0.04313887
C	1.41704964	-0.7205925	-0.2285615
N	-1.132036	0.60690311	-1.293305
N	-0.4403341	0.82672045	1.57842502
N	1.70595767	0.51846503	-0.4332223
O	-1.9642167	-1.4149129	-1.6384747
O	-0.9195079	-1.063767	2.62131036
O	2.45278981	-1.5610925	-0.3049655
C	-0.1113964	-2.8986421	0.16023396
C	-0.3143053	-3.6932925	1.29376116
C	-0.2867785	-5.085095	1.22833453
C	-0.0522064	-5.7280649	0.02083637
C	0.15634695	-4.9630241	-1.1224414
C	0.12584906	-3.5773058	-1.0447337
H	-0.5017655	-3.2249114	2.25257534
H	-0.4505518	-5.6678744	2.13127547
H	-0.0308099	-6.8131612	-0.0316021

H	0.34301949	-5.4487021	-2.0768284
H	0.29319078	-3.007122	-1.9563523
Cl	0.22228092	3.96228256	-0.3382602

Table S4. Calculated vibrational frequencies (cm^{-1}) for $To^{M}CoCl$-calc.

	232.64	653.33	1021.41	1360.22	1627.89
-158.3	240.62	665.81	1024.42	1389.98	1646.63
-135.65	253.27	691.58	1033.47	1409.5	1668.12
-124.55	270.26	729.78	1034.12	1413.17	1677.98
-101.73	278.79	733.32	1047.69	1414.23	3047.18
-96.38	286.08	772.81	1050.12	1415.59	3047.96
-89.93	292.71	830.66	1051.05	1423.93	3048.62
-77.36	313.02	837.07	1052.52	1431.41	3052.85
-64.73	319.06	848.81	1060.82	1435.15	3054.14
-52.63	328.65	856.32	1073.35	1439.87	3057.06
-33.17	341.49	874.81	1111.05	1452.64	3082.55
-17.81	346.31	878.22	1169.04	1490.39	3083.78
27.61	355.33	883.81	1181.72	1491.73	3084.97
28.68	361.44	916.83	1185.78	1494.3	3123.1
52.78	372.81	934.78	1193.43	1495.63	3124.56
59.84	395.36	939.61	1210.32	1503.74	3126.64
72.71	414.4	944.74	1216.42	1505.86	3129.06
85.56	416.5	947.87	1219.61	1508.34	3131.51
92.84	437.36	949.61	1221.48	1517.75	3131.91
100.85	450.15	959.13	1224.15	1518.26	3134.9
122.18	465.23	968.4	1232.63	1521.86	3135.62
138.22	478.97	978.38	1237.67	1523.66	3138.4
143.7	494.82	979.44	1267.87	1525.25	3140.36
156.42	537.98	985.28	1275.03	1533.75	3141.46
172.43	549.17	989.88	1292.5	1536.86	3143.92
189.32	613.04	1003.56	1299.01	1538.29	3144.24
218.63	626.56	1007.77	1302.36	1548	3145.81
222.6	632.05	1009.72	1324.93	1558.01	3149.88
227.88	647.08	1010.66	1343.37	1606.3	3157.11

3170.33 3185.96 3202.51 3236.09

Table S5. xyz-coordinates for To^{M}CoBn-calc (**1-calc**). $CoBC_{28}H_{36}N_3O_3$. Calculated electronic energy for quartet (high spin) configuration is –1647.914454986070 Hartree (–1034082.154 kcal/mol); doublet (low spin) configuration is –1647.839882286510 Hartree (–1034035.359 kcal/mol). Quartet configuration is 46.79 kcal/mol lower than the doublet configuration. ZPE correction is 378.84 kcal/mol.

Atom	**x**	**y**	**z**
Co	0.56059071	1.00016582	0.39428164
B	-0.23378992	-1.94594282	-0.20345713
C	-1.97640967	1.10166899	3.22896256
H	-1.39979407	0.38185811	3.81622172
H	-2.87035332	1.37280506	3.79967523
H	-1.3698367	2.00236428	3.10647544
C	-2.35437952	0.51865893	1.87472673
C	-3.11966656	1.53434701	1.03117993
H	-2.50721595	2.41633625	0.82615959
H	-4.02578903	1.86352333	1.55046759
H	-3.4165851	1.09670614	0.07359277
C	-3.12244968	-0.81145317	2.00598303
H	-3.08852844	-1.22246316	3.0197652
H	-4.16167685	-0.7535398	1.67739518
C	-1.29380556	-1.13628299	0.75417467
C	1.37702011	1.42515675	-3.30075323
H	1.68001893	2.24181573	-2.64149217
H	1.30571864	1.82321622	-4.31808403
H	2.16010571	0.66195313	-3.28484125
C	0.04179248	0.84367477	-2.85376463
C	-1.04351166	1.91515024	-2.83923329
H	-1.99994669	1.49389824	-2.51655422
H	-1.1784112	2.33934764	-3.83967611
H	-0.78062655	2.73243114	-2.16225096
C	-0.36600781	-0.38276696	-3.69596363
H	-1.31288601	-0.2526775	-4.22428389
H	0.4041202	-0.68777927	-4.40983249

C	-0.17241164	-0.99273993	-1.54036473
C	3.2587537	-0.20616889	2.75586719
H	3.13061474	0.87832101	2.70328444
H	4.25254724	-0.40883187	3.16796448
H	2.51271614	-0.60434575	3.44887916
C	3.1062062	-0.83167764	1.3762997
C	4.10969088	-0.23318175	0.39435509
H	4.00538502	-0.6875488	-0.5950518
H	5.13572438	-0.39540424	0.74014738
H	3.9533944	0.84398998	0.29243981
C	3.1837961	-2.37202068	1.41410917
H	4.05593642	-2.78077542	0.90027397
H	3.14613371	-2.77339639	2.43127772
C	1.232297	-1.75392007	0.50474797
C	-0.59580654	-3.50765894	-0.36748664
C	-0.65070678	-4.20154045	-1.58143938
H	-0.48864409	-3.67047377	-2.51177548
C	-0.91659392	-5.56847696	-1.63521559
H	-0.95311498	-6.07031437	-2.59895461
C	-1.13411788	-6.28932141	-0.46918231
H	-1.34226209	-7.35508566	-0.5095382
C	-1.07996568	-5.62711305	0.75321939
H	-1.2450944	-6.17485835	1.67762152
C	-0.81506649	-4.2648387	0.79337972
H	-0.778411	-3.77684925	1.76506809
C	1.26475186	2.83621213	0.90787652
H	1.28276618	2.85480252	2.00694934
H	2.31089941	2.8816368	0.57418235
C	0.50648506	3.99237599	0.37881557
C	-0.61377115	4.51360231	1.04741463
H	-0.89645715	4.09048096	2.00905687
C	-1.35364201	5.56749723	0.52680451
H	-2.21054239	5.94484729	1.07927684
C	-0.99896727	6.14954638	-0.6866304

H	-1.57410795	6.9758369	-1.0931304
C	0.11900051	5.66468499	-1.35842782
H	0.42734326	6.11858871	-2.29693372
C	0.85530513	4.61012054	-0.83370126
H	1.73877356	4.26213318	-1.3650821
N	-1.15096764	0.08433696	1.14276561
N	0.17135074	0.24898571	-1.51188171
N	1.74131323	-0.62727098	0.86428868
O	-0.53292416	-1.45093305	-2.74832331
O	-2.43269208	-1.72651482	1.1395206
O	2.00848477	-2.82353538	0.72170305

Table S6. Calculated vibrational frequencies (cm^{-1}) for To^{M}CoBn-calc (**1-calc**).

	150.99	418.79	780.03
-249.61	174.32	422.04	821.93
-195.85	178.32	424.2	824.62
-172.19	190.52	428.74	835.23
-159.1	208.69	452.2	853.99
-136.92	218.62	462.47	859.88
-115.53	229.15	472.16	865.19
-95.66	232.98	480.85	870.2
-89.46	242.7	485.05	881.42
-83.88	255.06	515.28	890.9
-59.3	260.39	537.29	902.42
-31.1	265.27	562.7	919.71
39.3	278.42	613.12	926.13
48.04	291.87	625.1	943.74
62.79	308.98	627.63	945.31
69.81	313.93	636.67	947.79
77.46	326.55	643.45	951.78
80.75	331.7	653.92	963.93
83.81	338.77	665.57	973.81
100.9	347.68	674.77	979.47
107.03	349.77	685.68	982.57
117.35	358.95	691.76	984.51
123.76	363.18	700.32	989.9
132.39	375.3	733.13	990.95
144.4	383.77	775.67	994.19

1000.42	1235.1	1501.51	3087.83
1006.87	1243.57	1503.65	3089.72
1008.59	1250.12	1505.59	3130.4
1012.41	1251.46	1513.74	3137.97
1017.32	1255.16	1517.05	3139.22
1019.47	1291.66	1518.67	3140.23
1022.33	1296.83	1520.78	3143.16
1028.2	1299.44	1521.41	3143.8
1030.93	1306.17	1526	3146.28
1042.49	1317.96	1528.19	3146.98
1044.41	1331.74	1532.74	3151.21
1046.76	1341.46	1538.41	3153.27
1052.21	1355.58	1545.41	3153.95
1055.64	1374.59	1567.59	3157.33
1063.15	1377.09	1609.88	3159.11
1071.44	1402.46	1625.13	3162.39
1075.46	1404.85	1636.77	3163.72
1076.13	1408.64	1639.28	3176.54
1109.73	1412.95	1661.24	3177.72
1141.37	1414.39	1667.02	3179.54
1182.02	1419.38	1672.51	3187.03
1184.3	1431.94	3024.22	3195.43
1186.55	1434.37	3058.45	3199.75
1202.66	1436.13	3060.45	3200.59
1204.77	1476.98	3062.37	3212.59
1207.11	1477.47	3062.82	3218.09
1214.89	1489.8	3066.41	3247.7
1219.82	1492.92	3068.76	
1225.94	1493.82	3076.55	
1231.78	1500.4	3081.65	

Table S7. xyz-coordinates for To^{M}CoMe-calc (**6-calc**). $CoBC_{22}H_{32}N_3O_3$. Calculated electronic energy for quartet (high spin) configuration is –1418.483290970870 Hartree (–890111.894 kcal/mol); doublet (low spin) configuration is –1418.407613576880 Hartree (–890064.405 kcal/mol). Quartet configuration is 47.49 kcal/mol lower than the doublet configuration. ZPE correction is 326.67 kcal/mol.

Atom	**x**	**y**	**z**
Co	0.15651852	1.94540046	-0.2417756
B	-0.0844536	-1.1474657	0.1672626

C	-1.9458514	1.64555321	-3.3799921
H	-1.5125583	2.62858554	-3.1769621
H	-2.7952476	1.78264459	-4.0570793
H	-1.1926265	1.04092551	-3.8923659
C	-2.3870118	0.97861342	-2.0838946
C	-3.3994905	1.84918339	-1.3452305
H	-3.7249667	1.36818558	-0.4183671
H	-4.2830242	2.03062372	-1.9658608
H	-2.9585922	2.81689809	-1.090726
C	-2.9057504	-0.4580846	-2.305056
H	-3.9610008	-0.5868653	-2.0558298
H	-2.7316088	-0.8204712	-3.3225228
C	-1.1776181	-0.5059881	-0.8772316
C	-1.9075551	2.29084949	2.84088158
H	-1.7920062	3.15549687	2.1817113
H	-2.2012054	2.65472525	3.83086781
H	-2.7182307	1.66959471	2.4495833
C	-0.6044594	1.50061836	2.91796817
C	0.51989748	2.36691325	3.47076398
H	1.46261182	1.81345801	3.49486408
H	0.29117119	2.7001312	4.48826316
H	0.66132848	3.25397638	2.84758853
C	-0.7687999	0.18015372	3.6976593
H	0.03053946	0.01305959	4.42532645
H	-1.7346905	0.08297365	4.19757934
C	-0.3378738	-0.2778046	1.53891183
C	3.2709706	1.39959246	-2.3202379
H	2.7128933	0.87813844	-3.1026024
H	4.32471987	1.43475003	-2.6153123
H	2.90045772	2.42673092	-2.2647776
C	3.10616189	0.69982722	-0.9779595
C	3.84272754	1.45864468	0.1223799
H	3.44279624	2.47141285	0.2224168
H	4.91094521	1.53546276	-0.1052048

H	3.73283738	0.95228099	1.08566807
C	3.51244551	-0.7879537	-1.0320584
H	3.69006655	-1.1422087	-2.0518315
H	4.37951189	-1.0291366	-0.4138829
C	1.38032276	-0.6270536	-0.3605754
N	-1.2263964	0.73568063	-1.2133748
N	-0.2543083	1.00630952	1.57794734
N	1.68184764	0.59591162	-0.6252624
O	-2.1358354	-1.2775382	-1.4098725
O	-0.6793662	-0.8548284	2.70309952
O	2.38195578	-1.5051447	-0.5098297
C	0.298957	3.93037902	-0.4845057
C	-0.1480519	-2.7561844	0.22818691
C	-0.2428615	-3.5206029	1.39631093
C	-0.2507145	-4.9139401	1.36386075
C	-0.1612512	-5.5901181	0.15501154
C	-0.0617029	-4.8561194	-1.0228772
C	-0.0555931	-3.4686073	-0.9772215
H	-0.3163031	-3.0258643	2.35741011
H	-0.3276166	-5.4717682	2.29389097
H	-0.1678191	-6.6764396	0.12807535
H	0.01108102	-5.3676816	-1.9793681
H	0.0241079	-2.9233074	-1.9155161
H	1.09116343	4.38056125	0.13203464
H	-0.6267241	4.4636784	-0.2211536
H	0.5260448	4.21506298	-1.5224372

Table S8. Calculated vibrational frequencies (cm^{-1}) for To^{M}CoMe-calc (**6-calc**).

	-78.35	5.47	79.66
-148.67	-60.12	32.74	94.17
-130.42	-48.61	46.98	103.94
-121.93	-34.57	59.55	121.73
-103.87	-11.32	64.61	143.9
-92.14			

154.06	610.58	1018.39	1405.2
156.11	616.13	1022.01	1408.44
164.21	621.23	1024.35	1414.1
174.54	630.56	1031.55	1415.14
185.58	634.1	1036.12	1421.97
188.05	637.81	1038.76	1431.22
198.49	650.64	1045.62	1433.18
205.16	679.39	1050.37	1434.82
226.44	688.29	1057.07	1476.88
243.69	694.58	1059.28	1479.2
257.16	730.83	1075.55	1479.41
264.86	772.5	1111.48	1491.42
275.79	820.81	1183.64	1493.65
285.82	836.66	1192.07	1494.22
295.55	847.92	1198.36	1501.76
304.74	868.56	1204.74	1506.06
316.52	879.34	1213.89	1507.72
326.46	887.17	1214.71	1514.35
328.76	892.05	1224.45	1516.21
344.94	929.85	1227.95	1520.05
351.02	936.42	1233.2	1523.27
355.46	941.39	1240.4	1528.73
366.73	945.55	1241.08	1531.16
374.9	947.45	1245.98	1537.59
398.08	948.53	1258.55	1546.92
416.17	961.73	1285.38	1550.61
417.67	971.7	1290.44	1566.53
435.34	979.73	1301.19	1615.33
454.25	987.97	1304.37	1636.21
471.88	990.19	1319.02	1639.38
477.72	1000.05	1325.37	1666.71
483.14	1007.07	1342.55	1693.98
502.39	1008.41	1386.38	3003.66
509.87	1009.99	1391.77	3058.02

3058.82	3089.4	3150.65	3199.86
3059.75	3136.74	3153.56	3211.31
3064.66	3138.06	3153.95	3247.81
3064.83	3139.16	3154.78	
3067.06	3139.68	3158.82	
3073.79	3143.08	3161.44	
3076.01	3144.13	3163.17	
3082.99	3145.67	3176.81	
3089.24	3148.25	3186.55	

Table S9. xyz-coordinates for To^{M}Co(Me)CO-calc (**12a-calc**). $CoBC_{23}H_{32}N_3O_4$. Calculated electronic energy for doublet (low spin) configuration is –1531.844720748800 Hartree (–961247.280 kcal/mol); quartet (high spin) configuration is –1531.7887097632 Hartree (–961212.132 kcal/mol); doublet configuration is 35.15 kcal/mol lower than the quartet configuration. ZPE correction is 334.292 kcal/mol.

Atom	**x**	**y**	**z**
Co	0.18895951	1.80355962	0.20859267
B	-0.0003142	-1.3552262	-0.1256967
C	-3.6577186	1.36572856	0.66204991
H	-3.3258988	2.34803735	0.31806156
H	-4.6386217	1.48919393	1.13307444
H	-3.77747	0.72094877	-0.213457
C	-2.6590894	0.76263196	1.64836538
C	-2.521271	1.64268236	2.88069384
H	-1.762211	1.24840182	3.56097389
H	-3.4722496	1.69386715	3.42143611
H	-2.2354992	2.66060266	2.60862157
C	-3.0409832	-0.6826519	2.01716623
H	-2.8492312	-0.9095052	3.07147812
H	-4.0736385	-0.9427625	1.77691571
C	-1.2148165	-0.698856	0.73353062
C	3.04540154	0.90224625	2.75681712
H	2.63092017	1.88211944	2.99030916
H	4.08126838	0.87977618	3.1119579
H	2.48021024	0.1496752	3.31426915

C	3.00437946	0.60756285	1.25823266
C	3.74622578	1.67613225	0.4674928
H	3.70214136	1.46793183	-0.6051518
H	4.79970047	1.71285336	0.76357443
H	3.31755478	2.66552591	0.64142288
C	3.56841724	-0.7979742	0.97691435
H	4.21395222	-0.8283111	0.09279739
H	4.10184455	-1.2319765	1.82428855
C	1.38131339	-0.7837984	0.52042556
C	-1.3984666	1.78393423	-3.2513495
H	-2.160226	1.0252742	-3.0507959
H	-1.4723706	2.07356921	-4.3046999
H	-1.6298059	2.6635324	-2.6486031
C	-0.002956	1.24281286	-2.9458166
C	1.06606842	2.28402566	-3.2381709
H	0.88805342	3.20046308	-2.6693617
H	1.0683067	2.54955298	-4.3001716
H	2.05951566	1.90889746	-2.9779074
C	0.24839262	-0.0731829	-3.6980399
H	-0.4206957	-0.2341878	-4.5445737
H	1.2865404	-0.1756307	-4.0319122
C	0.00506855	-0.5090009	-1.5192541
N	-1.3660746	0.5553729	0.96332616
N	1.60961843	0.45951339	0.7742402
N	0.06313519	0.77720136	-1.5437083
O	-2.174658	-1.5036488	1.22490737
O	2.41973705	-1.6097274	0.70530824
O	-0.000892	-1.0991552	-2.7255678
C	0.51659335	2.94588732	1.80726631
C	-0.10646	-2.9584755	-0.1950404
C	0.27741808	-3.728444	0.91221374
C	0.12828431	-5.1096384	0.9417095
C	-0.419718	-5.7750193	-0.1497163
C	-0.8165216	-5.0384389	-1.2582449

C	-0.6625675	-3.6544541	-1.2751288
H	0.70808069	-3.2383321	1.7818744
H	0.44073458	-5.6693055	1.81982529
H	-0.5377361	-6.8551754	-0.1339611
H	-1.2505914	-5.5421901	-2.1184226
H	-0.9819177	-3.1110021	-2.1577488
C	-0.6961484	3.23655439	-0.2426695
O	-1.261331	4.20651674	-0.458594
H	0.50856316	2.24577846	2.64444104
H	1.50897232	3.40489848	1.73044498
H	-0.1824665	3.75343505	2.0438029

Table S10. Calculated vibrational frequencies (cm^{-1}) for $To^{M}Co(Me)CO$-calc (**12a-calc**).

151.32	351	636.97	953.71	1112.02
-126.33	168.69	356.47	652.79	967.25	1188.21
-114.59	187.76	359.62	681.34	975.57	1198.48
-90.32	189.75	367.18	699.04	983.81	1203.73
-69.14	204.04	377.81	709.24	986.64	1206.55
-47.89	207.09	384.06	730.43	990.57	1212.61
-39.78	217.11	401.54	762.85	992.06	1216.39
-28.9	224.74	418.45	775.71	1004.62	1222.36
-19.67	237.93	447.71	819.26	1007.89	1226.52
-4.13	247.47	459.7	828.19	1011.05	1234.04
4.73	249.61	469.46	834.22	1015.59	1239.01
16.86	259.36	483.43	851.98	1020.96	1245.08
36.06	260.12	494.17	860.77	1021.73	1248.1
50.03	272.2	494.76	869.64	1040.11	1260.27
59.27	277.21	511.32	872.44	1042.63	1286.75
67.43	287.2	523.64	876.89	1047.69	1296.94
82.47	297.54	543.76	921.27	1050.28	1298.81
97.77	305.33	615.83	932.31	1052.95	1307.48
104.11	312.62	623.66	939.57	1056.88	1326.21
125.78	323.24	628.78	947.79	1065.59	1339.63
139.33	343.65	631.25	951.53	1078.08	1348.55

1377.46	1485.36	1527.95	3061.55	3139.88	3170.62
1405.03	1493.37	1530.52	3062.67	3143.5	3185.21
1409.01	1495.77	1532.05	3064.07	3144.2	3192.93
1411.46	1496.61	1537.07	3067.34	3147.29	3196.17
1414.45	1502.74	1540.46	3069.07	3147.77	3205.9
1416.69	1503.51	1615.07	3070.51	3151.87	3215.51
1418.18	1512.15	1637.61	3077.2	3153.1	3237.35
1432.73	1515.07	1641.43	3080.47	3158.72	
1434.35	1515.87	1670.42	3080.88	3160.27	
1436.73	1517.89	1674.59	3125.24	3162	
1468.36	1520.06	2030.6	3137.75	3164.61	
1476.95	1522.37	3044.59	3138.9	3168.03	

Table S11. xyz-coordinates for To^{M}Co{(C=O)Me}CO-calc (**12c-calc**). $CoBC_{24}H_{32}N_3O_5$. Calculated electronic energy for doublet (low spin) configuration is –1645.196497983730 Hartree (–1032376.60 kcal/mol); quartet (high spin) configuration is –1645.133273682140 Hartree (–1032336.936 kcal/mol); doublet configuration is 39.67 kcal/mol lower than the quartet configuration. ZPE correction is 340.177 kcal/mol.

Atom	**x**	**y**	**z**
Co	0.00457031	1.66928008	-0.0702197
B	0.07960781	-1.5100017	-0.0794258
C	-3.7233323	1.57353909	0.64370148
H	-3.3186138	2.54852565	0.92590027
H	-4.7671378	1.54545447	0.97298879
H	-3.7109536	1.4997161	-0.4468366
C	-2.9358281	0.44107389	1.27918959
C	-2.9006248	0.58807133	2.79967738
H	-2.3446091	-0.236263	3.2555426
H	-3.9173032	0.5785838	3.20672639
H	-2.4292715	1.52410137	3.099527
C	-3.4984481	-0.9340809	0.89436855
H	-4.0955665	-1.4040551	1.67752914
H	-4.0795901	-0.9049858	-0.0349543
C	-1.3067438	-0.8891752	0.49424341
C	2.78766589	1.60805434	2.6456827

H	2.50522254	2.64929256	2.49875016
H	3.7939657	1.60112791	3.07836297
H	2.11092611	1.15023579	3.37246954
C	2.79621211	0.82064342	1.33995169
C	3.59808017	1.55356637	0.26846241
H	3.65373351	0.95891354	-0.6484658
H	4.62020345	1.73856023	0.61532692
H	3.13919131	2.51693492	0.03558332
C	3.34251625	-0.5982109	1.59589868
H	4.2953813	-0.7946142	1.09945729
H	3.44179127	-0.8245132	2.66139173
C	1.31299133	-0.7546662	0.66522419
C	-1.1259669	1.10214812	-3.7236063
H	-1.8313758	0.28327721	-3.5554697
H	-1.0606168	1.28108394	-4.801727
H	-1.5350889	2.00317441	-3.2634251
C	0.25002967	0.75578034	-3.1574976
C	1.24477308	1.87956926	-3.4048675
H	0.89128229	2.82101913	-2.9757871
H	1.38923002	2.03997996	-4.4780867
H	2.21632437	1.65045052	-2.9596281
C	0.74319665	-0.5914488	-3.7097863
H	0.23324705	-0.9108642	-4.6197535
H	1.82558271	-0.6084296	-3.8752002
C	0.20669876	-0.83494	-1.5545919
N	-1.5507402	0.34836018	0.74893743
N	1.43553212	0.52154704	0.81738787
N	0.13620594	0.4397907	-1.716836
O	-2.3385953	-1.7383808	0.66490395
O	2.36342175	-1.4863555	1.04882609
O	0.44644762	-1.5390499	-2.6715246
C	0.35085187	3.0727064	1.17985062
C	0.11106508	-3.1122663	0.0591664
C	0.29064213	-3.6820599	1.32772045

C	0.25378026	-5.0550337	1.53571453
C	0.03076316	-5.915	0.46526493
C	-0.1561187	-5.3794878	-0.8021362
C	-0.1176689	-4.0007582	-0.997309
H	0.46552882	-3.0349927	2.18459802
H	0.39957937	-5.4560102	2.53557116
H	0.00101622	-6.9902677	0.61926148
H	-0.3341824	-6.0378963	-1.6486979
H	-0.2677439	-3.6162585	-2.0001157
C	-0.3167562	3.19504359	2.52490579
O	1.20807385	3.85736695	0.8323658
H	-0.2996303	2.23519746	3.04444193
H	-1.3679384	3.4629666	2.3753822
H	0.16665092	3.96806782	3.12861428
C	-1.0466294	2.89557525	-0.7889372
O	-1.7120803	3.71951773	-1.2108068

Table S12. Calculated vibrational frequencies (cm^{-1}) for $To^{M}Co\{(C=O)Me\}CO$-calc (**12c-calc**).

	59.45	221.88	345.69
-152.28	78.85	231.43	349.94
-141.49	83.62	235.43	359.7
-129.6	92.71	240.4	364.87
-95.87	100.9	249.79	369.93
-76.21	107.42	258.66	388.74
-66.41	124.13	268.44	419.05
-47.71	136.29	286.87	429.72
-36.24	142.15	293.67	436.29
1.69	153.87	302.64	446.67
3.42	173.42	306.91	459.24
28.97	176.24	311.95	460.89
39.39	189.5	322.7	472.96
44.56	203.58	331.88	489.59
50.7	207.59	335.33	505.2

514.29	995.18	1336.03	1641.25
528.88	1002.6	1338.12	1670.03
565.82	1007.33	1364.87	1679.62
609.1	1009.34	1375.17	1731.6
617.7	1014.28	1388.98	2117.71
625.82	1018.64	1405.71	3056.2
632.27	1022.58	1412.31	3060.57
634.8	1028.77	1415.26	3063.51
659.79	1037.75	1420.34	3064.19
679.88	1050.16	1422.22	3065.59
683.44	1053.3	1433.1	3068.07
705.74	1056.62	1435.88	3068.79
730.23	1060.91	1454.95	3070.7
773.51	1072.51	1473.98	3082.09
805.27	1076.08	1476.16	3086.72
822.72	1112.37	1477.27	3131.15
828.96	1142.94	1491.17	3137.85
846.23	1181.28	1493.57	3138.32
863.3	1193.37	1497.6	3139.52
875.19	1200.9	1500.16	3141.55
879.3	1210.12	1506.13	3142.25
912.68	1213.4	1509.27	3142.91
922.41	1226.36	1515.68	3147.29
941.06	1227.28	1516.49	3148.68
945.38	1228.27	1519.47	3153.4
948.95	1231.67	1523.08	3158.66
952.91	1240.18	1525.97	3160.67
956.4	1242.77	1528.72	3167.03
958.02	1258.43	1531.23	3173.55
976.91	1293.85	1537.22	3175.82
980.52	1295.37	1538.99	3178.61
984.6	1299.06	1553.38	3182.99
989.77	1307.74	1612.09	3188.61
992.05	1310.96	1631.34	3195.58

3197.93 3232.16

3212.07

Table S13. xyz-coordinates for To^{M}Co{(C=O)Et}CO-calc (**10c-calc**). $CoBC_{25}H_{34}N_3O_5$. Calculated electronic energy for doublet (low spin) configuration is –1682.825750973980 Hartree (–1055989.327 kcal/mol); quartet (high spin) configuration is –1682.771754515140 Hartree (–1055955.444 kcal/mol); doublet configuration is 33.88 kcal/mol lower than the quartet configuration. ZPE correction is 358.392 kcal/mol.

Atom	**x**	**y**	**z**
Co	-0.3260752	-1.4852775	-0.0490225
B	-0.0415979	1.68169689	0.08691172
C	-3.4018743	-1.4366609	1.76834679
H	-3.1418107	-2.3985689	1.31761146
H	-4.4385142	-1.5048615	2.11317325
H	-2.7607999	-1.2836447	2.64079952
C	-3.2385697	-0.3034581	0.76721781
C	-4.0887132	-0.5412681	-0.4798514
H	-3.9702835	0.28123331	-1.1907897
H	-5.147696	-0.6098318	-0.210153
H	-3.8159912	-1.4681969	-0.9860477
C	-3.5556402	1.06803	1.38396418
H	-4.5100355	1.48745155	1.06231141
H	-3.5139847	1.05906785	2.47849727
C	-1.5249022	1.13287079	0.45295975
C	0.12289914	-1.4437062	-3.7930296
H	0.32711628	-2.4331782	-3.3773408
H	0.44977647	-1.4536321	-4.8378573
H	-0.957043	-1.272221	-3.7787683
C	0.86531407	-0.3713578	-3.0171416
C	2.36237335	-0.6726612	-2.9651332
H	2.90141201	0.14881365	-2.4827335
H	2.76210594	-0.7931046	-3.978051
H	2.54678917	-1.5840608	-2.3964744
C	0.61366993	1.03597736	-3.5688694
H	1.41392446	1.4115479	-4.2081084

H	-0.3444127	1.11689115	-4.0965824
C	0.29268727	1.03730202	-1.3663148
C	1.24933898	-1.8809747	3.28853345
H	0.24444051	-1.6081543	3.62306452
H	1.88674438	-1.9735373	4.17398596
H	1.2049309	-2.8641136	2.81955934
C	1.8140012	-0.8322851	2.34446716
C	3.1502986	-1.2738119	1.75072098
H	3.04811287	-2.1614306	1.12800133
H	3.86175919	-1.4934301	2.55407071
H	3.57408166	-0.4809835	1.12762666
C	1.96988738	0.51711041	3.05618787
H	1.3180809	0.60970604	3.93249273
H	2.99677563	0.74761993	3.34328413
C	0.83049339	0.8231864	1.16545093
N	-1.8198469	-0.1180087	0.39044377
N	0.34324336	-0.1929969	-1.5945128
N	0.86078572	-0.4665797	1.26078522
O	-2.5052152	1.92616355	0.91415024
O	0.54377091	1.86338174	-2.3993113
O	1.54067969	1.48140216	2.09024262
C	0.86875123	-3.0099366	-0.1388194
C	0.23501323	3.26647544	0.11738223
C	1.5578475	3.73228168	0.09553069
C	1.86634254	5.0855937	0.04327772
C	0.84721226	6.0317502	0.00828217
C	-0.4726707	5.60087442	0.02091001
C	-0.7690015	4.2407341	0.07298211
H	2.3774817	3.01785445	0.11830734
H	2.90574932	5.40381622	0.02852259
H	1.08121991	7.09217787	-0.0318251
H	-1.2817074	6.32647514	-0.0108855
H	-1.8109891	3.94064331	0.08252146
O	1.88245738	-3.0429075	-0.7914258

C	0.44889903	-4.2446456	0.66733617
C	1.5901649	-5.1749129	1.0445745
H	-0.2629904	-4.7708368	0.01420363
H	-0.1440232	-3.9398568	1.53732693
H	1.21451974	-6.076364	1.53645885
H	2.15263486	-5.4740768	0.15841542
H	2.29623365	-4.6919093	1.72639954
C	-1.3596821	-2.5164745	-1.0265505
O	-2.0008891	-3.1860051	-1.6920105

Table S14. Calculated vibrational frequencies (cm^{-1}) for $To^{M}Co\{(C=O)Et\}CO$-calc (**10c-calc**).

	140.87	329.85	633.09
-137.63	149.43	335.37	642.78
-132.47	163.65	340.28	651.21
-125.85	171.88	352.32	671.84
-119.03	186.18	357.33	694.07
-114.08	196.38	366.45	701.23
-89.47	201.28	372.32	726.2
-80.44	213.48	393.4	731.85
-78.26	217.99	414.9	774.11
-68.76	230.2	422.27	789.93
-44.79	235.62	426.67	818.91
-31.07	240.5	455.9	833.84
29.46	250.04	460.35	834.99
45.63	251.95	477.96	857.28
54.9	257.17	481.31	861.35
62.63	274.33	501.92	868.3
77.09	283.13	511.89	879.56
81.61	294.11	529.93	895.56
91.08	297.74	544.2	924.3
102.74	303.12	606.86	930.46
112.07	306.23	622.45	943.71
117.35	320.84	626.62	947.21
129.11			

954.04	1216.61	1491.49	3065.75
957.32	1219.19	1492.73	3066.55
962.02	1221.26	1495.08	3068.69
981.84	1231.81	1499.92	3071.98
982.79	1235.01	1503.59	3076.21
985.08	1240.32	1506.53	3076.46
990.13	1249.82	1513.97	3098.92
996.82	1254.51	1515.84	3130.33
1000.3	1284.94	1516.77	3135.41
1003.33	1291.51	1517.56	3136.35
1006.76	1295.16	1518.27	3139.48
1007.32	1298.12	1521.24	3139.75
1010.69	1315.54	1525.52	3144.18
1012.8	1317.62	1531.52	3148.06
1017.91	1331.65	1531.93	3149.66
1031.69	1341.54	1532.8	3154.71
1038.52	1352.5	1536.16	3155.22
1040.97	1376.62	1539.55	3158.89
1042.9	1389.09	1602.37	3160.47
1054.4	1404.97	1634.52	3172.19
1058.77	1408.2	1639.5	3173.85
1063.67	1411.98	1661.3	3181.35
1065.18	1415.81	1670.24	3183.11
1081.77	1419.8	1772.64	3185.63
1107.27	1420.97	2119.66	3190.26
1113.88	1437.49	3050.63	3193.8
1186.24	1442.57	3056.44	3194.12
1200.31	1448.44	3059.97	3208.49
1203.48	1471.92	3062.56	3233.6
1206.02	1476.51	3063.66	