Supplementary Information

Synthesis, Structure, and Characterizations of a Heterobimetallic Heptanuclear Complex [$Pb_2Co_5(acac)_{14}$]

Yuxuan Zhang[1], Zheng Wei[1], Evgeny V. Dikarev[1*]

[1]*Department of Chemistry, University at Albany, State University of New York, Albany, NY, 12222, USA*

*Author to whom correspondence should be addressed.

E-mail: edikarev@albany.edu

Table of Content

1. Direct Analysis in Real Time Mass Spectrometry (DART-MS) of $[Pb_2Co_5(acac)_{14}]$

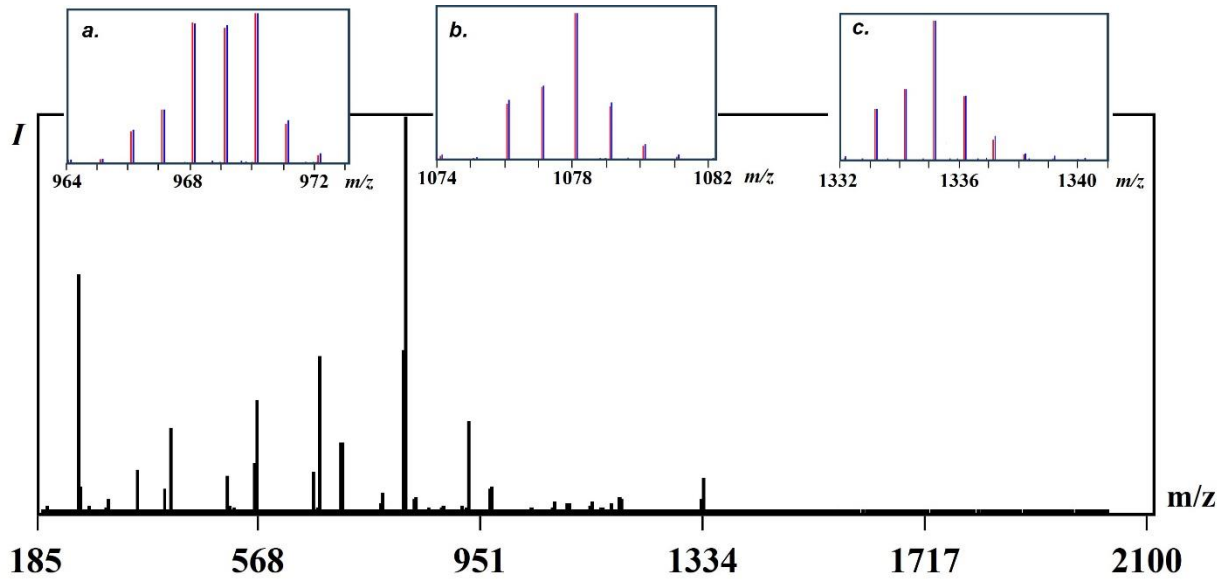

Figure S1. DART-MS spectrum of $[Pb_2Co_5(acac)_{14}]$ in a positive mode. The isotope distribution patterns for *a)* $[Pb_2Co(acac)_5]^+$, *b)* $[PbCo_3(acac)_7]^+$, and *c)* $[PbCo_4(acac)_9]^+$ peaks are shown in the inset. Blue and red lines are experimental and calculated patterns, respectively.

Table S1. Assignment of ions detected in a positive-ion DART mass spectrum of $[Pb_2Co_5(acac)_{14}]$ (acac = $C_5H_7O_2$). All ions having relative intensity higher than 2% are shown in the table.

Ions	Measured, *m/z*	Calculated, *m/z*	*Δ*	% Base
$[PbCo_4(acac)_9]^+$	1335.1158	1335.1109	0.0049	8.76
$[PbCo_3(acac)_7]^+$	1078.0908	1078.0885	0.0023	3.00
$[Pb_2Co(acac)_5]^+$	970.1122	970.1095	0.0027	6.41
$[Co_4(acac)_7]^+$	929.0517	929.0450	0.0067	22.88
$[PbCo_2(acac)_5]^+$	821.0725	821.0661	0.0064	100
$[Pb_2(acac)_3]^+$	713.0949	713.0871	0.0078	17.71
$[Co_3(acac)_5]^+$	672.0242	672.0226	0.0016	39.28
$[PbCo(acac)_3]^+$	564.0454	564.0437	0.0017	28.20
$[Co_2(acac)_3]^+$	415.0054	415.0002	0.0052	21.25
$[HPb(acac)_2]^+$	407.0775	407.0737	0.0038	6.05
$[HCo(acac)_2]^+$	258.0373	258.0302	0.0051	60.13

2. ATR-IR Spectrum of $[Pb_2Co_5(acac)_{14}]$

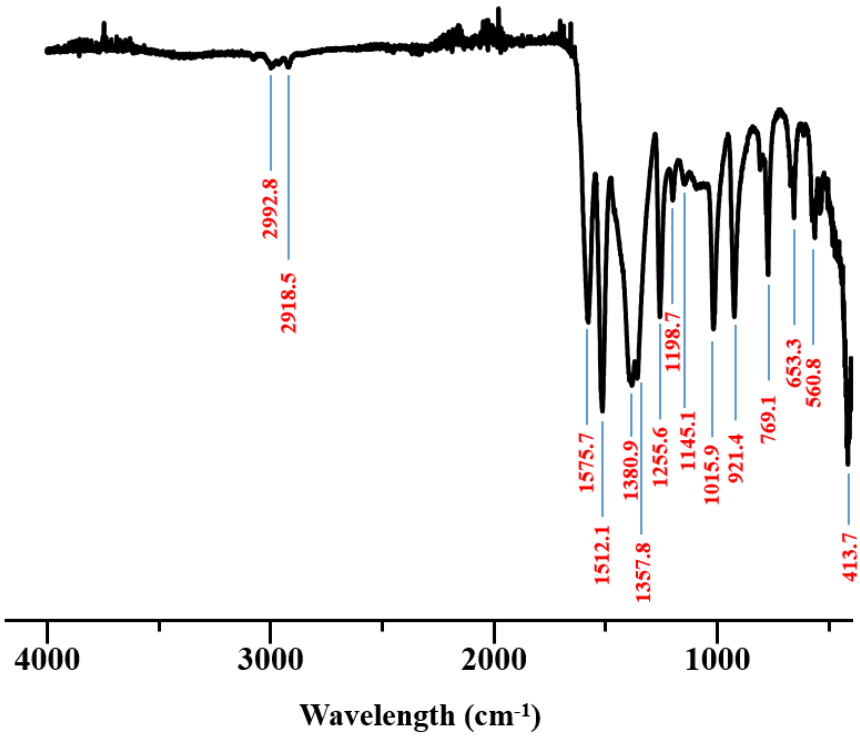

Figure S2. The attenuated total reflection (ATR) spectrum of $[Pb_2Co_5(acac)_{14}]$.

3. Crystal Structure of $[Pb_2Co_5(acac)_{14}]$

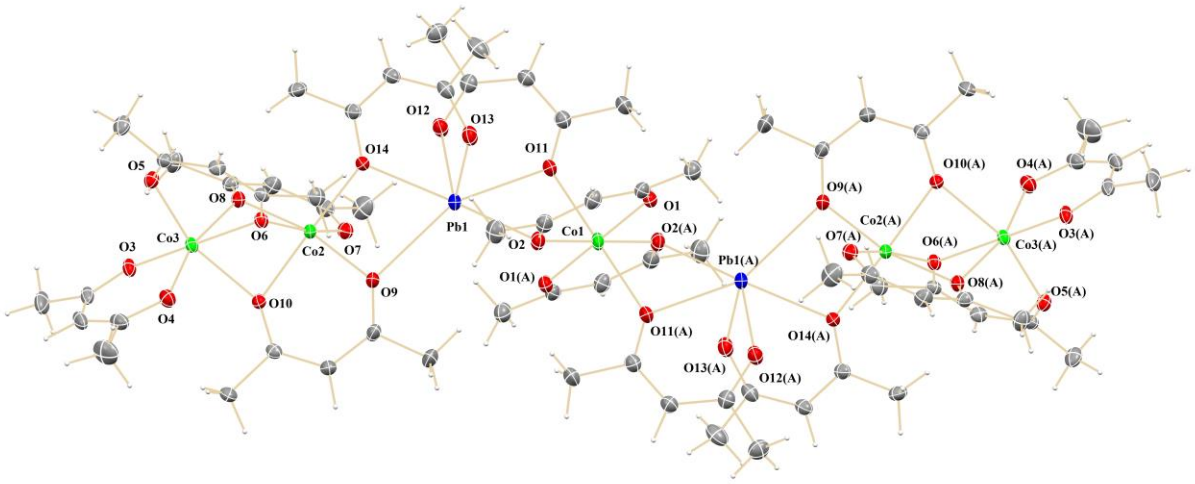

Figure S3. Crystal structure of $[Pb_2Co_5(acac)_{14}]$. The Pb, Co, O and C atoms are represented by thermal ellipsoids at the 40% probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

Table S2. Bond distances (Å) and angles (°) in the structure of $[Pb_2Co_5(acac)_{14}]$.

Bond distances							
Pb(1)-O(2)*	2.7904(15)	Co(1)-O(1)	2.0127(15)	Co(2)-O(6)*	2.0911(14)	Co(3)-O(3)	1.9813(14)
Pb(1)-O(9)*	2.8581(14)	Co(1)-O(2)**	2.0186(14)	Co(2)-O(7)	2.0483(15)	Co(3)-O(4)	2.0193(15)
Pb(1)-O(11)**	2.4844(14)	Co(1)-O(11)*	2.2638(15)	Co(2)-O(8)**	2.0589(14)	Co(3)-O(5)	2.0509(14)
Pb(1)-O(12)	2.3402(16)			Co(2)-O(9)**	2.0241(14)	Co(3)-O(6)**	2.0355(13)
Pb(1)-O(13)	2.3458(17)			Co(2)-O(10)**	2.0726(14)	Co(3)-O(8)*	2.1957(14)
Pb(1)-O(14)**	2.4905(14)			Co(2)-O(14)*	2.0965(15)	Co(3)-O(10)*	2.2186(13)

Angles					
O(2)-Pb(1)-O(9)	94.74(4)	O(6)-Co(2)-O(14)	94.02(6)	O(3)-Co(3)-O(4)	91.67(7)
O(11)-Pb(1)-O(2)	65.72(5)	O(7)-Co(2)-O(6)	167.65(6)	O(3)-Co(3)-O(5)	96.19(6)
O(11)-Pb(1)-O(9)	156.36(5)	O(7)-Co(2)-O(8)	88.82(6)	O(3)-Co(3)-O(6)	173.09(6)
O(11)-Pb(1)-O(14)	138.95(5)	O(7)-Co(2)-O(10)	103.29(6)	O(3)-Co(3)-O(8)	95.95(6)
O(12)-Pb(1)-O(2)	137.70(5)	O(7)-Co(2)-O(14)	86.22(6)	O(3)-Co(3)-O(10)	100.54(6)
O(12)-Pb(1)-O(9)	126.85(5)	O(8)-Co(2)-O(6)	79.34(5)	O(4)-Co(3)-O(5)	91.54(6)
O(12)-Pb(1)-O(11)	75.06(5)	O(8)-Co(2)-O(10)	78.19(6)	O(4)-Co(3)-O(6)	94.40(6)
O(12)-Pb(1)-O(13)	86.58(6)	O(8)-Co(2)-O(14)	107.65(6)	O(4)-Co(3)-O(8)	165.62(6)
O(12)-Pb(1)-O(14)	76.05(5)	O(9)-Co(2)-O(6)	103.07(6)	O(4)-Co(3)-O(10)	94.31(6)
O(13)-Pb(1)-O(2)	70.57(5)	O(9)-Co(2)-O(7)	89.26(6)	O(5)-Co(3)-O(8)	99.71(6)
O(13)-Pb(1)-O(9)	109.43(5)	O(9)-Co(2)-O(8)	166.11(6)	O(5)-Co(3)-O(10)	162.09(5)
O(13)-Pb(1)-O(11)	77.67(5)	O(9)-Co(2)-O(10)	88.87(6)	O(6)-Co(3)-O(5)	86.94(6)
O(13)-Pb(1)-O(14)	72.07(5)	O(9)-Co(2)-O(14)	85.94(6)	O(6)-Co(3)-O(8)	77.42(5)
O(14)-Pb(1)-O(2)	125.65(5)	O(10)-Co(2)-O(6)	77.84(5)	O(6)-Co(3)-O(10)	75.75(5)
O(14)-Pb(1)-O(9)	62.93(4)	O(10)-Co(2)-O(14)	169.12(6)	O(8)-Co(3)-O(10)	72.34(5)
O(1)-Co(1)-O(2)	91.33(6)				
O(1)-Co(1)-O(2A)	88.67(6)				
O(1)-Co(1)-O(11)	81.37(6)				
O(1)-Co(1)-O(11A)	98.63(6)				
O(2)-Co(1)-O(11A)	84.09(6)				
O(2)-Co(1)-O(11)	95.91(6)				

* – bridging oxygen; ** – chelating-bridging oxygen.

Symmetry code: (A) -*x*+1, -*y*+1, -*z*+1

4. Crystal Structure of [PbCo(acac)$_4$]

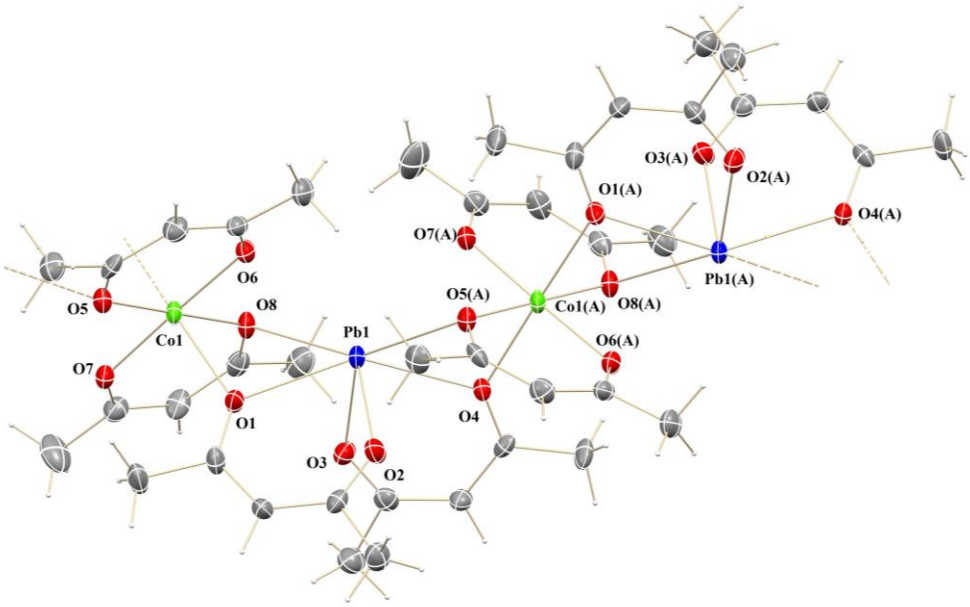

Figure S4. Fragment of the solid-state structure of polymeric [PbCo(acac)$_4$] drawn with thermal ellipsoids at the 40% probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

Table S3. Bond distances (Å) and angles (°) in the structure of [$PbCo(acac)_4$].

Bond distances			
Pb(1)-O(1)**	2.517(6)	Co(1)-O(1)*	2.237(6)
Pb(1)-O(2)	2.315(7)	Co(1)-O(4A)*	2.218(6)
Pb(1)-O(3)	2.310(6)	Co(1)-O(5)**	2.036(6)
Pb(1)-O(4)**	2.512(6)	Co(1)-O(6)	2.031(6)
Pb(1)-O(5A)*	2.884(6)	Co(1)-O(7)	2.017(6)
Pb(1)-O(8)*	2.860(6)	Co(1)-O(8)**	2.036(7)
Angles			
O(1)-Pb(1)-O(5A)	124.55(19)	O(4A)-Co(1)-O(1)	179.0(2)
O(1)-Pb(1)-O(8)	64.58(2)	O(5)-Co(1)-O(1)	94.7(2)
O(2)-Pb(1)-O(1)	74.3(2)	O(5)-Co(1)-O(4A)	85.5(2)
O(2)-Pb(1)-O(4)	81.0(2)	O(6)-Co(1)-O(1)	82.1(2)
O(2)-Pb(1)-O(5A)	70.4(2)	O(6)-Co(1)-O(4)	96.9(2)
O(2)-Pb(1)-O(8)	133.13(18)	O(6)-Co(1)-O(5)	90.3(3)
O(3)-Pb(1)-O(1)	79.0(2)	O(6)-Co(1)-O(8)	89.1(3)
O(3)-Pb(1)-O(2)	79.7(2)	O(7)-Co(1)-O(1)	96.5(2)
O(3)-Pb(1)-O(4)	75.0(2)	O(7)-Co(1)-O(4A)	84.5(2)
O(3)-Pb(1)-O(5A)	132.26(19)	O(7)-Co(1)-O(5)	90.5(3)
O(3)-Pb(1)-O(8)	71.42(2)	O(7)-Co(1)-O(6)	178.5(2)
O(4)-Pb(1)-O(1)	146.9(2)	O(7)-Co(1)-O(8)	90.1(3)
O(4)-Pb(1)-O(5A)	64.34(18)	O(8)-Co(1)-O(1)	84.9(2)
O(4)-Pb(1)-O(8)	123.75(19)	O(8)-Co(1)-O(4)	94.9(2)
O(5A)-Pb(1)-O(8)	153.59(18)	O(8)-Co(1)-O(5)	179.3(3)

* – bridging oxygen; ** – chelating-bridging oxygen.

Symmetry codes: (A) *x*, -*y*+1/2, *z*-1/2