Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

Structure investigations of group 13 organometallic carboxylates

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X-ray Structure Determination

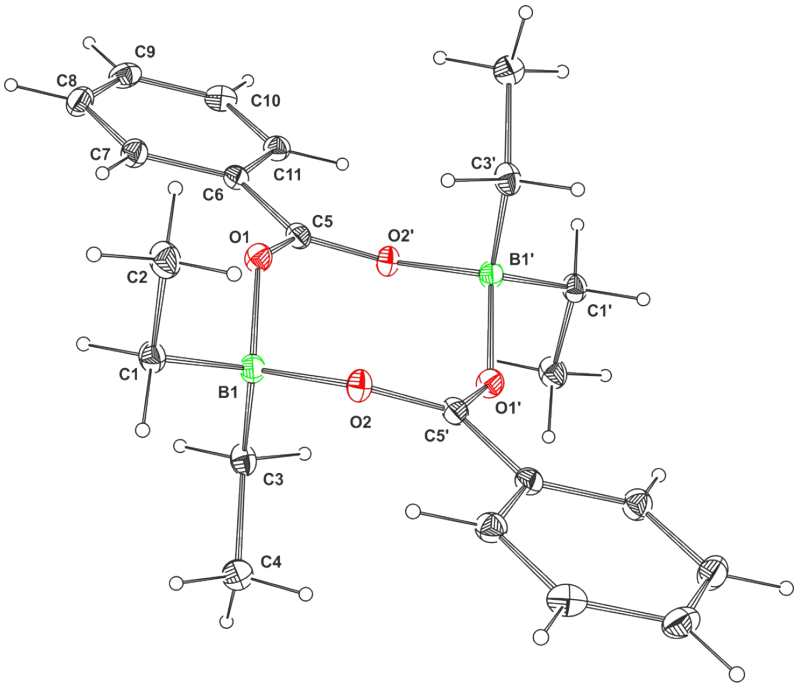

Figure 1S. Molecular structure of **1** with thermal ellipsoids set at 35% probability. Atoms labeled with a prime belong to the centrosymmetric counterpart of the dimeric units with the symmetry code: (*-x+1, -y+1, -z*).

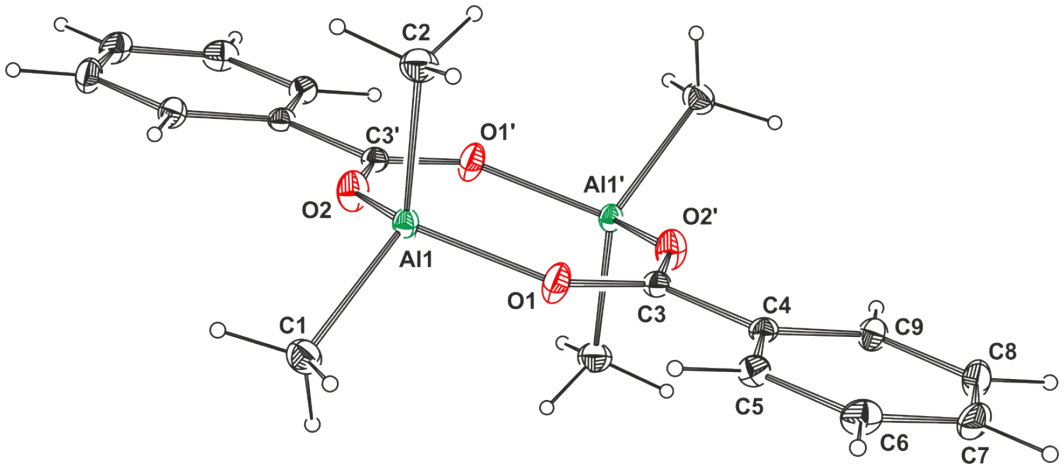

Figure 2S. Molecular structure of **2** with thermal ellipsoids set at 35% probability. Atoms labeled with a prime belong to the centrosymmetric counterpart of the dimeric units with the symmetry code: (*-x+1, -y+2, -z+1*).

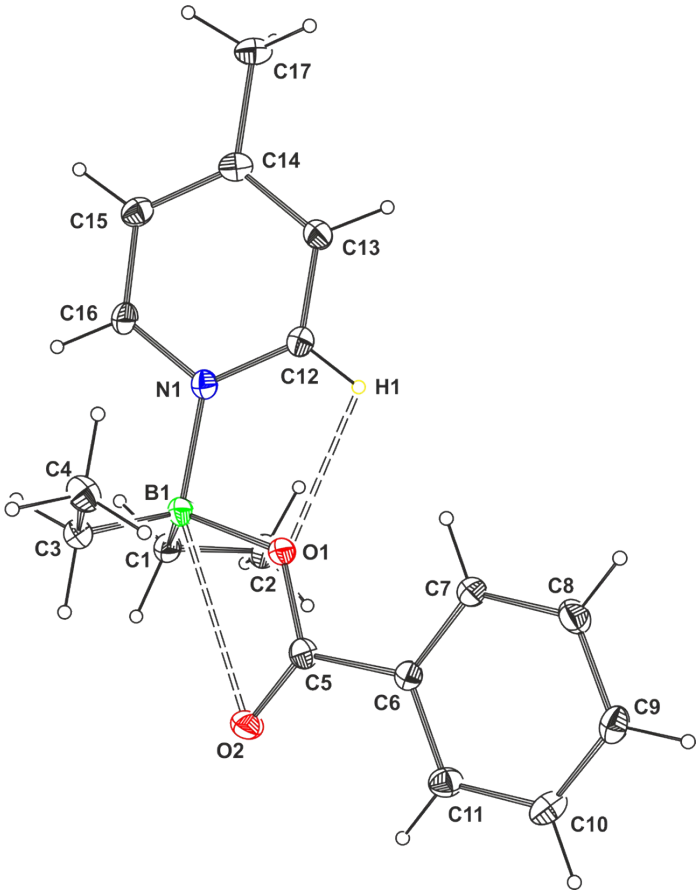

Figure 3S. Molecular structure of **4** with thermal ellipsoids set at 35% probability.

Table 1S. Selected Intra- and Intermolecular bond lengths (Å) and angles (deg) for comp. **4**.

contact	H···A	D···A	D–H···A	symmetry
C12–H12···O1	2.31	2.706(2)	104	*x, y, z*
C29–H29···O3	2.30	2.700(2)	104	*x, y, z*
C13–H13···O2	2.50	3.328(2)	146	*-x+1,+y-1/2,-z+1/2*
C17–H17···O4	2.56	3.525(2)	168	*-x+1,+y-1/2,-z+1/2*
C30–H30···O4	2.31	3.210(2)	158	*-x+2, +y-1/2, -z+1/2*
C34–H34···O2	2.68	3.653(2)	173	*x+1, -y+1/2+1, +z+1/2*

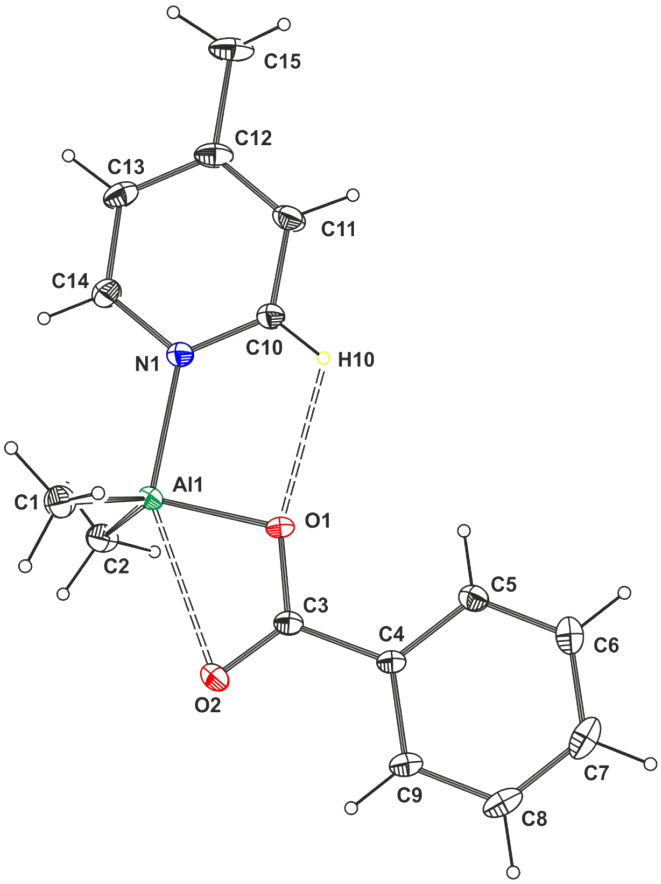

Figure 4S. Molecular structure of **5** with thermal ellipsoids set at 35% probability.

Table 2S. Selected Intra- and Intermolecular bond lengths (Å) and angles (deg) for comp. **5**.

contact	H···A	D···A	D–H···A	symmetry
C10–H10···O1	2.39	2.911(3)	115	*-x+1, -y+1, -z+1*
C9–H9···O2	2.49	3.298(3)	145	*-x+1, -y+1, z*

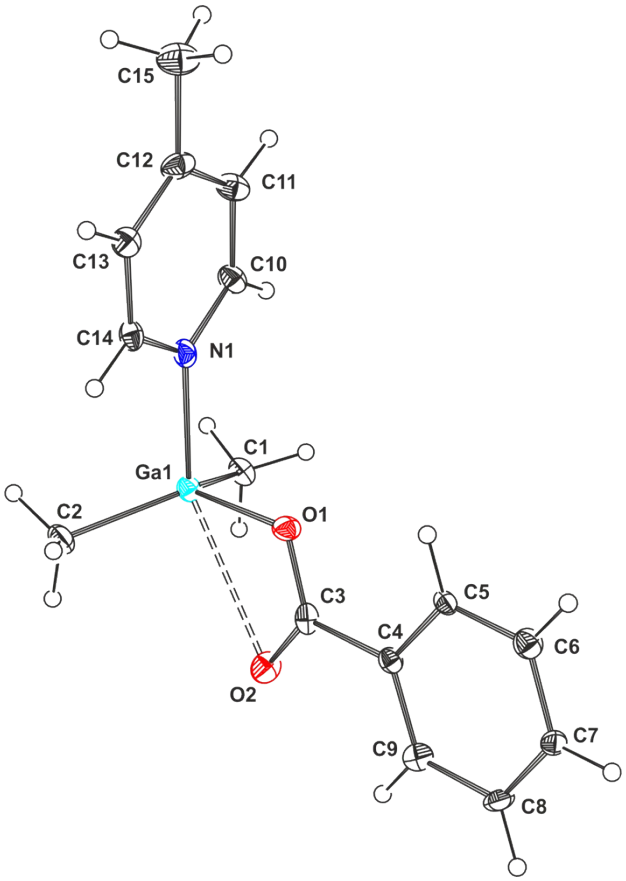

Figure 5S. Molecular structure of **6** with thermal ellipsoids set at 35% probability.

Table 3S. Selected Intra- and Intermolecular bond lengths (Å) and angles (deg) for comp. **6**.

contact	H···A	D···A	D–H···A	symmetry
C11–H11···O2	2.66	3.551(13)	157	*x-1/2, +y-1/2, +z*
C6–H6···O2	2.70	3.294(12)	121.5	*x-1/2, -y+1/2, +z-1/2*

Theoretical Section

a. Energies (Hartree) and coordinates of the calculated molecular systems

4'

E=-580.9183535

ZPE= 0.222825

C	2.04580000	-0.98939700	-0.00010700
C	3.35737800	-0.55483300	-0.00016500
C	3.61398300	0.81276800	-0.00004700
C	2.53847500	1.68914600	0.00013400
C	1.24939300	1.17729000	0.00018200
N	1.01109000	-0.13849800	0.00005100
H	4.63281900	1.18432700	-0.00010100
H	1.78805100	-2.04048000	-0.00018900
H	4.15948600	-1.28238400	-0.00030200
H	2.68223500	2.76265300	0.00024000
H	0.36681700	1.80277800	0.00031400
C	-0.66461800	-1.60344200	1.36793600
H	-1.68261500	-1.99919300	1.42316100
H	-0.50088400	-0.98208100	2.25746800
C	-0.66472700	-1.60315500	-1.36802600
H	0.01627300	-2.46071800	-1.43416100
H	-1.68277300	-1.99878500	-1.42327000
O	-1.32861600	0.48081100	0.00015500
C	-2.64967200	0.45095100	0.00003000
O	-3.32221000	-0.55499500	0.00007800
C	-3.24137300	1.83844300	-0.00016800
H	-4.32813600	1.77683200	-0.00027400
H	-2.89998700	2.38813900	0.88118000
H	-2.89979300	2.38796100	-0.88155000
B	-0.50917300	-0.76803400	0.00004500
H	0.01648600	-2.46094500	1.43385100
H	-0.50097700	-0.98161000	-2.25742800

5'

E= -798.4428395

ZPE=0.215038

C	2.18509300	0.90281700	-0.00083700
C	3.52008200	0.53305800	-0.00097900
C	3.83582700	-0.82114100	-0.00012200
C	2.80095400	-1.74699800	0.00088400
C	1.49062300	-1.28839700	0.00099600
N	1.18663300	0.01327800	0.00015400
H	4.87044500	-1.14729100	-0.00022500
H	1.89033300	1.94729900	-0.00152500
H	4.29039300	1.29467700	-0.00175300
H	2.99570100	-2.81274400	0.00158000
H	0.64578800	-1.96690100	0.00183800
C	-0.65114300	1.67113500	-1.75883900
H	-1.46921900	2.38425200	-1.90952400

H	-0.72212600	0.92967700	-2.56583400
C	-0.65028000	1.67417400	1.75737900
H	0.28985700	2.21766700	1.91233700
H	-1.46829400	2.38755900	1.90715700
O	-1.39637000	-1.02281800	0.00143100
C	-2.63570400	-0.67728500	0.00117200
O	-2.89312200	0.54148700	0.00075100
C	-3.69140300	-1.73438800	-0.00061400
H	-4.68246400	-1.28525400	0.02179200
H	-3.57881800	-2.35213800	-0.89504300
H	-3.55131600	-2.38623200	0.86494600
Al	-0.79180900	0.79390600	0.00009600
H	0.28896000	2.21411300	-1.91569800
H	-0.72051500	0.93439000	2.56593400

6'

E= -2478.9748422

ZPV=0.215051

C	-1.64344600	1.35718700	-0.00046300
C	-2.95223600	1.82148300	-0.00033400
C	-3.99158200	0.90023600	-0.00015300
C	-3.68309100	-0.45567400	-0.00010400
C	-2.34877600	-0.83007700	-0.00021900
N	-1.34831700	0.05463100	-0.00039200
H	-5.02460400	1.23145400	-0.00004800
H	-0.79320900	2.02930200	-0.00061600
H	-3.14324200	2.88799100	-0.00040400
H	-4.45750300	-1.21325800	0.00003300
H	-2.05974700	-1.87701300	-0.00020600
C	0.62049800	-1.56327200	-1.78942200
H	1.46412900	-2.24593100	-1.92215500
H	0.68956900	-0.78979000	-2.56105700
C	0.61824400	-1.56117700	1.79046300
H	-0.30497100	-2.12473300	1.96147900
H	1.46329900	-2.24115100	1.92744300
O	1.26138200	1.16040600	-0.00082700
C	2.52203200	0.90421700	-0.00004700
O	2.89718600	-0.27850900	0.00087900
C	3.47864300	2.05782700	-0.00012200
H	4.50736700	1.70213200	-0.00158000
H	3.29525200	2.68031400	-0.87931800
H	3.29736500	2.67835200	0.88092700
H	-0.30360800	-2.12473200	-1.96237600
H	0.68224500	-0.78595900	2.56084900
Ga	0.68179400	-0.74287300	0.00005700

b. Estimated barriers of rotation around the C-N-M-O angle in the [(MMe_2)(μ-O_2CMe)(*py*-*Me*)] molecular systems.

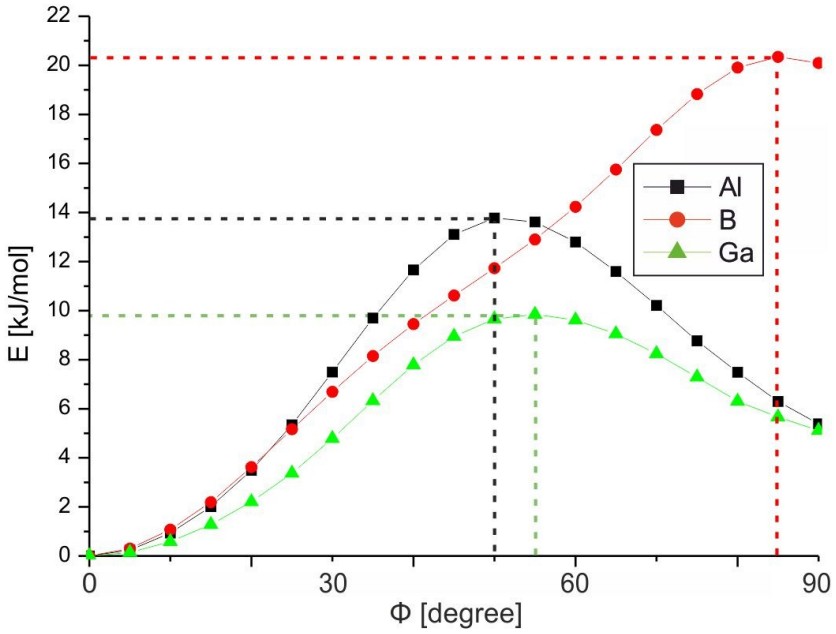

Figure 6S. PES scan of the [(MMe_2)(μ-O_2CMe)(*py*-*Me*)] system run for the C-N-M-O dihedral angle. Values acquired for Boron, Aluminum and Gallium atoms.