Electronic Supplementary Material (ESI) for Dalton Transactions. This journal is © The Royal Society of Chemistry 2017

E	III _C ¹¹	III _{Si} 12	III _{Ge} ^{10c}	III _{Sn} ¹³	III _{Pb} ¹⁴	o-C ₆ H ₄ (NHMe) ₂
EI–N ₁	1.361(2)	1.752(3)	1.861(3)	2.051(5)	2.180(4)	
$EI-N_2$	1.374(2)	1.747(3)	1.866(3)	2.067(5)	2.180(4)	
	1.363	1.768	1.876	2.068	2.210	
$N_1 - C_1$	1.397(2)	1.385(5)	1.393(5)	1.382(8)	1.373(7)	
$N_2 - C_6$	1.388(2)	1.380(5)	1.391(5)	1.376(7)		
-	1.390	1.389	1.383	1.397	1.401	1.40
$C_1 - C_6$	1.395(2)	1.417(5)	1.433(9)	1.433(10)	1.441(10)	
-	1.400	1.411	1.417	1.427	1.447	1.42
$C_1 - C_2$	1.390(2)	1.395	1.399(8)	1.397(10)	1.416(7)	
$C_5 - C_6$	1.382(2)	1.392	1.397(10)	1.398	1.416(7)	
	1.390	1.394	1.398	1.404	1.419	1.39
$C_2 - C_3$	1.369(2)	1.373	1.382(11)	1.379(10)	1.371(7)	
$C_4 - C_5$	1.376(2)	1.382	1.379(11)	1.382	1.371(7)	
	1.389	1.391	1.390	1.391	1.390	1.39
$C_3 - C_4$	1.390(3)	1.374	1.371(11)	1.371(11)	1.440(10)	
	1.399	1.391	1.391	1.393	1.399	1.38
N_1 –El– N_2	103.49(13)	88.2(1)	84.9(1)	78.49	75.8(2)	
	107.07	89.05	85.68	80.79	77.41	
$EI-N_1-C_1$	112.36(13)	111.9(3)	114.0(2)	115.32	115.3(3)	
$EI-N_2-C_6$	112.80(12)	111.3(3)	114.2(2)	115.07	115.3(3)	
	112.32	112.88	112.97	112.95	113.29	
$N_1 - C_1 - C_6$	106.17(14)	111.92	115.2(5)	115.10	116.4(3)	
$N_2 - C_6 - C_1$	105.73(14)	111.33	115.1(5)	115.16	116.4(3)	
	105.63	112.60	114.19	116.65	118.01	
*marked by italics						

Table S1. Experimental and calculated* (PBE0) geometry parameters for IIIC-Pb.

Table S2 Frontier MOs for III at PBE0 level.

El=	HOMO[-2]	HOMO[-1]	НОМО	LUMO
IIIc				
	1(p)+2(s)%*	13(p)%	50(s)+42(p)%	19(p)%
III _{si}	58(s)+26(p)%	0%	14(p)%	68(p)%





* The AOs contribution of E^{II} atom for each type

IIIa C	IIIb Si	lllc Ge	IIId Sn	Ille Pb	assignment
767 vs* (759)	702 vs (649)	670 vs (613)	647 vs (619)	629 vs (615)	«breathing» of both rings
					with some
					from the N–E ^{II} bonds
	1033 s	1034 s	1036 s	1037 s	#3 (Fig. 4)
2 s	(1050)	(1041)	(1050)	(1059)	
(1013)					
1182 s	1132 s	1117 s	1094 s	1082 s	complex mode
(1100)	(1130)	(1112)	(1180)	(1076)	
12/2 sm	12/5 sm	12/9 sm	12/2 sm	1269 sm	complex mode
(1314?)	(1276)	(1284)	(1251)	(1270)	$v(C_{ar}N)+\delta CH$
1386 s	1365 s	1360 s	1359 s	1361 s	complex mode
(1349)	(1367)	(1386)	(1377)	(1376)	$\nu(CC)_{ar}+\delta CH$
1446 w	1475	1471 m	1473 s	1472	complex mode
	(1455)	(1460)	(1480)	(1484)	ν(ĊC) _{ar} +δCH
					+vCN
1606 sm	1579 sh, 1587	1568 sh,	1550, 1556	1542, 1550	#1, #2 (Fig. 4)
(1595s, 1596	(1573s,	1581	(1556s,	sh	
as)	1580as)	(1562s,	1577as)	(1550s,	
,	,	1577as)	, ,	1575as)	

 Table S3 Experimental and calculated (in brackets) frequencies (cm⁻¹) of prominent Raman lines.

* - relative intensities

Fig. S1 ACID isosurface plotted for silylene $\rm III_{SI}$ at isovalue 0.06.

		<u>1</u>

Fig. S2 ACID isosurface plotted for stannylene III_{sn} at isovalue 0.02.





Fig. S3 ACID isosurface plotted for plumbylene III_{Pb} at isovalue 0.02.

Fig. S4 ACID isosurface plotted for carbene II_c at isovalue 0.05.





Fig. S5 ACID isosurface plotted for silylene II_{si} at isovalue 0.05.