Structure and bonding of proximity-enforced main-group dimers stabilized by a rigid naphthyridine diimine ligand

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Supporting Information

Table S1. Geometric parameters (Figure 1), sums of covalent single bond radii[1] and sums of Van der Waals radii[2].

E	E–E distance (Å)	Absolute value of E1–N5–N4–E2 dihedral angle (°)	Sum of covalent E-E single bond radii (Å)	Sum of E–E Van der Waals radii (Å)	E–E Mayer bond order
B	1.72	3.67	1.70	3.84	0.99
Al	2.54	22.88	2.52	3.68	0.95
Ga	2.89	41.36	2.48	3.74	0.47
In	3.27	51.63	2.84	3.86	0.27
Tl	3.41	57.21	2.88	3.92	0.12
C	2.87	20.59	1.50	3.40	-
Si	2.94	0.03	2.32	4.20	0.21
Ge	2.94	0.02	2.42	4.22	0.26
Sn	3.06	0.02	2.80	4.34	0.49
Pb	3.10	0.05	2.88	4.04	0.55
N	2.72	25.73	1.42	3.10	-
P	2.10	0.73	2.22	3.6	1.42
As	2.31	3.73	2.42	3.70	1.45
Sb	2.81	20.51	2.80	4.12	1.33
Bi	2.98	26.00	3.02	4.14	1.36

Table S2. N–E bond lengths.

Group 13		Group 14		Group 15	
Bond	**Bond length (Å)**	**Bond**	**Bond length (Å)**	**Bond**	**Bond length (Å)**
B1–N5	1.45	C1–N5	1.38	N1–N5	1.35
B1–N6	1.44	C1–N6	1.36	N1–N6	1.36
B2–N4	1.44	C2–N4	1.38	N2–N4	1.35
B2–N3	1.44	C2–N3	1.36	N2–N3	1.36
Al1–N5	1.89	Si1–N5	1.84	P1–N5	1.78
Al1–N6	1.88	Si1–N6	1.79	P1–N6	2.57
Al2–N4	1.89	Si2–N4	1.84	P2–N4	1.78
Al2–N3	1.88	Si2–N3	1.79	P2–N3	2.57
Ga1–N5	2.07	Ge1–N5	1.97	As1–N5	1.93
Ga1–N6	2.10	Ge1–N6	1.90	As1–N6	2.53
Ga2–N4	2.08	Ge2–N4	1.97	As2–N4	1.93
Ga2–N3	2.15	Ge2–N3	1.90	As2–N3	2.53
In1–N5	2.33	Sn1–N5	2.22	Sb1–N5	2.22
In1–N6	2.35	Sn1–N6	2.14	Sb1–N6	2.36
In2–N4	2.34	Sn2–N4	2.24	Sb2–N4	2.24
In2–N3	2.39	Sn2–N3	2.15	Sb2–N3	2.38
Tl1–N5	2.47	Pb1–N5	2.35	Bi1–N5	2.38
Tl1–N6	2.50	Pb1–N6	2.26	Bi1–N6	2.46
Tl2–N4	2.47	Pb2–N4	2.37	Bi2–N4	2.39
Tl2–N3	2.53	Pb2–N3	2.27	Bi2–N3	2.47

Figure S1. Optimized geometries of group 13 compounds. Geometric details are given according to Table S1.

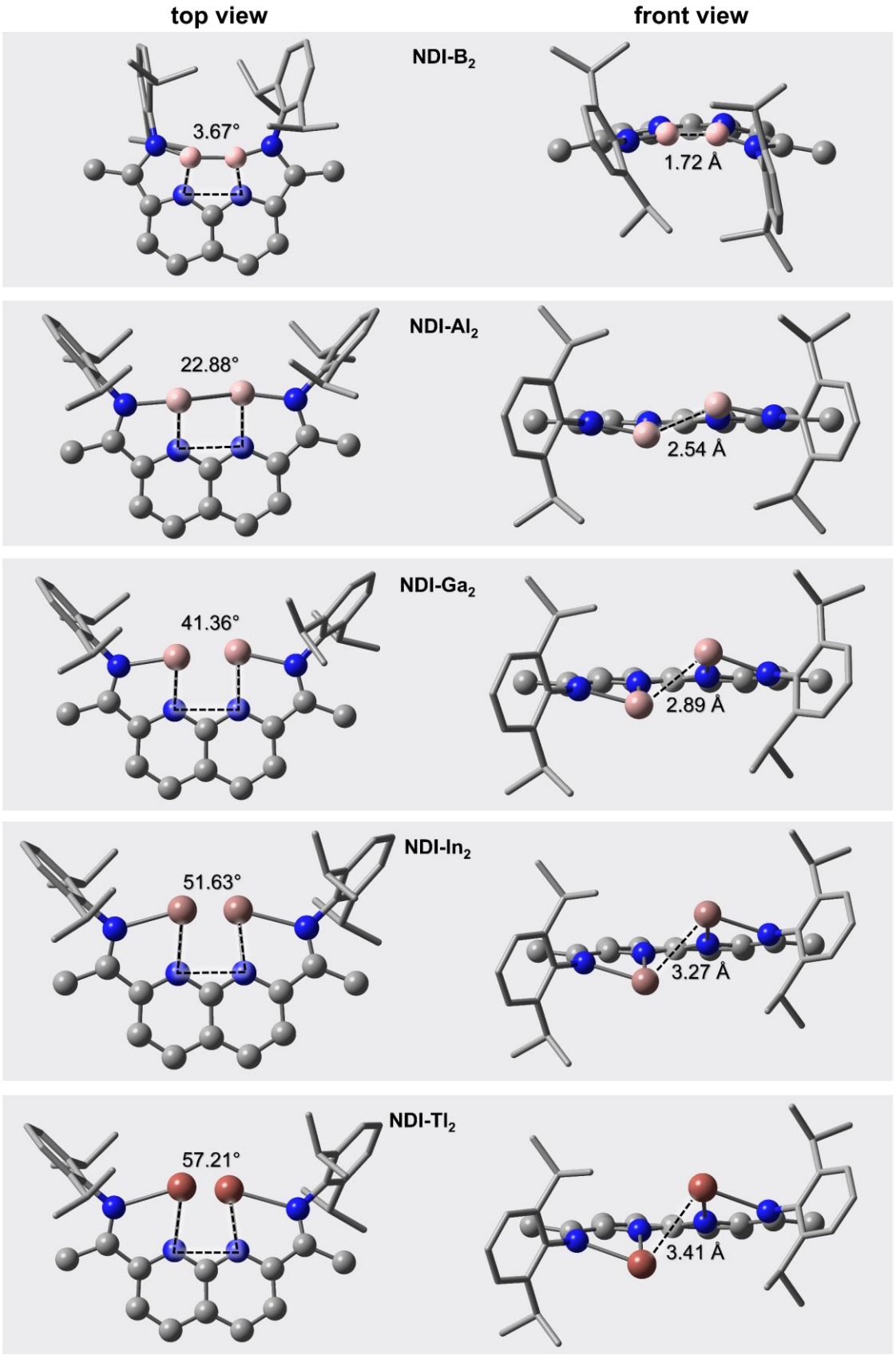


Figure S2. Optimized geometries of group 14 compounds. Geometric details are given according to Table S1.

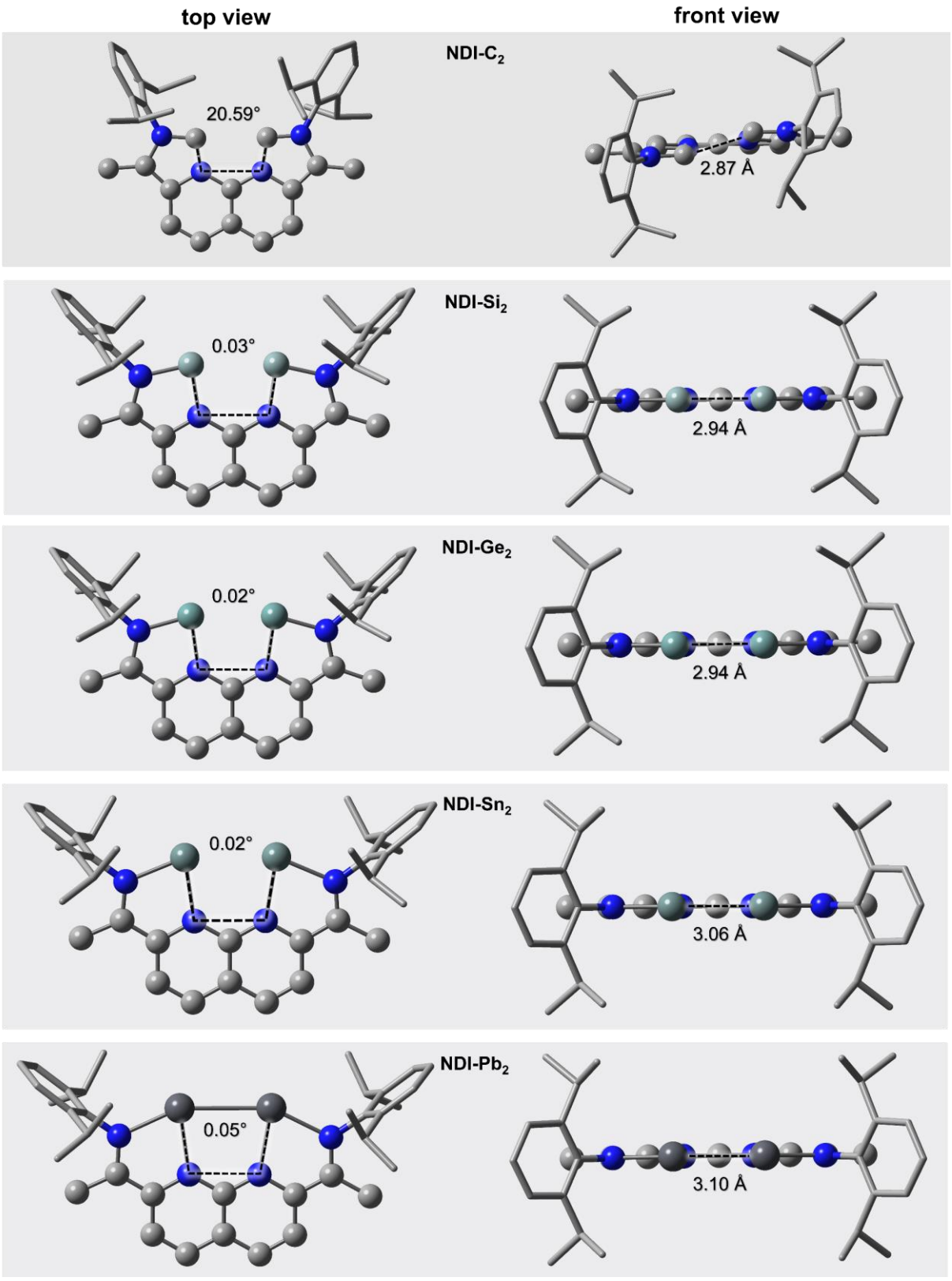


Figure S3. Optimized geometries of group 15 compounds. Geometric details are given according to Table S1.

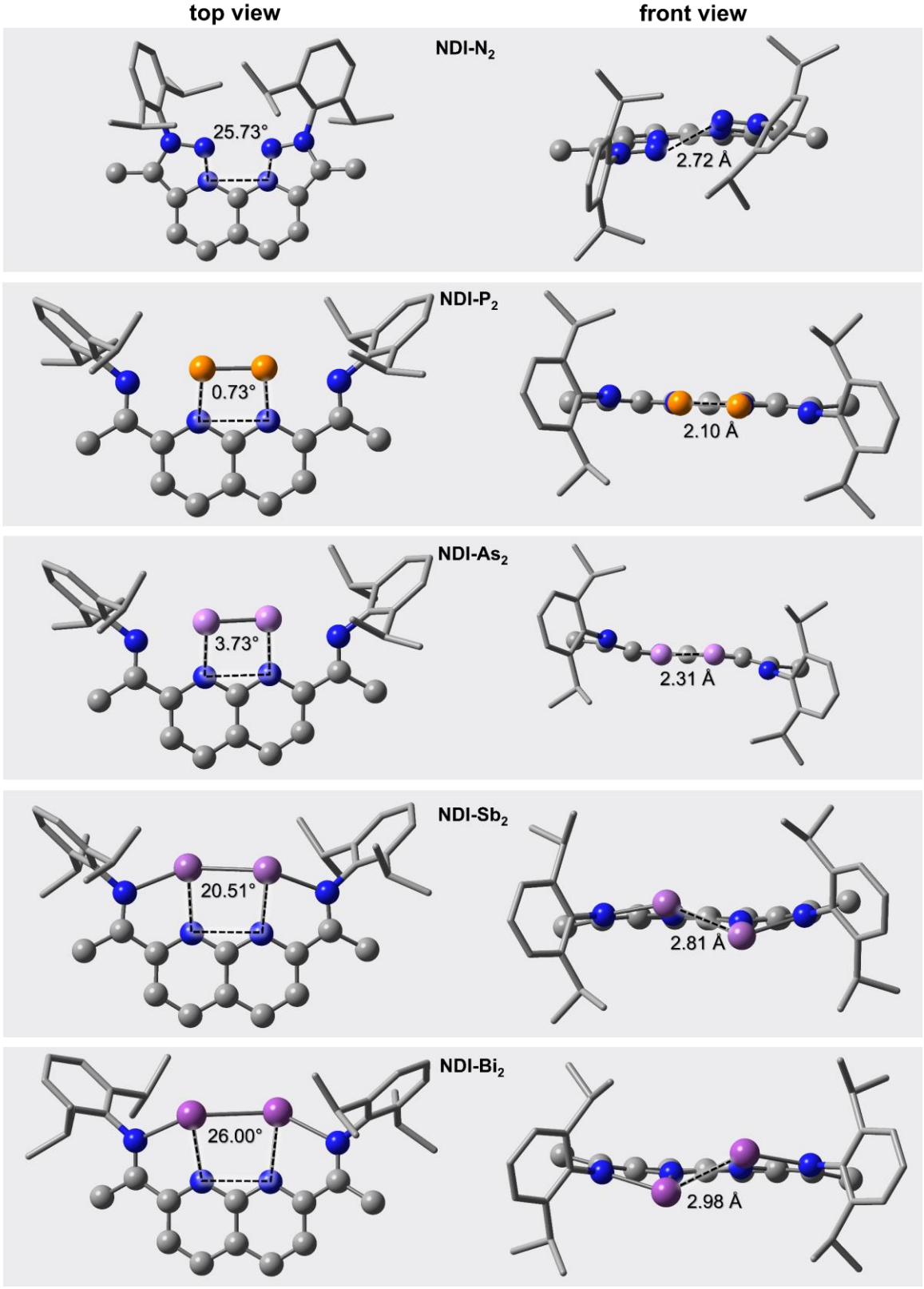


Table S3. Electron density and Laplacian of electron density at E–E bond critical points (BCPs).

E	ρ at BCP_{E-E} [e/a.u.^{3}]	$\nabla^2\rho$ at BCP_{E-E} [e/a.u.^{5}]
B	0.14	-0.26
Al	0.05	-0.06
Ga	0.03	0.01
In	0.02	0.02
Tl	0.01	0.03
C	0.01	0.05
Si	0.02	0.02
Ge	0.02	0.03
Sn	0.03	0.03
Pb	0.02	0.06
N	0.01	0.06
P	0.14	-0.26
As	0.11	-0.87
Sb	0.06	-0.01
Bi	0.05	0.02

Figure S4. Selected plots of electron density (left) and Laplacian of electron density (right; dark blue indicates negative value of the Laplacian) with given Isovalues.

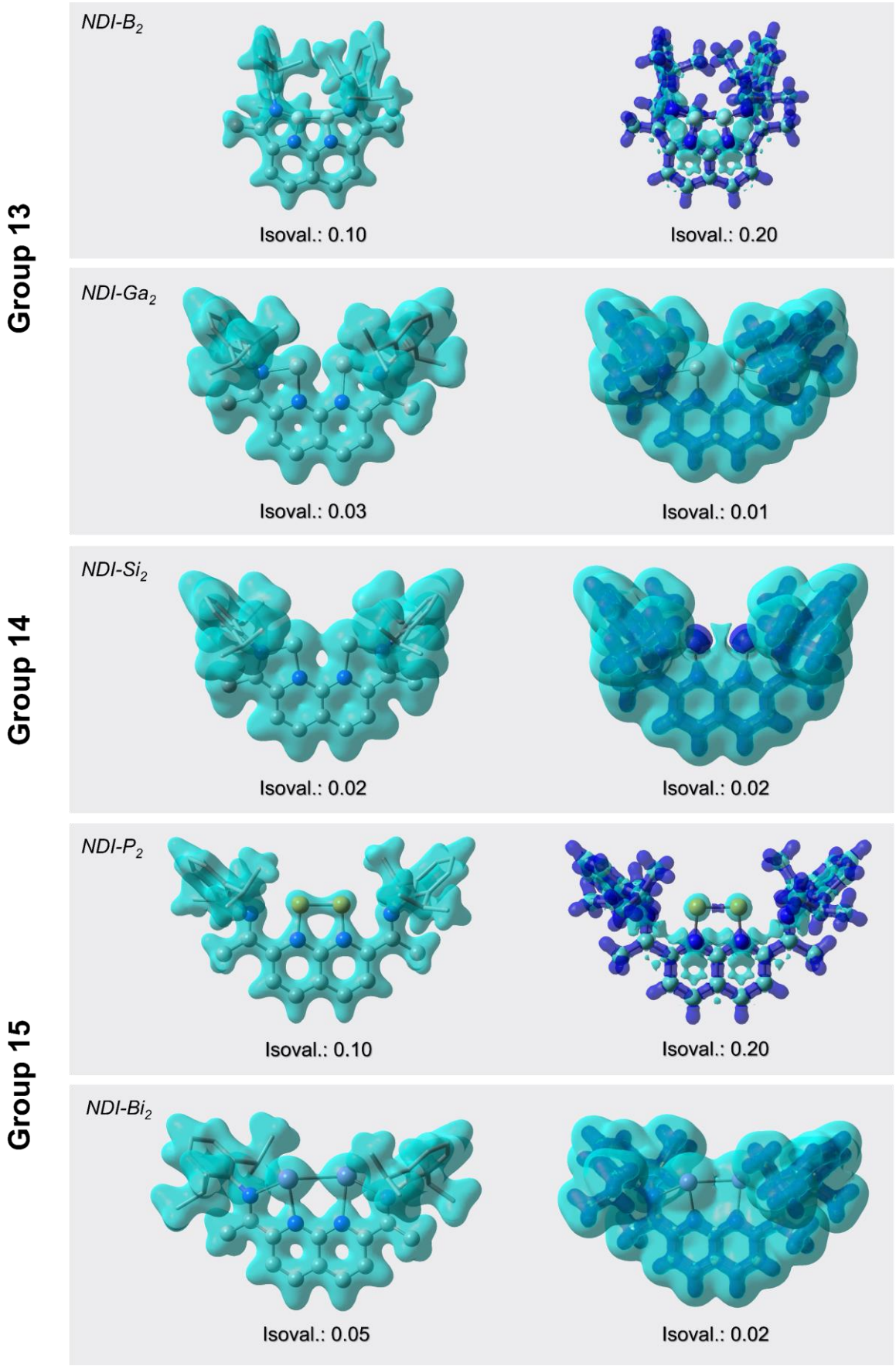


Table S4. ELF values, basin population N, variance σ^2 and fluctuation λ for valence basins of E.

E		ELF	N	$\sigma^2(N; \Omega)$	$\lambda(\Omega)$
B	V(B1, B2)	0.99	2.42	1.03	0.43
Al	V(Al1)	0.98	0.88	0.62	0.70
	V(Al2)	0.98	0.88	0.62	0.70
	V(Al1, Al2)	0.98	1.42	0.80	0.56
Ga	V(Ga1)	0.95	2.45	1.42	0.58
	V(Ga2)	0.96	2.33	1.35	0.58
In	V(In1)	0.89	2.22	1.35	0.61
	V(In2)	0.88	2.19	1.33	0.61
Tl	V(Tl1)	0.64	1.77	1.26	0.71
	V(Tl2)	0.63	1.77	1.26	0.71
C	V(C1)	0.99	2.48	1.00	0.40
	V(C2)	0.99	2.48	1.00	0.40
Si	V(Si1)	0.98	2.53	1.12	0.44
	V(Si2)	0.98	2.53	1.12	0.44
Ge	V(Ge1)	0.92	2.94	1.62	0.55
	V(Ge2)	0.92	2.94	1.62	0.55
Sn	V_1(Sn1)	0.83	1.50	1.06	0.71
	V_2(Sn1)	0.83	1.50	1.06	0.71
	V_1(Sn2)	0.84	1.52	1.06	0.70
	V_2(Sn2)	0.84	1.52	1.06	0.70
Pb	V_1(Pb1)	0.71	1.32	0.98	0.74
	V_2(Pb1)	0.70	1.30	0.98	0.75
	V_1(Pb2)	0.73	1.36	1.01	0.74
	V_2(Pb2)	0.73	1.32	0.98	0.74
N	V(N1)	0.95	3.73	1.42	0.38
	V(N2)	0.95	3.75	1.42	0.38
P	V(P1)	0.97	3.29	1.44	0.44
	V(P1)	0.97	3.29	1.44	0.44

	V(P1, P2)	0.91	1.93	1.07	0.55
As	V(As1)	0.94	3.51	1.84	0.52
	V(As1)	0.94	3.51	1.83	0.52
	V(As1, As2)	0.80	2.00	1.22	0.61
Sb	V_1(Sb1)	0.93	2.34	1.38	0.59
	V_2(Sb1)	0.84	2.02	1.32	0.65
	V_1(Sb2)	0.82	1.91	1.26	0.66
	V_2(Sb2)	0.93	2.37	1.39	0.59
Bi	V_1(Bi1)	0.74	1.82	1.25	0.69
	V_2(Bi1)	0.82	2.19	1.44	0.66
	V_1(Bi2)	0.83	2.16	1.42	0.66
	V_2(Bi2)	0.76	1.89	1.29	0.68

Table S5. Fraction of electrons of the doubly-occupied NBOs and IBOs given in Figures 4 and 5, assigned to the individual center atoms. Occupation numbers are given for NBOs. Top and bottom refers to relative position of the orbitals in Figure 5, center atoms are enumerated as E1 and E2 from left to right corresponding to their positions in Figures 4 and 5.

Orbital	E	NBO	IBO
		Occ. 1.957	
	B1	50.1 %	49.4 %
	B2	49.9 %	49.3 %
		Occ. 1.979	
	Al1	50.0 %	49.7 %
	Al2	50.0 %	49.7 %
		Occ. 1.560	
	Pb1	48.9 %	35.0 %
	Pb2	51.1 %	38.0 %
		Occ. 1.959	
Top	P1	50 %	49.4 %
	P2	50 %	49.4 %
		Occ. 1.871	
Bottom	P1	50 %	46.4 %
	P2	50 %	46.4 %
		Occ. 1.956	
Top	As1	50.0 %	54.7 %
	As2	50.0 %	41.6 %
		Occ. 1.880	
Bottom	As1	50.0 %	54.6 %
	As2	50.0 %	41.6 %
		Occ. 1.929	
Top	Sb1	50.8 %	63.7 %
	Sb2	49.2 %	31.5 %
		Occ. 1.773	
Bottom	Sb1	46.2 %	27.7 %
	Sb2	53.8 %	65.8 %

		Occ. 1.936	
Top	Bi1	50.7 %	64.1 %
	Bi2	49.3 %	31.5 %
		Occ. 1.808	
Bottom	Bi1	48.1 %	29.6 %
	Bi2	51.9 %	65.1 %

Figure S5. Relevant non-bonding natural bond orbitals (NBOs, red and blue) and intrinsic bond orbitals (IBOs, orange and pink).

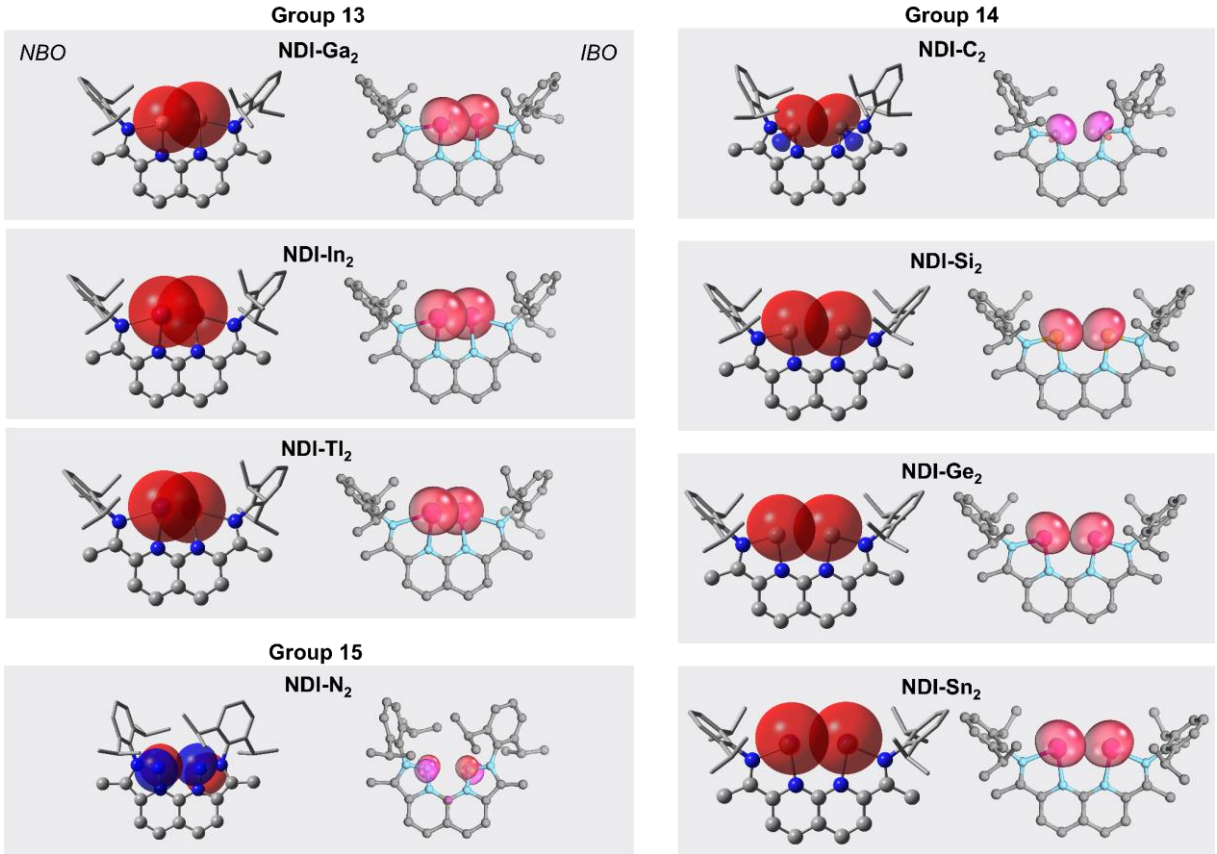


Table S6. Occupation numbers of NBOs and IBOs given in Figure S5. Center atoms are enumerated as E1 and E2 from left to right corresponding to their positions in Figure S5.

E	NBO	IBO
Ga1	1.778	1.716
Ga2	1.802	1.752
In1	1.873	1.818
In2	1.881	1.833
Tl1	1.932	1.890
Tl2	1.935	1.896
C1	1.899	1.906
C2	1.899	1.907
Si1	1.903	1.892
Si2	1.903	1.892
Ge1	1.909	1.901
Ge2	1.909	1.901
Sn1	1.882	1.876
Sn2	1.888	1.870
N1	0.894	1.777
N2	0.886	1.759

Figure S6. N–E electronegativity[3] difference plotted against average electron pair fraction of E in the N–E IBO. A linear fit was applied.

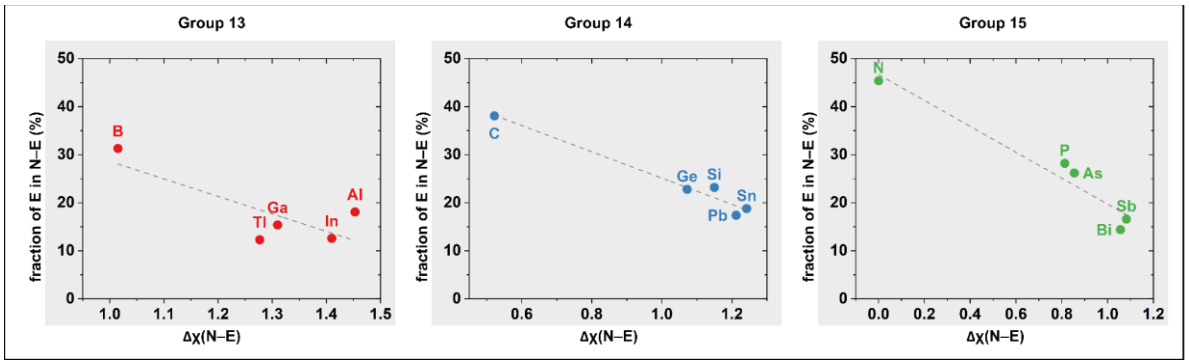


Table S7. $NICS_{ZZ}$ (min.) values (Figure 5).

E	C_2N_2E/CN_2E_2 $NICS_{ZZ}$ (min.) (ppm)	C_5N $NICS_{ZZ}$ (min.) (ppm)
B	-32.15	-14.42
Al	-25.69	-13.32
Ga	-18.19	-7.37
In	-15.04	-5.33
Tl	-14.37	-5.67
C	-36.21	-9.78
Si	-28.07	-10.99
Ge	-29.53	-12.88
Sn	-27.73	-14.43
Pb	-25.76	-13.57
N	-14.96	-6.08
P	-25.00	-3.76
As	-22.58	-3.02
Sb	-13.14	-3.29
Bi	-2.66	-3.52
NDI	-3.83	-26.25

Figure S7. $NICS_{ZZ}$ curves of the NDI. The values of the pink and purple color-coded pseudo-ring structures are attributed to an artifact of the method due to the presence of adjacent aromatic rings.[4]

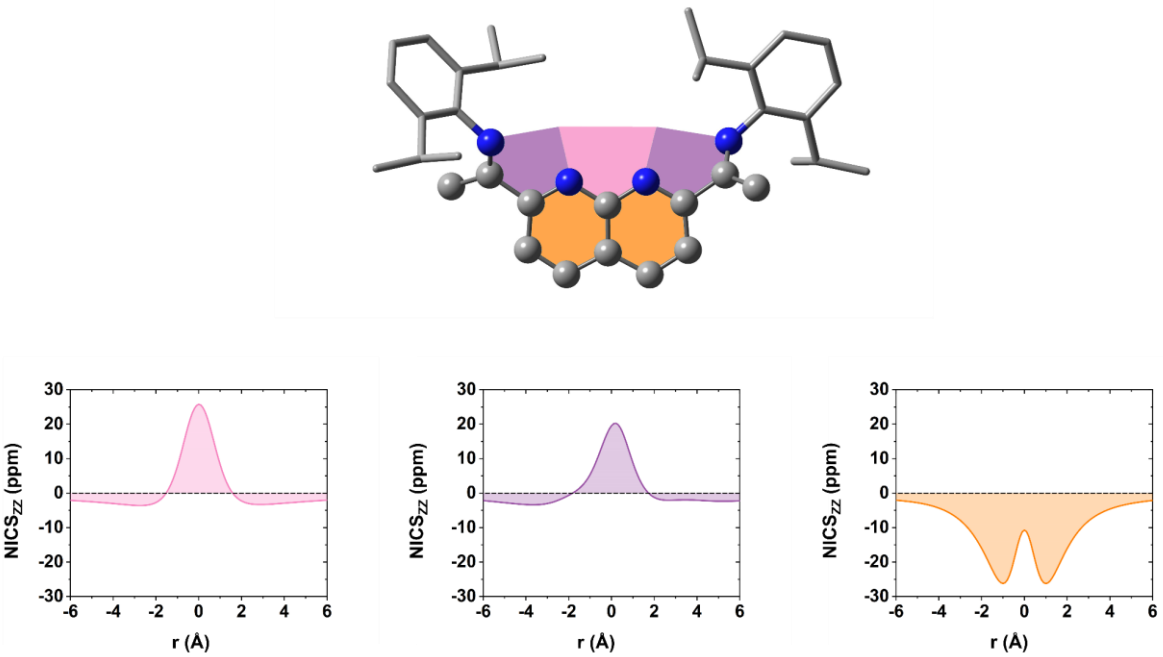


Figure S8. $NICS_{ZZ}$ curves of group 13 compounds. The values of the pink color-coded pseudo-ring structure of E = Ga, In and Tl compounds are attributed to an artifact of the method due to the presence of adjacent aromatic rings.[4]

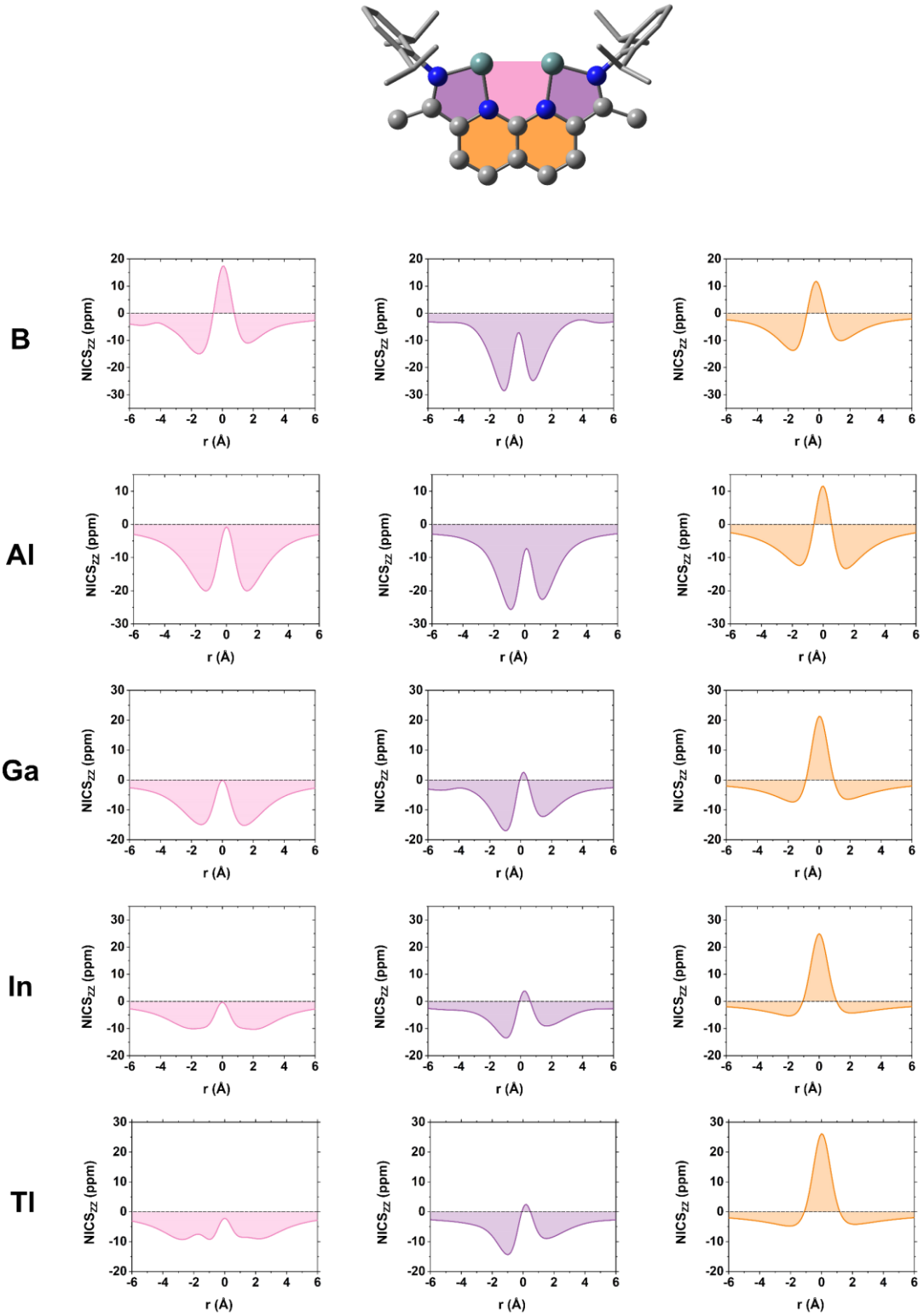


Figure S9. $NICS_{ZZ}$ curves of group 14 compounds. The values of the pink color-coded pseudo-ring structure of E = C, Si, Ge and Sn compounds are attributed to an artifact of the method due to the presence of adjacent aromatic rings.[4]

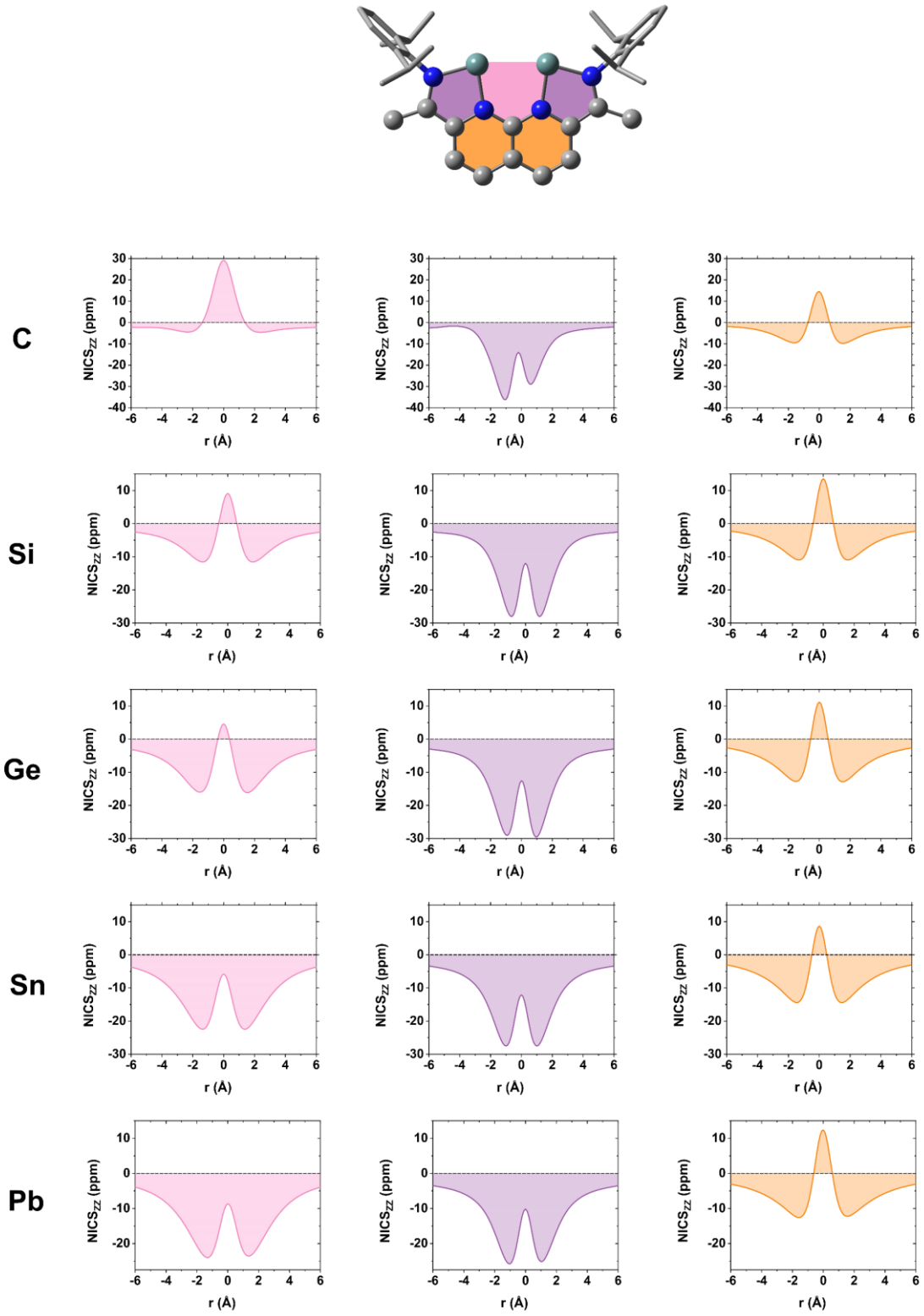


Figure S10. $NICS_{ZZ}$ curves of group 15 compounds. The values of the pink color-coded pseudo-ring structure for the E = N compound and the purple color-coded pseudo-ring structures for the E = P and As compounds are attributed to an artifact of the method due to the presence of adjacent aromatic rings.[4]

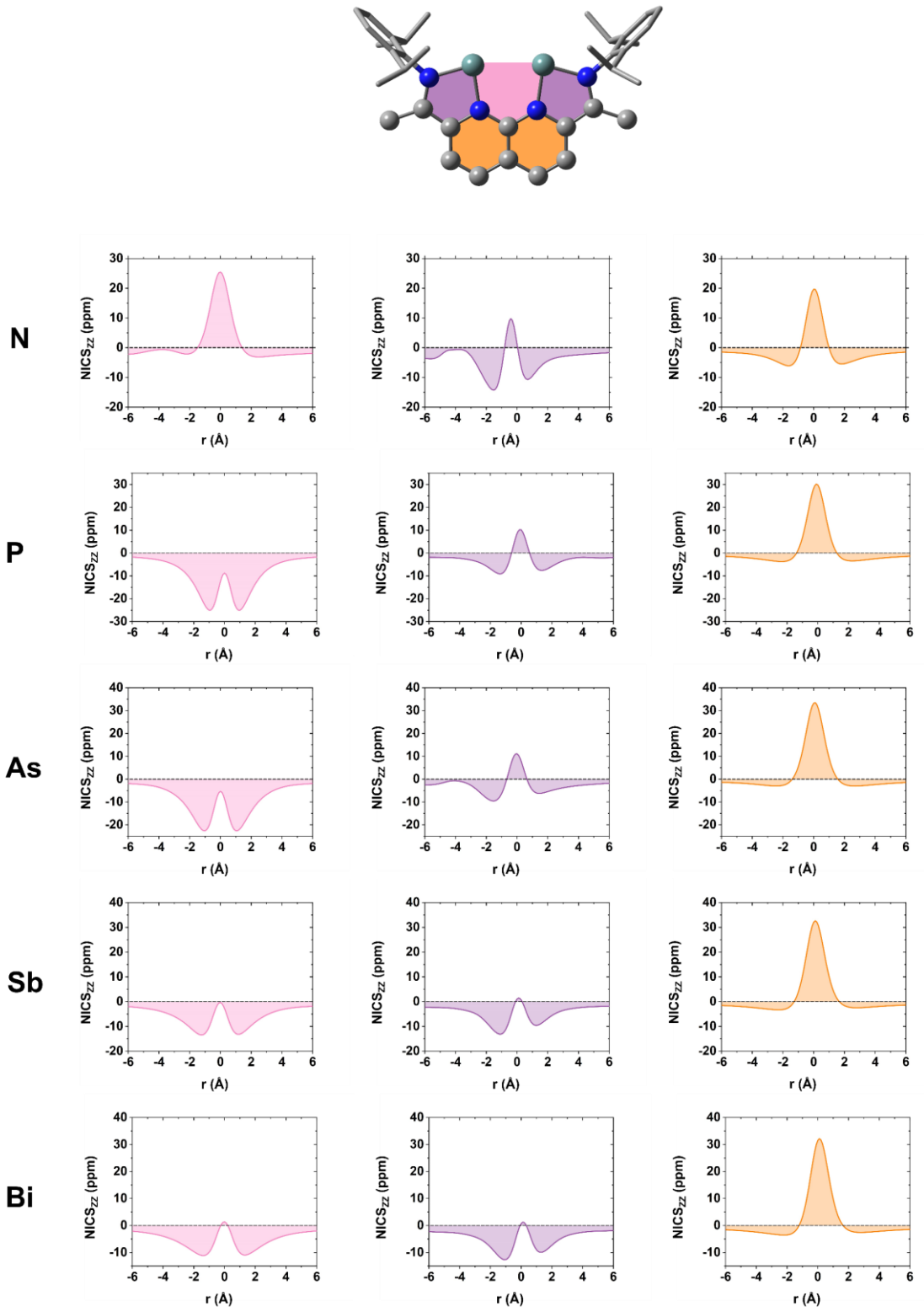


Figure S11. π ACID plot of the NDI.

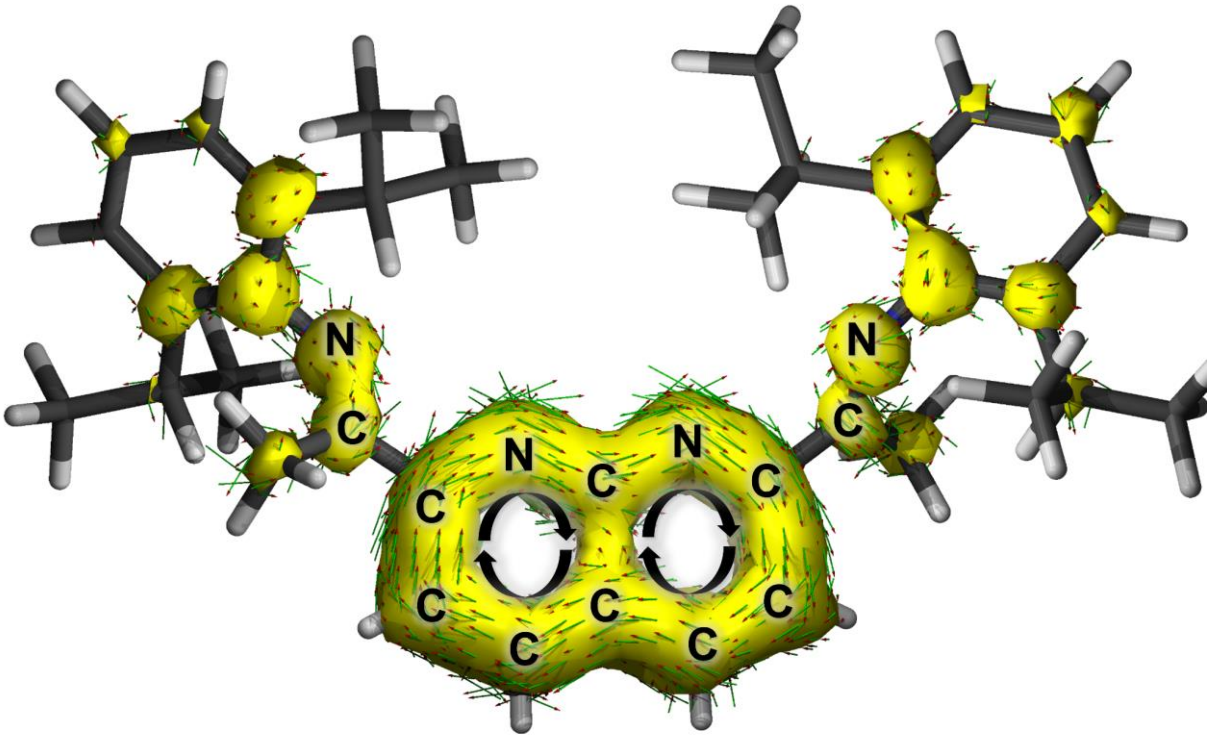


Figure S12. π ACID plots of group 13 compounds.

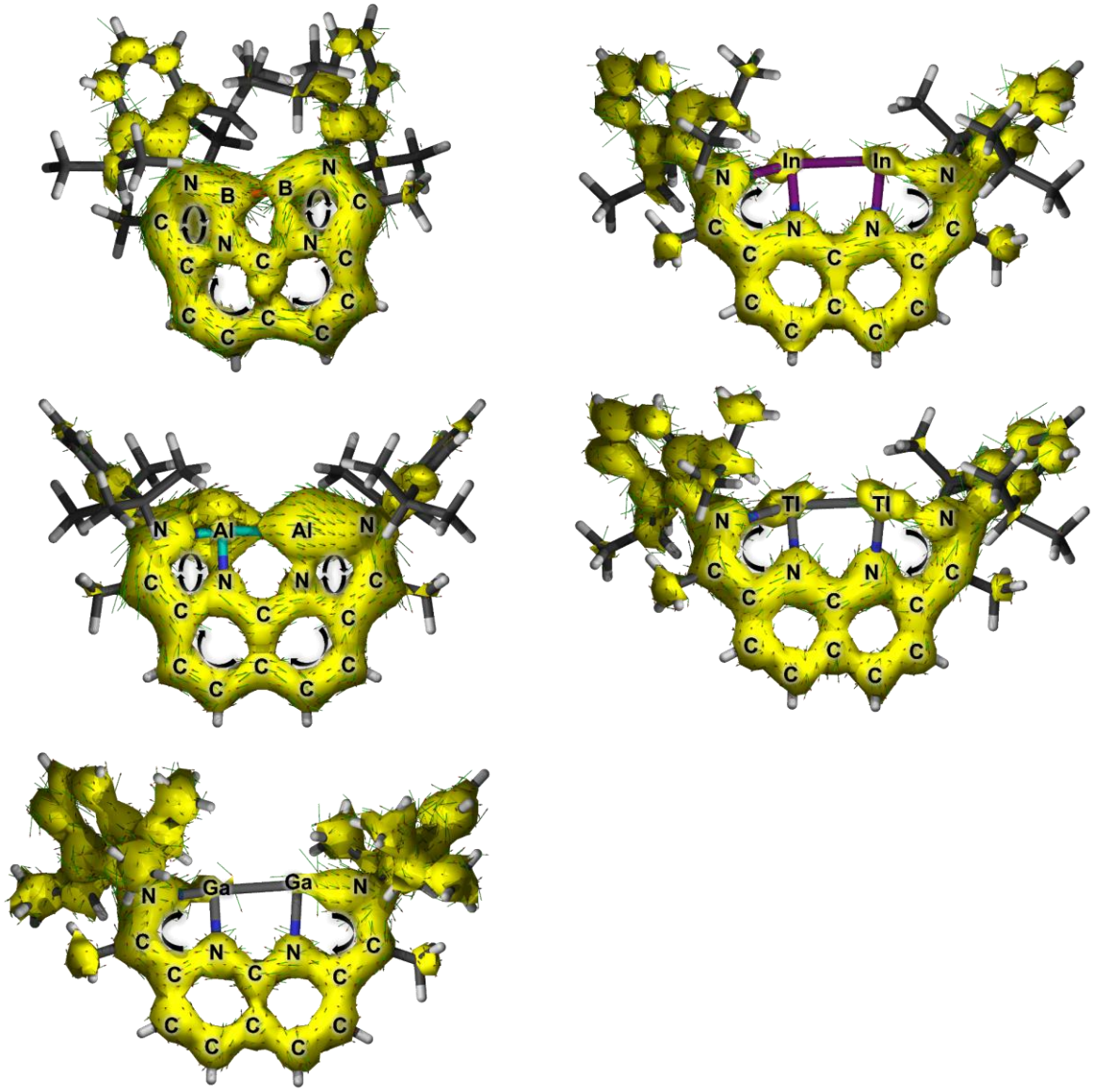


Figure S13. π ACID plots of group 14 compounds.

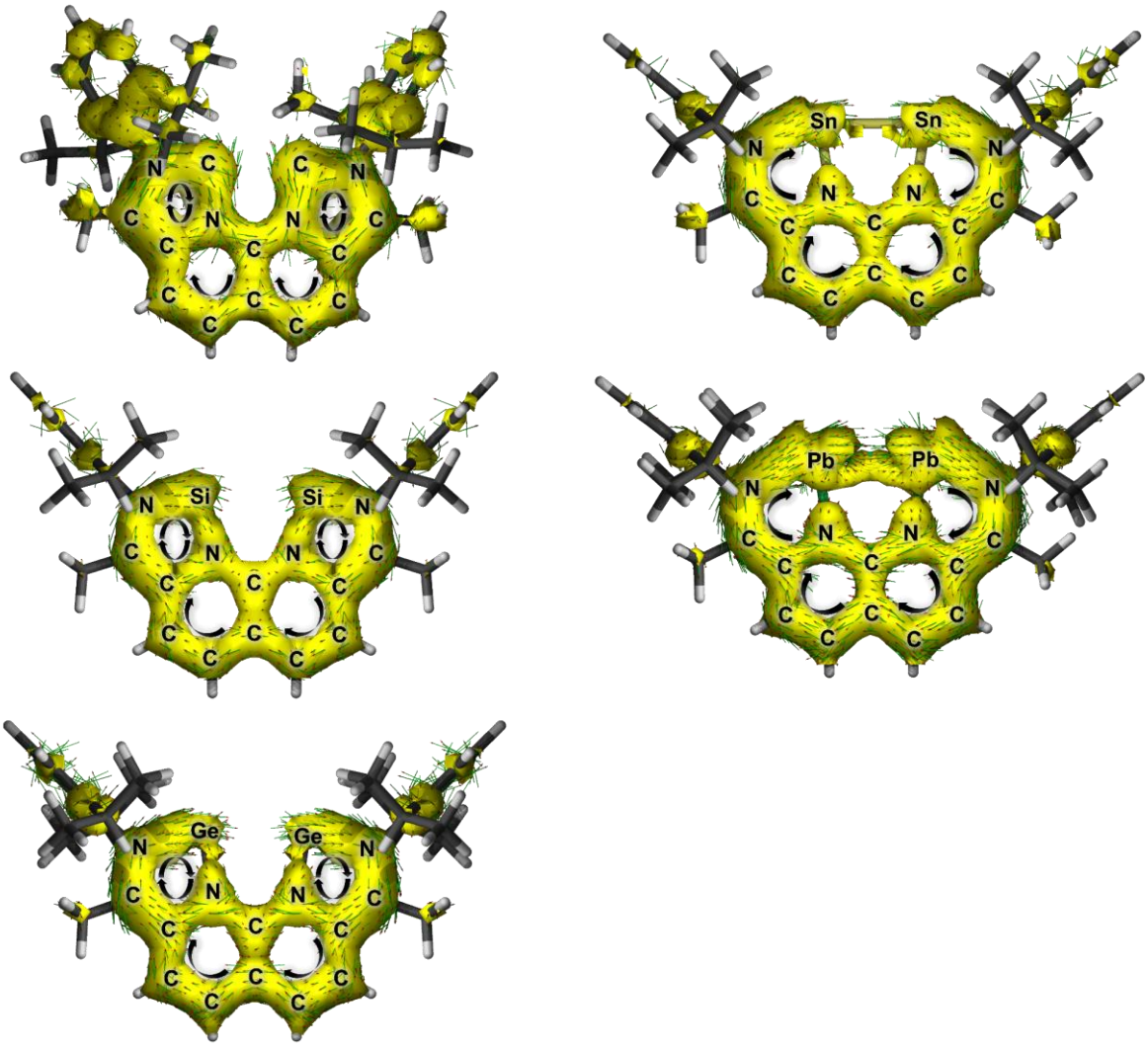


Figure S14. π ACID plots of group 15 compounds. Due to its triplet ground state, no π ACID calculation could be executed for the E = N compound.

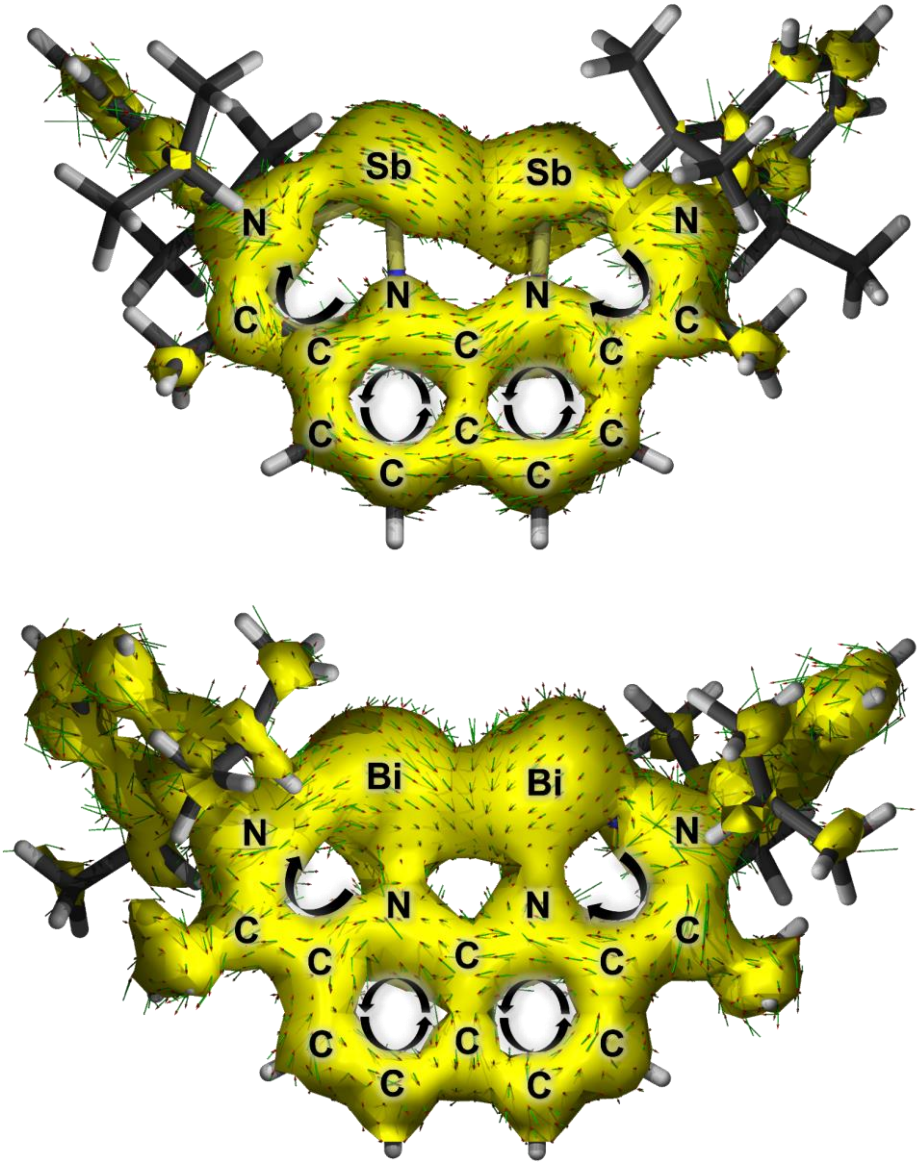


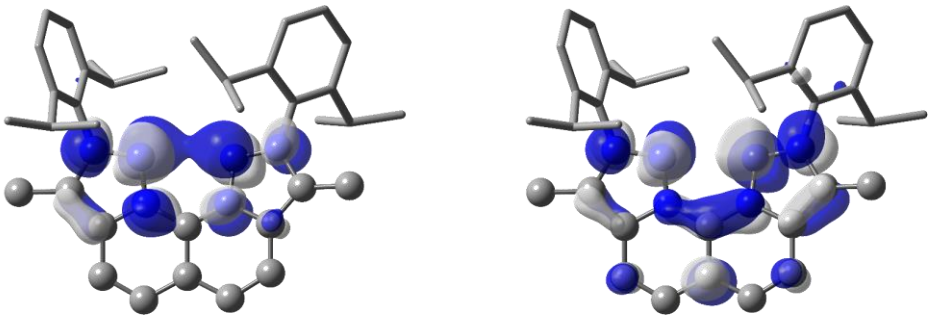
Table S8. Singlet-triplet gaps and corresponding HOMO-LUMO gaps (Figure 8).

E	HOMO-LUMO gap (eV)	singlet-triplet gap (kcal mol^{-1})
B	3.72	42.00
Al	2.11	10.71
Ga	2.25	15.20
In	2.16	13.63
Tl	2.11	13.31
C	3.74	39.82
Si	3.01	30.88
Ge	2.75	29.00
Sn	2.36	25.72
Pb	2.30	22.92
N	1.57	-2.68
P	2.85	25.26
As	2.65	7.98
Sb	2.20	13.98
Bi	1.94	11.08

Table S9. Net enthalpy of reduction and main-group-element exchange (Figure 9).

E	$\Delta H_{red.}$ (kcal mol^{-1})	$\Delta H_{ex.}$ (kcal mol^{-1})
B	-64.53	-0.75
Al	23.48	20.36
Ga	-12.59	16.69
In	-43.30	-10.29
Tl	-35.32	-37.81
C	-69.23	112.57
Si	-25.54	10.52
Ge	-30.00	0
Sn	-19.76	-24.55
Pb	-8.32	-65.79
N	-56.34	222.86
P	-32.25	122.63
As	-40.12	112.16
Sb	-33.82	79.91
Bi	-30.60	58.25

Figure S15. CASSCF-SOMOs of the E = N compound and the corresponding orbital energies.



SOMO 1
-1.21 eV

SOMO 2
-1.45 eV

Figure S16. Relaxed scan of transition from Isomer I to Isomer II for E = P and As. Depicted energy differences between isomers were calculated from separate optimizations.

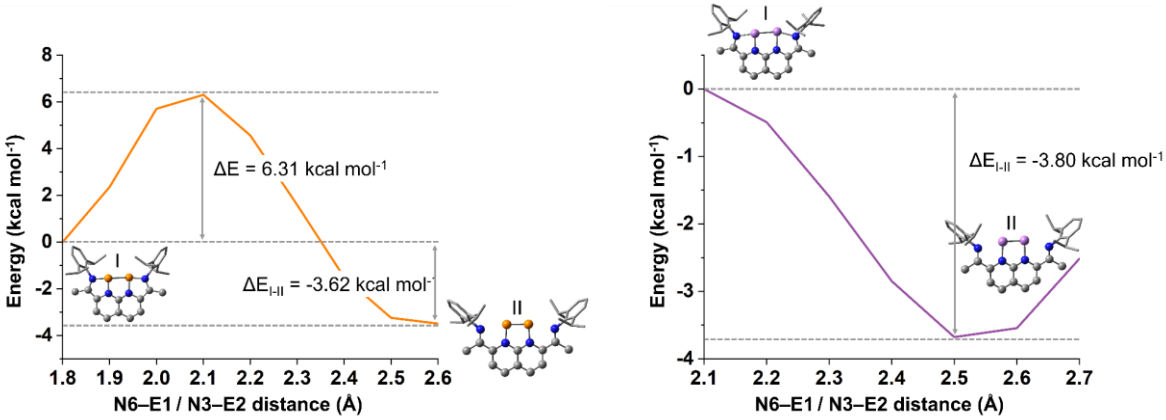


Table S10. Scan data (Figure S16).

P		As	
N6–E1 / N3–E2 distance (Å)	**Energy (kcal mol^{-1})**	**N6–E1 / N3–E2 distance (Å)**	**Energy (kcal mol^{-1})**
1.80	0	2.10	0
1.90	2.35	2.20	-0.49
2.00	5.71	2.30	-1.59
2.10	6.31	2.40	-2.85
2.20	4.57	2.50	-3.68
2.30	1.59	2.60	-3.54
2.40	-1.51		
2.50	-3.24		

Cartesian coordinates of optimized main-group dimer geometries in Ångstrøm.

NDI-B_2 **$E_{el.}$(a.u.)** = -1664.74336772

Atom	x	y	z
B	-0.7891633	0.86869451	0.19361462
C	3.09252784	1.20913506	1.20164131
N	2.1400026	0.17967066	0.94725941
B	0.81291208	0.73353618	0.81906692
C	4.50760918	0.907999	1.52850902
H	5.05589317	1.84361451	1.71465444
H	5.03882978	0.35901399	0.73076553
H	4.5862851	0.28661565	2.43899019
N	1.10550862	2.13769365	1.02610383
N	-2.0209106	0.53007483	-0.482997
C	2.73723372	3.84914987	1.06467744
H	3.74797196	4.21431128	1.26810271
N	-0.8688027	2.3061769	0.13176037
C	2.44934401	2.43605732	1.1708824
C	0.21075138	2.99771607	0.51561631
C	0.43153636	4.31690118	0.25724107
C	1.77541748	4.73792725	0.62647458
H	2.05572848	5.78980649	0.50953373
C	-0.6834826	4.93827744	-0.4456039
H	-0.6297564	6.00514883	-0.6857244
C	-1.796863	4.23278847	-0.857625
H	-2.5831702	4.75476374	-1.410069
C	-1.9158611	2.81257512	-0.6117602
C	-3.9170567	1.63984337	-1.7636953
H	-4.1579467	2.63710269	-2.1611342
H	-4.7857	1.3005401	-1.1703045
H	-3.8329153	0.94411188	-2.6169562
C	-2.6654963	1.7023938	-0.9717094
C	-2.6273502	-0.7601541	-0.5016958
C	-3.7208669	-1.0039134	0.35360087
C	-4.2891334	-2.2805288	0.35215639
H	-5.1391146	-2.4936968	1.00762564
C	-3.7738721	-3.2916231	-0.448755
H	-4.2297505	-4.2859947	-0.4365803
C	-2.6617808	-3.0475863	-1.2462436
H	-2.2469492	-3.8620485	-1.845673
C	-2.0600152	-1.7868605	-1.283774
C	-0.8232486	-1.5355164	-2.1224863
H	-0.1492604	-0.9017835	-1.5168647
C	-1.1661701	-0.7566548	-3.3892142
H	-0.267934	-0.5956639	-4.0087303

H	-1.5908747	0.23366155	-3.1583299
H	-1.9007022	-1.3120171	-3.9991547
C	-0.0431835	-2.7972704	-2.4536886
H	0.91769961	-2.5326875	-2.9264709
H	-0.5827175	-3.4505047	-3.1617184
H	0.18985739	-3.3838699	-1.5482869
C	-4.1859911	0.03655623	1.35401124
H	-3.9290321	1.03617403	0.9628408
C	-3.4165409	-0.1394195	2.66227643
H	-3.705401	0.62955299	3.39793889
H	-2.3271949	-0.0663831	2.5054264
H	-3.6251511	-1.1301365	3.10422803
C	-5.6873034	0.01791549	1.60339882
H	-5.9813004	0.87344838	2.23269923
H	-6.0079908	-0.8933457	2.1368891
H	-6.2615578	0.07435159	0.66349734
C	2.51389244	-1.1208959	0.49638328
C	2.09224872	-2.2542609	1.21586393
C	2.43784225	-3.5190974	0.72589576
H	2.11663738	-4.4109426	1.27407295
C	3.17290463	-3.6611288	-0.4410327
H	3.44048568	-4.6572561	-0.8053306
C	3.55131708	-2.5317067	-1.1607823
H	4.10256709	-2.6584992	-2.0967031
C	3.2200291	-1.247291	-0.7251166
C	3.52238737	-0.0453762	-1.605959
H	3.74227713	0.81791436	-0.9574931
C	4.72839222	-0.2400008	-2.5128267
H	4.98361596	0.70870343	-3.0115865
H	4.53374968	-0.9761137	-3.3120072
H	5.61608364	-0.5777602	-1.9520859
C	2.29628561	0.34194789	-2.4307215
H	2.51622167	1.21040182	-3.073302
H	1.43570512	0.61186489	-1.7939495
H	1.98538657	-0.4935172	-3.0840079
C	1.21514679	-2.1526503	2.44545384
H	1.20728139	-1.0965674	2.76616248
C	-0.2201204	-2.5419323	2.09169935
H	-0.88643	-2.446415	2.96578732
H	-0.2736199	-3.5887969	1.7428161
H	-0.6281107	-1.910158	1.28299734
C	1.73823024	-2.9801081	3.61288987
H	1.12802068	-2.8042913	4.51393178
H	2.78285727	-2.7255067	3.85530073
H	1.69753496	-4.0628585	3.40401793

NDI-Al_2 **$E_{el.}$(a.u.)** = -2099.80078122

Atom	x	y	z
Al	-1.1928255	-0.0246757	-0.437585
C	3.42117652	1.48031334	-0.0977478
N	3.01210477	0.16855247	-0.0177292
Al	1.19231975	-0.025005	0.4348396
C	4.8667724	1.8258759	-0.1668534
H	5.01997374	2.91220417	-0.2159055
H	5.34665897	1.37415895	-1.0532004
H	5.422448	1.44148699	0.70673661
N	1.13546801	1.82482377	0.05774868
N	-3.0122995	0.16858195	0.01625856
C	2.44007506	3.8411279	-0.0727369
H	3.40917312	4.34558559	-0.1150668
N	-1.1357322	1.82490231	-0.0590871
C	2.38766032	2.42164339	-0.0652933
C	-0.0001272	2.54946526	-0.000344
C	-0.0001077	3.95231676	0.00044218
C	1.2818667	4.5834834	-0.0189401
H	1.331665	5.67690219	-0.0142176
C	-1.2820534	4.58349387	0.02064939
H	-1.3318385	5.67691716	0.01709438
C	-2.4402633	3.84108956	0.0739876
H	-3.409345	4.34550565	0.11712769
C	-2.387852	2.42162243	0.06513613
C	-4.8668805	1.82577481	0.16802613
H	-5.0200069	2.91205898	0.21817436
H	-5.3461326	1.37326833	1.05430903
H	-5.4232369	1.4422114	-0.705498
C	-3.4213481	1.48025223	0.09754547
C	-3.976308	-0.8751047	0.11691718
C	-4.2646166	-1.4003656	1.39502133
C	-5.1772781	-2.4525743	1.49337007
H	-5.4049563	-2.8774307	2.47656107
C	-5.7942974	-2.9756363	0.36232863
H	-6.5040627	-3.8025939	0.45739
C	-5.505426	-2.4456547	-0.8884095
H	-5.9937673	-2.8633465	-1.7754449
C	-4.6023433	-1.3881181	-1.0370924
C	-4.3005218	-0.8504736	-2.4213314
H	-3.7194279	0.0818517	-2.2988508
C	-5.5635758	-0.5027443	-3.200545
H	-5.3074302	-0.0212376	-4.1585414
H	-6.2152845	0.18685266	-2.6384765

H	-6.1599324	-1.3998518	-3.4391422
C	-3.4310476	-1.830612	-3.203621
H	-3.1811229	-1.43052	-4.2005635
H	-3.9511901	-2.7938464	-3.3469802
H	-2.4836579	-2.0406639	-2.6777257
C	-3.5513328	-0.887394	2.6295001
H	-3.1374288	0.10835829	2.38894893
C	-2.375586	-1.8014128	2.96634707
H	-1.7985744	-1.4125978	3.82217568
H	-1.6805617	-1.9040054	2.11545184
H	-2.7308715	-2.8145415	3.22523854
C	-4.4729489	-0.7220019	3.83027469
H	-3.9362779	-0.2389081	4.66298712
H	-4.8413662	-1.6915076	4.20738247
H	-5.3521281	-0.1021399	3.58854727
C	3.97632223	-0.8750475	-0.1172269
C	4.60066373	-1.3882387	1.03761858
C	5.50386858	-2.4458449	0.8901291
H	5.99084935	-2.863695	1.77784542
C	5.79454522	-2.9756725	-0.3602449
H	6.50436279	-3.8026901	-0.4543833
C	5.17926238	-2.4523697	-1.492134
H	5.40839569	-2.8770807	-2.4750441
C	4.26652531	-1.4001243	-1.3949805
C	3.55503393	-0.8868445	-2.6303617
H	3.14168629	0.1092908	-2.3904445
C	4.4780227	-0.7224253	-3.8302159
H	3.94266444	-0.2388351	-4.6634836
H	4.84584243	-1.6923069	-4.20694
H	5.35758023	-0.1034275	-3.5876368
C	2.37888921	-1.7999496	-2.9682851
H	1.80322993	-1.4109501	-3.8249342
H	1.68274838	-1.9016816	-2.1181935
H	2.73362793	-2.8134707	-3.2263884
C	4.29711849	-0.8506551	2.42150933
H	3.71529845	0.08113859	2.29839328
C	3.42791552	-1.831426	3.20328958
H	3.17669332	-1.4312886	4.19988526
H	3.94885361	-2.7941114	3.34742784
H	2.48121649	-2.0425561	2.67658432
C	5.55926466	-0.5015948	3.20162701
H	5.3019573	-0.0204945	4.15951507
H	6.21054458	0.1888277	2.64006626
H	6.15650712	-1.3980559	3.44043752

NDI-Ga_2 **$E_{el.}$(a.u.)** = -5464.23477727

Atom	x	y	z
Ga	-1.2153093	-0.2513646	-0.5711511
C	3.48231916	1.40452408	-0.4499706
N	3.17223771	0.16376839	-0.1166169
Ga	1.27933126	-0.0789538	0.8667139
C	4.87338672	1.85024944	-0.7696252
H	4.88591818	2.5325504	-1.6330762
H	5.52627199	0.99369181	-0.9937188
H	5.31928002	2.39484339	0.0819373
N	1.17863179	1.75101932	-0.1255907
N	-3.1266238	0.23298478	0.14197537
C	2.4581489	3.69944729	-0.6915462
H	3.42075069	4.1656565	-0.9198391
N	-1.1047315	1.76538916	-0.1108827
C	2.38957086	2.3264497	-0.4517831
C	0.04056978	2.45369452	-0.204057
C	0.05334467	3.87868556	-0.3829918
C	1.30670626	4.47869664	-0.6226271
H	1.35784902	5.55938822	-0.7855525
C	-1.1981506	4.53835139	-0.3041707
H	-1.23401	5.62676794	-0.4086861
C	-2.3569314	3.81580729	-0.0716453
H	-3.3114832	4.34162072	0.0146189
C	-2.3197008	2.41725308	0.02916791
C	-4.8249369	2.00484666	0.34949754
H	-4.9099348	3.09860668	0.35378683
H	-5.242641	1.6227895	1.29731947
H	-5.4756392	1.60720101	-0.4476696
C	-3.4196582	1.5346733	0.17722447
C	-4.1383246	-0.7443403	0.31298649
C	-4.3824387	-1.232095	1.61611643
C	-5.3363642	-2.2362807	1.78553833
H	-5.5333261	-2.6279129	2.78871929
C	-6.0339521	-2.7555505	0.69944146
H	-6.7754887	-3.5454794	0.85006279
C	-5.7816799	-2.2694139	-0.5763087
H	-6.3294291	-2.6850588	-1.4292342
C	-4.8396314	-1.2590168	-0.7960873
C	-4.5829607	-0.7728072	-2.2083368
H	-3.9145673	0.10561815	-2.1461655
C	-5.8620773	-0.3256435	-2.9075281
H	-5.6351964	0.10622351	-3.8962224
H	-6.4059892	0.43483718	-2.3225486

H	-6.5535986	-1.1694164	-3.0728859
C	-3.8591793	-1.8379727	-3.0267077
H	-3.6407757	-1.4742731	-4.0448754
H	-4.4731783	-2.7506683	-3.1202311
H	-2.9037405	-2.1266176	-2.5569202
C	-3.5697206	-0.7280949	2.79121602
H	-3.1931291	0.27792514	2.532493
C	-2.3530324	-1.6268101	2.99814578
H	-1.7064199	-1.248083	3.80747941
H	-1.7381547	-1.6983635	2.08441879
H	-2.6695914	-2.6512675	3.26267033
C	-4.3761653	-0.5973151	4.07516881
H	-3.772642	-0.1136414	4.86036536
H	-4.6867768	-1.579107	4.47214708
H	-5.2872357	0.00625796	3.92625987
C	4.07510379	-0.9215438	-0.178155
C	5.03378382	-1.1493053	0.8287977
C	5.85026981	-2.2793999	0.72122052
H	6.59948505	-2.4744607	1.49596726
C	5.72216023	-3.1633631	-0.3428556
H	6.37410676	-4.0391422	-0.4096297
C	4.75335863	-2.9389133	-1.315735
H	4.64795988	-3.6454413	-2.1450679
C	3.90896977	-1.8299488	-1.248247
C	2.87229749	-1.5683315	-2.3211474
H	2.06777576	-0.9656402	-1.8596378
C	3.47047996	-0.7255451	-3.4446327
H	2.71733542	-0.5050042	-4.21927
H	4.30911612	-1.2591576	-3.926469
H	3.85853636	0.23674057	-3.0716122
C	2.23114839	-2.8333677	-2.8699591
H	1.3885931	-2.57562	-3.5322181
H	1.83977024	-3.4730523	-2.0620151
H	2.93818857	-3.4346575	-3.4678175
C	5.1428461	-0.2493156	2.04226189
H	4.57886885	0.67664643	1.82950044
C	4.48047273	-0.908907	3.24932871
H	4.51986224	-0.2504397	4.13327046
H	4.9888161	-1.8540555	3.50825457
H	3.42201782	-1.1458217	3.04767906
C	6.57946643	0.14910916	2.35732059
H	6.60688686	0.88968369	3.17350115
H	7.0868202	0.58691322	1.4816941
H	7.18046218	-0.7148765	2.68868638

NDI-In_2 **$E_{el.}$(a.u.)** = -1995.52204973

Atom	x	y	z
In	-1.3420504	-0.4436758	-0.8929826
C	3.50107973	1.43529729	-0.6061256
N	3.33324164	0.18461779	-0.2329012
In	1.33762728	-0.3286905	0.97029173
C	4.82974801	1.98029181	-1.0378533
H	4.73436513	2.60515893	-1.9386131
H	5.54110314	1.16981846	-1.2537351
H	5.27609038	2.6112666	-0.2487943
N	1.16436521	1.69395405	-0.1864223
N	-3.3164457	0.25152651	0.17792546
C	2.40010271	3.67311562	-0.7646035
H	3.34277169	4.14927334	-1.0470533
N	-1.1291461	1.72066242	-0.0439644
C	2.35131551	2.29327021	-0.554075
C	0.02225639	2.40062	-0.1609653
C	0.03743097	3.84000379	-0.2515284
C	1.26427841	4.45091721	-0.5743722
H	1.30535934	5.53797713	-0.6920877
C	-1.1827202	4.50813832	-0.0058068
H	-1.2056376	5.60190502	-0.0227519
C	-2.3263488	3.78160703	0.28098818
H	-3.2554345	4.31239203	0.50114347
C	-2.310676	2.37990191	0.24815299
C	-4.7904751	2.09928222	0.81758398
H	-4.7743924	3.17700275	1.01638548
H	-5.1389933	1.58931592	1.73226612
H	-5.5578712	1.89646771	0.0515754
C	-3.4615901	1.54910581	0.40524022
C	-4.395983	-0.6441112	0.34930438
C	-4.5260039	-1.3141724	1.58694755
C	-5.549631	-2.2508638	1.73782756
H	-5.6573804	-2.7801157	2.6905441
C	-6.4293351	-2.5305146	0.69731588
H	-7.2244177	-3.2694225	0.83263606
C	-6.288774	-1.8690576	-0.5157088
H	-6.9792002	-2.0960317	-1.3357167
C	-5.2817947	-0.9195299	-0.714094
C	-5.1487955	-0.2422551	-2.0635723
H	-4.383019	0.54930382	-1.9682659
C	-6.4449338	0.42634056	-2.5084913
H	-6.2936382	0.98580905	-3.4464091
H	-6.8241215	1.13245628	-1.7509491

H	-7.2422582	-0.3129363	-2.6963649
C	-4.6572752	-1.2272816	-3.1202681
H	-4.5193497	-0.728824	-4.0945437
H	-5.3801096	-2.0493113	-3.2630129
H	-3.6942723	-1.6831243	-2.8327496
C	-3.5322321	-1.0750121	2.70583683
H	-3.0324284	-0.1089459	2.51094955
C	-2.4539952	-2.1550991	2.6802694
H	-1.6865376	-1.9767763	3.45237824
H	-1.9437128	-2.1958179	1.70164589
H	-2.8950868	-3.1513968	2.8602812
C	-4.1814605	-0.9866612	4.08015622
H	-3.437386	-0.6975491	4.84029279
H	-4.6064094	-1.9533389	4.40096844
H	-4.9948	-0.2422912	4.10081799
C	4.35374586	-0.7870905	-0.2537589
C	5.34381056	-0.8328405	0.75098578
C	6.28470756	-1.8654375	0.71054248
H	7.05782165	-1.9160624	1.4851245
C	6.25442856	-2.8327044	-0.286479
H	7.00402798	-3.629077	-0.3026458
C	5.25881383	-2.7898918	-1.2568947
H	5.23154135	-3.5586433	-2.0362935
C	4.29051042	-1.7843322	-1.2536978
C	3.22539384	-1.7255572	-2.3292377
H	2.39930194	-1.1036396	-1.9358625
C	3.76171971	-1.0179367	-3.5705303
H	2.98480046	-0.9343438	-4.3487484
H	4.61414614	-1.5745541	-3.9990728
H	4.11465671	-0.0001832	-3.3359246
C	2.64586428	-3.0878904	-2.6798692
H	1.7929074	-2.9757363	-3.3692789
H	2.28699551	-3.6189119	-1.7825425
H	3.38253971	-3.7372903	-3.1838282
C	5.37020788	0.15928487	1.89623695
H	4.65219913	0.96647671	1.66521872
C	4.89863204	-0.5048882	3.18723989
H	4.8725502	0.21769224	4.02008183
H	5.57326489	-1.3291407	3.47687812
H	3.88733438	-0.9321267	3.07561789
C	6.73892172	0.80340492	2.08364276
H	6.69889681	1.58516623	2.86008513
H	7.10486138	1.26610235	1.15227114
H	7.49588453	0.06790955	2.40543983

NDI-Tl_2 **$E_{el.}$(a.u.)** = -1960.20578886

Atom	x	y	z
Tl	-1.3572117	-0.4530561	-1.0310144
C	3.49614246	1.49874098	-0.7199353
N	3.36948835	0.25683775	-0.3186811
Tl	1.33433258	-0.3329337	1.06010067
C	4.80028274	2.06058149	-1.2082863
H	4.66510041	2.66287563	-2.1193648
H	5.52044623	1.25867049	-1.4275962
H	5.25996634	2.71738476	-0.4483363
N	1.15935633	1.74992953	-0.2510452
N	-3.3562321	0.3383965	0.24314298
C	2.37694799	3.72505751	-0.874067
H	3.31022249	4.19825901	-1.1904088
N	-1.1261102	1.78443793	-0.015136
C	2.33232627	2.34549874	-0.6498449
C	0.02186937	2.46084283	-0.1793793
C	0.03781192	3.90118235	-0.270074
C	1.25167093	4.50757796	-0.6464081
H	1.29194471	5.5943308	-0.7687511
C	-1.1673891	4.57240023	0.03012892
H	-1.1886581	5.66641448	0.01580914
C	-2.3001296	3.84713548	0.36253891
H	-3.2178142	4.3805572	0.62044682
C	-2.2891431	2.44477147	0.31858004
C	-4.7450546	2.19793175	1.00945231
H	-4.690293	3.26520848	1.25211676
H	-5.062289	1.65992349	1.91946001
H	-5.5553968	2.0472725	0.2759896
C	-3.4529698	1.62686827	0.50913142
C	-4.4376119	-0.5384323	0.45525366
C	-4.5110262	-1.2362983	1.68316741
C	-5.5367573	-2.1638434	1.86878476
H	-5.5997813	-2.7129275	2.81436351
C	-6.4755108	-2.4099709	0.87189032
H	-7.2719133	-3.1419857	1.03399425
C	-6.3913988	-1.7223672	-0.3321092
H	-7.1281822	-1.9222658	-1.1182254
C	-5.3847743	-0.7801514	-0.5632879
C	-5.3070027	-0.0762241	-1.9031435
H	-4.5458612	0.72074493	-1.8185493
C	-6.6227748	0.58742256	-2.2930817
H	-6.506882	1.16754262	-3.2235147
H	-6.9827443	1.27382835	-1.5086905

H	-7.4191875	-0.1552421	-2.4713118
C	-4.8412905	-1.0377333	-2.9927079
H	-4.7401011	-0.523344	-3.9632917
H	-5.5596956	-1.8656227	-3.1238591
H	-3.8653327	-1.4900742	-2.7444992
C	-3.452863	-1.0339984	2.74899734
H	-2.9585445	-0.0656671	2.55132922
C	-2.3852278	-2.1184468	2.63056055
H	-1.5713034	-1.9655888	3.35979142
H	-1.9357966	-2.1342519	1.62160506
H	-2.820801	-3.1173448	2.8096307
C	-4.0194003	-0.9810807	4.16099785
H	-3.2301511	-0.7187002	4.88447567
H	-4.4332995	-1.9535685	4.47873569
H	-4.823816	-0.2320799	4.24970641
C	4.40258049	-0.6940781	-0.344596
C	5.42162264	-0.6989678	0.63290983
C	6.37569921	-1.7194035	0.59706916
H	7.16987123	-1.7362163	1.35173883
C	6.33387611	-2.7155876	-0.3709107
H	7.09455857	-3.5013871	-0.3851599
C	5.31168929	-2.7136205	-1.3146819
H	5.2751803	-3.5044724	-2.0713595
C	4.32912098	-1.7223883	-1.3134866
C	3.23297173	-1.7081646	-2.358706
H	2.4072183	-1.0953863	-1.9498896
C	3.71573004	-1.0147016	-3.6295875
H	2.91475445	-0.9645139	-4.3861728
H	4.56757105	-1.5612422	-4.0720666
H	4.05217271	0.01517658	-3.4268407
C	2.67420263	-3.0893458	-2.6672287
H	1.80003712	-3.0100762	-3.3346016
H	2.35410303	-3.6125804	-1.7507393
H	3.41051533	-3.7317725	-3.1806104
C	5.45895895	0.32570335	1.74871531
H	4.72815232	1.11807791	1.50735335
C	5.01661668	-0.3064978	3.06582921
H	4.99496916	0.43810345	3.87922775
H	5.70446227	-1.1155769	3.36710964
H	4.00862565	-0.7486019	2.98267601
C	6.82308773	0.98953054	1.89317031
H	6.78960298	1.79013854	2.6505427
H	7.16325387	1.43314872	0.94290499
H	7.59550887	0.27113594	2.21695206

NDI-C_2 **$E_{el.}$(a.u.)** = -1691.00014411

Atom	x	y	z
C	-1.4441298	0.47788291	-0.0232619
C	3.35271907	1.45983764	-0.7068866
N	2.72744494	0.28940203	-0.2689482
C	1.42238372	0.42827722	0.07617195
C	4.76662834	1.53866684	-1.1376365
H	4.99638356	2.54599774	-1.5149037
H	4.98186236	0.81815856	-1.9458522
H	5.4732869	1.31542572	-0.3188897
N	1.20499711	1.76253216	-0.1961841
N	-2.7656161	0.42460374	0.28026103
C	2.39400575	3.83912609	-0.7973309
H	3.31379563	4.33366306	-1.1200327
N	-1.1815719	1.82314017	0.13005644
C	2.38772899	2.42542219	-0.6325663
C	0.02535383	2.47985338	-0.0598084
C	0.05132503	3.86460356	-0.1253327
C	1.2698658	4.53595976	-0.5005412
H	1.24979787	5.62732627	-0.5728558
C	-1.1430711	4.61340839	0.17244187
H	-1.0800838	5.70527191	0.14806473
C	-2.3002136	3.99017146	0.50442171
H	-3.2048176	4.54714893	0.76169751
C	-2.3485324	2.56840227	0.46483685
C	-4.7844108	1.8066157	0.93497004
H	-5.0228913	2.86220262	1.1305959
H	-5.0478887	1.22734031	1.83772267
H	-5.4485685	1.45047347	0.12766026
C	-3.3550049	1.65060169	0.58673493
C	-3.4816485	-0.813691	0.29498945
C	-3.4856325	-1.5651552	1.48043361
C	-4.1909815	-2.771814	1.47705028
H	-4.2121721	-3.3881849	2.38084239
C	-4.8614896	-3.2032903	0.3377705
H	-5.4086825	-4.1505772	0.3548783
C	-4.8357208	-2.4410964	-0.825191
H	-5.3586052	-2.7996352	-1.7170516
C	-4.1433332	-1.2281891	-0.8707257
C	-4.0282437	-0.4313228	-2.1524271
H	-3.8547168	0.62544819	-1.8748779
C	-5.2833581	-0.4790899	-3.0106799
H	-5.1913774	0.21425831	-3.8622547
H	-6.1844489	-0.1991824	-2.4394583

H	-5.4539704	-1.4831153	-3.4358848
C	-2.8016963	-0.900792	-2.9336755
H	-2.6769265	-0.3162867	-3.8608333
H	-2.9087121	-1.9641666	-3.2124587
H	-1.8867033	-0.7959556	-2.3266812
C	-2.6887804	-1.1188608	2.68799314
H	-2.6118263	-0.0156144	2.64790437
C	-1.2674983	-1.6768996	2.60770358
H	-0.6769936	-1.3614393	3.48445517
H	-0.7461687	-1.3313659	1.69825383
H	-1.2917112	-2.7811537	2.59557778
C	-3.3496351	-1.4812203	4.00993431
H	-2.8035671	-1.0193475	4.84823362
H	-3.3421949	-2.570264	4.1890637
H	-4.3975991	-1.1398968	4.05657958
C	3.39208249	-0.9765751	-0.2059562
C	4.30615756	-1.2020329	0.83519133
C	5.00188373	-2.4141077	0.8405497
H	5.72501879	-2.6213472	1.63481506
C	4.77258665	-3.3669573	-0.1443432
H	5.328309	-4.3093127	-0.1306678
C	3.81948464	-3.1420018	-1.1320175
H	3.62916389	-3.9210253	-1.874583
C	3.09763217	-1.9458993	-1.1832684
C	2.02141209	-1.7073166	-2.2263528
H	1.17010536	-1.2463668	-1.6879913
C	2.48093203	-0.7279471	-3.3048601
H	1.691705	-0.5911649	-4.0626003
H	3.38078453	-1.1084544	-3.8213928
H	2.71626525	0.26844275	-2.8981161
C	1.51410888	-2.9869933	-2.8717116
H	0.64921979	-2.7647894	-3.5167474
H	1.19099004	-3.7288243	-2.1240347
H	2.27923781	-3.4588784	-3.5138058
C	4.43108584	-0.2185076	1.98032979
H	4.23199687	0.79472244	1.58624616
C	3.34335031	-0.5180421	3.01155694
H	3.38069845	0.20284827	3.84545424
H	3.48019176	-1.5309434	3.42951778
H	2.33975193	-0.472849	2.55653542
C	5.80878046	-0.1957674	2.62371323
H	5.87242731	0.61904601	3.36279182
H	6.60990846	-0.0443465	1.88053004
H	6.02618722	-1.1325905	3.1649391

NDI-Si$_2$ **$E_{el.}$(a.u.)** = -2193.84530791

Atom	x	y	z
Si	-1.4700557	-0.2258302	-2.847E-05
C	3.53748169	1.51208733	0.00061895
N	3.21299786	0.17698706	-0.0001238
Si	1.47011193	-0.2258401	-0.0008182
C	4.95747979	1.95310037	0.00142803
H	5.04741631	3.04711559	0.00139624
H	5.49974238	1.56923411	-0.8805879
H	5.49871159	1.56941083	0.88416429
N	1.19547011	1.59772116	-0.0000309
N	-3.2129425	0.17695683	-0.000233
C	2.41682618	3.74221089	0.00104465
H	3.37206334	4.27141415	0.00159663
N	-1.195429	1.59771819	-0.0003269
C	2.42022244	2.32085831	0.00061408
C	2.1001E-05	2.3014958	-9.672E-05
C	1.5604E-05	3.6988537	0.00010241
C	1.24029199	4.4125884	0.00071051
H	1.20920546	5.50595862	0.00096151
C	-1.240265	4.41258185	-0.000262
H	-1.2091823	5.50595217	-0.0002156
C	-2.4167962	3.74220131	-0.000664
H	-3.372035	4.27140282	-0.0009531
C	-2.4201881	2.32084517	-0.0006137
C	-4.9574385	1.95308757	-0.0008179
H	-5.0473588	3.04710227	-0.0009506
H	-5.499302	1.56940242	0.88152757
H	-5.4990844	1.56921695	-0.8832171
C	-3.5374403	1.51206652	-0.0005933
C	-4.2285549	-0.8268215	-0.0001645
C	-4.7108398	-1.3179377	1.22899451
C	-5.6741881	-2.3299412	1.20303523
H	-6.0546451	-2.7339379	2.14693598
C	-6.1518746	-2.8356316	0.0000173
H	-6.9036429	-3.6303223	9.6122E-05
C	-5.6738249	-2.3305097	-1.2030941
H	-6.0539842	-2.7349588	-2.1469202
C	-4.710449	-1.3185348	-1.229244
C	-4.1801475	-0.8101936	-2.5543868
H	-3.6439335	0.13637781	-2.3604989
C	-5.2883068	-0.5105018	-3.5564314
H	-4.8720079	-0.0333565	-4.4586019
H	-6.0507387	0.16610804	-3.13615

H	-5.8045059	-1.4275249	-3.8885038
C	-3.1706853	-1.7963966	-3.1361974
H	-2.7573985	-1.4238747	-4.0883802
H	-3.6459974	-2.7735827	-3.3326152
H	-2.3290218	-1.9676195	-2.4440442
C	-4.1809491	-0.8088967	2.55403157
H	-3.6450832	0.13781327	2.35985332
C	-3.1711711	-1.7944819	3.13634067
H	-2.7581888	-1.4214665	4.08846265
H	-2.3293264	-1.9656039	2.44438176
H	-3.6461209	-2.7717932	3.33301226
C	-5.289361	-0.5092577	3.5558083
H	-4.8733753	-0.0316037	4.45785425
H	-5.8052438	-1.4263546	3.88816896
H	-6.0520084	0.16688905	3.13517001
C	4.22856682	-0.8268379	9.2821E-05
C	4.70998265	-1.3186675	1.22930767
C	5.67325933	-2.3307514	1.20342793
H	6.0530201	-2.7353362	2.14735965
C	6.15172748	-2.8357944	0.00045495
H	6.90342969	-3.6305479	0.00059175
C	5.67455127	-2.3299406	-1.2027018
H	6.05535023	-2.733874	-2.1464877
C	4.71126637	-1.317891	-1.2289312
C	4.18183583	-0.8087246	-2.5541017
H	3.64600446	0.13802612	-2.3600296
C	5.29055471	-0.509151	-3.5555592
H	4.87486168	-0.0313541	-4.4576634
H	5.80636763	-1.4262989	-3.887889
H	6.05320473	0.16683647	-3.1346733
C	3.17214436	-1.7941846	-3.1367828
H	2.75948779	-1.4210673	-4.0890058
H	2.33006904	-1.9653003	-2.4450982
H	3.64708465	-2.7715161	-3.3333777
C	4.17929614	-0.8103215	2.55430375
H	3.643191	0.13628021	2.36025366
C	3.16959659	-1.7964514	3.13581587
H	2.75597346	-1.4238471	4.08782004
H	3.64479339	-2.7736423	3.33248911
H	2.32818047	-1.9676919	2.44337012
C	5.28717886	-0.5106665	3.55666807
H	4.87063005	-0.0336228	4.4587798
H	6.04968142	0.16601327	3.13664248
H	5.80333941	-1.4276933	3.8887815

NDI-Ge_2 **$E_{el.}$(a.u.)** = -5768.46681031

Atom	x	y	z
Ge	-1.4722567	-0.3393777	-0.0280517
C	3.5552591	1.52742187	0.06968424
N	3.29978166	0.18853819	0.01301898
Ge	1.47231986	-0.3393034	-0.0271849
C	4.9607043	2.02016116	0.1013581
H	5.01988823	3.11498483	0.13731444
H	5.52434631	1.68092099	-0.7853498
H	5.50473696	1.62449446	0.97706314
N	1.1918876	1.60553221	0.05633566
N	-3.2997244	0.18849132	0.01252194
C	2.41406751	3.73530322	0.15068497
H	3.36804972	4.26535377	0.17619037
N	-1.1918161	1.60547721	0.05623228
C	2.4150021	2.31700738	0.09354243
C	2.3183E-05	2.30155638	0.08438546
C	-8.5E-08	3.70581524	0.1427234
C	1.23859837	4.41257998	0.1732552
H	1.21333268	5.50528255	0.2170699
C	-1.2386075	4.41254205	0.17345901
H	-1.2133733	5.50524407	0.21727878
C	-2.4140514	3.73520812	0.15109926
H	-3.3680569	4.26520765	0.17681576
C	-2.4149324	2.31692497	0.09376952
C	-4.9606321	2.02004321	0.10235682
H	-5.0198721	3.11492278	0.13666491
H	-5.5036457	1.62571645	0.97931969
H	-5.5252604	1.67934857	-0.7831433
C	-3.5551918	1.52732968	0.06980834
C	-4.352231	-0.7699133	-0.025893
C	-4.846676	-1.3025415	1.18228109
C	-5.8422104	-2.280798	1.11618586
H	-6.2317568	-2.7142794	2.04331848
C	-6.3418109	-2.7163792	-0.1053859
H	-7.11901	-3.4855638	-0.1366256
C	-5.8525253	-2.1724497	-1.2868201
H	-6.2506616	-2.5204471	-2.2458443
C	-4.8570611	-1.1917763	-1.2728873
C	-4.3237774	-0.6360006	-2.5777377
H	-3.7224435	0.25983954	-2.3386776
C	-5.4350666	-0.2031769	-3.5268628
H	-5.0119171	0.29585441	-4.4139499
H	-6.1362662	0.49854387	-3.0457199

H	-6.0236945	-1.0624175	-3.8913285
C	-3.3959138	-1.6436235	-3.2507882
H	-2.9812505	-1.2352935	-4.1875332
H	-3.9369764	-2.5738616	-3.4981043
H	-2.5504306	-1.9145421	-2.5961768
C	-4.2975032	-0.8688317	2.52623716
H	-3.7197407	0.05962178	2.36749014
C	-3.3339083	-1.9184315	3.07345236
H	-2.9071674	-1.5993455	4.03900169
H	-2.4973835	-2.1010583	2.37771835
H	-3.8503983	-2.8812627	3.23334345
C	-5.3944688	-0.5589057	3.53759804
H	-4.9606584	-0.1371592	4.45895756
H	-5.9534204	-1.4638714	3.83136909
H	-6.1234885	0.16783339	3.14267629
C	4.35225797	-0.7698808	-0.0259972
C	4.84724217	-1.3027064	1.1818746
C	5.84264823	-2.2810483	1.11517605
H	6.23259868	-2.7146917	2.04206247
C	6.34160369	-2.7165379	-0.1066915
H	7.11870508	-3.4858017	-0.1384124
C	5.85178982	-2.1724267	-1.2878217
H	6.24943763	-2.5203776	-2.2470702
C	4.856434	-1.1916501	-1.2732913
C	4.32257721	-0.6356817	-2.5778271
H	3.72090126	0.25981362	-2.338352
C	5.43351526	-0.202043	-3.5269886
H	5.01000861	0.29683393	-4.4139921
H	6.02268793	-1.0608712	-3.8915434
H	6.13430866	0.50006355	-3.0458092
C	3.39496678	-1.6434521	-3.2510015
H	2.97985739	-1.2349232	-4.1874582
H	2.54979846	-1.9149405	-2.59622
H	3.93632273	-2.5733733	-3.4988576
C	4.29873867	-0.8691201	2.52614065
H	3.72155714	0.05977576	2.36787819
C	3.3346039	-1.918287	3.07322602
H	2.9083213	-1.599277	4.03900252
H	3.85052556	-2.8815062	3.2326382
H	2.49778015	-2.1001491	2.37765489
C	5.39616503	-0.5603433	3.53735349
H	4.96287539	-0.1384572	4.45889262
H	6.12573477	0.16586178	3.14248173
H	5.95439845	-1.4658488	3.83082737

NDI-Sn_2 **$E_{el.}$(a.u.)** = -2043.85651427

Atom	x	y	z
Sn	-1.5347941	-0.6090071	-0.0003038
C	3.59858839	1.55687077	0.00170257
N	3.50176692	0.21538855	0.00047105
Sn	1.5301031	-0.6357347	-0.0005532
C	4.93210802	2.24175906	0.00273134
H	5.0633261	2.88607774	-0.8833909
H	5.7537373	1.51075284	0.00268204
H	5.06244068	2.88498607	0.88977271
N	1.17898583	1.57450345	0.00125604
N	-3.5047911	0.22643801	2.9958E-05
C	2.40843408	3.69308204	0.00300627
H	3.36558949	4.21767112	0.00367047
N	-1.199786	1.59027427	0.00090393
C	2.39636024	2.2823291	0.00205651
C	-0.0057786	2.2667405	0.00145002
C	0.00329942	3.69032626	0.00220706
C	1.23562705	4.38764117	0.00301552
H	1.21980031	5.48132685	0.00364741
C	-1.2249314	4.39863127	0.0021581
H	-1.1990336	5.49212037	0.00258373
C	-2.404465	3.71946179	0.00160649
H	-3.3489909	4.2643663	0.00155096
C	-2.4168967	2.30577402	0.00108068
C	-4.9775228	2.18095634	0.00065567
H	-4.9693719	3.27620263	0.00206191
H	-5.555652	1.8483511	0.8801063
H	-5.5546683	1.8505505	-0.8802888
C	-3.6124658	1.57139794	0.00066576
C	-4.6469503	-0.6181273	-0.0003515
C	-5.1895484	-1.0547497	1.22753455
C	-6.2701317	-1.9402337	1.20060061
H	-6.6966142	-2.2941073	2.14553112
C	-6.8092663	-2.3830095	-0.0011404
H	-7.6535387	-3.0785434	-0.0014448
C	-6.2700405	-1.9392739	-1.2024785
H	-6.6964411	-2.292373	-2.1477368
C	-5.189467	-1.0537402	-1.2286144
C	-4.6179065	-0.609063	-2.5599704
H	-3.8773392	0.18588629	-2.3590933
C	-5.6836883	-0.0231844	-3.479354
H	-5.2256162	0.37571664	-4.399279
H	-6.2372834	0.79765551	-2.9939962

H	-6.4224365	-0.7827589	-3.787669
C	-3.8812597	-1.7568493	-3.2438371
H	-3.4359852	-1.4288632	-4.1978832
H	-4.5662681	-2.5947573	-3.4621802
H	-3.0680025	-2.1499142	-2.6102572
C	-4.6180202	-0.61125	2.55930131
H	-3.8773985	0.1838325	2.35919022
C	-3.8814481	-1.7596938	3.24214298
H	-3.4361333	-1.4325824	4.19647101
H	-3.0682282	-2.1522163	2.60817323
H	-4.566497	-2.5977594	3.45974795
C	-5.6838059	-0.0261143	3.47915651
H	-5.2257506	0.37191879	4.399465
H	-6.4226523	-0.7858874	3.78674789
H	-6.2372812	0.79522358	2.99450372
C	4.63233379	-0.6426992	-0.000375
C	5.16938706	-1.0848993	1.22735059
C	6.2343729	-1.9892793	1.19994942
H	6.65849143	-2.3453644	2.14523423
C	6.76392799	-2.4427809	-0.0022172
H	7.59610821	-3.1527256	-0.0029439
C	6.2343112	-1.9868924	-1.2034556
H	6.65841332	-2.3410876	-2.149456
C	5.16932239	-1.0824573	-1.2290166
C	4.62803555	-0.6003034	-2.5593961
H	3.85163291	0.15765898	-2.3515462
C	5.7116985	0.07023301	-3.3973043
H	5.28456536	0.49332912	-4.321485
H	6.49636999	-0.6455022	-3.697765
H	6.20466431	0.8877285	-2.8458763
C	3.96064366	-1.7350513	-3.3293618
H	3.53427934	-1.369616	-4.2783698
H	3.14307813	-2.1910756	-2.7458928
H	4.68189256	-2.5344952	-3.573196
C	4.62813449	-0.6053995	2.55870215
H	3.85195788	0.15319405	2.35238951
C	3.96034499	-1.7416321	3.32611437
H	3.53418653	-1.3782122	4.2759862
H	4.68126484	-2.5419533	3.56803137
H	3.14255165	-2.1959249	2.74160006
C	5.71194505	0.06307368	3.39806897
H	5.28491774	0.48425984	4.32316969
H	6.20506024	0.88167813	2.84840532
H	6.49648736	-0.6534684	3.69694045

NDI-Pb_2 **$E_{el.}$(a.u.)** = -2000.89756001

Atom	x	y	z
Pb	-1.5539249	-0.6352153	0.03782159
C	3.61743557	1.66881902	-0.0056494
N	3.58118292	0.33440739	0.01176337
Pb	1.54920394	-0.6670984	0.04975935
C	4.93120115	2.39694947	-0.0156431
H	5.03789298	3.04375839	-0.9025573
H	5.77355001	1.68997545	-0.0190166
H	5.04758954	3.04268839	0.87121027
N	1.17559069	1.67564988	0.00467128
N	-3.5854458	0.34688807	-0.0115268
C	2.40607941	3.78363595	-0.0194424
H	3.36112343	4.31117182	-0.0234018
N	-1.1989118	1.692799	-0.0059
C	2.39196882	2.37648775	-0.0060586
C	-0.0067605	2.36127398	-0.0090616
C	0.00325894	3.79439688	-0.0271813
C	1.23332029	4.48551977	-0.0287366
H	1.22324371	5.57924607	-0.0400388
C	-1.222338	4.49789617	-0.0442772
H	-1.200843	5.5914334	-0.0571536
C	-2.4023551	3.81274347	-0.047234
H	-3.3437696	4.36167599	-0.0629807
C	-2.4144551	2.40236986	-0.0294548
C	-4.9808856	2.33861669	-0.0647321
H	-4.9511505	3.43245934	-0.0854314
H	-5.5780074	2.03532507	0.81242091
H	-5.5533676	2.00215531	-0.9461916
C	-3.6325832	1.68635397	-0.034338
C	-4.7525358	-0.4563345	-0.0153858
C	-5.3266679	-0.8586613	1.2108281
C	-6.4303297	-1.7149963	1.18188078
H	-6.8802437	-2.0402931	2.1263549
C	-6.9635935	-2.164344	-0.0201154
H	-7.8266729	-2.836369	-0.0218754
C	-6.3930758	-1.7565875	-1.2199109
H	-6.8139003	-2.1145555	-2.1659679
C	-5.2886734	-0.9011923	-1.2442494
C	-4.6833978	-0.4970269	-2.5736402
H	-3.9186732	0.27491504	-2.3735905
C	-5.7154175	0.11035059	-3.517301
H	-5.2317097	0.4775228	-4.4373392
H	-6.2457856	0.95817282	-3.0528696

H	-6.4768144	-0.6277723	-3.8227645
C	-3.976894	-1.6792615	-3.2299943
H	-3.5052531	-1.3808542	-4.1810785
H	-4.6865219	-2.4967147	-3.4473804
H	-3.1865926	-2.0908685	-2.578848
C	-4.7641777	-0.4076252	2.54390816
H	-3.9834828	0.34744335	2.34110211
C	-4.0960914	-1.5692056	3.27294583
H	-3.6527929	-1.2362668	4.22617939
H	-3.2901298	-2.0173217	2.66665623
H	-4.8230434	-2.368403	3.50056396
C	-5.8228033	0.24894612	3.42326465
H	-5.3695246	0.64607173	4.34638075
H	-6.6053694	-0.467392	3.72711495
H	-6.3236608	1.08439551	2.90645002
C	4.73491944	-0.4852056	-0.0199765
C	5.32260633	-0.9094451	1.19164672
C	6.40829151	-1.7871134	1.13398967
H	6.87083364	-2.1277264	2.06696737
C	6.91127755	-2.2331843	-0.0824711
H	7.76134995	-2.9211415	-0.1068748
C	6.33101009	-1.7975741	-1.2677871
H	6.73425474	-2.1459172	-2.2251223
C	5.24222426	-0.9216098	-1.2637921
C	4.65588224	-0.449152	-2.5787619
H	3.79625201	0.20518793	-2.3475853
C	5.66575613	0.38084891	-3.3658227
H	5.21089348	0.78309029	-4.2862023
H	6.53963732	-0.2232468	-3.6657931
H	6.040942	1.23125189	-2.7730721
C	4.12823622	-1.6105199	-3.4133406
H	3.65577921	-1.2437608	-4.3396096
H	3.37411699	-2.1951123	-2.8600703
H	4.93706857	-2.3021879	-3.706127
C	4.80892997	-0.4381213	2.53674546
H	4.01267227	0.30464614	2.35000467
C	4.18402864	-1.5859701	3.32293924
H	3.77728831	-1.230486	4.28425742
H	4.92625108	-2.3727514	3.54400877
H	3.35821041	-2.0561171	2.76233159
C	5.90114549	0.25135241	3.34749558
H	5.49035165	0.66536935	4.28312196
H	6.36469825	1.07842785	2.78497997
H	6.70629587	-0.4501986	3.62643035

NDI-N_2 **$E_{el.}$(a.u.)** = -1724.18705878

Atom	x	y	z
N	-1.2990943	0.62988073	0.19800731
C	3.19883856	1.55047612	-0.8381573
N	2.61651657	0.40903277	-0.3095738
N	1.42286873	0.65716717	0.29848439
C	4.45083784	1.53853306	-1.6274643
H	4.61275317	2.52083554	-2.0935433
H	4.39217126	0.78531625	-2.433308
H	5.34605851	1.29421355	-1.0298325
N	1.20456804	1.95963447	0.0156209
N	-2.59133	0.42552066	0.58362522
C	2.2914057	3.99385113	-0.7445147
H	3.1578602	4.50153387	-1.1731554
N	-1.1196346	1.94849378	0.44983676
C	2.32020036	2.57852041	-0.5844416
C	0.03965116	2.62162115	0.23975906
C	0.02754709	4.0469452	0.19894154
C	1.1872707	4.69277921	-0.3067952
H	1.174422	5.78538712	-0.3738685
C	-1.1610565	4.69944454	0.63176231
H	-1.1622878	5.79394625	0.65674002
C	-2.2879977	4.00701851	1.00795541
H	-3.1892244	4.52082523	1.34879182
C	-2.3022469	2.58745367	0.87705191
C	-4.6268372	1.58620938	1.47437384
H	-4.9020158	2.58629929	1.83713072
H	-4.7576539	0.87203303	2.30632234
H	-5.3483821	1.29640913	0.69010625
C	-3.2290899	1.57638781	0.99007953
C	-3.1085932	-0.887056	0.42653783
C	-2.7167257	-1.8787667	1.34229155
C	-3.1951474	-3.175376	1.13360687
H	-2.9081328	-3.973279	1.82571731
C	-4.027733	-3.4656288	0.05909296
H	-4.3946538	-4.4863052	-0.0842674
C	-4.3875351	-2.469636	-0.8440441
H	-5.0241983	-2.721559	-1.6973404
C	-3.9227009	-1.1622216	-0.6888929
C	-4.1728582	-0.1070929	-1.7465574
H	-4.151584	0.88291144	-1.2567502
C	-5.5200238	-0.2432579	-2.438967
H	-5.6957941	0.61618944	-3.1056509
H	-6.3518715	-0.2891256	-1.7161482

H	-5.5709166	-1.1484892	-3.0679809
C	-3.0268532	-0.1220588	-2.7578954
H	-3.1546696	0.67264704	-3.5117518
H	-2.992685	-1.0910021	-3.2885476
H	-2.0549385	0.02833141	-2.256902
C	-1.7674002	-1.5718619	2.47928312
H	-1.7803795	-0.4771753	2.63444368
C	-0.3398585	-1.9612441	2.09526173
H	0.35795266	-1.7421028	2.92070504
H	0.00418647	-1.3987552	1.21239114
H	-0.274585	-3.0429065	1.87805641
C	-2.1864869	-2.2290757	3.78753853
H	-1.5442268	-1.88019	4.61227873
H	-2.0845843	-3.3272565	3.74829377
H	-3.2324075	-1.9978335	4.04928872
C	3.02900555	-0.9412028	-0.4378875
C	4.22264616	-1.3400747	0.19606271
C	4.65240925	-2.6561843	0.01146663
H	5.58117196	-2.9944124	0.48017404
C	3.89229656	-3.5557187	-0.7267543
H	4.2404501	-4.5843772	-0.8592737
C	2.67226649	-3.1621948	-1.2689327
H	2.07037068	-3.8934488	-1.8150305
C	2.20540812	-1.8526364	-1.1399012
C	0.88164116	-1.4264222	-1.7439907
H	0.38119432	-0.7780938	-1.0032729
C	1.0970778	-0.5856207	-3.0007516
H	0.12877404	-0.261287	-3.4185329
H	1.62444364	-1.1652298	-3.7799243
H	1.68727292	0.32394776	-2.7977929
C	-0.0683634	-2.5799367	-2.0229189
H	-1.0620782	-2.1825802	-2.2901048
H	-0.2020597	-3.2243625	-1.1377242
H	0.26568928	-3.2160988	-2.8625377
C	4.91192334	-0.4305059	1.19434942
H	4.77346608	0.61684708	0.87762628
C	4.20979748	-0.5714533	2.5448019
H	4.6634182	0.09407623	3.29834336
H	4.28587674	-1.6093483	2.91384446
H	3.1399212	-0.3196168	2.4621047
C	6.40780387	-0.6712646	1.32151296
H	6.86457993	0.09290331	1.97083572
H	6.91511689	-0.6339419	0.34258489
H	6.63180158	-1.6504743	1.77827756

NDI-P_2 **$E_{el.}$(a.u.)** = -2297.45124003

Atom	x	y	z
P	-1.0486181	-0.3359569	-0.0368674
C	3.64559165	1.39095947	0.17290336
N	3.57684004	0.11691146	0.01718246
P	1.04843701	-0.3359622	0.037644
C	4.93947333	2.1279659	0.39057605
H	4.91470402	2.73093646	1.31217766
H	5.16047799	2.81098466	-0.4464466
H	5.7706997	1.41224592	0.46878217
N	1.17393291	1.44336136	0.05483434
N	-3.5768864	0.11693718	-0.0169749
C	2.39768626	3.52655425	0.179819
H	3.35542443	4.04451899	0.25397971
N	-1.1740686	1.4433896	-0.0540995
C	2.40965965	2.13852751	0.14454812
C	-6.108E-05	2.1555143	0.00035955
C	-3.781E-05	3.58562989	0.00034039
C	1.23270716	4.25668683	0.10421926
H	1.24108931	5.34884733	0.11859104
C	-1.2327668	4.25672162	-0.1035581
H	-1.2411145	5.34888193	-0.1179738
C	-2.3977652	3.52662274	-0.1791146
H	-3.3554846	4.04461511	-0.2533257
C	-2.4097792	2.13859334	-0.1437976
C	-4.9395953	2.1280388	-0.3898793
H	-4.915301	2.72993267	-1.3122128
H	-5.1599077	2.81206466	0.44648733
H	-5.7710142	1.41239888	-0.4667617
C	-3.645699	1.3910279	-0.1723195
C	-4.6449018	-0.7763807	-0.0640046
C	-5.371824	-1.0665888	1.1156789
C	-6.3827923	-2.0250125	1.05304126
H	-6.9581117	-2.2604934	1.95330045
C	-6.6781065	-2.6897316	-0.1348896
H	-7.4769815	-3.4362434	-0.162238
C	-5.9514507	-2.3990169	-1.2816683
H	-6.184043	-2.9232433	-2.2156233
C	-4.9259591	-1.449228	-1.2716417
C	-4.1495395	-1.1559816	-2.53878
H	-3.3752719	-0.4087756	-2.2893802
C	-5.0453599	-0.5494843	-3.6136989
H	-4.4624412	-0.2802413	-4.5104986
H	-5.5514163	0.36081824	-3.2505883

H	-5.83106	-1.2571511	-3.9309027
C	-3.4212994	-2.3933534	-3.0500973
H	-2.8162408	-2.1536889	-3.9405927
H	-4.126428	-3.1932494	-3.3357902
H	-2.746445	-2.8010993	-2.2800046
C	-4.9952602	-0.3876741	2.4163195
H	-4.7267352	0.65997628	2.1791849
C	-3.7552336	-1.0512327	3.01299696
H	-3.4387301	-0.5442263	3.9401702
H	-2.9092578	-1.0365633	2.30705408
H	-3.970568	-2.10599	3.25837629
C	-6.119919	-0.3436619	3.43853573
H	-5.8238298	0.26720412	4.30672338
H	-6.3600106	-1.3492356	3.8252048
H	-7.0451391	0.08531542	3.01999766
C	4.64497491	-0.7762963	0.06376893
C	4.92644962	-1.4494081	1.27116024
C	5.95206092	-2.3990771	1.28066315
H	6.18496966	-2.9235263	2.21441373
C	6.67844374	-2.6894118	0.13361721
H	7.47741381	-3.4358365	0.1605592
C	6.38273018	-2.0244209	-1.0540624
H	6.95784044	-2.259595	-1.9545348
C	5.37163095	-1.0661046	-1.1161792
C	4.99463959	-0.3869055	-2.4165489
H	4.72608323	0.66066153	-2.1790867
C	6.1190111	-0.3425432	-3.4390667
H	5.82262416	0.2685004	-4.3070277
H	6.35909411	-1.3480025	-3.8260389
H	7.0443052	0.08642328	-3.0206812
C	3.75450408	-1.0504263	-3.0130427
H	3.43769806	-0.5432167	-3.9400014
H	2.90872461	-1.0360026	-2.3068593
H	3.96986159	-2.1051037	-3.2587453
C	4.15027655	-1.1566828	2.53856987
H	3.37616705	-0.4091319	2.28971163
C	3.42179627	-2.3941972	3.04922195
H	2.81688209	-2.1549383	3.93992523
H	4.12679519	-3.1944093	3.3343511
H	2.74678158	-2.8013575	2.27896191
C	5.04635019	-0.5510804	3.61377926
H	4.46354505	-0.2821134	4.5107348
H	5.55272678	0.35923588	3.25115351
H	5.83180025	-1.2591892	3.93061304

NDI-As$_2$ **$E_{el.}$(a.u.)** = -6086.07057028

Atom	x	y	z
As	-1.126699	-0.467016	-0.2552835
C	3.62904444	1.44185038	0.31547867
N	3.57272486	0.17130857	0.1008533
As	1.12719762	-0.4658744	0.25922886
C	4.92560233	2.18344241	0.49183503
H	4.92830718	2.78044038	1.41737187
H	5.11339107	2.87376494	-0.3474081
H	5.76396227	1.47344815	0.53825187
N	1.1672773	1.46542956	0.19860668
N	-3.5729285	0.17075954	-0.1019408
C	2.36557743	3.55535826	0.43650145
H	3.30943353	4.08256985	0.58665183
N	-1.1671432	1.46464085	-0.2022167
C	2.38567146	2.16892963	0.3641202
C	4.2697E-05	2.15273638	-0.0030287
C	6.2914E-05	3.59086702	-0.0055452
C	1.20120805	4.27087541	0.2678476
H	1.19288961	5.36291847	0.30078547
C	-1.201095	4.26986977	-0.2812917
H	-1.1928394	5.36179137	-0.3180351
C	-2.3654151	3.55371026	-0.4475581
H	-3.3092488	4.08039992	-0.5996122
C	-2.3855236	2.1675306	-0.3704116
C	-4.9254152	2.18205545	-0.4984512
H	-4.9281404	2.77624274	-1.4257936
H	-5.112912	2.87495818	0.33872593
H	-5.7639505	1.47211735	-0.5425801
C	-3.629002	1.4407105	-0.3199705
C	-4.6600566	-0.6974799	-8.133E-05
C	-5.2954989	-0.8822186	1.25156048
C	-6.3252895	-1.8183044	1.34253008
H	-6.8289629	-1.972875	2.30168056
C	-6.7288721	-2.5604759	0.23545166
H	-7.5408409	-3.287419	0.32800767
C	-6.0942066	-2.3710515	-0.9847147
H	-6.4128443	-2.9548341	-1.8557614
C	-5.0530571	-1.4493327	-1.127861
C	-4.3859334	-1.2654491	-2.475254
H	-3.5646529	-0.5385828	-2.3428046
C	-5.3544342	-0.6869476	-3.5020094
H	-4.847476	-0.5006902	-4.4636503
H	-5.7900381	0.26603802	-3.1582261

H	-6.1925606	-1.3782032	-3.6986115
C	-3.758649	-2.5612034	-2.975792
H	-3.2234458	-2.3966183	-3.9259776
H	-4.5200116	-3.3396588	-3.1574717
H	-3.0381768	-2.9630186	-2.2447978
C	-4.8104033	-0.1215893	2.46856814
H	-4.4724928	0.87490005	2.12700653
C	-3.6006902	-0.8258849	3.0796666
H	-3.2120729	-0.2695806	3.94926429
H	-2.7812514	-0.9325901	2.34994052
H	-3.8812729	-1.8380784	3.4202348
C	-5.8849298	0.10393987	3.52120609
H	-5.5116534	0.77533501	4.3114856
H	-6.1772172	-0.8374711	4.01760132
H	-6.7953063	0.55434	3.09268713
C	4.65981556	-0.6972713	0.00139907
C	5.05396353	-1.4448484	1.13161727
C	6.09502699	-2.367063	0.99091955
H	6.41446108	-2.9476343	1.8638204
C	6.72859498	-2.5609798	-0.229092
H	7.54050041	-3.2882388	-0.3196927
C	6.32404135	-1.8228557	-1.3385149
H	6.8269512	-1.9808674	-2.2975065
C	5.29428391	-0.8864898	-1.2500889
C	4.80843959	-0.1300236	-2.4693772
H	4.4709733	0.86770808	-2.1310031
C	5.88230202	0.09167492	-3.5235174
H	5.50865594	0.76058449	-4.3157267
H	6.17385651	-0.8514935	-4.017004
H	6.79317477	0.54318057	-3.0972172
C	3.59826813	-0.8361383	-3.0774527
H	3.20938372	-0.2826817	-3.9487458
H	2.77910788	-0.940273	-2.347068
H	3.87853549	-1.8495095	-3.4147644
C	4.38791714	-1.2564649	2.47892441
H	3.5677025	-0.5286281	2.34520793
C	3.75892181	-2.5501332	2.98280676
H	3.22440053	-2.3826111	3.93286709
H	4.51936228	-3.3291761	3.16585742
H	3.03759163	-2.9527346	2.25310256
C	5.3576903	-0.6770743	3.50397174
H	4.85117253	-0.4873241	4.46515653
H	5.79504122	0.27417791	3.15762332
H	6.19452787	-1.3693381	3.70245811

NDI-Sb_2 **$E_{el.}$(a.u.)** = -2095.66982056

Atom	x	y	z
Sb	-1.3417206	0.34555686	-0.7963509
C	3.56451198	-1.5618868	0.18774163
N	3.4521383	-0.26816	0.04261929
Sb	1.25713983	0.64211111	0.24377956
C	4.87712389	-2.2775691	0.06118379
H	5.13172704	-2.8099157	0.99227685
H	5.69038848	-1.5694071	-0.1536802
H	4.85253861	-3.0279828	-0.7460543
N	1.14924798	-1.5946078	0.38933343
N	-3.4596364	-0.2441545	0.06584427
C	2.38550874	-3.6515255	0.73567924
H	3.34481503	-4.1697758	0.79424808
N	-1.1933298	-1.6578659	0.14077828
C	2.36652986	-2.2844402	0.46854618
C	-0.019722	-2.2834921	0.41547043
C	-0.0224743	-3.6893229	0.73274223
C	1.2094247	-4.3490983	0.90107421
H	1.20924764	-5.4199239	1.12168269
C	-1.2587009	-4.3575276	0.86817981
H	-1.2567204	-5.4216947	1.11879063
C	-2.4327372	-3.6483197	0.76182213
H	-3.3901064	-4.1348101	0.96247585
C	-2.4125823	-2.2939103	0.43000324
C	-4.878736	-2.037357	0.98209489
H	-4.782302	-2.4567075	1.99622884
H	-5.2355149	-2.8492192	0.32587445
H	-5.6561212	-1.2597224	1.00192504
C	-3.5788637	-1.4818968	0.48099858
C	-4.4735254	0.72904751	0.1067651
C	-5.3694577	0.85281968	-0.9772893
C	-6.313639	1.88185814	-0.9433687
H	-7.0148279	1.99181028	-1.7780365
C	-6.3771701	2.76895584	0.12515831
H	-7.1251267	3.56706108	0.13286683
C	-5.4838515	2.63829055	1.18247158
H	-5.5387059	3.33714439	2.0244382
C	-4.5178427	1.6296119	1.1934301
C	-3.5814786	1.48469372	2.37594376
H	-2.819689	0.72999443	2.10906455
C	-4.333818	0.96482048	3.59735409
H	-3.6487347	0.80469782	4.44654313
H	-4.838116	0.00785211	3.38230724

H	-5.1096218	1.67994488	3.92293625
C	-2.8374207	2.77639323	2.6889119
H	-2.1031396	2.615288	3.49564305
H	-3.5199969	3.57712627	3.02238942
H	-2.2913465	3.14631507	1.80549824
C	-5.3136235	-0.0800133	-2.1696566
H	-4.5850244	-0.8779238	-1.9396483
C	-4.8039502	0.64963992	-3.4086685
H	-4.7327427	-0.0362652	-4.269347
H	-3.8041444	1.0809203	-3.2346747
H	-5.4811534	1.47441637	-3.691759
C	-6.6585774	-0.7460724	-2.4395821
H	-6.5711516	-1.48712	-3.2512961
H	-7.421764	-0.0122832	-2.7511034
H	-7.0457102	-1.2639843	-1.546492
C	4.51301643	0.60774376	-0.2486153
C	4.85078647	0.88171616	-1.5915931
C	5.86520409	1.8077468	-1.8459566
H	6.14139895	2.02696843	-2.8833602
C	6.52937874	2.45352262	-0.8092716
H	7.32308164	3.17341013	-1.0289645
C	6.17639423	2.18286433	0.50759914
H	6.69975175	2.69493093	1.32265438
C	5.16479313	1.26976303	0.81441487
C	4.8139857	0.98882203	2.26122948
H	3.92784334	0.32916896	2.26753547
C	5.94853459	0.24961138	2.96462923
H	5.67197936	-0.0062337	4.00103913
H	6.86229802	0.86792587	3.00708378
H	6.2095437	-0.685403	2.44200754
C	4.43341875	2.2579412	3.01369907
H	4.11683035	2.01934741	4.04258426
H	3.60160085	2.78260465	2.51610229
H	5.28041985	2.96180912	3.08699118
C	4.1418676	0.2026588	-2.7457904
H	3.42632519	-0.5245678	-2.3210362
C	3.33081257	1.20530636	-3.5604236
H	2.7799788	0.69986855	-4.371172
H	3.98183131	1.96770625	-4.0227765
H	2.59547425	1.73064732	-2.9287893
C	5.11314427	-0.5683901	-3.6332844
H	4.57106837	-1.1214529	-4.4181824
H	5.70719076	-1.294991	-3.0545675
H	5.82352101	0.10684348	-4.1409901

NDI-Bi_2 **$E_{el.}$(a.u.)** = -2044.37007824

Atom	x	y	z
Bi	-1.3987622	-0.4645497	-0.7575227
C	3.58960891	1.69147402	-0.0400415
N	3.53923917	0.38620034	-0.007502
Bi	1.34404239	-0.6723726	0.38105525
C	4.87189318	2.4326557	-0.2913449
H	4.78177164	3.13551651	-1.1350123
H	5.68943618	1.73161514	-0.5137095
H	5.17042573	3.02119609	0.5923428
N	1.17124933	1.7037012	0.24681994
N	-3.5314839	0.34001302	0.16872075
C	2.3895607	3.7977366	0.33786075
H	3.34109602	4.33100955	0.29406686
N	-1.1869887	1.7138464	0.17017447
C	2.374792	2.40855277	0.19978319
C	-0.0076068	2.37383343	0.30018315
C	-0.0116508	3.80536131	0.4964881
C	1.21562089	4.49443233	0.51115233
H	1.210306	5.58167764	0.62798764
C	-1.2427356	4.46888562	0.66999422
H	-1.2407931	5.54935613	0.83817063
C	-2.4108058	3.7419004	0.68919301
H	-3.3615348	4.23615636	0.89968196
C	-2.3882586	2.36487632	0.45961255
C	-4.848226	2.19770866	1.09068621
H	-4.686591	2.76481191	2.01977576
H	-5.6033902	1.42221754	1.28558102
H	-5.278222	2.89433353	0.34958072
C	-3.5801338	1.5840503	0.5704363
C	-4.5987424	-0.5711908	0.23152453
C	-4.6878564	-1.4588898	1.32724157
C	-5.7133619	-2.4069787	1.33458842
H	-5.8008678	-3.0939996	2.18362378
C	-6.6252552	-2.4918695	0.28834677
H	-7.4213991	-3.2415719	0.31189983
C	-6.5177447	-1.6201512	-0.7892206
H	-7.2341491	-1.692421	-1.6152043
C	-5.5112477	-0.6528643	-0.843115
C	-5.4127707	0.2656233	-2.0441222
H	-4.5919989	0.9805454	-1.8545095
C	-6.6909477	1.07199915	-2.2483001
H	-6.5740794	1.78915601	-3.0776805
H	-6.9629673	1.63984232	-1.3431125

H	-7.5464226	0.4207177	-2.4977271
C	-5.0470877	-0.513262	-3.3036801
H	-4.9326108	0.16369255	-4.1667167
H	-5.826076	-1.2522951	-3.5602174
H	-4.0981951	-1.0598861	-3.1733835
C	-3.7322727	-1.3644222	2.49942324
H	-2.9310545	-0.6562641	2.22009013
C	-3.0636447	-2.6975099	2.81021307
H	-2.3108551	-2.5776636	3.60714387
H	-2.5529998	-3.1061683	1.92245171
H	-3.7900472	-3.4530063	3.15661369
C	-4.4374255	-0.8013636	3.73002182
H	-3.7332108	-0.6827944	4.57032791
H	-5.24933	-1.4706376	4.06504316
H	-4.8876961	0.18407346	3.52495265
C	4.62983878	-0.4720785	-0.2274051
C	5.38274706	-0.9273894	0.87775956
C	6.4168175	-1.8384163	0.64958153
H	7.01272194	-2.1935933	1.4978187
C	6.70201303	-2.3022414	-0.6293422
H	7.51627034	-3.0153189	-0.7873292
C	5.9435799	-1.8567681	-1.7059062
H	6.16816537	-2.2247644	-2.7133041
C	4.89897886	-0.9461931	-1.5308196
C	4.10721959	-0.4678996	-2.7310603
H	3.28258014	0.16606547	-2.3577332
C	4.97053756	0.38854158	-3.6527259
H	4.37779361	0.78479626	-4.4939693
H	5.80299338	-0.1979166	-4.0793659
H	5.41332069	1.24452918	-3.1173792
C	3.47359573	-1.6249329	-3.4945202
H	2.84521947	-1.250083	-4.3195203
H	2.83661527	-2.2390284	-2.8366469
H	4.23544092	-2.2895714	-3.937617
C	5.10606242	-0.4383413	2.28475504
H	4.21709655	0.21628983	2.24150926
C	4.77343446	-1.5881088	3.2287487
H	4.51678167	-1.2088764	4.23186383
H	5.62637396	-2.2788617	3.34625873
H	3.91646416	-2.1749234	2.85895449
C	6.26880282	0.39263782	2.81904736
H	6.03543946	0.80472269	3.81493976
H	6.50759283	1.23546974	2.14964353
H	7.18424548	-0.2163096	2.91889466

References

[1] P. Pyykkö, M. Atsumi, *Chem. Eur. J.* **2009**, 15, 186–197.

[2] M. Mantina, A. Chamberlin, R. Valero, C. Cramer, D. Truhlar, *J. Phys. Chem.* **2009**, *113*, 5806–5812.

[3] a) L. Allen, *J. Am. Chem. Soc.* **1989**, 111, 9003–9014; b) J. Mann, T. Meek, L. Allen, *J. Am. Chem. Soc.* **2000**, 122, 2780–2783; c) J. Mann, T. Meek, E. Knight, J. Capitani, L. Allen, *J. Am. Chem. Soc.* **2000**, 122, 5132–5137.

[4] M. Solà, F. Feixas, J. O. C. Jiménez-Halla, E. Matito, J. Poater, *Symmetry.* **2010**, *2*, 1156–1179.