Supplementary Material (ESI) for Dalton Transactions

Supplementary data

Arsacarborane chemistry. The 7,8,9,11-, 7,9,8,10-, and 7,8,9,10-isomers of *nido*-$As_2C_2B_7H_9$ and some of their halogenated derivatives.

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Selected bond lengths (Å) and angles (°) for 3-I-7,8,9,11-$As_2C_2B_7H_8$ (3-I-**2**).

bond lengths

B(11)-B(31)	1.765(6)
B(11)-B(21)	1.777(4)
B(11)-B(61)	1.804(5)
B(21)-C(111)	1.730(4)
B(21)-B(61)	1.778(4)
B(21)-B(31)	1.857(4)
B(21)-As(71)	2.159(3)
B(31)-I(1)	2.179(4)
B(31)-As(71)	2.230(3)
B(61)-C(111)	1.695(4)
B(61)-B(101)	1.813(5)
As(71)-C(111)	2.007(3)
As(71)-As(71)i	2.4111(6)
As(72)-As(72)i	2.4147(5)
B(101)-C(111)	1.608(4)
B(12)-B(22)	1.765(4)
B(12)-B(32)	1.774(6)
B(12)-B(62)	1.798(5)
B(22)-C(112)	1.722(4)
B(22)-B(62)	1.776(5)
B(22)-B(32)	1.849(4)
B(22)-As(72)	2.161(3)
B(32)-I(2)	2.185(4)
B(32)-As(72)	2.222(4)
B(62)-C(112)	1.696(4)
B(62)-B(102)	1.816(5)
As(72)-C(112)	2.002(3)

B(102)-C(112)	1.618(4)

Bond angles

C(111)-As(71)-B(21)	48.91(12)
C(111)-As(71)-B(31)	84.64(14)
B(21)-As(71)-B(31)	50.03(12)
C(111)-As(71)-As(71)^{i}	94.36(8)
B(21)-As(71)-As(71)^{i}	97.22(9)
B(31)-As(71)-As(71)^{i}	57.28(6)
C(111)^{i} -B(101)-C(111)	115.3(3)
C(111)^{i} -B(101)-B(61)	106.9(3)
C(111)-B(101)-B(61)	59.06(18)
C(111)-B(101)-B(61)^{i}	106.9(3)
B(61)-B(101)-B(61)^{i}	56.9(2)
B(101)-C(111)-B(61)	66.5(2)
B(101)-C(111)-B(21)	114.7(3)
B(61)-C(111)-B(21)	62.51(18)
B(101)-C(111)-As(71)	115.5(2)
B(61)-C(111)-As(71)	125.68(19)
B(21)-C(111)-As(71)	70.14(15)
C(112)-As(72)-B(22)	48.68(12)
C(112)-As(72)-B(32)	84.47(14)
B(22)-As(72)-B(32)	49.88(12)
C(112)-As(72)-As(72)^{ii}	94.37(8)
B(22)-As(72)-As(72)^{ii}	96.88(9)
B(32)-As(72)-As(72)^{ii}	57.09(6)
C(112)-B(102)-C(112)^{ii}	114.4(3)
C(112)-B(102)-B(62)^{ii}	106.5(3)
C(112)-B(102)-B(62)	58.86(18)
B(62)^{ii} -B(102)-B(62)	57.0(3)
B(102)-C(112)-B(62)	66.4(2)
B(102)-C(112)-B(22)	114.6(3)
B(62)-C(112)-B(22)	62.61(18)
B(102)-C(112)-As(72)	115.8(2)
B(62)-C(112)-As(72)	126.26(18)
B(22)-C(112)-As(72)	70.47(14)

Symmetry transformations used to generate equivalent atoms: i: x,y,-z ii: x,y,-z+1

Standard output orientation for 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.679557	0.000002	1.366409
2	5	0	0.863578	-1.471761	0.847352
3	5	0	-0.081453	-0.000013	1.516767
4	5	0	0.863560	1.471757	0.847362
5	5	0	2.216858	0.862172	-0.121249
6	5	0	2.216866	-0.862154	-0.121255
7	33	0	-1.042625	-1.200749	-0.082243
8	33	0	-1.042631	1.200744	-0.082241
9	6	0	0.786346	1.360396	-0.887830
10	5	0	1.396827	0.000007	-1.506188
11	6	0	0.786354	-1.360387	-0.887836
12	1	0	2.317484	0.000005	2.367787
13	1	0	0.919423	-2.515604	1.409159
14	1	0	-0.613284	-0.000012	2.575562
15	1	0	0.919402	2.515598	1.409175
16	1	0	3.178048	1.554704	-0.199744
17	1	0	3.178065	-1.554680	-0.199752
18	1	0	0.892402	2.299479	-1.423493
19	1	0	1.914338	0.000014	-2.579189
20	1	0	0.892414	-2.299462	-1.423507

Standard output orientation for 3-Cl-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.388520	-0.000285	2.013666
2	5	0	0.249154	-1.473225	1.053757
3	5	0	-0.872100	-0.000109	0.771291
4	5	0	0.249166	1.472921	1.054167
5	5	0	1.866213	0.861716	1.465069
6	5	0	1.866210	-0.862151	1.464826
7	33	0	-0.255028	-1.202771	-1.009218
8	33	0	-0.255009	1.203065	-1.008884
9	6	0	1.530205	1.359264	-0.125147
10	5	0	2.400408	-0.000009	-0.047079
11	6	0	1.530187	-1.359247	-0.125532
12	1	0	0.015685	-0.000441	3.139773

13	1	0	-0.148361	-2.512192	1.464128
14	17	0	-2.625858	-0.000159	1.174407
15	1	0	-0.148336	2.511776	1.464836
16	1	0	2.543210	1.553630	2.151582
17	1	0	2.543202	-1.554263	2.151147
18	1	0	2.005737	2.300917	-0.385241
19	1	0	3.553770	0.000027	-0.342273
20	1	0	2.005708	-2.300830	-0.385894

Standard output orientation for 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.055966	1.765888	1.129702
2	5	0	1.405372	1.421950	0.147963
3	5	0	0.890998	0.327977	1.538702
4	5	0	-0.911381	0.283145	1.550402
5	5	0	-1.481942	1.361065	0.151542
6	5	0	-0.034277	2.027551	-0.638329
7	33	0	1.692519	-0.678633	-0.192110
8	6	0	0.014470	-1.007666	0.883555
9	33	0	-1.619815	-0.752385	-0.192895
10	6	0	-0.832900	0.681617	-1.309780
11	5	0	0.786960	0.664090	-1.439043
12	1	0	-0.089845	2.685134	1.880435
13	1	0	2.390693	2.076713	0.252870
14	1	0	1.458549	0.172568	2.568254
15	1	0	-1.507401	0.109623	2.560218
16	1	0	-2.509781	1.951765	0.170431
17	1	0	-0.140670	3.084322	-1.168818
18	1	0	0.023680	-1.924070	1.466432
19	1	0	-1.434957	0.883454	-2.191737
20	1	0	1.322265	0.882057	-2.480257

Standard output orientation for 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	5	0	1.652320	-0.285579	1.382700
2	5	0	0.579820	-1.603830	0.846152
3	5	0	-0.086751	-0.008519	1.521385
4	5	0	1.073370	1.295982	0.883572
5	5	0	2.334394	0.481503	-0.069712
6	5	0	2.002750	-1.241994	-0.094134
7	33	0	-1.255375	-1.027079	-0.080399
8	33	0	-0.821208	1.349668	-0.091029
9	6	0	1.000255	1.171959	-0.875513
10	6	0	1.430273	-0.207289	-1.366255
11	5	0	0.509037	-1.486690	-1.026502
12	1	0	2.295196	-0.391135	2.375251
13	1	0	0.466213	-2.610398	1.466683
14	1	0	-0.628099	0.120167	2.567606
15	1	0	1.337529	2.319224	1.420335
16	1	0	3.405107	0.965395	-0.218589
17	1	0	2.933378	-1.961943	-0.246996
18	1	0	1.300946	2.033652	-1.463590
19	1	0	1.999574	-0.208148	-2.291358
20	1	0	0.509518	-2.454646	-1.718933

Standard output orientation for 3-Cl-5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.420756	-1.248693	1.581733
2	5	0	-0.231682	0.519749	1.740338
3	5	0	0.858661	-0.485341	0.627734
4	5	0	-0.264316	-1.790576	-0.086038
5	5	0	-1.880862	-1.557446	0.623931
6	5	0	-1.838152	-0.162017	1.685540
7	33	0	0.320502	1.586955	-0.028889
8	33	0	0.242181	-0.306530	-1.530537
9	6	0	-1.549855	-0.911482	-0.920662
10	6	0	-2.327908	-0.006028	0.030219
11	5	0	-1.582034	1.276429	0.668819
12	1	0	-0.092428	-1.970578	2.463609
13	1	0	0.218381	1.011544	2.722319
14	17	0	2.603657	-0.819479	0.903762

15	1	0	0.064276	-2.881248	-0.410194
16	1	0	-2.645948	-2.456015	0.718159
17	1	0	-2.625089	-0.141614	2.572742
18	1	0	-2.107276	-1.436928	-1.690322
19	1	0	-3.394832	0.055080	-0.162340
20	1	0	-2.185541	2.241409	1.015501

Standard output orientation for 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000001	1.762628	1.149048
2	5	0	-0.888000	0.270402	1.557485
3	5	0	-1.445771	1.372052	0.194808
4	5	0	-0.000007	2.050931	-0.587868
5	5	0	1.445763	1.372055	0.194798
6	5	0	0.888001	0.270402	1.557480
7	33	0	-1.671533	-0.722577	-0.192946
8	6	0	-0.758377	0.688256	-1.278239
9	6	0	0.758374	0.688262	-1.278238
10	33	0	1.671535	-0.722574	-0.192945
11	5	0	0.000002	-1.177809	0.906225
12	1	0	0.000003	2.681395	1.900870
13	1	0	-1.540243	0.182621	2.546073
14	1	0	-2.425307	2.038592	0.160950
15	1	0	-0.000007	3.082746	-1.168836
16	1	0	2.425299	2.038593	0.160945
17	1	0	1.540243	0.182626	2.546069
18	1	0	-1.254078	0.914625	-2.216904
19	1	0	1.254076	0.914632	-2.216905
20	1	0	0.000006	-2.208283	1.501111