Electronic Supplementary Information

The Electron Sextet on Carbon and the Electron Deficiency on Boron Readily Combine together: Boron-Based Octahedral Dication as a Result

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Experimental section

Instrumentation. NMR spectra were recorded on Bruker AVANCE III 500 (^{11}B 160.388 MHz, ^{31}P 202.363 MHz) and AVANCE III HD 600 (^{11}B 192.552 MHz, ^{31}P 242.945 MHz, *^{13}C 150.908 MHz*, *^{1}H 600.15 MHz)* at 293 K if not stated otherwise. Chemical shifts were referenced to ext. $BF_3{\cdot}OEt_2$ (^{11}B) and 85% H_3PO_4 (^{31}P) and TMS. Negative signs indicate an upfield shift. The NMR spectra were processed using SpinWorks 4 (v 4.2.3.0 Kirk Marat, University of Manitoba, Canada) software. High- and low-resolution mass spectra were obtained on a Finnigan Varian MAT 95 with electron ionization at 70 eV.

General Procedures and Materials. All manipulations were conducted using standard high vacuum or inert atmosphere techniques as described by Shriver.[1] Reaction vessels were constructed by sealing the Pyrex 13 mm glass tube of a right-angle PTFE high vacuum valve (J. Young Scientific Glassware, Acton, London) at one end and equipping the other end with an O-ring seal for greaseless connection to the vacuum-line. Solvents were reagent grade, dried and purified according to standard procedures and were finally degassed in repeated freeze-pump-thaw cycles before use. 3-Bis-(2,6-diisopropylphenyl)-imidazol-2-yliden („Idip") was obtained from Sigma-Aldrich and was used as received after degassing under high-vacuum. PBr_3 and $AsBr_3$ were freshly vacuum-distilled before use. BBr_3 was stirred over mercury, degassed, and condensed into a trap of -78°C prior to use. Diboron tetrabromide B_2Br_4 was prepared by co-condensation of BBr_3 with copper-vapor onto cooled walls (-196 ºC) of a metal-vapor reactor similar to that described by Timms.[2] After reaction, B_2Br_4 was separated from excess BBr_3 by repeated fractionation until the condensate exhibited a vapor pressure of less than 1 Torr. The pnictogenaboranes $Pn_2B_4Br_4$ (*Pn* = As or P) were prepared by co-pyrolyses of appropriate mixtures of B_2Br_4 with $PnBr_3$ and were separated according to the conditions given in the literatures as mentioned in the main text.

Reactions of *closo*-1,2-$Pn_2B_4Br_4$ (*Pn* = P, As) with 1,3-Bis-(2,6-diisopropylphenyl)-imidazol-2-yliden („Idip") to monocationic 1,6-$Idip_2$-$P_2B_4Br_3^+$, 4-Idip-*Pn*$_2B_4Br_3^+$ (1: *Pn* = P; 2: *Pn* = As) and dicationic 3,5-$Idip_2$-$P_2B_4Br_2^{2+}$ (3) : In typical reactions, 0.016 mmoles of *closo*-1,2-*Pn*$_2B_4Br_4$ (6.8 mg *Pn* = P; 8.2 mg *Pn* = As) were dissolved in 4 mL CH_2Cl_2 and a dilution of 12.4 mg (0.032 mmol) Idip in 2 mL CH_2Cl_2 was syringed into the stirred solution at -78°C under a constant flow of inert gas. After closure of the Teflon stopcock the mixture was allowed to slowly warm up to room temperature. The still clear solution was syringed under inert gas into an NMR tube and immediately thereafter was analyzed with NMR. After ca 1 h at room temperature a pale white solid started to precipitate. The reaction was completed after 16 h at 0°C for *Pn* = P. For *Pn* = As completion was not accomplished due to degradation reactions.

Data for **(1a+1b)/2**: ^{11}B NMR (ppm, CH_2Cl_2) -2.6 ppm (B3,5), 10.2 ppm (B4), 15.8 ppm (B6). ^{31}P NMR (ppm, CH_2Cl_2) -122.7 ppm (P2), d, ^1J(PP) = 218 Hz; -56.0 ppm (P1), d (br), ^1J(PP) =192 Hz.

Data for **2**: ^{11}B NMR (ppm, CH_2Cl_2) 7.2 ppm (B3,5), 21.5 ppm (B4), 23.5 ppm (B6).

Data for **3:** ^{11}B NMR (ppm, CH_2Cl_2) -1.2 ppm (B3,5), 17.4 ppm (B4,6). ^{31}P NMR (ppm, CH_2Cl_2) -145.7 ppm (P1,2). MS (neg. ESI) *m/z* 1272.6 as anionic adduct with $2Br^-/Cl^-$/HCl.

Computational details. Magnetic-property computations were obtained by means of the GIAO-PBE1PBE method incorporated into Gaussian16[3] utilizing the IGLO-II basis with the B3LYP/6-311+G(2d,p) + D3(BJ) geometries for IDip-based species and with the B3LYP/6-311+G(2d,p) geometries for NHC-based species. Second derivative analyses the confirmed them to be minima on the respective potential energy surfaces. Additional NMR calculations were performed using the same geometries as in the quasi-relativistic GIAO-PBE1PBE computations with the Amsterdam Density Functional (ADF) code[4] employing the PBE0 functional. The two-component relativistic zeroth-order regular approximation (ZORA) method[5] including scalar and spin–orbit (SO)[6] corrections was employed for these computations; the all-electron triple-zeta basis set plus one polarization function (denoted TZ2P; from the ADF library) was used for all atoms. Magnetic shieldings were converted into relative ^{11}B chemical shifts using the ^{11}B NMR of B_2H_6[7] and the ^{31}P NMR of PH_3[8] as the primary references, respectively. Reaction pathways were searched in terms of computing SMD energies in CH_2Cl_2 or THF at the B3LYP/6-311+G(2d,p) +D3(BJ) level. Zero-point, heat-capacity, and entropy corrections with frequencies were carried out at the B3LYP/6-31+G(d) + D3(BJ) level. Electrostatic potentials were computed on 0.001 a.u. at the HF/cc-pVDZ level using Gaussian16 and Molekel4.3[9] programs. It has recently been shown that this basis set size is sufficient for these purposes.[10] The IAO/IBO method[11] was used to connect quantitative SCF wave functions to a qualitative chemical picture, naturally revealing the nature of the orbitals. The IBOview program was used.[11] The corresponding input file for the latter were generated at the B3LYP/def2-TZVP//B3LYP/6-311+G** level using the Turbomole6.6[12] program package.

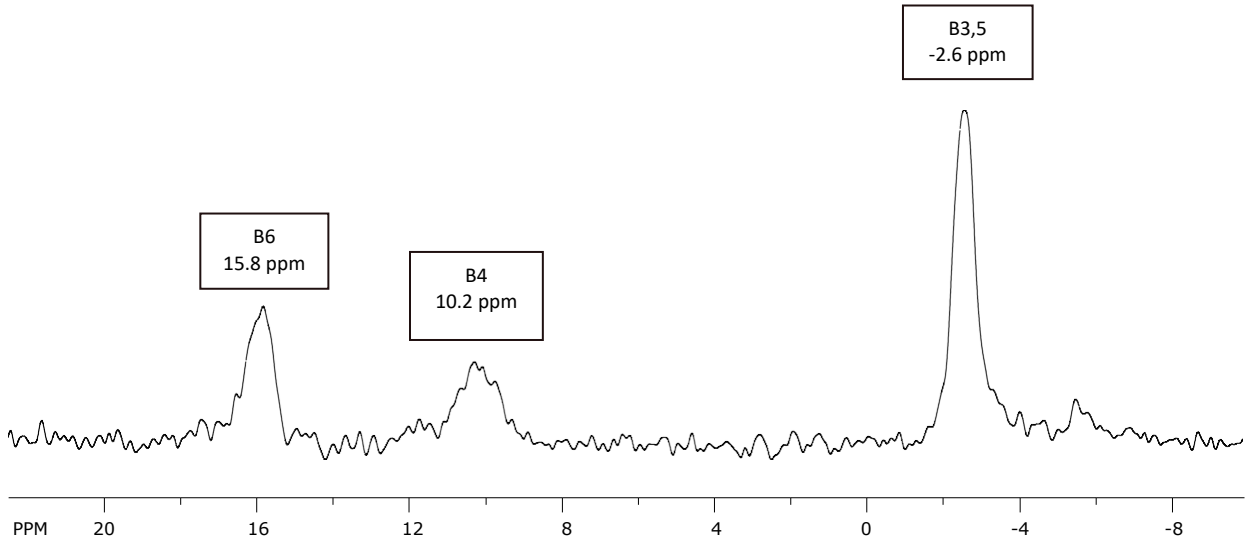

Fig. S1 160.388 MHz ^{11}B NMR spectrum of the reaction of $P_2B_4Br_4$ with IDip in CH_2Cl_2 immediately after warm-up with the exclusive formation of a mixture of [4-IDip-1,2-$P_2B_4Br_3$]$^+$ Br^- (**1a**) and [1,6-$Idip_2$-1,2-$P_2B_4Br_3$]$^+$ Br^- (**1b**).

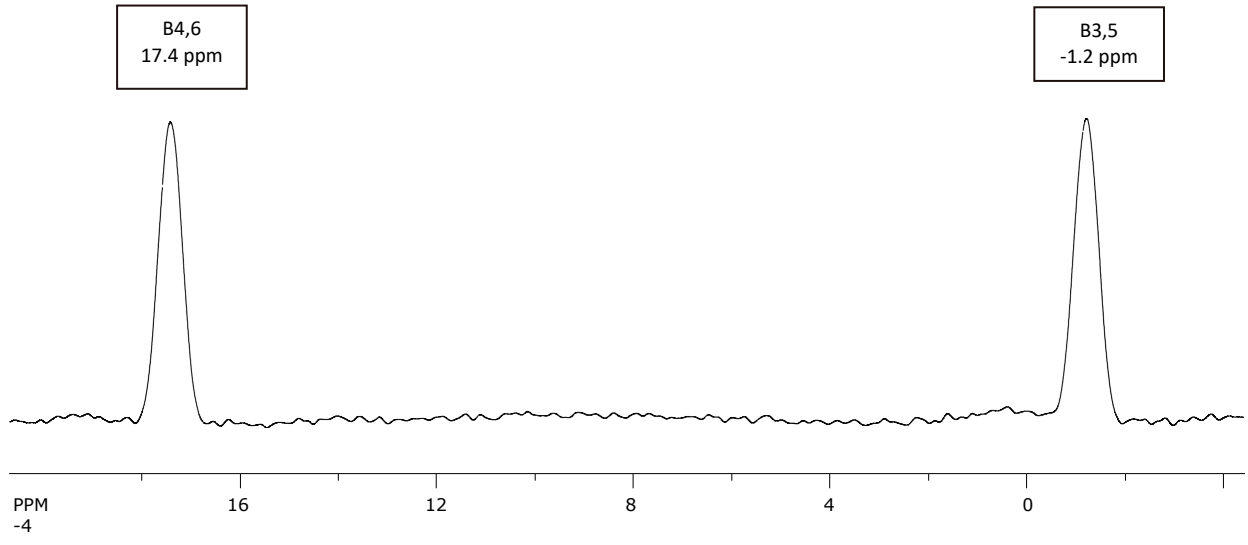

Fig. S2 160.388 MHz ^{11}B NMR spectrum of the reaction of $P_2B_4Br_4$ with Idip in CH_2Cl_2 after 1 day at 0°C. Formation of [3,5-$Idip_2$-1,2-$P_2B_4Br_2$]$^{2+}$ $2Br^-$ **(3)**.

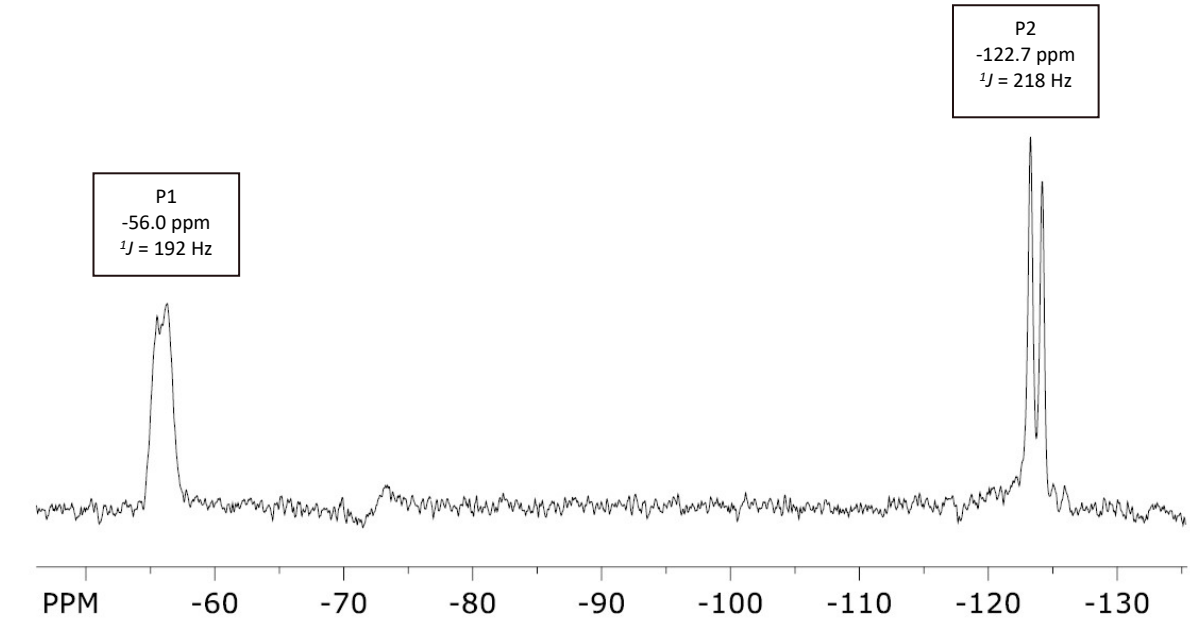

Fig. S3 242.945 MHz ^{31}P NMR spectrum of the reaction of $P_2B_4Br_4$ with Idip in CH_2Cl_2 immediately after warm-up. Formation of a mixture of [4-Idip-1,2-$P_2B_4Br_3$]$^+$ Br^- (**1a**) and [1,6-$Idip_2$-1,2-$P_2B_4Br_3$]$^+$ Br^- (**1b**).

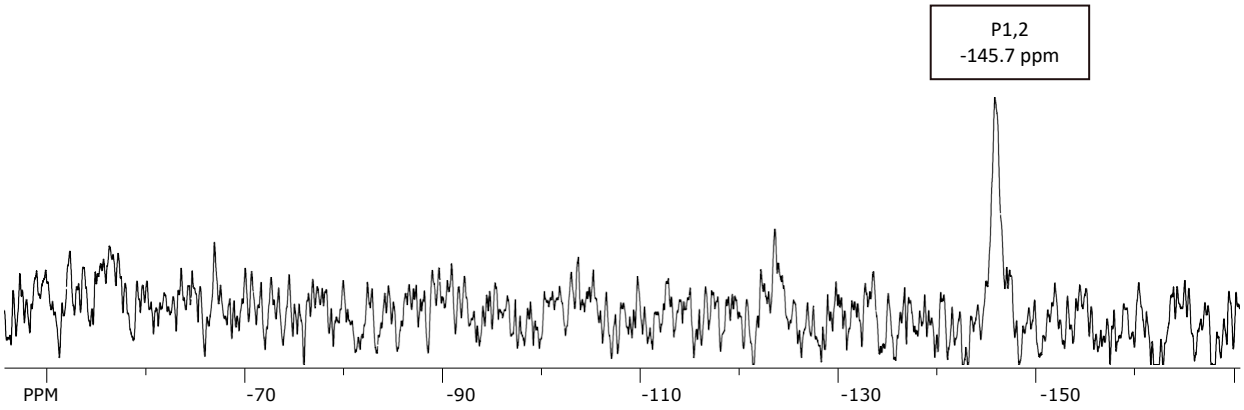

Fig. S4 242.945 MHz ^{31}P NMR spectrum of the reaction of $P_2B_4Br_4$ with Idip in CH_2Cl_2 after 1 day at 0°C. Formation of [3,5-$Idip_2$-1,2-$P_2B_4Br_2$]$^{2+}$ $2Br^-$.

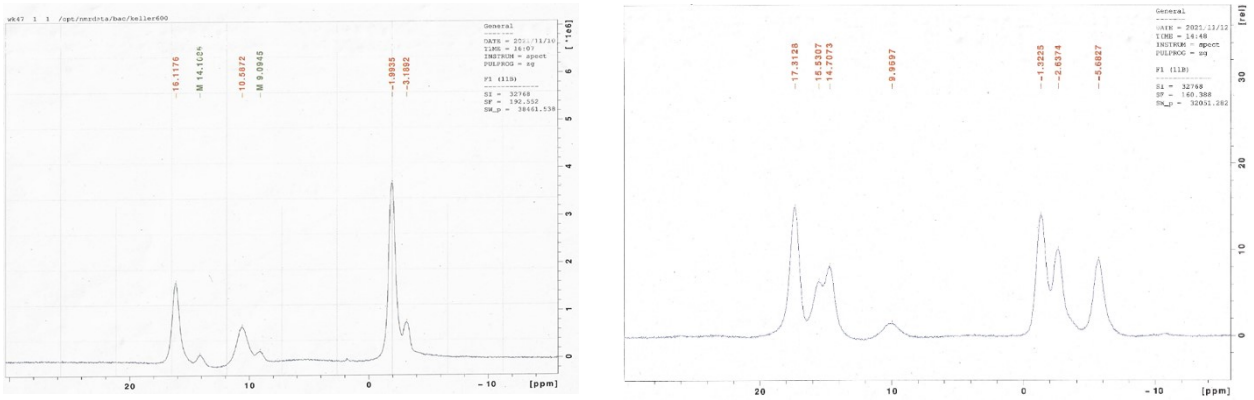

Fig. S5 160.388 MHz ^{11}B NMR spectrum of two reactions of $P_2B_4Br_4$ with Idip in THF in approximately 1:1 molar ratios immediately after warm-up. Left: 1st attempt, right: 2nd attempt. The differences in spectra between 1st and 2nd attempts could be caused by deviations of the molar amounts (the amount of only 8 mg of Idip could not be weighted exactly). Continuous formation of a mixture of [4-Idip-1,2-$P_2B_4Br_3$]$^+$ Br^- (**1a**) and [1,6-$Idip_2$-1,2-$P_2B_4Br_3$]$^+$ Br^- (**1b**).

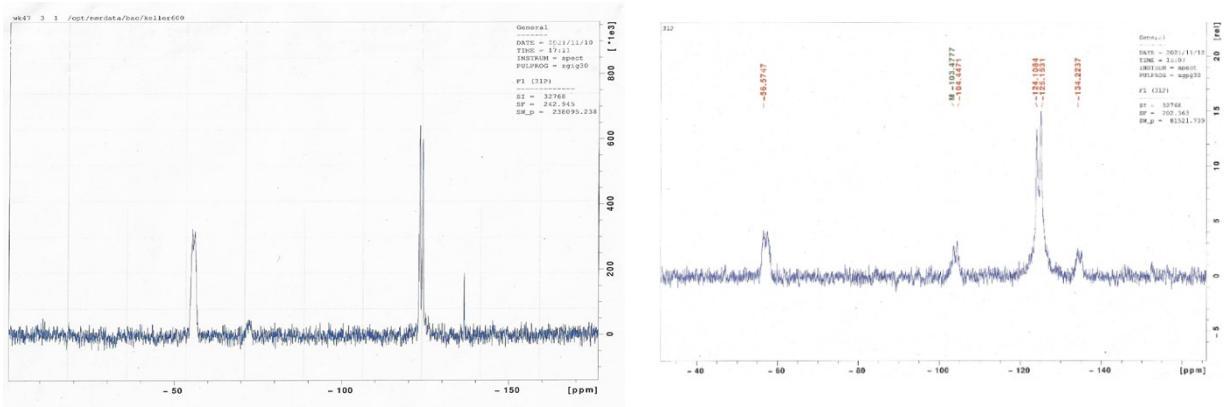

Fig. S6 202.363 MHz ^{31}P NMR spectrum of two reactions of $P_2B_4Br_4$ with Idip in THF immediately after recording of the ^{11}B spectra of Fig. S5. Left: 1st attempt, right: 2nd attempt. Continuous formation of a mixture of [4-Idip-1,2-$P_2B_4Br_3$]$^+$ Br^- (**1a**) and [1,6-$Idip_2$-1,2-$P_2B_4Br_3$]$^+$ Br^- (**1b**).

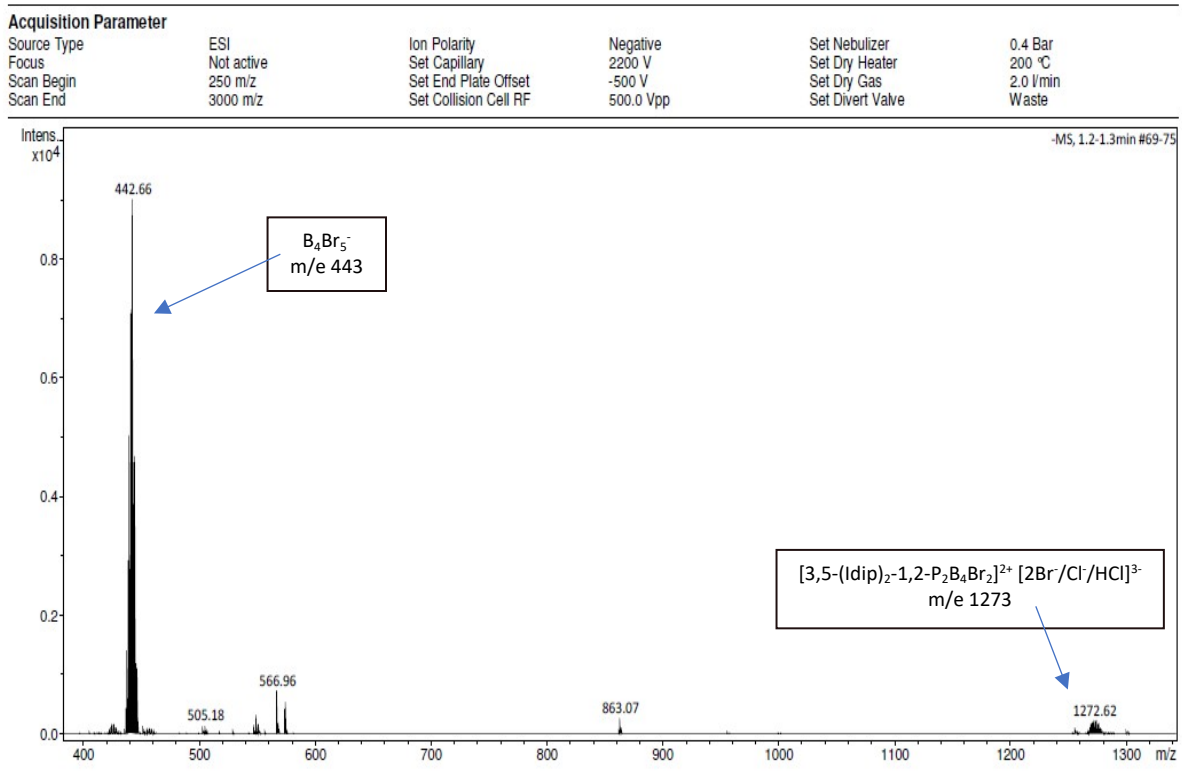

Fig. S7 ESI-MS (negative ion polarity) with the adduct of $[3,5\text{-}(Idip)_2\text{-}1,2\text{-}P_2B_4Br_2]^{2+}$ (**3**) with $2Br^-/Cl^-/HCl$ at m/e 1273.

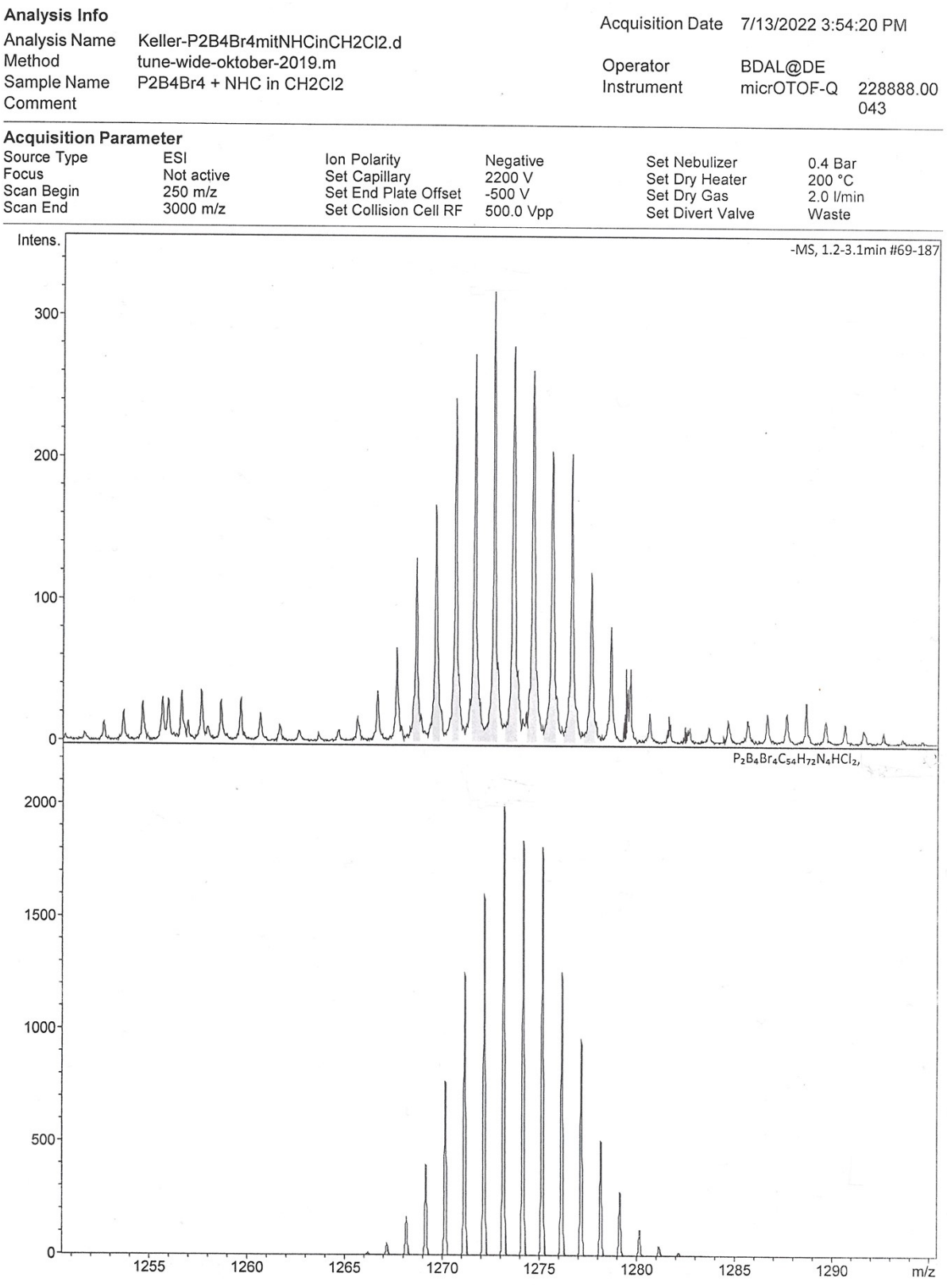

Fig. S8 Sector of ESI-MS (negative ion polarity) with the adduct of $[3,5\text{-Idip}_2\text{-}1,2\text{-}P_2B_4Br_2]^{2+}$ (**3**) with $2Br^-/Cl^-/HCl$ at m/e 1273 on top and calculated below.

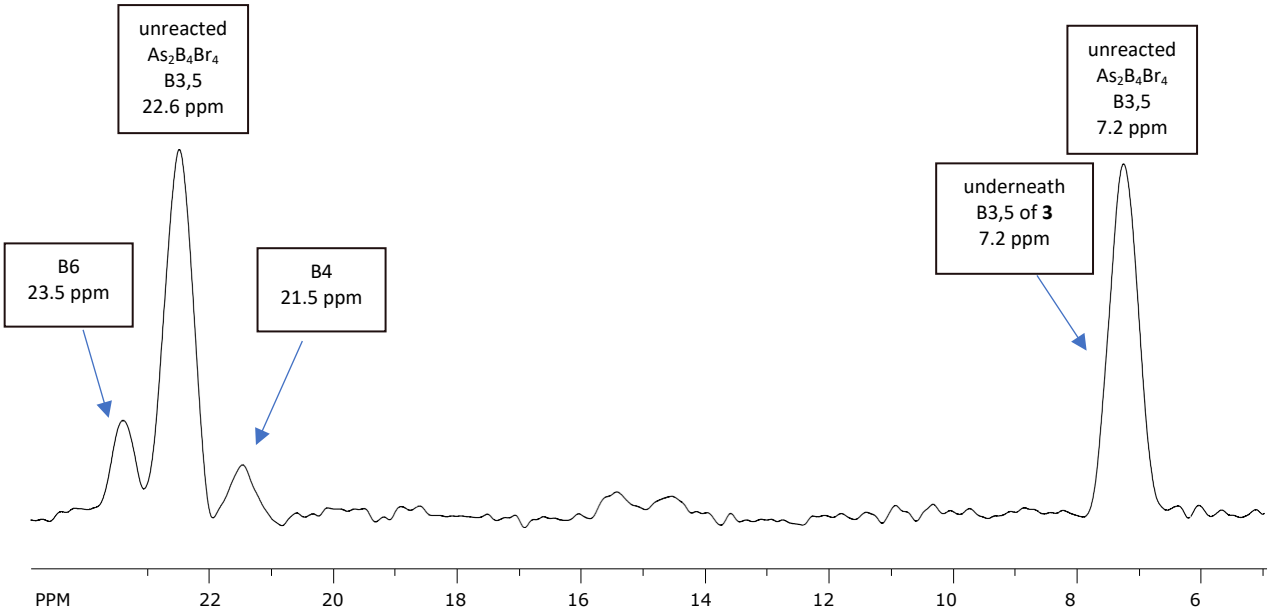

Fig. S9 192.55 MHz ^{11}B NMR spectrum of the reaction of $As_2B_4Br_4$ with Idip in CH_2Cl_2 after 10 min heating at 50°C. Formation of $[4\text{-Idip-}As_2B_4Br_3]^+Br^-$ (**2**) besides unreacted $As_2B_4Br_4$.

Table S1 Species related to the reaction of ID and Idip ligands with $P_2B_4Br_4$ in dichloromethane[a]

species	PG	B3LYP/ 6-311+G(2d) +D3BJ	ZPE	NIF[b]	Entropy	Cp	Solv[c]
Br^-	K	-2574.232916	0.00	0	39.01	1.48	-49.21
$P_2B_4Br_4$	C_{2v}	-11078.975677	15.23	0	114.78	8.05	-8.91
ID	C_{2v}	-688.462899	145.73	-2	102.64	7.52	-18.23
ID	C_2	-688.465093	145.78	0	113.28	8.60	-19.17
Idip	C_{2v}	-1160.380315	358.82	-2	184.08	18.33	-20.67
Idip	C_2	-1160.380441	358.94	0	196.60	19.43	-20.71
Br-Idip$^-$	C_{2v}	-3734.609491	358.06	-3	189.29	19.22	-58.47
Br-Idip$^-$	C_2	-3734.609368	358.20	-2	194.24	19.72	-58.62
Br-Idip$^-$	C_1	-3734.614001	358.37	0	205.22	20.75	-57.17
Br-Idip$_2^-$	D_{2d}	-4894.990173	716.44	0	303.25	35.95	-65.26
Br_2-Iip$_2^{-2}$	D_2	-7469.175268	716.50	0	371.23	42.04	-135.51
1-ID-$P_2B_4Br_4$	C_s	-11767.478268	162.23	0	181.43	16.97	-26.69
1,2-ID$_2$-$P_2B_4Br_4$	C_{2v}	-12455.954094	307.58	0	261.90	26.68	-32.49
1,2-ID$_2$-$P_2B_4Br_4$	C_1	-12455.954912	308.84	0	255.90	26.29	-38.89
TS1-ID-a	C_1	-12455.943766	308.28	194	242.43	25.64	-35.11
1,6-ID$_2$-$P_2B_4Br_4$	C_1	-12455.979391	309.38	0	242.58	25.82	-36.97

1,6-ID-$P_2B_4Br_3^+$	C_s	-9881.651361	310.33	0	234.01	24.32	-58.58
4-ID-$P_2B_4Br_3$-a^+	C_s	-9193.116562	162.63	-1	165.44	15.02	-53.43
4-ID-$P_2B_4Br_3$-b^+	C_s	-9193.121915	162.56	-1	168.85	15.17	-54.42
4-ID-$P_2B_4Br_3$-c^+	C_s	-9193.124588	162.65	-1	168.82	15.19	-54.58
4-ID-$P_2B_4Br_3$-d^+	C_1	-9193.124849	162.87	0	171.74	15.61	-52.99
TS2-ID	C_1	-12455.944898	308.46	181	247.18	25.75	-35.65
1,3-ID_2-$P_2B_4Br_4$-a	C_1	-12455.996757	310.60	0	247.66	25.84	-38.92
1,3-ID_2-$P_2B_4Br_4$-b	C_1	-12455.997531	309.71	0	246.63	25.85	-38.15
1,3-ID_2-$P_2B_4Br_3^+$	C_1	-9881.647344	310.37	0	234.81	24.44	-63.23
TS3(+)-ID	C_1	-9881.606339	309.01	34	236.58	24.32	-59.04
3,5-ID_2-$P_2B_4Br_3^+$	C_1	-9881.662383	310.68	0	233.76	24.31	-58.08
3-ID-$P_2B_4Br_3^+$	C_1	-9193.126005	162.75	0	172.83	15.67	-54.80
3,5-ID_2-$P_2B_4Br_2^{+2}$	C_2	-7307.211449	310.63	0	228.85	23.19	-137.63
[3,5-ID_2-$P_2B_4Br_2$][Br]$_2$	C_2	-12456.040311	311.54	0	248.27	28.62	-42.64
TS4(+)-ID	C_1	-9881.604703	309.58	127	234.36	24.26	-59.78
INT(+)-ID	C_1	-9881.623918	309.76	0	241.76	24.75	-59.25
TS5(+)-ID	C_1	-9881.605778	309.67	19	237.00	24.30	-62.49
1-Idip-$P_2B_4Br_4$	C_s	-12239.385003	375.39	0	262.50	27.93	-23.50
1-Idip-$P_2B_4Br_4$	C_s	-12239.402630	376.42	0	252.06	27.42	-27.35
1,2-$Idip_2$-$P_2B_4Br_4$	C_{2v}	-13399.795153	735.30	-3	385.10	46.15	-35.13
1,2-$Idip_2$-$P_2B_4Br_4$	C_s	-13399.800150	735.84	-1	395.81	46.91	-38.94
TS11-Idip-a	C_1	-13399.775217	737.47	156	377.01	45.95	-34.72
TS11-Idip-b	C_1	-13399.783915	737.24	160	377.89	46.10	-34.79
1,6-$Idip_2$-$P_2B_4Br_4$	C_1	-13399.829270	738.89	0	381.55	46.35	-39.65
3-Idip-$P_2B_4Br_4$	C_1	-12239.404132	377.05	0	248.50	27.16	-25.22
1,6-$Idip_2$-$P_2B_4Br_3^+$	C_s	-10825.500964	738.76	-1	368.20	44.55	-58.12
4-Idip-$P_2B_4Br_3$-a^+	C_s	-9665.056418	377.46	0	240.73	25.86	-51.76
4-Idip-$P_2B_4Br_3$-b^+	C_s	-9665.052019	377.15	0	240.08	25.94	-52.30
TS22-Idip	C_1	-13399.790019	736.98	82	382.75	46.35	-35.24
1,3-$Idip_2$-$P_2B_4Br_4$	C_1	-13399.837779	738.26	0	382.38	46.45	-37.03
1,3-$Idip_2$-$P_2B_4Br_3^+$	C_1	-10825.485110	738.86	0	375.72	45.27	-61.21
TS33(+)-Idip	C_1	-10825.457323	737.54	153	377.56	45.22	-59.56
3,5-$Idip_2$-$P_2B_4Br_3^+$	C_1	-10825.500224	739.12	0	372.84	45.15	-59.34
3-Idip-$P_2B_4Br_3^+$	C_s	-9665.045953	376.81	-2	233.55	25.07	-54.52
3-Idip-$P_2B_4Br_3^+$	C_1	-9665.057519	377.05	0	243.70	26.07	-54.39
1,2-$Idip_2$-$P_2B_4Br_2^{+2}$	C_{2v}	-8250.833115	735.36	-3	367.71	43.54	-134.30
1,2-$Idip_2$-$P_2B_4Br_2^{+2}$	C_2	-8250.923877	737.16	0	365.18	44.16	-133.71
3,5-$Idip_2$-$P_2B_4Br_2^{+2}$	C_{2v}	-8251.060705	738.47	-3	357.88	42.65	-134.54
3,5-$Idip_2$-$P_2B_4Br_2^{+2}$	C_2	-8251.087386	738.47	0	357.88	42.65	-133.72
[3,5-$Idip_2$-$P_2B_4Br_2$][Br]$_2$	C_2	-13399.872545	739.71	0	394.00	46.74	-43.60
TS44(+)-Idip	C_1	-10825.460278	737.83	143	378.78	45.27	-59.50
INT(+)-Idip-a	C_1	-10825.470544	738.69	0	375.12	45.34	-58.97
INT(+)-Idip-b	C_1	-10825.463969	738.58	0	375.18	45.31	-60.38
TS55(+)-Idip	C_1	-10825.453653	738.00	216	377.88	45.17	-60.70
$(ID)_2$	D_2	-1376.965565	292.79	0	176.24	17.38	-24.69
$(Idip)_2$	D_2	-2320.747067	721.27	2	307.52	36.94	-22.37

(a) Point Group, total energy at B3LYP/6-311+G(2d,p)+D3(BJ) (hartrees), zero-point energies (kcal.mol^{-1}), number of imaginary frequencies, entropies (cal.mol^{-1}.K^{-1}), heat capacity correction to 298K (kcal.mol^{-1}), and free energy of solvation in dichloromethane (kcal.mol^{-1}) using the SMD solvation model. Geometries, frequencies, and solvation at the B3LYP/6-31+G(d)+D3(BJ) level. Single-point energies at B3LYP/6-311+G(2d,p)+D3(BJ) level.

(b) Number of imaginary frequencies. For species labelled with "TS", the NIF value is the value of the single imaginary frequencies in cm^{-1}.

(c) Solvation free energies (kcal.mol^{-1}) determined by the difference in SMD(CH_2Cl_2)/B3LYP/6-31+G(d)+D3(BJ) and B3LYP/6-31+G(d)+D3(BJ) energies.

Table S2 Cartesian coordinates of all the detectable species at B3LYP/6-311+G** level

4-Idip-$P_2B_4Br_3^{(+)}$, 1a

P	-0.00066400	-0.00016500	-3.42571400
B	0.10824900	-1.25888800	-1.84480700
B	0.10792300	1.25880700	-1.84487600
B	0.15414100	-0.00008900	-0.64460000
P	1.70439300	0.00040700	-1.91574600
B	-1.10583500	-0.00013900	-1.76715400
Br	-3.01501900	-0.00043400	-1.77475200
Br	0.04053900	-3.17186300	-1.82933000
Br	0.03850700	3.17173500	-1.82928500
C	0.31492600	-0.00000900	0.90556500
N	1.49643900	0.00023700	1.57328900
N	-0.64954500	-0.00020700	1.85207400
C	1.26908600	0.00015400	2.93567100
C	-0.07697100	-0.00026000	3.10992500
H	2.07855300	0.00033900	3.64219700
H	-0.68165100	-0.00056700	3.99848600
C	-2.08724900	-0.00055200	1.65523700
C	-2.74250900	-1.23920900	1.60864100
C	-2.74315600	1.23776800	1.60883600
C	-4.13674200	-1.20831900	1.54974500
C	-4.13739700	1.20615500	1.54999500

C	-4.82487300	-0.00126000	1.53228000
H	-4.68997500	-2.13685800	1.50913600
H	-4.69113500	2.13439500	1.50961100
H	-5.90755600	-0.00155700	1.49016700
C	2.81278000	0.00070800	0.96813700
C	3.41539400	1.24168700	0.69582200
C	3.41632500	-1.23985400	0.69601200
C	4.68523200	1.20897100	0.11556000
C	4.68615700	-1.20630700	0.11575900
C	5.31118800	0.00153800	-0.17027300
H	5.18821200	2.13677600	-0.11955400
H	5.18978100	-2.13380700	-0.11917900
H	6.29578000	0.00191500	-0.62249600
C	-1.98912900	-2.56022800	1.63751000
C	-2.62096500	-3.61442500	0.71817100
C	-1.87631000	-3.09798200	3.07586400
H	-0.97541900	-2.38021700	1.26776300
H	-2.77864300	-3.22569100	-0.28880000
H	-1.96468300	-4.48422600	0.64760800
H	-3.58055700	-3.96267300	1.10663200
H	-1.36755300	-2.39463500	3.73835600
H	-2.86874300	-3.28992800	3.49121200
H	-1.31701100	-4.03677200	3.08818200
C	-1.99049700	2.55921000	1.63783700
C	-1.87774500	3.09678600	3.07626300
C	-2.62297800	3.61321200	0.71872300
H	-0.97673200	2.37982400	1.26795200
H	-1.36857600	2.39352800	3.73853500
H	-1.31888900	4.03583500	3.08865700
H	-2.87019100	3.28820300	3.49182600
H	-2.78046300	3.22455700	-0.28830600

H	-3.58275400	3.96084500	1.10727700
H	-1.96719400	4.48339600	0.64829400
C	2.74480100	-2.56199800	1.03614700
C	3.07564400	-2.98206200	2.48154100
C	3.12002900	-3.69043700	0.06688600
H	1.66211600	-2.41987900	0.96711000
H	2.75662900	-2.23821900	3.21293400
H	2.57840800	-3.92432200	2.72337300
H	4.15243500	-3.12719000	2.59837700
H	2.99048500	-3.39345800	-0.97447200
H	4.15425200	-4.01269500	0.20799600
H	2.48304400	-4.55787600	0.24934800
C	2.74286800	2.56333400	1.03582900
C	3.11746900	3.69210100	0.06669400
C	3.07313700	2.98362600	2.48130800
H	1.66030100	2.42044400	0.96659200
H	2.98832300	3.39510300	-0.97470400
H	2.47986300	4.55908300	0.24913200
H	4.15145100	4.01503900	0.20804200
H	2.75464400	2.23948300	3.21262600
H	4.14979400	3.12963800	2.59829500
H	2.57508000	3.92546000	2.72309700

1,6-Idip$_2$-P$_2$B$_4$Br$_3^{(+)}$, 1b

P	-1.6040	-1.1002	0.0000
P	-2.1983	1.4783	0.0000
B	-1.0265	0.4171	1.2183
B	-1.0265	0.4171	-1.2183
B	-0.2794	1.5314	0.0000
B	0.1524	-0.0547	0.0000

Br	1.8099	-1.0330	0.0000
Br	-0.8010	0.4970	3.1403
Br	-0.8010	0.4970	-3.1403
C	0.5839	2.8457	0.0000
C	1.0756	5.0457	0.0000
C	2.2499	4.3616	0.0000
C	-0.7094	-2.8550	0.0000
C	-0.6844	-5.0024	0.6787
C	-0.6844	-5.0024	-0.6787
C	-0.5904	-3.2570	2.4701
C	-1.7735	-2.9606	3.1696
C	0.6921	-3.2402	3.0611
C	-1.6438	-2.6128	4.5206
C	0.7594	-2.8562	4.4050
C	-0.3932	-2.5491	5.1278
C	-0.5904	-3.2570	-2.4701
C	0.6921	-3.2402	-3.0611
C	-1.7735	-2.9606	-3.1696
C	0.7594	-2.8562	-4.4050
C	-1.6438	-2.6128	-4.5206
C	-0.3932	-2.5491	-5.1278
C	2.9858	2.0234	0.0000
C	3.4941	1.6060	-1.2415
C	3.4941	1.6060	1.2415
C	4.6227	0.7781	-1.2110
C	4.6227	0.7781	1.2110
C	5.1884	0.3805	0.0000
C	-1.3291	4.5102	0.0000
C	-1.9556	4.7146	-1.2428
C	-1.9556	4.7146	1.2428
C	-3.2652	5.2083	-1.2110

C	-3.2652	5.2083	1.2110
C	-3.9075	5.4633	0.0000
C	-3.1572	-3.0853	-2.5417
C	-3.8524	-4.3674	-3.0441
C	-4.0364	-1.8462	-2.7924
C	-3.1572	-3.0853	2.5417
C	-4.0364	-1.8462	2.7924
C	-3.8524	-4.3674	3.0441
C	1.9379	-3.7536	-2.3423
C	3.2113	-2.9414	-2.6381
C	2.1829	-5.2332	-2.7155
C	1.9379	-3.7536	2.3423
C	2.1829	-5.2332	2.7155
C	3.2113	-2.9414	2.6381
C	2.8527	2.0195	2.5615
C	3.6247	3.1845	3.2110
C	2.7157	0.8354	3.5329
C	2.8527	2.0195	-2.5615
C	2.7157	0.8354	-3.5329
C	3.6247	3.1845	-3.2110
C	-1.2639	4.3896	2.5631
C	-2.2268	3.7829	3.5986
C	-0.5588	5.6310	3.1467
C	-1.2639	4.3896	-2.5631
C	-0.5588	5.6310	-3.1467
C	-2.2268	3.7829	-3.5986
N	0.0645	4.1076	0.0000
N	1.9333	3.0175	0.0000
N	-0.6895	-3.6738	1.0833
N	-0.6895	-3.6738	-1.0833
H	0.8601	6.1019	0.0000

H	3.2756	4.6936	0.0000
H	-0.6784	-5.8083	1.3942
H	-0.6784	-5.8083	-1.3942
H	-2.5327	-2.3881	5.1015
H	1.7235	-2.8192	4.9020
H	-0.3142	-2.2696	6.1751
H	1.7235	-2.8192	-4.9020
H	-2.5327	-2.3881	-5.1015
H	-0.3142	-2.2696	-6.1751
H	5.0564	0.4279	-2.1422
H	5.0564	0.4279	2.1422
H	6.0690	-0.2566	0.0000
H	-3.7955	5.3829	-2.1411
H	-3.7955	5.3829	2.1411
H	-4.9242	5.8470	0.0000
H	-3.0415	-3.1842	-1.4572
H	-3.2543	-5.2594	-2.8231
H	-4.8320	-4.4843	-2.5659
H	-4.0063	-4.3283	-4.1287
H	-3.5373	-0.9270	-2.4723
H	-4.2907	-1.7400	-3.8529
H	-4.9767	-1.9397	-2.2372
H	-3.0415	-3.1842	1.4572
H	-3.5373	-0.9270	2.4723
H	-4.9767	-1.9397	2.2372
H	-4.2907	-1.7400	3.8529
H	-3.2543	-5.2594	2.8231
H	-4.0063	-4.3283	4.1287
H	-4.8320	-4.4843	2.5659
H	1.7613	-3.7035	-1.2634
H	3.0655	-1.8741	-2.4662

H	4.0236	-3.2835	-1.9862
H	3.5476	-3.0795	-3.6722
H	1.3199	-5.8671	-2.4902
H	2.3909	-5.3280	-3.7877
H	3.0453	-5.6274	-2.1648
H	1.7613	-3.7035	1.2634
H	1.3199	-5.8671	2.4902
H	3.0453	-5.6274	2.1648
H	2.3909	-5.3280	3.7877
H	3.0655	-1.8741	2.4662
H	3.5476	-3.0795	3.6722
H	4.0236	-3.2835	1.9862
H	1.8346	2.3667	2.3527
H	3.6717	4.0577	2.5504
H	3.1386	3.4912	4.1446
H	4.6532	2.8845	3.4447
H	2.1947	0.0024	3.0564
H	3.6920	0.4840	3.8860
H	2.1320	1.1363	4.4090
H	1.8346	2.3667	-2.3527
H	2.1947	0.0024	-3.0564
H	2.1320	1.1363	-4.4090
H	3.6920	0.4840	-3.8860
H	3.6717	4.0577	-2.5504
H	4.6532	2.8845	-3.4447
H	3.1386	3.4912	-4.1446
H	-0.4980	3.6297	2.3670
H	-2.7963	2.9504	3.1743
H	-1.6567	3.3977	4.4501
H	-2.9326	4.5283	3.9825
H	0.1877	6.0399	2.4573

H	-1.2870	6.4219	3.3617
H	-0.0486	5.3738	4.0825
H	-0.4980	3.6297	-2.3670
H	0.1877	6.0399	-2.4573
H	-0.0486	5.3738	-4.0825
H	-1.2870	6.4219	-3.3617
H	-2.7963	2.9504	-3.1743
H	-2.9326	4.5283	-3.9825
H	-1.6567	3.3977	-4.4501

4-Idip-$As_2B_4Br_3^{(+)}$, 2

As	0.10756	-0.00039	-3.3528
B	0.11309	-1.28181	-1.60058
B	0.11358	1.28154	-1.60094
B	0.12132	0.00004	-0.42388
As	1.87658	-0.00052	-1.61442
B	-1.07811	0.00009	-1.6211
Br	-2.99159	0.00043	-1.68861
Br	-0.0016	-3.19375	-1.53512
Br	0.	3.19358	-1.53652
C	0.16986	-0.00025	1.13776
N	1.30461	-0.00091	1.88583
N	-0.85432	-0.0006	2.0219
C	0.98805	-0.0018	3.2307
C	-0.36521	-0.0016	3.31506
H	1.74975	-0.0024	3.98855
H	-1.02777	-0.00194	4.16119
C	-2.28021	0.00036	1.74937
C	-2.93472	-1.23748	1.67537
C	-2.93301	1.23912	1.67512

C	-4.3246	-1.20518	1.5507
C	-4.3229	1.20872	1.55041
C	-5.01006	0.00223	1.49935
H	-4.87627	-2.13313	1.48506
H	-4.8733	2.1374	1.48454
H	-6.0895	0.00298	1.40552
C	2.66336	-0.00037	1.38625
C	3.28797	1.24052	1.16721
C	3.28884	-1.24072	1.16687
C	4.60494	1.20817	0.70278
C	4.60585	-1.20734	0.70253
C	5.25453	0.00066	0.47479
H	5.1265	2.13629	0.51354
H	5.12806	-2.13507	0.51312
H	6.27608	0.00109	0.11373
C	-2.18668	-2.56019	1.74236
C	-2.78884	-3.62095	0.81082
C	-2.12739	-3.08824	3.18763
H	-1.16026	-2.38573	1.40699
H	-2.91179	-3.24017	-0.20392
H	-2.13173	-4.49198	0.76961
H	-3.76123	-3.96509	1.17017
H	-1.63739	-2.38424	3.86317
H	-3.13493	-3.2717	3.56913
H	-1.57469	-4.0303	3.22541
C	-2.18309	2.56079	1.74205
C	-2.1214	3.08786	3.18759
C	-2.78476	3.623	0.81189
H	-1.15729	2.38513	1.40542
H	-1.63161	2.38279	3.86214
H	-1.56736	4.02914	3.22532

H	-3.12826	3.27249	3.57033
H	-2.90943	3.24305	-0.20296
H	-3.75621	3.96839	1.17258
H	-2.1264	4.49307	0.77045
C	2.58661	-2.56247	1.43801
C	2.8133	-3.00762	2.89569
C	3.01862	-3.67591	0.47515
H	1.51279	-2.41027	1.29676
H	2.45089	-2.27053	3.61391
H	2.29121	-3.94783	3.08791
H	3.87787	-3.16595	3.08519
H	2.95152	-3.36099	-0.56719
H	4.04197	-4.00342	0.67208
H	2.36992	-4.54423	0.60353
C	2.58479	2.56166	1.43892
C	3.01731	3.67639	0.4778
C	2.80957	3.00541	2.89733
H	1.51121	2.40908	1.29627
H	2.95158	3.36261	-0.56497
H	2.368	4.54421	0.60643
H	4.04025	4.00422	0.6763
H	2.44665	2.26745	3.61439
H	3.87384	3.16405	3.08822
H	2.28681	3.94517	3.0899

3,5-Idip$_2$-P$_2$B$_4$Br$_2^{(2+)}$, 3

P	-0.06569500	0.08698400	1.69253300
B	-1.24691900	0.11697900	0.05217400
B	1.25028400	0.02190800	0.15029700
B	0.04846300	0.04682300	-1.10092600
P	0.06641700	1.66894100	0.08926800
B	-0.04439100	-1.15082500	0.09528000
Br	-0.12694400	-3.04981700	0.07366500
Br	0.11453400	-0.00828200	-3.00843400
C	2.79999500	0.06097400	0.22760100
N	3.56594900	1.18190400	0.17994600
N	3.65624100	-0.96889500	0.40187800
C	4.89674600	0.85009300	0.33033400
C	4.95328500	-0.50177800	0.46647100
H	5.66963300	1.59714400	0.33030300
H	5.78401100	-1.17148100	0.60137700
C	-2.78793200	0.27498200	-0.04749600
N	-3.45542500	1.45723000	-0.01844900
N	-3.72872800	-0.68187300	-0.20739500
C	-4.80987600	1.23920500	-0.16426900
C	-4.98106200	-0.10486200	-0.28128500
H	-5.51681500	2.04936100	-0.16129000
H	-5.86715600	-0.70335700	-0.39648900
C	-2.85108800	2.74566900	0.24676100
C	-2.69892000	3.12669900	1.59048500
C	-2.42719100	3.52380200	-0.84161700
C	-2.08182200	4.35680800	1.82885300
C	-1.82916800	4.75005300	-0.54178800
C	-1.65642300	5.15815000	0.77529800
H	-1.94596900	4.69786200	2.84672800
H	-1.48869100	5.38796500	-1.34602200
H	-1.19128300	6.11411100	0.98411300

C	-3.53278700	-2.11943900	-0.16687200
C	-3.40852700	-2.81239300	-1.37837100
C	-3.56411100	-2.73678700	1.09150900
C	-3.34665600	-4.20470600	-1.29871000
C	-3.49659200	-4.13089900	1.11021800
C	-3.40045800	-4.85574900	-0.07125600
H	-3.25489400	-4.78733000	-2.20559000
H	-3.52454600	-4.65419300	2.05758300
H	-3.36172200	-5.93791600	-0.03595400
C	3.32190600	-2.37426300	0.52461500
C	3.37149800	-3.16204700	-0.63241100
C	3.04884300	-2.87388700	1.80559100
C	3.17085200	-4.53373600	-0.46500400
C	2.85203000	-4.25124200	1.91263900
C	2.92516100	-5.07198000	0.79244000
H	3.20716200	-5.18706000	-1.32716300
H	2.64502000	-4.68867600	2.88069400
H	2.78313500	-6.14061300	0.90045700
C	3.06155300	2.53239700	0.04294100
C	2.69858400	3.21526900	1.21528300
C	2.93833400	3.07088200	-1.24905800
C	2.18815600	4.50615500	1.06119900
C	2.41008000	4.36130100	-1.34015500
C	2.04297800	5.06855600	-0.20063100
H	1.89861400	5.07400100	1.93513000
H	2.29280700	4.82127800	-2.31184100
H	1.64597500	6.07181800	-0.29889000
C	-3.68048900	-1.95466700	2.39008300
C	-2.56380700	-2.32487300	3.37863300
C	-5.06954300	-2.13701900	3.02390400
H	-3.56573400	-0.89196200	2.16359500

H	-1.57790700	-2.24304300	2.91486300
H	-2.59403200	-1.66486900	4.24885800
H	-2.67067800	-3.34964000	3.73997400
H	-5.86378600	-1.82847800	2.34005200
H	-5.24493600	-3.18287100	3.28594300
H	-5.15566700	-1.54282800	3.93694000
C	-3.36241900	-2.09942100	-2.71999700
C	-4.75936300	-2.05580900	-3.36576800
C	-2.34268300	-2.72964400	-3.67935900
H	-3.04351600	-1.06766400	-2.54258800
H	-5.48942400	-1.55197500	-2.72844700
H	-4.72223600	-1.52519400	-4.32006900
H	-5.12623400	-3.06732100	-3.55558400
H	-1.36422100	-2.83935800	-3.20849800
H	-2.66887500	-3.71352200	-4.02280500
H	-2.22819700	-2.10053800	-4.56454600
C	2.86760800	2.59973900	2.59564800
C	1.71754600	2.95504800	3.54817400
C	4.22225200	3.00513900	3.20550400
H	2.87068800	1.51130600	2.48440600
H	0.74237300	2.77585300	3.09045700
H	1.78616400	2.35403700	4.45728300
H	1.75403800	4.00327500	3.85199600
H	5.05890900	2.70488900	2.57170000
H	4.27488600	4.08863400	3.33553300
H	4.35494400	2.53891800	4.18443300
C	3.40201900	2.31761700	-2.48710600
C	4.90278300	2.56996500	-2.73541200
C	2.60527700	2.67219400	-3.74889100
H	3.26464600	1.24731000	-2.30201600
H	5.52177300	2.26813400	-1.88979100

H	5.23880900	2.01257000	-3.61249300
H	5.08386500	3.63162600	-2.91934500
H	1.52997800	2.59333700	-3.58994500
H	2.82979100	3.68366200	-4.09464200
H	2.87648400	1.98987000	-4.55673700
C	2.99332700	-1.97974300	3.03423700
C	4.29878400	-2.07626400	3.84282500
C	1.77429700	-2.28537400	3.91724800
H	2.89506100	-0.94322700	2.69791000
H	5.16687000	-1.80261900	3.23868800
H	4.26465500	-1.41146500	4.70938900
H	4.45381200	-3.09533900	4.20462100
H	0.84943200	-2.29766100	3.33532200
H	1.86577200	-3.25640100	4.40780300
H	1.67964300	-1.53248100	4.70317900
C	3.64075800	-2.57691700	-2.00927900
C	2.61279500	-3.05725500	-3.04533100
C	5.07638200	-2.88917000	-2.46590500
H	3.54399500	-1.48936400	-1.94391000
H	1.59141700	-2.87193600	-2.70833500
H	2.76257300	-2.53145700	-3.99091000
H	2.71487900	-4.12569600	-3.24639500
H	5.81748100	-2.50677700	-1.75972900
H	5.22923200	-3.96731200	-2.55478300
H	5.27354200	-2.43963400	-3.44191000
C	-2.61023100	3.06511000	-2.27917300
C	-1.44045800	3.47754200	-3.18235100
C	-3.94389200	3.58478000	-2.84732200
H	-2.65051900	1.97159600	-2.28141200
H	-0.47860800	3.20525900	-2.74357400
H	-1.52457000	2.97983500	-4.15004600

H	-1.43471600	4.55343100	-3.37009300
H	-4.79798200	3.24747000	-2.25668600
H	-3.95648900	4.67730000	-2.85778500
H	-4.08304300	3.23392400	-3.87227300
C	-3.23554700	2.28286200	2.73662600
C	-4.63755900	2.77630100	3.14189300
C	-2.30462700	2.24722600	3.95544600
H	-3.33962800	1.25379500	2.38319500
H	-5.33145700	2.76435600	2.29904100
H	-5.05094600	2.14392500	3.93078400
H	-4.58984100	3.80093200	3.51811600
H	-1.29573000	1.92720200	3.68785600
H	-2.23111000	3.22229200	4.44110600
H	-2.69443500	1.54700700	4.69726500

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