Persistent 2*c*-3*e* σ-Bonded Heteronuclear Radical Cations Between S/Se and P/As Atoms

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Experimental section

General considerations: All operations were performed on a dry nitrogen Schlenck line or in the glovebox. Solvents were dried following standard methods and degassed prior to use. All commercial chemicals were purchased from Alfa Aesar and used without further purification. $NOAl(OC(CF_3)_3)_4$,[S1] chlorodimesitylphosphane (Mes_2PCl)[S2] and chlorodimesitylarsane (Mes_2AsCl)[S3], 1-bromine-8 benzene sulfonium naphthalene[S4] and (8-bromonaphthalen-1-yl)(phenyl)selane[S4] were synthesized according to the reported procedures. X-ray single crystal diffraction analyses were performed on Bruker D8 Venture and Bruker D8 VENTURE PHOTONII detectors at 193 K using ω–scan techniques. The structures were solved by direct method and all refined on F^2 with the SHELX-2018 programs. The positions of the H atoms were placed in calculated positions using an appropriate riding model. The NMR spectra were collected using a Bruker DRX-400 and Bruker DRX-500 (Germany) at room temperature in ppm downfield from internal Me_4Si using CD_2Cl_2 as solvent. EPR spectra were obtained using a Bruker EMX-10/12 X-band variable-temperature apparatus and were simulated with the software of WINEPR SimFonia. Element analyses of radical salts ($[\mathbf{1}^{\bullet+}][Al(OR_F)_4]^-$ - $[\mathbf{4}^{\bullet+}][Al(OR_F)_4]^-$) and neutral compounds (**1 - 4**) were performed on Vario EL III elemental analyser and Vario MICRO elemental analyser, respectively. High resolution mass spectra (HRMS) were obtained on Agilent HPLC units.

Synthesis of **1**: Under an argon atmosphere, *n*-BuLi (6.87 mL, 1.60 M in hexane, 11.00 mmol) was added to the solution of 1-bromine-8 benzene sulfonium naphthalene (3.47 g, 11.00 mmol) in ether (140 mL) at -78 ℃ and kept stirring for 1 hour. Chlorodimesitylphosphane (3.35 g, 11.00 mmol) in ether (20 mL) was added dropwise to the (8-(phenylthio)naphthalen-1-yl)lithium solution, then warmed up to room temperature and kept stirring for 24 h. The crude product was treated with 0.10 M sodium hydroxide solution (3×50 ml) and extracted with CH_2Cl_2. The organic phase was dried by anhydrous Na_2SO_4, and the solvent was removed under vacuum and then purified by silica gel column chromatography (petroleum ether/CH_2Cl_2, 3:1). The orange solid **1** (2.33 g) was obtained, and the yield was 42%. ^{1}H NMR (400 MHz, CD_2Cl_2): δ (ppm) 1.82 (s, 12H, CH_3), 2.14 (s, 6H, CH_3), 6.66 (d, ^{3}J(H, H) = 8.1 Hz, 4H, Ar-H), 6.73 (d, ^{3}J(H, H) = 8.1 Hz, 2H, Ar-H), 7.00 (m, 2H, Ar-H), 7.05 (m, 2H, Ar-H), 7.16 (m, 2H, Ar-H), 7.44 (m, 1H, Ar-H), 7.77-7.90 (m, 2H, Ar-H). ^{13}C NMR (125 MHz, CD_2Cl_2): δ (ppm) 53.42, 125.08, 125.59, 127.18, 128.57, 129.73, 129.76, 142.59. ^{31}P NMR {^{1}H, ^{13}C}(162.0 MHz, $CDCl_3$): δ (ppm) 23.16. ^{31}P NMR {^{1}H, ^{13}C}(162.0 MHz, CD_2Cl_2): δ (ppm) -23.38. ESI-HRMS: *m*/*z* calcd for $C_{34}H_{34}PS+H^+$: 505.2113, found 505.2108. Elemental analysis calcd (%) for $C_{34}H_{33}PS$: C 80.92, H 6.59; found: C 80.71, H 5.97.

The syntheses of **2**, **3** and **4** followed can be referred to the synthetic procedure for compound **1**.

Compound **2**: (8-bromonaphthalen-1-yl)(phenyl)selane (3.98 g, 11.00 mmol), chlorodimesitylphosphane (3.35 g, 11.00 mmol), yield : 2.31 g, 38%. ^{1}H NMR(400 MHz, CD_2Cl_2): δ (ppm) 2.01 (s, 12H，CH_3), 2.25 (s，6H，CH_3), 6.81 (d, ^{3}J(H, H) = 8.1 Hz, 4H, Ar-H), 7.23(d, ^{3}J(H, H) = 8.1 Hz, 2H, Ar-H), 7.27 (m, 2H, Ar-H), 7.60 (m, 2H, Ar-H), 7.62 (m，2H, Ar-H)，7.78 (m，1H, Ar-H), 7.83 (m, 2H, Ar-H). ^{13}C NMR (125 MHz, CD_2Cl_2): δ (ppm) 53.44, 124.97, 125.64, 127.29, 129.17, 129.86, 133.84, 138.75, 142.09. ^{31}P NMR {^{1}H, ^{13}C}(162.0 MHz, CD_2Cl_2): δ (ppm) -29.26. ESI-HRMS: *m*/*z* calcd for $C_{34}H_{34}PSe+H^+$: 553.1558, found 553.1561. Elemental analysis calcd (%) for $C_{34}H_{33}PSe$: C 74.04, H 6.03; found: C 73.77, H 6.38.

Compound **3**: 1-bromine-8 benzene sulfonium naphthalene (3.47 g, 11.00 mmol), chlorodimesitylarsane (3.84 g, 11.00 mmol), yield: 1.81 g, 30%. ^{1}H NMR(400 MHz, CD_2Cl_2): δ (ppm) 1.96 (s, 12H, CH_3), 2.22 (s, 6H, CH_3), 6.74 (d, ^{3}J(H, H) =8.1 Hz, 4H, Ar-H), 6.87(d, ^{3}J(H, H) = 8.1 Hz, 2H, Ar-H), 7.08 (m, 2H, Ar-H), 7.14 (m, 2H, Ar-H), 7.25 (m, 2H, Ar-H)，7.67 (m, 1H, Ar-H), 7.98 (m, 2H, Ar-H). ^{13}C NMR (125 MHz, CD_2Cl_2): δ (ppm) 53.43, 125.11, 125.52, 126.01, 126.95, 128.48, 129.41, 131.89,138.76, 142.71. Elemental analysis calcd (%) for $C_{34}H_{33}SAs$: C 74.44, H 6.06; found: C 73.96, H 5.99.

Compound **4**: (8-bromonaphthalen-1-yl)(phenyl)selane (3.98 g, 11.00 mmol), chlorodimesitylarsane (3.84 g, 11.00 mmol), yield : 1.83 g, 28%. ^{1}H NMR (400 MHz, CD_2Cl_2): δ (ppm) 2.03 (s, 12H, CH_3), 2.23 (s, 6H, CH_3), 6.77 (d, ^{3}J(H, H) = 8.1 Hz, 4H, Ar-H), 7.18(d, ^{3}J(H, H) = 8.1 Hz, 2H, Ar-H), 7.21 (m, 2H, Ar-H), 7.34 (m, 2H, Ar-H), 7.72 (m, 2H, Ar-H), 7.80 (m，1H, Ar-H), 7.86 (m, 2H, Ar-H). ^{13}C NMR (125 MHz, CD_2Cl_2): δ (ppm) 53.43, 125.56, 126.66, 129.05, 129.49, 130.48, 136.13, 137.41, 137.82, 142.45. Elemental analysis calcd (%) for $C_{34}H_{33}AsSe$: C 68.57, H 5.59; found: C 67.91, H 5.90.

Syntheses of [**1**$^{\bullet+}$][$Al(OR_F)_4$]$^-$ - [**4**$^{\bullet+}$][$Al(OR_F)_4$]$^-$: Under anaerobic and anhydrous conditions, CH_2Cl_2 (35 ml) was added dropwise to a mixture of neutral precursors (**1** - **4**) and $NOAl(OC(CF_3)_3)_4$, which was stirred at room temperature for 12 hours. The resultant deep blue or purple solution was filtered and the filtrate was then concentrated in vacuo to afford a blue or purple powder.

[**1**$^{\bullet+}$][$Al(OR_F)_4$]$^-$: **1** (0.05 g, 0.1 mmol), $NOAl(OC(CF_3)_3)_4$ (0.10 g, 0.1 mmol). Dark blue powder, yield: 0.03 g, 21.1%. Elemental analysis calcd (%) for $C_{50}H_{33}AlF_{36}O_4PS$: C 40.80, H 2.26; found: C 41.2, H 2.18.

[**2**$^{\bullet+}$][$Al(OR_F)_4$]$^-$: **2** (0.06 g, 0.1 mmol), $NOAl(OC(CF_3)_3)_4$ (0.10 g, 0.1 mmol). Dark purple powder, yield: 0.06 g, 40.0%. Elemental analysis calcd (%) for $C_{50}H_{33}AlF_{36}O_4PSe$: C 39.54, H 2.19; found: C 39.06, H 2.25.

[**3**$^{\bullet+}$][$Al(OR_F)_4$]$^-$: **3** (0.05 g, 0.1 mmol), $NOAl(OC(CF_3)_3)_4$ (0.1 g, 0.1 mmol). Dark blue powder, yield: 0.05 g, 34.0%. Elemental analysis calcd (%) for $C_{50}H_{33}AlF_{36}O_4AsS$: C 39.62, H 2.19; found: C 39.70, H 2.28.

[4$^{\bullet+}$][$Al(OR_F)_4$]$^-$: **4** (0.06 g, 0.1 mmol), $NOAl(OC(CF_3)_3)_4$ (0.10 g, 0.1 mmol). Dark blue powder, yield: 0.04 g, 28.0%. Elemental analysis calcd (%) for $C_{50}H_{33}AlF_{36}O_4AsSe$: C 38.43, H 2.13; found: C 38.28, H 2.08.

References:

S1 A. Decken, H. D. B. Jenkins, G. B. Nikiforov and J. Passmore, *Dalton Trans.*, 2004, 2496.

S2 M. Wang, F. Nudelman, R. R. Matthes and M. P. Shaver, *J. Am. Chem. Soc.*, 2017, **139**, 14232.

S3 C. G. Pitt, A. P. Purdy, K. T. Higa and R. L. Wells, *Organometallics*, 1986, **5**, 1266.

S4 F. R. Knight, A. L. Fuller, M. Bühl, A. M. Z. Slawin and J. D. Woollins, *Chem. Eur. J.*, 2010, **16**, 7503.

Table S1. Crystal data and structure refinement for compounds **1** – **4**

	1	2	3	4
formula	C34H33PS	C34H33PSe	C34H33AsS	C34H33AsSe
Mr/g mol-1	504.63	551.53	548.58	595.48
crystal system	Triclinic	Triclinic	Triclinic	Triclinic
space group	*P* -1	*P* -1	*P* -1	*P* -1
a, Å	10.4680(4)	10.4597(5)	10.4570(6)	10.4307(4)
b, Å	11.2779(4)	11.3320(5)	11.3972(7)	11.4296(4)
c, Å	13.2284(5)	13.2801(6)	13.2662(8)	13.3226(4)
α, deg	66.2850(10)	66.2890(10)	66.746(2)	66.9580(10)
β, deg	69.1860(10)	69.7310(10)	68.9940(10)	69.6880(10)
γ, deg	78.1630(10)	78.7920(10)	78.780(2)	79.6480(10)
V, Å3	1332.98(9)	1349.18(11)	1353.50(14)	1368.93(8)
Z	2	2	2	2
Temperature, K	193(2)	193(2)	193(2)	193(2)
*R*1 (*I*>2*σ*(*I*))	0.0383	0.0320	0.0234	0.0258
*wR*2 (all data)	0.1017	0.0840	0.0630	0.0713

$R_1 = \Sigma||F_o| - |F_c||/\Sigma F_o|$, $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

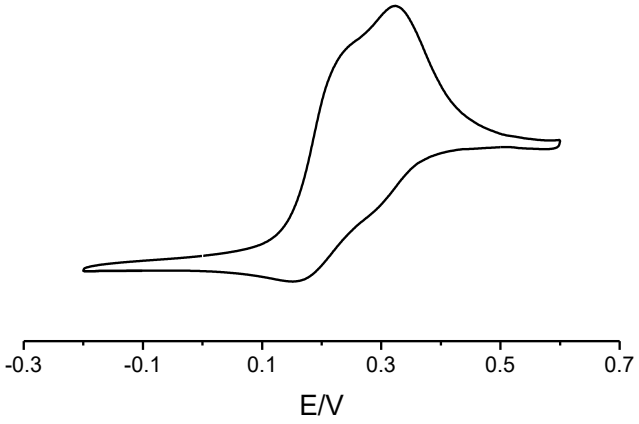

Fig. S1 The cyclic voltammogram of **1** (1×10^{-3} M) in CH_2Cl_2 at 298 K containing 0.1 M $^{n}Bu_4NPF_6$. Scan rate: 100 mV s^{-1}.

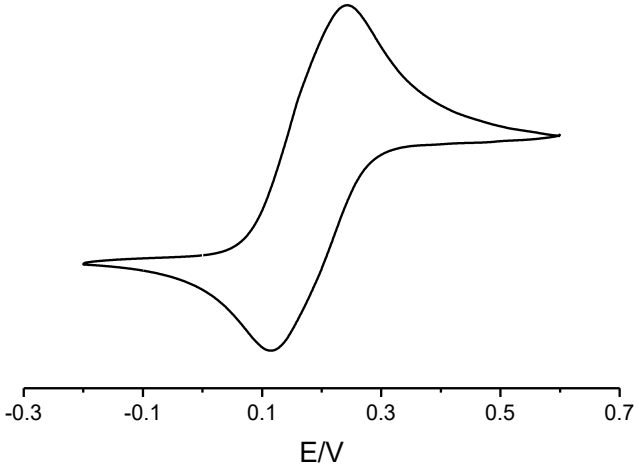

Fig. S2 The cyclic voltammogram of **2** (1×10^{-3} M) in CH_2Cl_2 at 298 K containing 0.1 M $^{n}Bu_4NPF_6$. Scan rate: 100 mV s^{-1}.

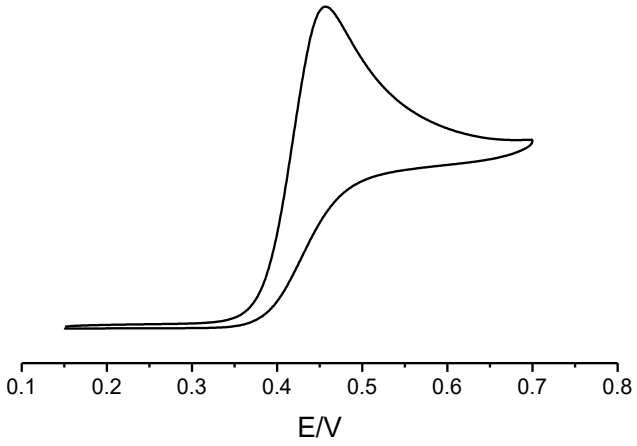

Fig. S3 The cyclic voltammogram of **3** (1×10^{-3} M) in CH_2Cl_2 at 298 K containing 0.1 M $^{n}Bu_4NPF_6$. Scan rate: 100 mV s^{-1}.

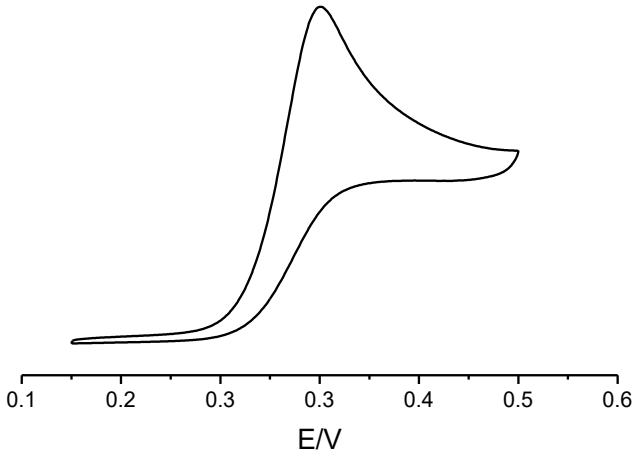

Fig. S4 The cyclic voltammogram of **4** (1×10^{-3} M) in CH_2Cl_2 at 298 K containing 0.1 M $^{n}Bu_4NPF_6$. Scan rate: 100 mV s^{-1}.

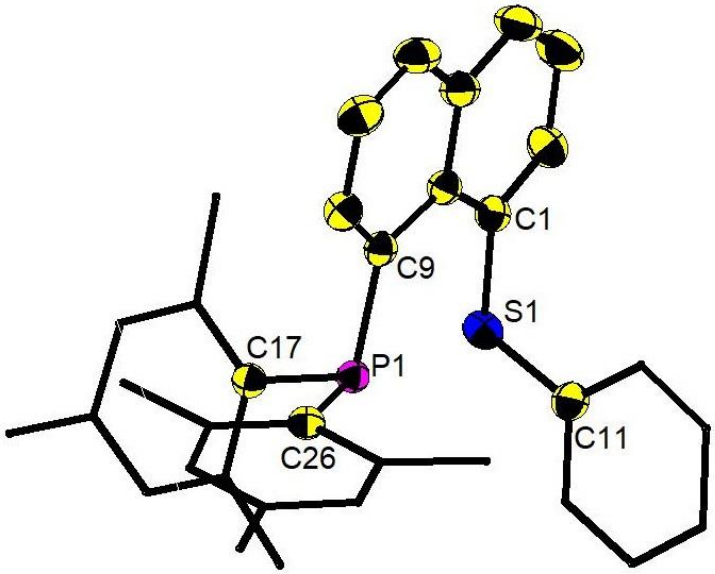

Fig. S5 Stick and Thermal ellipsoid (50%) drawing of **1**. Yellow, C; blue, S; pink P. Hydrogen atoms are omitted for clarity. Selected bond distances (Å) and angles (deg): P1–S1 3.039(4), S1–C1 1.777(1), S1–C11 1.766(1) , P1–C9 1.851(1), P1–C17 1.840(1), P1–C26 1.855(1), C17–P1–C26 106.36(6), C17–P1–C9 109.66(6), C26–P1–C9 100.96(6), C1–S1–C11 103.81(7).

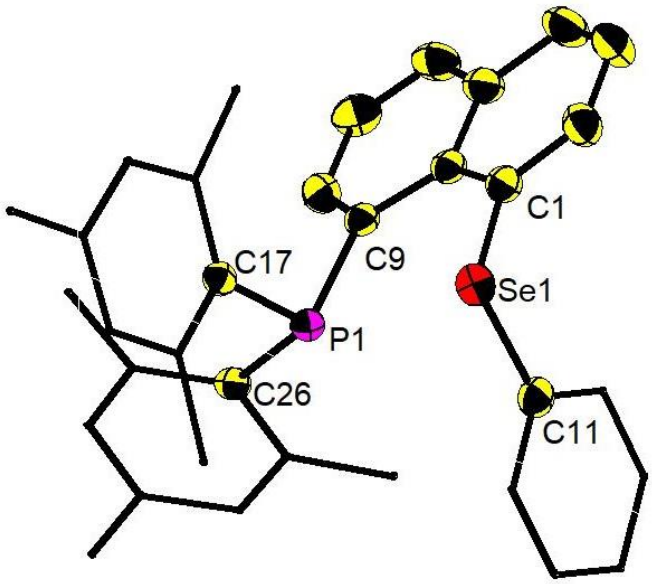

Fig. S6 Stick and Thermal ellipsoid (50%) drawing of **2**. Yellow, C; red, Se; pink P. Hydrogen atoms are omitted for clarity. Selected bond distances (Å) and angles (deg): P1–Se1 3.122(5), Se1–C1 1.928(2), Se1–C11 1.914(2), P1–C9 1.855(2), P1–C17 1.848(2), P1–C26 1.854(2), C17–P1–C26 106.88(9), C17–P1–C9 109.14(9), C26–P1–C9 101.27(9), C1–Se1–C11 100.76(9).

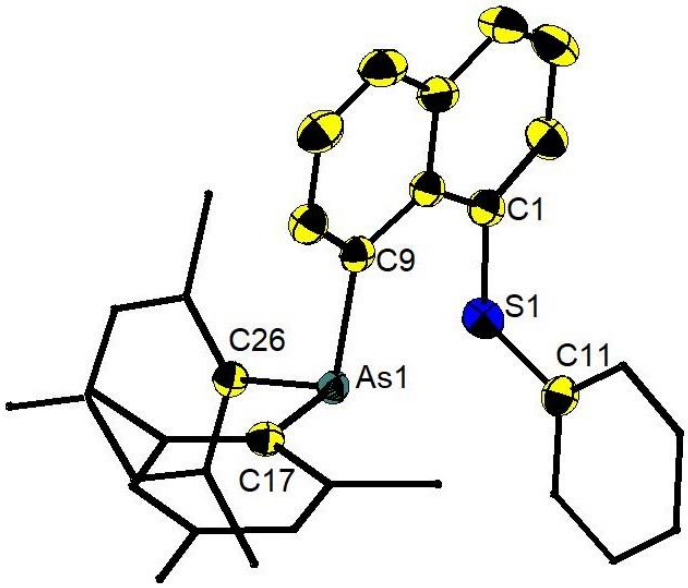

Fig. S7 Stick and Thermal ellipsoid (50%) drawing of **3**. Yellow, C; blue, S; gray As. Hydrogen atoms are omitted for clarity. Selected bond distances (Å) and angles (deg): S1–As1 3.048(4), S1–C1 1.776(1), S1–C11 1.769(1), As1–C9 1.985(1), As1–C17 1.989(1), As1–C26 1.972(1), C17–As1–C26 103.98(5), C9–As1–C26 107.35(5), C9–As1–C17 98.38(5), C1–S1–C11 103.79(7).

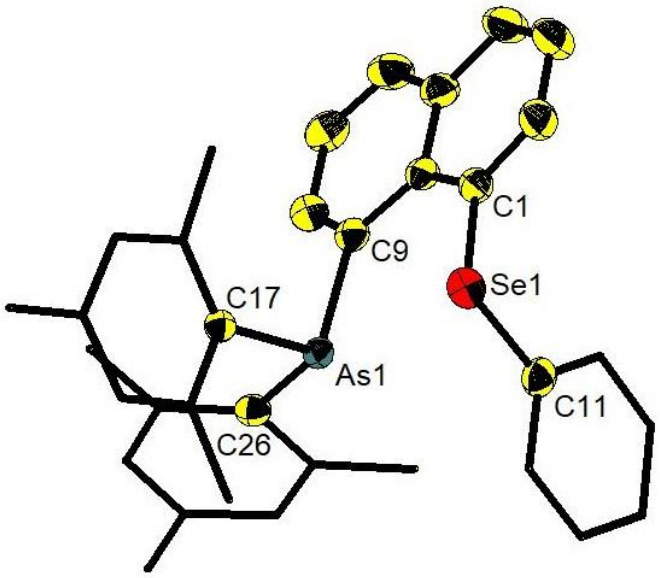

Fig. S8 Stick and Thermal ellipsoid (50%) drawing of **4**. Yellow, C; red, Se; gray As. Hydrogen atoms are omitted for clarity. Selected bond distances (Å) and angles (deg): As1–Se1 3.127(3), Se1–C1 1.925(2), Se1–C11 1.919(2), As1–C9 1.992(1), As1–C17 1.983(1), As1–C26 1.992(1), C17–As1–C26 104.45(7), C17–As1–C9 106.96(7), C26–As1–C9 98.56(8), C1–Se1–C11 100.74(8).

Table S2 Selected bonds in **1** - **4** and $\mathbf{1}^{\bullet+}$ - $\mathbf{4}^{\bullet+}$.

	1 - 4		$\mathbf{1}^{\bullet+}$ - $\mathbf{4}^{\bullet+}$
	X-ray	DFT	DFT
S–P, Å	3.039	3.097	2.796
Se–P, Å	3.122	3.164	2.867
S–As, Å	3.048	3.118	2.851
Se–As, Å	3.127	3.192	2.911

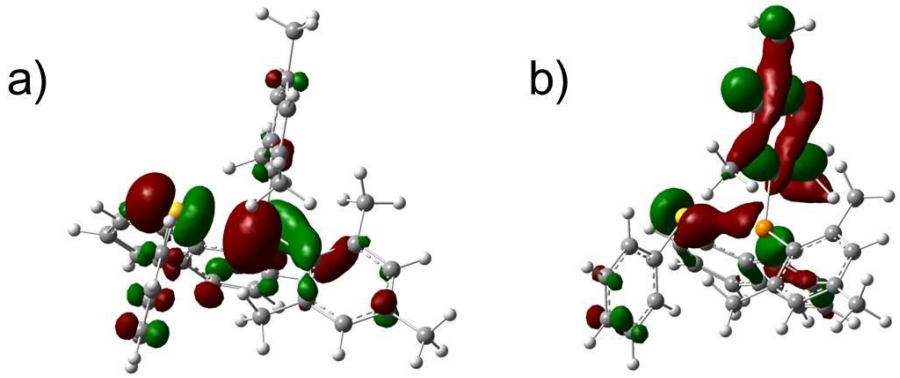

Fig. S9 a) S-P σ*-antibonding orbital (SOMO) of $\mathbf{1}^{\bullet+}$; b) S-P σ*-antibonding orbital (SOMO-12) of $\mathbf{1}^{\bullet+}$.

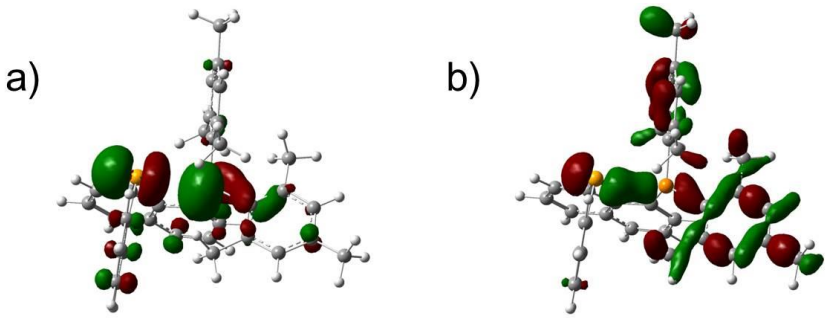

Fig. S10 a) Se-P σ*-antibonding orbital (SOMO) of $\mathbf{2}^{\bullet+}$; b) Se-P σ-bonding orbital (SOMO-11) of $\mathbf{2}^{\bullet+}$.

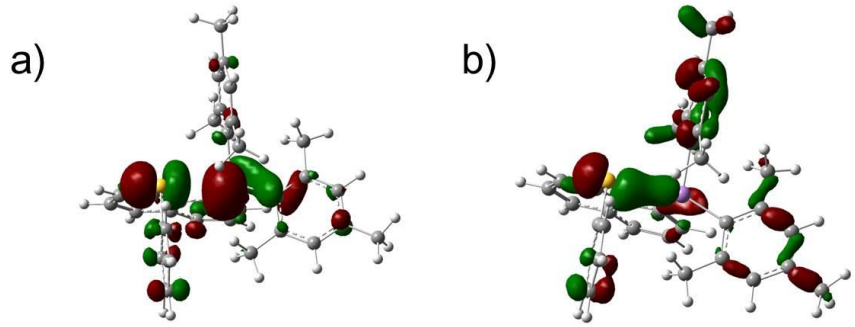

Fig. S11 a) S-As σ*-antibonding orbital (SOMO) of $\mathbf{3}^{\bullet+}$; b) S-As σ-bonding orbital (SOMO-12) of $\mathbf{3}^{\bullet+}$.

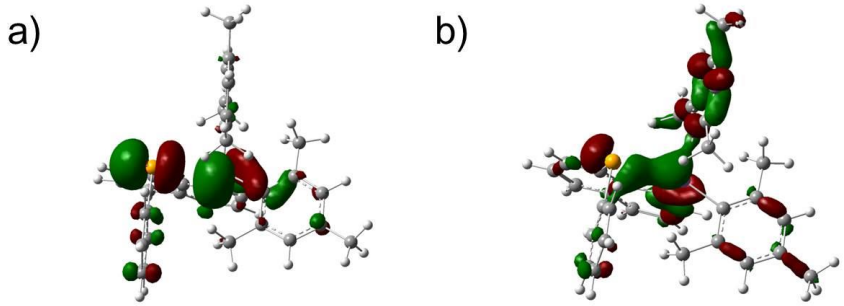

Fig. S12 a) Se-As σ*-antibonding orbital (SOMO) $\mathbf{4}^{\bullet+}$; b) Se-As σ-bonding orbital (SOMO-12) $\mathbf{4}^{\bullet+}$.

Table S3 Bond lengths (Å), dissociation energies (kcal/mol), vibrational frequencies (cm^{-1}) of rare gas dimer cations radicals

	He_2^+		Ne_2^+		Ar_2^+	
	EXP	DFT	EXP	DFT	EXP	DFT
Bond length (Å)	1.081[S6]	1.126	1.75[S6]	1.773	2.42[S7]	2.502
Dissociation energy (kcal/mol)	56.9	62.9	31.4	50.5	29.3	40.6
Vibrational frequency (cm^{-1})	1698.5	1464.7	598.5	530.6	304	283.4

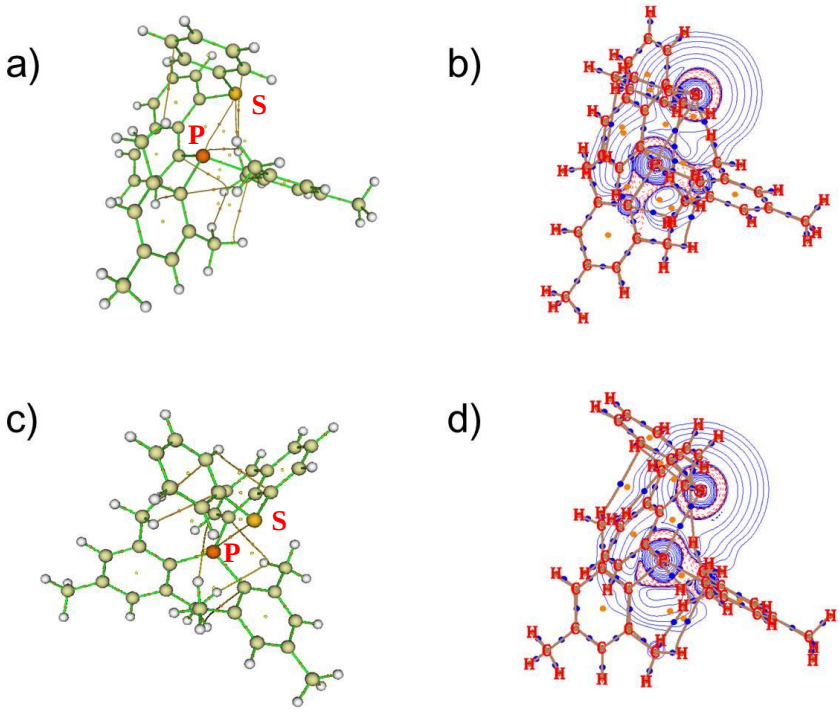

Fig. S13 Plots of Laplacian distribution [$\nabla^2\rho(r)$] in P−S−C plane for **1**: a) and b); $\mathbf{1}^{\bullet+}$: c) and d). Solid blue lines mean the charge depletion ($\nabla^2\rho(r) > 0$), while red dashed lines indicate the areas of charge concentration ($\nabla^2\rho(r) < 0$). Brown lines indicate bond paths and blue dots are bond critical points (BCPs).

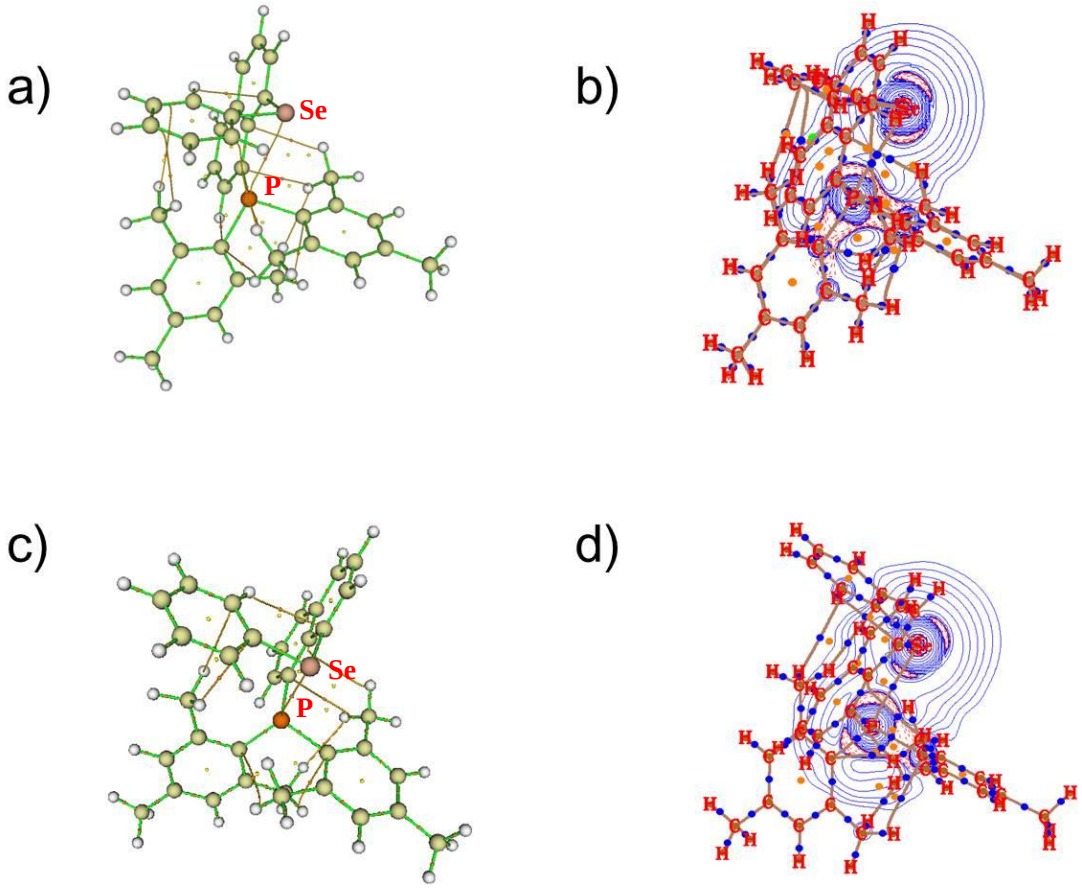

Fig. S14 Plots of Laplacian distribution [$\nabla^2\rho$(r)] in P−Se−C plane for **2**: a) and b); **2**$^{+}$: c) and d). Solid blue lines mean the charge depletion ($\nabla^2\rho$(r) > 0), while red dashed lines indicate the areas of charge concentration ($\nabla^2\rho$(r) < 0). Brown lines indicate bond paths and blue dots are bond critical points (BCPs).

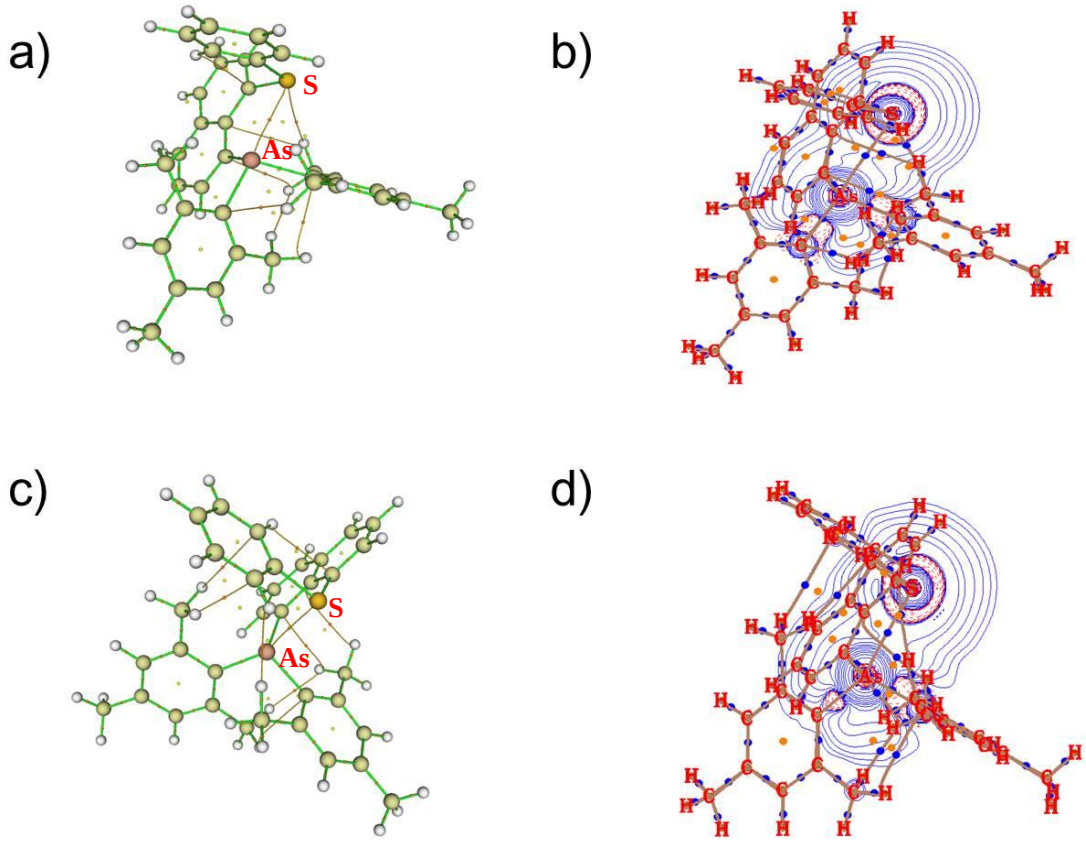

Fig. S15 Plots of Laplacian distribution [$\nabla^2\rho(r)$] in S−As−C plane for **3**: a) and b); $\mathbf{3}^{\bullet+}$: c) and d). Solid blue lines mean the charge depletion ($\nabla^2\rho(r) > 0$), while red dashed lines indicate the areas of charge concentration ($\nabla^2\rho(r) < 0$). Brown lines indicate bond paths and blue dots are bond critical points (BCPs).

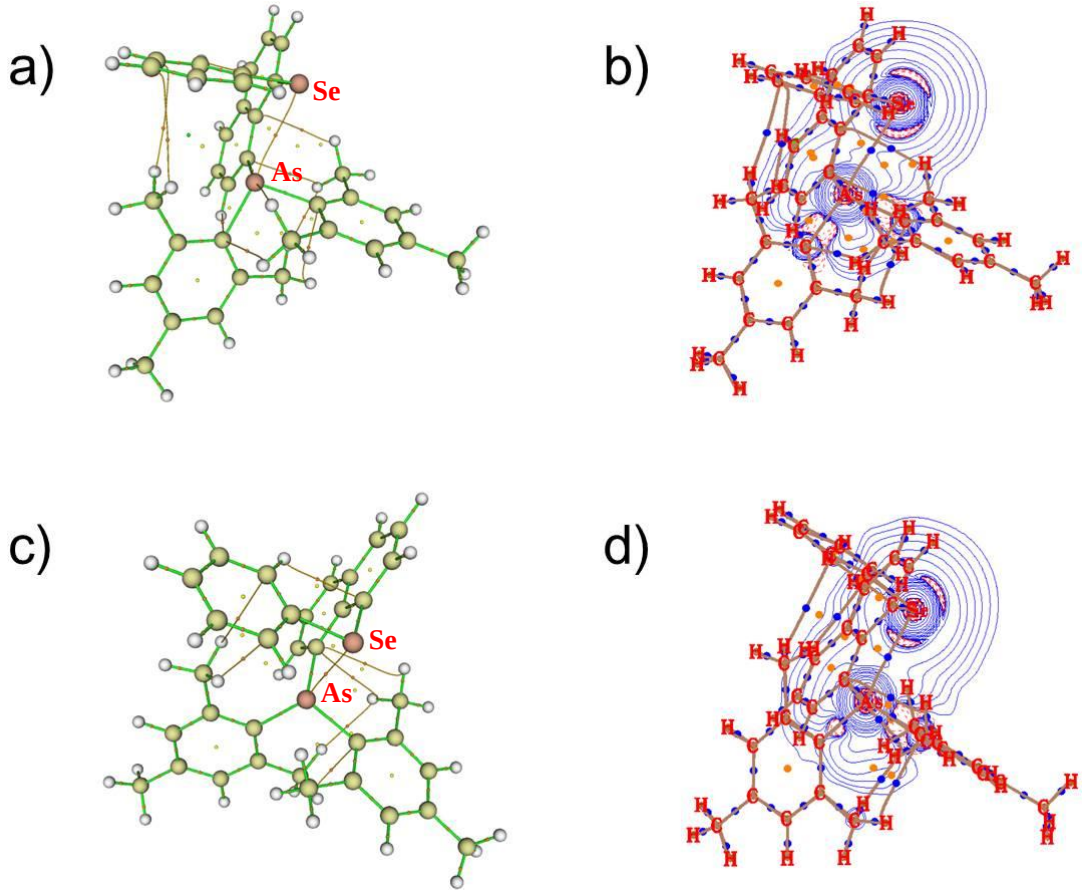

Fig. S16 Plots of Laplacian distribution [$\nabla^2\rho(r)$] in Se−As−C plane for **4** a) and b); $\mathbf{4}^{\bullet+}$ c) and d). Solid blue lines mean the charge depletion ($\nabla^2\rho(r) > 0$), while red dashed lines indicate the areas of charge concentration ($\nabla^2\rho(r) < 0$). Brown lines indicate bond paths and blue dots are bond critical points (BCPs).

Table S4 The calculated ρ(r) values at the (3, −1) bond critical points and Wiberg bond orders of selected bonds (Ch-Pn) in **1** - **4** and $\mathbf{1}^{\bullet+}$ - $\mathbf{4}^{\bullet+}$.

	Ch-Pn	ρ(r)	Wiberg Bond Order
1	S–P	0.020	0.063
$\mathbf{1}^{\bullet+}$	S–P	0.052	0.327
2	Se–P	0.020	0.085
$\mathbf{2}^{\bullet+}$	Se–P	0.039	0.392
3	S–As	0.020	0.102
$\mathbf{3}^{\bullet+}$	S–As	0.037	0.354
4	Se–As	0.021	0.126
$\mathbf{4}^{\bullet+}$	Se–As	0.038	0.432

Computational details:

All calculations were performed with the Gaussian 09 program suite.[S5] The geometry optimizations were carried out at the (U)M062x/SVP level of theory. The obtained stationary points were characterized by frequency calculations. The molecular orbitals were calculated at the level of (U)M062x/SVP on the optimized geometries.

S5 Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G.Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, Jr. J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Kieth, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

Coordinates for calculated geometries

1:

P	0.25018800	-0.16416700	0.06645700
S	-2.30827100	1.53152200	0.48057100
C	0.87580900	1.47852000	-0.50848300
C	1.02507200	3.45606400	-1.90270700
H	0.71589500	3.99406300	-2.80317200
C	1.79946600	2.07415200	0.38390300
C	0.47620400	2.19495800	-1.66007700
C	2.76310100	-0.17686000	-2.14753300
H	3.05631200	0.85119400	-1.88450700
H	1.74912000	-0.11867400	-2.56412000
H	3.44259600	-0.53615800	-2.93207400
C	1.77223500	-1.22349400	-0.01472800
C	-2.50610500	-2.72839300	-2.71989900
H	-3.14387900	-3.38855700	-3.31078000
C	1.95333600	4.05009400	-1.04612000
C	-2.02105700	0.86223200	2.10103900
C	1.89869900	-2.15392500	1.04200900
C	2.28456000	1.39583000	1.64451800
H	3.04245400	0.62811600	1.42251600
H	1.46427000	0.89286100	2.17937000
H	2.73712700	2.13394700	2.31996400
C	-2.32947100	-0.81645300	-1.14190900
C	-0.88910400	-0.98645700	-1.15822800
C	4.13121500	-2.76554600	0.26811000
C	-1.22720100	1.64185200	2.95012500
H	-0.83452500	2.59815500	2.59524600
C	-3.06697300	0.18609100	-0.41313500
C	-0.35696000	-1.99970300	-1.93860000
H	0.72071200	-2.15893200	-1.94220700
C	2.82390700	-1.09509700	-0.95139500
C	-3.12109400	-1.71916400	-1.93129000
C	2.32261500	3.33906500	0.09188900
H	3.04267600	3.77829500	0.78798100
C	3.98056700	-1.86226600	-0.78478600
H	4.78997200	-1.75410700	-1.51264400
C	-1.14679600	-2.86371300	-2.72820200
H	-0.66288900	-3.63599300	-3.32747300
C	3.07149900	-2.90541400	1.16290900
H	3.15862100	-3.61868400	1.98669300
C	-4.53947100	-1.63239800	-1.94626400
H	-5.09081200	-2.34777900	-2.55969200
C	-0.51073300	1.66429900	-2.66896200

H	-0.61858900	2.37414700	-3.49906800
H	-1.50546300	1.51485400	-2.22505400
H	-0.20138700	0.69519500	-3.08540700
C	-2.50609200	-0.37221200	2.53680700
H	-3.12000200	-0.98593700	1.87550600
C	2.50119800	5.42412800	-1.32740400
H	1.80257000	6.20195200	-0.98142000
H	2.65641400	5.57812400	-2.40428800
H	3.45856900	5.58487600	-0.81392900
C	0.80052500	-2.36280300	2.05857700
H	1.07036100	-3.17083200	2.75133000
H	-0.15203900	-2.62746400	1.57490500
H	0.60369500	-1.44860000	2.64045000
C	-2.18584500	-0.82386900	3.81693300
H	-2.56113900	-1.79304200	4.15065900
C	-5.20115000	-0.68154300	-1.21750300
H	-6.28950100	-0.61720300	-1.23005900
C	-4.44710500	0.23672100	-0.45974500
H	-4.95130400	1.02342000	0.10289800
C	-1.39053200	-0.05529400	4.66545400
H	-1.14098000	-0.41700000	5.66364900
C	5.39183000	-3.57730600	0.40861500
H	5.39494800	-4.15165700	1.34411800
H	6.28074300	-2.93015900	0.39931200
H	5.49604500	-4.28776500	-0.42541200
C	-0.91623200	1.18194300	4.22633500
H	-0.29056900	1.79327100	4.87921000

2:

P	-0.44398900	-0.14496300	-0.01286000
Se	2.26752000	1.02924200	-1.14421500
C	-1.01076900	1.61349800	-0.14125900
C	-1.16078500	3.97121200	0.40162900
H	-0.88419300	4.80149700	1.05728900
C	-1.84309100	1.85162500	-1.26138300
C	-0.65042100	2.70198400	0.68587500
C	-3.08963900	0.76686700	1.84624300
H	-3.30181200	1.61161100	1.17337500
H	-2.10734800	0.95930600	2.29813500
H	-3.84496300	0.76649900	2.64359500
C	-2.01207500	-1.05809500	0.38620800
C	1.99556700	-1.24064600	3.84757400
H	2.55253400	-1.53270600	4.73987300
C	-2.01148400	4.21704000	-0.67612900
C	2.09563200	-0.62315400	-2.09662100
C	-2.10290900	-2.34176900	-0.20101600
C	-2.24307400	0.76147700	-2.22805200
H	-2.98591400	0.07751100	-1.78853100
H	-1.37660800	0.14585400	-2.51706400
H	-2.67940600	1.20025200	-3.13484400
C	2.02727900	-0.22488400	1.57545800
C	0.59230700	-0.43036200	1.51232200
C	-4.40087400	-2.56685500	0.58951000
C	1.42556500	-0.58288800	-3.32421100
H	1.02363000	0.36263100	-3.69705000
C	2.86727600	0.36482500	0.56011600
C	-0.03248100	-1.04743300	2.58466100
H	-1.10550700	-1.22888600	2.54138200
C	-3.11390300	-0.55220700	1.11376100
C	2.70410000	-0.63137300	2.77809400
C	-2.33512700	3.13986600	-1.49649500
H	-2.98888700	3.30088400	-2.35813000
C	-4.28403000	-1.31374700	1.19250700
H	-5.13165400	-0.91451600	1.75709200
C	0.65006600	-1.45522400	3.74965700
H	0.09569100	-1.92941500	4.56060900
C	-3.29143500	-3.06922500	-0.08835200
H	-3.34960000	-4.05932600	-0.54798700
C	4.10258800	-0.43589500	2.94216700
H	4.55850200	-0.76135300	3.87943400
C	0.25738600	2.58152200	1.88392000
H	0.31154700	3.54198900	2.41236900

H	1.28058100	2.30463200	1.59084600
H	-0.08632200	1.81810400	2.59521300
C	2.59206000	-1.83500800	-1.61438900
H	3.11598800	-1.87472700	-0.65773200
C	-2.52093800	5.60509000	-0.96102900
H	-1.77058700	6.19008900	-1.51554600
H	-2.73793300	6.14782000	-0.03052900
H	-3.43623200	5.57875600	-1.56731800
C	-0.94304500	-2.96364100	-0.94197400
H	-1.19956500	-3.97744900	-1.27714200
H	-0.04849500	-3.02922100	-0.30379800
H	-0.64919200	-2.36530000	-1.81848200
C	2.41370100	-3.00045600	-2.36073200
H	2.80059200	-3.94564500	-1.97526900
C	4.85727000	0.14356400	1.96065100
H	5.92943500	0.29666600	2.08702500
C	4.22324700	0.53739800	0.76403400
H	4.81558000	0.98580600	-0.03413200
C	1.75118400	-2.96559000	-3.58615500
H	1.61555400	-3.88052400	-4.16419500
C	-5.68677200	-3.34549700	0.67945800
H	-5.56972300	-4.35887700	0.27395700
H	-6.48725700	-2.84435600	0.11430700
H	-6.02692200	-3.42855600	1.72186400
C	1.26033000	-1.75026200	-4.06601400
H	0.73641700	-1.70935800	-5.02260200

3:

As	0.25213600	-0.12145700	0.22505100
S	-2.41828900	1.45478100	0.55437700
C	-3.08681800	0.28500500	-0.61555500
C	-4.45059800	0.38518000	-0.81031300
H	-5.00465200	1.10891700	-0.21131900
C	-5.12728400	-0.41197300	-1.75502700
H	-6.20571900	-0.31305200	-1.88182100
C	-4.40319600	-1.29300800	-2.51212400
H	-4.89266500	-1.91594900	-3.26350500
C	-2.99671300	-1.42095800	-2.35255400
C	-2.28460000	-0.63869000	-1.37961600
C	-0.85502500	-0.83393300	-1.26706900
C	-0.24853800	-1.75619500	-2.10076000
H	0.82376300	-1.93081400	-2.01596200
C	-0.95762500	-2.50598700	-3.06603700
H	-0.41869300	-3.21153500	-3.69971200
C	-2.30881400	-2.34370100	-3.18547900
H	-2.88473800	-2.91536000	-3.91567200
C	1.87541600	-1.23655200	0.00706100
C	1.98240400	-2.29508800	0.93616100
C	0.87911900	-2.61779000	1.91855500
H	1.13537800	-3.51278100	2.50071300
H	-0.07635600	-2.80499200	1.40517600
H	0.69582500	-1.78652200	2.61645100
C	3.13830300	-3.08313900	0.95281900
H	3.21099800	-3.89880500	1.67713300
C	4.19572600	-2.85761600	0.07302900
C	4.06505200	-1.82061700	-0.85158500
H	4.87446300	-1.63871400	-1.56465800
C	2.92753300	-1.00855400	-0.90727200
C	2.88325700	0.06164100	-1.96981300
H	3.17582700	1.04368600	-1.56805900
H	1.87369400	0.17774200	-2.38595400
H	3.56999600	-0.18994500	-2.78930300
C	5.43078300	-3.71979500	0.09045400
H	5.45399200	-4.36599200	0.97769200
H	6.34208300	-3.10488700	0.08737900
H	5.46880100	-4.36649200	-0.79950300
C	0.96067200	1.65912400	-0.23437300
C	1.85688100	2.17166900	0.72908500
C	2.41577300	3.44253800	0.54301500
H	3.11691500	3.82202600	1.29132200
C	2.10073400	4.23367100	-0.55764200

C	1.19128500	3.71986000	-1.48435000
H	0.92237500	4.32508800	-2.35484500
C	0.61175600	2.45640500	-1.34696300
C	-0.34666400	2.01069400	-2.42138400
H	-0.43478600	2.78294900	-3.19639600
H	-1.35164800	1.82651800	-2.01703800
H	-0.02458300	1.07698200	-2.90391700
C	2.69303200	5.60647100	-0.73957900
H	1.92625100	6.38490700	-0.60686000
H	3.11006500	5.72744000	-1.74977100
H	3.49384400	5.79473500	-0.01251300
C	2.25867000	1.39644500	1.96327700
H	1.37728500	1.02839900	2.51245100
H	2.84514100	2.03212300	2.63907800
H	2.86972000	0.51636400	1.70878200
C	-2.36773100	0.53520700	2.07537100
C	-1.73222900	1.16711500	3.15071400
H	-1.32718600	2.17419800	3.02434700
C	-1.59354400	0.50134700	4.36462200
H	-1.09258200	1.00019400	5.19615000
C	-2.08268400	-0.79724300	4.51727900
H	-1.96782000	-1.31982300	5.46764700
C	-2.71864100	-1.41885800	3.44471700
H	-3.10614100	-2.43351100	3.55271700
C	-2.86708300	-0.75966100	2.22388700
H	-3.35837300	-1.25958800	1.38775200

4:

As	0.39706400	-0.18298300	0.16985400
Se	-2.38989100	1.12843500	1.00846700
C	-2.95337100	0.38044700	-0.67258700
C	-4.29671000	0.56716800	-0.93582700
H	-4.90883400	1.07213400	-0.18794100
C	-4.89282300	0.11787400	-2.13250600
H	-5.95653600	0.28145100	-2.30778300
C	-4.11260300	-0.52499900	-3.05321300
H	-4.53933700	-0.89139800	-3.98914100
C	-2.72532400	-0.73600200	-2.82580700
C	-2.08718000	-0.28153600	-1.61896600
C	-0.66496200	-0.52006800	-1.48219500
C	-0.00937600	-1.20201800	-2.49270800
H	1.05507700	-1.41113700	-2.39279700
C	-0.65143000	-1.64755700	-3.66868800
H	-0.07468600	-2.17128300	-4.43212700
C	-1.98638000	-1.41085400	-3.83368600
H	-2.51240600	-1.73532600	-4.73362300
C	2.06647300	-1.15591700	-0.28046800
C	2.20943100	-2.39874300	0.37779800
C	1.10360100	-2.99634300	1.21828600
H	1.38719400	-3.99778900	1.56785700
H	0.16525200	-3.08519900	0.64987200
H	0.87366100	-2.37258300	2.09579800
C	3.40590100	-3.11106300	0.25300600
H	3.50628900	-4.06935200	0.76986900
C	4.47195900	-2.63315500	-0.50869300
C	4.30516300	-1.41779000	-1.17180500
H	5.12022600	-1.03411000	-1.79222600
C	3.12440700	-0.67196800	-1.08002500
C	3.04787200	0.60976900	-1.87255100
H	3.30769000	1.48394200	-1.25642800
H	2.03663100	0.78363800	-2.26275600
H	3.74571500	0.57095800	-2.71990600
C	5.74727900	-3.42181300	-0.64912700
H	5.87156700	-4.13068700	0.18024400
H	6.62363600	-2.75955700	-0.67317100
H	5.74659900	-4.00145000	-1.58541000
C	1.06359900	1.67497500	0.16498000
C	1.93588300	1.95529900	1.23999000
C	2.47707500	3.24001900	1.37281400
H	3.16087000	3.43742400	2.20290500
C	2.16633500	4.26765300	0.48745900

C	1.27610700	3.97976100	-0.54833300
H	1.00876300	4.77239000	-1.25289900
C	0.71390400	2.71291100	-0.72594800
C	-0.23351200	2.53273700	-1.88449300
H	-0.30330400	3.46193800	-2.46458100
H	-1.24632800	2.27465500	-1.54292700
H	0.08555700	1.72874300	-2.56235000
C	2.73751600	5.65163000	0.65064700
H	1.97793100	6.34567400	1.04220000
H	3.08260700	6.05384100	-0.31255100
H	3.58546600	5.65425000	1.34806600
C	2.33107000	0.91787200	2.26590200
H	1.44948300	0.40272200	2.67894700
H	2.87253300	1.39080600	3.09537300
H	2.98284400	0.14352400	1.83252600
C	-2.31936900	-0.46522000	2.07080900
C	-1.73501800	-0.35627100	3.33704300
H	-1.36403700	0.61005000	3.68793900
C	-1.60712700	-1.48443100	4.14327300
H	-1.15006000	-1.39015600	5.12997600
C	-2.05115500	-2.72800100	3.69102000
H	-1.94511000	-3.61215900	4.32081900
C	-2.63188700	-2.83005400	2.42846600
H	-2.98352500	-3.79735400	2.06496700
C	-2.77237100	-1.70408700	1.61617000
H	-3.22610600	-1.79831200	0.62799100

1$^{\bullet+}$:

P	0.48833800	-0.01052500	0.14075900
S	-1.73328100	-0.72673100	-1.39844300
C	1.27529400	-1.50151500	-0.50464900
C	1.97834700	-3.80275500	-0.49470600
H	2.02495400	-4.77222300	0.00701200
C	1.86858700	-1.32738200	-1.77865900
C	1.31084000	-2.75684200	0.14464800
C	3.50117000	-0.37538700	1.29034500
H	3.74546300	-0.92949700	0.37159800
H	2.75578200	-0.97056100	1.83661000
H	4.40780600	-0.32115900	1.90496300
C	1.68887000	1.29081200	0.52389400
C	-2.16005600	-0.66554200	3.84944600
H	-2.75956400	-0.86707200	4.73918600
C	2.59272700	-3.65639700	-1.74145900
C	-2.44697500	0.84726500	-1.83037100
C	1.26429500	2.62030700	0.29795300
C	1.83284300	-0.01118100	-2.51625300
H	2.50033100	0.73242300	-2.05305900
H	0.81945400	0.42338200	-2.52873100
H	2.15310600	-0.14764000	-3.55624500
C	-1.91970500	-0.79627600	1.39985500
C	-0.61608200	-0.21878600	1.55065200
C	3.46303600	3.41845600	0.98810400
C	-2.11745500	1.31996700	-3.10578200
H	-1.51989900	0.70454900	-3.78259000
C	-2.52618700	-1.12320300	0.14636700
C	-0.16914300	0.18511200	2.79755500
H	0.81248700	0.65487100	2.89516100
C	2.99705200	1.01388500	0.99053700
C	-2.67925400	-1.05041900	2.58304800
C	2.52319100	-2.40982300	-2.36560700
H	2.98885800	-2.27486900	-3.34464700
C	3.85243100	2.09381700	1.20988100
H	4.86128200	1.89320700	1.57926800
C	-0.94479800	-0.03617600	3.95503300
H	-0.56419800	0.27795200	4.92702100
C	2.16290500	3.65928000	0.53965400
H	1.83828200	4.68765900	0.36685300
C	-3.95624600	-1.66626000	2.48876900
H	-4.50998200	-1.85948200	3.40928600
C	0.69343900	-3.03217900	1.49327000
H	0.97115900	-4.03804200	1.82986400

H	-0.40470500	-2.98508800	1.45774500
H	1.02499400	-2.31723800	2.25910700
C	-3.23437900	1.61062400	-0.96661600
H	-3.50010800	1.23874900	0.02429600
C	3.27788500	-4.81981100	-2.40205600
H	2.53981500	-5.45413800	-2.91680300
H	3.79472800	-5.44746200	-1.66423700
H	4.00751900	-4.48249100	-3.14894800
C	-0.12333400	2.93745400	-0.19781900
H	-0.27599000	4.02183900	-0.26026600
H	-0.89647700	2.52941600	0.47194300
H	-0.30407200	2.51376900	-1.19917800
C	-3.67848300	2.86487200	-1.38613600
H	-4.29629200	3.46502400	-0.71664000
C	-4.48737500	-2.00787600	1.27049600
H	-5.46546500	-2.48439600	1.20243100
C	-3.76840700	-1.72039500	0.08971300
H	-4.20239600	-1.95571900	-0.88357800
C	-3.33981500	3.35310000	-2.64730200
H	-3.69089200	4.33516600	-2.96564000
C	4.41992200	4.54664800	1.25386800
H	4.03780300	5.49852000	0.86526700
H	5.39779700	4.34874400	0.79368700
H	4.58489000	4.66217100	2.33574200
C	-2.56228000	2.57654500	-3.50756100
H	-2.30620400	2.94557700	-4.50146200

2$^{\bullet+}$:

P	0.62754300	0.04963800	0.16632900
Se	-1.64574300	-0.77185400	-1.37519300
C	1.48353400	-1.41539200	-0.46151500
C	2.30242500	-3.67990200	-0.42212800
H	2.41281100	-4.63297200	0.10051200
C	2.03665200	-1.24358400	-1.75513300
C	1.60514200	-2.65156600	0.21482800
C	3.71177000	-0.11214700	1.19503900
H	3.94066400	-0.67709200	0.27907100
H	3.03633600	-0.73594300	1.79795500
H	4.64551400	0.01567600	1.75591400
C	1.76766900	1.42512800	0.47654100
C	-1.77792800	-0.69700200	4.02397900
H	-2.31600400	-0.91903500	4.94741500
C	2.87019200	-3.53583800	-1.69041500
C	-2.58353000	0.88002100	-1.62756500
C	1.25371600	2.72315200	0.25395900
C	1.93881500	0.05624700	-2.51597300
H	2.59399600	0.82794700	-2.08204700
H	0.91406500	0.46264600	-2.51120100
H	2.23778800	-0.09036600	-3.56083800
C	-1.65720800	-0.86500600	1.56557100
C	-0.38953500	-0.19784000	1.63798100
C	3.42996400	3.66463900	0.82227700
C	-2.44111500	1.47612400	-2.88506400
H	-1.86624100	0.98341800	-3.67323700
C	-2.30977800	-1.26418900	0.35641200
C	0.09277200	0.26008900	2.85197300
H	1.04515500	0.79420600	2.88817000
C	3.10949900	1.23635000	0.88862600
C	-2.33249600	-1.14624100	2.79436400
C	2.72410600	-2.30797400	-2.33786900
H	3.15847200	-2.17203600	-3.33113300
C	3.90714500	2.37004500	1.04926600
H	4.94059100	2.23678600	1.37859000
C	-0.60554200	0.01544400	4.05343000
H	-0.19775700	0.37683100	4.99766800
C	2.09663500	3.81867700	0.43776000
H	1.69914700	4.82245700	0.27216000
C	-3.56248200	-1.85770900	2.78522100
H	-4.04886400	-2.06680500	3.73976000
C	1.05543100	-2.92492600	1.59276200
H	1.39739400	-3.90699300	1.94040000

H	-0.04398500	-2.93298200	1.60227100
H	1.38086800	-2.17546900	2.32737400
C	-3.33394400	1.49368000	-0.62388400
H	-3.45136800	1.02579300	0.35512800
C	3.58970800	-4.68045000	-2.34728900
H	2.87238200	-5.33077100	-2.87143800
H	4.11515700	-5.29746300	-1.60680000
H	4.31756300	-4.32325900	-3.08687100
C	-0.17324600	2.94852100	-0.17492500
H	-0.39656200	4.02056400	-0.23815100
H	-0.88714500	2.49959300	0.53326900
H	-0.37299300	2.50436700	-1.16305200
C	-3.93525600	2.72475500	-0.88554300
H	-4.52419300	3.20918300	-0.10548400
C	-4.13173800	-2.26979000	1.60742100
H	-5.07174700	-2.82167500	1.60481700
C	-3.50457900	-1.95313100	0.38197400
H	-3.98200200	-2.23965800	-0.55659900
C	-3.78916900	3.33471800	-2.13102700
H	-4.26410500	4.29684600	-2.32595100
C	4.33804200	4.85137700	0.98356600
H	3.77257300	5.79116700	0.99571900
H	5.05651400	4.89866600	0.15133800
H	4.91886700	4.78013500	1.91329300
C	-3.04469200	2.70725000	-3.13056100
H	-2.93662900	3.17350000	-4.11076000

3$^{\bullet+}$:

As	-0.43412900	-0.01572100	0.00271800
S	1.86708100	0.85107500	-1.44061200
C	2.66922000	1.11452000	0.12805300
C	3.89757900	1.74015500	0.11179500
H	4.30896100	2.07949900	-0.84020200
C	4.63315600	1.92356300	1.30403800
H	5.60014900	2.42549500	1.26828700
C	4.13371700	1.44710300	2.48914800
H	4.70210100	1.55502600	3.41471000
C	2.86926800	0.79987700	2.54340000
C	2.09063500	0.65273900	1.35411300
C	0.80000100	0.04776200	1.47522300
C	0.37273000	-0.47316600	2.68141700
H	-0.60559700	-0.95522600	2.75283900
C	1.16964700	-0.35919900	3.84217000
H	0.80838100	-0.76767700	4.78616900
C	2.37824000	0.28669800	3.77535500
H	2.99316000	0.40557200	4.66938900
C	-1.73272700	-1.38067800	0.42861500
C	-1.35038600	-2.70701100	0.13438100
C	0.00470100	-3.04175800	-0.43729100
H	0.10908100	-4.12381700	-0.58257800
H	0.81680800	-2.71827800	0.23337400
H	0.17398700	-2.55651200	-1.41290800
C	-2.25991200	-3.73209500	0.39707600
H	-1.97261700	-4.76195500	0.17312900
C	-3.52450700	-3.47573600	0.93177400
C	-3.86884800	-2.15081600	1.21360300
H	-4.85102700	-1.93820900	1.64300600
C	-3.00043700	-1.08336800	0.97475200
C	-3.45623200	0.31037600	1.32915200
H	-3.70361400	0.89987100	0.43359500
H	-2.68470300	0.86824400	1.87936000
H	-4.35132800	0.26378900	1.96094400
C	-4.48267100	-4.59511100	1.23024400
H	-4.23420600	-5.49841800	0.65929800
H	-5.51598100	-4.30594600	0.99712100
H	-4.44612500	-4.85286100	2.29990300
C	-1.26452200	1.65406700	-0.46346100
C	-1.92692600	1.63849900	-1.70867700
C	-2.57763900	2.79898100	-2.12999200
H	-3.10281000	2.79042500	-3.08781300
C	-2.57221400	3.96531900	-1.36231900

C	-1.89122800	3.94864700	-0.14179000
H	-1.88110600	4.85321400	0.47108700
C	-1.22526600	2.81754700	0.33322700
C	-0.52407700	2.90519500	1.66507300
H	-0.76010500	3.85882900	2.15211500
H	0.56889000	2.85135500	1.55158400
H	-0.81957100	2.09536400	2.34674900
C	-3.25304900	5.21662500	-1.84209500
H	-2.51522800	5.91126700	-2.27186300
H	-3.75196700	5.73832200	-1.01453700
H	-3.99773000	4.99721800	-2.61717200
C	-1.96349300	0.40931500	-2.58432700
H	-0.94732300	0.04014100	-2.80208300
H	-2.44910600	0.63019300	-3.54208600
H	-2.51994400	-0.41428000	-2.10883500
C	2.43227600	-0.78091600	-1.90365100
C	2.02832300	-1.22173000	-3.16869800
H	1.45547900	-0.56193300	-3.82499300
C	2.37211900	-2.50327700	-3.59138800
H	2.05968800	-2.84570900	-4.57875100
C	3.12025700	-3.33940500	-2.76116400
H	3.39338600	-4.34071900	-3.09549100
C	3.53147700	-2.88433200	-1.50978300
H	4.12925600	-3.52855300	-0.86333300
C	3.19106900	-1.60410200	-1.07113900
H	3.52202100	-1.25782800	-0.09093100

4$^{\bullet+}$:

As	0.53104000	0.03578300	0.06774700
Se	-1.84299300	-0.84223500	-1.37101700
C	-2.59542600	-1.06702400	0.37960300
C	-3.84531600	-1.64664600	0.43642800
H	-4.33012700	-1.97243400	-0.48527500
C	-4.51480400	-1.80856200	1.67009300
H	-5.50006900	-2.27435100	1.69232900
C	-3.92397200	-1.35974100	2.82275600
H	-4.43498600	-1.45628200	3.78245000
C	-2.63718000	-0.75683400	2.80056800
C	-1.92550900	-0.62340800	1.56589700
C	-0.61209200	-0.05546300	1.61778500
C	-0.10073900	0.43617000	2.80356600
H	0.89180200	0.89316800	2.82172500
C	-0.82870900	0.33002700	4.00954900
H	-0.39960400	0.71564400	4.93454900
C	-2.05908400	-0.27512300	4.00667600
H	-2.62503100	-0.38499800	4.93356800
C	1.84609800	1.40388800	0.45085400
C	1.46452600	2.72850800	0.15037700
C	0.09014200	3.06476100	-0.37162700
H	-0.02234000	4.14762400	-0.50502800
H	-0.69768700	2.73280300	0.32348400
H	-0.10963900	2.58582100	-1.34430000
C	2.39240600	3.74992700	0.35741000
H	2.10498400	4.77830000	0.12664900
C	3.67537600	3.49136400	0.84522600
C	4.01629000	2.16942200	1.14343300
H	5.01131100	1.95525300	1.54151700
C	3.12858100	1.10635800	0.96001700
C	3.58204900	-0.28322500	1.33378400
H	3.83161500	-0.88454200	0.44665100
H	2.80749300	-0.83295400	1.88801800
H	4.47544500	-0.22929800	1.96759100
C	4.65580900	4.60680600	1.08035600
H	4.40176300	5.49482200	0.48808900
H	5.67822300	4.29695700	0.82695100
H	4.65331800	4.89940800	2.14167300
C	1.38713800	-1.61533500	-0.43629300
C	2.03604000	-1.56468600	-1.68806700
C	2.69391900	-2.70846200	-2.14410800
H	3.20722600	-2.67110400	-3.10771600
C	2.70911200	-3.89302800	-1.40595700

C	2.04021500	-3.91261400	-0.17888000
H	2.04308900	-4.83220000	0.41132900
C	1.36825900	-2.79980500	0.32995800
C	0.68112300	-2.92757300	1.66590000
H	0.88518800	-3.91328200	2.10076000
H	-0.40995800	-2.82402100	1.57417600
H	1.02092600	-2.16600400	2.38236500
C	3.39705900	-5.12521000	-1.92405800
H	2.65984000	-5.82626700	-2.34425100
H	3.92753200	-5.65077400	-1.11880000
H	4.11618400	-4.88039400	-2.71546600
C	2.05324000	-0.31774300	-2.53941100
H	1.03330000	0.05738800	-2.72933000
H	2.51819400	-0.52008600	-3.51147700
H	2.61866300	0.49689000	-2.05956800
C	-2.44294400	0.93680700	-1.77988500
C	-2.08717100	1.42200300	-3.04152700
H	-1.54316900	0.79076000	-3.74877900
C	-2.43773000	2.72236500	-3.39847700
H	-2.16319500	3.10260800	-4.38327100
C	-3.14167300	3.52904900	-2.50357000
H	-3.41785900	4.54566200	-2.78554100
C	-3.50366900	3.02873900	-1.25404300
H	-4.06562900	3.65248900	-0.55742200
C	-3.15800400	1.72825600	-0.88205000
H	-3.44953600	1.34473900	0.09758700

$He_2^{\bullet+}$:

He	0.00000000	0.00000000	0.56321800
He	0.00000000	0.00000000	-0.56321800

$Ne_2^{\bullet+}$:

Ne	0.00000000	0.00000000	0.88628400
Ne	0.00000000	0.00000000	-0.88628400

$Ar_2^{\bullet+}$:

Ar	0.00000000	0.00000000	1.25117700
Ar	0.00000000	0.00000000	-1.25117700

$Ph_3P^{\bullet+}$:

C	0.00000000	1.72910400	0.21449300
C	1.03141100	2.53739900	0.73057200
C	1.04778200	3.89518700	0.43777600
H	1.84514800	4.52547800	0.83275100
C	0.03585600	4.45191200	-0.34926900
C	-0.99374600	3.65312700	-0.85108500
H	-1.77642100	4.09342800	-1.46955900
C	-1.02195700	2.29095000	-0.57137200
H	1.81166900	2.10456800	1.36128200
H	0.04886800	5.51990600	-0.57124500
H	-1.82038000	1.66491500	-0.97411500
P	0.00000000	0.00000000	0.63083800
C	1.49744800	-0.86455200	0.21449300
C	-1.49744800	-0.86455200	0.21449300
C	1.68174700	-2.16192800	0.73057200
C	2.49500000	-0.26043500	-0.57137200
C	-2.71315800	-0.37547200	0.73057200
C	-1.47304300	-2.03051600	-0.57137200
C	2.84944000	-2.85499900	0.43777600
H	0.91677500	-2.62123500	1.36128200
C	3.66057400	-0.96595500	-0.85108500
H	2.35204900	0.74403800	-0.97411500
C	-3.89722200	-1.04018800	0.43777600
H	-2.72844400	0.51666700	1.36128200
C	-2.66682800	-2.68717300	-0.85108500
H	-0.53166900	-2.40895300	-0.97411500
H	2.99660500	-3.86068400	0.83275100
C	3.83754100	-2.25700900	-0.34926900
H	4.43322300	-0.50828800	-1.46955900
H	-4.84175300	-0.66479400	0.83275100
C	-3.87339700	-2.19490400	-0.34926900
H	-2.65680200	-3.58513900	-1.46955900
H	4.75594500	-2.80227400	-0.57124500
H	-4.80481300	-2.71763200	-0.57124500

(2,6-dimethylphenyl)$_3$P$^{\bullet+}$:

C	0.00000000	1.76842600	0.06847600
C	0.86226800	2.51692400	0.90943500
C	0.87252300	3.90406900	0.76415200
H	1.52714800	4.49998000	1.40197400
C	0.05549900	4.53085800	-0.17326600
C	-0.78588500	3.77979500	-0.99004200
H	-1.41244900	4.28041000	-1.72981500
C	-0.83712200	2.38825600	-0.89284200
C	1.76620100	1.86962700	1.92742500
H	1.23355200	1.12472100	2.53874200
H	2.61072300	1.35290800	1.44431500
H	2.18047300	2.62528700	2.60518800
H	0.07629800	5.61730100	-0.27018000
C	-1.74959300	1.62422900	-1.81824700
H	-1.25069800	0.75292300	-2.26841500
H	-2.64133900	1.24905900	-1.29305100
H	-2.08936300	2.27651000	-2.63130500
P	0.00000000	0.00000000	0.28639900
C	1.53150200	-0.88421300	0.06847600
C	-1.53150200	-0.88421300	0.06847600
C	1.74858600	-2.00520800	0.90943500
C	2.48685100	-0.46915900	-0.89284200
C	-2.61085400	-0.51171600	0.90943500
C	-1.64973000	-1.91909700	-0.89284200
C	2.94476200	-2.70766100	0.76415200
C	0.73604500	-2.46438800	1.92742500
C	3.66634100	-1.20930100	-0.99004200
C	2.28142000	0.70307700	-1.81824700
C	-3.81728500	-1.19640800	0.76415200
C	-2.50224500	0.59476100	1.92742500
C	-2.88045600	-2.57049400	-0.99004200
C	-0.53182700	-2.32730600	-1.81824700
H	3.13352300	-3.57253900	1.40197400
C	3.89608800	-2.31349200	-0.17326600
H	0.35726100	-1.63064800	2.53874200
H	4.41316800	-0.91698800	-1.72981500
H	1.27739900	0.70667400	-2.26841500
H	-4.66067100	-0.92744100	1.40197400
C	-3.95158700	-2.21736500	-0.17326600
H	-1.59081300	0.50592700	2.53874200
H	-3.00071900	-3.36342200	-1.72981500
H	-0.02670200	-1.45959700	-2.26841500
H	-0.13370900	-2.93740600	1.44431500

H	1.18332900	-3.20098800	2.60518800
H	2.40238600	1.66293800	-1.29305100
H	3.01619700	0.67118700	-2.63130500
H	-2.47701400	1.58449800	1.44431500
H	-3.36380100	0.57570100	2.60518800
H	0.23895300	-2.91199600	-1.29305100
H	-0.92683400	-2.94769600	-2.63130500
H	4.82657700	-2.87472700	-0.27018000
H	-4.90287500	-2.74257500	-0.27018000

(2,6-diisopropylphenyl)$_3$P$^{\bullet+}$:

C	0.00000000	0.00000000	1.79117900
C	0.78380700	0.96230500	2.47253600
C	0.75338200	0.94527900	3.86837900
H	1.33726000	1.67801400	4.42724600
C	0.00000000	0.00000000	4.55845600
C	-0.75338200	-0.94527900	3.86837900
H	-1.33726000	-1.67801400	4.42724600
C	-0.78380700	-0.96230500	2.47253600
C	1.63841300	2.00118000	1.76049400
H	1.73455400	1.70632300	0.70298000
C	0.96857300	3.37944800	1.78139800
H	-0.00390800	3.36219600	1.26739100
H	1.60640000	4.12188400	1.27970200
H	0.80496900	3.71673300	2.81614300
C	3.06118300	2.05779800	2.32434300
H	3.07719500	2.46739900	3.34434600
H	3.68675700	2.71176200	1.70022400
H	3.52257000	1.05936400	2.35231500
H	0.00000000	0.00000000	5.64935400
C	-1.63841300	-2.00118000	1.76049400
H	-1.73455400	-1.70632300	0.70298000
C	-0.96857300	-3.37944800	1.78139800
H	0.00390800	-3.36219600	1.26739100
H	-1.60640000	-4.12188400	1.27970200
H	-0.80496900	-3.71673300	2.81614300
C	-3.06118300	-2.05779800	2.32434300
H	-3.07719500	-2.46739900	3.34434600
H	-3.68675700	-2.71176200	1.70022400
H	-3.52257000	-1.05936400	2.35231500
P	0.00000000	0.00000000	0.00230700
C	-0.49620500	1.46802500	-0.89263700
C	0.49620500	-1.46802500	-0.89263700
C	0.42013300	2.05249600	-1.79999000
C	-1.78958500	1.99916100	-0.66916500
C	1.78958500	-1.99916100	-0.66916500
C	-0.42013300	-2.05249600	-1.79999000
C	0.00000000	3.18690300	-2.49683500
C	1.81715600	1.50246600	-2.04972100
C	-2.14146900	3.15167800	-1.37496500
C	-2.79383300	1.37892600	0.29173000
C	2.14146900	-3.15167800	-1.37496500
C	2.79383300	-1.37892600	0.29173000
C	0.00000000	-3.18690300	-2.49683500

C	-1.81715600	-1.50246600	-2.04972100
H	0.67551900	3.65745300	-3.21276100
C	-1.26172900	3.73432200	-2.28277200
H	2.04974300	0.77202700	-1.25796400
C	1.88725000	0.75370600	-3.38511900
C	2.88749500	2.59370100	-1.95887700
H	-3.12666400	3.59538900	-1.22268600
H	-2.43961200	0.37061000	0.56067100
C	-2.88935500	2.18159000	1.59377600
C	-4.16965300	1.19743500	-0.35696900
H	3.12666400	-3.59538900	-1.22268600
C	1.26172900	-3.73432200	-2.28277200
H	2.43961200	-0.37061000	0.56067100
C	2.88935500	-2.18159000	1.59377600
C	4.16965300	-1.19743500	-0.35696900
H	-0.67551900	-3.65745300	-3.21276100
H	-2.04974300	-0.77202700	-1.25796400
C	-1.88725000	-0.75370600	-3.38511900
C	-2.88749500	-2.59370100	-1.95887700
H	1.19129600	-0.09814500	-3.40685700
H	2.90346800	0.36837200	-3.55426900
H	1.63606400	1.42424000	-4.22085800
H	2.80295500	3.31460700	-2.78462600
H	3.88869800	2.14374600	-2.01966800
H	2.81415500	3.15159000	-1.01346300
H	-1.92553400	2.20863800	2.12359200
H	-3.63505400	1.73185200	2.26557400
H	-3.19876500	3.21786100	1.38963300
H	-4.65992900	2.16400900	-0.54209500
H	-4.82576000	0.62059900	0.31039200
H	-4.09662900	0.66494100	-1.31707800
H	1.92553400	-2.20863800	2.12359200
H	3.63505400	-1.73185200	2.26557400
H	3.19876500	-3.21786100	1.38963300
H	4.65992900	-2.16400900	-0.54209500
H	4.82576000	-0.62059900	0.31039200
H	4.09662900	-0.66494100	-1.31707800
H	-1.19129600	0.09814500	-3.40685700
H	-2.90346800	-0.36837200	-3.55426900
H	-1.63606400	-1.42424000	-4.22085800
H	-2.80295500	-3.31460700	-2.78462600
H	-3.88869800	-2.14374600	-2.01966800
H	-2.81415500	-3.15159000	-1.01346300
H	-1.56329100	4.62724100	-2.83240500

H	1.56329100	-4.62724100	-2.83240500

(2,6-diisopropylphenyl)$_3$As$^{\bullet+}$:

As	0.04938500	-0.00362800	-0.28297500
C	1.89947700	-0.34489800	0.09277400
C	-1.21441000	-1.44362600	-0.37319200
C	-1.22655800	-2.47486800	0.59082400
C	-0.30469700	2.79927900	-0.61238700
C	-0.67823500	1.70476100	0.20059400
C	-2.14307200	-1.37677200	-1.43440900
C	2.47342200	0.06625000	1.31578800
C	-1.59128100	1.82664300	1.27051500
C	-2.21604900	-3.45336700	0.46602600
H	-2.25855800	-4.26992800	1.18777400
C	-2.01808300	0.67140600	2.16512000
H	-1.34336500	-0.17735800	1.98221200
C	-3.12159100	-2.37317900	-1.49553500
H	-3.86542900	-2.34588800	-2.29307000
C	-2.13292700	3.09384500	1.50748000
H	-2.85001800	3.22573100	2.31906100
C	-0.86364300	4.04416800	-0.31345400
H	-0.59298200	4.91337500	-0.91374900
C	-0.21468900	-2.56779100	1.72282800
H	0.23628500	-1.57243600	1.86201000
C	-3.15654100	-3.40009300	-0.55941700
C	2.65753400	-0.92751400	-0.94698400
C	0.69247700	2.68418200	-1.75719600
H	0.70246800	1.63160900	-2.09452600
C	1.67958700	0.66363000	2.46745500
H	0.60923400	0.52556500	2.25664200
C	-2.15869500	-0.27042300	-2.48105700
H	-1.20061500	0.27793100	-2.42980100
C	-0.85854100	-2.94482100	3.05905600
H	-1.71740800	-2.29756300	3.29175100
H	-0.12322500	-2.84881900	3.87051000
H	-1.20775200	-3.98721600	3.06128100
C	-1.77199200	4.18938700	0.73034600
C	3.85307800	-0.09858700	1.46233700
H	4.33327800	0.21521400	2.39071300
C	-1.88522500	1.02071200	3.65096300
H	-0.88321900	1.40909600	3.88641100
H	-2.06423100	0.12676800	4.26563800
H	-2.62102200	1.77813100	3.95657100
C	1.96120300	-0.06609600	3.78495300
H	1.83143100	-1.15349300	3.67824100
H	1.27616700	0.29010200	4.56777700

H	2.98589700	0.11864300	4.13785500
C	4.03048500	-1.08157300	-0.73509900
H	4.64671300	-1.52765600	-1.51762700
C	-3.43543900	0.19622700	1.82841100
H	-4.16397100	1.00716200	1.97862300
H	-3.72133600	-0.64182500	2.48131700
H	-3.51059300	-0.14501700	0.78538800
C	4.62426000	-0.66211100	0.45021200
C	1.92237800	2.17078100	2.59774400
H	2.98752300	2.37898400	2.77991700
H	1.34896300	2.57857900	3.44336100
H	1.61693100	2.70974600	1.68881900
C	0.92415900	-3.52685800	1.36016900
H	1.66419300	-3.56798500	2.17292900
H	1.44141300	-3.20483500	0.44477300
H	0.53623600	-4.54359900	1.19731900
C	0.29784300	3.51817600	-2.97819400
H	-0.74555800	3.33595400	-3.27279100
H	0.94782100	3.26541900	-3.82768000
H	0.41908700	4.59429300	-2.78878300
C	-2.25270000	-0.82621200	-3.90501000
H	-1.47175500	-1.57622600	-4.09643600
H	-2.14012500	-0.01203000	-4.63432800
H	-3.22897300	-1.29656700	-4.08976500
C	-3.27724600	0.73907400	-2.19799800
H	-3.28057200	1.53126200	-2.96056700
H	-3.15757500	1.21267300	-1.21208000
H	-4.25884200	0.24166200	-2.22150500
C	2.07584900	-1.35794000	-2.28662700
H	0.97606200	-1.27393100	-2.24419400
C	2.11158700	3.02960300	-1.28914100
H	2.14291500	4.05738800	-0.89654800
H	2.81864200	2.96614500	-2.12945500
H	2.46189000	2.35076200	-0.49713900
C	2.56271800	-0.43228800	-3.40768100
H	2.34879100	0.62351500	-3.18444100
H	2.07898300	-0.69306700	-4.35980500
H	3.65012300	-0.52847200	-3.54382200
C	2.38312300	-2.82331100	-2.60730000
H	3.46329500	-2.98765100	-2.73024300
H	1.89621200	-3.11115500	-3.54963300
H	2.02275400	-3.49574800	-1.81652000
H	-2.20581000	5.16851600	0.93844500
H	5.69976000	-0.77982700	0.58990400

H	-3.92523500	-4.17097300	-0.63001200

(2,4,6-triisopropylphenyl)$_3$As$^{\bullet+}$:

As	-0.08595300	-0.07922700	0.32796400
C	-1.95221200	-0.27113800	-0.04670300
C	1.11509400	-1.54345600	0.05369100
C	1.05795500	-2.33766800	-1.11006000
C	0.32773600	2.58355800	1.22912600
C	0.66696500	1.67606700	0.20274600
C	2.07860200	-1.75796300	1.06551700
C	-2.54610000	0.39604900	-1.13919000
C	1.56285900	2.01681800	-0.83534800
C	2.00039600	-3.36093000	-1.23593600
H	1.98139200	-3.99628300	-2.12407600
C	1.95277200	1.07388300	-1.96568000
H	1.25678000	0.22222500	-1.96362800
C	3.00478400	-2.78149800	0.86661500
H	3.76971300	-2.95446500	1.62691700
C	2.11582600	3.29679500	-0.81116500
H	2.81749400	3.57990500	-1.59896800
C	0.89971600	3.85696800	1.18111400
H	0.64798700	4.58477500	1.95508700
C	0.02828900	-2.13166200	-2.21114500
H	-0.39597200	-1.12219800	-2.09666900
C	2.98251800	-3.59410600	-0.27098900
C	-2.71265300	-1.02929500	0.87163300
C	-0.65246400	2.24920400	2.34607500
H	-0.70622900	1.14865000	2.43464500
C	-1.76629200	1.20237200	-2.16768800
H	-0.69458000	1.00146400	-2.02463000
C	2.17861900	-0.91020100	2.32798000
H	1.23596400	-0.34567400	2.44622700
C	0.64738200	-2.18937600	-3.60996100
H	1.52303000	-1.52804300	-3.69076900
H	-0.09183600	-1.87882900	-4.36216700
H	0.96657700	-3.20857700	-3.87046500
C	1.79639400	4.23105100	0.17907500
C	-3.93288800	0.29815800	-1.27454700
H	-4.42179300	0.81082600	-2.10642000
C	1.81951800	1.74085600	-3.33843500
H	0.83019100	2.20453900	-3.46749100
H	1.96078200	0.99619800	-4.13502200
H	2.57958500	2.52151700	-3.48454900
C	-2.10346000	0.77125900	-3.59873500
H	-2.00700700	-0.31758700	-3.72407900
H	-1.42662400	1.26380100	-4.31177300

H	-3.12989800	1.05256900	-3.87469600
C	2.07557200	6.36850900	-1.12145000
H	2.47192000	7.39265100	-1.07811100
H	0.98932100	6.42568300	-1.27800100
H	2.52233000	5.87685400	-1.99897900
C	-4.09029700	-1.10208800	0.66751000
H	-4.69396500	-1.68716700	1.36577900
C	3.35959700	0.50145600	-1.76019900
H	4.10702000	1.30905000	-1.73377000
H	3.61977900	-0.17646600	-2.58686500
H	3.43157100	-0.06537200	-0.82050600
C	-4.72175100	-0.43837300	-0.38852200
C	-1.96962500	2.70887500	-1.97573200
H	-3.03296900	2.97378800	-2.07822200
H	-1.40626000	3.26970100	-2.73639300
H	-1.62641600	3.04069800	-0.98475700
C	-1.13308600	-3.12109800	-2.07194300
H	-1.88165800	-2.94950500	-2.85970000
H	-1.63337400	-3.01274700	-1.09880200
H	-0.77215200	-4.15674500	-2.16176000
C	4.00564300	-4.69662500	-0.45277300
H	3.77836300	-5.19301500	-1.40944000
C	-0.19648300	2.76310700	3.71349300
H	0.83681200	2.45975100	3.93523500
H	-0.85267400	2.36325100	4.49932800
H	-0.25267100	3.85943500	3.77274200
C	2.32234000	-1.76370900	3.59076300
H	1.53372800	-2.52723800	3.65284100
H	2.26062900	-1.12612600	4.48379300
H	3.29494600	-2.27520300	3.62412700
C	-6.22429600	-0.51632600	-0.56428500
H	-6.47556900	0.07924800	-1.45614000
C	3.31166700	0.11625500	2.21515800
H	3.37824100	0.71457700	3.13551600
H	3.15576500	0.80426400	1.37095300
H	4.27719600	-0.39155000	2.06882100
C	-2.11927000	-1.74533100	2.07780800
H	-1.02578800	-1.59269700	2.08331000
C	2.41532100	5.61367600	0.16705400
H	1.97715900	6.16892400	1.01128300
C	-2.06250100	2.74940600	2.00924200
H	-2.05534100	3.84077000	1.86677800
H	-2.75777600	2.51910700	2.82991800
H	-2.45411800	2.28665100	1.09094900

C	-2.65867200	-1.15652400	3.38595500
H	-2.49371100	-0.07006100	3.43798700
H	-2.16601600	-1.62631300	4.24919700
H	-3.74004200	-1.33441300	3.48005500
C	-6.68166400	-1.95665000	-0.81321200
H	-6.47621700	-2.59358700	0.06073400
H	-6.17164100	-2.39557200	-1.68201000
H	-7.76462900	-1.98573700	-0.99804500
C	-2.34658500	-3.25797900	2.01054600
H	-3.41982000	-3.49869600	2.02644400
H	-1.88074200	-3.75077900	2.87573300
H	-1.91397200	-3.68945100	1.09689500
C	3.92980100	5.53867400	0.38594100
C	5.42304300	-4.12267700	-0.54385000
H	5.71322100	-3.63429400	0.39905800
H	5.50416500	-3.38068300	-1.35062600
H	6.14822300	-4.92506300	-0.73934600
C	-6.95213400	0.09915900	0.63501000
H	-8.03788400	0.09703300	0.46480600
H	-6.63251300	1.13619000	0.80883800
H	-6.75798100	-0.47637000	1.55310600
C	3.89866700	-5.74361600	0.65995900
H	4.60796800	-6.56372100	0.48063800
H	2.88664500	-6.16817700	0.71548500
H	4.13837700	-5.30432200	1.64041500
H	4.42309600	5.01291900	-0.44600100
H	4.35842600	6.54921000	0.44291400
H	4.17402900	5.00780000	1.31673200