Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Monocyclic Aromatic Compounds $B_nRg_n^{(n-2)+}$ of Boron and Rare Gases

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Supporting Materials

The bond lengths of the monocyclic aromatic compounds $B_nRg_n^{(n-2)+}$ calculate by the MP2, B3LYP and CCSD methods are listed in S1, S2, S3 and S4. Some selected vibrational frequencies of the BRg compounds calculated by the B3LYP, MP2 and CCSD methods are listed in Tables S5~S8. The breathing modes and the infrared-active BB bond stretch mode of the pure boron clusters $B_3^+(D_{3h})$, $B_4^{2+}(D_{4h})$, $B_5^{3+}(D_{5h})$ and $B_6^{4+}(D_{6h})$, calculated by B3LYP/def2-QZVPPD, MP2/def2-QZVPPD and MP2/aug-cc-pVDZ, are listed in Table S9. The geometry, relative energies and the lowest frequencies of the isomers optimized by the B3LYP/aug-cc-pVDZ method are listed in Table S10. Some CMOs for $B_6Ne_6^{4+}$ (D_{6h}) are shown in Figure S1. Contour line diagrams of electron density Laplacian for $B_3Rg_3^+$, $B_4Rg_4^{2+}$, $B_5Rg_5^{3+}$, and $B_6Rg_6^{4+}$ are shown in Fig S2~S5 respectively. The Cartesian coordinates of the monocyclic geometries optimized by MP2 and CCSD methods are also listed in the end.

Table S1 Bond lengths of $B_3Rg_3^+(D_{3h})$, $B_4Rg_4^{2+}(D_{4h})$, $B_5Rg_5^{3+}(D_{5h})$, and $B_6Rg_6^{4+}(D_{6h})$ optimized by *a*: MP2/def2-QZVPPD, and *b*: MP2/def2-TZVPPD

	^{a}**$B_3Rg_3^+$**		^{a}**$B_4Rg_4^{2+}$**		^{a}**$B_5Rg_5^{3+}$**		^{b}**$B_5Rg_5^{3+}$**		**$B_6Rg_6^{4+}$**		
Rg	BB	BRg	BB	BRg	BB	BRg	BB	BRg	Rg	BB	BRg
$B_n^{(n-2)+}$	1.596		1.593		1.650					1.698	
He	1.593	2.607	1.590	1.365	1.635	1.356	1.639	1.357	He^a	1.678	1.360
Ne	1.579	2.243	1.592	1.678	1.638	1.652	1.640	1.651	He^b	1.681	1.361
Ar	1.544	1.975	1.601	1.921	1.638	1.912	1.641	1.913	Ne^b	1.682	1.642
Kr	1.546	2.091	1.603	2.056	1.638	2.050	1.640	2.052			
Xe	1.549	2.228	1.606	2.217	1.637	2.217	1.641	2.220			
Rn	1.552	2.316	1.606	2.304			1.640	2.308			

Table S2 Bond lengths of $B_3Rg_3^+(D_{3h})$, $B_4Rg_4^{2+}(D_{4h})$, $B_5Rg_5^{3+}(D_{5h}$ for He~Kr, C_1 for Xe, Rn), and $B_6Rg_6^{4+}(D_{6h}$ for He, Ne, D_{3d} for Ar~Rn) optimized by MP2/aug-cc-pVDZ and B3LYP/aug-cc-pVDZ (in the parentheses) levels.

	$B_3Rg_3^+$		$B_4Rg_4^{2+}$		$B_5Rg_5^{3+}$		$B_6Rg_6^{4+}$	
Rg	**BB**	**BRg**	**BB**	**BRg**	**BB**	**BRg**	**BB**	**BRg**
$B_n^{(n-2)+}$	1.641(1.581)	-(-)	1.622(1.598)	-(-)	1.678(1.656)	-(-)	1.724(1.704)	-(-)
He	1.638(1.553)	2.647(2.409)	1.615(1.595)	1.406(1.399)	1.656(1.640)	1.394(1.392)	1.699(1.683)	1.396(1.395)
Ne	1.632(1.564)	2.480(2.042)	1.617(1.597)	1.746(1.748)	1.660(1.643)	1.713(1.718)	1.700(1.683)	1.700(1.706)
Ar	1.582(1.552)	2.063(2.078)	1.624(1.604)	1.962(1.986)	1.657(1.641)	1.951(1.974)	1.687(1.673)	1.951(1.974)
Kr	1.581(1.555)	2.147(2.191)	1.626(1.607)	2.087(2.123)	1.657(1.642)	2.081(2.118)	1.679(1.665)	2.080(2.115)
Xe	1.582(1.558)	2.283(2.350)	1.629(1.610)	2.255(2.314)	1.656(1.642)	2.255(2.314)	1.664(1.655)	2.245(2.310)
Rn	1.585(1.560)	2.371(2.446)	1.629(1.610)	2.344(2.410)	1.654(1.641)	2.348(2.413)	1.660(1.650)	2.338(2.407)

Table S3 Bond lengths of $B_3Rg_3^+(D_{3h})$, $B_4Rg_4^{2+}(D_{4h})$, $B_5Rg_5^{3+}(D_{5h})$, and $B_6Rg_6^{4+}(D_{6h})$ optimized by the B3LYP-D3/def2-QZVPPD method.

	$B_3Rg_3^+$		**$B_4Rg_4^{2+}$**		**$B_5Rg_5^{3+}$**		**$B_6Rg_6^{4+}$**	
Rg	BB	BRg	BB	BRg	BB	BRg	BB	BRg
He	1.522	1.502	1.522	1.502	1.630	1.374	1.377	1.673
Ne	1.538	1.976	1.538	1.976	1.631	1.674	1.673	1.666
Ar	1.530	2.021	1.530	2.021	1.632	1.952	1.664	1.955
Kr	1.532	2.154	1.532	2.154	1.631	2.105	1.662	2.114
Xe	1.537	2.313	1.537	2.313	1.630	2.295	1.642	2.290
Rn	1.538	2.401	1.538	2.401	1.627	2.387	1.636	2.383

Table S4 Bond lengths of $B_3Rg_3^+(D_{3h})$, $B_4Rg_4^{2+}(D_{4h})$, $B_5Rg_5^{3+}(D_{5h})$, and $B_6Rg_6^{4+}(D_{6h})$ optimized by the CCSD/aug-cc-pVDZ method

	$B_3Rg_3^+$		$B_4Rg_4^{2+}$		$B_5Rg_5^{3+}$		$B_6Rg_6^{4+}$	
Rg	BB	BRg	BB	BRg	BB	BRg	BB	BRg
He	1.616	2.665	1.616	1.418	1.657	1.405		
Ne	1.611	2.484	1.617	1.756				
Ar	1.575	1.611	1.622	1.977	1.656	1.965	1.686	1.964
Kr	1.574	2.162	1.624	2.105	1.655	1.657		
Xe	1.575	2.298						
Rn	1.576	2.387						

Table S5 Selected vibrational frequencies ν (cm^{-1}) of $B_3Rg_3^+(D_{3h})$, $B_4Kr_4^{2+}(D_{4h})$, $B_5Ar_5^{3+}(D_{5h})$ and $B_5Kr_5^{3+}(D_{5h})$ calculated at the CCSD/aug-cc-pVDZ level

$B_3Rg_3^+$	He	Ne	Ar	Kr	Xe	Rn	$B_4Rg_4^{2+}$	Kr	$B_5Rg_5^{3+}$	Ar	Kr
$\nu_1(a_1')$	1111.93	1145.18	1361.47	1373.56	1377.99	1369.31	$\nu_1(a_{1g})$	1151.95	$\nu_1(a_1')$	989.02	980.33
$\nu_2(e')$	924.83	935.94	987.77	987.92	984.39	977.91	$\nu_2(e_u)$	1107.58	$\nu_2(e_1')$	1009.87	1000.85
$\nu_5(e')$	81.23	61.94	224.98	252.75	279.54	269.82	$\nu_{11}(e_u)$	326.95	$\nu_{11}(e_1')$	392.70	359.54
$\nu_6(a_2')$	50.63	94.10	317.16	324.29	320.24	309.40	$\nu_{12}(a_{2g})$	413.54	$\nu_{13}(a_2')$	437.57	421.35
$\nu_7(a_2'')$	23.86	27.79	75.30	74.60	75.21	70.91	$\nu_{14}(a_{2u})$	94.62	$\nu_{14}(a_2'')$	108.31	99.72
$\nu_4(e')$	21.54	22.07	65.03	49.00	39.25	29.12	$\nu_{10}(b_{2u})$	15.38	$\nu_9(e_2'')$	22.45	11.45

Table S6 Selected vibrational frequencies (cm^{-1}) of $B_3Rg_3^+(D_{3h})$, $B_4Rg_4^{2+}(D_{4h})$, $B_5Rg_5^{3+}(D_{5h})$ and $B_6Rg_6^{4+}(D_{6h})$ calculated by B3LYP/def2-QZVPPD. The Infrared active modes are the B–B and B–Rg bond stretch modes.

Vib-Modes	**Symmetry**	**He**	**Ne**	**Ar**	**Kr**	**Xe**	**Rn**
$B_3Rg_3^+(D_{3h})$							
B_3 breathing	$\nu_1(a_1')$	1403.9	1315.0	1386.4	1376.9	1368.0	1355.9
BB bond stretch	$\nu_2(e')$	1055.4	1022.9	1021.0	1011.9	1001.8	995.7
Rg–B bond stretch	$\nu_5(e')$	311.4	139.5	262.3	249.0	268.5	256.2
Rg_3–B_3 relative rotation	$\nu_6(a_2')$	391.4	241.5	353.5	344.4	334.7	319.5
Rg_3–B_3 relative translation vertical to the molecular plane	$\nu_7(a_2'')$	151.3	67.3	85.0	78.0	71.5	65.6
Rg_3 deformation	$\nu_4(e')$	177.0	60.6	74.1	49.9	39.5	27.9
$B_4Rg_4^{2+}(D_{4h})$							
B_4 breathing	$\nu_1(a_{1g})$	1193.3	1150.1	1134.9	1122.4	1103.8	1097.2
BB bond stretch	$\nu_2(e_u)$	1171.8	1132.4	1115.1	1104.2	1087.3	1080.5
B-Rg stretch	$\nu_{11}(e_u)$	620.5	331.7	342.9	310.6	295.3	283.1
Rg_4-B_4 relative rotation	$\nu_{12}(a_{2g})$	542.4	401.5	427.7	408.1	385.9	368.2

Rg_4-B_4 relative translation vertical to molecular plane	$\nu_{14}(a_{2u})$	206.8	109.8	102.3	88.7	83.1	71.0
Rg_4 out-of-plane	$\nu_{10}(b_{2u})$	125.0	50.5	24.9	13.2	7.8	-3.4
$B_5Rg_5^{3+}(D_{5h})$							
B_5 breathing	$\nu_1(a_1')$	1039.0	960.5	957.8	947.5	-	-
BB bond stretch	$\nu_2(e_1')$	1066.0	999.4	1002.9	995.2	-	-
B–Rg stretch	$\nu_{11}(e_1')$	689.0	383.3	379.2	343.7	-	-
Rg_5-B_5 relative rotation	$\nu_{13}(a_2')$	576.6	417.3	437.8	415.3		
Rg_5-B_5 relative translation vertical to molecular plane	$\nu_{14}(a_2'')$	207.7	112.4	106.0	95.9		
Rg_5 out of plane	$\nu_9(e_2'')$	124.6	48.1	20.5	9.9	-	-
$B_6Rg_6^{4+}(D_{6h})$							
B_6 breathing	$\nu_1(a_{1g})$	942.6	822.2	821.6	-	-	-
BB bond stretch	$\nu_2(e_{1u})$	948.8	852.6	871.9	-	-	-
B–Rg bond stretch	$\nu_{17}(e_{1u})$	688.5	407.9	390.9	-	-	-
B_6 triangle mode	$\nu_6(b_{1u})$	533.5	524.7	535.2	-	-	-
B_6-Rg_6 relative rotation	$\nu_{19}(b_{2g})$	589.7	419.1	432.8	-	-	-
B_6-Rg_6 relative translation vertical to the plane	$\nu_{18}(a_{2u})$	202.9	112.8	109.4	-	-	-
Rg_6 boat twist	$\nu_{12}(e_u)$	117.8	45.5	15.3	-	-	-
Rg_6 chair twist	$\nu_{13}(b_{2g})$	133.9	50.7	1.2	-	-	-
B_6 boat-style twist	$\nu_4(e_{2u})$	451.6	406.6	432.0			
B_6 chair-style twist	$\nu_5(a_{2g})$	541.4	517.3	551.2			

Table S7 Selected vibrational frequencies (cm^{-1}) of $B_3Rg_3^+(D_{3h})$ (mp2/def2-QZVPPD), $B_4Rg_4^{2+}$ (D_{4h}) (He, Ne and Ar: mp2/def2-QZVPPD; Kr, Xe and Rn: mp2/def2-TZVPPD), $B_5Rg_5^{3+}$ (D_{5h}) (mp2/def2-TZVPPD), $B_6Rg_6^{4+}(D_{6h})$(He, Ne: mp2/def2-TZVPPD, Ar: mp2/def2-TZVP)

$B_3Rg_3^+$	He	Ne	Ar	Kr	Xe	Rn	$B_5Rg_5^{3+}$	He	Ne	Ar
$\nu_1(a_1')$	1082.0	1154.4	1386.1	1385.3	1382.0	1368.7	$\nu_1(a_1')$	1065.3	983.0	999.6
$\nu_2(e')$	936.4	958.4	1014.2	1006.7	1004.0	996.9	$\nu_2(e_1')$	1098.5	1031.5	1048.9
$\nu_5(e')$	78.2	64.6	301.6	300.5	321.6	309.3	$\nu_{11}(e_1')$	715.1	409.2	426.0
$\nu_6(a_2')$	56.0	144.1	366.4	349.3	345.2	337.1	$\nu_{13}(a_2')$	593.7	432.9	449.4
$\nu_7(a_2'')$	26.4	42.4	88.7	80.5	76.8	73.6	$\nu_{14}(a_2'')$	217.4	120.4	111.4
$\nu_4(e')$	23.8	28.0	79.8	54.6	41.9	31.1	$\nu_9(e_2'')$	119.9	47.5	19.7
$B_4Rg_4^{2+}$	He	Ne	Ar	Kr	Xe	Rn	$B_6Rg_6^{4+}$	He	Ne	Ar
$\nu_1(a_{1g})$	1209.7	1162.6	1163.1	1154.6	1138.7	1132.0	$\nu_1(a_{1g})$	974.4	849.7	871.3
$\nu_2(e_u)$	1192.5	1151.7	1141.6	1131.6	1117.8	1112.7	$\nu_2(e_{1u})$	991.0	896.4	941.0
$\nu_{11}(e_u)$	642.5	348.5	387.8	359.2	342.0	329.9	$\nu_{17}(e_{1u})$	713.6	434.7	438.2
$\nu_{12}(a_{2g})$	558.8	417.5	440.7	424.3	405.8	387.6	$\nu_6(b_{1u})$	522.6	513.7	563.0
$\nu_{14}(a_{2u})$	212.8	115.6	104.5	95.6	85.0	79.6	$\nu_{19}(b_{2g})$	606.2	429.1	446.2
$\nu_{10}(b_{2u})$	121.5	50.6	22.3	13.0	8.7	6.3	$\nu_{18}(a_{2u})$	210.5	118.8	113.9
							$\nu_{12}(e_u)$	112.9	43.0	14.4
							$\nu_{13}(b_{2g})$	132.2	49.7	4.9

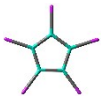
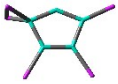
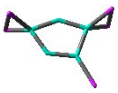
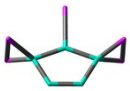
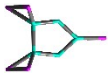
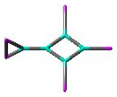
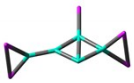
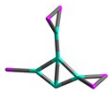
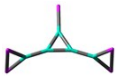
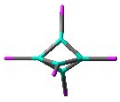
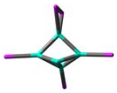
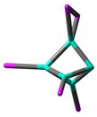
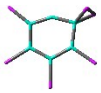
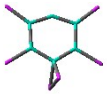
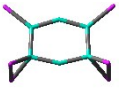
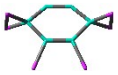
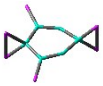
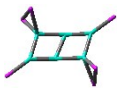
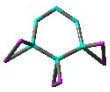
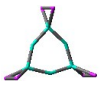
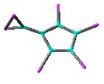
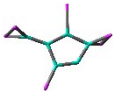
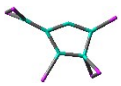
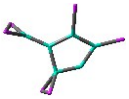
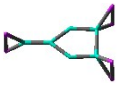
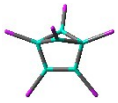
Table S8 Selected vibrational frequencies ν (cm^{-1}) of $B_3Rg_3^+(D_{3h})$, $B_4Rg_4^{2+}(D_{4h})$, $B_5Rg_5^{3+}(D_{5h})$ and $B_6Rg_6^{4+}$ (He, Ne: D_{6h}, Ar ~Rn: D_{3d}) at the mp2/aug-cc-pVDZ level .

$B_3Rg_3^+$	He	Ne	Ar	Kr	Xe	Rn	$B_4Rg_4^{2+}$	He	Ne	Ar	Kr	Xe	Rn
$\nu_1(a_1')$	1049.2	1069.5	1338.5	1353.5	1357.6	1345.2	$\nu_1(a_{1g})$	1180.2	1150.8	1159.1	1150.2	1135.6	1127.8
$\nu_2(e')$	882.5	891.6	972.7	973.9	970.0	961.2	$\nu_2(e_u)$	1165.6	1130.5	1128.7	1120.2	1105.1	1099.2
$\nu_5(e')$	94.4	65.0	236.3	264.6	291.7	282.8	$\nu_{11}(e_u)$	544.7	328.6	363.3	340.3	331.6	317.5
$\nu_6(a_2')$	42.1	87.1	318.9	325.0	318.6	307.1	$\nu_{12}(a_{2g})$	526.8	372.4	414.1	416.0	403.9	391.9
$\nu_7(a_2'')$	16.0	28.7	78.6	77.1	76.3	71.3	$\nu_{14}(a_{2u})$	201.0	102.6	102.0	95.5	90.2	86.8
$\nu_4(e')$	10.9	20.6	66.0	49.4	39.2	29.0	$\nu_{10}(b_{2u})$	123.6	47.3	23.4	14.5	8.9	7.3
$B_5Rg_5^{3+}$	He	Ne	Ar	Kr		$B_6Rg_6^{4+}$	He	Ne	D_{3d}	Ar	Kr	Xe	Rn
$\nu_1(a_1')$	1023.7	972.3	991.8	983.0		$\nu_1(a_{1g})$	924.7	841.1	a_{1g}	865.7	874.4	905.5	899.9
$\nu_2(e_1')$	1072.8	1016.8	1043.3	1034.7		$\nu_2(e_{1u})$	955.9	876.9	e_u	935.7	943.5	963.2	959.7
$\nu_{11}(e_1')$	639.6	386.0	404.8	372.4		$\nu_{17}(e_{1u})$	655.2	413.0	e_u	411.1	368.4	324.1	300.0
$\nu_{13}(a_2')$	566.6	381.7	439.8	423.1		$\nu_6(b_{1u})$	474.3	502.4	a_{2u}	570.6	571.5	549.1	524.3
$\nu_{14}(a_2'')$	206.3	105.5	108.4	99.2		$\nu_{19}(b_{2g})$	570.5	374.6	a_{2g}	434.0	403.3	354.1	323.1
$\nu_9(e_2'')$	120.4	44.8	21.5	10.1		$\nu_{18}(a_{2u})$	203.7	106.8	a_{2u}	103.5	72.9	43.0	31.9
						$\nu_{12}(e_u)$	112.3	43.9	e_u	19.7	11.7	11.2	8.7
						$\nu_{13}(b_{2g})$	98.0	24.4	a_{1g}	23.6	17.6	22.0	17.6

Table S9 The breathing modes and infrared-active BB bond stretch mode of $B_3^+(D_{3h})$, $B_4^{2+}(D_{4h})$, $B_5^{3+}(D_{5h})$ and $B_6^{4+}(D_{6h})$, calculated by the methods B3LYP/def2-QZVPPD, mp2/def2-QZVPPD and mp2/aug-cc-pVDZ

		B_3^+	B_4^{2+}	B_5^{3+}	B_6^{4+}
B3LYP/def2-QZVPPD	breathing mode	1191.7	1089.9	839.3	675.8
	BB bond stretch	997.8	1081.4	906.5	728.0
mp2/def2-QZVPPD	breathing mode	1068.9	1083.7	839.5	678.1
	BB bond stretch	930.2	1090.6	932.3	767.6
mp2/aug-cc-pVDZ	breathing mode	1041.9	1068.3	816.6	665.2
	BB bond stretch	876.5	1067.5	913.1	757.8

Table S10 Geometric strucutres of all the isomers for $B_4Ar_4^{2+}$, $B_5Ar_5^{3+}$ and $B_6Ar_6^{4+}$, their relative energies (kcal/mol) with respect to that of the desired monocyclic structure, and the lowest frequencies (cm^{-1}) calculated by B3LYP/aug-cc-pVDZ; the relative energies are also refined by the method MP4(SDQ)/aug-cc-pVDZ. The data in the parentheses were calculated by MP2/aug-cc-pVDZ level for further confirmation.

$B_4Ar_4^{2+}$	**4-1**	**4-2**					
							
ΔE_{B3LYP}	0.00	53.37					
$\Delta E_{MP4(SDQ)}$	0.00	54.47					
ν_{min}	26.25	16.00					
$B_5Ar_5^{3+}$	**5-1**	**5-2**	**5-3**	**5-4**	**5-5**	**5-6**	**5-7**
							
ΔE_{B3LYP}	0.00	16.96	33.73	51.03	34.77	25.88	32.66
$\Delta E_{MP4(SDQ)}$	0.00	17.39	34.69	51.62	35.77	27.55	33.00
ν_{min}	22.51	21.15	26.40	14.6	26.18	10.96	27.00
Name	**5-8**	**5-9**	**5-10**	**5-11**	**5-12**	**5-13**	
							
ΔE_{B3LYP}	47.39	56.15	27.76	61.85	64.70	91.93	
$\Delta E_{MP4(SDQ)}$	44.08	56.17	21.54	56.05	62.19	91.82	
ν_{min}	15.20	14.48	64.57	37.40	42.69	29.72	
$B_6Ar_6^{4+}$	**6-1**	**6-2**	**6-3**	**6-4**	**6-5**	**6-6**	**6-7**
							
ΔE_{B3LYP}	0.00	16.20	17.97	18.53	49.27	53.28	33.03
$\Delta E_{MP4(SDQ)}$	0.00	16.64	19.09	19.84	49.79	55.40	34.91
ν_{min}	16.57	15.83	14.53	11.70	7.84	19.58	16.78
Name	**6-8**	**6-9**	**6-10**	**6-11**	**6-12**	**6-13**	**6-14**
							
ΔE_{B3LYP}	33.01	45.99	33.36	27.22	43.61	84.32	52.06
$\Delta E_{MP4(SDQ)}$	34.02	45.39	34.07	20.88	40.39	85.23	52.38
ν_{min}	18.05	11.04	12.71	9.34	18.31	16.83	38.82
Name	**6-15**	**6-16**	**6-17**	**6-18**	**6-19**	**6-20**	**6-21**
							
ΔE_{B3LYP}	6.99	10.10	26.37	13.74	32.83	20.18	27.45
$\Delta E_{MP4(SDQ)}$	6.10(6.06)	8.77(8.54)	24.89.	13.01	32.20	18.27	20.03
ν_{min}	9.67	16.19	6.02	15.18	11.98	12.23	30.89

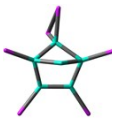
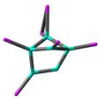
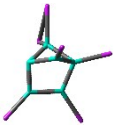
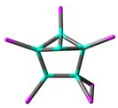
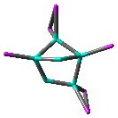
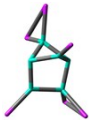
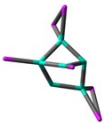
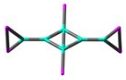
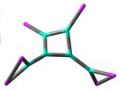
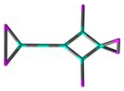
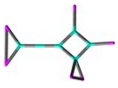
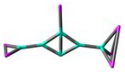
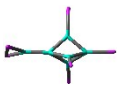
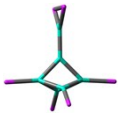
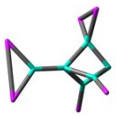
Name	6-22	6-23	6-24	6-25	6-26	6-27	6-28
							
ΔE_{B3LYP}	56.35	55.41	53.90	56.05	77.26	70.91	69.19
$\Delta E_{MP4(SDQ)}$	47.90	47.16	49.31	48.99	68.06	68.68	63.09
ν_{min}	32.44	41.60	32.76	33.10	43.69	38.66	47.90
Name	**6-29**	**6-30**	**6-31**	**6-32**	**6-33**	**6-34**	**6-35**
							
ΔE_{B3LYP}	7.71	27.16	28.44	27.34	33.16	46.68	6.08
$\Delta E_{MP4(SDQ)}$	9.56(9.16)	24.62	22.81	31.79	39.00	50.26	5.59(5.25)
ν_{min}	3.55	20.98	16.59	4.92	4.11	23.04	7.07
Name	**6-36**	**6-37**	**6-38**	**6-39**	**6-40**		
							
ΔE_{B3LYP}	23.65	23.42	64.91	29.45	1.57		
$\Delta E_{MP4(SDQ)}$	13.20	14.19	58.34	28.28	-23.35(-23.64)		
ν_{min}	1.20	39.80	8.46	12.54	80.20		

Fig.S1 CMOs corresponding to the BB and BNe bonds for $B_6Ne_6^{4+}$ (D_{6h})

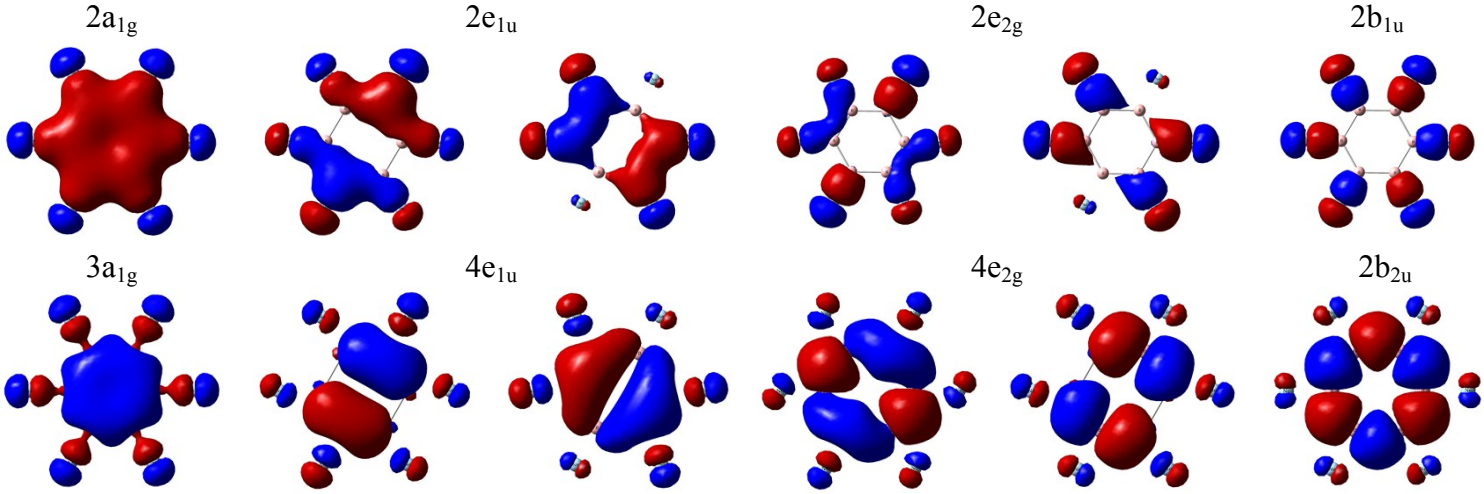


Fig.S2 Contour line diagrams of electron density Laplacian for $B_3Rg_3^+$ calculated by B3LYP/def2-QZVPPD. Green solid lines show areas of charge depletion ($\nabla^2\rho>0$) and blue dotted lines show areas of charge concentration ($\nabla^2\rho<0$).

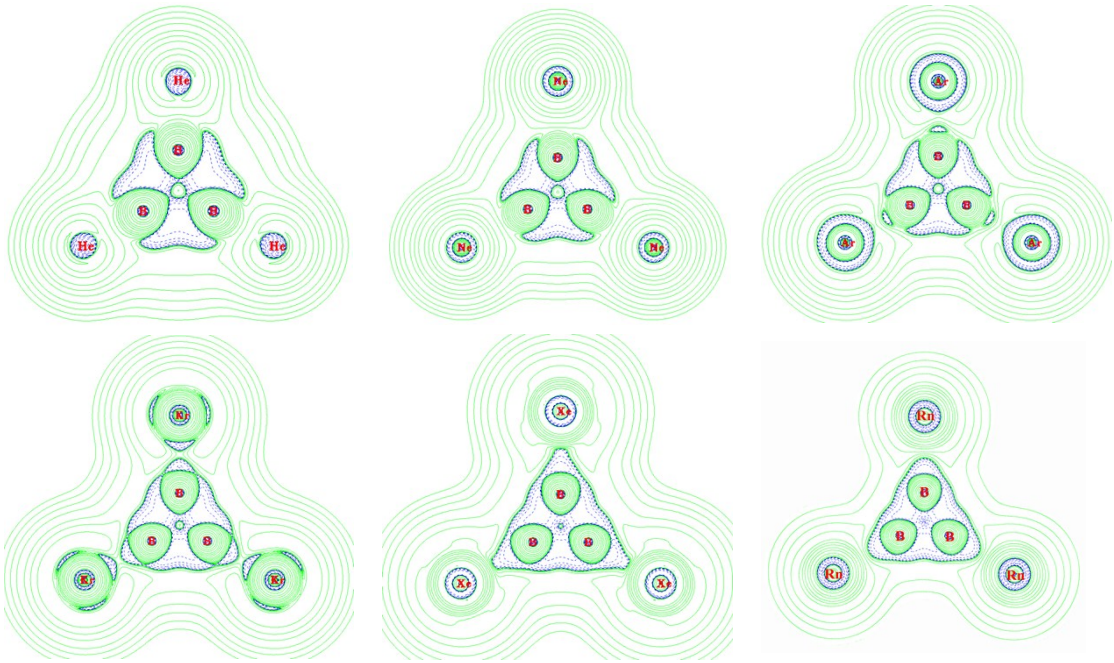
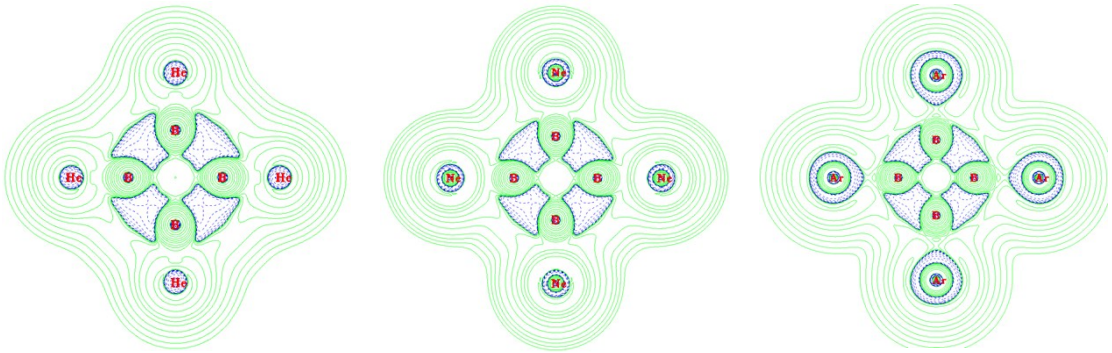


Fig.S3 Contour line diagrams of electron density Laplacian for $B_4Rg_4^{2+}$ calculated by MP2/aug-cc-pVDZ . Green solid lines show areas of charge depletion ($\nabla^2\rho>0$) and blue dotted lines show areas of charge concentration ($\nabla^2\rho<0$).



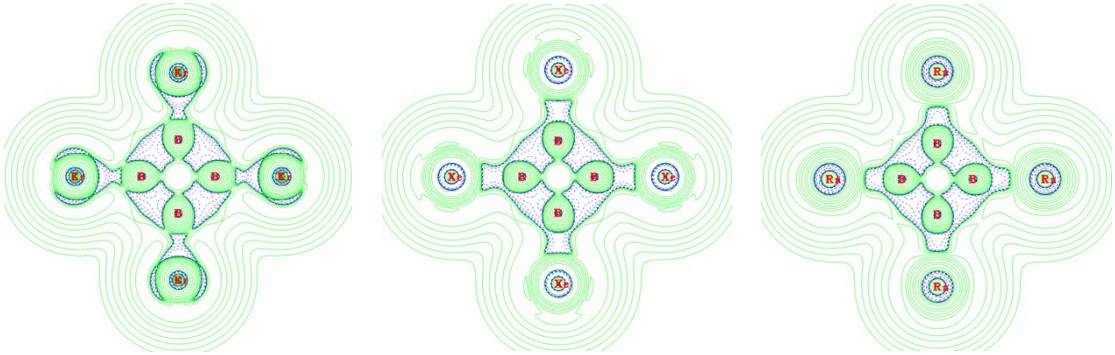


Fig.S4 Contour line diagrams of electron density Laplacian for $B_5Rg_5^{3+}$ calculated by MP2/aug-cc-pVDZ. Green solid lines show areas of charge depletion ($\nabla^2\rho>0$) and blue dotted lines show areas of charge concentration ($\nabla^2\rho<0$).

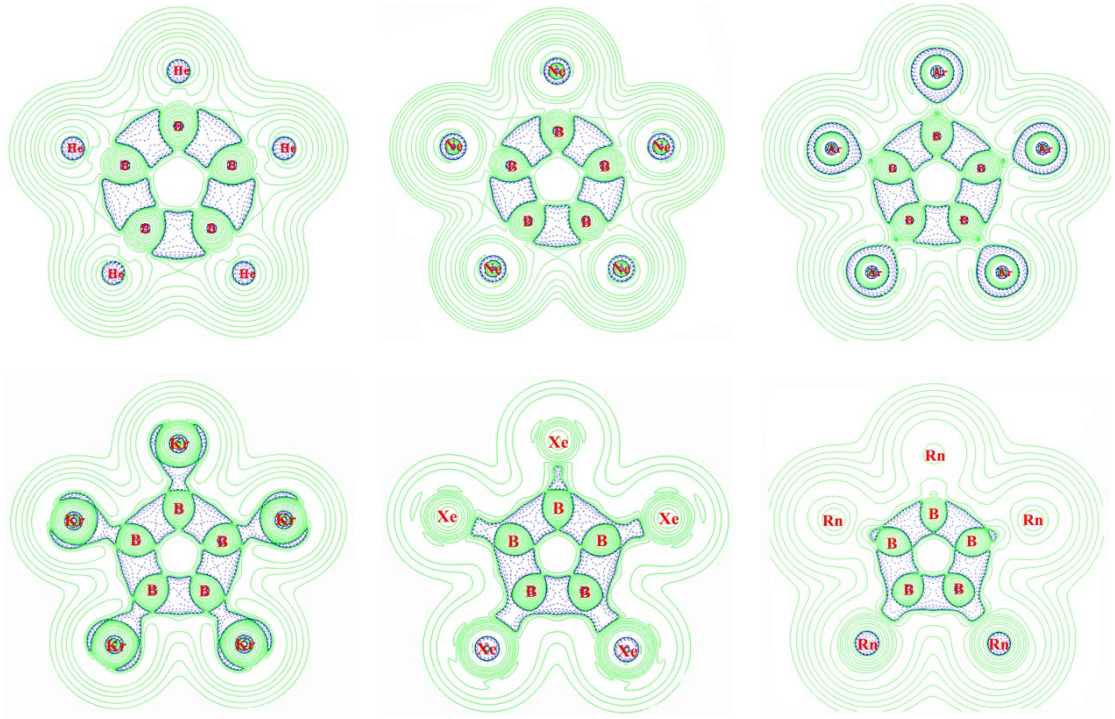
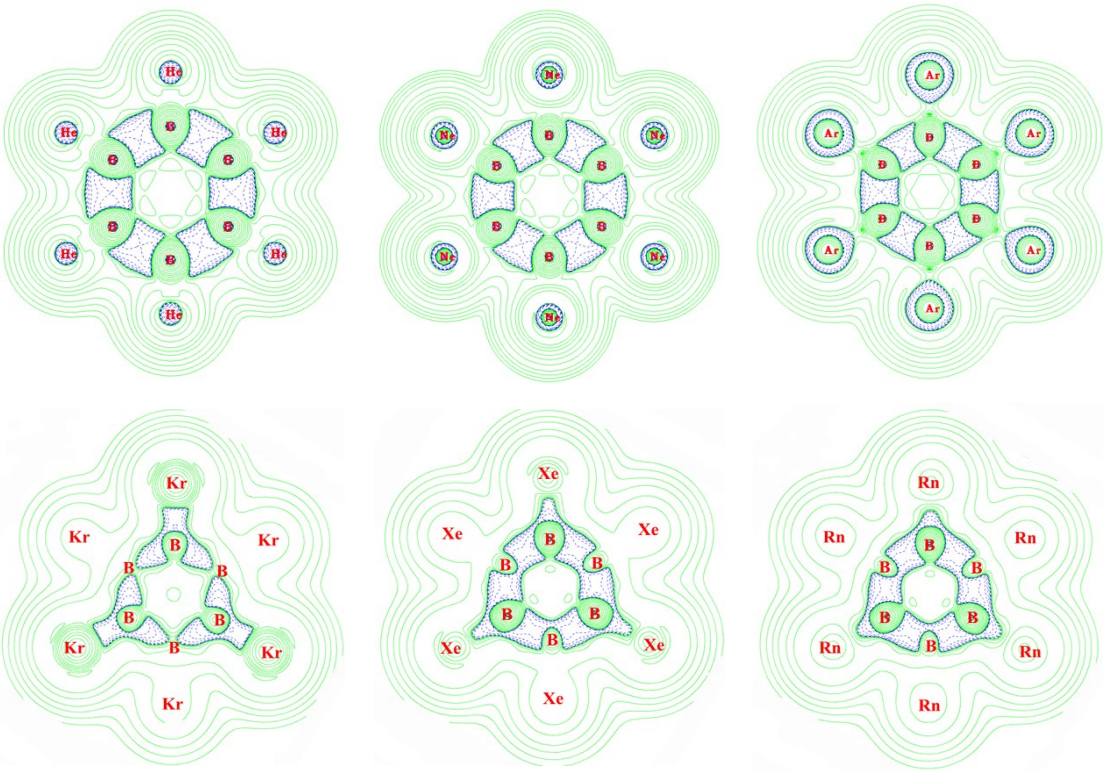


Fig.S5 Contour line diagrams of electron density Laplacian for $B_6Rg_6^{4+}$ calculated by MP2/aug-cc-pVDZ. Green solid lines show areas of charge depletion ($\nabla^2\rho>0$) and blue dotted lines show areas of charge concentration ($\nabla^2\rho<0$).



Cartesian coordinates of the monocyclic geometries calculated by MP2/aug-cc-pVDZ

	$B_3He_3^+$				$B_3Ne_3^+$		
B	0.00000000	0.94563800	0.00000000	B	0.00000000	0.94225500	0.00000000
B	0.81894700	-0.47281900	0.00000000	B	-0.81601700	-0.47112800	0.00000000
B	-0.81894700	-0.47281900	0.00000000	B	0.81601700	-0.47112800	0.00000000
He	-3.11121700	-1.79626200	0.00000000	Ne	2.96413700	-1.71134500	0.00000000
He	3.11121700	-1.79626200	0.00000000	Ne	-2.96413700	-1.71134500	0.00000000
He	0.00000000	3.59252400	0.00000000	Ne	0.00000000	3.42269100	0.00000000
	$B_3Ar_3^+$				$B_3Kr_3^+$		
B	0.00000000	0.91309000	0.00000000	B	0.00000000	0.91243800	0.00000000
B	-0.79075900	-0.45654500	0.00000000	B	0.79033300	-0.45649000	0.00000000
B	0.79075900	-0.45654500	0.00000000	B	-0.79033300	-0.45649000	0.00000000
Ar	2.57775100	-1.48826500	0.00000000	Kr	-2.65031100	-1.52983700	0.00000000
Ar	-2.57775100	-1.48826500	0.00000000	Kr	2.65031300	-1.52983800	0.00000000
Ar	0.00000000	2.97653000	0.00000000	Kr	-0.00000200	3.05975000	0.00000000
	$B_3Xe_3^+$				$B_3Rn_3^+$		
B	0.00000000	0.00000000	0.91323600	B	0.00000000	0.00000000	0.91532500
B	0.00000000	0.79091100	-0.45666500	B	0.00000000	0.79249300	-0.45729800
B	0.00000000	-0.79091100	-0.45666500	B	0.00000000	-0.79249300	-0.45729800
Xe	0.00000000	-2.76811200	-1.59812600	Rn	0.00000000	-2.84566100	-1.64325000
Xe	0.00000000	2.76811200	-1.59812600	Rn	0.00000000	2.84566100	-1.64325000
Xe	0.00000000	0.00000000	3.19626100	Rn	0.00000000	0.00000000	3.28645800
	$B_4He_4^{2+}$				$B_4Ne_4^{2+}$		
B	0.00000000	1.14216200	0.00000000	B	0.00000000	1.14370600	0.00000000

B	0.00000000	-1.14216200	0.00000000	B	0.00000000	-1.14370600	0.00000000
B	1.14216200	0.00000000	0.00000000	B	1.14370600	0.00000000	0.00000000
B	-1.14216200	0.00000000	0.00000000	B	-1.14370600	0.00000000	0.00000000
He	0.00000000	2.54847600	0.00000000	Ne	0.00000000	2.88960300	0.00000000
He	-2.54847600	0.00000000	0.00000000	Ne	-2.88960300	0.00000000	0.00000000
He	0.00000000	-2.54847600	0.00000000	Ne	0.00000000	-2.88960300	0.00000000
He	2.54847600	0.00000000	0.00000000	Ne	2.88960300	0.00000000	0.00000000
		$B_4Ar_4^{2+}$				$B_4Kr_4^{2+}$	
B	0.00000000	1.14799300	0.00000000	B	0.00000000	0.00000000	1.14961000
B	0.00000000	-1.14799300	0.00000000	B	0.00000000	0.00000000	-1.14961000
B	1.14799300	0.00000000	0.00000000	B	0.00000000	1.14960800	0.00000000
B	-1.14799300	0.00000000	0.00000000	B	0.00000000	-1.14960800	0.00000000
Ar	-3.10975700	0.00000000	0.00000000	Kr	0.00000000	-3.23676300	0.00000000
Ar	3.10975700	0.00000000	0.00000000	Kr	0.00000000	0.00000000	3.23676400
Ar	0.00000000	3.10975700	0.00000000	Kr	0.00000000	3.23676300	0.00000000
Ar	0.00000000	-3.10975700	0.00000000	Kr	0.00000000	0.00000000	-3.23676400
		$B_4Xe_4^{2+}$				$B_4Rn_4^{2+}$	
B	0.00000000	1.15185400	0.00000000	B	0.00000000	1.15204000	0.00000000
B	0.00000000	-1.15185400	0.00000000	B	0.00000000	-1.15204000	0.00000000
B	1.15185400	0.00000000	0.00000000	B	0.00000000	0.00000000	1.15204200
B	-1.15185400	0.00000000	0.00000000	B	0.00000000	0.00000000	-1.15204200
Xe	0.00000000	3.40640100	0.00000000	Rn	0.00000000	3.49558800	0.00000000
Xe	-3.40640100	0.00000000	0.00000000	Rn	0.00000000	-3.49558800	0.00000000
Xe	0.00000000	-3.40640100	0.00000000	Rn	0.00000000	0.00000000	3.49558900
Xe	3.40640100	0.00000000	0.00000000	Rn	0.00000000	0.00000000	-3.49558900
		$B_5He_5^{3+}$				$B_5Ne_5^{3+}$	
B	0.00000000	1.40888500	0.00000000	B	-1.19926100	0.74501400	0.00018300
B	1.33992900	0.43536900	0.00000000	B	0.33793100	1.37074600	-0.00009100
B	0.82812200	-1.13981200	0.00000000	B	1.40800900	0.10214900	-0.00000800
B	-0.82812200	-1.13981200	0.00000000	B	0.53224600	-1.30762000	0.00011500
B	-1.33992900	0.43536900	0.00000000	B	-1.07917100	-0.91032400	-0.00020200
He	1.64767800	-2.26783400	0.00000000	Ne	3.11702400	0.22614000	-0.00003600
He	0.00000000	2.80319700	0.00000000	Ne	-2.65449100	1.64904000	0.00063600
He	-2.66599900	0.86623600	0.00000000	Ne	-2.38866900	-2.01491800	-0.00068600
He	2.66599900	0.86623600	0.00000000	Ne	0.74806100	3.03427400	-0.00034100
He	-1.64767800	-2.26783400	0.00000000	Ne	1.17819700	-2.89451900	0.00042900
		$B_5Ar_5^{3+}$				$B_5Kr_5^{3+}$	
B	0.00000000	1.40926500	0.00000000	B	-0.43544300	1.34015200	0.00000000
B	1.34034900	0.43550100	0.00000000	B	1.14000500	0.82826500	0.00000000
B	0.82836000	-1.14013100	0.00000000	B	1.14000100	-0.82825800	0.00000000
B	-0.82837000	-1.14014500	0.00000000	B	-0.43544300	-1.34015600	0.00000000
B	-1.34034300	0.43549300	0.00000000	B	-1.40912300	-0.00000200	0.00000000
Ar	1.97505100	-2.71844800	0.00000000	Kr	2.82339200	-2.05131400	0.00000000
Ar	-0.00000900	3.36017100	0.00000000	Kr	-1.07843800	3.31909700	0.00000000

Ar -3.19571200 1.03836400 0.00000000	Kr -3.48990500 -0.00000100 0.00000000
Ar 3.19570400 1.03838100 0.00000000	Kr 2.82339200 2.05131500 0.00000000
Ar -1.97503300 -2.71846400 0.00000000	Kr -1.07843900 -3.31909700 0.00000000
$B_5Xe_5^{3+}$	$B_5Rn_5^{3+}$
B 0.43989400 1.32862700 -0.10682600	B -1.31038100 -0.43655600 -0.16844600
B 1.39650700 -0.00077300 0.13662100	B -0.00652400 -1.36974700 0.22596900
B 0.43842100 -1.32912200 -0.10677800	B 1.30687200 -0.44863400 -0.16516300
B -1.13346000 -0.82767000 0.03723100	B 0.83169900 1.11937200 0.04658800
B -1.13254000 0.82894100 0.03729600	B -0.82173600 1.12636400 0.04977400
Xe1.15237400 -3.42324300 -0.55329900	Rn-3.39780100-1.20365100 -0.89424500
Xe1.15615700 3.42192000 -0.55353000	Rn -2.22771500 2.98605200 0.32333300
Xe -2.94408300 2.17082500 0.20612000	Rn 2.25317500 2.96964200 0.30456200
Xe 3.58126900 -0.00196700 0.69516300	Rn 3.39060400 -1.23665300 -0.87994100
Xe -2.94653300 -2.16753600 0.20577300	Rn -0.01826000 -3.51485600 1.14694600
$B_6He_6^{4+}$	$B_6Ne_6^{4+}$
He -2.68002100 1.54731100 0.00000000	Ne -2.94457900 1.70006700 0.00000000
He -2.68002100 -1.54731100 0.00000000	Ne 0.00000300 3.40011300 0.00000000
He 0.00000000 -3.09462200 0.00000000	Ne 2.94457900 1.70006000 0.00000000
He 2.68002100 -1.54731100 0.00000000	Ne 2.94457900 -1.70006700 0.00000000
He 2.68002100 1.54731100 0.00000000	Ne -0.00000300 -3.40011300 0.00000000
He 0.00000000 3.09462200 0.00000000	Ne -2.94457900 -1.70006000 0.00000000
B -1.47092900 0.84924100 0.00000000	B -1.47244500 0.85012000 0.00000000
B -1.47092900 -0.84924100 0.00000000	B 0.00000300 1.70022800 0.00000000
B 0.00000000 -1.69848300 0.00000000	B 1.47244700 0.85011200 0.00000000
B 1.47092900 -0.84924100 0.00000000	B 1.47244500 -0.85012000 0.00000000
B 1.47092900 0.84924100 0.00000000	B -0.00000300 -1.70022800 0.00000000
B 0.00000000 1.69848300 0.00000000	B -1.47244700 -0.85011200 0.00000000
$B_6Ar_6^{4+}$	$B_6Kr_6^{4+}$
Ar 0.00000000 3.62537000 0.24389300	B -0.30505000 -1.64179100 0.00000000
Ar 3.13966200 1.81268500 -0.24389300	B 0.00000100 -0.83964600 1.44344200
Ar 3.13966200 -1.81268500 0.24389300	B 0.00000100 0.83964400 1.44344300
Ar 0.00000000 -3.62537000 -0.24389300	B 0.30504200 1.64179100 0.00000000
Ar -3.13966200 -1.81268500 0.24389300	B 0.00000100 0.83964400 -1.44344300
Ar -3.13966200 1.81268500 -0.24389300	B 0.00000100 -0.83964600 -1.44344200
B 0.00000000 1.68480500 0.04365800	Kr -1.07399200 -3.57394600 0.00000000
B 1.45908400 0.84240300 -0.04365800	Kr -0.40077400 1.90225500 -3.18549400
B 1.45908400 -0.84240300 0.04365800	Kr -0.40077400 1.90225500 3.18549400
B 0.00000000 -1.68480500 -0.04365800	Kr 1.07396200 3.57395700 0.00000000
B -1.45908400 -0.84240300 0.04365800	Kr 0.40078900 -1.90226000 -3.18548800
B -1.45908400 0.84240300 -0.04365800	Kr 0.40078900 -1.90226000 3.18548800
$B_6Xe_6^{4+}$	$B_6Rn_6^{4+}$
B 0.00000000 1.63169400 0.16770700	B 0.18256100 1.61936000 0.00000000
B -1.41308800 0.81584700 -0.16770700	B -0.18256900 0.80967900 1.40240400
B -1.41308800 -0.81584700 0.16770700	B 0.18256900 -0.80967900 1.40240400

B 0.00000000 -1.63169400 -0.16770700	B -0.18256100 -1.61936000 0.00000000
B 1.41308800 -0.81584700 0.16770700	B 0.18256900 -0.80967900 -1.40240400
B 1.41308800 0.81584700 -0.16770700	B -0.18256900 0.80967900 -1.40240400
Xe -3.19557500 1.84496600 -1.06813100	Rn -1.20902000 1.86016300 -3.22189600
Xe 0.00000000 3.68993300 1.06813100	Rn 1.20903700 3.72032500 0.00000000
Xe 3.19557500 1.84496600 -1.06813100	Rn -1.20901900 1.86016300 3.22189600
Xe 3.19557500 -1.84496600 1.06813100	Rn 1.20902000 -1.86016300 3.22189600
Xe -3.19557500 -1.84496600 1.06813100	Rn -1.20903700 -3.72032500 0.00000000
Xe 0.00000000 -3.68993300 -1.06813100	Rn 1.20901900 -1.86016300 -3.22189600

Cartesian coordinates of the monocylic geometries calculated by CCSD/aug-cc-pVDZ

$B_3He_3^+$	$B_3Ne_3^+$
B 0.00000000 0.93327300 0.00000000	B 0.00000000 0.92993400 0.00000000
B 0.80823800 -0.46663700 0.00000000	B 0.80534600 -0.46496700 0.00000000
B -0.80823800 -0.46663700 0.00000000	B -0.80534600 -0.46496700 0.00000000
He -3.11649500 -1.79930900 0.00000000	Ne -2.95621800 -1.70677300 0.00000000
He 3.11649500 -1.79930900 0.00000000	Ne 2.95621800 -1.70677300 0.00000000
He 0.00000000 3.59861900 0.00000000	Ne 0.00000000 3.41354600 0.00000000
$B_3Ar_3^+$	$B_3Kr_3^+$
B 0.00000000 0.90918900 0.00000000	B 0.00000000 0.90883100 0.00000000
B 0.78738100 -0.45459400 0.00000000	B 0.78707100 -0.45441600 0.00000000
B -0.78738100 -0.45459400 0.00000000	B -0.78707100 -0.45441600 0.00000000
Ar -2.58522100 -1.49257800 0.00000000	Kr -2.65939300 -1.53540400 0.00000000
Ar 2.58522100 -1.49257800 0.00000000	Kr 2.65939500 -1.53540000 0.00000000
Ar 0.00000000 2.98515600 0.00000000	Kr -0.00000200 3.07080400 0.00000000
$B_3Xe_3^+$	$B_3Rn_3^+$
B 0.90914900 0.00000000 0.00000000	B 0.91018700 0.00000000 0.00000000
B -0.45457400 -0.78734600 0.00000000	B -0.45509300 0.78824500 0.00000000
B -0.45457400 0.78734600 0.00000000	B -0.45509300 -0.78824500 0.00000000
Xe -1.60355800 2.77744400 0.00000000	Rn -1.64881700 -2.85583500 0.00000000
Xe -1.60355900 -2.77744400 0.00000000	Rn -1.64881800 2.85583500 0.00000000
Xe 3.20711700 0.00000000 0.00000000	Rn 3.29763500 0.00000000 0.00000000
$B_4He_4^{2+}$	$B_4Ne_4^{2+}$
B 0.00000000 1.14272300 0.00000000	B 0.00000000 1.14350200 0.00000000
B 0.00000000 -1.14272300 0.00000000	B 0.00000000 -1.14350200 0.00000000
B 1.14272300 0.00000000 0.00000000	B 1.14350200 0.00000000 0.00000000
B -1.14272300 0.00000000 0.00000000	B -1.14350200 0.00000000 0.00000000
He 0.00000000 2.56096200 0.00000000	Ne 0.00000000 2.89938000 0.00000000
He -2.56096200 0.00000000 0.00000000	Ne -2.89938000 0.00000000 0.00000000
He 0.00000000 -2.56096200 0.00000000	Ne 0.00000000 -2.89938000 0.00000000
He 2.56096200 0.00000000 0.00000000	Ne 2.89938000 0.00000000 0.00000000
$B_4Ar_4^{2+}$	$B_4Kr_4^{2+}$
Ar 3.12382000 0.00000000 0.00000000	Kr -3.25272300 0.00000100 0.00000000
Ar 0.00000000 3.12382000 0.00000000	Kr 0.00000000 -3.25272300 0.00000000

Ar 0.00000000 -3.12382000 0.00000000	Kr 0.00000000 3.25272300 0.00000000
Ar -3.12382000 0.00000000 0.00000000	Kr 3.25272300 -0.00000100 0.00000000
B 0.00000000 1.14704900 0.00000000	B 0.00000000 -1.14822600 0.00000000
B -1.14704900 0.00000000 0.00000000	B 1.14822700 0.00000000 0.00000000
B 0.00000000 -1.14704900 0.00000000	B 0.00000000 1.14822600 0.00000000
B 1.14704900 0.00000000 0.00000000	B -1.14822700 0.00000000 0.00000000
$B_5He_5^{3+}$	$B_5Ar_5^{3+}$
B 0.00000000 1.40941400 0.00000000	B -1.13960400 -0.82797100 0.00000000
B 1.34043300 0.43553300 0.00000000	B 0.43529000 -1.33968500 0.00000000
B 0.82843300 -1.14024000 0.00000000	B 1.40862900 0.00000000 0.00000000
B -0.82843300 -1.14024000 0.00000000	B 0.43529000 1.33968500 0.00000000
B -1.34043300 0.43553300 0.00000000	B -1.13960400 0.82797100 0.00000000
He 1.65424200 -2.27686800 0.00000000	Ar 3.37338700 0.00000000 0.00000000
He 0.00000000 2.81436400 0.00000000	Ar -2.72912700 -1.98282700 0.00000000
He -2.67661900 0.86968600 0.00000000	Ar -2.72912800 1.98282700 0.00000000
He 2.67661900 0.86968600 0.00000000	Ar 1.04243400 -3.20828200 0.00000000
He -1.65424200 -2.27686800 0.00000000	Ar 1.04243400 3.20828200 0.00000000
$B_5Kr_5^{3+}$	$B_6Ar_6^{4+}$
B 0.00000000 1.40814000 0.00000000	Ar 0.00000000 3.63919300 0.23341200
B 1.33922100 0.43513900 0.00000000	Ar 3.15163400 1.81959700 -0.23341200
B 0.82768400 -1.13920900 0.00000000	Ar 3.15163400 -1.81959700 0.23341200
B -0.82768400 -1.13920900 0.00000000	Ar 0.00000000 -3.63919300 -0.23341200
B -1.33922100 0.43513900 0.00000000	Ar -3.15163400 -1.81959700 0.23341200
Kr 2.06104800 -2.83678900 0.00000000	Ar -3.15163400 1.81959700 -0.23341200
Kr 0.00000000 3.50646400 0.00000000	B 0.00000000 1.68430100 0.04166800
Kr -3.33484600 1.08355700 0.00000000	B 1.45864700 0.84215000 -0.04166800
Kr 3.33484600 1.08355700 0.00000000	B 1.45864700 -0.84215000 0.04166800
Kr -2.06104800 -2.83678900 0.00000000	B 0.00000000 -1.68430100 -0.04166800
	B -1.45864700 -0.84215000 0.04166800
	B -1.45864700 0.84215000 -0.04166800

Cartesian coordinates of the selected isomers of $B_6Ar_6^{2+}$ calculated by MP2/aug-cc-pVDZ.

6-15	6-16
B 0.38019800 -1.20127400 -0.22256600	B 1.58825800 0.74048400 -0.00019200
B 1.96793300 -0.83067000 0.12493500	B 0.15030200 -0.92569100 -0.00002400
B 1.96793000 0.83068200 0.12496100	B 1.82324300 -0.94866500 -0.00004000
B 0.38018700 1.20129600 -0.22249400	B -1.21212300 -0.07329600 0.00001700
B -0.76711300 -0.00000100 -0.00430200	Ar 2.98496700 2.10262800 -0.00048500
Ar 3.42576100 2.04194100 0.38281500	B -2.81405200 -0.41636900 -0.00005400
Ar -0.08501800 -3.05065300 -0.88704300	Ar -3.93227500 -0.69169700 1.49898100
Ar 3.42577900 -2.04193100 0.38269200	Ar -3.93212900 -0.69171500 -1.49918800
Ar -0.08503600 3.05067800 -0.88695600	Ar 2.79284100 -1.81456700 1.51319700
B -2.40222500 -0.00001700 0.27923800	Ar 2.79299700 -1.81510800 -1.51272400
Ar -3.27213600 -0.00019200 1.96599700	B -0.04664600 1.11865200 0.00000900

Ar	-3.83349100	0.00015200	-0.97966400	Ar	-0.56445200	3.05070700	0.00029700
	6-29				6-35		
Ar	4.34413400	-0.00016100	-1.05911100	B	-0.48432500	-0.87777300	0.00024200
Ar	3.87277900	-0.00056300	1.90805900	B	2.58729600	-0.31495800	0.00005800
Ar	0.00093100	2.85653500	-0.84684800	B	0.90877200	-0.09538900	0.00006400
Ar	-3.87295000	-0.00028600	1.90800600	B	-0.47795400	0.87272300	-0.00007300
Ar	-4.34408800	0.00053900	-1.05919400	B	-1.88376200	-0.07308200	0.00008200
Ar	-0.00077200	-2.85621300	-0.84764700	Ar	-0.55911600	2.83640200	-0.00050600
B	2.96332000	-0.00038700	0.24556700	B	-3.47654500	-0.34955400	0.00008000
B	1.36442000	-0.00024800	-0.00487000	Ar	-4.60154200	-0.59777300	1.50315400
B	0.00018400	0.90066300	-0.24653700	Ar	-4.60133400	-0.59896000	-1.50295500
B	-2.96335800	0.00031200	0.24562200	Ar	3.86416800	1.24867500	-0.00023400
B	-1.36445200	0.00050100	-0.00483800	Ar	3.34152200	-1.32752500	1.53436600
B	-0.00023600	-0.90030400	-0.24670100	Ar	3.34144600	-1.32803100	-1.53395100
	6-40						
Ar	-2.19639800	0.13191900	-2.17976300				
Ar	2.17270400	0.46359700	-2.15814000				
Ar	0.23509600	-3.05947500	-0.42101900				
Ar	-2.17332800	-0.46348800	2.15746500				
Ar	2.19569600	-0.13215600	2.18047700				
Ar	-0.23381500	3.05958700	0.42099900				
B	-0.87706000	0.05285400	-0.87203900				
B	0.86841000	0.18538200	-0.86259500				
B	0.09322900	-1.22288200	-0.16843700				
B	-0.86781300	-0.18541800	0.86309600				
B	0.87768200	-0.05269000	0.87146100				
B	-0.09428500	1.22281300	0.16844400				

Cartesian coordinates of the isomer of $B_4Ar_4^{2+}$ calculated by MP2/aug-cc-pVDZ.

$B_4Ar_4^{2+}$			
Ar	-2.61750100	-2.23811300	0.18542200
Ar	2.72062500	0.25390300	1.43022500
Ar	2.60874900	-0.97627900	-1.36070700
Ar	-2.10231800	2.84636200	-0.23938800
B	-1.74847700	-0.52001800	-0.04688700
B	1.34455400	-0.14422100	0.01970900
B	-0.21401500	0.09567000	-0.01198300
B	-1.59415900	0.99712600	-0.00974400

Cartesian coordinates of the isomers of $B_5Ar_5^{3+}$ calculated by B3LYP/aug-cc-pVDZ.

	5-1				5-2		
B	0.00000000	1.39602300	0.00000000	B	0.10737800	-1.47372100	0.00034100
B	-1.32791900	0.43135400	0.00000000	B	1.66415500	-1.12210300	0.00014200
B	-0.82086200	-1.12948400	0.00000000	B	1.32717200	0.46945300	0.00002900

B 0.82051400 -1.12951700 0.00000000	B -0.29620600 0.74207400 0.00002800
B 1.32783000 0.43134200 0.00000000	B -1.28056200 -0.62096500 0.00043000
Ar -1.98122600 -2.72683900 0.00000000	Ar 2.68608100 1.93107800 -0.00007500
Ar 0.00013700 3.37032700 0.00000000	Ar -2.64001100 -0.91234600 1.53663900
Ar 3.20560200 1.04136900 0.00000000	Ar 3.22597500 -2.17247600 0.00013600
Ar -3.20548400 1.04190000 0.00000000	Ar -1.05508700 2.62421800 -0.00037300
Ar 1.98109300 -2.72667900 0.00000000	Ar -2.63971800 -0.91345600 -1.53659700
5-3	**5-4**
B 1.16309100 -0.51562800 0.00121800	B -1.59707200 -0.00008800 -0.65839700
B 0.83821600 1.13336600 -0.00116400	B -0.79475600 -0.00012300 -2.03145800
B -0.76334100 1.25097900 -0.00134700	B 0.79566200 0.00018400 -2.03119100
B -1.88534500 0.10411700 0.00034500	B 1.59784900 0.00000900 -0.65794500
B -0.44402200 -0.71544000 0.00167200	Ar -2.88417000 -1.52954400 -0.15828000
Ar 2.08583700 2.61744100 -0.00312100	Ar -2.88405200 1.52966200 -0.15840300
Ar 2.32403900 -1.33958700 1.53809300	Ar 2.88376900 -1.52963100 -0.15859200
Ar 2.32256100 -1.34412600 -1.53557900	Ar 2.88367300 1.52969900 -0.15821300
Ar -3.21473800 -0.13954600 1.52290000	B 0.00007900 -0.00007700 -0.04966100
Ar -3.21453200 -0.14345800 -1.52249400	Ar 0.00029100 -0.00016000 2.14144700
5-5	**5-6**
B 0.34699000 -0.86642000 0.00440900	Ar 2.32891200 -0.97825500 1.77851300
B -1.28825900 -1.02031400 0.00908400	Ar -0.84265900 -4.18646900 -1.07115800
B -2.50039600 -0.00009300 -0.00086000	Ar -2.40920300 -3.40821200 1.40516200
B -1.28859900 1.02039500 -0.01499800	Ar -2.36934900 0.87973000 -1.77689600
B 0.34652500 0.86609700 -0.01558800	B 0.49324300 1.15071500 -0.05086400
Ar -4.34354700 -0.00006200 0.00143100	B 0.72856900 -0.31337400 0.55892800
Ar 1.38589800 -1.87753800 -1.53579000	B -1.15512300 -2.69529500 0.11903600
Ar 1.39481400 -1.84557500 1.55706300	B -0.52813600 -1.23061100 0.05450100
Ar 1.39484700 1.85038900 -1.55576700	B -0.74718700 0.27015500 -0.55764900
Ar 1.38569300 1.87287900 1.53805100	Ar 1.23103000 2.87186300 -0.12607000
5-7	**5-8**
B -0.82813600 -0.00018000 -0.12044300	Ar -2.02086000 -1.74422800 -1.51884900
B 1.86750700 0.00033100 -0.52908100	Ar -2.01890300 -1.74416800 1.51972900
B 0.39268400 0.00070400 -1.11892500	Ar -1.97620200 3.07089800 0.00006300
B 0.63566900 -0.00084800 0.61348100	B 1.00756800 1.82896500 -0.00034700
B -2.40733000 0.00011400 -0.22170900	B 1.69738100 0.42051000 -0.00041800
Ar 0.86509100 -0.00279200 2.62107500	B -1.11446800 -0.85912400 0.00005600
Ar 3.21026700 -1.52417300 -0.75138300	B -0.03614200 0.31183700 -0.00022900
Ar -3.59558000 -1.51326100 -0.37105700	B -0.53159500 1.89862600 0.00001400
Ar 3.20969400 1.52600500 -0.74803500	Ar 2.86633000 -0.29093700 1.52474500
Ar -3.59513700 1.51418600 -0.36818900	Ar 2.86553900 -0.29179100 -1.52543100
5-9	**5-10**
Ar 3.50544400 -0.80093200 1.51824200	B -0.00047500 -0.48508500 1.00090100
Ar 3.49924200 -0.80766600 -1.52040700	B 0.00044300 -0.62396600 -0.92073900
Ar -0.00525200 3.19766500 -0.00117800	B -1.23047300 0.00020100 -0.00050300

B -0.81013200 -0.05695600 -0.00112700	B 0.00000200 1.10964100 -0.08034300
B 2.29435800 -0.54279400 0.00136400	B 1.23049300 0.00028200 0.00034800
B 0.81249100 -0.05290100 0.00231000	Ar -3.12449100 0.00032100 -0.00069200
B -0.00199700 1.28817900 -0.00016700	Ar -0.00121600 -1.32023800 2.72169900
B -2.29196700 -0.54639700 0.00009300	Ar 3.12447300 0.00013700 0.00117900
Ar -3.50203100 -0.80501500 -1.51803700	Ar 0.00101200 -1.69794900 -2.50394700
Ar -3.49816800 -0.80881100 1.52069400	Ar 0.00022300 3.01743000 -0.21814600
5-11	**5-12**
B 0.01300300 1.31287200 -0.17561700	B -0.93765500 1.04150400 -0.51382300
B 0.00439700 0.19533100 -1.65127700	B -0.94250700 -1.03683000 -0.51462400
B 1.24819900 0.24100300 -0.62924600	B -0.20319900 0.00088000 -1.56006500
B -0.00337700 -0.77691500 -0.00270700	B 0.97693800 -0.00214700 -0.41459200
B -1.24043900 0.26632600 -0.63686200	B -0.41304000 0.00075600 0.67219800
Ar 3.13211400 0.24217500 -0.73063100	Ar -1.93991000 2.64232800 -0.67099300
Ar 0.02767200 3.04224800 0.60608700	Ar -0.51098900 -0.00016700 2.59439900
Ar -3.12346800 0.29751800 -0.73665200	Ar 2.41720800 1.51213500 -0.30152300
Ar -0.01776900 -1.09800300 2.11668100	Ar 2.40959800 -1.52354300 -0.30204100
Ar -0.02460000 -2.82799800 -0.39556700	Ar -1.95383400 -2.63190900 -0.67236900
5-13	
B -0.00110200 1.60985600 0.00724200	
B -1.20778700 -0.36210300 -0.00593400	
B -0.00144300 0.28553600 -1.00162500	
B 1.20846700 -0.36039000 -0.00029000	
B 0.00131500 0.28799400 1.00350500	
Ar -0.00312300 3.47844900 0.00326800	
Ar 3.13468600 0.37660900 -0.00575500	
Ar 1.77441300 -2.31508500 0.00374900	
Ar -3.13502900 0.37188900 -0.00372200	
Ar -1.77079400 -2.31766600 0.00165500	

Cartesian coordinates of the isomers of $B_6Ar_6^{4+}$ calculated by B3LYP/aug-cc-pVDZ.

6-1	**6-2**
Ar 0.00000000 3.63850400 0.20144100	Ar -3.78359700 0.67427600 -0.00020600
Ar 3.15090000 1.81917100 -0.20156700	Ar -2.68186600 -3.01715600 -0.00025100
Ar 3.15090100 -1.81917000 0.20156700	Ar 2.31121100 2.30148900 -0.00166600
Ar 0.00000000 -3.63850400 -0.20144100	Ar -1.14578300 3.14990900 0.00081100
Ar -3.15090000 -1.81917100 0.20156700	B -1.89768800 0.09359700 -0.00005500
Ar -3.15090100 1.81917000 -0.20156700	B -1.51696900 -1.51785100 -0.00012600
B -0.00000100 1.67146400 0.03226700	B 0.11213700 -1.59782700 0.00002200
B 1.44747100 0.83572200 -0.03228700	B 1.56788300 -0.79555900 0.00011000
B 1.44747200 -0.83572200 0.03228800	B 0.97519200 0.81497600 -0.00036000
B 0.00000100 -1.67146400 -0.03226700	B -0.66494800 1.21751300 0.00011000
B -1.44747100 -0.83572200 0.03228700	Ar 2.84806400 -1.30713700 -1.53898300
B -1.44747200 0.83572200 -0.03228800	Ar 2.84763600 -1.30550600 1.54037800

6-3			6-4		
Ar	2.41684500	2.92374700	0.00048400	Ar	-3.06604200	2.78379600	0.00139200
Ar	-3.65831600	2.23829700	-0.00056500	Ar	3.18688900	-1.03488900	-0.01460500
Ar	-3.31007700	-1.58697800	0.00107300	Ar	3.06651900	2.78342100	0.00130500
Ar	-0.04308100	-2.99816300	-0.00136500	B	0.00009900	2.16258100	-0.00024500
B	1.06436900	1.58108300	0.00020100	B	-1.53862200	1.66111700	-0.00188300
B	-0.53878000	1.91653000	-0.00005700	B	-0.00024100	-0.89004500	-0.00936400
B	-2.02409400	1.28858600	-0.00017800	B	1.47855300	-0.01559300	-0.00793200
B	-1.75775900	-0.35015300	0.00018100	B	1.53882200	1.66130900	-0.00190500
B	-0.19487400	-0.99744100	-0.00029100	Ar	0.00007500	-2.39668500	-1.56614400
B	1.27908600	-0.11105000	-0.00005300	Ar	0.00007700	-2.36862900	1.60086600
Ar	2.59928300	-0.74988800	-1.57408000	B	-1.47915100	-0.01580100	-0.00793500
Ar	2.59869300	-0.75133600	1.57450700	Ar	-3.18736700	-1.03467100	-0.01468500
6-5				**6-6**			
Ar	2.49674800	1.79487500	-0.00038900	Ar	-3.69246600	1.49696700	0.41902300
Ar	4.17001200	-1.56976600	-0.00003200	B	0.79438500	2.61599800	-0.08271000
B	1.14268000	-2.40636300	-0.00010300	B	-0.88070300	-0.08142100	0.01944800
B	-0.45988900	-2.21568200	-0.00013000	B	-1.81671800	1.36332800	0.18183300
B	-0.32862000	0.34286400	0.00033700	B	-0.79406200	2.61687700	0.08679200
B	1.39353900	0.08169300	-0.00001600	Ar	-1.71001200	-1.71976900	0.97346700
B	2.30924600	-1.32911700	-0.00004400	Ar	-1.57970200	-0.86012000	-2.10804300
Ar	-0.78605900	1.78952600	1.58651800	B	0.88007700	-0.08113300	-0.02529600
Ar	-0.78681000	1.79029200	-1.58568700	Ar	1.57880600	-0.86006200	2.11005000
B	-1.54000500	-0.95940300	-0.00005600	Ar	1.71099500	-1.72015500	-0.97362800
Ar	-2.89670200	-1.00170900	1.52906100	B	1.81723000	1.36310500	-0.18252600
Ar	-2.89634200	-1.00154900	-1.52946700	Ar	3.69231900	1.49737400	-0.42018700
6-7				**6-8**			
Ar	3.03033400	2.42798700	-0.00078700	Ar	3.39333200	0.85383700	-0.00356400
Ar	-3.03034000	2.42798100	-0.00079400	Ar	0.86104000	3.67146400	0.00395400
B	1.55772200	1.20903300	-0.00041000	B	-1.15439500	1.30893200	0.00009800
B	0.00000100	-0.87839900	0.00034500	B	-0.80594500	-0.92328300	-0.00434200
B	-1.55772500	1.20903300	-0.00036400	B	1.43985600	0.52474600	-0.00221700
B	-0.00000200	1.67506800	-0.00042300	B	0.38736600	1.81763500	0.00069800
B	-1.63394600	-0.49115800	0.00013300	B	0.86226400	-1.08209700	-0.00515100
Ar	-2.73357300	-1.36793300	1.54163000	Ar	1.58370900	-2.30784300	-1.54079700
Ar	-2.73295100	-1.37011200	-1.54075300	Ar	1.57915000	-2.30485100	1.54537600
Ar	2.73358400	-1.36790100	1.54162600	Ar	-3.50772300	-0.18439000	-1.52346000
Ar	2.73294700	-1.37013900	-1.54075500	Ar	-3.50539300	-0.18997600	1.52208900
B	1.63394800	-0.49115800	0.00011900	B	-2.18395900	0.01639900	-0.00203700
6-9				**6-10**			
Ar	-1.68312200	2.32334700	-0.00127300	Ar	-1.10961600	-3.21124300	-0.00029200
Ar	1.68311500	2.32327100	0.00004400	Ar	-1.10961600	3.21124400	-0.00027000
B	0.81233900	-1.82577000	0.00101000	B	-0.47874800	-1.38802400	-0.00028300
B	-0.81229900	-1.82560000	0.00115700	B	1.14084500	-1.08497700	-0.00015700

B -0.84872700 0.44827600 -0.00009800	B 1.14084400 1.08497700 -0.00013000
B 0.84867500 0.44822900 0.00013100	B -0.47874800 1.38802500 -0.00026900
Ar -3.38350500 -0.85792100 1.52729100	Ar 3.71497300 0.00002000 -1.52089700
Ar -3.38312600 -0.85991300 -1.52666900	Ar 3.71461000 -0.00002000 1.52110800
Ar 3.38379600 -0.85841600 1.52684100	Ar -2.91720000 0.00000700 -1.56131200
Ar 3.38286500 -0.85934700 -1.52712300	Ar -2.91644100 -0.00000800 1.56203700
B 2.05874600 -0.80241300 0.00047900	B -1.46462900 0.00000000 -0.00039900
B -2.05881400 -0.80239700 0.00051700	B 2.38428400 0.00000000 -0.00010900
6-11	**6-12**
Ar -1.37246200 2.97137400 -0.00256200	B 0.19901700 0.81816600 -0.24750500
Ar 1.37252000 -2.97120000 0.00019600	B 1.53366800 -0.52031200 -0.00661400
B -1.10367800 1.07197000 -0.00163200	B -0.19870400 -0.81899600 -0.24599700
B 0.56352600 0.63491100 -0.00170000	B -1.53381800 0.52104100 -0.01003800
B 1.10450800 -1.07226000 -0.00074800	B 1.76371400 1.13579300 -0.12077400
B -0.56272400 -0.63504000 0.00002900	Ar -2.50300200 1.71195900 -1.40607700
Ar 3.35962400 0.61951800 1.52511200	Ar -2.26827700 1.56156800 1.68391100
Ar 3.36167900 0.61895800 -1.52361200	Ar 3.04271200 2.44775800 -0.17222200
Ar -3.36037300 -0.61645600 1.52505300	Ar 2.26849500 -1.56287600 1.68279300
Ar -3.36167000 -0.62198300 -1.52265900	Ar 2.50323000 -1.71098900 -1.40657200
B -2.15914900 -0.24238000 -0.00103800	B -1.76393000 -1.13536500 -0.12121800
B 2.15997600 0.24203800 -0.00041100	Ar -3.04314300 -2.44751100 -0.17290400
6-13	**6-14**
B -1.28588400 -0.63385300 2.24334400	B 1.28951100 0.43572800 -0.00019800
B 0.00045200 -0.82780100 3.14578100	B -1.02217000 0.89861000 0.00061100
Ar -2.58349100 -1.84492500 -0.32633600	B -0.26719100 -1.33469700 -0.00026900
Ar -3.11424600 1.09816700 0.40627600	Ar 0.63107500 3.15655500 -1.52224500
B -1.57111400 -0.23535100 0.64024800	Ar 2.41757200 -2.12536700 -1.52263200
B 1.28660700 -0.63277100 2.24332500	Ar -3.04998000 -1.03035900 -1.52204200
Ar -0.00026900 -0.21847900 -2.19422700	Ar 2.41784600 -2.12510400 1.52187800
Ar -0.00106700 2.37721100 -0.40928100	Ar -3.04911000 -1.03162500 1.52261300
Ar 3.11423500 1.09901400 0.40541200	Ar 0.63253600 3.15607400 1.52247500
Ar 2.58438700 -1.84457700 -0.32591500	B 1.38800600 -1.22041400 -0.00066700
B 0.00004700 0.16496800 -0.11420500	B -1.75080800 -0.59185000 0.00017100
B 1.57151000 -0.23427100 0.64016400	B 0.36287500 1.81199500 0.00018600
6-15	**6-16**
B -0.38904200 1.19548300 -0.13458500	B 1.56770000 0.74381500 0.00048700
B -1.98348500 0.82444400 0.08732600	B 0.15997100 -0.92670800 -0.00165500
B -1.98348000 -0.82445300 0.08728900	B 1.80972600 -0.92876100 -0.00095400
B -0.38903000 -1.19547200 -0.13460900	B -1.19774800 -0.09115500 -0.00056500
B 0.76247100 0.00001000 -0.00578600	Ar 2.98333800 2.11877200 0.00178500
Ar -3.47358000 -2.03720700 0.25576700	B -2.79850300 -0.43156800 -0.00000100
Ar 0.10359900 3.15672400 -0.60719400	Ar -3.93398700 -0.70741400 1.50633800
Ar -3.47360400 2.03717700 0.25578100	Ar -3.93318900 -0.71166000 -1.50593400
Ar 0.10363600 -3.15671000 -0.60722300	Ar 2.81427200 -1.81228500 1.52980200

B 2.40853100 0.00001200 0.18856900	Ar 2.81863600 -1.81130800 -1.52878700
Ar 3.39134800 -0.00003600 1.83341600	B -0.05644200 1.09891300 -0.00037600
Ar 3.78583200 0.00004500 -1.15504800	Ar -0.60593200 3.07263400 -0.00235300
6-17	**6-18**
B 0.32067300 1.77486600 -0.00012000	Ar 4.06008900 0.38652500 -1.50555200
B -1.27844700 1.62680700 0.00050000	B 0.13280300 1.35544000 -0.00005200
B -2.24189600 0.31285200 0.00051100	B 2.89394700 0.28964500 -0.00006100
B -0.73101100 -0.48659700 -0.00032300	B -1.47692600 1.53739000 -0.00002100
B 0.79406400 0.17718800 0.00008000	Ar 4.05978600 0.38666200 1.50568500
B 2.33998700 -0.44470700 0.00051800	B -0.11772400 -0.69554800 -0.00008200
Ar -0.92056800 -2.63684400 -0.00225600	B -1.72229700 -0.13125700 -0.00008900
Ar 1.28603600 3.45076400 -0.00085100	Ar -2.96276500 -0.89017500 -1.56042700
Ar 3.46909500 -0.84824800 1.50817300	B 1.25693700 0.24255800 -0.00005700
Ar 3.46971700 -0.84830600 -1.50699400	Ar -2.96255000 -0.89075000 1.56048800
Ar -3.54096300 0.02938200 1.52770900	Ar 0.12297000 -2.76779300 -0.00017200
Ar -3.54203100 0.03091700 -1.52610500	Ar -2.58607000 3.05380200 0.00007700
6-19	**6-20**
B 1.27232500 -0.79587400 -0.12361200	B 1.56111900 -0.00062400 -0.00010700
B 2.60281500 0.07911700 0.24990600	B 0.29200700 0.95655400 -0.04207500
B 1.64604600 1.35828900 0.26854300	B 0.29201700 -0.95744700 0.04173000
B 0.05663000 1.57723800 0.00886400	Ar -2.35737500 1.91691600 1.45712400
B -0.26057300 -0.13305900 0.01434600	Ar -2.36363600 1.78393800 -1.60977000
B -1.73788300 -0.91617500 0.16123700	Ar -2.35786800 -1.91628500 -1.45698800
Ar -2.60675200 -1.53468400 1.76544000	Ar -2.36306000 -1.78431700 1.61017900
Ar -2.99569000 -1.40686700 -1.22088100	B -1.36584000 0.88293500 -0.03694200
Ar 1.54864900 -2.77508900 -0.72612800	B -1.36584400 -0.88307000 0.03634900
Ar 4.41912200 -0.20949300 0.51402400	Ar 4.35879700 0.06660800 1.50281900
Ar -0.44309300 2.67889200 -1.76495800	Ar 4.35837100 -0.06637300 -1.50310800
Ar -0.91650400 2.92237100 1.27159000	B 3.19571400 -0.00009800 0.00012200
6-21	**6-22**
Ar 0.00686100 1.05589000 -2.98574700	Ar -2.90551300 2.00215400 0.17230100
Ar 2.02264100 1.56039700 2.32090800	Ar 0.78451700 3.14464600 -0.88094000
Ar 3.14614700 -0.57074100 -0.83341500	Ar 1.42695600 -0.00897500 2.25365900
Ar -0.00148700 -3.16477900 -0.13848300	Ar 0.78083600 -3.14270500 -0.88962000
Ar -3.14076900 -0.56584500 -0.85272900	Ar -2.91143800 -1.99661300 0.17741900
Ar -2.03076600 1.56873400 2.31315000	B 0.11880700 0.00074400 -1.33722400
B 0.00406600 0.35245000 -1.20696000	B -1.34943800 0.87903200 -0.02681600
B 0.85392900 0.69701000 1.03719700	B 0.18275900 1.38233600 -0.44561200
B 1.33084100 -0.19255300 -0.28090200	B 1.12915600 0.00377200 0.23736400
B -0.00033900 -1.25213900 -0.12530800	B 0.17592900 -1.38258700 -0.45462400
B -1.32901700 -0.18919600 -0.28385300	B -1.35281200 -0.87773300 -0.02866400
B -0.86210700 0.70077400 1.03614100	Ar 3.12897500 -0.00005300 -0.26182600
6-23	**6-24**
Ar -0.45363000 -2.85394600 -0.04946300	Ar 0.68454500 2.48365500 -1.45179700

Ar 2.00717700 0.27626900 2.10737300	B 0.51361900 -0.74004700 1.18388700
Ar 3.50922700 -0.06924100 -1.66421900	B 0.43822800 -0.72371600 -0.49578700
B -0.27304800 1.22680500 -0.08151000	B 0.86877500 0.94530100 -0.07796100
B 0.26782100 0.04773300 -1.84779000	B -0.18485600 0.82613300 1.28136100
B -1.17129000 0.21566200 -1.10759300	Ar 2.84675200 1.36561800 0.34419700
B -0.50809900 -0.76957500 0.18516700	Ar -2.49223300 -1.37359600 -1.71080800
B 0.98303600 0.15797900 0.42513300	Ar 1.37942700 -1.89609000 -1.76789800
B 1.74313000 0.00576600 -1.07623500	B -1.23877300 -0.50253700 -0.48693900
Ar -1.73105700 -0.91816800 1.90567800	B -1.71996700 0.58450800 0.81722800
Ar -0.73149400 2.96618500 0.58208000	Ar -3.39317500 1.13150300 1.46544800
Ar -2.88954200 0.35324300 -1.90844100	Ar 1.34217700 -1.81932300 2.50369400
6-25	**6-26**
B 0.51228000 0.47113700 -1.44053100	Ar -1.42759500 -0.97393900 2.06423600
B 0.89117300 1.27691000 0.17943800	B -0.37213900 0.55130300 -1.36819200
B 1.67913200 -0.18071400 -0.44164600	B -1.09882600 -0.42166800 0.10885000
B -1.05167700 -0.44145500 0.00778500	B -1.25575200 1.38862600 -0.23438100
B -0.66771000 1.18365300 -0.57235100	Ar -2.65711500 -1.56695800 -0.64864900
Ar -2.56092800 -1.40615800 -1.04762000	B 1.57493200 0.64562400 0.14546200
Ar -2.06505500 -0.48187400 1.86838600	B 0.24415300 1.65626600 0.33777300
Ar -1.90742000 2.57809600 -0.98826100	B 0.47117300 -0.65002700 -0.68321300
Ar 1.69260600 2.66066000 1.17463300	Ar 3.10407300 1.33667000 -0.95004000
B 0.49549700 -1.25867100 0.03656200	Ar 2.61455600 0.05304400 1.76786300
Ar 0.78761000 -3.15225900 0.38906200	Ar 1.21516700 -2.28269200 -1.38116100
Ar 3.53688300 -0.49037100 -0.77654900	Ar -2.72784700 2.55328500 -0.38177700
6-27	**6-28**
Ar -1.33607200 -2.76410000 0.09325400	Ar -0.65762100 -2.84849900 -0.06124700
B -0.98827300 1.50018900 0.04923700	B -0.55753900 1.33379900 -0.28906900
B -1.42252000 -0.73656700 0.00150800	B -0.77986900 -0.81635100 -0.40553900
B -0.68855100 0.29792500 1.21651400	B -0.93964100 0.31618200 1.01354700
Ar -3.43870000 -0.63450600 -0.23321200	Ar -2.42653700 -0.97833400 -1.63728000
B 1.22668500 0.05909300 -0.61898200	B 1.92398200 0.09944100 0.10023500
B 0.94819100 0.07559900 1.17596800	B 0.68524700 0.19675000 1.25412900
Ar 2.21134600 -0.05985800 2.59768900	B 0.51095900 0.16818600 -0.91821800
B -0.42172700 0.27960700 -0.98291400	Ar 3.27235900 1.55917800 0.00004500
Ar 2.57187100 1.47061600 -1.30006500	Ar 3.15922200 -1.46110000 0.06066200
Ar 2.22835200 -1.56798000 -1.37789000	Ar -2.29989900 0.41108500 2.36170900
Ar -1.86285400 3.14587000 -0.01347900	Ar -1.28172800 2.95711200 -0.93363500
6-29	**6-30**
Ar 0.85474000 4.20672700 1.06615200	Ar -3.35474900 -1.76889700 -1.05421100
Ar 2.41516300 3.43302600 -1.39965200	Ar -3.15727000 -1.16140600 1.89280500
Ar 2.31041900 -0.91314900 1.74634300	Ar -1.45508200 2.77405100 -1.71866400
Ar -0.85677300 -4.20795800 -1.06411200	B 0.60989600 1.51346500 0.50229800
Ar -2.41590100 -3.43082800 1.40143000	B 0.83958100 -0.03489500 0.01668700
Ar -2.30851000 0.91311400 -1.74892000	B -2.18781400 -0.91374600 0.24292100

B 1.17608000 2.74592300 -0.12043600	B -0.83988400 -0.03462800 -0.01739800
B 0.54015500 1.25935500 -0.05576700	B -0.60899300 1.51384800 -0.50157800
B 0.67444500 -0.26675500 0.50934400	B 2.18757000 -0.91387200 -0.24354300
B -1.17667200 -2.74581700 0.12127500	Ar 3.35345000 -1.77088500 1.05306700
B -0.53970100 -1.25975200 0.05512100	Ar 3.15807600 -1.15954900 -1.89325200
B -0.67344500 0.26611300 -0.51077700	Ar 1.45547500 2.77274900 1.72042500
6-31	**6-32**
Ar 3.93690200 -0.17837000 -1.50539000	B -1.04279700 1.06039700 -0.00038200
Ar 3.93590000 -0.17874600 1.50625900	B -1.04268000 -1.06021000 0.00026700
B -1.27022300 -1.55718400 -0.00128900	B -2.37794600 -0.00001800 0.00013200
B -0.51390500 0.08517000 -0.00037100	B 1.84956700 0.00008200 0.00001100
B 2.75360600 -0.06858300 0.00011700	B 0.27188700 0.00015100 -0.00006400
B 1.15501600 -0.12308800 -0.00027600	Ar -1.08496200 3.08612100 -0.00060800
B 0.28744800 -1.42656000 -0.00117700	Ar -1.08440300 -3.08587700 -0.00093100
B -1.18345000 1.55795000 0.00037700	B 3.50860800 0.00005400 0.00011500
Ar -1.73126400 2.65939300 1.50868900	Ar 4.63991200 1.51111000 -0.00070100
Ar -1.72791200 2.66195900 -1.50736500	Ar 4.63982400 -1.51105600 0.00102300
Ar -2.37689000 -2.27043600 1.51481900	Ar -3.71761600 -0.00079600 -1.54165400
Ar -2.37798400 -2.26816200 -1.51628500	Ar -3.71682100 0.00037100 1.54285000
6-33	**6-34**
B 1.13832500 1.46115100 -0.00138300	B -1.61677700 1.39172300 -0.00006400
B -0.01440200 0.22158500 -0.00205100	B -1.61793400 -1.39089000 0.00025900
B 2.51692700 0.50217000 -0.01339400	B -0.47371500 -0.00015300 -0.00006600
B -1.59706100 0.11305000 -0.00360500	B 1.09334200 -0.00036600 0.00016500
Ar 1.00355600 3.44067500 0.01182200	B -2.42973900 0.00075600 0.00033800
B -3.24989600 0.01333600 -0.00500300	B 2.73530000 -0.00086400 0.00004400
Ar -4.28296500 -1.56896600 -0.00946700	Ar 3.88500600 1.50670000 0.00000500
Ar -4.48043500 1.44599100 -0.00150600	Ar 3.88425500 -1.50888100 -0.00038000
Ar 1.64420800 -2.26010100 -1.56788100	Ar -1.78273700 -2.67483300 1.52955400
Ar 1.65667200 -2.22285000 1.60722100	Ar -1.78342700 -2.67459900 -1.52937900
B 1.40296000 -0.77974900 -0.00683100	Ar -1.78046700 2.67588800 1.52938600
Ar 4.40428200 0.73982200 -0.03122700	Ar -1.78109600 2.67566800 -1.52937300
6-35	**6-36**
B -0.47652300 -0.90103100 -0.00001700	B 0.77622000 0.96121400 -0.53865700
B 2.56323900 -0.32246900 0.00004200	B 0.77597600 -0.95894700 -0.54234400
B 0.89571800 -0.12221600 -0.00001300	B 2.00286200 0.00007300 -0.00209300
B -0.48465200 0.82098400 0.00000600	B 0.69013000 -0.00214400 1.06456800
B -1.86699900 -0.12768600 -0.00001500	B -0.55861900 0.00031100 -0.06440500
Ar -0.57560500 2.83162100 0.00004000	Ar 3.88145300 -0.00034200 0.08176400
B -3.46477300 -0.36585600 -0.00002700	Ar 0.89324700 2.62006100 -1.48672500
Ar -4.60686100 -0.58933300 1.50999300	Ar 0.89283100 -2.61407100 -1.49695000
Ar -4.60687900 -0.58921500 -1.51004800	Ar 0.73326800 -0.00592700 2.98262700
Ar 3.85626700 1.28507900 -0.00108000	B -2.17692900 0.00019800 -0.04802300
Ar 3.36019600 -1.32672300 1.55249600	Ar -3.40990500 -1.49271700 -0.02213200

Ar 3.36010100 -1.32857500 -1.55139500	Ar -3.41023900 1.49280000 -0.02220800
6-37	**6-38**
B 1.25882700 0.00002700 -0.96057400	B 0.35708500 1.35749400 1.01054600
B 1.25883100 0.00009500 0.96056900	B 0.35448700 1.35995400 -1.00911500
B 0.74812600 1.23714900 -0.00004800	B 1.64459400 1.44788300 -0.00081300
B -0.47275300 -0.00009000 0.00000600	B -0.24579400 0.11035200 -0.00002400
B 0.74834900 -1.23711900 0.00004500	Ar -0.12087500 2.28510800 2.59582500
Ar 0.84269400 3.12367400 -0.00011000	Ar -0.12739800 2.29243000 -2.59036800
Ar 2.23574300 0.00005100 -2.61147700	B -1.59103500 -0.79401300 0.00019700
Ar 0.84328200 -3.12362600 0.00011600	Ar -1.82746500 -2.71917400 -0.00106000
Ar 2.23569300 0.00025500 2.61150400	Ar -3.44990200 -0.21427600 0.00193000
B -2.10491100 -0.00027400 -0.00000700	Ar 2.47324700 -1.27853800 -1.51750400
Ar -3.27820400 -0.00021000 -1.50590300	Ar 2.47566200 -1.28058700 1.51162300
Ar -3.27822600 -0.00008500 1.50587300	B 1.55689300 -0.18753800 -0.00239600
6-39	**6-40**
Ar -3.72815200 -0.30638500 1.49642400	Ar 2.22295000 0.15143300 2.16483500
Ar -3.73850300 0.07179200 -1.49804900	Ar -2.17353900 0.12959200 2.21635600
B 0.43950000 0.82010300 -0.00035500	Ar 0.01774700 -3.10057700 0.19836300
B -2.51652800 -0.07926000 0.00000300	Ar 2.17362300 -0.12940900 -2.21554800
B -0.93012500 -0.02920700 0.00033500	Ar -2.22270000 -0.15168400 -2.16567800
B 0.49027600 -0.79074200 -0.00025200	Ar -0.01795400 3.10061600 -0.19838500
B 1.18957200 2.21883100 0.00025500	B 0.87540400 0.05972600 0.85528800
Ar 1.93146500 3.20323700 -1.49638400	B -0.85739200 0.05129400 0.87413500
Ar 1.59881900 3.37990300 1.49838300	B 0.00825600 -1.22291100 0.07853700
B 1.32662100 -2.13967500 -0.00009500	B 0.85589100 -0.05137700 -0.87518500
Ar 1.81010200 -3.27231200 -1.49784000	B -0.87695200 -0.05958600 -0.85398300
Ar 2.12645800 -3.07625000 1.49749600	B -0.00566200 1.22295800 -0.07858700