Electronic Supplementary Information (ESI)

Regioisomer-specific electron affinities and electronic structures of C_{70} *para*-adducts at polar and equatorial positions with (bromo)benzyl radicals: photoelectron spectroscopy and theoretical study

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1. Low-Temperature Negative Ion Photoelectron Spectroscopy (LT-NIPES)

The LT-NIPES experiments were performed with a low temperature apparatus that couples an electrospray ionization source and a temperature-controlled cryogenic ion trap to a magnetic-bottle time-of-flight photoelectron spectrometer.[S1] Fresh spray solutions were prepared by adding an aliquot of an acetonitrile solution of an electron-donor compound, tetrakis(dimethyamino)ethylene (TDAE), to 0.1 mM toluene stock solutions of 2,5–/7,23–$(ArCH_2)_2C_{70}$. The produced $[(ArCH_2)_2C_{70}]^-$ anions were guided by two RF-only quadrupoles and directed by a 90° ion bender into the 3-D ion trap, where they were accumulated and thermalized via collisions with a background buffer gas (ca. 0.1 mTorr 20/80 H_2/He) for a period of 20 to 100 ms before being pulsed out into the extraction zone of a time-of-flight mass spectrometer at a repetition rate of 10 Hz. The trap was operated at 10 K in the current experiments in order to achieve the best instrument resolution, as well as to eliminate vibrational hot bands. For each NIPES experiment, the anions were mass selected and decelerated before being intercepted by a 266 nm (4.661 eV) laser beam from a Nd:YAG laser in the photodetachment zone. The laser was operated at a 20 Hz repetition rate with the ion beam off at alternating laser shots to enable shot-by-shot background subtraction. Photoelectrons were collected at nearly 100% efficiency by the magnetic bottle, analyzed in a 5.2 m long calibrated flight tube, and converted to kinetic energy spectra. The electron binding energy (EBE) spectra were obtained by subtracting the kinetic energy spectra from the detachment photon energy used. The energy resolution ($\Delta E/E$) was ca. 2% (i.e., ca. 20 meV for 1 eV kinetic energy electrons).

2. Theoretical Methods

The structures of $(ArCH_2)_2C_{70}$ anions and neutrals were optimized with density functional theory (DFT) employing the B3LYP exchange–correlation functional[S2] with the Pople's all-electron basis set 6-31+G(d).[S3] The theoretical adiabatic detachment energies (ADEs) of the anions, i.e., the EAs of the neutrals were calculated as the energy differences between the neutrals and the anions at their respective optimized structures. To obtain more accurate EAs, single-point energy calculations were performed with B3LYP functional and triple–ζ quality basis set of 6-311+G(d). The nucleus-independent chemical shifts (NICS) calculations[S4] were performed for $NICS(1)_{zz}$ at 1 Å above the center of 2,5–hexagon and 7,23–hexagon in C_{70} at the

B3LYP/6-311+G(d) level using GIAO method as implemented in the Gaussian program. All calculations were conducted with the GAUSSIAN09 program package. [S5]

3. Details of the Density of States (DOS) Spectra Simulations

In Koopmans' theorem (the single particle approximation),[S6, S7] the observed spectral features can be viewed as originating from an electron removal from a specific occupied orbital of the anion. The simulated density of states (DOS) spectra can be obtained by setting the highest occupied molecular orbital (HOMO) transition of the anions as the first experimental VDE, and shifting the deeper orbitals' transitions by the orbital energy differences relative to the HOMO. It should be pointed out that, in comparison of the simulated DOS spectra with the experimental ones, the important part is how well the electron binding energies correspond to spectral features but not the relative intensities.[S8, S9]

References

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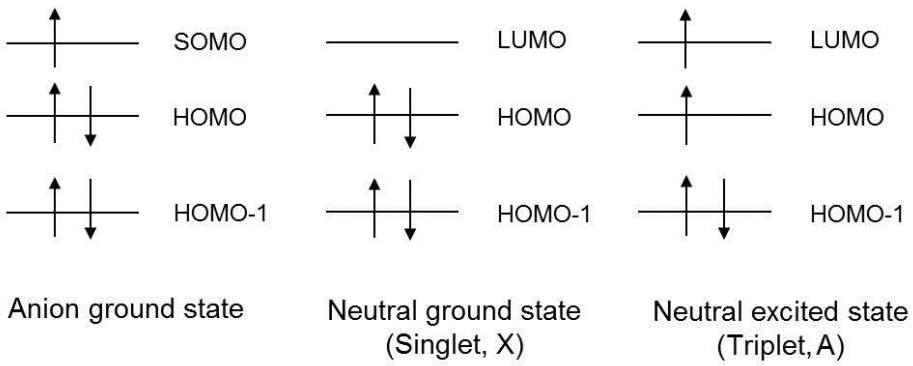

Figure S1. Diagram of the correlations between the anion and neutral occupied molecular orbitals. Under Koopmans' theorem (the single particle approximation), the SOMO-HOMO energy separation of the anion can be viewed as the HOMO-LUMO gap of the neutral. Removal of one electron from the anion SOMO will result in the neutral singlet ground state, and removal of one electron from the anion HOMO will result in the neutral triplet state.

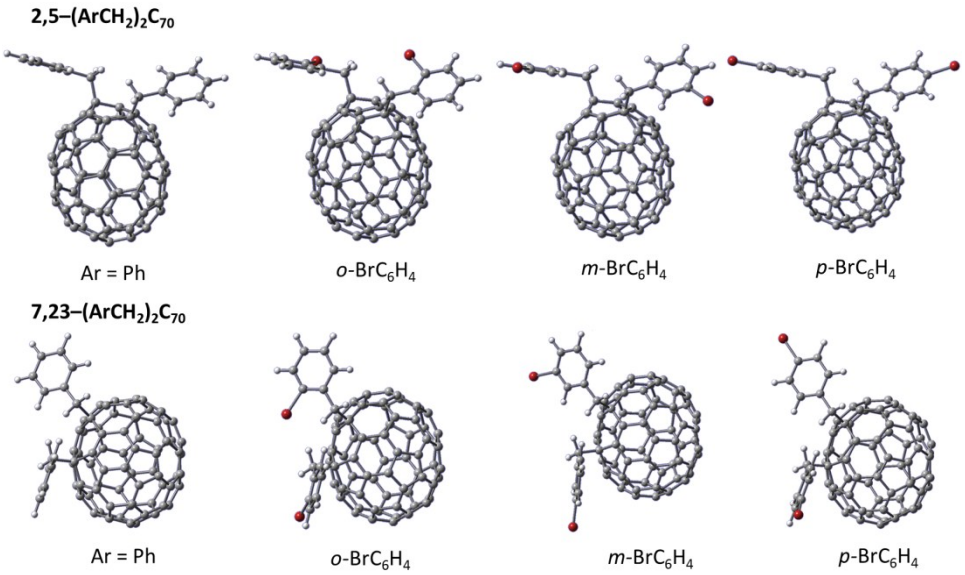

Figure S2. DFT optimized structures for $(ArCH_2)_2C_{70}$ (Ar = Ph, *o*-, *m*-, and *p*-BrC_6H_4) anions and neutrals. Their detailed Cartesian coordinates are provided in the following parts.

Table S1. The calculated C2–C5 and C7–C23 distances in C_{70} and $(ArCH_2)_2C_{70}$ (Ar = Ph, *o*-, *m*-, and *p*-BrC_6H_4).

	Anions		Neutrals	
	C2–C5	C7–C23	C2–C5	C7–C23
C_{70}	2.855	2.816	2.847	2.808
2,5–$(ArCH_2)_2C_{70}$				
Ar = Ph	3.098	2.824	3.092	2.808
o-BrC_6H_4	3.095	2.824	3.09	2.809
m-BrC_6H_4	3.095	2.822	3.089	2.807
p-BrC_6H_4	3.096	2.822	2.089	2.807
7,23–$(ArCH_2)_2C_{70}$				
Ar = Ph	2.842	3.007	2.834	3.007
o-BrC_6H_4	2.842	3.009	2.833	3.009
m-BrC_6H_4	2.843	3.004	2.835	3.004
p-BrC_6H_4	2.843	3.005	2.835	3.004

Table S2. The measured EAs and ΔE_{ST} of the C_{70} derivatives and their comparison with the theoretically calculated results. The experimental uncertainty is ±0.010 eV.

	EAs (eV)			ΔE_{ST} (eV)[e]		
	Exptl.	Theo.[b]		Exptl.[c]	Theo.[d]	
		6-31+G(d)	6-311+G(d)		6-31+G(d)	6-311+G(d)
C_{70}[a]	2.765	2.647	2.692	1.55	1.86	1.75
2,5–$(ArCH_2)_2C_{70}$						
Ar = Ph	2.820	2.737	2.777	1.33	1.35	1.35
o-BrC_6H_4	2.835	2.744	2.803	1.31	1.36	1.35
m-BrC_6H_4	2.905	2.837	2.883	1.32	1.35	1.35
p-BrC_6H_4	2.915	2.862	2.906	1.33	1.35	1.35
7,23–$(ArCH_2)_2C_{70}$						
Ar = Ph	2.770	2.688	2.730	1.32	1.28	1.27
o-BrC_6H_4	2.780	2.697	2.742	1.31	1.27	1.26
m-BrC_6H_4	2.860	2.776	2.829	1.32	1.28	1.27
p-BrC_6H_4	2.890	2.811	2.856	1.32	1.28	1.27

[a] Experimental values are taken from *Phys. Rev. Lett.*, 2006, **96**, 143002. [b] From the calculated EA values, it can be seen that the 6-311+G(d) basis set has improved the agreement between calculations and experiments much compared to the 6-31+G(d) basis set. [c] Measured X–A separations from the spectra. [d] MO energy gaps between singly occupied and first occupied MOs from the anions. [e] See Fig. S1 for how the ΔE_{ST} were determined experimentally by X-A separations, and how they can approximate the HOMO-LUMO gaps.

Cartesian coordinates for C_{70} anions and neutrals.

C_{70} anion

C	-3.98430200	-1.02464100	-0.69349800
C	3.98310200	-0.98596400	0.74533900
C	-2.44697800	-2.92340000	0.77237300
C	-3.21998100	0.80636600	2.26916300
C	-2.44183100	-0.32600600	-2.99393100
C	-2.44248700	-0.16666700	3.00641300
C	2.44183100	-0.32600600	-2.99393100
C	2.44821000	-1.50782900	2.61373000
C	1.20956500	0.27409600	-3.44876500
C	-1.20981400	1.66067000	-3.04766000
C	-1.20834100	-2.26001500	2.62834000
C	-2.44821100	-1.50782900	2.61373000
C	-2.45164800	2.82491800	1.08467400
C	0.00000000	2.32457200	-2.70397000
C	-3.22640500	-1.92394700	1.47295800
C	3.22640500	-1.92394700	1.47295800
C	-2.44146500	2.03022800	2.22851700
C	-1.20794200	3.38723800	-0.80494100
C	1.20932900	0.45686800	3.42905500
C	1.20877500	-3.22232100	-1.33035800
C	-2.44716900	-2.96056400	-0.61765300
C	-1.20847700	-2.39694400	-2.50588900
C	2.44062300	1.90980300	-2.33210900
C	1.20981400	1.66066900	-3.04766000
C	3.22659800	-2.00005900	-1.37050200
C	3.98430200	-1.02464100	-0.69349800
C	3.97320000	0.41594400	1.15523900
C	0.00000000	-1.86038500	-3.03187900
C	1.20953000	1.81940500	2.95639800
C	2.45207200	2.76449700	-1.23142400
C	-3.99189600	1.24192400	-0.03253600
C	3.97243400	0.35344300	-1.17588900
C	0.00000000	-3.48184100	0.82833500
C	-3.23140900	2.43289400	-0.06422400
C	-3.21863900	0.68487900	-2.30757900
C	-1.20953000	1.81940500	2.95639800
C	-1.20873800	-3.14640300	1.49802300
C	-2.44888100	-1.64531000	-2.53156000
C	3.23140900	2.43289500	-0.06422400
C	0.00000000	-0.28421800	3.54002600
C	0.00000000	3.30305500	1.36763100
C	3.21863900	0.68487900	-2.30757900
C	-1.20877500	-3.22232100	-1.33035800
C	1.20798600	3.42637100	0.62690200
C	1.20873800	-3.14640300	1.49802300
C	0.00000000	-0.47134700	-3.51947000
C	2.44716900	-2.96056400	-0.61765300
C	2.44888100	-1.64531000	-2.53156000

C	-2.45207200	2.76449700	-1.23142400
C	1.20834100	-2.26001400	2.62834000
C	0.00000000	3.22472100	-1.53845700
C	2.44697900	-2.92340000	0.77237300
C	-1.20798600	3.42637100	0.62690200
C	2.45164800	2.82491800	1.08467400
C	-1.20956500	0.27409600	-3.44876500
C	1.20847700	-2.39694400	-2.50588900
C	-3.97320000	0.41594400	1.15523900
C	-3.98310100	-0.98596400	0.74533900
C	-3.22659800	-2.00005800	-1.37050200
C	0.00000000	-1.69695400	3.12599100
C	-2.44062300	1.90980300	-2.33210900
C	3.21998100	0.80636600	2.26916300
C	3.99189600	1.24192400	-0.03253600
C	2.44146500	2.03022800	2.22851700
C	0.00000000	2.46477700	2.57849300
C	-1.20932900	0.45686800	3.42905600
C	-3.97243400	0.35344300	-1.17588900
C	2.44248600	-0.16666700	3.00641300
C	0.00000000	-3.52132900	-0.64391300
C	1.20794100	3.38723800	-0.80494000

C_{70} neutral

C	-3.97197600	-0.07766900	-1.23307900
C	3.97226800	-1.19687400	-0.30720600
C	-2.44385400	-2.40740900	-1.81997400
C	-3.22332100	-1.29441700	2.03974000
C	-2.44350100	2.15997200	-2.10745700
C	-2.44364400	-2.47472400	1.72708700
C	2.44350100	2.15997900	-2.10745400
C	2.44389800	-2.98643100	0.43529700
C	1.20715600	2.89290200	-1.91741700
C	-1.20713700	3.42110900	-0.58302100
C	-1.20722900	-3.46689900	-0.14921700
C	-2.44389000	-2.98643400	0.43529300
C	-2.44351600	0.87778200	2.88732800
C	-0.00000600	3.56135000	0.15466100
C	-3.22378300	-2.34025800	-0.60076100
C	3.22379100	-2.34025200	-0.60075600
C	-2.44374400	-0.50901900	2.97486900
C	-1.20713800	2.71724700	2.15871200
C	1.20705000	-2.42505400	2.48209700
C	1.20702400	-0.92948400	-3.34309200
C	-2.44362000	-1.33672200	-2.70550800
C	-1.20702900	0.50267000	-3.43322400
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C	3.22345200	-0.15184600	-2.41107800
C	3.97197700	-0.07766000	-1.23307200
C	3.97202900	-0.66197900	1.04328400

C	0.00000200	1.24793800	-3.33931900
C	1.20698800	-1.21321300	3.25071900
C	2.44380200	2.67215200	1.40333200
C	-3.97204000	0.78774800	0.95206300
C	3.97199800	1.14891800	-0.45489600
C	0.00000600	-2.79067800	-2.21867200
C	-3.22326600	1.54001400	1.86146000
C	-3.22320000	2.24619400	-0.88948600
C	-1.20699200	-1.21321500	3.25071800
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C	-0.00000500	0.95371100	3.43600200
C	3.22319600	2.24620100	-0.88948100
C	-1.20701400	-0.92948800	-3.34309600
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C	1.20724800	-3.11009500	-1.53914300
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C	1.20723900	-3.46689900	-0.14921600
C	-0.00000700	3.19537000	1.57976600
C	2.44386400	-2.40740400	-1.81997000
C	-1.20716300	1.61159300	3.07366100
C	2.44350700	0.87778700	2.88733000
C	-1.20715900	2.89289700	-1.91741900
C	1.20703600	0.50267200	-3.43322300
C	-3.97203000	-0.66198800	1.04327800
C	-3.97226400	-1.19688200	-0.30721300
C	-3.22344700	-0.15185300	-2.41108300
C	0.00000400	-3.51437600	0.60017100
C	-2.44376000	3.01761600	0.05728400
C	3.22332100	-1.29441000	2.03974600
C	3.97203500	0.78775600	0.95207000
C	2.44373900	-0.50901400	2.97487200
C	-0.00000300	-0.51492300	3.52724300
C	-1.20704800	-2.42505700	2.48209500
C	-3.97199900	1.14891000	-0.45490300
C	2.44364800	-2.47472000	1.72709100
C	0.00000500	-1.65735100	-3.15718800
C	1.20712500	2.71724800	2.15871400

Cartesian coordinates for 2,5–$(ArCH_2)_2C_{70}$ anions and neutrals.

Ar = Ph anion

C	-5.25986500	-0.03747300	-0.61075800
C	2.14082500	-0.18166400	2.56918900
C	-4.37870200	1.13242000	1.83606200
C	-3.28540000	2.70674500	-1.78683500
C	-4.02830000	-2.60568300	-0.78073300
C	-2.84708700	3.28652500	-0.53537200
C	0.33830300	-3.54542500	1.15093100
C	0.92421500	1.94141300	2.59619800
C	-0.60598600	-3.78280300	0.08879500
C	-2.14286000	-2.92725300	-2.11682000
C	-2.65246200	2.70180800	1.84426400
C	-3.45926600	2.91810500	0.65877200
C	-1.99532600	1.35997000	-3.38969500
C	-0.72966000	-2.83414900	-2.22352900
C	-4.54029600	1.95358100	0.65479200
C	1.23682400	0.68199900	3.20751900
C	-2.10398100	2.49623700	-2.59393800
C	-1.02761200	-0.75469600	-3.55650400
C	0.75530000	2.93104200	0.35270500
C	-1.61587700	-1.64554000	3.42506400
C	-4.65221300	-0.23030900	1.78003700
C	-3.67082700	-2.33626100	1.63384500
C	1.36468500	-2.95783200	-0.86157400
C	0.03290400	-3.39983400	-1.15502000
C	0.67401000	-2.10346800	3.09635600
C	1.85768600	-1.60076600	2.51112600
C	2.81292700	0.21302600	1.35666500
C	-2.47041200	-3.09831000	1.58797800
C	1.22771000	2.49605800	-0.90348600
C	1.90564100	-1.86928200	-1.55376800
C	-4.21645900	0.58577500	-2.62830600
C	2.33774800	-2.10705700	1.26206100
C	-2.40137200	0.71306200	3.32049900
C	-3.07161300	0.38673800	-3.41324600
C	-4.18758800	-1.79224400	-1.97476400
C	-0.94408300	2.95736700	-1.85215700
C	-3.22040200	1.60254800	2.57516500
C	-4.48669100	-2.13154900	0.45128000
C	2.68292100	-0.85952000	-0.86844000
C	-0.60637600	3.31534900	0.57426700
C	0.43626200	1.14316800	-2.85031600
C	1.57327800	-3.04660500	0.58071000
C	-3.78281400	-1.16844000	2.46435900
C	1.42062900	0.17855500	-2.50408000
C	-1.05216400	1.12477600	3.53200000
C	-2.00271700	-3.60274100	0.28464600
C	-0.26878600	-1.19491900	3.71675000
C	-0.09551300	-3.09147300	2.39728700
C	-2.45825300	-0.91940200	-3.49953600

C	-0.48714800	2.21831000	2.79916600
C	-0.15284900	-1.70487300	-2.96577500
C	0.00716100	0.16630100	3.77625400
C	-0.73051100	0.66331200	-3.49459100
C	2.36872300	0.36820000	-1.43134300
C	-2.77966700	-3.31702200	-0.87244600
C	-1.50652500	-2.81218000	2.59590500
C	-4.32750000	1.76641900	-1.80037500
C	-4.96691000	1.37944400	-0.55026600
C	-5.10340500	-0.83069600	0.53964500
C	-1.24981900	2.93611800	1.83914100
C	-3.01083400	-1.99796600	-2.79476200
C	2.52009200	1.43282300	0.78340000
C	3.20656900	-1.04343900	0.54590300
C	2.53487500	1.69624000	-0.73404100
C	0.33059600	2.34743000	-1.99441000
C	-1.40462100	3.44882700	-0.58284700
C	-4.78912000	-0.53311500	-1.89179900
C	1.53367200	2.28173300	1.39194000
C	-2.69288700	-0.72790000	3.26396800
C	1.13202600	-1.22921400	-2.57993200
C	4.74720200	-1.32518800	0.64637000
H	5.26174100	-0.46379500	0.20335800
H	5.01067300	-1.34386800	1.71133600
C	3.80314000	2.46397100	-1.26020500
H	3.68675100	2.56298100	-2.34593600
H	4.66452100	1.80678400	-1.09211600
C	5.22683500	-2.59877000	-0.01520300
C	5.33568300	-3.79069100	0.71687100
C	5.57757800	-2.62018200	-1.37381300
C	5.77962500	-4.96979500	0.11267300
H	5.06482400	-3.79472000	1.77051400
C	6.02157200	-3.79617400	-1.98330500
H	5.49358600	-1.70807500	-1.95982300
C	6.12461500	-4.97652900	-1.24166200
H	5.85219300	-5.88262900	0.69964400
H	6.28320600	-3.79033800	-3.03899100
H	6.46815500	-5.89327900	-1.71534400
C	4.06621400	3.82213800	-0.64743800
C	3.53043200	4.98635700	-1.21936900
C	4.85323400	3.95371500	0.50693600
C	3.76776500	6.24212800	-0.65480800
H	2.91838800	4.90588300	-2.11503300
C	5.09482500	5.20679300	1.07594400
H	5.27786000	3.06364900	0.96635600
C	4.55123300	6.35710500	0.49703300
H	3.33864800	7.12958300	-1.11440200
H	5.70630000	5.28330600	1.97222400
H	4.73649800	7.33334200	0.93900300

Ar = Ph neutral

C	-5.24806700	-0.04070000	-0.62414500
C	2.14165500	-0.15974400	2.59675600
C	-4.38008100	1.14164200	1.81842300
C	-3.27572700	2.68924200	-1.80497300
C	-4.02534600	-2.60659800	-0.78377200
C	-2.84086900	3.28033400	-0.55634100
C	0.35578000	-3.52928800	1.18124200
C	0.91831100	1.95920600	2.60076200
C	-0.59135700	-3.75529000	0.10296800
C	-2.12828500	-2.94505200	-2.10395300
C	-2.65577800	2.71158800	1.82639500
C	-3.45713800	2.92192400	0.63597900
C	-1.98605100	1.33124200	-3.39918300
C	-0.71454300	-2.85712800	-2.21471200
C	-4.53832500	1.95723300	0.63231300
C	1.22955500	0.70473500	3.21973900
C	-2.08843500	2.46596400	-2.60461600
C	-1.01211200	-0.78403000	-3.54560300
C	0.75626000	2.93178100	0.34936800
C	-1.62008300	-1.62588000	3.42341200
C	-4.65345600	-0.21964500	1.76623200
C	-3.66454700	-2.32919800	1.63294800
C	1.37547100	-2.93753000	-0.82829300
C	0.03680700	-3.40147500	-1.13330300
C	0.67100400	-2.07661100	3.11654300
C	1.85843600	-1.57960200	2.54670000
C	2.81779600	0.22546400	1.38400900
C	-2.46469600	-3.08930900	1.59796400
C	1.22998400	2.48077300	-0.89964300
C	1.91224200	-1.88296600	-1.52505800
C	-4.20737600	0.56506200	-2.64169600
C	2.34477100	-2.09123700	1.29857600
C	-2.40909900	0.73097300	3.31019200
C	-3.06435600	0.36361900	-3.42242500
C	-4.18836300	-1.80787400	-1.98112500
C	-0.93414500	2.93459500	-1.86187100
C	-3.22623100	1.61672100	2.55999300
C	-4.46646100	-2.12519700	0.44050700
C	2.69557000	-0.85612400	-0.83270100
C	-0.60601300	3.31678800	0.56095200
C	0.44677200	1.10969900	-2.83541400
C	1.58779500	-3.03312000	0.62457500
C	-3.78028900	-1.15569400	2.45007900
C	1.41867500	0.14352200	-2.48950700
C	-1.06261100	1.14549800	3.52719900
C	-1.99140700	-3.59265000	0.29819200
C	-0.27614500	-1.17139500	3.73009800
C	-0.09355100	-3.07235400	2.41565500
C	-2.45335500	-0.94729300	-3.49540700
C	-0.49487900	2.23445800	2.79250600
C	-0.13713100	-1.73603100	-2.96392700
C	-0.00372500	0.18941600	3.78163200

C	-0.72356100	0.62259200	-3.48024900
C	2.37626400	0.34736000	-1.39908100
C	-2.75504700	-3.30714100	-0.86540500
C	-1.50665000	-2.79870900	2.60762600
C	-4.31638000	1.75514500	-1.81557100
C	-4.96270900	1.38149100	-0.56974800
C	-5.09521200	-0.82075700	0.52491500
C	-1.25387200	2.94681000	1.82513300
C	-3.00295900	-2.01150300	-2.79011600
C	2.51920100	1.43683800	0.79856000
C	3.21860300	-1.03497100	0.58293000
C	2.53458700	1.68436700	-0.71961500
C	0.34127300	2.32421400	-1.99130800
C	-1.39899200	3.44044600	-0.60070900
C	-4.78396000	-0.54553800	-1.90700100
C	1.53063700	2.28883600	1.39537600
C	-2.69677400	-0.71022300	3.25572900
C	1.14241800	-1.25175000	-2.57294400
C	4.75746700	-1.32822500	0.67723400
H	5.27575700	-0.46375200	0.24605600
H	5.01998600	-1.36000700	1.74135500
C	3.80185600	2.44712400	-1.26049100
H	3.68801200	2.53002700	-2.34768000
H	4.66492300	1.79602800	-1.08032800
C	5.21955400	-2.59814600	-0.00522400
C	5.28684600	-3.80803400	0.70145600
C	5.59732200	-2.59300000	-1.35647000
C	5.71187000	-4.98270800	0.07543400
H	5.00896900	-3.83031200	1.75315300
C	6.02230500	-3.76480800	-1.98713800
H	5.56216800	-1.66260300	-1.91915500
C	6.07909100	-4.96476400	-1.27277800
H	5.75940700	-5.90928200	0.64209900
H	6.31290400	-3.73898800	-3.03443700
H	6.41256400	-5.87680800	-1.76114400
C	4.05023400	3.81488100	-0.66241800
C	3.52790500	4.96798200	-1.26710400
C	4.81444400	3.96206600	0.50478300
C	3.75516100	6.23250200	-0.71843200
H	2.94187800	4.87562500	-2.17914400
C	5.04491700	5.22440300	1.05751500
H	5.23694200	3.08132400	0.98394900
C	4.51346700	6.36428200	0.44811300
H	3.34327000	7.11338800	-1.20447300
H	5.64242300	5.31679700	1.96104000
H	4.69384000	7.34737600	0.87527100

Ar = *o*-BrC_6H_4 anion

C	5.90781300	-0.34060600	0.11891400
C	-1.81946900	-0.19319300	-2.14394000
C	4.80692000	0.69824500	-2.29813700

C	4.26894900	2.62097100	1.28000000
C	4.54791500	-2.79235900	0.65155600
C	3.71707700	3.13311400	0.04416200
C	-0.07329300	-3.56096000	-0.66664000
C	-0.48998100	1.83011800	-2.49856100
C	0.97801700	-3.78271300	0.29398700
C	2.82469300	-2.87209200	2.22260500
C	3.19460400	2.38373100	-2.23809200
C	4.15258800	2.63029300	-1.17755200
C	3.10486000	1.50037900	3.13408200
C	1.44421400	-2.66991800	2.48743200
C	5.16413900	1.59388700	-1.21863800
C	-0.95177900	0.55232500	-2.95814300
C	3.18567200	2.56001700	2.23589100
C	2.03429100	-0.51987500	3.59264200
C	0.01817800	2.97012200	-0.38122000
C	1.70129400	-1.98592700	-3.30777500
C	4.99906700	-0.67236500	-2.15834500
C	3.91313800	-2.68371700	-1.71816900
C	-0.80445400	-2.74593900	1.39538800
C	0.52239600	-3.25893000	1.56700100
C	-0.55437900	-2.25166900	-2.67522900
C	-1.61619200	-1.61789400	-1.99559500
C	-2.30636300	0.33918200	-0.89868100
C	2.68275900	-3.35203300	-1.46686500
C	-0.32031700	2.66852800	0.95449100
C	-1.18569800	-1.56968900	2.05107500
C	5.16215500	0.51017800	2.18499000
C	-1.97687200	-1.99398600	-0.66405000
C	2.63928900	0.31037600	-3.49928700
C	4.11267500	0.45607500	3.11351900
C	4.90331800	-1.90236100	1.74425300
C	1.97473600	3.04424300	1.59865900
C	3.59781200	1.19256800	-2.93302700
C	4.87962900	-2.44867100	-0.66187000
C	-1.97439700	-0.56275500	1.37729600
C	1.36310500	3.23714300	-0.79256500
C	0.61641200	1.41919700	2.90534000
C	-1.19352300	-2.92877300	-0.00009900
C	3.99537200	-1.59489200	-2.65314500
C	-0.46271000	0.50531800	2.76133900
C	1.30267400	0.80159700	-3.58574700
C	2.34839000	-3.72020700	-0.07937400
C	0.36005300	-1.46277900	-3.47593200
C	0.23222600	-3.23570400	-1.98874800
C	3.43372000	-0.79163700	3.38223600
C	0.90134900	1.98686800	-2.88766200
C	1.03583500	-1.44682200	3.19259300
C	0.16364800	-0.09376000	-3.62009800
C	1.82123500	0.90722800	3.44603500
C	-1.52198800	0.68000100	1.79571100
C	3.27810700	-3.40207100	0.95013400

C	1.62184600	-3.07464900	-2.37455300
C	5.24394000	1.61206900	1.25144400
C	5.69915000	1.08488100	-0.02755800
C	5.56088300	-1.20652800	-0.93278500
C	1.82054700	2.71803000	-2.08813400
C	3.82609700	-1.95842500	2.71182600
C	-1.87680200	1.57619200	-0.47058000
C	-2.67775800	-0.81564000	0.05526800
C	-1.68690100	1.95727200	1.00979700
C	0.69179800	2.54124900	1.94181400
C	2.30445300	3.40271300	0.24690200
C	5.56764900	-0.70053100	1.48419200
C	-0.92225700	2.29990300	-1.26111400
C	2.84486700	-1.13928700	-3.35363600
C	-0.25406100	-0.90984000	2.92056400
C	-4.23505300	-0.97671500	0.17256000
H	-4.62036900	-0.05149000	0.61432600
H	-4.64650200	-1.04927100	-0.83850100
C	-2.81942400	2.86387500	1.62216800
H	-2.57040000	3.00531700	2.67979200
H	-3.75381000	2.29615100	1.58563800
C	-4.69186700	-2.14696500	1.01114900
C	-4.97524500	-3.41910600	0.49264600
C	-4.83178400	-1.99012900	2.40160300
C	-5.40958000	-4.47283700	1.29886200
C	-5.24305100	-3.03416700	3.22835000
H	-4.60474700	-1.01950400	2.83449600
C	-5.53308400	-4.28347300	2.67517100
H	-5.63449000	-5.43541800	0.85112300
H	-5.33259100	-2.87230000	4.29940300
H	-5.85831700	-5.10732000	3.30549000
C	-2.99346700	4.22075000	0.97894000
C	-2.25494500	5.31355600	1.46916500
C	-3.83363900	4.47585300	-0.11441900
C	-2.34884100	6.58608000	0.90848000
H	-1.58779000	5.14623900	2.31112600
C	-3.95263200	5.74475100	-0.68519700
C	-3.20073500	6.80358300	-0.17703400
H	-1.75732900	7.40187600	1.31583400
H	-4.62393200	5.89662000	-1.52421100
H	-3.28622700	7.78964400	-0.62656100
Br	-4.95552700	3.09705400	-0.83724000
Br	-4.89011700	-3.75133300	-1.39739300

Ar = *o*-BrC_6H_4 neutral

C	5.89843400	-0.33146000	0.12924600
C	-1.82556200	-0.18455200	-2.16288800
C	4.80554100	0.70578500	-2.28911800
C	4.25929700	2.62011100	1.28481400
C	4.55032900	-2.78136000	0.66481400
C	3.70898300	3.13654600	0.04899100

C	-0.09032900	-3.54738900	-0.67300500
C	-0.49084400	1.83609700	-2.50809800
C	0.96870000	-3.75067100	0.30090100
C	2.81580500	-2.87297300	2.22692200
C	3.19310800	2.38980600	-2.23410300
C	4.14753200	2.63780400	-1.17073100
C	3.09872600	1.49489400	3.13854000
C	1.43498700	-2.67546600	2.49728600
C	5.16050700	1.60232300	-1.20895400
C	-0.95094000	0.55977900	-2.96880600
C	3.17051600	2.54957100	2.23741000
C	2.02319900	-0.52617000	3.58925300
C	0.01259300	2.97201400	-0.38727900
C	1.70283600	-1.97865500	-3.29663900
C	4.99945000	-0.66270100	-2.14696300
C	3.90758100	-2.67752000	-1.70650200
C	-0.81168400	-2.71825800	1.38144100
C	0.52314800	-3.25102100	1.56601700
C	-0.55504100	-2.23886600	-2.68085700
C	-1.62208400	-1.60961900	-2.01599800
C	-2.31398600	0.34410600	-0.91788400
C	2.67799000	-3.34533600	-1.46051800
C	-0.32636500	2.66057200	0.94507700
C	-1.19165000	-1.57434900	2.04093800
C	5.15706800	0.51125200	2.19369100
C	-1.98884300	-1.98571800	-0.68234100
C	2.64210900	0.31685900	-3.49312700
C	4.11025500	0.45721100	3.12021400
C	4.90979800	-1.90026700	1.75672900
C	1.96337600	3.03621800	1.59790300
C	3.59902200	1.19981900	-2.92751700
C	4.86321900	-2.43466700	-0.64178600
C	-1.98902400	-0.55476000	1.35539600
C	1.35849800	3.23981200	-0.79278400
C	0.60547100	1.40269100	2.89119500
C	-1.20847000	-2.91607100	-0.02068500
C	3.99210700	-1.58656700	-2.63440600
C	-0.46047500	0.48447900	2.75316400
C	1.30689600	0.80804400	-3.58551000
C	2.34084100	-3.70602500	-0.07357800
C	0.36198100	-1.45553800	-3.48010300
C	0.22929200	-3.22535500	-1.98747900
C	3.43404800	-0.79590900	3.38327200
C	0.90258100	1.99207800	-2.88978300
C	1.02590200	-1.45739900	3.20533500
C	0.16834000	-0.08747400	-3.62353300
C	1.81514500	0.88787200	3.43331600
C	-1.53250700	0.66615000	1.77109100
C	3.25948200	-3.37959600	0.96032200
C	1.62060700	-3.06970700	-2.37012100
C	5.23450900	1.61821800	1.25613000
C	5.69575200	1.09833100	-0.01901100

C	5.55506900	-1.18996200	-0.91798700
C	1.81914200	2.72368500	-2.08729800
C	3.82474700	-1.95137800	2.71659800
C	-1.88104700	1.57698200	-0.48507200
C	-2.69364100	-0.80987000	0.03341100
C	-1.69101800	1.95012900	0.99561700
C	0.67933700	2.53182200	1.93318600
C	2.29632500	3.40286300	0.25000300
C	5.56737600	-0.69446100	1.49855700
C	-0.92497900	2.30148300	-1.26982900
C	2.84565100	-1.13197500	-3.34209000
C	-0.26027700	-0.91587700	2.92701200
C	-4.24963800	-0.97301500	0.15741900
H	-4.63361600	-0.04392600	0.59095800
H	-4.65964200	-1.05114700	-0.85345100
C	-2.81957700	2.85162200	1.62439800
H	-2.56514300	2.98832400	2.68126300
H	-3.75304000	2.28255800	1.59003800
C	-4.70243500	-2.13969700	1.00428500
C	-4.94401000	-3.42388000	0.49362500
C	-4.89120700	-1.96234500	2.38583800
C	-5.38004600	-4.47440500	1.30279000
C	-5.30703100	-3.00286700	3.21507700
H	-4.71292600	-0.97721600	2.81011500
C	-5.55073500	-4.26616500	2.67147000
H	-5.57630900	-5.44715700	0.86399800
H	-5.44482000	-2.82592900	4.27822300
H	-5.88335100	-5.08556200	3.30289000
C	-2.99744000	4.21057700	0.98562700
C	-2.28369400	5.30971600	1.49559700
C	-3.83073900	4.45742400	-0.11505000
C	-2.39341700	6.58484400	0.94354000
H	-1.63033100	5.15115300	2.35032100
C	-3.96368700	5.72848200	-0.67711000
C	-3.23528900	6.79494300	-0.15097900
H	-1.82721500	7.40932700	1.36793800
H	-4.63030200	5.87824500	-1.51999500
H	-3.33537500	7.78344200	-0.59091700
Br	-4.92762400	3.06719500	-0.85255900
Br	-4.80554500	-3.77223300	-1.38969800

Ar = *m*-BrC_6H_4 anion

C	-5.39222600	-1.57631900	-1.40679400
C	1.05332300	0.05052600	3.14449000
C	-5.30344100	-0.15758700	1.06465400
C	-3.85056600	1.49958600	-2.39029200
C	-3.63405100	-3.80708500	-1.13544000
C	-3.81179800	2.20408100	-1.12667300
C	0.34042000	-3.67799100	1.66984600
C	-0.56703800	1.84627300	2.76888700
C	-0.29269200	-4.15636900	0.46711800

C	-1.48981900	-3.74199300	-2.05300200
C	-3.99084500	1.75901300	1.28385200
C	-4.56330500	1.74819400	-0.04845500
C	-2.00195400	0.42489000	-3.60488600
C	-0.13808500	-3.33751400	-1.89199700
C	-5.39025600	0.56663700	-0.18582200
C	-0.12549600	0.71040200	3.52607100
C	-2.51147100	1.53295200	-2.93542600
C	-0.59239100	-1.42346900	-3.41481100
C	-0.47924000	2.69618800	0.46437000
C	-2.39828500	-2.18940000	3.36718600
C	-5.26203400	-1.54810400	1.06312400
C	-3.84630400	-3.38460900	1.27420800
C	1.60982000	-2.94251900	-0.14653700
C	0.49145900	-3.68105100	-0.65548700
C	-0.04620800	-2.13344800	3.52568600
C	1.09765600	-1.39735400	3.14300800
C	1.85967100	0.54512500	2.05696300
C	-2.52791100	-3.85903600	1.52025300
C	0.32256900	2.33702700	-0.63948700
C	2.03786000	-1.78431700	-0.80549300
C	-4.11477300	-0.80270100	-3.22792500
C	1.91963100	-1.82406200	2.05281500
C	-3.63046600	-0.07272900	2.93084300
C	-2.81767900	-0.76545700	-3.75891200
C	-3.71445600	-3.09055900	-2.39741000
C	-1.65446100	2.26720700	-2.02221800
C	-4.44875400	0.58480600	1.97429000
C	-4.42580600	-3.40731200	-0.05612500
C	2.41966100	-0.60290000	-0.06280000
C	-1.90677300	2.77535500	0.38831200
C	0.25577100	0.77659400	-2.59136600
C	1.53061000	-2.93333500	1.31105300
C	-4.37228100	-2.24389800	1.97311100
C	1.33016100	0.06944500	-1.98713100
C	-2.47266100	0.63802900	3.36518600
C	-1.70552100	-4.28858300	0.37494900
C	-1.26794500	-1.43875800	3.87819500
C	-0.42708300	-3.29059600	2.76893600
C	-1.93562700	-1.90284000	-3.62162000
C	-2.01595300	1.80571200	2.67284000
C	0.32468500	-2.13284500	-2.59487700
C	-1.30708600	-0.04932100	3.88394700
C	-0.62373400	0.02610700	-3.40878100
C	1.97425200	0.50343100	-0.77072600
C	-2.27064000	-4.22363500	-0.92902500
C	-1.87502700	-3.32864600	2.66881200
C	-4.64302700	0.34997500	-2.53154500
C	-5.42766300	-0.12860700	-1.40184200
C	-5.31008300	-2.27532700	-0.19006300
C	-2.70003200	2.30182700	1.53070100
C	-2.37794200	-3.05349700	-2.95563900

C	1.43663500	1.64658600	1.34323300
C	2.66738200	-0.61631300	1.43571700
C	1.70576600	1.85552600	-0.15872100
C	-0.27762100	1.95472200	-1.86868200
C	-2.45948300	2.68588400	-0.90798200
C	-4.57388800	-1.99614100	-2.53026100
C	0.18952000	2.27343200	1.68169200
C	-3.58944700	-1.54319300	2.93064200
C	1.37194500	-1.36862200	-2.00760200
C	4.17994500	-0.54750200	1.84735100
H	4.57608200	0.40565200	1.47661600
H	4.22941000	-0.51513900	2.94262000
C	2.86018100	2.87434700	-0.48304400
H	2.92890700	2.94742500	-1.57473000
H	3.79661300	2.42463800	-0.13342800
C	5.02757300	-1.68788600	1.33102700
C	5.26882600	-2.82433000	2.11520300
C	5.56972100	-1.63249000	0.03865800
C	6.03090900	-3.88467700	1.62063400
H	4.85069000	-2.88031000	3.11709900
C	6.31461200	-2.70368600	-0.44499400
H	5.39274700	-0.76524600	-0.58890300
C	6.56478800	-3.83410000	0.33082200
H	6.20983800	-4.76036900	2.23975600
H	7.15931400	-4.65302400	-0.06087900
C	2.69555700	4.24946500	0.12352100
C	1.93060700	5.22688700	-0.53028900
C	3.27464900	4.56418500	1.36123300
C	1.74057000	6.46984400	0.06744500
H	1.47449700	5.00931500	-1.49079300
C	3.09237100	5.82252200	1.93752700
H	3.86953500	3.81471700	1.87723700
C	2.31738500	6.79089600	1.29500500
H	3.54983500	6.05280100	2.89661900
H	2.16648400	7.77036500	1.73699000
Br	0.70694100	7.79226900	-0.84962900
Br	7.07377600	-2.58360000	-2.19601700

Ar = *m*-BrC_6H_4 neutral

C	-5.36428400	-1.58262600	-1.43086000
C	1.04223600	0.06415800	3.17867400
C	-5.29808700	-0.15947600	1.03585600
C	-3.82005400	1.48203500	-2.40805600
C	-3.61620400	-3.81213600	-1.15035300
C	-3.79080400	2.19418700	-1.14725500
C	0.35286900	-3.66358400	1.70101100
C	-0.57910100	1.85333400	2.77854800
C	-0.27795300	-4.13059300	0.47832500
C	-1.45819700	-3.75653800	-2.04280800
C	-3.98966800	1.75785600	1.26191700
C	-4.55085600	1.74443900	-0.07541600

C	-1.96661900	0.40017000	-3.60975800
C	-0.10461400	-3.35632300	-1.88041200
C	-5.37647500	0.56220800	-0.21715500
C	-0.14290600	0.72087700	3.54154900
C	-2.47264400	1.50646100	-2.93956800
C	-0.55467800	-1.44599000	-3.39858500
C	-0.47375800	2.69116400	0.47071300
C	-2.40661800	-2.18319600	3.35810500
C	-5.25646900	-1.54838200	1.03556000
C	-3.83471700	-3.38527700	1.26171100
C	1.61827900	-2.92048200	-0.10949700
C	0.50363600	-3.68330700	-0.63412200
C	-0.05993300	-2.11757100	3.54404200
C	1.08608900	-1.38412900	3.18243100
C	1.85729700	0.55319400	2.09582700
C	-2.51989400	-3.85694200	1.52127300
C	0.33449400	2.31894600	-0.62260800
C	2.05223100	-1.79579200	-0.76753900
C	-4.08085600	-0.82202600	-3.24615700
C	1.91855900	-1.81196200	2.09622200
C	-3.64019400	-0.06933900	2.91264300
C	-2.78412900	-0.78556500	-3.76957500
C	-3.69303100	-3.10821600	-2.41401900
C	-1.62600000	2.24535900	-2.02278500
C	-4.45254600	0.58583200	1.95063400
C	-4.39504600	-3.40406100	-0.07713400
C	2.43194500	-0.59694000	-0.01435900
C	-1.89962600	2.77058700	0.38051900
C	0.28497500	0.74772900	-2.56437300
C	1.53822500	-2.92002600	1.36016200
C	-4.36573700	-2.24219000	1.94711400
C	1.34728700	0.03648700	-1.96223400
C	-2.48861800	0.64389800	3.35645800
C	-1.68943700	-4.28111900	0.38193900
C	-1.28529900	-1.42908500	3.88741600
C	-0.43097100	-3.28023300	2.78402100
C	-1.90582800	-1.92713000	-3.61935900
C	-2.02685100	1.80933100	2.66670600
C	0.36337300	-2.15833200	-2.58608100
C	-1.32699700	-0.04103500	3.88694600
C	-0.59326900	-0.00922300	-3.38731700
C	1.98893700	0.48492200	-0.72381600
C	-2.23706400	-4.21184100	-0.92752500
C	-1.87786500	-3.32544500	2.67325800
C	-4.61168100	0.33823100	-2.55124100
C	-5.40777400	-0.13188900	-1.43112300
C	-5.29118600	-2.27214900	-0.21804200
C	-2.70187400	2.30230100	1.51740900
C	-2.34958900	-3.06499400	-2.95636500
C	1.43476100	1.64607100	1.37084900
C	2.67399800	-0.60814300	1.48603100
C	1.71214900	1.84247200	-0.12959200

C	-0.25147100	1.93327600	-1.85277800
C	-2.44024100	2.67447900	-0.92032300
C	-4.54605200	-2.01003000	-2.55494400
C	0.18554900	2.27301500	1.69458600
C	-3.59462600	-1.53907500	2.91251600
C	1.40037500	-1.38690200	-1.99106400
C	4.18674100	-0.54937300	1.89712700
H	4.58026000	0.41303100	1.54963600
H	4.23541600	-0.54055500	2.99212600
C	2.86859000	2.85808700	-0.46333000
H	2.94491500	2.91920500	-1.55522700
H	3.80350400	2.41550400	-0.10198600
C	5.02859100	-1.67972100	1.34712000
C	5.26076700	-2.84218600	2.09424000
C	5.57287600	-1.58278900	0.05885100
C	6.01456000	-3.89054600	1.56163900
H	4.85296100	-2.92667100	3.09853000
C	6.30447600	-2.64392400	-0.46749900
H	5.41749600	-0.68740900	-0.53482800
C	6.54323400	-3.80162400	0.27201300
H	6.19480100	-4.78451800	2.15289800
H	7.13209400	-4.61153500	-0.14579100
C	2.68655200	4.23751700	0.12998100
C	1.89987000	5.19193800	-0.52972900
C	3.27208700	4.57420400	1.35806000
C	1.68450100	6.43677600	0.05672100
H	1.44742400	4.96075500	-1.48901000
C	3.06987800	5.83583700	1.92126600
H	3.89211600	3.84589300	1.87500400
C	2.26784100	6.77945000	1.27597300
H	3.53595100	6.08852700	2.87001200
H	2.10329700	7.76054900	1.70901800
Br	0.61573800	7.72059500	-0.86441600
Br	7.05806600	-2.46850900	-2.21088700

Ar = *p*-BrC_6H_4 anion

C	-3.57125000	-4.71065500	-0.77793200
C	0.72724900	1.15897900	2.68213900
C	-4.27670100	-3.11616600	1.47815800
C	-4.23218900	-1.54213000	-2.30536000
C	-0.81494500	-5.38367600	-0.47518000
C	-4.58644300	-0.74765100	-1.14891600
C	2.36375000	-2.45499200	1.76116200
C	-1.65934400	1.55448300	2.31222500
C	2.10940600	-3.41180600	0.71393900
C	0.82396900	-4.22272400	-1.66217000
C	-4.38032800	-0.79247700	1.29994200
C	-4.87320300	-1.36694800	0.06324200
C	-2.14955000	-1.50553300	-3.61222700
C	1.66186400	-3.07808400	-1.72511600
C	-4.82305500	-2.81057700	0.17300300

C	-0.59723500	1.04874900	3.13340500
C	-3.20346100	-0.81792800	-3.01878700
C	0.09520500	-2.09738300	-3.39092900
C	-2.17714500	1.88263700	-0.06803800
C	-0.66239300	-2.60851400	3.61126700
C	-3.40461300	-4.18826200	1.63448300
C	-1.16151200	-4.76255300	1.87490100
C	2.87201300	-1.43610400	-0.27722300
C	2.41129300	-2.76617200	-0.54832100
C	1.18171200	-1.14716700	3.45576900
C	1.63628000	0.04297000	2.84517800
C	1.03632000	1.84010700	1.45022800
C	0.18284800	-4.31632500	2.00339800
C	-1.35703500	1.88329600	-1.21605800
C	2.49134100	-0.38232500	-1.11622300
C	-3.07932100	-3.65699000	-2.82595400
C	2.51430700	0.00544000	1.71680500
C	-2.93598200	-1.74132100	3.09144600
C	-2.08551100	-2.95214400	-3.51974000
C	-1.35241300	-5.08143200	-1.79106800
C	-2.93457800	0.42364100	-2.31575800
C	-4.01454000	-1.87026300	2.17661100
C	-1.65225800	-5.35122600	0.64255500
C	2.10731800	0.90207200	-0.57314600
C	-3.36305700	1.08624800	0.03131100
C	-0.53162400	0.28004400	-2.94708900
C	2.85094300	-1.22628000	1.16715200
C	-2.24671500	-4.05578600	2.49818300
C	0.77040000	0.45959700	-2.40626600
C	-2.42839100	-0.42252300	3.28616300
C	1.06057900	-4.36607200	0.82055000
C	-0.19892800	-1.26096100	3.87973300
C	1.55321100	-2.41419200	2.89629400
C	-0.69184100	-3.30443900	-3.36557500
C	-2.79197200	0.65001800	2.40907400
C	1.28015500	-1.97523800	-2.61799700
C	-1.06835200	-0.18720000	3.72753700
C	-0.80512700	-0.97163400	-3.55049500
C	1.06145900	1.39003900	-1.34237300
C	0.52915800	-4.87156300	-0.39849800
C	0.41981100	-3.31688600	2.98899500
C	-4.17368900	-2.94108500	-2.20753000
C	-4.47330700	-3.58904100	-0.93828600
C	-3.04416800	-5.00427000	0.49163400
C	-3.67207900	0.44035900	1.31372300
C	-0.32821200	-4.35884200	-2.51744100
C	0.01104900	2.33812000	0.67341300
C	2.36165000	1.29438000	0.87178700
C	0.05113300	2.40307900	-0.86466600
C	-1.64430800	1.01730200	-2.30464300
C	-3.79241000	0.46845100	-1.16374200
C	-2.70212200	-4.75023900	-1.94026500

C	-1.35014800	2.15363400	1.09434400
C	-2.01563000	-2.87714100	3.25898500
C	1.67068900	-0.65357900	-2.26248300
C	3.53517100	2.31569200	1.07602500
H	3.27150700	3.22794000	0.52706900
H	3.56684400	2.57835300	2.14070300
C	0.35047200	3.82717500	-1.45968000
H	0.34444000	3.72508400	-2.55120900
H	1.37638700	4.08459800	-1.17127900
C	4.89613400	1.82973800	0.63179700
C	5.76180200	1.19468900	1.53304600
C	5.32144000	1.98904000	-0.69505300
C	7.01777800	0.73431400	1.13261600
H	5.45112500	1.05264500	2.56534400
C	6.57302200	1.53562100	-1.11534200
H	4.66269400	2.46724900	-1.41534500
C	7.40901900	0.91042000	-0.19266500
H	7.67822800	0.24479400	1.84113900
H	6.88937700	1.66460100	-2.14539800
C	-0.59062000	4.93393900	-1.04119900
C	-1.75060800	5.21486400	-1.77759700
C	-0.32953800	5.70732500	0.09910400
C	-2.62451700	6.23561600	-1.39743200
H	-1.97800700	4.62718600	-2.66373100
C	-1.18916000	6.73338200	0.49616800
H	0.56158200	5.50757300	0.68955900
C	-2.33138900	6.98592900	-0.26063000
H	-3.51709900	6.44261900	-1.97901600
H	-0.97141000	7.32622900	1.37866100
Br	9.13557800	0.30579300	-0.75039900
Br	-3.50123200	8.40911500	0.25351700

Ar = *p*-BrC_6H_4 neutral

C	5.89843400	-0.33146000	0.12924600
C	-1.82556200	-0.18455200	-2.16288800
C	4.80554100	0.70578500	-2.28911800
C	4.25929700	2.62011100	1.28481400
C	4.55032900	-2.78136000	0.66481400
C	3.70898300	3.13654600	0.04899100
C	-0.09032900	-3.54738900	-0.67300500
C	-0.49084400	1.83609700	-2.50809800
C	0.96870000	-3.75067100	0.30090100
C	2.81580500	-2.87297300	2.22692200
C	3.19310800	2.38980600	-2.23410300
C	4.14753200	2.63780400	-1.17073100
C	3.09872600	1.49489400	3.13854000
C	1.43498700	-2.67546600	2.49728600
C	5.16050700	1.60232300	-1.20895400
C	-0.95094000	0.55977900	-2.96880600
C	3.17051600	2.54957100	2.23741000
C	2.02319900	-0.52617000	3.58925300

C	0.01259300	2.97201400	-0.38727900
C	1.70283600	-1.97865500	-3.29663900
C	4.99945000	-0.66270100	-2.14696300
C	3.90758100	-2.67752000	-1.70650200
C	-0.81168400	-2.71825800	1.38144100
C	0.52314800	-3.25102100	1.56601700
C	-0.55504100	-2.23886600	-2.68085700
C	-1.62208400	-1.60961900	-2.01599800
C	-2.31398600	0.34410600	-0.91788400
C	2.67799000	-3.34533600	-1.46051800
C	-0.32636500	2.66057200	0.94507700
C	-1.19165000	-1.57434900	2.04093800
C	5.15706800	0.51125200	2.19369100
C	-1.98884300	-1.98571800	-0.68234100
C	2.64210900	0.31685900	-3.49312700
C	4.11025500	0.45721100	3.12021400
C	4.90979800	-1.90026700	1.75672900
C	1.96337600	3.03621800	1.59790300
C	3.59902200	1.19981900	-2.92751700
C	4.86321900	-2.43466700	-0.64178600
C	-1.98902400	-0.55476000	1.35539600
C	1.35849800	3.23981200	-0.79278400
C	0.60547100	1.40269100	2.89119500
C	-1.20847000	-2.91607100	-0.02068500
C	3.99210700	-1.58656700	-2.63440600
C	-0.46047500	0.48447900	2.75316400
C	1.30689600	0.80804400	-3.58551000
C	2.34084100	-3.70602500	-0.07357800
C	0.36198100	-1.45553800	-3.48010300
C	0.22929200	-3.22535500	-1.98747900
C	3.43404800	-0.79590900	3.38327200
C	0.90258100	1.99207800	-2.88978300
C	1.02590200	-1.45739900	3.20533500
C	0.16834000	-0.08747400	-3.62353300
C	1.81514500	0.88787200	3.43331600
C	-1.53250700	0.66615000	1.77109100
C	3.25948200	-3.37959600	0.96032200
C	1.62060700	-3.06970700	-2.37012100
C	5.23450900	1.61821800	1.25613000
C	5.69575200	1.09833100	-0.01901100
C	5.55506900	-1.18996200	-0.91798700
C	1.81914200	2.72368500	-2.08729800
C	3.82474700	-1.95137800	2.71659800
C	-1.88104700	1.57698200	-0.48507200
C	-2.69364100	-0.80987000	0.03341100
C	-1.69101800	1.95012900	0.99561700
C	0.67933700	2.53182200	1.93318600
C	2.29632500	3.40286300	0.25000300
C	5.56737600	-0.69446100	1.49855700
C	-0.92497900	2.30148300	-1.26982900
C	2.84565100	-1.13197500	-3.34209000
C	-0.26027700	-0.91587700	2.92701200

C	-4.24963800	-0.97301500	0.15741900
H	-4.63361600	-0.04392600	0.59095800
H	-4.65964200	-1.05114700	-0.85345100
C	-2.81957700	2.85162200	1.62439800
H	-2.56514300	2.98832400	2.68126300
H	-3.75304000	2.28255800	1.59003800
C	-4.70243500	-2.13969700	1.00428500
C	-4.94401000	-3.42388000	0.49362500
C	-4.89120700	-1.96234500	2.38583800
C	-5.38004600	-4.47440500	1.30279000
C	-5.30703100	-3.00286700	3.21507700
H	-4.71292600	-0.97721600	2.81011500
C	-5.55073500	-4.26616500	2.67147000
H	-5.57630900	-5.44715700	0.86399800
H	-5.44482000	-2.82592900	4.27822300
H	-5.88335100	-5.08556200	3.30289000
C	-2.99744000	4.21057700	0.98562700
C	-2.28369400	5.30971600	1.49559700
C	-3.83073900	4.45742400	-0.11505000
C	-2.39341700	6.58484400	0.94354000
H	-1.63033100	5.15115300	2.35032100
C	-3.96368700	5.72848200	-0.67711000
C	-3.23528900	6.79494300	-0.15097900
H	-1.82721500	7.40932700	1.36793800
H	-4.63030200	5.87824500	-1.51999500
H	-3.33537500	7.78344200	-0.59091700
Br	-4.92762400	3.06719500	-0.85255900
Br	-4.80554500	-3.77223300	-1.38969800

Cartesian coordinates for 7,23–$(ArCH_2)_2C_{70}$ anions and neutrals.

Ar = Ph anion

C	1.21979400	3.19284100	0.07923300
C	0.04437700	3.97545900	0.11087000
C	-0.80713600	4.00148600	-1.05144600
C	-0.43979400	3.26949500	-2.18678400
C	-0.81428500	3.93259600	1.28100500
C	-2.19519900	4.00071800	-0.60705900
C	-2.19953200	3.96236000	0.83522900
C	-1.42905700	2.51536000	-2.92289900
C	-0.45499300	3.15352600	2.38260500
C	-0.81467400	1.29661600	-3.40103500
C	0.76746000	2.37012000	2.35125900
C	-3.16071300	3.18801200	1.51576600
C	1.57943200	2.38099100	1.21672300
C	-3.14948800	3.26242500	-1.33122300
C	-4.13206300	2.46416700	-0.62768200
C	0.53566100	1.12909700	3.02386200
C	-0.83820700	1.11929600	3.48307900
C	-4.13690000	2.42711900	0.76313400
C	-2.78069600	2.38161800	2.64891900
C	1.19328500	-0.06114300	2.61219600
C	-3.51797900	1.27765800	-2.53318700
C	-2.76173300	2.51592400	-2.50353600
C	-1.57176600	-0.09122300	3.53201300
C	-2.97095900	0.08264900	-3.08090200
C	-1.57176800	0.09122200	-3.53201300
C	-4.37442300	1.24765900	-1.38216200
C	-3.52588100	1.13978200	2.60428300
C	-4.37870900	1.16956500	1.44733400
C	-4.69272700	-0.01977300	0.73575000
C	-4.69272800	0.01977100	-0.73574800
C	-4.37870900	-1.16956700	-1.44733200
C	-3.52588100	-1.13978400	-2.60428100
C	-4.37442100	-1.24766200	1.38216400
C	-3.51797700	-1.27766000	2.53318800
C	-2.97095700	-0.08265100	3.08090300
C	-0.83820800	-1.11929600	-3.48307900
C	0.55051900	-1.28306000	2.96470600
C	-0.81467200	-1.29661600	3.40103500
C	1.62140500	-2.49190400	1.09716500
C	0.78808800	-2.49950400	2.20108000
C	-1.42905400	-2.51536100	2.92289900
C	-0.43979100	-3.26949500	2.18678300
C	-1.44810600	-2.36141600	-3.07690400
C	-2.78069600	-2.38161900	-2.64891800
C	-4.13689900	-2.42712100	-0.76313300
C	-4.13206200	-2.46416900	0.62768300
C	-3.14948600	-3.26242600	1.33122400
C	-2.19519700	-4.00071900	0.60705900
C	-2.19953000	-3.96236100	-0.83522800

C	-3.16071200	-3.18801400	-1.51576500
C	-0.80713400	-4.00148600	1.05144600
C	-2.76173100	-2.51592600	2.50353700
C	-1.44810600	2.36141600	3.07690400
C	1.21979600	-3.19284000	-0.07923500
C	0.04437900	-3.97545900	-0.11087100
C	-0.81428300	-3.93259600	-1.28100500
C	-0.45499200	-3.15352600	-2.38260500
C	4.03444700	1.59146400	-1.12713500
H	4.62199200	0.71003300	-0.84932700
H	4.07245200	1.66178100	-2.22103100
C	4.65504900	2.83093700	-0.51916100
C	4.60779300	4.06222700	-1.19052200
C	5.29802200	2.77982900	0.72690000
H	4.11245100	4.12233900	-2.15695000
C	5.17942400	5.20878800	-0.63338800
C	5.87256500	3.92281400	1.28881600
H	5.34464400	1.83583100	1.26523200
H	5.12614900	6.15310800	-1.17030000
C	5.81405000	5.14330700	0.61021600
H	6.36326300	3.85920600	2.25732900
H	6.25827700	6.03488900	1.04654900
C	4.03444800	-1.59146100	1.12713300
H	4.62199300	-0.71003000	0.84932300
H	4.07245400	-1.66177700	2.22102900
C	4.65505100	-2.83093400	0.51916000
C	4.60779600	-4.06222400	1.19052300
C	5.29802300	-2.77982800	-0.72690200
H	4.11245400	-4.12233600	2.15695100
C	5.17942800	-5.20878500	0.63338900
C	5.87256700	-3.92281300	-1.28881600
H	5.34464500	-1.83583000	-1.26523400
H	5.12615300	-6.15310500	1.17030300
C	5.81405300	-5.14330500	-0.61021500
H	6.36326500	-3.85920600	-2.25732900
H	6.25828000	-6.03488800	-1.04654600
C	2.23715200	1.18245500	0.77189900
C	2.08106800	-0.01164200	1.44978000
C	2.53220100	-1.30464100	0.74758500
C	2.23715200	-1.18245300	-0.77190100
C	1.57943300	-2.38099000	-1.21672400
C	0.76746000	-2.37011900	-2.35126000
C	0.53566000	-1.12909700	-3.02386300
C	1.19328400	0.06114400	-2.61219700
C	0.55051700	1.28306100	-2.96470700
C	0.78808500	2.49950500	-2.20108100
C	1.62140300	2.49190500	-1.09716600
C	2.53220000	1.30464300	-0.74758700
C	2.08106800	0.01164300	-1.44978200

Ar = Ph neutral

C	1.21852000	3.19337800	0.07663200
C	0.04381400	3.96310800	0.10464300
C	-0.80094100	4.00603200	-1.06479400
C	-0.42985400	3.27271900	-2.19660600
C	-0.80766100	3.93966900	1.28092900
C	-2.18422100	3.99538600	-0.62075300
C	-2.18879900	3.95722400	0.83239700
C	-1.41907300	2.51230200	-2.92895200
C	-0.44544000	3.16353900	2.38249600
C	-0.80242300	1.28590400	-3.40631000
C	0.77248200	2.37871300	2.35121800
C	-3.14416000	3.18889300	1.50464900
C	1.57931100	2.38194900	1.21723900
C	-3.13278400	3.25829300	-1.33463500
C	-4.11693100	2.46124400	-0.63351700
C	0.54058300	1.13537100	3.02825100
C	-0.82696600	1.12480000	3.48823800
C	-4.12304900	2.42676600	0.75632700
C	-2.76298000	2.38249400	2.64742900
C	1.19828200	-0.05287800	2.61406400
C	-3.50335900	1.26991100	-2.54288500
C	-2.74243700	2.50696900	-2.51208900
C	-1.56209900	-0.08042600	3.54189200
C	-2.95984300	0.07430100	-3.09059600
C	-1.56213100	0.08041400	-3.54188900
C	-4.34652100	1.24246000	-1.38672200
C	-3.51318200	1.14541200	2.60947100
C	-4.35549900	1.17203800	1.44496900
C	-4.66837800	-0.01691800	0.73513900
C	-4.66838500	0.01686600	-0.73510800
C	-4.35549800	-1.17208600	-1.44494100
C	-3.51319100	-1.14544900	-2.60945000
C	-4.34649200	-1.24250800	1.38675000
C	-3.50332000	-1.26994900	2.54290500
C	-2.95981400	-0.07433100	3.09061200
C	-0.82698300	-1.12480300	-3.48824200
C	0.54664900	-1.27102700	2.96069600
C	-0.80237600	-1.28590700	3.40630700
C	1.61713900	-2.48515000	1.10238500
C	0.79252900	-2.50126500	2.20472400
C	-1.41901600	-2.51231200	2.92895400
C	-0.42979400	-3.27271700	2.19659900
C	-1.43939200	-2.37068400	-3.07712400
C	-2.76297400	-2.38252200	-2.64741500
C	-4.12302600	-2.42681200	-0.75630100
C	-4.11689400	-2.46128900	0.63354300
C	-3.13273200	-3.25832600	1.33465200
C	-2.18416500	-3.99540600	0.62076100
C	-2.18875800	-3.95724500	-0.83238900
C	-3.14413400	-3.18892600	-1.50463200
C	-0.80088200	-4.00603200	1.06478900
C	-2.74238400	-2.50699700	2.51210300

C	-1.43939400	2.37067400	3.07712600
C	1.21855900	-3.19335400	-0.07665600
C	0.04386100	-3.96309900	-0.10465500
C	-0.80762200	-3.93967300	-1.28093400
C	-0.44542100	-3.16353700	-2.38250200
C	4.03299200	1.60239900	-1.12308100
H	4.62491000	0.72805900	-0.83378800
H	4.07783900	1.66373500	-2.21694200
C	4.63013700	2.85486200	-0.51718300
C	4.58932400	4.07474700	-1.20896600
C	5.24565400	2.82358500	0.74312700
H	4.12642500	4.11677400	-2.19258500
C	5.13817200	5.23355700	-0.65429900
C	5.79675200	3.97939400	1.30204800
H	5.29756200	1.88585500	1.29217800
H	5.09722800	6.16828800	-1.20785400
C	5.74202800	5.18966200	0.60527000
H	6.27138500	3.93287000	2.27897900
H	6.17198900	6.08953600	1.03747300
C	4.03300800	-1.60235700	1.12305700
H	4.62493500	-0.72802600	0.83375300
H	4.07786300	-1.66367800	2.21691900
C	4.63016200	-2.85482900	0.51717600
C	4.58933500	-4.07471300	1.20896000
C	5.24570800	-2.82355400	-0.74312000
H	4.12641200	-4.11674100	2.19256800
C	5.13819800	-5.23352200	0.65430700
C	5.79681900	-3.97936200	-1.30202700
H	5.29762300	-1.88582500	-1.29217200
H	5.09724500	-6.16825300	1.20786400
C	5.74208100	-5.18962900	-0.60524800
H	6.27147200	-3.93283900	-2.27894800
H	6.17205300	-6.08950400	-1.03743900
C	2.23492000	1.18233100	0.76977400
C	2.08142100	-0.00968500	1.44805200
C	2.53030800	-1.30310000	0.74949600
C	2.23494100	-1.18230000	-0.76981400
C	1.57933600	-2.38192500	-1.21726800
C	0.77249300	-2.37869800	-2.35123700
C	0.54057000	-1.13535800	-3.02826700
C	1.19825600	0.05290000	-2.61408300
C	0.54660600	1.27104100	-2.96070900
C	0.79247800	2.50128100	-2.20474000
C	1.61710400	2.48518200	-1.10241400
C	2.53027900	1.30313500	-0.74952000
C	2.08140700	0.00971500	-1.44808400

Ar = *o*-BrC_6H_4 anion

C	-0.25907200	3.36236300	-0.19820600
C	0.98600400	3.98252900	-0.44127800
C	1.96452400	4.01843700	0.61602200

C	1.65107300	3.45978600	1.86046900
C	1.69104800	3.70951000	-1.68072700
C	3.28138900	3.79318500	0.03332800
C	3.11269000	3.60805200	-1.38763700
C	2.62488600	2.66641200	2.57455700
C	1.11623200	2.87520300	-2.64118700
C	1.93314500	1.59333600	3.25321800
C	-0.17758200	2.26303500	-2.39360200
C	3.89070200	2.65053200	-2.06940000
C	-0.84554100	2.49313700	-1.19044100
C	4.22214400	3.01820000	0.73614300
C	5.01547500	2.03152900	0.03167300
C	-0.17235700	0.94013900	-2.93777700
C	1.12832800	0.70621300	-3.53074700
C	4.85309500	1.85205400	-1.33859900
C	3.28812900	1.78722500	-3.05420300
C	-0.90956500	-0.10685900	-2.32128600
C	4.49459900	1.13708700	2.11564200
C	3.89088800	2.45268300	2.02166900
C	1.70547600	-0.58699200	-3.51482000
C	3.87968100	0.08527700	2.85212100
C	2.55414700	0.32008800	3.44264400
C	5.20158500	0.87866500	0.89329600
C	3.88499500	0.47112400	-2.94452800
C	4.86373100	0.50977300	-1.89237500
C	5.12053300	-0.63047200	-1.08377100
C	5.29695800	-0.43998100	0.36536800
C	4.93184500	-1.49938000	1.23955800
C	4.22916600	-1.24096900	2.46712600
C	4.58608600	-1.86674200	-1.54541000
C	3.60361100	-1.90434900	-2.58992900
C	3.13871800	-0.71183900	-3.21350000
C	1.68384100	-0.78462700	3.61174900
C	-0.45755600	-1.43042900	-2.59211400
C	0.83441300	-1.66481800	-3.16538000
C	-1.43881200	-2.29489200	-0.49842500
C	-0.74027800	-2.51818000	-1.66912200
C	1.35496900	-2.89717800	-2.61392100
C	0.37810100	-3.43591300	-1.69463900
C	2.09331900	-2.12966800	3.29280600
C	3.35566000	-2.36542800	2.73443800
C	4.46695000	-2.77901900	0.73579400
C	4.29428000	-2.95819100	-0.63314400
C	3.15070900	-3.69225800	-1.13286700
C	2.20775800	-4.22205500	-0.23266300
C	2.38577200	-4.03771700	1.18751600
C	3.50233400	-3.32548700	1.66862800
C	0.78717000	-4.09121700	-0.52728000
C	2.71750200	-3.02608200	-2.33779800
C	1.92206400	1.89547600	-3.33913000
C	-0.98546100	-2.91663300	0.70305400
C	0.08630800	-3.83661000	0.70570400

C	1.07498500	-3.78296200	1.76758600
C	0.94039700	-2.85461300	2.80166600
C	-3.07740700	2.28631400	1.48455500
H	-3.83822500	1.54107100	1.23919500
H	-3.01090700	2.32583500	2.57777300
C	-3.49539400	3.65529400	0.99151500
C	-3.11136500	4.79077100	1.72871700
C	-4.23945400	3.89153500	-0.17268000
H	-2.52699700	4.64242700	2.63308400
C	-3.44813100	6.08400400	1.33382200
C	-4.60185400	5.17743200	-0.57956500
H	-3.12530200	6.93289100	1.93079400
C	-4.19539000	6.28025600	0.17021900
H	-5.18945700	5.30945700	-1.48220800
H	-4.46759500	7.28182600	-0.15279800
C	-3.71857800	-1.09286300	-0.36264300
H	-4.14700100	-0.10415800	-0.18539300
H	-3.91471100	-1.33704200	-1.41101100
C	-4.40727200	-2.08367700	0.54829100
C	-4.66931400	-3.41972500	0.21126200
C	-4.82563400	-1.66622300	1.82472100
C	-5.32943300	-4.29191900	1.07963400
C	-5.46864000	-2.52440000	2.71457400
H	-4.63581400	-0.63738700	2.11855100
H	-5.52383600	-5.31358100	0.76972100
C	-5.71891500	-3.84726800	2.34253600
H	-5.77089000	-2.16122500	3.69347800
H	-6.22172500	-4.52950500	3.02328600
C	-1.58314100	1.44275600	-0.54341200
C	-1.64559600	0.17467200	-1.08908300
C	-2.15763000	-0.97113400	-0.19688500
C	-1.67085200	-0.73072600	1.25676100
C	-1.11108500	-1.95156600	1.76814100
C	-0.17773800	-1.92801500	2.80467100
C	0.27376600	-0.66430100	3.29970300
C	-0.28364700	0.55174800	2.82189000
C	0.53249100	1.71091900	2.96573700
C	0.35245100	2.85926900	2.09119200
C	-0.59783100	2.84515100	1.08679400
C	-1.67908100	1.75949100	0.97403600
C	-1.30223700	0.49701300	1.77135200
Br	-4.90812400	2.43742800	-1.23040200
Br	-4.22996700	-4.09846900	-1.52802100

Ar = *o*-BrC_6H_4 neutral

C	-0.24361300	3.36601700	-0.18354700
C	1.00179500	3.96792700	-0.42538800
C	1.98107700	4.01525300	0.63398000
C	1.66500600	3.45591300	1.87614600
C	1.69498900	3.71256100	-1.67537200
C	3.28850300	3.77540500	0.04808700

C	3.11222500	3.59179200	-1.38318500
C	2.63623500	2.64939300	2.58191900
C	1.10983000	2.88533900	-2.63418900
C	1.93806700	1.57038700	3.26137100
C	-0.18206000	2.27780400	-2.38314400
C	3.87846700	2.63894700	-2.06108900
C	-0.84028600	2.50157800	-1.17706800
C	4.22127600	2.99525000	0.73642300
C	5.00868700	2.00711800	0.03014300
C	-0.18676500	0.95372600	-2.93411900
C	1.10465900	0.71395100	-3.53271600
C	4.84161000	1.83214900	-1.33903300
C	3.26577000	1.77954000	-3.05440200
C	-0.92530000	-0.08816300	-2.31290500
C	4.49167500	1.10684100	2.11914000
C	3.88848700	2.42506200	2.02800900
C	1.67680200	-0.57784600	-3.52569100
C	3.87753000	0.05592200	2.85574100
C	2.55661800	0.29397400	3.45188500
C	5.17852800	0.85070500	0.88993600
C	3.86056800	0.46397200	-2.95570200
C	4.83476600	0.49477700	-1.89885300
C	5.08703700	-0.64779100	-1.09470500
C	5.26860800	-0.46632000	0.35348800
C	4.90185800	-1.52505000	1.22544900
C	4.21692500	-1.26893000	2.46281600
C	4.54122600	-1.87854500	-1.56125100
C	3.56647900	-1.90903700	-2.60877700
C	3.10857700	-0.71279100	-3.22858300
C	1.67975800	-0.80141500	3.61655200
C	-0.47238000	-1.41093600	-2.58417400
C	0.79963300	-1.65124100	-3.17006700
C	-1.45117800	-2.27963900	-0.49645900
C	-0.76783600	-2.51146100	-1.66767100
C	1.31692600	-2.89450000	-2.62315600
C	0.33946300	-3.43606500	-1.70386500
C	2.08252700	-2.15330200	3.28930700
C	3.33302600	-2.38490400	2.72417000
C	4.43833900	-2.80112800	0.71573500
C	4.25881800	-2.97348300	-0.65219200
C	3.10784500	-3.69889600	-1.14668200
C	2.17056300	-4.22690100	-0.25486500
C	2.35633200	-4.04423100	1.17534600
C	3.47190500	-3.34603900	1.64731600
C	0.75263100	-4.09755100	-0.54279900
C	2.67160000	-3.02446200	-2.35435000
C	1.90852400	1.90205100	-3.33798900
C	-0.99973400	-2.91186400	0.70545700
C	0.06730200	-3.82619900	0.69742200
C	1.05206300	-3.79657300	1.76454100
C	0.92295700	-2.87202200	2.80154300
C	-3.05874600	2.31265600	1.50542800

H	-3.82631400	1.57318800	1.26446600
H	-2.98896000	2.35523600	2.59805200
C	-3.46083300	3.68384800	1.00344700
C	-3.09313300	4.81849400	1.74956700
C	-4.18424600	3.91612900	-0.17487000
H	-2.53642300	4.67270800	2.67196700
C	-3.42154500	6.11112900	1.34488500
C	-4.53314000	5.20151300	-0.59367400
H	-3.11927600	6.96103500	1.95044500
C	-4.14296000	6.30451800	0.16481400
H	-5.10489700	5.33374800	-1.50619700
H	-4.41090500	7.30510900	-0.16328000
C	-3.72741800	-1.07674300	-0.34127200
H	-4.15064500	-0.08916500	-0.14729700
H	-3.93101200	-1.30489900	-1.39168600
C	-4.40691500	-2.08143000	0.56195300
C	-4.65411300	-3.41655100	0.20944500
C	-4.83373700	-1.67716300	1.83922900
C	-5.31117100	-4.30150700	1.06667000
C	-5.47294300	-2.54950400	2.71817400
H	-4.66363400	-0.64672600	2.14062300
H	-5.50101600	-5.32057100	0.74609400
C	-5.70854000	-3.87092400	2.33218800
H	-5.78905800	-2.19763300	3.69640000
H	-6.21222200	-4.56215800	3.00240900
C	-1.57948600	1.45376900	-0.52659000
C	-1.65035100	0.18865100	-1.07399500
C	-2.16423000	-0.95694400	-0.18605700
C	-1.67089100	-0.72279900	1.26630800
C	-1.11742400	-1.94839200	1.77655000
C	-0.18542500	-1.93841000	2.80960300
C	0.27566800	-0.67500200	3.30902900
C	-0.27789400	0.54250400	2.83285600
C	0.55252900	1.69127800	2.96882300
C	0.36906900	2.85829700	2.10365900
C	-0.57811800	2.84195800	1.10565200
C	-1.66840200	1.76719500	0.99222200
C	-1.29715100	0.50038600	1.78257400
Br	-4.83511000	2.46043700	-1.24090300
Br	-4.20906200	-4.07009600	-1.53821900

Ar = *m*-BrC_6H_4 anion

C	0.09380000	3.38129400	0.49286700
C	1.38156300	3.93673100	0.32683800
C	2.38047900	3.69257300	1.33635400
C	2.04590300	2.93209000	2.46306300
C	2.03661800	3.85370200	-0.96650100
C	3.66218500	3.48295700	0.67554900
C	3.45053000	3.58696900	-0.74789800
C	2.96537200	1.94279300	2.97758100
C	1.37678000	3.26498600	-2.04706600

C	2.20107700	0.81516600	3.46376900
C	0.04250000	2.71818900	-1.87475100
C	4.13349000	2.72123500	-1.62560800
C	-0.57697200	2.76367000	-0.62583900
C	4.54904400	2.51637200	1.18425100
C	5.24424300	1.62543100	0.27863000
C	-0.07135000	1.52731700	-2.65946900
C	1.19300500	1.31330600	-3.33277500
C	5.04073900	1.72526300	-1.09403100
C	3.44442000	2.11332300	-2.73665700
C	-0.88249000	0.44180700	-2.23245100
C	4.69329200	0.38958700	2.17176600
C	4.19681200	1.74143400	2.34927600
C	1.66128400	0.00030900	-3.58351300
C	4.00992600	-0.73396400	2.71721600
C	2.71959500	-0.51495600	3.38727100
C	5.35107000	0.31744100	0.89854300
C	3.93173700	0.75809200	-2.89841000
C	4.93191800	0.51830400	-1.89372100
C	5.10802100	-0.77222800	-1.32516900
C	5.32884700	-0.87834100	0.12649400
C	4.89539400	-2.05479900	0.79568400
C	4.24131000	-1.98409900	2.07429100
C	4.46549500	-1.85181000	-1.99455200
C	3.46227000	-1.61191600	-2.99172800
C	3.08567700	-0.28995800	-3.36207200
C	1.76521000	-1.56136500	3.37342600
C	-0.54803300	-0.83592000	-2.76685900
C	0.71081700	-1.05448400	-3.41655800
C	-1.54922600	-2.00650000	-0.83593200
C	-0.90268100	-2.05658600	-2.05748400
C	1.13885200	-2.40584500	-3.12727500
C	0.13988900	-3.03475000	-2.29328800
C	2.05585800	-2.84744400	2.78897900
C	3.28273800	-3.06771000	2.15224600
C	4.31629000	-3.17378400	0.07414600
C	4.10232700	-3.07203200	-1.29677200
C	2.89191300	-3.60487700	-1.88636700
C	1.92738900	-4.22518200	-1.07115700
C	2.14767100	-4.32926200	0.35088900
C	3.32928300	-3.81390400	0.91955300
C	0.51689600	-3.92944700	-1.28526300
C	2.49174600	-2.68873700	-2.92662600
C	2.08564400	2.37788400	-2.94505000
C	-1.12711400	-2.88149200	0.20938800
C	-0.13680600	-3.86574000	-0.00207400
C	0.87424600	-4.09350000	1.01481000
C	0.83759700	-3.37408700	2.21100800
C	-2.77547800	2.21157300	2.00744800
H	-3.56175000	1.49300400	1.75224600
H	-2.66066600	2.18081600	3.09720200
C	-3.18973300	3.60274000	1.58143000

C	-2.96666300	4.70895000	2.41245000
C	-3.78861900	3.81100700	0.33014000
H	-2.50084200	4.56123900	3.38353400
C	-3.32680700	5.99466300	2.00325200
C	-4.12280500	5.10001300	-0.07282100
H	-3.97205400	2.97265500	-0.33336500
H	-3.14851000	6.84344700	2.65881100
C	-3.91171100	6.20332800	0.75237700
H	-4.19374000	7.19899100	0.42622300
C	-3.72084100	-0.69122300	-0.40631600
H	-4.08436600	0.26112200	-0.00686400
H	-3.94249400	-0.68956700	-1.48039400
C	-4.44502400	-1.83482700	0.26867200
C	-4.59362500	-3.06538300	-0.38804000
C	-4.95234600	-1.69994400	1.56850100
H	-4.21277200	-3.19475000	-1.39584500
C	-5.20916600	-4.12861700	0.26649400
C	-5.58605500	-2.76947300	2.20386600
H	-4.84535400	-0.75204200	2.08973400
C	-5.71971500	-3.99988800	1.55692100
H	-5.97521100	-2.64920400	3.21187400
H	-6.20863800	-4.83737200	2.04365300
C	-1.38037500	1.66477800	-0.16497600
C	-1.56486600	0.53675400	-0.94098600
C	-2.15089900	-0.71411800	-0.26340400
C	-1.62154800	-0.79756400	1.19400400
C	-1.15405000	-2.13375200	1.44354800
C	-0.19989800	-2.38184900	2.43059800
C	0.36425100	-1.27579400	3.14133300
C	-0.10137300	0.04877800	2.92476500
C	0.81041100	1.09332100	3.25346500
C	0.70669900	2.40092600	2.62184600
C	-0.26253200	2.65392000	1.66805600
C	-1.42557300	1.68985000	1.38626200
C	-1.14099800	0.27526900	1.91981700
Br	-4.95517000	5.34870100	-1.77471800
Br	-5.41574800	-5.79070100	-0.65685100

Ar = *m*-BrC_6H_4 neutral

C	0.16150600	3.37825200	0.51483900
C	1.45873300	3.89137600	0.35154700
C	2.45157700	3.63638400	1.36740500
C	2.09690600	2.87836800	2.48819600
C	2.10564300	3.82028000	-0.94678300
C	3.72019400	3.39127800	0.70357700
C	3.50716700	3.50818100	-0.72960800
C	2.99219500	1.85993900	2.99249000
C	1.42814800	3.25605000	-2.02834500
C	2.19866100	0.74087400	3.47338500
C	0.08573000	2.73741000	-1.85710000
C	4.16520600	2.63740200	-1.60323300

C	-0.52593200	2.78179700	-0.60826900
C	4.57844700	2.40543000	1.19707000
C	5.25334000	1.50362400	0.28824600
C	-0.05818300	1.55136100	-2.65180000
C	1.19322800	1.31190200	-3.32864600
C	5.05147400	1.61657600	-1.08257500
C	3.45765800	2.05222100	-2.72519100
C	-0.89240100	0.48446700	-2.22534900
C	4.67702000	0.26648100	2.17989100
C	4.20743400	1.62863100	2.36427500
C	1.63244400	-0.00536400	-3.59041100
C	3.97167900	-0.84476800	2.72037300
C	2.68895600	-0.60169300	3.39359800
C	5.31771300	0.19086400	0.90249800
C	3.91754300	0.69106600	-2.90066300
C	4.90386500	0.42147300	-1.89011100
C	5.04977900	-0.87471100	-1.32969500
C	5.26932000	-0.99834400	0.11930600
C	4.81070700	-2.16730600	0.78184500
C	4.17136100	-2.09356100	2.06738300
C	4.37771900	-1.93237900	-2.00756400
C	3.39087100	-1.66398600	-3.00858000
C	3.04802200	-0.33197000	-3.37247200
C	1.70952200	-1.61965000	3.37278000
C	-0.57899800	-0.79677100	-2.76214700
C	0.65602200	-1.03865800	-3.42185700
C	-1.60526000	-1.95703300	-0.84387900
C	-0.97279900	-2.02312600	-2.06477600
C	1.05352300	-2.40870300	-3.14111100
C	0.03990000	-3.02378400	-2.31238500
C	1.97001300	-2.91313600	2.77618800
C	3.18317400	-3.14878000	2.13654400
C	4.21351900	-3.26780900	0.05027300
C	3.99899500	-3.15162900	-1.31836700
C	2.77458200	-3.65222900	-1.90560700
C	1.80165900	-4.25279900	-1.10245100
C	2.02372300	-4.37043700	0.32924200
C	3.21009100	-3.88932100	0.89055400
C	0.40043000	-3.93362600	-1.31354100
C	2.39186200	-2.71630500	-2.94512900
C	2.11522100	2.35597800	-2.93233400
C	-1.20608400	-2.85324000	0.19882800
C	-0.23802100	-3.84671300	-0.02180500
C	0.75899600	-4.12107400	0.99781700
C	0.73768700	-3.40895200	2.19779000
C	-2.73104300	2.27747800	2.02295600
H	-3.53565000	1.58217100	1.76183200
H	-2.62118700	2.23849900	3.11266200
C	-3.09552300	3.68313700	1.59609400
C	-2.85590400	4.77745500	2.43764300
C	-3.66230300	3.91247800	0.33426800
H	-2.42464500	4.61363700	3.42217400

C	-3.16684000	6.07492400	2.02393900
C	-3.94147500	5.21267600	-0.07684500
H	-3.86995200	3.08217100	-0.33244100
H	-2.98405300	6.91525000	2.68843600
C	-3.71289800	6.30480200	0.75951200
H	-3.95652500	7.31006900	0.43230500
C	-3.75105700	-0.61095300	-0.39625400
H	-4.09557400	0.34310300	0.01472400
H	-3.97866000	-0.59424900	-1.46876100
C	-4.48147500	-1.75417300	0.27434600
C	-4.63347700	-2.97974000	-0.38939900
C	-4.98782200	-1.62211700	1.57451400
H	-4.26551400	-3.10319900	-1.40302700
C	-5.24384900	-4.04948300	0.26089600
C	-5.62258000	-2.69474800	2.20428200
H	-4.88787300	-0.67472700	2.09839500
C	-5.75305100	-3.92278000	1.55271100
H	-6.01819200	-2.57739300	3.20970400
H	-6.24359700	-4.76093500	2.03635500
C	-1.35176200	1.69800400	-0.14898800
C	-1.56643800	0.58136000	-0.92974300
C	-2.17989500	-0.65887500	-0.26098800
C	-1.65007300	-0.76302100	1.19515700
C	-1.21455700	-2.11185600	1.43983100
C	-0.27137500	-2.39337000	2.42353500
C	0.32106200	-1.30235800	3.14287200
C	-0.11478000	0.03214300	2.93084900
C	0.82854900	1.04874300	3.25512200
C	0.75005200	2.37605200	2.64011900
C	-0.20803500	2.64599300	1.68895500
C	-1.39569800	1.71635400	1.40231800
C	-1.14550900	0.29309300	1.92540600
Br	-4.72325000	5.48773100	-1.79371600
Br	-5.44534800	-5.70317500	-0.66845400

Ar = *p*-BrC_6H_4 anion

C	0.46079200	-3.17854500	0.31871400
C	-0.71452800	-3.95863300	0.38448800
C	-1.56617700	-3.83853600	1.54101400
C	-1.19923100	-2.97122800	2.57655700
C	-1.57328300	-4.06180200	-0.78181800
C	-2.95390300	-3.89333200	1.10032100
C	-2.95830100	-4.03502800	-0.33542300
C	-2.18827000	-2.13233900	3.21428200
C	-1.21417300	-3.42587800	-1.97182200
C	-1.57366500	-0.86338900	3.53778800
C	0.00873900	-2.64488100	-2.03854200
C	-3.91937900	-3.35194900	-1.10701600
C	0.82070100	-2.51473700	-0.91146800
C	-3.90825200	-3.07110300	1.72694900
C	-4.89013200	-2.36632800	0.92927500

C	-0.22406500	-1.49640200	-2.85933800
C	-1.59742100	-1.54409200	-3.31613600
C	-4.89579800	-2.50339800	-0.45518400
C	-3.54001300	-2.69336400	-2.33228100
C	0.43354800	-0.26408600	-2.60038100
C	-4.27562900	-0.95178900	2.67157800
C	-3.52044700	-2.18460900	2.79739700
C	-2.33081300	-0.34916000	-3.51677700
C	-3.72951700	0.30192200	3.06717500
C	-2.33081200	0.34915900	3.51677700
C	-5.13203300	-1.06558400	1.52632200
C	-4.28532100	-1.45562100	-2.44294600
C	-5.13745700	-1.34074900	-1.29061500
C	-5.45100300	-0.07209300	-0.73233700
C	-5.45100300	0.07209200	0.73233800
C	-5.13745700	1.34074800	1.29061500
C	-4.28532100	1.45562100	2.44294700
C	-5.13203300	1.06558300	-1.52632100
C	-4.27563000	0.95178800	-2.67157700
C	-3.72951800	-0.30192200	-3.06717400
C	-1.59742100	1.54409100	3.31613600
C	-0.20789000	0.90463200	-3.10407100
C	-1.57366600	0.86338900	-3.53778800
C	0.86136500	2.33608500	-1.39885700
C	0.02866000	2.20586900	-2.49555400
C	-2.18827100	2.13233900	-3.21428200
C	-1.19923200	2.97122700	-2.57655700
C	-2.20726700	2.72627100	2.75915400
C	-3.54001300	2.69336300	2.33228200
C	-4.89579800	2.50339700	0.45518500
C	-4.89013300	2.36632700	-0.92927400
C	-3.90825300	3.07110300	-1.72694800
C	-2.95390400	3.89333200	-1.10032000
C	-2.95830200	4.03502800	0.33542300
C	-3.91937900	3.35194800	1.10701700
C	-1.56617800	3.83853600	-1.54101400
C	-3.52044800	2.18460900	-2.79739700
C	-2.20726700	-2.72627100	-2.75915400
C	0.46079100	3.17854500	-0.31871500
C	-0.71452900	3.95863300	-0.38448900
C	-1.57328400	4.06180200	0.78181800
C	-1.21417300	3.42587800	1.97182200
C	3.27316800	-1.43660500	1.31127100
H	3.86202200	-0.60093600	0.91847100
H	3.31824200	-1.36632800	2.40467900
C	3.88290200	-2.74620500	0.86369000
C	3.85357300	-3.87422000	1.69587400
C	4.49132700	-2.86939900	-0.39361700
H	3.38284600	-3.80575700	2.67360000
C	4.41350300	-5.08902400	1.29555200
C	5.05713600	-4.07465700	-0.81403300
H	4.52491700	-2.01192500	-1.06133000

H	4.38371800	-5.95325100	1.95120800
C	5.01037700	-5.17467400	0.03964800
H	5.52571000	-4.15403100	-1.78961400
C	3.27316700	1.43660600	-1.31127200
H	3.86202100	0.60093700	-0.91847300
H	3.31824100	1.36632900	-2.40468000
C	3.88290200	2.74620600	-0.86369100
C	3.85357200	3.87422100	-1.69587400
C	4.49132700	2.86939900	0.39361600
H	3.38284500	3.80575800	-2.67360000
C	4.41350200	5.08902500	-1.29555200
C	5.05713600	4.07465800	0.81403300
H	4.52491700	2.01192500	1.06133000
H	4.38371800	5.95325200	-1.95120700
C	5.01037700	5.17467400	-0.03964800
H	5.52571000	4.15403100	1.78961300
C	1.47587900	-1.26912500	-0.61900300
C	1.32011700	-0.16895300	-1.44039700
C	1.77025600	1.20057200	-0.90329100
C	1.47587900	1.26912600	0.61900200
C	0.82070100	2.51473700	0.91146800
C	0.00873900	2.64488100	2.03854100
C	-0.22406400	1.49640200	2.85933800
C	0.43354800	0.26408600	2.60038100
C	-0.20788900	-0.90463200	3.10407100
C	0.02866100	-2.20586900	2.49555400
C	0.86136500	-2.33608500	1.39885700
C	1.77025600	-1.20057200	0.90329000
C	1.32011800	0.16895300	1.44039700
Br	5.80554700	-6.82402300	-0.51173800
Br	5.80554600	6.82402300	0.51173800

Ar = *p*-BrC_6H_4 neutral

C	0.47365700	3.17725400	-0.33342000
C	-0.70095400	3.94415700	-0.40418900
C	-1.54580500	3.83533300	-1.56938400
C	-1.17502500	2.96335100	-2.59802300
C	-1.55250700	4.07179400	0.76527600
C	-2.92891900	3.88216600	-1.12804700
C	-2.93361100	4.03104600	0.31786700
C	-2.16406400	2.11629700	-3.22801400
C	-1.19045800	3.44327700	1.95727500
C	-1.54712000	0.83854800	-3.54478400
C	0.02797100	2.66115000	2.02726200
C	-3.88886600	3.35580800	1.08309300
C	0.83469000	2.51900300	0.90219400
C	-3.87746400	3.05996400	-1.74148100
C	-4.86100600	2.35919000	-0.94375200
C	-0.20487500	1.51412000	2.85724100
C	-1.57200100	1.56292100	3.31472000
C	-4.86783700	2.50388400	0.43891800

C	-3.50830300	2.70309600	2.32053400
C	0.45283000	0.28248400	2.60011700
C	-4.24679400	0.93268600	-2.68380400
C	-3.48698000	2.16394700	-2.81309600
C	-2.30693300	0.37458900	3.52376700
C	-3.70419900	-0.32314400	-3.07450500
C	-2.30693400	-0.37459300	-3.52376700
C	-5.09013700	1.05406400	-1.53430600
C	-4.25838900	1.47121500	2.44168600
C	-5.10020200	1.34786700	1.28282600
C	-5.41254400	0.07764800	0.73108000
C	-5.41254400	-0.07765700	-0.73107800
C	-5.10020100	-1.34787600	-1.28282400
C	-4.25838800	-1.47122300	-2.44168400
C	-5.09013500	-1.05407300	1.53430800
C	-4.24679000	-0.93269300	2.68380600
C	-3.70419800	0.32313800	3.07450600
C	-1.57200000	-1.56292400	-3.31472000
C	-0.19755800	-0.88129400	3.10181000
C	-1.54711600	-0.83855000	3.54478400
C	0.87125300	-2.32323400	1.41191800
C	0.04747100	-2.19770400	2.50783600
C	-2.16405900	-2.11630000	3.22801400
C	-1.17501800	-2.96335300	2.59802200
C	-2.18445100	-2.74597400	-2.74765400
C	-3.50830000	-2.70310200	-2.32053300
C	-4.86783300	-2.50389300	-0.43891700
C	-4.86100100	-2.35919800	0.94375400
C	-3.87745800	-3.05997100	1.74148200
C	-2.92891100	-3.88217100	1.12804800
C	-2.93360400	-4.03105000	-0.31786700
C	-3.88886100	-3.35581500	-1.08309200
C	-1.54579700	-3.83533500	1.56938400
C	-3.48697400	-2.16395300	2.81309700
C	-2.18445500	2.74597000	2.74765400
C	0.47366300	-3.17725200	0.33341800
C	-0.70094600	-3.94415700	0.40418800
C	-1.55250000	-4.07179600	-0.76527600
C	-1.19045300	-3.44327800	-1.95727500
C	3.28677300	1.44370600	-1.31393900
H	3.87915200	0.61506700	-0.91252100
H	3.33778400	1.36603900	-2.40633400
C	3.87486000	2.76432100	-0.86791300
C	3.84599800	3.88365000	-1.71148600
C	4.46208400	2.90327700	0.39769500
H	3.40443500	3.80001100	-2.70183600
C	4.37868200	5.10958200	-1.30895200
C	4.99968700	4.12063600	0.81877600
H	4.50728800	2.04941100	1.06962800
H	4.35350200	5.96665100	-1.97396100
C	4.94865900	5.21674000	-0.04126300
H	5.45481500	4.21290600	1.79945500

C	3.28677600	-1.44369900	1.31393600
H	3.87915400	-0.61506100	0.91251700
H	3.33778800	-1.36603100	2.40633100
C	3.87486500	-2.76431400	0.86791100
C	3.84600500	-3.88364200	1.71148500
C	4.46208900	-2.90327000	-0.39769700
H	3.40444300	-3.80000300	2.70183500
C	4.37869100	-5.10957400	1.30895200
C	4.99969300	-4.12062900	-0.81877700
H	4.50729100	-2.04940500	-1.06963100
H	4.35351200	-5.96664200	1.97396200
C	4.94866700	-5.21673200	0.04126300
H	5.45482100	-4.21289900	-1.79945600
C	1.48802100	1.27088900	0.61210100
C	1.33514600	0.17613300	1.43788200
C	1.78332700	-1.19545400	0.90968500
C	1.48802300	-1.27088600	-0.61210300
C	0.83469500	-2.51900100	-0.90219600
C	0.02797500	-2.66114900	-2.02726300
C	-0.20487400	-1.51412000	-2.85724100
C	0.45282900	-0.28248300	-2.60011800
C	-0.19756200	0.88129400	-3.10181100
C	0.04746600	2.19770400	-2.50783700
C	0.87124800	2.32323600	-1.41191900
C	1.78332400	1.19545800	-0.90968700
C	1.33514600	-0.17613000	-1.43788400
Br	5.69822200	6.87865600	0.51377900
Br	5.69823300	-6.87864800	-0.51377800