

Imidazolium-fulleride Ionic Liquids - A DFT Prediction

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Structure and energetics of $(C_{60}X)^-$

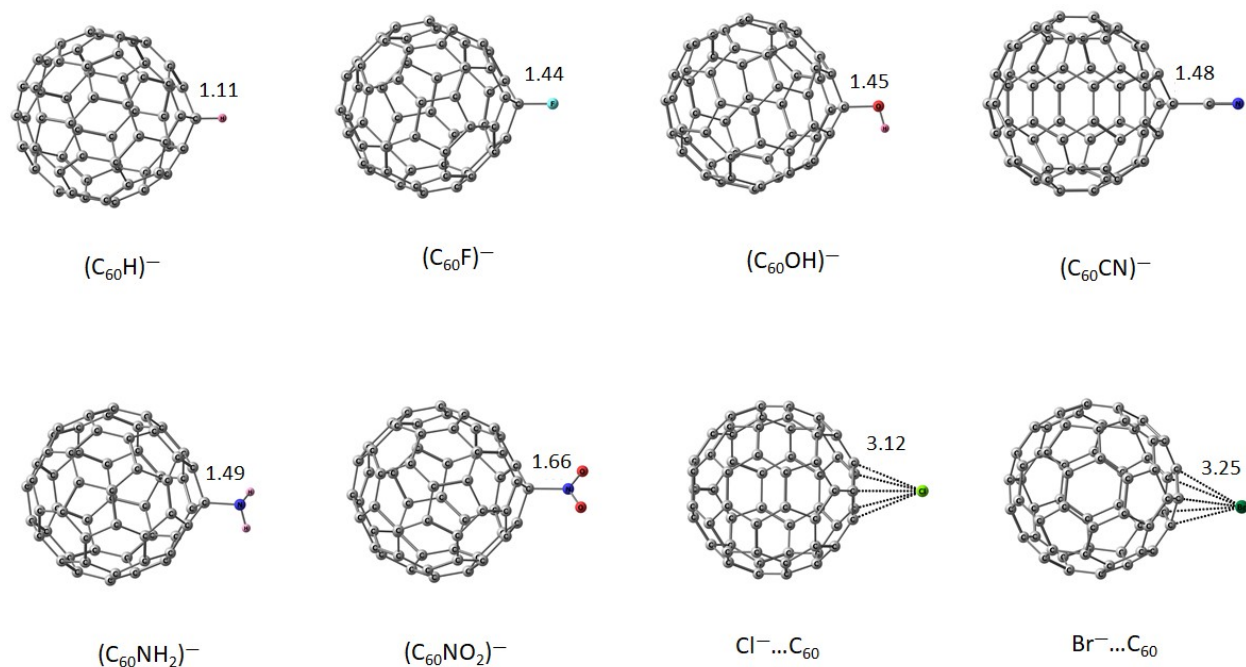


Fig. S1 Optimized geometries of X-fullerides and X⁻...C₆₀ at the M06L/6-31G(d,p) level with their local-minimum distances in Å.

The optimized geometries of X-fullerides (X = H, F, OH, CN, NH₂, and NO₂), with their respective C – X distance, are given in Fig. S1. The smallest anion (H⁻) is found to interact with the fullerene ring at the shortest interaction distance (d_{int}) 1.11 Å, which indicates the formation of a strong C-H covalent bond. Similarly, for the anions *viz.* F⁻, OH⁻, CN⁻, NH₂⁻, and NO₂⁻ the d_{int} observed is 1.44 Å, 1.45 Å, 1.48 Å, 1.49 Å, and 1.66 Å, respectively suggesting strong C–X covalent bond formation in all. The C-X bond features observed for these (C₆₀X)⁻ are very much similar to that observed for the IM⁺...(C₆₀X)⁻ ion-pairs. This shows that the anionic exohedral modifications are only weakly influenced by IM⁺ and the X-fullerides can be isolated as independent large anions. In the case of Cl⁻ and Br⁻, multiple C atoms of the fullerene cage are found to interact with the halide with average d_{int} 3.12 Å and 3.25 Å, respectively. The QTAIM analysis (Table S6) also shows that the ρ_b values for the C–X bond are in the range of 0.2131 to 0.2651 au for X = H, F, OH, CN, and NH₂, indicate the covalent nature of the C–X bond. While in the case of X = NO₂, the value is 0.1777 indicates a weak covalent bond interaction between C₆₀ and NO₂. The energy required for the dissociation of (C₆₀X)⁻ into C₆₀ and X⁻ (E_d) ranges from 97 to 33.5 kcal/mol for X = H, F, OH, CN, NH₂, and NO₂ (Table S1).

These results propose that irrespective of the nature of the anion, $(C_{60}X)^-$ may exist as a chemically stable anionic entity. Very similar features were observed for $X^-@C_{60}$ systems.⁵³ Whereas the dissociation energy values observed for $X = Cl$ and Br are 24.4 and 22.7 kcal/mol respectively, shows that $Cl^-...C_{60}$ and $Br^-...C_{60}$ exist as noncovalent complexes of fullerene as observed in the ion-pair $(IM^+...X^-)...C_{60}$, for $X = Cl$ and Br . Here $C...X$ interaction is completely noncovalent in nature and the anionic character remains in the halides itself.

The energy for dissociation (E_d) of each $(C_{60}X)^-$ into C_{60} and anion X^- is calculated as

$$E_d = (E_5 + E_8) - E_3 \quad (1)$$

where E_3 , E_5 and E_8 stand for the ZPE-corrected energy of $(C_{60}X)^-$, C_{60} and anion X^- . The free energy associated with the dissociation reaction (G_d) is also calculated in a similar fashion.

Table S1. ZPE-corrected E_d and G_d values (kcal/mol) of X-fullerides at the M06L/6-311++G(d,p)//M06L/6-31G(d,p) level.

System	E_d (kcal/mol)	G_d (kcal/mol)
$(C_{60}H)^-$	97.0	90.9
$(C_{60}F)^-$	56.8	48.7
$(C_{60}OH)^-$	73.5	64.5
$(C_{60}CN)^-$	48.3	38.0
$(C_{60}NH_2)^-$	86.5	76.4
$(C_{60}NO_2)^-$	33.5	22.4
$Cl^-...C_{60}$	24.4	18.8
$Br^-...C_{60}$	22.7	16.7

Table S2. Energetics of IM^+ , $(\text{C}_{60}\text{X})^-$ and $\text{X}^- \dots \text{C}_{60}$ systems in au.

System	E_{SCF} M06L/6- 311++G(d,p)	ZPE at M06L/6- 31G(d,p)	G_{corr} at M06L/6- 31G(d,p)
IM^+	-305.25535	0.14016	0.10835
$(\text{C}_{60}\text{H})^-$	-2287.16996	0.38724	0.34388
$(\text{C}_{60}\text{F})^-$	-2386.43335	0.37903	0.33473
$(\text{C}_{60}\text{OH})^-$	-2362.40468	0.39112	0.34629
$(\text{C}_{60}\text{CN})^-$	-2379.42545	0.38545	0.33972
$(\text{C}_{60}\text{NH}_2)^-$	-2342.52945	0.40413	0.35949
$(\text{C}_{60}\text{NO}_2)^-$	-2491.72997	0.38890	0.34049
$\text{Cl}^- \dots \text{C}_{60}$	-2746.79308	0.37845	0.32927
$\text{Br}^- \dots \text{C}_{60}$	-4860.60890	0.37809	0.32849

Molecular electrostatic potential (MESP) analysis

Table S3. V_m in kcal/mol for X at M06L/6-311++G(d,p)//M06L/6-31G(d,p) level.

System	V_m	ΔV_m	% ΔV_m
H	-188.4	116.2	61.7
F	-240.3	147.0	61.2
CN	-186.0	84.8	45.6
OH	-241.5	138.0	57.1
NH_2	-237.6	121.2	51.0
NO_2	-186.4	90.6	48.6
Cl	-171.0	51.5	30.1
Br	-155.6	50.3	32.3

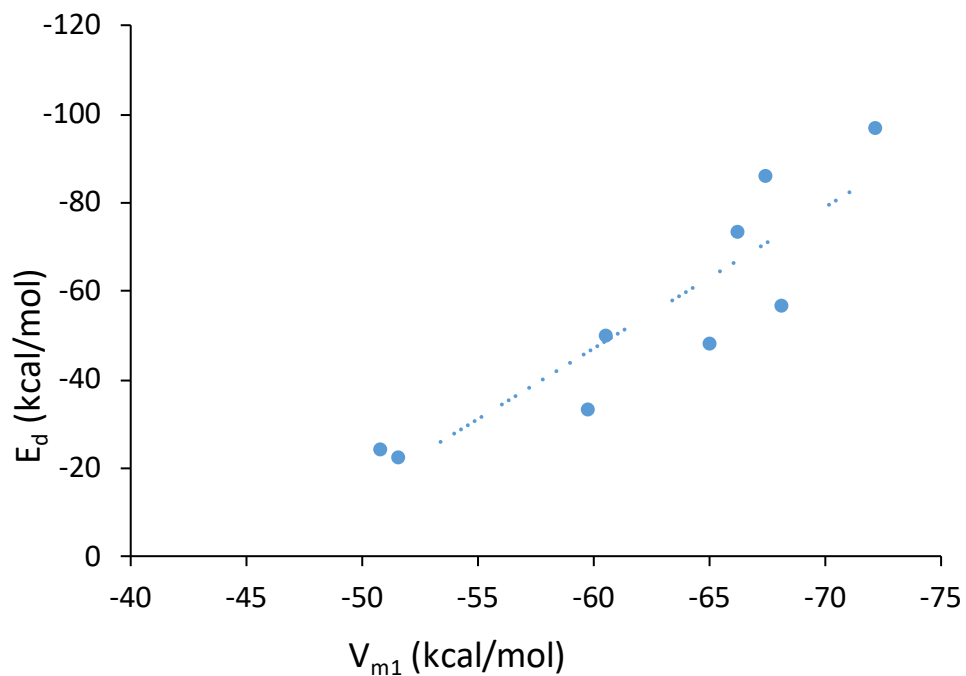


Fig. S2 Correlation between V_{m1} (kcal/mol) and E_d (kcal/mol) of exohedral fullerides at the M06L/6-311++G(d,p)//M06L/6-31G(d,p) level.

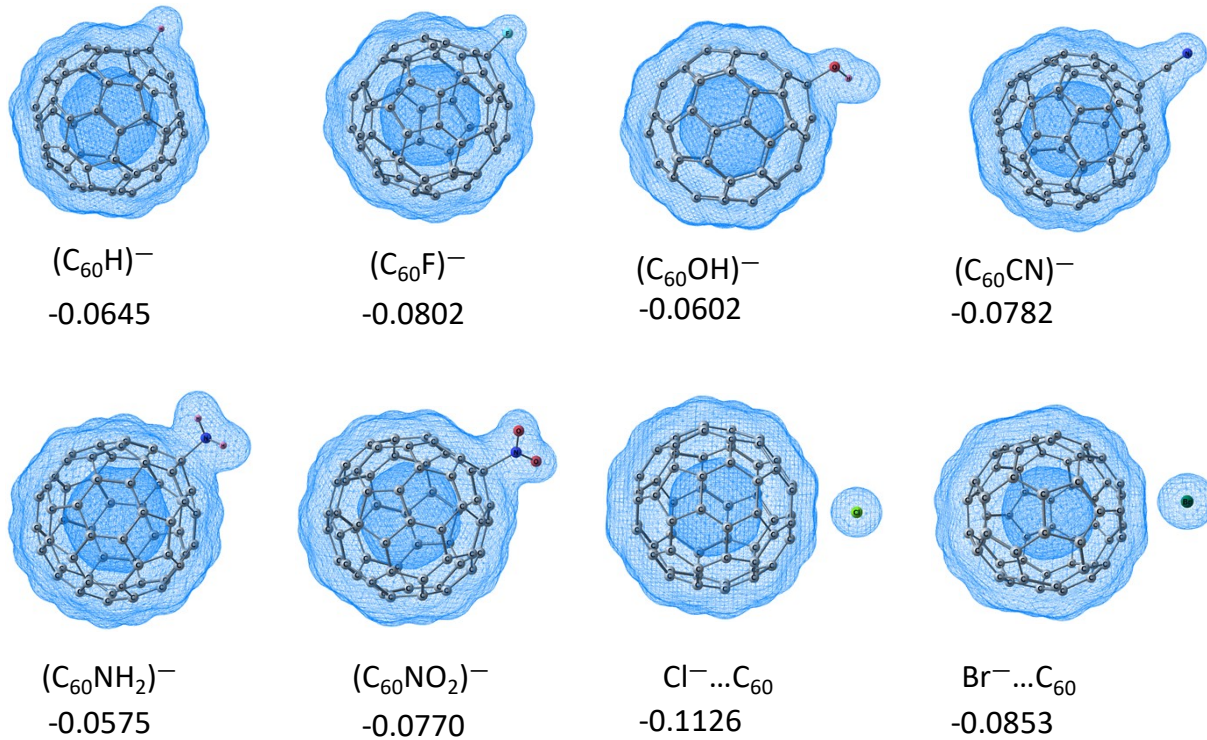


Fig. S3 MESP of exohedral fullerides that engulfs the whole anion at M06L/6-311++G(d,p)//M06L/6-31G(d,p) level. The minimum value of MESP that engulfs the whole anion is also depicted in au.

Table S4. ZPE-corrected $E_{\text{ion-pair}}$ and $G_{\text{ion-pair}}$ values (kcal/mol) of $\text{IM}^+\dots(\text{C}_{60}\text{X})^-$ systems at the M06L/6-311++G(d,p)//M06L/6-31G(d,p) level.

System	Structure	$E_{\text{ion-pair}}$	$G_{\text{ion-pair}}$
$\text{IM}^+\dots(\text{C}_{60}\text{F})^-$	i	-71.8	-59.1
	ii	-62.4	-51.5
	iii	-58.7	-47.3
	iv	-58.4	-46.9
$\text{IM}^+\dots(\text{C}_{60}\text{CN})^-$	i	-69.6	-57.1
	ii	-69.2	-56.8
	iii	-66.0	-53.6
	iv	-57.2	-45.7
	v	-56.9	-45.5
$\text{IM}^+\dots(\text{C}_{60}\text{NH}_2)^-$	i	-73.0	-61.3
	ii	-68.8	-56.4
	iii	-60.1	-49.0
	iv	-60.0	-48.6
$\text{IM}^+\dots(\text{C}_{60}\text{NO}_2)^-$	i	-71.0	-57.7
	ii	-68.3	-54.7
	iii	-66.9	-53.1
	iv	-56.3	-44.4
	v	-56.1	-44.1

Table S5. Energetics of $\text{IM}^+\dots(\text{C}_{60}\text{X})^-$ systems in au.

System	Structure	E_{SCF} M06L/6-311++G(d,p)	ZPE at M06L/6-31G(d,p)	G_{corr} at M06L/6-31G(d,p)
$\text{IM}^+\dots(\text{C}_{60}\text{H})^-$	i	-2592.52814	0.52824	0.47201
	ii	-2592.52737	0.52834	0.47228
	iii	-2592.52693	0.52877	0.47226
	iv	-2592.52331	0.52789	0.46861

	v	-2592.52349	0.52817	0.47148
	vi	-2592.52205	0.52786	0.47017
IM ⁺ ...(C ₆₀ F) ⁻	i	-2691.80467	0.52073	0.46493
	ii	-2691.78936	0.52049	0.46174
	iii	-2691.78300	0.52002	0.46198
	iv	-2691.78264	0.52011	0.46230
IM ⁺ ...(C ₆₀ OH) ⁻	i	-2667.77681	0.53326	0.47749
	ii	-2667.77504	0.53287	0.47718
	iii	-2667.77045	0.53284	0.47688
	iv	-2667.75644	0.53230	0.47501
	v	-2667.75523	0.53240	0.47445
IM ⁺ ...(C ₆₀ CN) ⁻	i	-2684.79322	0.52707	0.46944
	ii	-2684.79262	0.52714	0.46942
	iii	-2684.78725	0.52685	0.46908
	iv	-2684.77264	0.52637	0.46709
	v	-2684.77216	0.52630	0.46696
IM ⁺ ...(C ₆₀ NH ₂) ⁻	i	-2647.90259	0.54573	0.48794
	ii	-2647.88110	0.54502	0.48665
	iii	-2647.88110	0.54502	0.48665
	iv	-2647.88118	0.54492	0.48615
IM ⁺ ...(C ₆₀ NO ₂) ⁻	i	-2797.09980	0.53038	0.47130
	ii	-2797.09540	0.53022	0.47178
	iii	-2797.09342	0.53060	0.47231
	iv	-2797.07622	0.53016	0.46902
	v	-2797.07587	0.53021	0.46913

QTAIM analysis

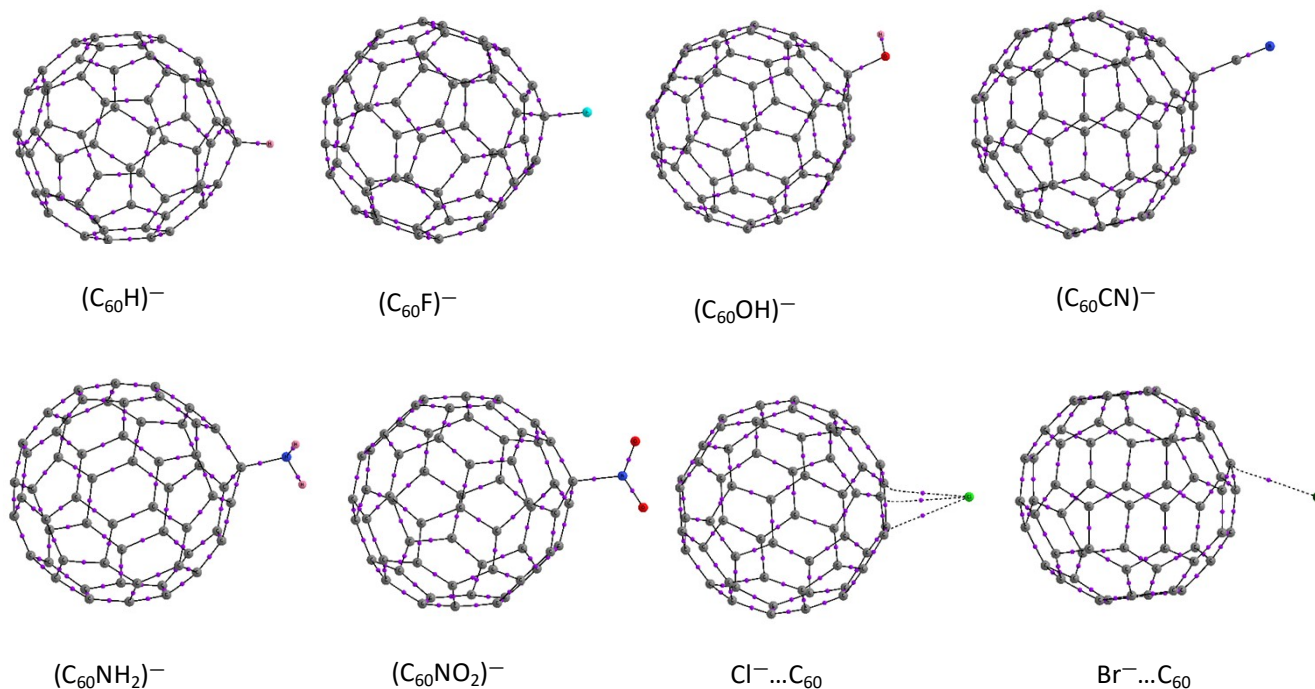


Fig. S4 QTAIM plots of exohedral fullerides at the M06L/6-311++G(d,p)//M06L/6-31G(d,p) level.

Table S6. QTAIM parameters (au) of exohedral fullerides at the M06L/6-311++G(d,p)//M06L/6-31G(d,p) level.

System	Bond	ρ	$\nabla^2\rho$	H
$(C_{60}H)^-$	C-H	0.2651	-0.8441	-0.2557
$(C_{60}F)^-$	C-F	0.2131	-0.1983	-0.2463
$(C_{60}OH)^-$	C-O	0.2423	-0.4899	-0.2949
$(C_{60}CN)^-$	C-C	0.2600	-0.6755	-0.2459
$(C_{60}NH_2)^-$	C-N	0.2542	-0.6226	-0.2583
$(C_{60}NO_2)^-$	C-N	0.1777	-0.1957	-0.1241
$(C_{60}Cl)^-$	C...Cl	0.0125	0.0448	0.0022
$(C_{60}Br)^-$	C...Br	0.0152	0.0471	0.0018

Table S7. QTAIM parameters (au) of $IM^+ \dots (C_{60}X)^-$ systems at the M06L/6-311++G(d,p)//M06L/6-31G(d,p) level.

System	Bond	ρ	$\nabla^2\rho$	H
$IM^+ \dots (C_{60}H)^-$	C-H	0.2627	-0.8293	-0.2526
$IM^+ \dots (C_{60}F)^-$	C-F	0.1636	-0.0260	-0.1229
$IM^+ \dots (C_{60}OH)^-$	C-O	0.2193	-0.3854	-0.2422
$IM^+ \dots (C_{60}CN)^-$	C-C	0.2592	-0.6719	-0.2502
$IM^+ \dots (C_{60}NH_2)^-$	C-N	0.2419	-0.5631	-0.2411
$IM^+ \dots (C_{60}NO_2)^-$	C-N	0.1647	-0.1388	-0.1074
$(IM^+ \dots Cl^-) \dots C_{60}$	C...Cl	0.0093	0.0295	0.0387
$(IM^+ \dots Br^-) \dots C_{60}$	C...Br	0.0092	0.0290	0.0382

Cartesian coordinates of optimized geometry of $IM^+ \dots (C_{60}X)^-$ complexes at M06L/6-31G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.

$IM^+ \dots (C_{60}H)^-$				$IM^+ \dots (C_{60}F)^-$			
6	1.404708000	1.893246000	2.945198000	6	3.978597000	1.211489000	1.313784000
6	0.610977000	0.787071000	3.443432000	6	3.887258000	1.933783000	0.064912000
6	0.827527000	2.850312000	2.113925000	6	2.872675000	2.953850000	0.212632000
6	-0.732883000	0.666292000	3.066292000	6	2.340312000	2.863700000	1.555387000
6	-1.311942000	-0.607596000	2.767403000	6	3.025844000	1.787665000	2.236178000
6	1.439132000	-0.384485000	3.468700000	6	2.325779000	0.966387000	3.120569000
6	0.887357000	-1.624344000	3.122212000	6	2.561713000	-0.461897000	3.119185000
6	-0.504834000	-1.730672000	2.762830000	6	3.483911000	-1.016221000	2.228963000
6	2.831094000	2.856344000	0.686180000	6	4.209842000	-0.165365000	1.312957000
6	3.430910000	1.863453000	1.550346000	6	4.344986000	-0.870776000	0.058353000
6	1.552511000	3.342707000	0.965220000	6	4.251899000	-0.175552000	-1.149281000
6	2.729312000	1.391945000	2.661520000	6	4.015800000	1.252407000	-1.145982000
6	2.749662000	-0.019154000	2.986803000	6	3.145168000	1.569489000	-2.255566000
6	4.176700000	0.943707000	0.721702000	6	2.161101000	2.550347000	-2.111281000
6	4.196473000	-0.418523000	1.035451000	6	2.028089000	3.257875000	-0.854627000
6	3.465753000	-0.905826000	2.179759000	6	0.619718000	3.483258000	-0.617980000
6	0.967236000	3.233384000	-1.422987000	6	0.106709000	3.399193000	0.677790000
6	2.290623000	2.739060000	-1.712910000	6	0.981930000	3.081894000	1.783946000
6	0.602693000	3.538489000	-0.109436000	6	0.254167000	2.227311000	2.699330000
6	3.206719000	2.548133000	-0.675149000	6	0.918743000	1.192554000	3.363304000

6	4.043662000	1.370480000	-0.651606000	6	0.280371000	-0.096988000	3.493599000
6	2.171905000	1.750027000	-2.765632000	6	1.295665000	-1.118580000	3.346480000
6	2.980229000	0.612452000	-2.742294000	6	0.997216000	-2.312523000	2.687229000
6	3.923945000	0.415570000	-1.666174000	6	1.954485000	-2.888105000	1.766793000
6	-1.599995000	2.499816000	-0.466230000	6	3.176560000	-2.251071000	1.542844000
6	-1.228063000	2.192504000	-1.822735000	6	3.708525000	-2.160821000	0.200805000
6	-0.704094000	3.167325000	0.378700000	6	2.998669000	-2.710349000	-0.868570000
6	0.034679000	2.554233000	-2.300158000	6	2.902060000	-1.990003000	-2.120151000
6	0.781022000	1.649386000	-3.140112000	6	3.514723000	-0.742964000	-2.254119000
6	-1.803699000	0.905127000	-2.166624000	6	2.827346000	0.334074000	-2.934788000
6	-1.074875000	0.028114000	-2.990623000	6	1.545418000	0.125663000	-3.446622000
6	0.232878000	0.399639000	-3.458776000	6	0.525359000	1.146585000	-3.304825000
6	-1.331731000	1.659091000	2.199821000	6	0.839523000	2.349298000	-2.655639000
6	-2.293943000	1.012865000	1.360312000	6	-0.110489000	2.914739000	-1.729767000
6	-0.569521000	2.743077000	1.742690000	6	-1.328054000	2.271173000	-1.497765000
6	-2.397526000	1.404625000	0.034589000	6	-1.853295000	2.180086000	-0.161498000
6	-2.572793000	0.429325000	-1.049294000	6	-1.156460000	2.735180000	0.913945000
6	-2.505161000	-0.434158000	1.822846000	6	-1.071820000	2.024571000	2.167508000
6	-2.414437000	-1.392836000	0.650470000	6	-1.689943000	0.771029000	2.285456000
6	-2.457608000	-0.935021000	-0.681770000	6	-0.996436000	-0.304952000	2.967098000
6	0.284467000	-1.886463000	-2.947285000	6	-1.302881000	-1.535580000	2.281532000
6	-1.037367000	-1.378866000	-2.655135000	6	-0.324943000	-2.523627000	2.144589000
6	-1.724324000	-1.855687000	-1.541413000	6	-0.189152000	-3.224999000	0.894253000
6	0.863024000	-2.845196000	-2.112621000	6	1.221885000	-3.454965000	0.658333000
6	3.019098000	-1.669725000	-2.221770000	6	1.733318000	-3.367112000	-0.633995000
6	2.418348000	-0.676146000	-3.085306000	6	0.854947000	-3.048509000	-1.741869000
6	1.074104000	-0.780952000	-3.440252000	6	1.576883000	-2.201888000	-2.655031000
6	2.256225000	-2.734037000	-1.743042000	6	0.909917000	-1.159947000	-3.303110000
6	3.291753000	-2.510526000	0.480450000	6	-0.499294000	-0.937989000	-3.068444000
6	4.077422000	-1.404875000	-0.018038000	6	-0.740434000	0.497483000	-3.099531000
6	3.950493000	-0.992755000	-1.345135000	6	-1.645425000	1.026510000	-2.172780000
6	2.386371000	-3.160446000	-0.364627000	6	-2.425129000	0.197800000	-1.295733000
6	0.693276000	-3.226292000	1.424891000	6	-2.476245000	0.876058000	-0.034759000
6	1.629811000	-2.540910000	2.296352000	6	-2.446794000	0.208091000	1.199065000
6	2.900718000	-2.194601000	1.834513000	6	-2.179679000	-1.222711000	1.174144000
6	1.081637000	-3.543762000	0.111252000	6	-2.070099000	-1.915452000	-0.025286000
6	-1.136315000	-2.847590000	-0.686919000	6	-1.032361000	-2.898583000	-0.170350000
6	-1.529118000	-2.520064000	0.673642000	6	-0.502082000	-2.809305000	-1.514254000
6	-0.627972000	-2.754087000	1.719864000	6	-1.206764000	-1.771437000	-2.215031000
6	0.140766000	-3.340112000	-0.961517000	6	-2.339829000	-1.269955000	-1.359776000
1	-3.459718000	-0.531932000	2.381024000	9	-3.653174000	-1.880935000	-1.913440000
6	-5.425889000	0.003021000	-0.920359000	6	-5.355280000	-0.086081000	-0.559095000
7	-5.508306000	-1.087440000	-0.144388000	7	-5.621903000	-0.799478000	0.537645000
7	-5.732176000	1.077394000	-0.175332000	7	-5.571320000	1.203935000	-0.283203000
6	-5.978797000	0.660866000	1.114884000	6	-5.979844000	1.316892000	1.028355000
1	-6.206930000	1.361044000	1.901204000	1	-6.189745000	2.273011000	1.478111000
6	-5.851411000	-0.693115000	1.132748000	6	-6.015406000	0.058434000	1.543550000
1	-5.960605000	-1.405727000	1.933270000	1	-6.265075000	-0.297466000	2.529103000
1	-5.138693000	0.019659000	-1.957404000	1	-4.928437000	-0.501075000	-1.466613000
6	-5.566660000	2.452381000	-0.615413000	6	-5.254712000	2.295440000	-1.192120000
1	-4.521030000	2.750025000	-0.487881000	1	-4.712792000	3.067493000	-0.645068000
1	-5.844722000	2.533274000	-1.665937000	1	-4.598768000	1.908103000	-1.973575000
1	-6.215702000	3.097116000	-0.024285000	1	-6.165192000	2.709454000	-1.628714000
6	-5.281847000	-2.452757000	-0.595344000	6	-5.463231000	-2.245655000	0.635709000
1	-4.851024000	-3.024832000	0.225052000	1	-4.895706000	-2.479057000	1.537024000

1	-6.219992000	-2.903537000	-0.929832000	1	-6.442285000	-2.727208000	0.671591000
1	-4.552695000	-2.439661000	-1.407023000	1	-4.897056000	-2.578120000	-0.235718000
IM ⁺ ... (C ₆₀ OH) ⁻				IM ⁺ ... (C ₆₀ CN) ⁻			
6	0.697993000	-3.132398000	0.460261000	6	-1.692009000	1.955262000	2.860595000
6	-0.547986000	-3.310493000	1.152028000	6	-0.361707000	2.399980000	2.519106000
6	1.635340000	-2.213679000	0.951688000	6	-1.887469000	0.661913000	3.349896000
6	-0.811399000	-2.654034000	2.364410000	6	0.726424000	1.535315000	2.681554000
6	-2.114435000	-2.086527000	2.607682000	6	1.763941000	1.472748000	1.680236000
6	-1.606693000	-3.436207000	0.167900000	6	-0.450721000	3.216009000	1.341207000
6	-2.872277000	-2.902430000	0.419561000	6	0.552253000	3.125543000	0.368411000
6	-3.136587000	-2.216934000	1.663023000	6	1.696012000	2.290655000	0.565329000
6	2.310491000	-1.446883000	-1.388903000	6	-3.892302000	0.402621000	1.951211000
6	1.097165000	-2.263374000	-1.829298000	6	-3.690047000	1.738424000	1.437841000
6	2.400486000	-1.353388000	0.101464000	6	-3.008453000	-0.124209000	2.896281000
6	0.404417000	-3.099140000	-0.967334000	6	-2.609456000	2.501587000	1.883677000
6	-1.015619000	-3.307609000	-1.138746000	6	-1.842194000	3.284361000	0.942454000
6	0.367654000	-1.548474000	-2.837301000	6	-4.042453000	1.735408000	0.034700000
6	-1.001301000	-1.753959000	-3.033043000	6	-3.300305000	2.494880000	-0.871794000
6	-1.708055000	-2.651201000	-2.159920000	6	-2.180315000	3.280490000	-0.407798000
6	2.468125000	1.138684000	0.098956000	6	-3.036501000	-2.298575000	1.742890000
6	2.145176000	1.111295000	-1.322673000	6	-3.946959000	-1.749346000	0.764167000
6	2.496859000	-0.099945000	0.768456000	6	-2.568203000	-1.500383000	2.787516000
6	1.997013000	-0.085598000	-2.011883000	6	-4.376565000	-0.423744000	0.868949000
6	0.919321000	-0.213504000	-2.950091000	6	-4.461973000	0.397582000	-0.316642000
6	1.278315000	2.234468000	-1.609045000	6	-3.606400000	-2.303474000	-0.526091000
6	0.264360000	2.113410000	-2.563959000	6	-3.687293000	-1.509707000	-1.671144000
6	0.082953000	0.864778000	-3.254805000	6	-4.127494000	-0.133884000	-1.564967000
6	1.258332000	0.879700000	2.668662000	6	-0.300738000	-2.422478000	2.523489000
6	1.171738000	2.135342000	1.959059000	6	-0.788144000	-3.254154000	1.441082000
6	1.916820000	-0.208998000	2.096902000	6	-1.183905000	-1.568106000	3.193175000
6	1.748075000	2.236651000	0.682176000	6	-2.126979000	-3.189431000	1.056730000
6	1.028041000	2.928260000	-0.371720000	6	-2.480111000	-3.193211000	-0.347211000
6	-0.136151000	2.688435000	2.202507000	6	0.245632000	-3.325981000	0.433818000
6	-0.826174000	3.364935000	1.190603000	6	-0.094654000	-3.328598000	-0.920648000
6	-0.231996000	3.478225000	-0.120203000	6	-1.482504000	-3.261392000	-1.318863000
6	0.173635000	-1.743178000	2.893837000	6	0.525959000	0.204746000	3.193597000
6	-0.517050000	-0.617926000	3.484443000	6	1.448320000	-0.684844000	2.510920000
6	1.371609000	-1.533278000	2.209065000	6	-0.758608000	-0.228906000	3.526768000
6	0.015312000	0.668280000	3.377180000	6	1.034740000	-1.992807000	2.196954000
6	-0.850509000	1.788427000	3.085283000	6	1.362799000	-2.534177000	0.900153000
6	-1.935862000	-0.830396000	3.306992000	6	2.245548000	0.091443000	1.605313000
6	-2.771510000	0.250567000	3.028398000	6	2.502638000	-0.419072000	0.319439000
6	-2.219187000	1.583307000	2.915136000	6	2.092396000	-1.774003000	-0.015329000
6	-2.530761000	3.143648000	-0.405269000	6	-0.233270000	-2.005079000	-2.849958000
6	-2.243716000	3.143627000	1.013985000	6	0.669351000	-2.543988000	-1.865250000
6	-2.930483000	2.273693000	1.861554000	6	1.745127000	-1.778988000	-1.408785000
6	-3.487617000	2.267954000	-0.923926000	6	-0.017471000	-0.698844000	-3.325394000
6	-2.032719000	1.774418000	-2.846852000	6	-2.441959000	-0.243205000	-3.182897000
6	-1.039587000	2.679744000	-2.308626000	6	-2.658264000	-1.581234000	-2.682245000
6	-1.284536000	3.345861000	-1.106136000	6	-1.565170000	-2.435455000	-2.506735000
6	-3.235417000	1.573573000	-2.166459000	6	-1.152576000	0.189600000	-3.494970000
6	-3.115892000	-0.841849000	-2.624556000	6	-1.618861000	2.388158000	-2.493292000
6	-1.870325000	-0.630833000	-3.324987000	6	-2.952529000	1.944229000	-2.164497000

6	-1.339654000	0.651706000	-3.434337000	6	-3.354629000	0.649193000	-2.497551000
6	-3.787403000	0.241196000	-2.053708000	6	-0.733895000	1.521859000	-3.144538000
6	-4.284407000	-1.094810000	-0.046451000	6	1.120602000	2.288706000	-1.746727000
6	-3.585469000	-2.212770000	-0.635578000	6	0.201577000	3.123638000	-1.035235000
6	-3.015851000	-2.093621000	-1.904386000	6	-1.142353000	3.209651000	-1.417022000
6	-4.380297000	0.113171000	-0.741715000	6	0.653704000	1.463259000	-2.753381000
6	-3.918224000	1.366504000	1.322037000	6	1.959291000	-0.429519000	-1.909374000
6	-3.823880000	0.118246000	2.044638000	6	2.517866000	0.366056000	-0.864303000
6	-3.997168000	-1.092203000	1.372314000	6	2.274737000	1.872724000	-0.807878000
6	-4.199983000	1.367220000	-0.046157000	6	1.108897000	0.079270000	-2.900565000
1	3.416443000	-2.212585000	-2.855112000	7	4.623059000	2.991094000	-1.252750000
8	3.577941000	-2.014464000	-1.922687000	6	3.546311000	2.564675000	-1.084836000
6	5.313292000	-0.100120000	-0.526395000	6	5.516435000	0.056261000	-0.371140000
7	5.604582000	1.192144000	-0.347676000	7	5.491544000	-1.257313000	-0.619006000
7	5.689748000	-0.768191000	0.567575000	7	5.586724000	0.236195000	0.950499000
6	6.210457000	0.123080000	1.478373000	6	5.569244000	-0.997734000	1.566193000
1	6.565093000	-0.193672000	2.445082000	1	5.580242000	-1.095532000	2.638878000
6	6.157606000	1.355692000	0.904167000	6	5.509467000	-1.934127000	0.582641000
1	6.452003000	2.323978000	1.273339000	1	5.457856000	-3.009163000	0.628613000
1	4.795549000	-0.564450000	-1.368654000	1	5.483236000	0.854179000	-1.100948000
6	5.455024000	-2.190005000	0.789567000	6	5.539623000	1.528879000	1.622626000
1	4.801292000	-2.310340000	1.655343000	1	6.307682000	1.563708000	2.395656000
1	4.943238000	-2.593316000	-0.084828000	1	5.708624000	2.314314000	0.886563000
1	6.407635000	-2.695648000	0.957984000	1	4.549320000	1.660715000	2.067254000
6	5.261120000	2.264591000	-1.269049000	6	5.281420000	-1.850776000	-1.930571000
1	4.544198000	2.933720000	-0.788803000	1	6.026410000	-2.626850000	-2.109240000
1	6.161500000	2.810160000	-1.556444000	1	4.273330000	-2.270854000	-1.977506000
1	4.785918000	1.832643000	-2.148472000	1	5.374741000	-1.074491000	-2.688197000
IM ⁺ ... (C ₆₀ NH ₂) ⁻				IM ⁺ ... (C ₆₀ NO ₂) ⁻			
6	-3.354091000	-2.282993000	-1.208036000	6	-1.548311000	-1.720849000	3.091835000
6	-3.125277000	-2.768239000	0.134211000	6	-1.153786000	-0.399670000	3.524291000
6	-2.358757000	-2.417072000	-2.179089000	6	-0.611790000	-2.551690000	2.469895000
6	-1.908038000	-3.368818000	0.462190000	6	0.156266000	0.041157000	3.328011000
6	-1.266919000	-3.060603000	1.719336000	6	0.405800000	1.391858000	2.891814000
6	-3.745113000	-1.841440000	1.055830000	6	-2.260593000	0.502377000	3.284120000
6	-3.124170000	-1.547752000	2.271512000	6	-2.018768000	1.812476000	2.866469000
6	-1.862851000	-2.167504000	2.605807000	6	-0.661747000	2.264751000	2.666927000
6	-2.824513000	-0.145311000	-3.002849000	6	-2.298023000	-3.246895000	0.813443000
6	-3.851141000	-0.007873000	-1.994629000	6	-3.264208000	-2.382181000	1.453275000
6	-2.085733000	-1.325781000	-3.091654000	6	-0.998777000	-3.333174000	1.313299000
6	-4.120005000	-1.060757000	-1.116330000	6	-2.892112000	-1.630653000	2.568692000
6	-4.356149000	-0.784438000	0.282279000	6	-3.337191000	-0.258553000	2.695854000
6	-3.826863000	1.353967000	-1.511971000	6	-4.083033000	-1.787383000	0.420896000
6	-4.053749000	1.620271000	-0.161090000	6	-4.515910000	-0.465528000	0.542835000
6	-4.327934000	0.530898000	0.752900000	6	-4.131486000	0.312465000	1.699356000
6	-0.015783000	-0.041921000	-3.451174000	6	-0.094614000	-3.309462000	-0.977111000
6	-0.784250000	1.183742000	-3.363007000	6	-1.441475000	-3.220369000	-1.495133000
6	-0.661576000	-1.277973000	-3.330024000	6	0.122384000	-3.365199000	0.401178000
6	-2.159559000	1.132011000	-3.139737000	6	-2.522935000	-3.189072000	-0.615131000
6	-2.779426000	2.059468000	-2.217725000	6	-3.628174000	-2.288232000	-0.856572000
6	0.020576000	2.167320000	-2.674331000	6	-1.418419000	-2.344891000	-2.648763000
6	-0.576758000	3.060967000	-1.783112000	6	-2.488661000	-1.478258000	-2.884121000
6	-2.002732000	3.006210000	-1.550976000	6	-3.606374000	-1.445745000	-1.968752000
6	1.181732000	-2.106349000	-1.921248000	6	2.004659000	-1.802187000	0.187602000

6	1.856933000	-0.828034000	-2.056726000	6	1.783244000	-1.745889000	-1.232035000
6	-0.049732000	-2.323286000	-2.544114000	6	1.194883000	-2.599842000	0.999082000
6	1.264018000	0.184563000	-2.831023000	6	0.752814000	-2.489280000	-1.815033000
6	1.279324000	1.540892000	-2.335538000	6	-0.059483000	-1.904372000	-2.852167000
6	2.528784000	-0.532948000	-0.824007000	6	2.040855000	-0.381392000	-1.655486000
6	2.483804000	0.780064000	-0.314555000	6	1.279204000	0.172130000	-2.690997000
6	1.887392000	1.838451000	-1.115193000	6	0.196119000	-0.583734000	-3.254766000
6	-0.875582000	-3.506255000	-0.543204000	6	1.131232000	-0.823589000	2.690993000
6	0.399755000	-3.280434000	0.095158000	6	2.001256000	-0.010453000	1.886066000
6	-1.098051000	-3.030817000	-1.837531000	6	0.748486000	-2.110527000	2.280930000
6	1.408888000	-2.589637000	-0.584029000	6	2.385911000	-0.469028000	0.616785000
6	2.214326000	-1.609861000	0.111147000	6	2.491681000	0.382909000	-0.527511000
6	0.163064000	-3.005885000	1.485769000	6	1.528513000	1.365700000	1.982467000
6	0.941226000	-2.039206000	2.133004000	6	1.562544000	2.223063000	0.891765000
6	2.017742000	-1.369302000	1.463473000	6	2.193742000	1.822723000	-0.418682000
6	1.517895000	2.254525000	1.142024000	6	-0.527672000	1.632236000	-3.045650000
6	2.341293000	1.087844000	1.066765000	6	0.818908000	1.548005000	-2.531667000
6	2.273848000	-0.001079000	2.115954000	6	1.192876000	2.316374000	-1.440911000
6	0.540030000	2.439564000	2.130323000	6	-1.464582000	2.472030000	-2.436470000
6	-0.962458000	3.517681000	0.482154000	6	-3.197179000	0.744578000	-2.671163000
6	0.061533000	3.369323000	-0.522281000	6	-2.228623000	-0.121728000	-3.310121000
6	1.275808000	2.760662000	-0.199687000	6	-0.916436000	0.317257000	-3.489845000
6	-0.718889000	3.029014000	1.777076000	6	-2.822898000	2.020561000	-2.246005000
6	-3.012531000	2.112695000	1.867944000	6	-4.106289000	1.725690000	-0.165107000
6	-3.255319000	2.605094000	0.532134000	6	-4.494824000	0.406509000	-0.609724000
6	-2.236651000	3.280777000	-0.147614000	6	-4.051538000	-0.073870000	-1.844291000
6	-1.772929000	2.317464000	2.477112000	6	-3.284274000	2.518771000	-0.967944000
6	-1.814362000	0.034197000	3.391489000	6	-1.993583000	3.223728000	1.001336000
6	-3.093673000	-0.184908000	2.759011000	6	-2.843382000	2.404943000	1.835125000
6	-3.680026000	0.834605000	2.006467000	6	-3.881656000	1.667673000	1.262662000
6	-1.164507000	1.264396000	3.247343000	6	-2.210321000	3.280281000	-0.373024000
6	1.000553000	0.146433000	2.962608000	6	0.216551000	3.141002000	-0.787337000
6	0.321233000	-1.111460000	3.056399000	6	0.440527000	3.082059000	0.640155000
6	-1.055036000	-1.182144000	3.297534000	6	-0.643540000	3.133151000	1.519739000
6	0.261585000	1.316216000	3.021875000	6	-1.084926000	3.246553000	-1.285608000
7	3.540913000	-0.040211000	2.927197000	7	3.589181000	2.742936000	-0.628988000
1	3.580444000	0.831851000	3.453665000	8	3.648201000	3.825458000	-0.072651000
1	3.442678000	-0.769665000	3.633929000	8	4.487070000	2.269707000	-1.334334000
6	5.328983000	-0.021069000	0.491994000	6	5.286825000	-0.430583000	-0.422013000
7	5.636664000	-1.079789000	-0.264360000	7	5.232051000	-1.758424000	-0.572669000
7	5.588830000	1.079636000	-0.222120000	7	5.506511000	-0.163667000	0.870789000
6	6.047920000	0.713461000	-1.468351000	6	5.555190000	-1.353033000	1.567139000
1	6.301620000	1.443648000	-2.218854000	1	5.687198000	-1.377886000	2.636007000
6	6.080177000	-0.645791000	-1.495527000	6	5.392930000	-2.354274000	0.662866000
1	6.363863000	-1.333463000	-2.274750000	1	5.364800000	-3.424112000	0.784769000
1	4.848947000	-0.052272000	1.492271000	1	5.118323000	0.319312000	-1.184451000
6	5.279776000	2.435496000	0.207769000	6	5.450972000	1.168176000	1.457811000
1	4.591850000	2.887722000	-0.510022000	1	6.088855000	1.195131000	2.340478000
1	4.768558000	2.382733000	1.168681000	1	5.795428000	1.900241000	0.727918000
1	6.195179000	3.024703000	0.283309000	1	4.418069000	1.395712000	1.742856000
6	5.405408000	-2.464226000	0.116769000	6	5.008358000	-2.448052000	-1.833855000
1	4.701350000	-2.918224000	-0.583164000	1	5.940300000	-2.885107000	-2.198760000
1	6.347547000	-3.015268000	0.118069000	1	4.258643000	-3.225766000	-1.687222000
1	4.958270000	-2.481857000	1.109876000	1	4.621207000	-1.734070000	-2.559935000

(IM ⁺ ...X ⁻)...C ₆₀ C ₆₀ Cl ⁻				(IM ⁺ ...Br ⁻)...C ₆₀			
6	-2.413089000	3.302043000	0.367870000	6	-4.023129000	-1.947377000	0.982427000
6	-2.979520000	2.654419000	1.530190000	6	-4.016070000	-2.139758000	-0.451025000
6	-2.871436000	2.971157000	-0.907509000	6	-4.353512000	-0.702029000	1.517408000
6	-3.984954000	1.699408000	1.376291000	6	-4.340311000	-1.080547000	-1.299151000
6	-3.961240000	0.490346000	2.169171000	6	-3.574894000	-0.859029000	-2.505929000
6	-1.913747000	2.435010000	2.482826000	6	-2.912979000	-3.015690000	-0.778695000
6	-1.890858000	1.268386000	3.247774000	6	-2.174303000	-2.802128000	-1.943130000
6	-2.933181000	0.278682000	3.088462000	6	-2.510906000	-1.704728000	-2.822522000
6	-0.566724000	2.985270000	-1.770479000	6	-2.538867000	-0.898748000	3.168057000
6	-0.090882000	3.327524000	-0.447918000	6	-2.195385000	-2.188905000	2.612661000
6	-1.933056000	2.811318000	-1.996229000	6	-3.599306000	-0.168506000	2.630153000
6	-0.997476000	3.482687000	0.602444000	6	-2.924004000	-2.704121000	1.539985000
6	-0.689124000	2.947771000	1.909308000	6	-2.238291000	-3.364889000	0.451828000
6	1.156620000	2.631424000	-0.228439000	6	-0.755187000	-2.316762000	2.636749000
6	1.455153000	2.116938000	1.034726000	6	-0.094041000	-2.955992000	1.587387000
6	0.515876000	2.275408000	2.121846000	6	-0.848620000	-3.490140000	0.475353000
6	-1.473466000	0.845783000	-3.402553000	6	-2.285040000	1.905969000	2.792012000
6	-0.058627000	1.026585000	-3.169585000	6	-1.185669000	1.148598000	3.348807000
6	-2.394672000	1.722587000	-2.827492000	6	-3.470063000	1.258795000	2.438616000
6	0.387055000	2.079169000	-2.369560000	6	-1.311639000	-0.228501000	3.535713000
6	1.452704000	1.857829000	-1.416455000	6	-0.208749000	-1.104575000	3.206186000
6	0.546222000	-0.282570000	-3.049427000	6	0.046553000	1.702275000	2.832720000
6	1.573235000	-0.495253000	-2.131804000	6	1.110479000	0.856247000	2.511590000
6	2.029960000	0.594464000	-1.300327000	6	0.979280000	-0.571558000	2.704543000
6	-3.880697000	-0.160302000	-2.276989000	6	-3.608667000	2.590164000	0.374426000
6	-2.927292000	-1.068874000	-2.874821000	6	-2.381382000	3.260448000	0.741135000
6	-3.619692000	1.210218000	-2.254147000	6	-4.144080000	1.607452000	1.208060000
6	-1.744502000	-0.574849000	-3.426771000	6	-1.731282000	2.924542000	1.928614000
6	-0.496933000	-1.271750000	-3.209334000	6	-0.290025000	2.797273000	1.953435000
6	-2.903601000	-2.277201000	-2.081967000	6	-1.615088000	3.482087000	-0.465804000
6	-1.698448000	-2.948111000	-1.869582000	6	-0.227126000	3.355464000	-0.442222000
6	-0.473960000	-2.437976000	-2.444014000	6	0.449173000	3.006567000	0.787978000
6	-4.461061000	1.357459000	0.054210000	6	-4.684379000	0.210100000	-0.744290000
6	-4.731995000	-0.062660000	0.030318000	6	-4.130783000	1.228893000	-1.608489000
6	-3.914551000	1.982214000	-1.067482000	6	-4.690749000	0.395880000	0.638299000
6	-4.446315000	-0.807928000	-1.114259000	6	-3.601676000	2.397302000	-1.058942000
6	-3.842573000	-2.116482000	-0.993663000	6	-2.370135000	2.948106000	-1.578358000
6	-4.423085000	-0.598572000	1.337249000	6	-3.445460000	0.568384000	-2.696857000
6	-3.840181000	-1.860984000	1.453604000	6	-2.256696000	1.100774000	-3.198134000
6	-3.545097000	-2.633815000	0.267468000	6	-1.709741000	2.311879000	-2.629335000
6	0.025053000	-3.304501000	-0.328498000	6	1.559099000	1.941898000	-0.973174000
6	-1.389776000	-3.483986000	-0.562080000	6	0.460126000	2.694695000	-1.530279000
6	-2.297236000	-3.330786000	0.487470000	6	-0.268648000	2.183721000	-2.605474000
6	0.484018000	-2.977028000	0.947469000	6	1.894165000	0.700395000	-1.512258000
6	2.068788000	-1.362296000	-0.016482000	6	2.221084000	-0.210705000	0.753219000
6	1.597112000	-1.703291000	-1.339354000	6	1.879286000	1.079378000	1.310309000
6	0.592895000	-2.657022000	-1.491932000	6	1.551950000	2.134438000	0.459940000
6	1.526853000	-1.986193000	1.105743000	6	2.227488000	-0.396514000	-0.630372000
6	1.492811000	0.157367000	2.319728000	6	1.145405000	-2.598637000	-0.364181000
6	2.057654000	0.804813000	1.154377000	6	1.138801000	-2.405958000	1.068290000
6	2.332422000	0.059155000	0.007620000	6	1.663555000	-1.231707000	1.614139000
6	1.230607000	-1.213150000	2.293432000	6	1.677135000	-1.609611000	-1.196569000
6	-0.913996000	-0.848290000	3.443836000	6	-0.180755000	-1.909605000	-2.782694000

6	-0.643199000	0.571182000	3.468381000	6	-0.733743000	-2.928979000	-1.918391000
6	0.539496000	1.065735000	2.914995000	6	-0.083053000	-3.268003000	-0.731355000
6	0.006313000	-1.724796000	2.866156000	6	1.003782000	-1.261540000	-2.429374000
6	-1.821405000	-2.989404000	1.808789000	6	0.074874000	0.895984000	-3.161446000
6	-2.774610000	-2.080111000	2.406215000	6	-1.153104000	0.224166000	-3.524729000
6	-2.329564000	-1.029622000	3.209294000	6	-1.279320000	-1.153533000	-3.342275000
6	-0.455082000	-2.814538000	2.033902000	6	1.135635000	0.166775000	-2.619243000
17	4.959737000	-1.020455000	-1.691184000	35	4.870028000	2.267494000	-0.207039000
6	5.734546000	0.093004000	0.642694000	6	5.552419000	-0.754208000	-0.123594000
7	6.855514000	-0.605893000	0.865909000	7	5.136814000	-1.721866000	-0.950384000
7	6.070940000	1.322355000	0.231298000	7	5.339011000	-1.170132000	1.130519000
6	7.442720000	1.362636000	0.062676000	6	4.790375000	-2.436014000	1.101854000
1	7.940188000	2.245304000	-0.302621000	1	4.521450000	-2.962022000	2.003116000
6	7.932010000	0.160028000	0.457713000	6	4.661467000	-2.785021000	-0.206650000
1	8.940687000	-0.214700000	0.504372000	1	4.255733000	-3.670402000	-0.667829000
1	4.733602000	-0.232440000	0.871073000	1	5.786386000	0.293236000	-0.389566000
6	5.107752000	2.243599000	-0.346008000	6	5.506559000	-0.303232000	2.290624000
1	4.721142000	1.789416000	-1.266440000	1	6.488220000	-0.449752000	2.744669000
1	4.286647000	2.413033000	0.354136000	1	5.390255000	0.731122000	1.937529000
1	5.602684000	3.190809000	-0.556264000	1	4.725957000	-0.536681000	3.016237000
6	6.847432000	-2.046793000	1.045499000	6	5.071290000	-1.572737000	-2.394275000
1	6.460659000	-2.493422000	0.121784000	1	5.876750000	-2.124783000	-2.882588000
1	7.861217000	-2.386790000	1.252581000	1	4.104775000	-1.940522000	-2.745480000
1	6.202054000	-2.313588000	1.883539000	1	5.149955000	-0.510492000	-2.630468000

Cartesian coordinates of optimized geometry of ligands C₆₀, C₆₀^{•-}, exohedral fullerenes at Mo6L/6-31G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.

C ₆₀				C ₆₀ ^{•-}			
6	-1.694235000	2.876716000	1.169945000	6	0.380145000	-1.173229000	3.323467000
6	-1.015488000	3.388762000	0.000000000	6	1.224350000	-0.002102000	3.308739000
6	-0.960156000	2.512413000	2.298722000	6	0.752439000	-2.314339000	2.587588000
6	0.373217000	3.517998000	0.000000000	6	2.411940000	0.002744000	2.574611000
6	1.134317000	3.139925000	-1.170085000	6	2.801629000	1.174034000	1.826508000
6	-1.694235000	2.876716000	-1.169945000	6	0.376089000	1.175160000	3.316484000
6	-0.960156000	2.512413000	-2.298722000	6	0.750520000	2.309672000	2.584891000
6	0.479726000	2.646349000	-2.298675000	6	1.977755000	2.314914000	1.830297000
6	-2.355773000	0.506869000	2.590892000	6	-1.572897000	-2.594783000	1.818278000
6	-3.116859000	0.884873000	1.420643000	6	-1.954966000	-1.416712000	2.576109000
6	-1.296790000	1.305962000	3.021957000	6	-0.242644000	-3.027923000	1.825186000
6	-2.791989000	2.048222000	0.723095000	6	-0.988694000	-0.723252000	3.310450000
6	-2.791989000	2.048222000	-0.723095000	6	-0.992779000	0.729035000	3.314082000
6	-3.453682000	-0.321387000	0.697505000	6	-2.957186000	-0.700043000	1.828208000
6	-3.453682000	-0.321387000	-0.697505000	6	-2.960587000	0.708910000	1.829515000
6	-3.116859000	0.884873000	-1.420643000	6	-1.961244000	1.424974000	2.582096000
6	0.064754000	-0.694450000	3.468855000	6	-0.365079000	-3.477731000	-0.595501000
6	-1.033200000	-1.522858000	3.021722000	6	-1.741560000	-3.029340000	-0.600269000
6	-0.064754000	0.694450000	3.468855000	6	0.368624000	-3.477168000	0.591735000
6	-2.221456000	-0.932987000	2.590584000	6	-2.330337000	-2.595376000	0.592953000
6	-2.900087000	-1.444751000	1.420397000	6	-3.177587000	-1.416831000	0.596075000
6	-0.479726000	-2.646349000	2.298675000	6	-1.977755000	-2.314914000	-1.830297000
6	-1.134317000	-3.139925000	1.170085000	6	-2.801629000	-1.174034000	-1.826508000

6	-2.366154000	-2.528337000	0.723070000	6	-3.402315000	-0.723120000	-0.595668000
6	2.221456000	0.932987000	2.590584000	6	2.336100000	-2.597330000	-0.594746000
6	2.355773000	-0.506869000	2.590892000	6	1.576522000	-2.598247000	-1.824291000
6	1.033200000	1.522858000	3.021722000	6	1.743276000	-3.029105000	0.592576000
6	1.296790000	-1.305962000	3.021957000	6	0.249422000	-3.030292000	-1.825529000
6	0.960156000	-2.512413000	2.298722000	6	-0.750520000	-2.309672000	-2.584891000
6	3.116859000	-0.884873000	1.420643000	6	1.961244000	-1.424974000	-2.582096000
6	2.791989000	-2.048222000	0.723095000	6	0.992779000	-0.729035000	-3.314082000
6	1.694235000	-2.876716000	1.169945000	6	-0.376089000	-1.175160000	-3.316484000
6	1.134317000	3.139925000	1.170085000	6	2.798235000	-1.174543000	1.818926000
6	2.366154000	2.528337000	0.723070000	6	3.408830000	-0.728949000	0.594373000
6	0.479726000	2.646349000	2.298675000	6	1.975272000	-2.308821000	1.827117000
6	2.900087000	1.444751000	1.420397000	6	3.187242000	-1.424843000	-0.600484000
6	3.453682000	0.321387000	0.697505000	6	2.960587000	-0.708910000	-1.829515000
6	2.366154000	2.528337000	-0.723070000	6	3.402315000	0.723120000	0.595668000
6	2.900087000	1.444751000	-1.420397000	6	3.177587000	1.416831000	-0.596075000
6	3.453682000	0.321387000	-0.697505000	6	2.957186000	0.700043000	-1.828208000
6	1.694235000	-2.876716000	-1.169945000	6	-0.380145000	1.173229000	-3.323467000
6	2.791989000	-2.048222000	-0.723095000	6	0.988694000	0.723252000	-3.310450000
6	3.116859000	-0.884873000	-1.420643000	6	1.954966000	1.416712000	-2.576109000
6	0.960156000	-2.512413000	-2.298722000	6	-0.752439000	2.314339000	-2.587588000
6	-1.134317000	-3.139925000	-1.170085000	6	-2.798235000	1.174543000	-1.818926000
6	-0.373217000	-3.517998000	0.000000000	6	-2.411940000	-0.002744000	-2.574611000
6	1.015488000	-3.388762000	0.000000000	6	-1.224350000	0.002102000	-3.308739000
6	-0.479726000	-2.646349000	-2.298675000	6	-1.975272000	2.308821000	-1.827117000
6	-2.221456000	-0.932987000	-2.590584000	6	-2.336100000	2.597330000	0.594746000
6	-2.900087000	-1.444751000	-1.420397000	6	-3.187242000	1.424843000	0.600484000
6	-2.366154000	-2.528337000	-0.723070000	6	-3.408830000	0.728949000	-0.594373000
6	-1.033200000	-1.522858000	-3.021722000	6	-1.743276000	3.029105000	-0.592576000
6	-0.064754000	0.694450000	-3.468855000	6	0.365079000	3.477731000	0.595501000
6	-1.296790000	1.305962000	-3.021957000	6	-0.249422000	3.030292000	1.825529000
6	-2.355773000	0.506869000	-2.590892000	6	-1.576522000	2.598247000	1.824291000
6	0.064754000	-0.694450000	-3.468855000	6	-0.368624000	3.477168000	-0.591735000
6	2.355773000	-0.506869000	-2.590892000	6	1.572897000	2.594783000	-1.818278000
6	2.221456000	0.932987000	-2.590584000	6	2.330337000	2.595376000	-0.592953000
6	1.033200000	1.522858000	-3.021722000	6	1.741560000	3.029340000	0.600269000
6	1.296790000	-1.305962000	-3.021957000	6	0.242644000	3.027923000	-1.825186000
		(C ₆₀ H) ⁻				(C ₆₀ F) ⁻	
6	0.178693000	-3.470223000	0.692438000	6	3.664930000	0.007178000	0.000301000
6	1.320127000	-2.952969000	1.422203000	6	3.372753000	0.810540000	-1.165530000
6	0.176692000	-3.468922000	-0.701080000	6	2.891207000	2.097662000	-0.711122000
6	2.408186000	-2.415823000	0.717856000	6	2.890954000	2.089065000	0.735977000
6	3.093324000	-1.246310000	1.173880000	6	3.372558000	0.796881000	1.175373000
6	0.836666000	-2.265701000	2.585358000	6	2.810154000	0.192268000	2.301205000
6	1.468828000	-1.085594000	3.002402000	6	2.534854000	-1.229988000	2.293853000
6	2.608179000	-0.569749000	2.279881000	6	2.823638000	-1.992010000	1.158302000
6	-2.170300000	-2.726089000	-0.723815000	6	3.406203000	-1.366806000	-0.007900000
6	-2.168197000	-2.727675000	0.723132000	6	2.823542000	-1.978000000	-1.181164000
6	-1.017331000	-3.091966000	-1.422507000	6	2.535404000	-1.202987000	-2.308099000
6	-1.013462000	-3.095219000	1.418041000	6	2.810260000	0.219336000	-2.298369000
6	-0.603816000	-2.350465000	2.591046000	6	1.759120000	0.891371000	-3.028455000
6	-2.954325000	-1.599917000	1.170377000	6	1.282595000	2.129513000	-2.579487000
6	-2.559335000	-0.880237000	2.303150000	6	1.868258000	2.744807000	-1.404880000
6	-1.363352000	-1.255758000	3.015022000	6	0.811673000	3.412402000	-0.678083000

6	-1.371448000	-1.248776000	-3.014406000	6	0.811566000	3.404201000	0.718112000
6	-2.565619000	-0.874936000	-2.298698000	6	1.868034000	2.728128000	1.437163000
6	-0.610790000	-2.344561000	-2.594994000	6	1.282328000	2.099139000	2.604449000
6	-2.957468000	-1.597197000	-1.166409000	6	1.758756000	0.855761000	3.038730000
6	-3.450703000	-0.908786000	0.003448000	6	0.816821000	-0.153108000	3.463650000
6	-2.640813000	0.573851000	-2.294441000	6	1.298430000	-1.441298000	3.009334000
6	-3.116522000	1.240454000	-1.163302000	6	0.394724000	-2.415177000	2.577694000
6	-3.514154000	0.491007000	0.005207000	6	0.694615000	-3.204026000	1.401094000
6	1.460941000	-1.078538000	-3.008910000	6	1.888926000	-2.997959000	0.705948000
6	0.677782000	0.044906000	-3.445589000	6	1.888956000	-2.989362000	-0.740696000
6	0.829602000	-2.259517000	-2.592821000	6	0.694791000	-3.187228000	-1.438366000
6	-0.717329000	-0.033053000	-3.458008000	6	0.395052000	-2.384610000	-2.605657000
6	-1.513430000	1.092644000	-3.031469000	6	1.298830000	-1.405956000	-3.026084000
6	1.345171000	1.260301000	-3.005270000	6	0.817257000	-0.112504000	-3.465224000
6	0.563878000	2.360759000	-2.598128000	6	-0.554083000	0.156662000	-3.451414000
6	-0.868489000	2.259097000	-2.589408000	6	-1.046518000	1.446057000	-2.998615000
6	2.406189000	-2.414244000	-0.729788000	6	-0.126575000	2.424732000	-2.585661000
6	3.089952000	-1.243410000	-1.184805000	6	-0.421392000	3.202935000	-1.404713000
6	1.316132000	-2.949275000	-1.432521000	6	-1.605170000	2.985348000	-0.700796000
6	2.602215000	-0.564708000	-2.288183000	6	-1.605280000	2.976909000	0.735521000
6	2.545632000	0.897447000	-2.319284000	6	-0.421558000	3.186214000	1.442044000
6	3.769984000	-0.538465000	-0.005672000	6	-0.126870000	2.394288000	2.613822000
6	3.450564000	0.944207000	-0.003244000	6	-1.046831000	1.410848000	3.015229000
6	2.910318000	1.586989000	-1.145521000	6	-0.554480000	0.116218000	3.452927000
6	-0.226861000	3.476934000	-0.693894000	6	-1.485147000	-0.884909000	3.002569000
6	0.964406000	3.097473000	-1.420835000	6	-1.021901000	-2.132829000	2.575525000
6	2.108716000	2.727515000	-0.717119000	6	-1.599091000	-2.741663000	1.406827000
6	-0.224935000	3.475126000	0.702441000	6	-0.538581000	-3.408215000	0.676528000
6	-2.460024000	2.451678000	0.729419000	6	-0.538488000	-3.399939000	-0.716423000
6	-2.462193000	2.453580000	-0.717147000	6	-1.598858000	-2.724871000	-1.439009000
6	-1.363983000	2.953109000	-1.417030000	6	-1.021534000	-2.102407000	-2.600405000
6	-1.360024000	2.949739000	1.427566000	6	-1.484773000	-0.849591000	-3.012915000
6	-1.505445000	1.085588000	3.038384000	6	-2.547297000	-0.186885000	-2.287585000
6	-2.634722000	0.568439000	2.302770000	6	-2.288165000	1.245213000	-2.310019000
6	-3.113438000	1.237699000	1.174425000	6	-2.552740000	1.968640000	-1.133679000
6	-0.861321000	2.252780000	2.596836000	6	-3.176749000	1.391282000	0.007994000
6	1.353309000	1.253218000	3.004611000	6	-2.552967000	1.955344000	1.156529000
6	0.686963000	0.036778000	3.444024000	6	-2.288437000	1.218045000	2.324219000
6	-0.708141000	-0.041075000	3.459819000	6	-2.547517000	-0.213738000	2.284911000
6	0.570930000	2.354688000	2.602264000	6	-3.126719000	-0.809876000	1.174882000
6	2.110705000	2.725804000	0.717667000	6	-2.606378000	-2.062633000	0.712557000
6	2.913448000	1.583952000	1.141274000	6	-2.606156000	-2.054010000	-0.736943000
6	2.552404000	0.892075000	2.315482000	6	-3.126677000	-0.796068000	-1.184687000
6	0.968304000	3.093826000	1.425156000	6	-3.679188000	-0.011422000	-0.000263000
1	4.858381000	-0.735026000	-0.007702000	9	-5.114045000	-0.077942000	-0.000685000
$(C_{60}OH)^-$				$(C_{60}CN)^-$			
6	2.297793000	1.244958000	2.297549000	6	-0.464196000	-2.404225000	-2.592446000
6	1.059094000	1.469848000	2.980807000	6	0.950245000	-2.115442000	-2.586324000
6	2.571374000	1.949255000	1.110388000	6	-1.370791000	-1.428497000	-3.014835000
6	0.150884000	2.455769000	2.554863000	6	1.408205000	-0.860157000	-3.004678000
6	-1.260753000	2.177439000	2.550445000	6	2.466459000	-0.188677000	-2.285376000
6	0.550090000	0.191654000	3.448849000	6	1.528165000	-2.730023000	-1.424995000
6	-0.824718000	-0.059632000	3.464078000	6	2.533620000	-2.050212000	-0.724221000
6	-1.753671000	0.950405000	3.014677000	6	3.047186000	-0.800234000	-1.188713000
6	3.703721000	-0.061559000	-0.000191000				

6	3.109005000	-0.820512000	1.197128000	6	-2.894313000	-1.997108000	-1.169225000
6	3.194394000	1.355289000	-0.022374000	6	-1.956240000	-3.003012000	-0.724113000
6	2.539390000	-0.192786000	2.293325000	6	-2.607869000	-1.227115000	-2.300866000
6	1.468408000	-0.832195000	3.026335000	6	-0.762067000	-3.201655000	-1.421080000
6	2.576972000	-2.078080000	0.767099000	6	0.471667000	-3.405453000	-0.697222000
6	1.560485000	-2.728758000	1.477219000	6	-1.956205000	-3.003386000	0.722662000
6	0.989909000	-2.085671000	2.630107000	6	-0.762001000	-3.202388000	1.419480000
6	2.305006000	1.159482000	-2.336093000	6	0.471702000	-3.405815000	0.695458000
6	2.546308000	-0.277728000	-2.278043000	6	-3.453791000	0.789468000	-1.169382000
6	2.577410000	1.910377000	-1.178565000	6	-3.742474000	-0.008146000	0.000084000
6	3.114774000	-0.867886000	-1.160940000	6	-2.887535000	0.195354000	-2.299077000
6	2.577747000	-2.105027000	-0.682175000	6	-3.480940000	-1.383288000	-0.000278000
6	1.475725000	-0.943520000	-2.987156000	6	-2.894251000	-1.997705000	1.168331000
6	0.996022000	-2.181396000	-2.546194000	6	-3.453739000	0.788874000	1.169939000
6	1.563167000	-2.781871000	-1.369856000	6	-2.887435000	0.194178000	2.299305000
6	0.460072000	3.162415000	-1.482549000	6	-2.607765000	-1.228296000	2.300351000
6	0.157548000	2.358672000	-2.643964000	6	-1.369420000	2.111955000	-2.591829000
6	1.640335000	2.947686000	-0.771713000	6	-1.959445000	2.730657000	-1.420921000
6	1.067259000	1.358119000	-3.030298000	6	-1.841958000	0.867891000	-3.034120000
6	0.558657000	0.063421000	-3.450325000	6	-2.978184000	2.082116000	-0.722869000
6	-1.254518000	2.080951000	-2.632940000	6	-2.978146000	2.081743000	0.724061000
6	-1.746030000	0.837385000	-3.051759000	6	-0.907573000	3.408318000	-0.697237000
6	-0.815905000	-0.188593000	-3.460896000	6	-0.907540000	3.407954000	0.699006000
6	0.456694000	3.214800000	1.364206000	6	-1.959371000	2.729921000	1.422397000
6	-0.772696000	3.430341000	0.633198000	6	0.475333000	0.140598000	-3.446743000
6	1.638303000	2.974129000	0.664151000	6	0.963988000	1.436547000	-3.005699000
6	-0.771072000	3.404605000	-0.762837000	6	-0.894550000	-0.134136000	-3.460595000
6	-1.834506000	2.731787000	-1.474697000	6	0.035937000	2.414247000	-2.599804000
6	-1.837691000	2.784344000	1.367245000	6	0.326001000	3.199309000	-1.422463000
6	-2.867330000	2.140876000	0.680298000	6	2.206470000	1.248411000	-2.320617000
6	-2.865718000	2.114053000	-0.766483000	6	2.463772000	1.978530000	-1.145144000
6	-2.548944000	-1.229398000	-2.281423000	6	1.509537000	2.993364000	-0.716457000
6	-2.805603000	0.196497000	-2.306851000	6	0.036060000	2.412922000	2.601027000
6	-3.362520000	0.821886000	-1.189567000	6	0.326067000	3.198578000	1.424063000
6	-2.849082000	-1.973013000	-1.136160000	6	1.509571000	2.993002000	0.717897000
6	-0.735551000	-3.215317000	-1.360555000	6	0.964131000	1.435013000	3.006375000
6	-0.423698000	-2.445596000	-2.546848000	6	-0.894389000	-0.135903000	3.460549000
6	-1.314433000	-1.465290000	-2.991522000	6	-1.841821000	0.866337000	3.034637000
6	-1.927894000	-2.984938000	-0.669793000	6	-1.369297000	2.110631000	2.592963000
6	-0.738772000	-3.162176000	1.478516000	6	0.475494000	0.138836000	3.446793000
6	0.492634000	-3.399487000	0.761096000	6	0.950362000	-2.116771000	2.585198000
6	0.494063000	-3.425548000	-0.631734000	6	-0.464082000	-2.405552000	2.591234000
6	-1.929548000	-2.958075000	0.776720000	6	-1.370653000	-1.430037000	3.014166000
6	-2.554626000	-1.143704000	2.319848000	6	1.408339000	-0.861702000	3.004163000
6	-1.322132000	-1.352881000	3.041884000	6	3.047200000	-0.800803000	1.188083000
6	-0.429852000	-2.348800000	2.636154000	6	2.533651000	-2.050587000	0.723051000
6	-2.851913000	-1.929462000	1.202555000	6	1.528239000	-2.730764000	1.423526000
6	-3.666284000	0.051215000	-0.005091000	6	2.466533000	-0.189850000	2.285122000
6	-3.365713000	0.865633000	1.150453000	6	2.463831000	1.977955000	1.146014000
6	-2.811303000	0.282281000	2.291564000	6	3.090718000	1.426928000	0.000280000
6	-3.425786000	-1.326454000	0.020808000	6	3.630384000	0.002114000	-0.000063000
1	5.464199000	0.584554000	0.467356000	6	2.206573000	1.247211000	2.321130000
8	5.148241000	-0.163233000	-0.052400000	7	6.272175000	-0.062977000	0.000100000
				6	5.105061000	-0.038549000	-0.000069000
		(C ₆₀ NH ₂) ⁻				(C ₆₀ NO ₂) ⁻	

6	-2.843890000	-1.986929000	-1.130615000	6	-1.994327000	0.844545000	-3.032516000
6	-1.910857000	-2.994899000	-0.679614000	6	-1.033207000	-0.143043000	-3.463782000
6	-2.558180000	-1.232055000	-2.272671000	6	-1.542546000	2.094641000	-2.590746000
6	-0.722277000	-3.210782000	-1.381454000	6	0.332578000	0.152722000	-3.451109000
6	0.514339000	-3.416163000	-0.663311000	6	1.282198000	-0.833521000	-3.007629000
6	-1.901818000	-2.979232000	0.767065000	6	-1.489823000	-1.443321000	-3.017843000
6	-0.704492000	-3.179779000	1.458566000	6	-0.567886000	-2.402685000	-2.592587000
6	0.523150000	-3.401160000	0.729731000	6	0.842835000	-2.093396000	-2.587938000
6	-3.379204000	0.804082000	-1.158442000	6	-3.150297000	2.041008000	-0.722288000
6	-3.667700000	0.022075000	0.021879000	6	-3.606644000	0.742414000	-1.169920000
6	-2.825567000	0.192409000	-2.284982000	6	-2.140010000	2.704156000	-1.419424000
6	-3.417699000	-1.355009000	0.035281000	6	-3.032479000	0.156213000	-2.299496000
6	-2.829355000	-1.961501000	1.207590000	6	-2.730266000	-1.260565000	-2.301714000
6	-3.364906000	0.829645000	1.181117000	6	-3.883701000	-0.060289000	-0.000244000
6	-2.796985000	0.242510000	2.313677000	6	-3.598583000	-1.429215000	-0.001144000
6	-2.529541000	-1.182128000	2.329097000	6	-3.003880000	-2.035267000	-1.170994000
6	-1.292601000	2.092566000	-2.608363000	6	-1.097116000	3.394996000	0.700339000
6	-1.869566000	2.729435000	-1.440737000	6	-2.140148000	2.702233000	1.422897000
6	-1.778330000	0.847770000	-3.034184000	6	-1.097043000	3.395939000	-0.695822000
6	-2.889820000	2.097580000	-0.729229000	6	-3.150360000	2.040033000	0.724753000
6	-2.880670000	2.113197000	0.717438000	6	-3.606771000	0.740838000	1.170568000
6	-0.807136000	3.406321000	-0.731508000	6	-1.542828000	2.091129000	2.593460000
6	-0.798279000	3.421008000	0.664685000	6	-1.994675000	0.840431000	3.033471000
6	-1.851416000	2.759876000	1.401966000	6	-3.032736000	0.153094000	2.299401000
6	0.530234000	0.095738000	-3.454022000	6	1.327699000	3.017088000	-0.716185000
6	1.032250000	1.392037000	-3.028375000	6	1.327626000	3.016110000	0.720465000
6	-0.842573000	-0.167084000	-3.455980000	6	0.139957000	3.206917000	-1.421164000
6	0.115638000	2.382058000	-2.627689000	6	0.139808000	3.204997000	1.425565000
6	0.420462000	3.179485000	-1.461887000	6	-0.139612000	2.412957000	2.601137000
6	2.276366000	1.199158000	-2.346503000	6	2.294223000	2.016879000	1.148603000
6	2.551045000	1.942935000	-1.183231000	6	2.044198000	1.278901000	2.317682000
6	1.607226000	2.970521000	-0.761843000	6	0.798930000	1.450128000	3.008494000
6	-0.425426000	-2.429594000	-2.564376000	6	0.799253000	1.454190000	-3.006383000
6	0.991809000	-2.153693000	-2.572320000	6	2.044448000	1.282049000	-2.315677000
6	-1.327201000	-1.452000000	-2.992910000	6	-0.139328000	2.416479000	-2.597841000
6	1.458317000	-0.907218000	-3.006772000	6	2.294331000	2.018434000	-1.145581000
6	2.528468000	-0.237778000	-2.301040000	6	2.929603000	1.461826000	0.001167000
6	1.572110000	-2.758313000	-1.406027000	6	2.329691000	-0.145653000	-2.285429000
6	2.585381000	-2.075691000	-0.719837000	6	2.915385000	-0.743194000	-1.179594000
6	3.109482000	-0.831519000	-1.192716000	6	3.415289000	0.065886000	0.000297000
6	2.563300000	1.964577000	1.104338000	6	1.281852000	-0.837597000	3.006683000
6	3.175063000	1.385139000	-0.036549000	6	2.329434000	-0.148745000	2.285537000
6	3.714151000	-0.028357000	-0.028313000	6	2.915220000	-0.744740000	1.178899000
6	2.304277000	1.248981000	2.290781000	6	0.842553000	-2.096894000	2.585221000
6	0.147864000	2.438535000	2.572153000	6	-1.490145000	-1.447397000	3.015746000
6	0.438439000	3.209302000	1.384179000	6	-1.033589000	-0.147728000	3.463507000
6	1.615927000	2.985768000	0.673561000	6	0.332197000	0.148056000	3.451400000
6	1.069045000	1.457042000	2.983477000	6	-0.568165000	-2.406194000	2.589307000
6	-0.799943000	-0.091950000	3.467751000	6	-2.050563000	-3.027514000	0.721089000
6	-1.740823000	0.913591000	3.035444000	6	-3.003984000	-2.036850000	1.167945000
6	-1.259981000	2.148642000	2.576004000	6	-2.730505000	-1.263693000	2.299739000
6	0.573000000	0.170365000	3.444856000	6	-0.852951000	-3.207810000	1.417516000
6	1.024257000	-2.098121000	2.605921000	6	0.383961000	-3.392810000	-0.698834000
6	-0.392894000	-2.372946000	2.620352000	6	-0.852803000	-3.205893000	-1.421917000
6	-1.289939000	-1.386524000	3.039238000	6	-2.050493000	-3.026537000	-0.725388000

6	1.495815000	-0.842733000	3.008986000	6	0.383889000	-3.393730000	0.694316000
6	3.117863000	-0.801546000	1.165192000	6	2.425469000	-2.011666000	0.722074000
6	2.594073000	-2.060006000	0.729887000	6	2.425542000	-2.010719000	-0.724503000
6	1.590457000	-2.727447000	1.444474000	6	1.431245000	-2.701469000	-1.425272000
6	2.554891000	-0.187490000	2.272804000	6	1.431108000	-2.703388000	1.421801000
7	5.197549000	-0.040937000	-0.101441000	7	5.068487000	-0.011390000	0.000083000
1	5.535984000	0.489321000	0.698819000	8	5.554578000	-1.136569000	0.000327000
1	5.507390000	-0.998969000	0.059343000	8	5.690701000	1.038712000	-0.000485000
Cl ⁻ ...C ₆₀				Br ⁻ ...C ₆₀			
6	-2.083523000	-2.419578000	1.848451000	6	-2.355472000	-1.981107000	2.316597000
6	-2.852486000	-2.347422000	0.625215000	6	-3.067697000	-2.246707000	1.085346000
6	-2.080815000	-1.340950000	2.734994000	6	-2.437992000	-0.720177000	2.911109000
6	-3.593385000	-1.200817000	0.331444000	6	-3.837115000	-1.243589000	0.492159000
6	-3.604120000	-0.672506000	-1.014716000	6	-3.802809000	-1.060353000	-0.941906000
6	-2.096852000	-3.007965000	-0.416407000	6	-2.238754000	-3.103694000	0.267245000
6	-2.107149000	-2.498099000	-1.716228000	6	-2.205365000	-2.926699000	-1.117281000
6	-2.873327000	-1.309355000	-2.020013000	6	-3.000804000	-1.886462000	-1.731677000
6	0.341537000	-1.604215000	3.088098000	6	-0.026853000	-0.771576000	3.407981000
6	0.338859000	-2.722152000	2.169301000	6	0.058245000	-2.079105000	2.793737000
6	-0.848570000	-0.926792000	3.369266000	6	-1.253239000	-0.104464000	3.468827000
6	-0.854045000	-3.125559000	1.561773000	6	-1.089085000	-2.676259000	2.259679000
6	-0.862244000	-3.488571000	0.164089000	6	-1.015647000	-3.366973000	0.994148000
6	1.563907000	-2.674982000	1.405820000	6	1.314961000	-2.159989000	2.089788000
6	1.555999000	-3.026348000	0.054476000	6	1.385459000	-2.825681000	0.863940000
6	0.322841000	-3.435048000	-0.575758000	6	0.200406000	-3.436588000	0.307655000
6	0.334202000	1.227181000	3.258334000	6	-0.149639000	2.013934000	2.878938000
6	1.564461000	0.526119000	2.975519000	6	1.118448000	1.325648000	2.823394000
6	-0.852359000	0.514588000	3.455974000	6	-1.316328000	1.313249000	3.199598000
6	1.568085000	-0.867796000	2.891692000	6	1.179149000	-0.045316000	3.082112000
6	2.326819000	-1.528118000	1.851080000	6	2.010655000	-0.901738000	2.265561000
6	2.319289000	1.310082000	2.021218000	6	1.886021000	1.887880000	1.732922000
6	3.041665000	0.672490000	1.014923000	6	2.678845000	1.058997000	0.940850000
6	3.045738000	-0.771083000	0.928589000	6	2.744458000	-0.359569000	1.212564000
6	-2.095777000	2.171423000	2.123678000	6	-2.555963000	2.532104000	1.455488000
6	-0.869992000	2.913209000	1.923871000	6	-1.351019000	3.261284000	1.126430000
6	-2.086839000	0.994764000	2.875088000	6	-2.538556000	1.575860000	2.472800000
6	0.325144000	2.446650000	2.479192000	6	-0.167617000	3.004711000	1.824637000
6	1.550266000	2.497966000	1.716188000	6	1.089806000	2.927910000	1.117867000
6	-0.880631000	3.440430000	0.579605000	6	-1.316768000	3.443630000	-0.306177000
6	0.304421000	3.482951000	-0.160884000	6	-0.100878000	3.363110000	-0.990197000
6	1.540024000	3.008328000	0.416461000	6	1.122753000	3.103411000	-0.267088000
6	-3.590324000	-0.083699000	1.249647000	6	-3.921067000	0.062348000	1.107331000
6	-3.599457000	1.134718000	0.471291000	6	-3.938578000	1.052406000	0.053884000
6	-2.846757000	-0.152573000	2.429600000	6	-3.232866000	0.318896000	2.295618000
6	-2.864706000	2.241943000	0.900387000	6	-3.267575000	2.265674000	0.224595000
6	-2.112835000	3.026196000	-0.054441000	6	-2.501212000	2.828635000	-0.864674000
6	-3.607884000	0.771093000	-0.928318000	6	-3.865417000	0.358896000	-1.212653000
6	-2.880674000	1.527449000	-1.849956000	6	-3.123693000	0.901365000	-2.264277000
6	-2.120784000	2.675299000	-1.405830000	6	-2.429458000	2.158607000	-2.087879000
6	1.526627000	2.419727000	-1.848315000	6	1.240944000	1.983365000	-2.318388000
6	0.296148000	3.119215000	-1.561496000	6	-0.026753000	2.670127000	-2.258568000
6	-0.896661000	2.725225000	-2.174988000	6	-1.173800000	2.080041000	-2.800171000
6	1.524038000	1.341095000	-2.735043000	6	1.322135000	0.719871000	-2.908276000
6	3.027082000	0.083739000	-1.249107000	6	2.804251000	-0.062806000	-1.109196000
6	3.030374000	1.200692000	-0.331099000	6	2.714471000	1.242774000	-0.492506000

6	2.298058000	2.348844000	-0.625468000	6	1.953708000	2.248232000	-1.086085000
6	2.292326000	0.152730000	-2.430839000	6	2.121643000	-0.318651000	-2.296770000
6	1.538801000	-2.171196000	-2.123357000	6	1.440457000	-2.530840000	-1.454728000
6	2.310409000	-2.243113000	-0.900793000	6	2.157189000	-2.266808000	-0.224512000
6	3.036737000	-1.134618000	-0.471008000	6	2.824053000	-1.054896000	-0.054260000
6	1.530088000	-0.994723000	-2.875281000	6	1.423375000	-1.575676000	-2.472926000
6	-0.891931000	-1.231757000	-3.262745000	6	-0.966892000	-2.019505000	-2.881484000
6	-0.882956000	-2.448811000	-2.485148000	6	-0.949088000	-3.007333000	-1.829948000
6	0.312115000	-2.906736000	-1.922749000	6	0.234895000	-3.254126000	-1.126762000
6	0.294587000	-0.516380000	-3.449678000	6	0.200536000	-1.313468000	-3.192778000
6	-0.899296000	1.609524000	-3.092110000	6	-1.089437000	0.775190000	-3.412718000
6	-2.124845000	0.867915000	-2.891703000	6	-2.295110000	0.045669000	-3.083557000
6	-2.121193000	-0.525940000	-2.975244000	6	-2.233587000	-1.324410000	-2.821791000
6	0.290781000	0.928038000	-3.362837000	6	0.136988000	0.106410000	-3.462344000
17	5.905055000	-0.000961000	-0.001307000	35	5.739134000	-0.000972000	-0.000210000