

Polyanionic Cyano-fullerides for CO₂ Capture: A DFT Prediction

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Table S1. The sp^2-sp^2 C—C and sp^3-sp^2 C—C bond lengths of the carbon cage in Å at M06L/6-31G(d,p) level.

System	sp^3-sp^2 C—C	sp^2-sp^2 C—C
$(C_{60}(CN))^-$	1.54	1.43
$(C_{60}(CN)_2)^{2-}$	1.54	1.43
$(C_{60}(CN)_3)^{3-}$	1.54	1.43
$(C_{60}(CN)_4)^{4-}$	1.54	1.43
$(C_{60}(CN)_5)^{5-}$	1.54	1.43
$(C_{60}(CN)_6)^{6-}$	1.55	1.43
$IM^+...((C_{60}(CN))^-)$	1.54	1.43
$(IM^+)_2...((C_{60}(CN)_2)^{2-})$	1.54	1.43
$(IM^+)_3...((C_{60}(CN)_3)^{3-})$	1.54	1.43
$(IM^+)_4...((C_{60}(CN)_4)^{4-})$	1.54	1.43
$(IM^+)_5...((C_{60}(CN)_5)^{5-})$	1.54	1.43
$(IM^+)_6...((C_{60}(CN)_6)^{6-})$	1.54	1.43

Table S2. The energetics (kcal/mol) of the imidazolium cation-polyanionic fulleride complexes in the solvent DCM at M06L/6-311++G(d,p)//M06L/6-31G(d,p) level.

System	E_b'	G_b'	E_b'/IM	G_b'/IM
$IM^+...((C_{60}(CN))^-)$	-62.4	-49.9	-62.4	-49.9
$(IM^+)_2...((C_{60}(CN)_2)^{2-})$	-129.4	-103.5	-64.7	-51.7
$(IM^+)_3...((C_{60}(CN)_3)^{3-})$	-201.9	-163.5	-67.3	-54.5
$(IM^+)_4...((C_{60}(CN)_4)^{4-})$	-279.3	-227.0	-69.8	-56.8
$(IM^+)_5...((C_{60}(CN)_5)^{5-})$	-367.4	-300.7	-73.5	-60.1
$(IM^+)_6...((C_{60}(CN)_6)^{6-})$	-458.5	-377.8	-76.4	-63.0
$[IM^+...((C_{60}(CN))^-)]_2$	-131.3	-92.5	-65.6	-46.2
$[(IM^+)_2...((C_{60}(CN)_2)^{2-})]_2$	-264.9	-199.3	-132.5	-99.7
$[(IM^+)_3...((C_{60}(CN)_3)^{3-})]_2$	-414.5	-319.5	-138.2	-106.5

Table S3. The minimum MESP of $(C_{60}(CN)_n)^{n-}$ at M06L/6-311++G(d,p)//M06L/6-31G(d,p) level. All the values are in kcal/mol.

System	$V_{\min\text{-on}}$	$V_{\min\text{-CN}}$	$V_{\min\text{-in}}$	V_{\max}
$(C_{60}(CN))^-$	-73.8	-104.7	-61.1	-50.3
$(C_{60}(CN)_2)^{2-}$	-128.5	-147.7	-115.1	-103.9
$(C_{60}(CN)_3)^{3-}$	-183.7	-193.3	-175.5	-158.1
$(C_{60}(CN)_4)^{4-}$	-241.7	-240.3	-235.3	-210.7
$(C_{60}(CN)_5)^{5-}$	-298.4	-284.5	-296.2	-257.0
$(C_{60}(CN)_6)^{6-}$	-347.5	-327.9	-349.5	-308.9

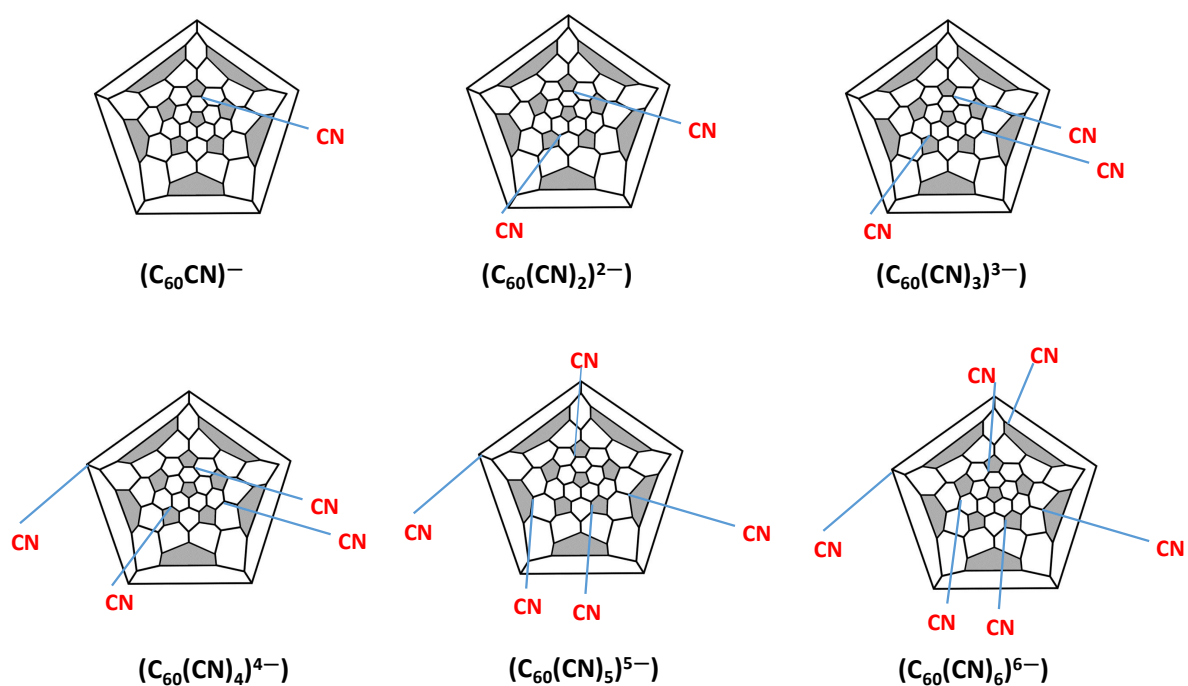


Fig. S1 The Schlegel diagram indicating the position of CN units.

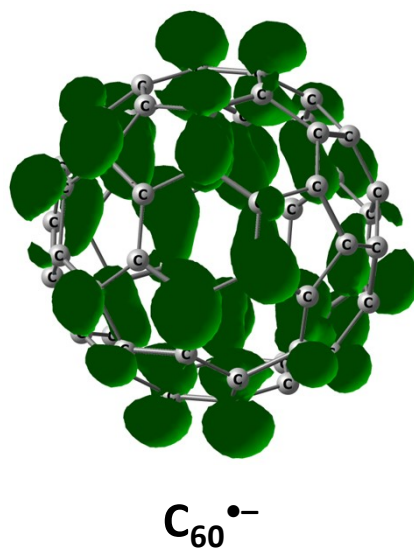


Fig.S2 The spin density distribution over $C_{60}^{\bullet-}$ at M06L/6-311++G(d,p)//M06L/6-31G(d,p) level (isosurface value = 0.001 au).

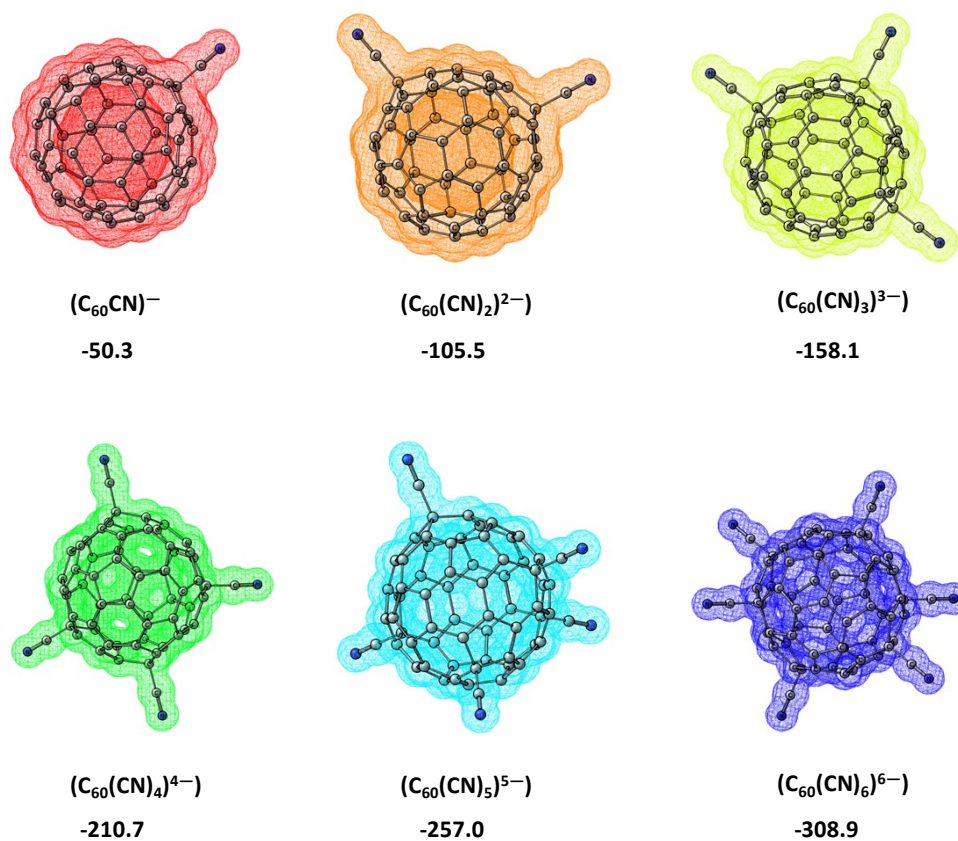


Fig. S3 MESP surfaces of $(C_{60}(CN)_n)^{n-}$ for $n = 1$ to 6 , that engulfs the whole anion at M06L/6-311++G(d,p)//M06L/6-31G(d,p) level. The minimum value of MESP that engulfs the whole anion in kcal/mol is also depicted.

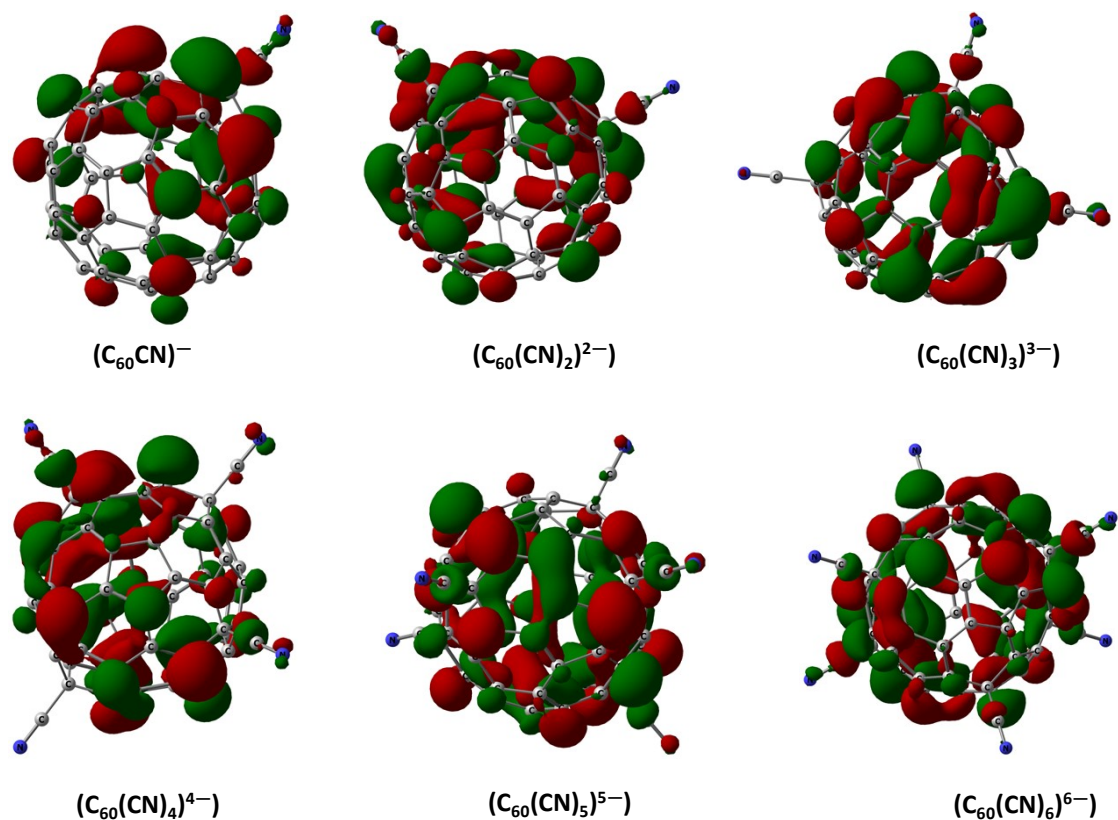


Fig. S4 HOMO plots of $(C_{60}(CN)_n)^{n-}$ for $n = 1$ to 6 at M06L/6-311++G(d,p)//M06L/6-31G(d,p) level (isosurface value = 0.02 au).

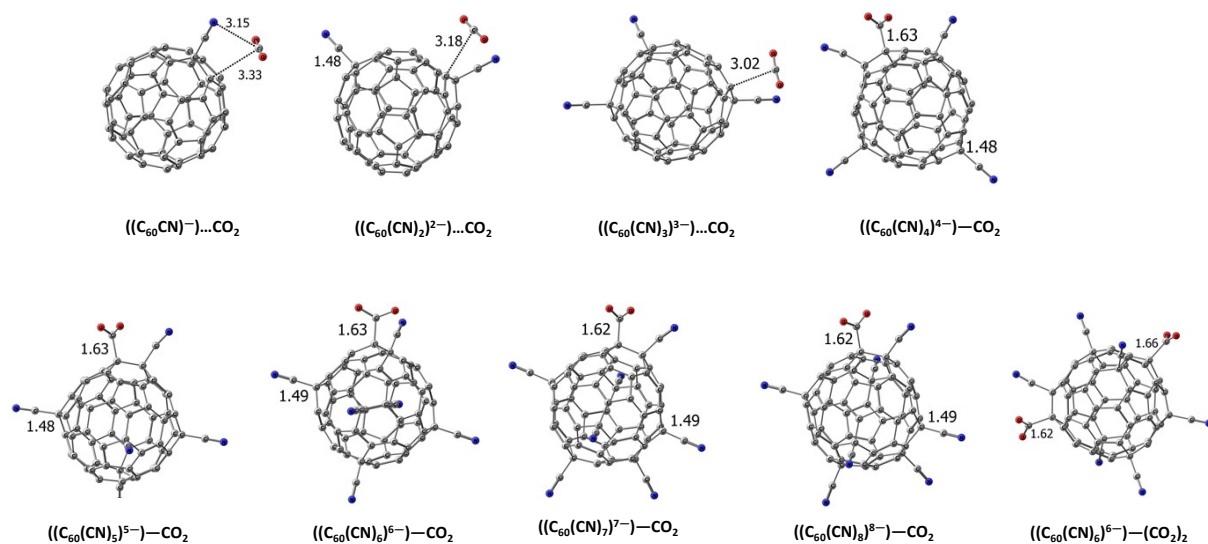


Fig. S5 The optimized geometry of $((C_{60}(CN)_n)^{n-}) - (CO_2)$ at M06L/6-31G(d,p) level. The distances are given in Å.

The binding energy of CO₂ with the bare fulleride anion (ΔE^a) is also calculated using equation,

$$\Delta E^a = E_8 - (E_4 + E_7) \quad (S1)$$

where E_8 , E_4 , and E_7 are the ZPE-corrected energy of the CO₂ complex of the bare fulleride, (C₆₀(CN)_{*n*})^{*n*-}, and '*n*' CO₂ respectively. The Gibbs energy change (ΔG) is also calculated in a similar fashion.

Table S4. Energetics of CO₂ complexes of ((C₆₀(CN)_{*n*})^{*n*-}) fullerides in kcal/mol.

<i>n</i>	ΔE^a	ΔG^a
((C ₆₀ (CN)) ⁻)...(CO ₂)	-3.7	4.0
((C ₆₀ (CN) ₂) ²⁻)...(CO ₂)	-4.3	3.5
((C ₆₀ (CN) ₃) ³⁻)...(CO ₂)	-5.6	1.9
((C ₆₀ (CN) ₃) ³⁻)—(CO ₂)	0.1	10.6
((C ₆₀ (CN) ₄) ⁴⁻)—(CO ₂)	-13.8	-3.4
((C ₆₀ (CN) ₅) ⁵⁻)—(CO ₂)	-21.9	-11.2
((C ₆₀ (CN) ₆) ⁶⁻)—(CO ₂)	-28.9	-18.1
((C ₆₀ (CN) ₆) ⁶⁻)—(CO ₂) ₂	-37.0	-13.7

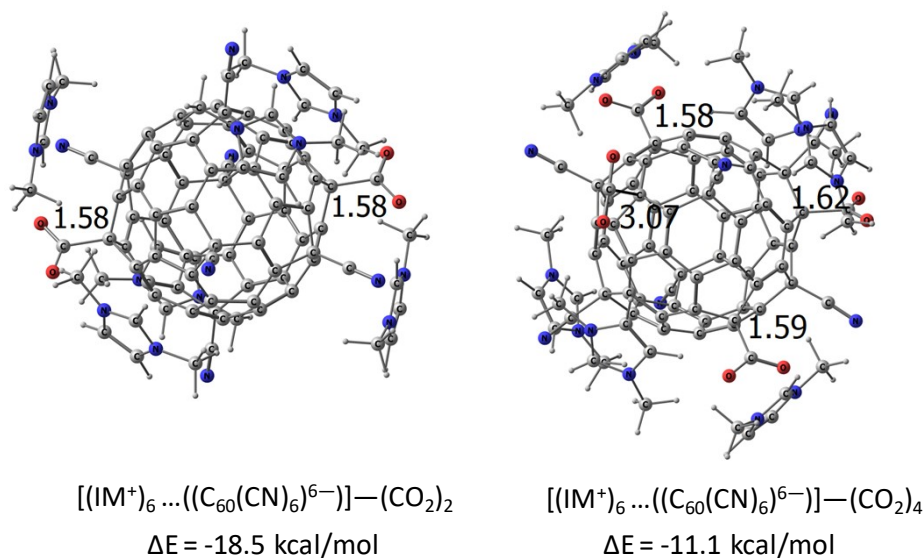


Fig. S6 The optimized geometries of $[(IM^+)_6 \dots ((C_{60}(CN)_6)^{6-})]-(CO_2)_2$ and $[(IM^+)_6 \dots ((C_{60}(CN)_6)^{6-})]-(CO_2)_4$ at M06L/6-31G(d,p) level. The distances are given in Å.

Basis set superposition error (BSSE)

The correction for the basis set superposition error (BSSE) with the ionic complex formation is also calculated made by the counterpoise (CP) approach of Boys and Bernardi. In the case of $(IM^{n+}) \cdots ((C_{60}(CN)_n)^{n-})$, for $n = 1, 2$, and 3 and but the BSSE calculation was not converging for the $n = 4, 5$, and 6 . Using the BSSE corrections of the systems $n = 1, 2$, and 3 a linear correlation graph in the form $Y = (0.0027)*X + 0.0007$ was obtained with correlation coefficient $R = 0.9998$. by extrapolating which the approximate values for the BSSE corrections of the systems with $n = 4, 5$, and 6 can be calculated. The BSSE was found to be $\sim 9\%$ of the E'_{rea} values.

Table S5. BSSE values of $[(IM^+)_{n \cdots} ((C_{60}(CN)_n)^{n-})]$ complexes.

n	BSSE (au)	BSSE (kcal/mol)
1	0.00336	2.1
2	0.00610	3.8
3	0.00869	5.5
4	0.01150	7.2
5	0.01420	8.9
6	0.01690	10.6

In the present study, we have not evaluated all the different attacks of CN^- on the carbon cage. There are too many possibilities when the number of CN increases. The reported ionic complex of fullerene represents one of the many such possible isomeric structures. The energetics will only improve with the identification of the global minimum (it could be more exothermic than the reported value) as the energetics of the reported structures give ample evidence for the fulleride formation.

Table S6. Energetics (kcal/mol) of CO_2 complexes of $[(IM^+)_{n \cdots} ((C_{60}(CN)_n)^{n-})]$ in the solvent DCM at M06L/SMD/6-311++G(d,p)// M06L/6-311++G(d,p) level.

System	$\Delta E'$	$\Delta G'$
1nc	-1.7	5.3
1'nc	-2.4	4.8
2nc	-2.0	7.1
3nc	-3.4	6.1
3c	-1.0	11.7
4nc	-4.0	3.4
4c	-15.7	-3.6
5nc	-2.7	5.8
5c	-12.7	-0.5
6nc	-3.4	5.5
6c	-17.9	-5.5

To understand the kinetic feasibility of this reaction, the transition state for the for the first addition of CN⁻ to C₆₀ is calculated in the presence of the solvent. The reaction intermediates involved in the formation (IM⁺)⁺...((C₆₀(CN))⁻) ion-pair from the reaction of IMCN and C₆₀ were discussed in our previous publication [*Phys. Chem. Chem. Phys.*, 2021, **23**, 20086-20094]. Based on which we have studied the solvation (DCM) effects and the solvation effect incorporated relative energy data given in the Table show that the transition states is stabilized in solvent due to its high ionic character and in the solvent, the reaction is expected to be barrierless.

Table S7. Relative energy (kcal/mol) of the reaction intermediates of [(IM⁺)...((C₆₀(CN))⁻)] formation in the solvent DCM at M06L/SMD/6-311++G(d,p)// M06L/6-311++G(d,p) level.

System	Relative energy (kcal/mol)
Reactant	0.0
ts1	-12.0
Intermediate	-26.0
ts2	-11.5
Product	-29.3

Cartesian coordinates of optimized geometry of (IM⁺)_n...((C₆₀(CN))_n)ⁿ⁻ for n = 1 to 6 at M06L/6-31G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.

IM ⁺ ...((C ₆₀ (CN)) ⁻)				(IM ⁺) ₂ ...((C ₆₀ (CN)) ₂) ²⁻			
6	-1.692009000	1.955262000	2.860595000	6	2.521001000	-1.268362000	-1.000715000
6	-0.361707000	2.399980000	2.519106000	6	1.367500000	-1.945721000	-1.576476000
6	-1.887469000	0.661913000	3.349896000	6	2.749948000	-1.235214000	0.367149000
6	0.726424000	1.535315000	2.681554000	6	0.407074000	-2.444033000	-0.665623000
6	1.763941000	1.472748000	1.680236000	6	-1.008465000	-2.265230000	-0.942742000
6	-0.450721000	3.216009000	1.341207000	6	0.924159000	-1.142372000	-2.673643000
6	0.552253000	3.125543000	0.368411000	6	-0.449899000	-0.951820000	-2.918964000
6	1.696012000	2.290655000	0.565329000	6	-1.416002000	-1.566063000	-2.059359000
6	-3.892302000	0.402621000	1.951211000	6	3.522467000	1.101762000	0.219949000
6	-3.690047000	1.738424000	1.437841000	6	3.319162000	1.062846000	-1.201314000
6	-3.008453000	-0.124209000	2.896281000	6	3.201048000	-0.031132000	0.986351000
6	-2.609456000	2.501587000	1.883677000	6	2.824415000	-0.102563000	-1.804864000
6	-1.842194000	3.284361000	0.942454000	6	1.831585000	-0.019509000	-2.839746000
6	-4.042453000	1.735408000	0.034700000	6	2.828925000	2.354934000	-1.620675000
6	-3.300305000	2.494880000	-0.871794000	6	1.856107000	2.432980000	-2.621525000
6	-2.180315000	3.280490000	-0.407798000	6	1.352684000	1.226536000	-3.246865000
6	-3.036501000	-2.298575000	1.742890000	6	2.209128000	1.397069000	2.729883000
6	-3.946959000	-1.749346000	0.764167000	6	2.505987000	2.559945000	1.917233000
6	-2.568203000	-1.500383000	2.787516000	6	2.533683000	0.114298000	2.266481000
6	-4.376565000	-0.423744000	0.868949000	6	3.162808000	2.424000000	0.693777000
6	-4.461973000	0.397582000	-0.316642000	6	2.724970000	3.193496000	-0.445463000
6	-3.606400000	-2.303474000	-0.526091000	6	1.412344000	3.490236000	2.058258000
6	-3.687293000	-1.509707000	-1.671144000	6	0.984248000	4.234893000	0.956257000

6	-4.127494000	-0.133884000	-1.564967000	6	1.655853000	4.086844000	-0.319910000
6	-0.300738000	-2.422478000	2.523489000	6	0.413334000	-0.795698000	3.035391000
6	-0.788144000	-3.254154000	1.441082000	6	0.053144000	0.527212000	3.504467000
6	-1.183905000	-1.568106000	3.193175000	6	1.669853000	-1.003215000	2.482740000
6	-2.126979000	-3.189431000	1.056730000	6	0.935168000	1.602758000	3.357854000
6	-2.480111000	-3.193211000	-0.347211000	6	0.436768000	2.896396000	2.948627000
6	0.245632000	-3.325981000	0.433818000	6	-1.350926000	0.708740000	3.261213000
6	-0.094654000	-3.328598000	-0.920648000	6	-1.838515000	1.957571000	2.866118000
6	-1.482504000	-3.261392000	-1.318863000	6	-0.924961000	3.068152000	2.699754000
6	0.525959000	0.204746000	3.193597000	6	0.586623000	-2.484227000	0.733282000
6	1.448320000	-0.684844000	2.510920000	6	-0.668326000	-2.215629000	1.353079000
6	-0.758608000	-0.228906000	3.526768000	6	1.898151000	-2.053915000	1.371622000
6	1.034740000	-1.992807000	2.196954000	6	-0.785444000	-1.460465000	2.551024000
6	1.362799000	-2.534177000	0.900153000	6	-1.846978000	-0.509582000	2.643121000
6	2.245548000	0.091443000	1.605313000	6	-1.691014000	-2.162944000	0.338982000
6	2.502638000	-0.419072000	0.319439000	6	-2.709545000	-1.204022000	0.442939000
6	2.092396000	-1.774003000	-0.015329000	6	-2.830593000	-0.397339000	1.641574000
6	-0.233270000	-2.005079000	-2.849958000	6	-2.556696000	3.218101000	1.033780000
6	0.669351000	-2.543988000	-1.865250000	6	-2.848285000	2.060730000	1.838923000
6	1.745127000	-1.778988000	-1.408785000	6	-3.306430000	0.886139000	1.230060000
6	-0.017471000	-0.698844000	-3.325394000	6	-2.753136000	3.155591000	-0.358295000
6	-2.441959000	-0.243205000	-3.182897000	6	-0.627584000	4.372731000	-0.721630000
6	-2.658264000	-1.581234000	-2.682245000	6	-0.424170000	4.425045000	0.707160000
6	-1.565170000	-2.435455000	-2.506735000	6	-1.368762000	3.843336000	1.561938000
6	-1.152576000	0.189600000	-3.494970000	6	-1.761349000	3.739209000	-1.239938000
6	-1.618861000	2.388158000	-2.493292000	6	-0.419386000	2.718978000	-3.032741000
6	-2.952529000	1.944229000	-2.164497000	6	0.759113000	3.362468000	-2.498944000
6	-3.354629000	0.649193000	-2.497551000	6	0.655644000	4.163325000	-1.354714000
6	-0.733895000	1.521859000	-3.144538000	6	-1.656797000	2.908562000	-2.410924000
6	1.120602000	2.288706000	-1.746727000	6	-2.238463000	0.555191000	-2.748188000
6	0.201577000	3.123638000	-1.035235000	6	-0.940181000	0.341657000	-3.318555000
6	-1.142353000	3.209651000	-1.417022000	6	-0.053305000	1.414919000	-3.512113000
6	0.653704000	1.463259000	-2.753381000	6	-2.572134000	1.802131000	-2.254436000
6	1.959291000	-0.429519000	-1.909374000	6	-3.513361000	0.834670000	-0.212701000
6	2.517866000	0.366056000	-0.864303000	6	-3.244411000	-0.491057000	-0.666995000
6	2.274737000	1.872724000	-0.807878000	6	-2.729343000	-0.748239000	-2.082370000
6	1.108897000	0.079270000	-2.900565000	6	-3.282655000	1.979673000	-0.985928000
7	4.623059000	2.991094000	-1.252750000	7	-4.662189000	-2.065506000	-3.303991000
6	3.546311000	2.564675000	-1.084836000	6	-3.780115000	-1.452226000	-2.838738000
6	5.516435000	0.056261000	-0.371140000	7	3.392860000	-4.093431000	2.139082000
7	5.491544000	-1.257313000	-0.619006000	6	2.698796000	-3.199991000	1.839395000
7	5.586724000	0.236195000	0.950499000	6	5.311077000	-3.155761000	-0.034185000
6	5.569244000	-0.997734000	1.566193000	7	5.244596000	-2.834763000	-1.329605000
1	5.580242000	-1.095532000	2.638878000	7	5.804446000	-2.110351000	0.634825000
6	5.509467000	-1.934127000	0.582641000	6	6.037864000	-1.084457000	-0.253893000
1	5.457856000	-3.009163000	0.628613000	1	6.396444000	-0.121754000	0.070208000
1	5.483236000	0.854179000	-1.100948000	6	5.681201000	-1.537155000	-1.486557000
6	5.539623000	1.528879000	1.622626000	1	5.664485000	-1.044138000	-2.444043000
1	6.307682000	1.563708000	2.395656000	6	5.921792000	-2.013946000	2.082713000
1	5.708624000	2.314314000	0.886563000	1	5.242283000	-1.230694000	2.432028000
1	4.549320000	1.660715000	2.067254000	1	5.621818000	-2.962356000	2.525240000
6	5.281420000	-1.850776000	-1.930571000	1	6.948851000	-1.768107000	2.355090000
1	6.026410000	-2.626850000	-2.109240000	6	4.581389000	-3.625982000	-2.355361000
1	4.273330000	-2.270854000	-1.977506000	1	3.551547000	-3.267787000	-2.469292000
1	5.374741000	-1.074491000	-2.688197000	1	4.960394000	-4.070210000	0.422194000

	1	5.122718000	-3.525424000	-3.295633000
	1	4.574187000	-4.672022000	-2.052553000
	6	-5.379024000	-2.516534000	-0.183329000
	7	-4.704342000	-3.651070000	0.027183000
	7	-5.704500000	-1.991701000	1.004311000
	6	-5.185292000	-2.794006000	1.998558000
	1	-5.282813000	-2.537572000	3.040149000
	6	-4.555562000	-3.831313000	1.387559000
	1	-3.992450000	-4.655803000	1.791224000
	6	-6.350688000	-0.701519000	1.181556000
	1	-5.986064000	-0.252474000	2.104587000
	1	-6.056997000	-0.053200000	0.353570000
	1	-7.436581000	-0.811630000	1.215780000
	6	-4.065778000	-4.444177000	-1.013816000
	1	-2.994995000	-4.218568000	-1.022913000
	1	-5.613674000	-2.111029000	-1.157859000
	1	-4.227881000	-5.503535000	-0.812103000
	1	-4.495985000	-4.172190000	-1.977504000
$(IM^+)_{3...}((C_{60}(CN)_3)^{3-})$				
6	-0.793235000	-3.587328000	0.251985000	
6	0.582301000	-3.658478000	0.692495000	
6	-1.079688000	-3.234542000	-1.071498000	
6	1.610339000	-3.373319000	-0.214988000	
6	2.755948000	-2.600040000	0.210299000	
6	0.649163000	-3.156608000	2.034181000	
6	1.757143000	-2.381713000	2.424775000	
6	2.837050000	-2.148951000	1.521215000	
6	-2.961996000	-1.846875000	-0.327991000	
6	-2.612265000	-2.142469000	1.020346000	
6	-2.180879000	-2.343096000	-1.370803000	
6	-1.583842000	-3.053634000	1.330274000	
6	-0.685681000	-2.769606000	2.434538000	
6	-2.827526000	-0.969417000	1.840108000	
6	-1.980789000	-0.733114000	2.943627000	
6	-0.879408000	-1.634334000	3.213670000	
6	-2.165733000	-0.178777000	-2.462770000	
6	-2.982179000	0.394129000	-1.474319000	
6	-1.821397000	-1.545960000	-2.528362000	
6	-3.629101000	-0.449749000	-0.390946000	
6	-3.309589000	0.088563000	1.020025000	
6	-2.453532000	1.695893000	-1.198708000	
6	-2.480158000	2.264793000	0.104186000	
6	-2.815336000	1.380846000	1.201202000	
6	0.452624000	-0.921981000	-3.295410000	
6	0.065884000	0.458785000	-3.357748000	
6	-0.474194000	-1.909980000	-2.888347000	
6	-1.200699000	0.843341000	-2.896324000	
6	-1.455107000	2.022123000	-2.163223000	
6	1.201936000	1.250289000	-2.895666000	
6	1.045553000	2.401926000	-2.140179000	
6	-0.344489000	3.015475000	-1.864707000	
6	1.317131000	-3.038793000	-1.583496000	
6	2.264963000	-2.041101000	-2.008717000	
6	-0.023398000	-2.957051000	-2.008810000	
$(IM^+)_{4...}((C_{60}(CN)_4)^{4-})$				
6	-0.571291000	-2.263318000	2.872043000	
6	0.720872000	-1.721406000	3.287148000	
6	-0.702981000	-3.011629000	1.704293000	
6	1.830081000	-1.918772000	2.449691000	
6	2.780311000	-0.843463000	2.242421000	
6	0.496535000	-0.429088000	3.843212000	
6	1.410209000	0.620979000	3.615181000	
6	2.593362000	0.389016000	2.859804000	
6	-2.766872000	-1.826538000	1.099629000	
6	-2.669111000	-1.081666000	2.331019000	
6	-1.794312000	-2.800183000	0.816260000	
6	-1.578178000	-1.290582000	3.191958000	
6	-0.929927000	-0.152805000	3.793335000	
6	-3.150452000	0.237104000	2.069982000	
6	-2.526188000	1.344458000	2.667590000	
6	-1.395600000	1.137807000	3.549362000	
6	-1.854017000	-2.075241000	-1.571669000	
6	-3.118575000	-1.210359000	-1.385068000	
6	-1.304965000	-2.861022000	-0.560327000	
6	-3.416814000	-1.026045000	0.102775000	
6	-3.534681000	0.279044000	0.664470000	
6	-2.708372000	0.106905000	-2.097354000	
6	-2.818638000	1.337934000	-1.444348000	
6	-3.329382000	1.454747000	-0.070730000	
6	0.951222000	-2.547216000	-1.435934000	
6	0.403713000	-1.701258000	-2.463910000	
6	0.088061000	-3.168300000	-0.539390000	
6	-0.972256000	-1.436164000	-2.489140000	
6	-1.460740000	-0.108428000	-2.786497000	
6	1.353507000	-0.655767000	-2.716818000	
6	0.862423000	0.632132000	-2.954891000	
6	-0.541337000	0.896417000	-3.087080000	
6	1.793541000	-2.727747000	1.278998000	

6	1.825889000	-1.000265000	-2.849739000	6	2.609253000	-2.097590000	0.304340000
6	2.281978000	0.338719000	-2.598623000	6	0.531853000	-3.496082000	0.906701000
6	3.184371000	-1.784903000	-0.922260000	6	2.281177000	-2.088444000	-1.091258000
6	3.564872000	-0.464575000	-0.646571000	6	2.477375000	-0.871414000	-1.822779000
6	3.145671000	0.604555000	-1.528382000	6	3.317331000	-0.989204000	0.904702000
6	1.112770000	3.188995000	0.074212000	6	3.468401000	0.200475000	0.153496000
6	1.889501000	2.628548000	-1.009556000	6	3.119996000	0.241293000	-1.250214000
6	2.954484000	1.767764000	-0.722995000	6	0.538225000	2.773235000	-2.078790000
6	1.445777000	2.858219000	1.406796000	6	1.518247000	1.776895000	-2.367973000
6	-0.967603000	2.632542000	1.887182000	6	2.608683000	1.562238000	-1.511607000
6	-1.281932000	2.973071000	0.518748000	6	0.622535000	3.452155000	-0.863957000
6	-0.240546000	3.296159000	-0.347176000	6	-1.771562000	3.120205000	-0.439252000
6	0.373216000	2.568307000	2.318710000	6	-1.954434000	2.440038000	-1.685942000
6	-0.125935000	0.530230000	3.598352000	6	-0.819090000	2.363777000	-2.705226000
6	-1.506288000	0.600921000	3.160954000	6	-0.561432000	3.689737000	-0.039897000
6	-1.909045000	1.636382000	2.306457000	6	-1.008152000	3.066434000	2.308768000
6	0.794889000	1.499937000	3.181134000	6	-2.295379000	2.539256000	1.910196000
6	2.520299000	-0.214561000	2.873668000	6	-2.666658000	2.555813000	0.548968000
6	1.557096000	-1.205239000	3.234191000	6	-0.157981000	3.625514000	1.341325000
6	0.259194000	-0.847343000	3.644461000	6	1.794802000	2.585919000	2.403436000
6	2.136722000	1.117618000	2.796254000	6	0.920933000	1.954123000	3.342897000
6	3.271062000	1.405169000	0.654305000	6	-0.457867000	2.220400000	3.329920000
6	3.750835000	0.062954000	0.669433000	6	1.260585000	3.362467000	1.387050000
6	3.550541000	-0.827468000	1.898979000	6	2.722375000	2.319909000	-0.285335000
6	2.559131000	1.991169000	1.709793000	6	3.355648000	1.506267000	0.708633000
7	5.969888000	-1.289566000	2.848767000	6	3.050660000	1.710354000	2.194822000
6	4.868231000	-1.091654000	2.504619000	6	1.750189000	3.285310000	0.011725000
6	6.553316000	-0.543836000	-0.230192000	7	5.271968000	2.635939000	3.285011000
7	6.507963000	0.354848000	-1.222733000	6	4.248521000	2.259748000	2.855789000
7	6.488091000	-1.766698000	-0.766362000	6	6.339422000	1.145125000	0.698177000
6	6.354721000	-1.644412000	-2.134093000	7	6.402281000	1.093397000	-0.637995000
1	6.228939000	-2.504631000	-2.769683000	7	6.453741000	-0.097040000	1.176161000
6	6.369448000	-0.316308000	-2.419762000	6	6.526156000	-0.973596000	0.113472000
1	6.260353000	0.209896000	-3.353266000	1	6.567405000	-2.038757000	0.265581000
1	6.627821000	-0.337739000	0.828619000	6	6.489771000	-0.229550000	-1.022941000
6	6.396518000	-3.004324000	-0.003469000	1	6.491675000	-0.514680000	-2.061284000
1	7.028597000	-3.762276000	-0.467521000	1	6.230014000	2.031345000	1.308948000
1	6.723770000	-2.811719000	1.018155000	6	6.337836000	-0.466662000	2.580267000
1	5.353703000	-3.334776000	0.012170000	1	7.114761000	-1.191340000	2.827790000
6	6.406036000	1.788825000	-1.011484000	1	6.448983000	0.430302000	3.189047000
1	7.389490000	2.224587000	-0.823231000	1	5.344617000	-0.895899000	2.748307000
1	5.959672000	2.241987000	-1.895082000	6	6.099495000	2.212722000	-1.512489000
1	5.739132000	1.961331000	-0.161674000	1	6.739805000	2.168880000	-2.394388000
7	-6.218665000	-0.839550000	-0.761432000	1	5.044558000	2.165460000	-1.801414000
1	-6.267808000	-3.007227000	-0.072505000	1	6.287651000	3.142236000	-0.976659000
6	-5.080975000	-0.618950000	-0.590623000	7	-5.285771000	-2.362484000	-2.375134000
6	-5.492957000	-3.749001000	-0.205804000	6	-4.303445000	-1.841357000	-2.003767000
7	-4.837277000	-4.397136000	0.761100000	6	-5.761159000	-2.355443000	0.852766000
7	-4.960629000	-4.091704000	-1.381247000	7	-5.949670000	-1.749065000	2.036362000
6	-3.916097000	-4.961210000	-1.155334000	7	-5.347281000	-3.611052000	1.089851000
1	-3.297747000	-5.326648000	-1.958038000	6	-5.197367000	-3.777907000	2.454086000
6	-3.840080000	-5.156427000	0.188794000	1	-4.803903000	-4.689104000	2.872228000
1	-3.138978000	-5.715779000	0.785377000	6	-5.585719000	-2.620008000	3.044621000
6	-5.244226000	-3.432829000	-2.649487000	1	-5.604341000	-2.323022000	4.079755000
1	-5.471561000	-4.179055000	-3.411640000	1	-5.992207000	-1.960836000	-0.125656000

1	-6.085208000	-2.754410000	-2.512964000	6	-4.881914000	-4.526731000	0.062470000
1	-4.359823000	-2.852162000	-2.936875000	1	-5.083013000	-5.550457000	0.380335000
6	-5.011068000	-4.183280000	2.188436000	1	-5.401669000	-4.307996000	-0.870704000
1	-5.357125000	-5.098720000	2.670866000	1	-3.806705000	-4.384442000	-0.087709000
1	-4.049860000	-3.871201000	2.606338000	6	-6.412318000	-0.382841000	2.197959000
1	-5.737603000	-3.386447000	2.341538000	1	-7.500079000	-0.352647000	2.307115000
7	-0.830155000	5.355725000	-2.989733000	1	-5.931054000	0.052074000	3.073337000
1	-1.402198000	6.208175000	-0.922668000	1	-6.098792000	0.193786000	1.326147000
6	-0.568776000	4.303665000	-2.546122000	7	0.931243000	-6.108214000	0.936692000
6	-2.058569000	5.902377000	-0.118251000	6	1.260247000	-5.527918000	-2.170757000
7	-1.789776000	5.937769000	1.190891000	7	2.544077000	-5.163030000	-2.173609000
7	-3.267870000	5.366453000	-0.289637000	7	0.684563000	-5.066013000	-3.286442000
6	-3.770521000	5.006774000	0.941539000	6	1.621319000	-4.345566000	-3.999761000
1	-4.720074000	4.508648000	1.040644000	1	1.365242000	-3.827922000	-4.908774000
6	-2.845210000	5.366917000	1.872883000	6	2.785824000	-4.407288000	-3.299975000
1	-2.823163000	5.233412000	2.941335000	1	3.747407000	-3.959581000	-3.484281000
6	-3.857082000	5.024842000	-1.577973000	1	0.779790000	-6.072632000	-1.368439000
1	-4.887539000	5.379989000	-1.613684000	6	-0.749807000	-5.033151000	-3.519255000
1	-3.265596000	5.485709000	-2.368362000	1	-0.953013000	-5.205398000	-4.576426000
1	-3.820225000	3.936390000	-1.690851000	1	-1.224930000	-5.814797000	-2.927760000
6	-0.477520000	6.203729000	1.756332000	1	-1.140003000	-4.056169000	-3.212729000
1	-0.575235000	6.843610000	2.634020000	6	3.467984000	-5.353020000	-1.063510000
1	-0.013323000	5.250641000	2.033229000	1	4.427152000	-5.702853000	-1.447727000
1	0.138912000	6.701135000	1.008949000	1	3.582233000	-4.393666000	-0.545699000
				1	3.044129000	-6.081998000	-0.373468000
				6	0.730020000	-4.954892000	0.993113000
				7	-1.416267000	4.040511000	-4.660261000
				6	-1.135010000	3.243431000	-3.848523000
				6	-1.698834000	5.893126000	-2.041626000
				7	-1.152990000	6.430159000	-0.945163000
				7	-3.001445000	5.697062000	-1.812157000
				6	-3.284684000	6.090893000	-0.524313000
				1	-4.269494000	5.978147000	-0.102934000
				6	-2.127514000	6.556379000	0.018157000
				1	-1.902308000	6.920789000	1.006599000
				1	-1.185718000	5.614816000	-2.953095000
				6	-3.895925000	4.960395000	-2.693310000
				1	-4.912358000	5.327359000	-2.553699000
				1	-3.575291000	5.099686000	-3.725036000
				1	-3.811961000	3.893185000	-2.444231000
				6	0.263906000	6.695080000	-0.750521000
				1	0.450453000	7.771159000	-0.743572000
				1	0.824380000	6.214257000	-1.551195000
				1	0.575456000	6.241951000	0.193159000
$(IM^+)_{5\dots}((C_{60}(CN)_5)^{5-})$				$(IM^+)_{6\dots}((C_{60}(CN)_6)^{6-})$			
6	2.747785000	1.157523000	-1.947127000	6	2.845255000	0.716943000	-1.964721000
6	3.502142000	0.946058000	-0.762979000	6	2.989022000	1.790223000	-1.050942000
6	1.775517000	2.181536000	-2.076714000	6	1.859841000	0.679816000	-2.978281000
6	3.370211000	1.878355000	0.441134000	6	2.118267000	3.038210000	-1.161009000
6	3.045459000	1.107706000	1.737391000	6	1.416851000	3.373001000	0.178494000
6	3.670180000	-0.459806000	-0.593057000	6	3.373628000	1.242827000	0.202026000
6	3.551054000	-1.083164000	0.661748000	6	2.836823000	1.730042000	1.416752000

6	3.208191000	-0.271788000	1.810451000	6	1.828688000	2.742427000	1.363987000
6	0.328686000	0.664430000	-3.416054000	6	1.603111000	-1.746598000	-2.594028000
6	1.336885000	-0.360704000	-3.289673000	6	2.674913000	-1.707468000	-1.648011000
6	0.532468000	1.904113000	-2.761737000	6	1.180847000	-0.558160000	-3.249332000
6	2.532944000	-0.120891000	-2.591805000	6	3.278170000	-0.502834000	-1.307586000
6	3.095114000	-1.131655000	-1.749511000	6	3.698281000	-0.168509000	0.041989000
6	0.688152000	-1.632950000	-3.145598000	6	2.478750000	-2.827220000	-0.598705000
6	1.256134000	-2.609289000	-2.308532000	6	2.647277000	-2.277327000	0.805918000
6	2.494958000	-2.393860000	-1.655155000	6	3.276484000	-1.069672000	1.052994000
6	-1.784506000	1.886154000	-1.929593000	6	-1.185040000	-1.201139000	-3.001432000
6	-1.999665000	0.616568000	-2.566778000	6	-0.764073000	-2.398758000	-2.317155000
6	-0.546905000	2.575083000	-2.086723000	6	-0.211033000	-0.303796000	-3.521256000
6	-0.947821000	0.010721000	-3.280770000	6	0.597424000	-2.660330000	-2.100027000
6	-0.743536000	-1.404737000	-3.157509000	6	1.030241000	-3.271579000	-0.888919000
6	-2.859583000	-0.163711000	-1.715822000	6	-1.708266000	-2.665115000	-1.265899000
6	-2.723604000	-1.566936000	-1.665344000	6	-1.297145000	-3.296145000	-0.079379000
6	-1.580867000	-2.136453000	-2.294783000	6	0.101532000	-3.449312000	0.138180000
6	-0.688568000	3.246862000	0.316424000	6	-1.604656000	1.599747000	-2.731481000
6	-2.147543000	2.754438000	0.449285000	6	-2.802087000	0.684037000	-2.392797000
6	0.008748000	3.166315000	-0.893534000	6	-0.424836000	1.100211000	-3.293248000
6	-2.578097000	1.928855000	-0.753619000	6	-2.420745000	-0.789578000	-2.431486000
6	-3.230750000	0.651643000	-0.588468000	6	-2.715291000	-1.650217000	-1.318180000
6	-2.066098000	1.901961000	1.734746000	6	-3.146079000	1.151249000	-0.951865000
6	-2.789165000	0.696506000	1.876451000	6	-3.556537000	0.249232000	0.060399000
6	-3.277286000	0.025139000	0.687783000	6	-3.250528000	-1.165474000	-0.101243000
6	2.107595000	2.772780000	0.325520000	6	0.893554000	2.779087000	-2.076663000
6	1.383127000	2.757376000	1.550876000	6	-0.290874000	3.199120000	-1.418291000
6	1.432530000	2.922007000	-0.887217000	6	0.849456000	1.715780000	-2.976913000
6	-0.011178000	2.935915000	1.530328000	6	-1.521728000	2.594233000	-1.719835000
6	-0.893815000	2.205240000	2.408226000	6	-2.529510000	2.368253000	-0.708511000
6	1.941812000	1.712075000	2.403998000	6	0.020257000	3.529043000	-0.038031000
6	1.143503000	0.969067000	3.272482000	6	-0.907277000	3.349201000	0.988442000
6	-0.344719000	1.298767000	3.496064000	6	-2.356823000	2.916513000	0.700360000
6	-2.351787000	-1.596293000	2.022811000	6	-2.726694000	-0.634463000	2.066215000
6	-2.152088000	-0.323245000	2.673032000	6	-3.147777000	0.581767000	1.404507000
6	-0.988642000	-0.108703000	3.411157000	6	-2.567175000	1.800189000	1.760101000
6	-1.394586000	-2.633185000	2.166968000	6	-1.739971000	-0.596172000	3.077426000
6	-1.733382000	-3.207394000	-0.218712000	6	-0.771655000	-2.693490000	2.174839000
6	-3.006678000	-2.326387000	-0.340994000	6	-1.997485000	-2.957597000	1.261926000
6	-3.111156000	-1.376122000	0.843985000	6	-2.872250000	-1.712381000	1.151971000
6	-1.058379000	-3.390132000	0.984413000	6	-0.727626000	-1.632036000	3.076493000
6	1.074099000	-3.675913000	-0.226274000	6	1.730224000	-1.518756000	2.835842000
6	0.389934000	-3.381602000	-1.434842000	6	1.640983000	-2.503280000	1.815861000
6	-0.996153000	-3.140667000	-1.428128000	6	0.413285000	-3.114661000	1.516689000
6	0.377615000	-3.618690000	0.983304000	6	0.545210000	-1.014999000	3.391456000
6	2.176846000	-2.344810000	2.032118000	6	1.305888000	1.281257000	3.099515000
6	2.966289000	-2.374863000	0.846330000	6	2.539391000	0.868949000	2.528191000
6	2.549879000	-3.230069000	-0.351785000	6	2.928094000	-0.602355000	2.494405000
6	0.935019000	-3.013644000	2.166517000	6	0.330250000	0.385600000	3.620564000
6	0.031062000	-1.094673000	3.467576000	6	-1.486377000	1.833709000	2.700293000
6	1.315699000	-0.436051000	3.350191000	6	-0.478356000	2.736955000	2.199565000
6	2.367048000	-1.061992000	2.662641000	6	0.883234000	2.476653000	2.414812000
6	-0.153178000	-2.351431000	2.840951000	6	-1.060856000	0.644203000	3.345092000
6	-0.621493000	1.853139000	4.832768000	6	-3.281617000	4.040738000	0.933025000
7	-0.956124000	2.238937000	5.887431000	7	-4.045674000	4.909876000	1.128047000

6	-3.109069000	3.853696000	0.645701000	6	-3.984208000	0.904137000	-3.244116000
7	-3.927623000	4.691667000	0.699985000	7	-4.966767000	0.972348000	-3.880538000
6	3.511020000	-4.340045000	-0.488841000	6	3.412849000	-3.943310000	-0.853366000
7	4.371612000	-5.132205000	-0.566114000	7	4.159843000	-4.817305000	-1.088007000
6	-4.188856000	-3.192854000	-0.490861000	6	4.099538000	-0.802171000	3.365348000
7	-5.081736000	-3.932562000	-0.664153000	7	5.062124000	-0.844571000	4.033258000
6	4.580318000	2.708310000	0.577902000	6	-2.744208000	-4.146391000	1.710017000
7	5.520427000	3.408176000	0.610470000	7	-3.279167000	-5.138268000	2.035451000
1	-4.761759000	3.499318000	-1.250449000	6	2.866345000	4.232820000	-1.592139000
6	-4.392174000	3.314446000	-2.247582000	7	3.398331000	5.233919000	-1.893387000
7	-4.785613000	2.331563000	-3.081334000	1	5.658971000	-3.532622000	-2.524765000
7	-3.632702000	4.179418000	-2.953296000	6	5.300924000	-2.738936000	-3.163376000
6	-3.442127000	3.660675000	-4.219814000	7	5.663045000	-1.452223000	-3.113211000
1	-2.786153000	4.134501000	-4.930536000	7	4.312962000	-2.862873000	-4.056432000
6	-4.171166000	2.520334000	-4.304909000	6	4.014531000	-1.618109000	-4.566615000
1	-4.289564000	1.814241000	-5.109372000	1	3.193985000	-1.462849000	-5.246613000
6	-2.859622000	5.243943000	-2.344461000	6	4.857298000	-0.731466000	-3.968825000
1	-2.572582000	5.955014000	-3.121007000	1	4.911719000	0.342299000	-4.031871000
1	-3.464637000	5.741685000	-1.585233000	6	3.510201000	-4.054264000	-4.261873000
1	-1.963992000	4.823672000	-1.868503000	1	3.484443000	-4.309140000	-5.322703000
6	-5.675923000	1.242887000	-2.727989000	1	3.932115000	-4.872159000	-3.679734000
1	-6.700191000	1.458575000	-3.052362000	1	2.497939000	-3.835776000	-3.897242000
1	-5.317654000	0.323967000	-3.193352000	6	6.509216000	-0.865988000	-2.089264000
1	-5.630583000	1.094868000	-1.648571000	1	7.097582000	-0.057362000	-2.524384000
1	5.632148000	-3.704538000	0.870353000	1	5.856904000	-0.483125000	-1.287783000
6	6.031872000	-2.699664000	0.876296000	1	7.179432000	-1.629582000	-1.694938000
7	6.157287000	-1.893194000	1.938867000	1	-4.985199000	-1.447028000	-3.792379000
7	6.444651000	-2.035181000	-0.208228000	6	-5.109224000	-2.191241000	-3.019434000
6	6.803443000	-0.756586000	0.165357000	7	-5.826798000	-2.023148000	-1.896145000
1	7.111024000	-0.018187000	-0.555916000	7	-4.509239000	-3.390937000	-2.955035000
6	6.622005000	-0.667364000	1.508774000	6	-4.831510000	-3.984139000	-1.752203000
1	6.737126000	0.165988000	2.182533000	1	-4.409638000	-4.930370000	-1.454245000
6	6.351210000	-2.536948000	-1.571641000	6	-5.654200000	-3.131832000	-1.089733000
1	7.284611000	-2.334872000	-2.099371000	1	-6.083007000	-3.191837000	-0.103052000
1	6.161327000	-3.609920000	-1.536179000	6	-3.476374000	-3.814262000	-3.881309000
1	5.510422000	-2.045315000	-2.071407000	1	-2.942744000	-4.658873000	-3.448048000
6	5.603601000	-2.200552000	3.246944000	1	-3.913164000	-4.102509000	-4.840988000
1	5.570503000	-1.285857000	3.836110000	1	-2.772294000	-2.982472000	-4.010794000
1	4.579565000	-2.566084000	3.108346000	6	-6.478948000	-0.785889000	-1.511881000
1	6.214681000	-2.948402000	3.756770000	1	-7.454811000	-1.010028000	-1.073119000
1	3.955593000	5.160393000	-0.000832000	1	-5.828692000	-0.260350000	-0.793418000
6	3.299222000	5.334581000	-0.841880000	1	-6.599101000	-0.158818000	-2.396247000
7	2.102168000	5.935593000	-0.811721000	1	5.031526000	1.572821000	3.950301000
7	3.549183000	4.945331000	-2.096307000	6	5.157336000	2.327415000	3.187479000
6	2.458958000	5.256133000	-2.878969000	7	4.539347000	3.518004000	3.124674000
1	2.414805000	4.979074000	-3.918675000	7	5.902907000	2.185291000	2.079730000
6	1.552736000	5.876569000	-2.077115000	6	5.729622000	3.300585000	1.283263000
1	0.563840000	6.251767000	-2.280146000	1	6.184903000	3.382527000	0.310466000
6	4.674983000	4.118366000	-2.505865000	6	4.878021000	4.131248000	1.936889000
1	5.003991000	4.430666000	-3.497507000	1	4.449169000	5.075199000	1.641586000
1	5.481432000	4.234610000	-1.782760000	6	6.583235000	0.961765000	1.694882000
1	4.352037000	3.069402000	-2.522040000	1	7.518024000	1.213847000	1.190157000
6	1.362573000	6.250048000	0.399379000	1	6.782780000	0.370012000	2.588268000
1	0.997222000	7.277876000	0.359671000	1	5.922890000	0.385485000	1.028382000
1	0.525433000	5.546563000	0.489252000	6	3.496117000	3.927433000	4.045706000

1	2.018721000	6.125542000	1.259398000	1	2.928348000	4.738833000	3.592413000
1	-3.563031000	-5.531274000	-1.488061000	1	2.821517000	3.076561000	4.198976000
6	-2.812701000	-5.493833000	-2.265664000	1	3.924910000	4.256553000	4.995773000
7	-1.584547000	-6.022118000	-2.218461000	1	1.213325000	6.017067000	-2.646138000
7	-2.954722000	-4.852289000	-3.431019000	6	0.228836000	6.101538000	-2.207686000
6	-1.766574000	-4.936742000	-4.126213000	7	-0.018718000	6.514082000	-0.955334000
1	-1.628009000	-4.442596000	-5.073156000	7	-0.935426000	5.769055000	-2.783699000
6	-0.907022000	-5.663783000	-3.362516000	6	-1.941405000	5.912904000	-1.850745000
1	0.126721000	-5.926715000	-3.513781000	1	-2.962188000	5.640407000	-2.063769000
6	-4.092392000	-4.018506000	-3.786123000	6	-1.369861000	6.380392000	-0.708933000
1	-4.249537000	-4.070689000	-4.863607000	1	-1.804121000	6.588025000	0.255865000
1	-4.973593000	-4.372334000	-3.252892000	6	-1.061912000	5.080701000	-4.057191000
1	-3.876785000	-2.988504000	-3.467404000	1	-1.809906000	5.579181000	-4.675990000
6	-0.981987000	-6.596750000	-1.025262000	1	-0.097898000	5.096636000	-4.563805000
1	-0.371817000	-7.456331000	-1.303983000	1	-1.352411000	4.039246000	-3.872023000
1	-0.362235000	-5.837916000	-0.534980000	6	1.009515000	6.781965000	0.034053000
1	-1.772741000	-6.916049000	-0.347882000	1	0.624595000	7.493534000	0.764408000
1	-2.502815000	0.495654000	6.026869000	1	1.286632000	5.831295000	0.515505000
6	-3.336287000	0.137151000	5.437748000	1	1.887104000	7.191924000	-0.466073000
7	-3.666560000	-1.140042000	5.211561000	1	-1.087948000	-5.843202000	2.940135000
7	-4.191330000	0.921399000	4.776894000	6	-0.105833000	-5.947841000	2.501679000
6	-5.060254000	0.123736000	4.064656000	7	1.060911000	-5.592136000	3.057794000
1	-5.803615000	0.544264000	3.408961000	7	0.134768000	-6.405418000	1.263681000
6	-4.733344000	-1.167824000	4.334814000	6	1.485619000	-6.286065000	1.007593000
1	-5.125419000	-2.093961000	3.949413000	1	1.913668000	-6.535542000	0.050274000
6	-4.086070000	2.369727000	4.667775000	6	2.062321000	-5.773966000	2.127506000
1	-5.061896000	2.821958000	4.849499000	1	3.083595000	-5.492656000	2.326768000
1	-3.358951000	2.724445000	5.397954000	6	-0.895569000	-6.718379000	0.289704000
1	-3.732064000	2.614715000	3.661071000	1	-0.518303000	-7.476673000	-0.396632000
6	-2.814270000	-2.275751000	5.518529000	1	-1.779893000	-7.084858000	0.810716000
1	-3.405034000	-3.072580000	5.973189000	1	-1.160280000	-5.795010000	-0.248354000
1	-2.349276000	-2.627485000	4.588694000	6	1.193724000	-4.844434000	4.297133000
1	-2.033237000	-1.958165000	6.207836000	1	1.955846000	-5.304993000	4.927679000
				1	1.470456000	-3.808614000	4.060657000
				1	0.236458000	-4.849275000	4.816500000
				1	-4.819502000	3.233910000	2.794440000
				6	-5.258292000	2.248500000	2.753469000
				7	-5.184169000	1.296100000	3.700647000
				7	-6.024218000	1.791966000	1.750509000
				6	-6.377406000	0.488710000	2.031495000
				1	-6.964844000	-0.096611000	1.344115000
				6	-5.852549000	0.176179000	3.243888000
				1	-5.871872000	-0.739749000	3.810111000
				6	-6.220938000	2.480108000	0.483702000
				1	-7.160943000	2.143518000	0.043316000
				1	-6.255550000	3.555307000	0.662597000
				1	-5.386723000	2.256611000	-0.193271000
				6	-4.250011000	1.310722000	4.812323000
				1	-4.772771000	1.086575000	5.744683000
				1	-3.460635000	0.573548000	4.623453000
				1	-3.788815000	2.295422000	4.873561000

Cartesian coordinates of optimized geometry of dimers of $(IM^+)_{n...}((C_{60}(CN)_n)^{n-})$ for $n = 1$ to 3 at M06L/6-31G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.

$[IM^+...((C_{60}(CN)^-)]_2$				$[(IM^+)_2...((C_{60}(CN)_2)^{2-})]_2$			
6	-4.966548000	1.916133000	-3.069221000	7	-6.029634000	4.085590000	-3.537358000
6	-4.785057000	0.520093000	-3.388048000	6	-10.007802000	1.548928000	-3.587971000
6	-3.950899000	2.616272000	-2.413702000	6	-7.626587000	0.791871000	-1.253456000
6	-3.593227000	-0.127626000	-3.042022000	6	-7.199297000	-0.291301000	-2.128203000
6	-3.617679000	-1.467971000	-2.505946000	6	-6.834346000	1.905762000	-1.019303000
6	-6.039602000	-0.149639000	-3.193906000	6	-5.873312000	-0.228473000	-2.614831000
6	-6.046705000	-1.439002000	-2.648250000	6	-5.054898000	-1.429178000	-2.639121000
6	-4.826645000	-2.124238000	-2.356411000	6	-7.656498000	-1.507048000	-1.528596000
6	-5.604503000	3.720793000	-0.966111000	6	-6.845638000	-2.658194000	-1.530818000
6	-6.657459000	2.995107000	-1.638630000	6	-5.550451000	-2.615072000	-2.138437000
6	-4.273759000	3.539286000	-1.353609000	6	-7.504718000	1.932236000	1.353566000
6	-6.344723000	2.107935000	-2.670484000	6	-8.352852000	0.798982000	1.110105000
6	-7.011513000	0.828756000	-2.749323000	6	-6.732401000	2.445780000	0.298196000
6	-7.651036000	2.633947000	-0.651275000	6	-8.412834000	0.234121000	-0.172333000
6	-8.294493000	1.397790000	-0.731348000	6	-8.429060000	-1.192090000	-0.338465000
6	-7.966431000	0.480700000	-1.798325000	6	-8.303359000	-0.057016000	2.272119000
6	-3.571197000	3.524524000	1.008671000	6	-8.309039000	-1.444939000	2.107957000
6	-4.948425000	3.710294000	1.404302000	6	-8.379606000	-2.023668000	0.781722000
6	-3.238752000	3.432801000	-0.345518000	6	-4.812561000	2.739151000	1.813377000
6	-5.949526000	3.815539000	0.433921000	6	-5.600115000	2.172188000	2.890274000
6	-7.210379000	3.137708000	0.629753000	6	-5.360067000	2.857747000	0.527647000
6	-5.176185000	2.941594000	2.606114000	6	-6.924739000	1.788504000	2.675158000
6	-6.393165000	2.284455000	2.792975000	6	-7.412788000	0.552950000	3.236679000
6	-7.431673000	2.388414000	1.788327000	6	-4.726246000	1.356026000	3.697330000
6	-1.672059000	1.588682000	0.131242000	6	-5.195545000	0.156713000	4.239078000
6	-2.012214000	1.689777000	1.537565000	6	-6.566648000	-0.251083000	4.008411000
6	-2.264306000	2.462804000	-0.793612000	6	-3.304732000	2.086245000	-0.518226000
6	-2.946507000	2.633803000	1.964921000	6	-2.727776000	1.938277000	0.803488000
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6	-2.831358000	-2.298460000	-0.344045000	6	-1.957125000	0.205028000	-0.548424000
6	-2.367941000	-1.789120000	0.939211000	6	-3.670638000	-1.017651000	-2.458600000
6	-5.039295000	-1.092987000	3.363609000	6	-2.872206000	-1.818392000	-1.622220000
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[[IM*] ₃ ...((C ₆₀ (CN) ₃) ³⁻)] ₂				
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6	4.996695000	1.014446000	3.301098000
6	4.235740000	-0.209308000	3.160587000
6	3.012328000	-0.151062000	2.492352000
6	4.526737000	2.225200000	2.755769000
6	6.797642000	2.794925000	2.010644000
6	7.282944000	1.553051000	2.576346000
6	6.382392000	0.675384000	3.197592000
6	5.438547000	3.119421000	2.098910000
6	5.457655000	3.994044000	-0.192918000
6	6.823777000	3.594585000	-0.300655000
6	7.516076000	3.049682000	0.798105000
6	4.752663000	3.717962000	0.972699000
6	2.845936000	2.873082000	-0.289762000
6	3.476447000	3.156399000	-1.527351000
6	4.791231000	3.929882000	-1.585986000
6	3.385642000	3.217316000	0.960531000
7	4.134011000	6.242153000	-2.678587000
6	4.504748000	5.252139000	-2.174157000
6	1.414355000	4.504625000	-3.072590000
7	0.367471000	3.878903000	-2.521673000
7	1.625215000	3.987387000	-4.286635000
6	0.714992000	2.970076000	-4.495095000
1	0.725554000	2.376903000	-5.394004000
6	-0.077869000	2.902825000	-3.393015000
1	-0.901069000	2.252715000	-3.139011000
1	1.995555000	5.305652000	-2.636761000
6	2.765062000	4.309640000	-5.132552000
1	2.436999000	4.385441000	-6.169991000
1	3.191773000	5.256969000	-4.802056000
1	3.516580000	3.521062000	-5.028421000

6	-0.122707000	4.123725000	-1.174991000
1	-1.190901000	4.357116000	-1.199330000
1	0.022787000	3.224784000	-0.568023000
1	0.455227000	4.942490000	-0.743604000
7	8.828803000	-4.537342000	2.202773000
1	10.697695000	-4.012497000	0.983997000
6	8.130910000	-3.654837000	1.877775000
6	10.699272000	-3.605056000	-0.017041000
7	11.239381000	-2.445867000	-0.404428000
7	10.061250000	-4.143072000	-1.058948000
6	10.170423000	-3.287667000	-2.133594000
1	9.680054000	-3.488002000	-3.071435000
6	10.912114000	-2.223282000	-1.724441000
1	11.186377000	-1.313546000	-2.231600000
6	9.174632000	-5.296496000	-0.994565000
1	9.448008000	-6.016277000	-1.767107000
1	9.250654000	-5.744846000	-0.005127000
1	8.148174000	-4.944483000	-1.148183000
6	11.878587000	-1.477260000	0.470971000
1	12.912191000	-1.312271000	0.163063000
1	11.312491000	-0.542770000	0.419454000
1	11.852601000	-1.850830000	1.493590000
7	0.567785000	-2.525661000	3.097925000
1	-0.221866000	-0.168251000	4.104029000
6	1.387631000	-1.996775000	2.449646000
6	0.576190000	0.424205000	4.539345000
7	0.802070000	1.719184000	4.294027000
7	1.529509000	-0.015328000	5.368845000
6	2.406330000	1.016080000	5.624520000
1	3.290525000	0.873858000	6.222965000
6	1.946068000	2.104995000	4.952780000
1	2.356202000	3.094620000	4.841062000
6	1.738444000	-1.394296000	5.780893000
1	1.863689000	-1.434035000	6.863896000
1	0.886789000	-1.995168000	5.469305000
1	2.636317000	-1.773903000	5.283921000
6	0.065739000	2.539117000	3.341540000
1	-0.800342000	3.006376000	3.817067000
1	0.753125000	3.291397000	2.948311000
1	-0.261339000	1.909280000	2.512381000
6	-1.483494000	-1.266976000	0.543113000
6	-1.489216000	0.002836000	1.235635000
6	-1.649847000	-1.300340000	-0.846128000
6	-1.669164000	1.185230000	0.504075000
6	-2.506187000	2.245609000	1.025880000
6	-2.163076000	-0.171001000	2.493644000
6	-3.003330000	0.857985000	2.972086000
6	-3.129940000	2.085983000	2.259607000
6	-3.104497000	-3.259560000	-0.651396000
6	-2.992199000	-3.177276000	0.767343000
6	-2.478534000	-2.314388000	-1.456495000
6	-2.155774000	-2.225539000	1.371454000
6	-2.587617000	-1.552852000	2.578938000
6	-4.262946000	-3.521410000	1.366578000
6	-4.656552000	-2.890576000	2.566728000

6	-3.813667000	-1.871628000	3.150882000
6	-4.483278000	-2.067156000	-2.806974000
6	-5.170796000	-3.048437000	-2.070711000
6	-3.129067000	-1.732261000	-2.620503000
6	-4.467030000	-3.892625000	-1.023604000
6	-5.193970000	-3.829060000	0.337672000
6	-6.500401000	-2.564152000	-1.877328000
6	-7.236781000	-2.818351000	-0.688584000
6	-6.506028000	-3.363210000	0.434956000
6	-3.674562000	0.650525000	-3.035253000
6	-5.026733000	0.302461000	-3.355052000
6	-2.735293000	-0.349905000	-2.676620000
6	-5.451895000	-1.026026000	-3.187130000
6	-6.709195000	-1.396222000	-2.675199000
6	-5.886482000	1.340141000	-2.797058000
6	-7.125960000	1.059654000	-2.242352000
6	-7.750615000	-0.350855000	-2.312778000
6	-1.812407000	1.153692000	-0.926845000
6	-2.763545000	2.172976000	-1.294087000
6	-1.816901000	-0.086012000	-1.600357000
6	-3.673635000	1.917547000	-2.336917000
6	-5.038695000	2.337486000	-2.185084000
6	-3.165654000	2.890744000	-0.101792000
6	-4.519209000	3.228115000	0.062409000
6	-5.455542000	2.991479000	-1.018432000
6	-8.201230000	0.725473000	-0.180303000
6	-7.512826000	1.682637000	-1.016592000
6	-6.713580000	2.669558000	-0.425826000
6	-8.056413000	0.801914000	1.223129000
6	-7.863924000	-1.660254000	1.277137000
6	-8.013830000	-1.711771000	-0.160130000
6	-8.232933000	-0.525462000	-0.853978000
6	-7.875852000	-0.423148000	1.952145000
6	-6.020498000	-1.174400000	3.379041000
6	-6.013159000	-2.449080000	2.688865000
6	-6.919575000	-2.674518000	1.644123000
6	-6.937811000	-0.180507000	3.013573000
6	-5.221178000	1.550474000	3.262386000
6	-4.274296000	0.525088000	3.569468000
6	-4.666235000	-0.820483000	3.677075000
6	-6.524057000	1.202960000	2.937440000
6	-6.541794000	2.719223000	1.021103000
6	-5.216910000	3.174454000	1.306560000
6	-4.496978000	2.733908000	2.584417000
6	-7.248407000	1.828284000	1.835733000
7	-4.123777000	4.906425000	4.037634000
6	-4.305692000	3.903309000	3.461091000
6	-4.644864000	6.076335000	1.076717000
7	-5.439426000	6.243544000	0.010932000
7	-3.372860000	6.171271000	0.673096000
6	-3.356761000	6.361474000	-0.694113000
1	-2.434010000	6.444598000	-1.243897000
6	-4.650148000	6.408169000	-1.107593000
1	-5.077465000	6.521365000	-2.089837000
1	-4.956851000	5.908340000	2.097588000

6	-2.211528000	5.931097000	1.519330000	
1	-1.416784000	6.625969000	1.244479000	
1	-2.497965000	6.077333000	2.561023000	
1	-1.878204000	4.896119000	1.382186000	
6	-6.884717000	6.093307000	0.042676000	
1	-7.366379000	7.032912000	0.321339000	
1	-7.225719000	5.774115000	-0.940976000	
1	-7.130038000	5.306805000	0.760875000	
7	-3.946002000	-6.369445000	-1.786033000	
1	-1.928468000	-6.033863000	-0.558378000	
6	-4.231739000	-5.283551000	-1.454828000	
6	-1.002739000	-5.475818000	-0.593674000	
7	-0.252262000	-5.106450000	0.448295000	
7	-0.431939000	-5.013014000	-1.710076000	
6	0.704904000	-4.312177000	-1.368313000	
1	1.333022000	-3.819181000	-2.094490000	
6	0.823120000	-4.375611000	-0.012741000	
1	1.585883000	-3.984057000	0.648857000	
6	-1.033344000	-5.075048000	-3.033779000	
1	-0.261957000	-5.301591000	-3.769911000	
1	-1.800948000	-5.848901000	-3.038600000	
1	-1.498189000	-4.110152000	-3.260732000	
6	-0.564360000	-5.377310000	1.844284000	
1	0.118337000	-6.132738000	2.238597000	
1	-0.463365000	-4.450215000	2.414572000	
1	-1.592064000	-5.734149000	1.909533000	
7	-9.908878000	-0.601047000	-3.814841000	
1	-11.014340000	-1.595997000	-2.051612000	
6	-8.932065000	-0.434106000	-3.190878000	
6	-10.797001000	-2.399224000	-1.359624000	
7	-11.015190000	-2.399416000	-0.040730000	
7	-10.203694000	-3.546547000	-1.692355000	
6	-9.997666000	-4.285636000	-0.548308000	
1	-9.489782000	-5.235002000	-0.572157000	
6	-10.509836000	-3.568934000	0.489562000	
1	-10.523739000	-3.763475000	1.548829000	
6	-9.680020000	-3.865707000	-3.014642000	
1	-10.004012000	-4.865762000	-3.304309000	
1	-10.045013000	-3.124724000	-3.725077000	
1	-8.587572000	-3.812429000	-2.971173000	
6	-11.406201000	-1.232687000	0.732460000	
1	-12.173270000	-1.507285000	1.457336000	
1	-10.522633000	-0.840643000	1.248054000	
1	-11.796843000	-0.472234000	0.057881000	

Cartesian coordinates of optimized geometry of $(C_{60}(CN)_n)^{n-}$ for $n = 1$ to 6 at M06L/6-31G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.

$(C_{60}(CN))^-$				$(C_{60}(CN)_2)^{2-}$			
6	0.464196000	-2.404225000	2.592446000	6	-1.866871000	1.696169000	-2.283661000
6	-0.950245000	-2.115442000	2.586324000	6	-0.750596000	2.597267000	-2.023227000

6	1.370791000	-1.428497000	3.014835000	6	-2.834342000	1.440249000	-1.324349000
6	-1.408205000	-0.860157000	3.004678000	6	-0.624980000	3.110720000	-0.715052000
6	-2.466459000	-0.188677000	2.285376000	6	0.685277000	3.184680000	-0.089126000
6	-1.528165000	-2.730023000	1.424995000	6	0.398336000	2.036902000	-2.653946000
6	-2.533620000	-2.050212000	0.724221000	6	1.662205000	2.089265000	-2.028256000
6	-3.047186000	-0.800234000	1.188713000	6	1.801678000	2.720296000	-0.750412000
6	2.894313000	-1.997108000	1.169225000	6	-2.879549000	-0.944882000	-1.950561000
6	1.956240000	-3.003012000	0.724113000	6	-1.900670000	-0.681427000	-2.965716000
6	2.607869000	-1.227115000	2.300866000	6	-3.301433000	0.107281000	-1.123133000
6	0.762067000	-3.201655000	1.421080000	6	-1.396107000	0.617462000	-3.125908000
6	-0.471667000	-3.405453000	0.697222000	6	0.007001000	0.822808000	-3.355523000
6	1.956205000	-3.003386000	-0.722662000	6	-1.007014000	-1.815366000	-3.031867000
6	0.762001000	-3.202388000	-1.419480000	6	0.359097000	-1.610086000	-3.251262000
6	-0.471702000	-3.405815000	-0.695458000	6	0.875928000	-0.267830000	-3.426277000
6	3.453791000	0.789468000	1.169382000	6	-3.252184000	-1.387520000	0.841255000
6	3.742474000	-0.008146000	-0.000084000	6	-2.773774000	-2.456523000	-0.010644000
6	2.887535000	0.195354000	2.299077000	6	-3.486145000	-0.113839000	0.298017000
6	3.480940000	-1.383288000	0.000278000	6	-2.605100000	-2.252143000	-1.382541000
6	2.894251000	-1.997705000	-1.168331000	6	-1.439624000	-2.783490000	-2.044486000
6	3.453739000	0.788874000	-1.169939000	6	-1.806930000	-3.224579000	0.737764000
6	2.887435000	0.194178000	-2.299305000	6	-0.675372000	-3.740610000	0.098066000
6	2.607765000	-1.228296000	-2.300351000	6	-0.490547000	-3.522090000	-1.324269000
6	1.369420000	2.111955000	2.591829000	6	-2.457378000	0.988606000	2.206313000
6	1.959445000	2.730657000	1.420921000	6	-2.181387000	-0.318831000	2.772627000
6	1.841958000	0.867891000	3.034120000	6	-3.161651000	1.077440000	1.010546000
6	2.978184000	2.082116000	0.722869000	6	-2.572997000	-1.483783000	2.103621000
6	2.978146000	2.081743000	-0.724061000	6	-1.678969000	-2.618877000	2.048437000
6	0.907573000	3.408318000	0.697237000	6	-0.899706000	-0.251014000	3.416650000
6	0.907540000	3.407954000	-0.699006000	6	-0.030561000	-1.347214000	3.370889000
6	1.959371000	2.729921000	-1.422397000	6	-0.426598000	-2.547340000	2.662176000
6	-0.475333000	0.140598000	3.446743000	6	-1.593009000	2.928480000	0.297427000
6	-0.963988000	1.436547000	3.005699000	6	-0.915266000	2.771343000	1.538693000
6	0.894550000	-0.134136000	3.460595000	6	-2.915897000	2.229345000	0.006930000
6	-0.035937000	2.414247000	2.599804000	6	-1.373060000	1.885822000	2.555772000
6	-0.326001000	3.199309000	1.422463000	6	-0.395568000	1.101470000	3.245106000
6	-2.206470000	1.248411000	2.320617000	6	0.493324000	3.005837000	1.340521000
6	-2.463772000	1.978530000	1.145144000	6	1.436464000	2.228587000	2.025993000
6	-1.509537000	2.993364000	0.716457000	6	0.983712000	1.278393000	3.032638000
6	-0.036060000	2.412922000	-2.601027000	6	1.857186000	-2.220840000	2.306508000
6	-0.326067000	3.198578000	-1.424063000	6	1.381271000	-1.151299000	3.150662000
6	-1.509571000	2.993002000	-0.717897000	6	1.856547000	0.153825000	2.961611000
6	-0.964131000	1.435013000	-3.006375000	6	2.811986000	-1.934344000	1.309413000
6	0.894389000	-0.135903000	-3.460549000	6	1.597962000	-3.405539000	-0.281159000
6	1.841821000	0.866337000	-3.034637000	6	0.616615000	-3.687392000	0.739708000
6	1.369297000	2.110631000	-2.592963000	6	0.744168000	-3.083944000	2.002398000
6	-0.475494000	0.138836000	-3.446793000	6	2.663293000	-2.537791000	-0.002913000
6	-0.950362000	-2.116771000	-2.585198000	6	2.446396000	-1.493424000	-2.221817000
6	0.464082000	-2.405552000	-2.591234000	6	1.339851000	-2.375587000	-2.516440000
6	1.370653000	-1.430037000	-3.014166000	6	0.915416000	-3.303077000	-1.553258000
6	-1.408339000	-0.861702000	-3.004163000	6	3.096886000	-1.581836000	-0.984874000
6	-3.047200000	-0.800803000	-1.188083000	6	3.266989000	0.856374000	-0.851872000
6	-2.533651000	-2.050587000	-0.723051000	6	2.540274000	0.950863000	-2.083047000
6	-1.528239000	-2.730764000	-1.423526000	6	2.177237000	-0.206053000	-2.800674000
6	-2.466533000	-0.189850000	-2.285122000	6	3.501147000	-0.382193000	-0.283790000
6	-2.463831000	1.977955000	-1.146014000	6	2.851737000	0.438443000	1.928369000

6	-3.090718000	1.426928000	-0.000280000	6	2.635426000	1.745814000	1.430920000
6	-3.630384000	0.002114000	0.000063000	6	3.014809000	2.121937000	0.002682000
6	-2.206573000	1.247211000	-2.321130000	6	3.361976000	-0.620417000	1.151680000
7	-6.272175000	-0.062976000	-0.000100000	7	5.100271000	3.747614000	-0.066394000
6	-5.105061000	-0.038549000	0.000069000	6	4.176799000	3.031441000	-0.042798000
				7	-4.941563000	3.930607000	-0.020997000
				6	-4.048866000	3.176138000	-0.008578000
				1	1.234032000	-2.656483000	1.351713000
				1	0.506009000	-1.264021000	2.179587000
$(C_{60}(CN)_3)^{3-}$				$(C_{60}(CN)_4)^{4-}$			
6	-0.563563000	2.449511000	-2.305902000	6	-0.643312000	3.208617000	1.493745000
6	0.855871000	2.649285000	-2.016025000	6	-2.002817000	2.820282000	1.114040000
6	-1.537918000	2.688270000	-1.334169000	6	0.328731000	3.481052000	0.524779000
6	1.225960000	3.034166000	-0.714013000	6	-2.299243000	2.672355000	-0.254079000
6	2.395668000	2.444878000	-0.087246000	6	-3.135793000	1.569287000	-0.703245000
6	1.582076000	1.601019000	-2.653636000	6	-2.444505000	1.814554000	2.026274000
6	2.701307000	1.012851000	-2.025379000	6	-3.232596000	0.729496000	1.579413000
6	3.143965000	1.489014000	-0.750026000	6	-3.637406000	0.648866000	0.211832000
6	-2.750772000	0.634581000	-1.932697000	6	2.038508000	2.214340000	1.763964000
6	-1.773477000	0.394693000	-2.970182000	6	1.052215000	1.959674000	2.796860000
6	-2.621542000	1.793517000	-1.142567000	6	1.655972000	2.992836000	0.650917000
6	-0.688111000	1.280939000	-3.132482000	6	-0.267801000	2.433843000	2.643875000
6	0.629507000	0.750408000	-3.356893000	6	-1.372310000	1.570585000	2.982514000
6	-1.569028000	-1.015622000	-3.028976000	6	1.293613000	0.644029000	3.289877000
6	-0.285720000	-1.535162000	-3.250808000	6	0.217799000	-0.195516000	3.629616000
6	0.833258000	-0.628813000	-3.422954000	6	-1.141834000	0.285797000	3.477409000
6	-3.348142000	0.482781000	0.850409000	6	2.989558000	1.470566000	-0.802334000
6	-3.755922000	-0.742927000	-0.005856000	6	3.668987000	0.760187000	0.393458000
6	-2.880021000	1.668307000	0.291345000	6	2.123028000	2.552558000	-0.663859000
6	-3.237741000	-0.613796000	-1.431402000	6	2.952745000	1.119191000	1.690932000
6	-2.444817000	-1.624976000	-2.024902000	6	2.431775000	0.110045000	2.539506000
6	-3.013800000	-1.876488000	0.750635000	6	3.508722000	-0.742608000	0.000434000
6	-2.265998000	-2.840856000	0.093514000	6	2.922504000	-1.659528000	0.888335000
6	-2.011721000	-2.786829000	-1.348017000	6	2.463317000	-1.262194000	2.229255000
6	-1.431453000	2.114351000	2.204845000	6	0.860250000	1.910816000	-2.653438000
6	-1.847607000	0.852069000	2.766674000	6	1.713015000	0.753670000	-2.771866000
6	-1.992529000	2.528696000	1.002616000	6	1.110744000	2.824185000	-1.634014000
6	-2.762356000	0.044509000	2.074702000	6	2.729537000	0.525904000	-1.834766000
6	-2.557755000	-1.386674000	2.019819000	6	3.000763000	-0.810608000	-1.347960000
6	-0.701049000	0.268572000	3.414307000	6	0.912127000	-0.338033000	-3.250094000
6	-0.499759000	-1.112426000	3.370592000	6	1.158683000	-1.616155000	-2.737981000
6	-1.447168000	-1.953530000	2.660263000	6	2.265828000	-1.882309000	-1.861486000
6	0.290058000	3.366903000	0.299250000	6	-1.397617000	3.015037000	-1.296514000
6	0.795812000	2.892313000	1.538347000	6	-1.567179000	2.051724000	-2.333348000
6	-1.205521000	3.405500000	0.001185000	6	-0.036274000	3.630112000	-0.978452000
6	-0.042935000	2.356797000	2.560255000	6	-0.475148000	1.560540000	-3.111351000
6	0.411245000	1.187524000	3.246803000	6	-0.446790000	0.157912000	-3.399634000
6	2.137865000	2.390177000	1.341814000	6	-2.709794000	1.215612000	-2.039511000
6	2.563735000	1.243220000	2.026928000	6	-2.644448000	-0.169445000	-2.337207000
6	1.699175000	0.650160000	3.037602000	6	-1.522173000	-0.695001000	-3.088200000
6	0.695069000	-2.817129000	2.312223000	6	0.426972000	-3.310449000	-1.296315000
6	0.820989000	-1.652840000	3.155064000	6	0.056792000	-2.491634000	-2.410786000
6	1.888800000	-0.759902000	2.964593000	6	-1.252552000	-2.008302000	-2.567640000

6	1.659011000	-3.044621000	1.308678000	6	-0.515508000	-3.510939000	-0.286420000
6	-0.130234000	-3.687682000	-0.286771000	6	1.142928000	-3.000066000	1.452342000
6	-1.114672000	-3.431419000	0.733831000	6	2.175538000	-2.795045000	0.483649000
6	-0.704934000	-2.995624000	2.003825000	6	1.937318000	-3.119082000	-0.988497000
6	1.228168000	-3.487682000	-0.004706000	6	-0.151588000	-3.429679000	1.130726000
6	1.565056000	-2.475759000	-2.218563000	6	-1.095795000	-1.968853000	2.900845000
6	0.172324000	-2.696397000	-2.536752000	6	0.244831000	-1.591645000	3.297800000
6	-0.681914000	-3.268857000	-1.561578000	6	1.349796000	-2.085626000	2.563433000
6	2.093782000	-2.884028000	-0.986292000	6	-1.279374000	-2.858462000	1.829818000
6	3.481319000	-0.861448000	-0.851779000	6	-3.212190000	-1.551731000	1.034826000
6	2.888112000	-0.414379000	-2.078780000	6	-2.972936000	-0.602154000	2.081816000
6	1.993550000	-1.229528000	-2.799126000	6	-1.963456000	-0.826193000	3.036701000
6	3.040732000	-2.047421000	-0.284166000	6	-2.339439000	-2.621631000	0.876543000
6	2.890814000	-1.013014000	1.928335000	6	-2.241372000	-2.276346000	-1.543927000
6	3.372178000	0.226978000	1.437223000	6	-3.158672000	-1.185406000	-1.482039000
6	3.891616000	0.362138000	0.006932000	6	-3.870763000	-0.836519000	-0.176221000
6	2.799492000	-2.186029000	1.151563000	6	-1.874887000	-3.062725000	-0.435161000
7	6.515621000	0.730346000	-0.041606000	7	-6.461063000	-1.402109000	-0.316036000
6	5.355914000	0.570760000	-0.027069000	6	-5.317980000	-1.148459000	-0.247010000
7	-6.377895000	-1.137175000	0.043645000	7	6.241897000	1.409076000	0.548728000
6	-5.220898000	-0.958637000	0.030680000	6	5.106981000	1.122050000	0.470851000
7	-2.105944000	5.895890000	-0.009568000	7	0.025946000	6.178336000	-1.716155000
6	-1.717099000	4.791703000	-0.006356000	6	0.012746000	5.052865000	-1.386419000
				7	3.327163000	-5.256328000	-1.735738000
				6	2.714962000	-4.310051000	-1.410872000
$(C_{60}(CN)_5)^{5-}$				$(C_{60}(CN)_6)^{6-}$			
6	-2.230972000	1.177467000	-2.375748000	6	-0.981197000	-2.523231000	-2.223544000
6	-2.669370000	2.004970000	-1.302439000	6	-0.677108000	-3.355207000	-1.106764000
6	-2.482574000	-0.216353000	-2.475943000	6	0.003301000	-1.906969000	-3.028129000
6	-3.491394000	1.399109000	-0.166794000	6	0.778820000	-3.682286000	-0.751494000
6	-2.831297000	1.664389000	1.209360000	6	1.098037000	-3.369102000	0.733494000
6	-1.623566000	2.960427000	-1.045021000	6	-1.665420000	-3.115568000	-0.106676000
6	-1.202619000	3.322441000	0.247326000	6	-1.354166000	-3.077337000	1.280088000
6	-1.803545000	2.596851000	1.358032000	6	0.040256000	-3.102313000	1.631541000
6	-0.276694000	-0.594576000	-3.526582000	6	-1.455165000	0.078472000	-3.244483000
6	-0.027823000	0.824338000	-3.438880000	6	-2.483995000	-0.609697000	-2.518598000
6	-1.491511000	-1.075268000	-3.029090000	6	-0.205502000	-0.555771000	-3.479636000
6	-0.987796000	1.693102000	-2.893044000	6	-2.258049000	-1.876151000	-1.985239000
6	-0.589772000	2.794713000	-2.061105000	6	-2.723313000	-2.286074000	-0.669379000
6	1.359616000	1.032737000	-3.137831000	6	-3.368464000	0.428434000	-1.770259000
6	1.732997000	2.105648000	-2.312393000	6	-3.593081000	0.018274000	-0.314058000
6	0.767962000	3.043635000	-1.827441000	6	-3.317582000	-1.287050000	0.123684000
6	-0.243213000	-3.036363000	-1.963976000	6	1.026364000	1.529805000	-2.991294000
6	0.966475000	-2.424775000	-2.420273000	6	-0.239215000	2.179359000	-2.719927000
6	-1.605021000	-2.490164000	-2.393714000	6	1.047736000	0.172009000	-3.467968000
6	0.987698000	-1.275473000	-3.234620000	6	-1.446665000	1.461785000	-2.811136000
6	1.983956000	-0.276768000	-3.000712000	6	-2.517256000	1.720001000	-1.903834000
6	1.999176000	-2.622808000	-1.420737000	6	-0.040227000	3.102330000	-1.631593000
6	3.031472000	-1.685454000	-1.278577000	6	-1.098084000	3.369271000	-0.733576000
6	2.985186000	-0.474934000	-2.023493000	6	-2.264928000	2.557430000	-0.805250000
6	-2.187507000	-2.668972000	0.093560000	6	3.014974000	-0.224360000	-1.970007000
6	-0.994367000	-3.416709000	0.398031000	6	3.193545000	1.290002000	-1.676162000
6	-2.515370000	-2.186567000	-1.174165000	6	2.004404000	-0.691010000	-2.829070000

6	-0.001206000	-3.468469000	-0.627229000	6	1.998177000	2.105701000	-2.151052000
6	1.403454000	-3.335129000	-0.312329000	6	1.354104000	3.077051000	-1.279971000
6	-0.585985000	-2.990364000	1.719340000	6	3.317615000	1.286998000	-0.123678000
6	0.793534000	-2.859477000	2.062169000	6	2.723522000	2.286131000	0.669401000
6	1.762159000	-2.926673000	1.003149000	6	1.665526000	3.115618000	0.106685000
6	-3.482026000	-0.156491000	-0.192942000	6	1.770309000	-2.727672000	-1.474140000
6	-3.208241000	-0.665029000	1.110036000	6	2.716756000	-2.211777000	-0.540348000
6	-3.080968000	-0.882197000	-1.320644000	6	1.388929000	-1.982928000	-2.588930000
6	-2.540169000	-1.893236000	1.268001000	6	3.277247000	-0.934661000	-0.760227000
6	-1.603729000	-2.182863000	2.306178000	6	3.593262000	-0.018294000	0.314064000
6	-2.769314000	0.445949000	1.955109000	6	2.264991000	-2.557436000	0.805222000
6	-1.821973000	0.265685000	2.961984000	6	2.517270000	-1.719996000	1.903769000
6	-1.282090000	-1.132742000	3.363199000	6	3.368537000	-0.428459000	1.770254000
6	2.403781000	-1.165641000	2.328685000	6	0.981220000	2.523193000	2.223502000
6	1.165525000	-1.709182000	2.866506000	6	2.258015000	1.876026000	1.985163000
6	0.243923000	-0.845507000	3.444090000	6	2.484070000	0.609709000	2.518638000
6	2.688073000	0.223758000	2.435572000	6	-0.003257000	1.906903000	3.028089000
6	3.659243000	0.144398000	0.141244000	6	-1.770184000	2.727588000	1.474074000
6	3.667472000	-1.410143000	0.113658000	6	-0.778744000	3.682254000	0.751477000
6	2.814355000	-1.978194000	1.247672000	6	0.677163000	3.355212000	1.106772000
6	3.251640000	0.863021000	1.263088000	6	-1.388927000	1.982951000	2.588987000
6	2.451540000	2.707426000	-0.164028000	6	-3.014963000	0.224382000	1.970024000
6	2.762036000	1.908633000	-1.307971000	6	-3.277238000	0.934639000	0.760179000
6	3.353192000	0.639381000	-1.157277000	6	-2.716629000	2.211745000	0.540292000
6	2.633271000	2.167872000	1.108490000	6	-2.004394000	0.690987000	2.829054000
6	0.447333000	2.956818000	1.830948000	6	-1.026326000	-1.529834000	2.991213000
6	0.175455000	3.581724000	0.586767000	6	-1.998230000	-2.105881000	2.151216000
6	1.263331000	3.657143000	-0.490899000	6	-3.193548000	-1.290079000	1.676148000
6	1.680494000	2.353034000	2.184587000	6	-1.047719000	-0.172057000	3.467928000
6	0.464735000	0.568765000	3.453710000	6	1.455169000	-0.078501000	3.244464000
6	-0.779044000	1.225189000	3.113406000	6	1.446635000	-1.461775000	2.811020000
6	-0.789862000	2.405970000	2.351898000	6	0.239278000	-2.179416000	2.719963000
6	1.668545000	1.105466000	2.929217000	6	0.205532000	0.555723000	3.479646000
6	-1.808141000	-1.533007000	4.690975000	6	4.669038000	-0.604405000	2.472919000
7	-2.230299000	-1.875831000	5.733190000	7	5.698965000	-0.737004000	3.028143000
6	1.732204000	5.054286000	-0.680954000	6	4.449852000	1.801523000	-2.290968000
7	2.094611000	6.162831000	-0.821794000	7	5.411632000	2.221225000	-2.825601000
6	5.054419000	-1.932725000	0.173001000	6	-4.669019000	0.604380000	-2.472908000
7	6.149695000	-2.354307000	0.236569000	7	-5.698925000	0.737618000	-3.028019000
6	-4.883983000	1.920191000	-0.194890000	6	-4.450014000	-1.801267000	2.290829000
7	-5.975881000	2.353023000	-0.237774000	7	-5.411827000	-2.220910000	2.825450000
6	-2.271963000	-3.422495000	-3.336070000	6	-1.083849000	5.101851000	1.067095000
7	-2.773394000	-4.182673000	-4.079770000	7	-1.312082000	6.228604000	1.322701000
				6	1.083799000	-5.101935000	-1.066999000
				7	1.311383000	-6.228881000	-1.322330000

Cartesian coordinates of optimized geometry of CO₂ complexes of [(IM⁺)_n...((C₆₀(CN)_n)ⁿ⁻)] for n = 1 to 6 at M06L/6-31G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.

1nc				1'nc			
6	0.755516000	-3.716125000	1.508236000	6	2.049325000	1.480079000	-3.165142000
6	-0.593562000	-3.629056000	1.001925000	6	0.637186000	1.744652000	-3.024306000

6	1.148264000	-2.910562000	2.579226000	6	2.496001000	0.167830000	-3.334867000
6	-1.502857000	-2.740652000	1.586533000	6	-0.278861000	0.687512000	-3.060474000
6	-2.399978000	-1.967447000	0.761929000	6	-1.393811000	0.656466000	-2.144942000
6	-0.544577000	-3.757249000	-0.427156000	6	0.472344000	2.794852000	-2.059590000
6	-1.404835000	-2.981505000	-1.213363000	6	-0.601066000	2.736530000	-1.162795000
6	-2.378713000	-2.123434000	-0.613384000	6	-1.573722000	1.691310000	-1.243748000
6	3.298617000	-2.446358000	1.481614000	6	4.357504000	0.568092000	-1.779749000
6	2.893384000	-3.274361000	0.368510000	6	3.895354000	1.925224000	-1.597286000
6	2.441572000	-2.272342000	2.571195000	6	3.672071000	-0.294195000	-2.639248000
6	1.644518000	-3.898000000	0.380642000	6	2.761505000	2.373925000	-2.276993000
6	0.840305000	-3.925359000	-0.819241000	6	1.785940000	3.190125000	-1.592053000
6	3.381775000	-2.659262000	-0.846195000	6	4.093678000	2.281471000	-0.209179000
6	2.603488000	-2.689872000	-2.004831000	6	3.150291000	3.072632000	0.448932000
6	1.309982000	-3.332910000	-1.987920000	6	1.976365000	3.532531000	-0.256346000
6	3.012839000	0.119780000	2.666889000	6	3.918934000	-2.135393000	-1.024392000
6	3.894484000	-0.062062000	1.536133000	6	4.623369000	-1.239705000	-0.135665000
6	2.292441000	-0.962874000	3.173149000	6	3.444183000	-1.671771000	-2.252128000
6	4.043799000	-1.324883000	0.956819000	6	4.848342000	0.088105000	-0.508097000
6	4.088703000	-1.452504000	-0.481765000	6	4.678292000	1.143734000	0.463774000
6	3.803536000	1.114161000	0.702107000	6	4.239995000	-1.559867000	1.220255000
6	3.845697000	0.990808000	-0.687262000	6	4.073897000	-0.540058000	2.158378000
6	3.995294000	-0.317058000	-1.291016000	6	4.301889000	0.837806000	1.774332000
6	0.287956000	0.443588000	3.429218000	6	1.335112000	-2.902574000	-1.941635000
6	1.037205000	1.568821000	2.906438000	6	1.829781000	-3.387151000	-0.668370000
6	0.913554000	-0.799966000	3.570768000	6	2.138485000	-2.066881000	-2.725353000
6	2.370177000	1.408237000	2.529857000	6	3.093461000	-3.007046000	-0.217908000
6	2.859430000	2.023237000	1.314234000	6	3.292004000	-2.651065000	1.170999000
6	0.146291000	2.352895000	2.081572000	6	0.719251000	-3.425694000	0.255857000
6	0.617626000	2.946657000	0.908712000	6	0.910486000	-3.081452000	1.595780000
6	1.998688000	2.778174000	0.518211000	6	2.220599000	-2.687562000	2.062507000
6	-1.100258000	-1.916325000	2.696131000	6	0.181405000	-0.664536000	-3.243430000
6	-1.756039000	-0.628095000	2.561915000	6	-0.656575000	-1.538200000	-2.442469000
6	0.202937000	-1.998401000	3.190414000	6	1.545888000	-0.925112000	-3.381990000
6	-1.064802000	0.536673000	2.943156000	6	-0.078107000	-2.655247000	-1.812400000
6	-1.145830000	1.703034000	2.097593000	6	-0.452701000	-2.960097000	-0.452834000
6	-2.592231000	-0.660786000	1.396154000	6	-1.657513000	-0.741029000	-1.792731000
6	-2.610839000	0.458279000	0.543986000	6	-1.965733000	-1.005656000	-0.446371000
6	-1.910682000	1.673242000	0.930631000	6	-1.384153000	-2.163270000	0.214526000
6	0.693335000	2.749848000	-1.425994000	6	0.635204000	-1.376203000	3.180417000
6	-0.182986000	2.918527000	-0.295204000	6	-0.062874000	-2.261898000	2.283599000
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6	2.538910000	0.941923000	-2.619725000	6	2.492737000	0.777748000	3.255693000
6	2.959839000	1.774739000	-1.516527000	6	2.967971000	-0.576270000	3.086679000
6	2.040632000	2.647947000	-0.925831000	6	2.046848000	-1.627131000	3.034584000
6	1.228790000	1.015336000	-3.094668000	6	1.125938000	1.032407000	3.373485000
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6	3.184653000	-0.347796000	-2.483887000	6	3.321322000	1.651561000	2.450260000
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6	-1.577979000	-1.111264000	-2.616524000	6	-1.248834000	2.278762000	1.043289000
6	-0.918018000	-2.367048000	-2.429287000	6	-0.403858000	3.093384000	0.225271000
6	0.415307000	-2.548163000	-2.815319000	6	0.861530000	3.494433000	0.669157000
6	-0.857852000	-0.023928000	-3.076881000	6	-0.768240000	1.781151000	2.240698000
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6	-1.016458000	1.314829000	-2.504783000	6	-1.014667000	0.402032000	2.666914000
7	-5.180115000	-1.144215000	-2.520391000	7	-4.737963000	2.258548000	0.214313000
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6	1.241030000	3.224744000	-0.324051000	6	2.989717000	0.740028000	0.929955000
6	1.956145000	2.618287000	-1.433453000	6	3.357855000	0.734577000	-0.492857000
6	1.029985000	-0.743886000	3.469186000	6	-1.453022000	-2.294711000	1.480121000
6	0.524290000	0.602154000	3.446534000	6	-0.631997000	-1.564708000	2.409878000
6	2.319114000	-1.031817000	2.971109000	6	-0.840673000	-3.089100000	0.516905000
6	1.278986000	1.613799000	2.829928000	6	0.762948000	-1.585624000	2.273800000
6	0.731101000	2.644303000	2.044225000	6	1.537189000	-0.382050000	2.466188000
6	-0.883584000	0.529925000	3.100718000	6	-1.317202000	-0.345049000	2.727975000
6	-1.500227000	1.483796000	2.294124000	6	-0.554331000	0.819327000	2.863827000
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6	1.457198000	-3.110183000	1.914410000	6	-2.621686000	-2.335694000	-1.116199000
6	0.143959000	-2.827137000	2.430760000	6	-3.177144000	-1.540663000	-0.080738000
6	2.512420000	-2.226821000	2.177216000	6	-1.505179000	-3.339386000	-0.858025000
6	-0.057985000	-1.649322000	3.182201000	6	-2.695222000	-1.580362000	1.269014000
6	-1.237154000	-0.864895000	2.958685000	6	-2.557351000	-0.339214000	1.973168000
6	-0.815631000	-3.212804000	1.431068000	6	-3.711653000	-0.318710000	-0.638980000
6	-1.948803000	-2.445064000	1.206154000	6	-3.532047000	0.886381000	0.080423000
6	-2.174247000	-1.257947000	1.994026000	6	-3.023565000	0.873826000	1.434812000
6	-2.159402000	1.860923000	0.067435000	6	0.090899000	2.841960000	1.885415000
6	-2.386929000	1.062015000	1.266643000	6	-1.029333000	2.067034000	2.313941000
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6	-2.344439000	1.313503000	-1.205901000	6	0.004501000	3.506685000	0.661846000
6	-0.313724000	2.496850000	-1.940904000	6	2.213197000	2.683677000	-0.017908000
6	-0.165691000	3.088054000	-0.631680000	6	2.391186000	1.991235000	1.220152000
6	-1.119182000	2.783755000	0.339692000	6	1.400085000	2.166172000	2.365278000
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6	1.219999000	1.056622000	-3.213702000	6	2.340058000	1.981564000	-2.386075000
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7	2.736675000	5.325667000	-2.382530000	6	-5.108413000	-3.190128000	-2.346746000
6	2.044160000	6.103828000	-1.480287000	7	-5.644656000	-3.131751000	-1.116244000
1	1.204908000	6.709846000	-1.779199000	7	-4.294270000	-4.257124000	-2.396195000
6	2.593787000	5.879218000	-0.257508000	6	-4.291854000	-4.870766000	-1.160823000
1	2.339780000	6.266253000	0.715128000	1	-3.656648000	-5.715026000	-0.947601000
6	2.343876000	5.084159000	-3.762495000	6	-5.134351000	-4.169904000	-0.360474000
1	2.076130000	6.032218000	-4.229802000	1	-5.372190000	-4.285084000	0.684029000
1	3.173336000	4.619120000	-4.294221000	6	-3.378733000	-4.510361000	-3.492283000
1	1.486206000	4.402272000	-3.771679000	1	-2.622386000	-5.219678000	-3.159869000
6	4.445448000	4.399813000	0.624254000	1	-3.912823000	-4.912878000	-4.356926000
1	3.866846000	4.402060000	1.548520000	1	-2.883764000	-3.565348000	-3.748628000
1	4.703856000	3.357619000	0.392874000	6	-6.440908000	-2.027582000	-0.615576000
1	5.345602000	5.008988000	0.743817000	1	-7.259149000	-2.418404000	-0.005098000
1	-4.428437000	4.972012000	1.037904000	1	-5.785929000	-1.364483000	-0.027174000
6	-5.099251000	4.247733000	0.596561000	1	-6.838028000	-1.464492000	-1.461058000
7	-5.758460000	3.274791000	1.236585000	1	4.643536000	2.218702000	3.590484000
7	-5.378366000	4.164546000	-0.708538000	6	4.431428000	3.120789000	3.037611000
6	-6.200598000	3.077650000	-0.913493000	7	3.586347000	4.104645000	3.407082000
1	-6.511808000	2.783917000	-1.901844000	7	5.127260000	3.557078000	1.967890000

6	-6.435931000	2.518941000	0.303751000	6	4.643990000	4.797852000	1.600650000
1	-6.994174000	1.642250000	0.587030000	1	4.998044000	5.302184000	0.717264000
6	-4.730880000	4.943799000	-1.754331000	6	3.693590000	5.144121000	2.503772000
1	-5.468245000	5.210914000	-2.511858000	1	3.066707000	6.017083000	2.575168000
1	-4.296381000	5.839110000	-1.311499000	6	5.996806000	2.716293000	1.167194000
1	-3.931302000	4.336810000	-2.196339000	1	6.665794000	3.355498000	0.589479000
6	-5.521131000	2.879314000	2.616183000	1	6.574500000	2.064750000	1.823550000
1	-6.472619000	2.743270000	3.132311000	1	5.393590000	2.097599000	0.489280000
1	-4.946572000	1.944867000	2.619171000	6	2.655350000	4.006331000	4.513008000
1	-4.941359000	3.655132000	3.113612000	1	1.930359000	4.815247000	4.430879000
1	3.806012000	-5.619635000	-1.253633000	1	2.128449000	3.050380000	4.444712000
6	4.219810000	-4.727623000	-1.700970000	1	3.182199000	4.077742000	5.468889000
7	4.978102000	-3.810455000	-1.096495000	1	-0.555500000	5.985352000	-3.224122000
7	3.964278000	-4.309146000	-2.943395000	6	-1.435428000	5.904306000	-2.600484000
6	4.570255000	-3.084616000	-3.129936000	7	-1.510448000	6.323631000	-1.330914000
1	4.442446000	-2.524534000	-4.041607000	7	-2.597900000	5.325636000	-2.926904000
6	5.207569000	-2.767629000	-1.967951000	6	-3.413005000	5.322976000	-1.814273000
1	5.705281000	-1.872103000	-1.615580000	1	-4.380585000	4.848198000	-1.815072000
6	3.030432000	-4.945418000	-3.857422000	6	-2.734757000	5.950923000	-0.816447000
1	3.527778000	-5.181195000	-4.799545000	1	-3.005884000	6.124122000	0.212611000
1	2.646793000	-5.852496000	-3.390933000	6	-2.826906000	4.555228000	-4.137979000
1	2.196377000	-4.258377000	-4.031494000	1	-3.773822000	4.851261000	-4.591933000
6	5.340794000	-3.810784000	0.314712000	1	-2.011567000	4.743101000	-4.835162000
1	6.335239000	-4.242392000	0.449850000	1	-2.844157000	3.488471000	-3.881674000
1	5.326092000	-2.765028000	0.643458000	6	-0.388577000	6.851972000	-0.572609000
1	4.599628000	-4.394971000	0.862727000	1	-0.760312000	7.564446000	0.163922000
1	2.857578000	0.750834000	5.347245000	1	0.128866000	6.012639000	-0.086094000
6	3.608558000	0.217691000	4.777690000	1	0.304687000	7.339475000	-1.257384000
7	4.531751000	0.750072000	3.972449000	1	0.552076000	-5.739517000	2.975192000
7	3.719730000	-1.111874000	4.727217000	6	1.442890000	-5.691385000	2.365370000
6	4.723899000	-1.433607000	3.840078000	7	2.597842000	-5.092589000	2.683745000
1	4.955898000	-2.457667000	3.598431000	7	1.544071000	-6.179847000	1.120980000
6	5.234916000	-0.265365000	3.360634000	6	2.779816000	-5.833833000	0.614009000
1	5.962826000	-0.062183000	2.585608000	1	3.071307000	-6.064073000	-0.397966000
6	2.808129000	-2.040584000	5.380064000	6	3.435083000	-5.150322000	1.590262000
1	3.372157000	-2.732271000	6.008248000	1	4.401014000	-4.671915000	1.587145000
1	2.105864000	-1.467316000	5.986780000	6	0.442217000	-6.752700000	0.367159000
1	2.243070000	-2.580242000	4.615983000	1	0.833975000	-7.498767000	-0.324575000
6	4.650759000	2.165723000	3.653513000	1	-0.264556000	-7.209084000	1.059587000
1	5.487624000	2.605841000	4.200691000	1	-0.069833000	-5.943734000	-0.174325000
1	4.814297000	2.232476000	2.572234000	6	2.806811000	-4.248567000	3.850519000
1	3.717982000	2.660919000	3.925765000	1	3.724992000	-4.538834000	4.363438000
6	4.940641000	0.293959000	0.341177000	1	2.871653000	-3.203684000	3.524284000
8	5.377910000	1.386153000	0.785532000	1	1.958481000	-4.356523000	4.524927000
8	5.596167000	-0.772383000	0.213929000	1	-4.870802000	2.403753000	3.313665000
				6	-5.122815000	1.354857000	3.350972000
				7	-4.726807000	0.465309000	4.280312000
				7	-5.944386000	0.732826000	2.490726000
				6	-6.006593000	-0.601252000	2.835651000
				1	-6.583141000	-1.305588000	2.259857000
				6	-5.245454000	-0.771482000	3.946613000
				1	-5.007892000	-1.655191000	4.514546000
				6	-6.468824000	1.330925000	1.272525000
				1	-7.383974000	0.808028000	0.990048000
				1	-6.681418000	2.385016000	1.454916000

	1	-5.725796000	1.249751000	0.469155000
	6	-3.631512000	0.681221000	5.208141000
	1	-3.908831000	0.319362000	6.200340000
	1	-2.741639000	0.155207000	4.840785000
	1	-3.410732000	1.746729000	5.254645000
	6	3.439646000	-0.285612000	5.376736000
	8	3.439851000	-1.448197000	5.492616000
	8	3.456839000	0.882299000	5.315037000
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6	0.685604000	2.221866000	-2.938899000	
6	-0.598788000	2.667438000	-2.527167000	
6	0.916731000	1.038632000	-3.666749000	
6	-1.846095000	1.880169000	-2.906850000	
6	-2.699846000	1.538090000	-1.663572000	
6	-0.449529000	3.281444000	-1.254304000	
6	-1.424833000	3.134148000	-0.221470000	
6	-2.484173000	2.192023000	-0.444052000	
6	3.011554000	0.691379000	-2.407194000	
6	2.801885000	1.941723000	-1.743982000	
6	2.053924000	0.222336000	-3.350019000	
6	1.664064000	2.696326000	-1.976621000	
6	0.956406000	3.428026000	-0.939828000	
6	3.473623000	1.918617000	-0.349446000	
6	2.519183000	2.446835000	0.708688000	
6	1.400422000	3.204146000	0.382616000	
6	2.199183000	-2.062958000	-2.443587000	
6	3.150295000	-1.587922000	-1.462795000	
6	1.694309000	-1.171660000	-3.432079000	
6	3.527861000	-0.240549000	-1.428709000	
6	3.762608000	0.412471000	-0.182572000	
6	2.907932000	-2.289982000	-0.230368000	
6	3.161556000	-1.662466000	1.005387000	
6	3.451177000	-0.272898000	0.994068000	
6	-0.556594000	-2.202877000	-3.124134000	
6	-0.002124000	-3.351943000	-2.254375000	
6	0.279986000	-1.222715000	-3.680001000	
6	1.438226000	-3.092494000	-1.835514000	
6	1.830143000	-3.198023000	-0.455016000	
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6	-0.532810000	-3.569570000	0.283726000	
6	0.884035000	-3.399127000	0.580004000	
6	-1.477431000	0.460822000	-3.405781000	
6	-2.283815000	-0.501099000	-2.744083000	
6	-0.203199000	0.129846000	-3.843055000	
6	-1.799249000	-1.806249000	-2.563838000	
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6	-3.007332000	0.156199000	-1.663400000	
6	-3.324240000	-0.523648000	-0.478586000	
6	-3.041321000	-2.034994000	-0.312779000	
6	-0.254215000	-2.352294000	2.266489000	
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6	-2.372975000	-2.068380000	1.079934000	
6	-0.480557000	-1.141123000	2.960623000	

6	1.924375000	-0.586882000	2.744957000
6	2.286829000	-2.004975000	2.237757000
6	1.031993000	-2.774547000	1.844173000
6	0.641621000	-0.246404000	3.174015000
6	0.968212000	2.042605000	2.423766000
6	2.247016000	1.679587000	1.890704000
6	2.718528000	0.375293000	2.070920000
6	0.168788000	1.103540000	3.023013000
6	-1.757568000	1.934425000	1.747889000
6	-0.981773000	2.910329000	1.133379000
6	0.427129000	3.211553000	1.588989000
6	-1.352416000	1.118491000	2.946288000
6	-2.533370000	-0.800911000	1.712801000
6	-3.108585000	0.130050000	0.754316000
6	-2.717354000	1.479453000	0.790053000
6	-1.619477000	-0.356234000	2.670586000
6	-4.315009000	-2.778991000	-0.278074000
7	-5.335553000	-3.352487000	-0.199740000
6	-0.089919000	-4.680249000	-2.885182000
7	-0.072548000	-5.771807000	-3.312133000
6	4.735766000	2.683875000	-0.360042000
7	5.743528000	3.283163000	-0.393457000
6	0.516193000	4.477499000	2.328970000
7	0.558553000	5.496041000	2.902327000
6	3.126063000	-2.717914000	3.219033000
7	3.862760000	-3.232450000	3.972505000
6	-2.716797000	2.512530000	-3.916752000
7	-3.480510000	2.903646000	-4.715528000
1	5.162160000	4.592278000	-2.378667000
6	4.564249000	4.192137000	-3.183862000
7	3.401592000	4.679361000	-3.628615000
7	4.823290000	3.055292000	-3.837122000
6	3.780134000	2.787695000	-4.695838000
1	3.732215000	1.875289000	-5.266356000
6	2.883659000	3.803633000	-4.558121000
1	1.910628000	3.951228000	-4.995661000
6	5.902627000	2.134416000	-3.527837000
1	6.484267000	1.925808000	-4.427251000
1	6.532458000	2.573047000	-2.755235000
1	5.447212000	1.212990000	-3.143568000
6	2.654132000	5.756394000	-2.999242000
1	2.112589000	6.313383000	-3.763932000
1	1.952655000	5.314005000	-2.275728000
1	3.347396000	6.423873000	-2.488378000
1	2.027208000	-6.048306000	-2.243963000
6	2.431988000	-6.026443000	-1.241776000
7	1.776462000	-6.420326000	-0.140993000
7	3.615211000	-5.520783000	-0.867448000
6	3.702992000	-5.571124000	0.506937000
1	4.543418000	-5.156112000	1.039497000
6	2.555032000	-6.136097000	0.963056000
1	2.207346000	-6.312868000	1.967113000
6	4.485981000	-4.781634000	-1.764007000
1	5.208428000	-4.225819000	-1.168643000
1	5.005714000	-5.462268000	-2.442457000

1	3.869678000	-4.069095000	-2.327490000
6	0.395197000	-6.871804000	-0.116658000
1	0.304302000	-7.732927000	0.547612000
1	-0.234548000	-6.037753000	0.227475000
1	0.097055000	-7.141564000	-1.129912000
1	-2.221441000	4.349288000	3.152586000
6	-3.048452000	4.686093000	2.521887000
7	-4.284403000	4.172740000	2.603383000
7	-3.056440000	5.603843000	1.542860000
6	-4.311666000	5.651512000	0.977191000
1	-4.535328000	6.313867000	0.157658000
6	-5.082496000	4.752440000	1.642809000
1	-6.117134000	4.476701000	1.525589000
6	-1.899898000	6.339317000	1.053561000
1	-2.250420000	7.260200000	0.586475000
1	-1.229289000	6.564917000	1.881474000
1	-1.371434000	5.718009000	0.322830000
6	-4.664798000	3.061892000	3.463335000
1	-4.411777000	2.129015000	2.949835000
1	-4.088004000	3.099070000	4.389310000
1	-5.738379000	3.118722000	3.651472000
1	-4.263310000	0.701844000	-5.241008000
6	-4.605965000	-0.140875000	-4.654796000
7	-5.408377000	-0.049010000	-3.591270000
7	-4.264418000	-1.422780000	-4.821230000
6	-4.812193000	-2.158036000	-3.791297000
1	-4.612144000	-3.210321000	-3.670122000
6	-5.538480000	-1.298749000	-3.025650000
1	-6.093325000	-1.469488000	-2.116701000
6	-3.212192000	-1.889624000	-5.710070000
1	-3.550408000	-2.775141000	-6.249338000
1	-2.969300000	-1.098634000	-6.418113000
1	-2.325983000	-2.125083000	-5.106954000
6	-5.915109000	1.195947000	-3.032790000
1	-7.006012000	1.169769000	-3.001057000
1	-5.495997000	1.317033000	-2.030518000
1	-5.569114000	2.021883000	-3.655313000
1	4.489348000	-0.934631000	4.685952000
6	4.876755000	-0.078982000	4.151279000
7	4.519358000	1.200453000	4.324001000
7	5.778243000	-0.139643000	3.160898000
6	5.952833000	1.130467000	2.649480000
1	6.587522000	1.326483000	1.800422000
6	5.161861000	1.965978000	3.375108000
1	4.977872000	3.023479000	3.276453000
6	6.273428000	-1.373428000	2.576065000
1	7.271351000	-1.200719000	2.173168000
1	6.302927000	-2.146073000	3.343937000
1	5.577530000	-1.688304000	1.784084000
6	3.415856000	1.646197000	5.160248000
1	3.707599000	2.544508000	5.705091000
1	2.546502000	1.857614000	4.527484000
1	3.164243000	0.856469000	5.866548000
1	-5.639262000	-3.023313000	2.240041000
6	-4.852046000	-2.919115000	2.971733000

7	-4.596121000	-1.842995000	3.720759000
7	-3.894561000	-3.822970000	3.197220000
6	-2.988250000	-3.291327000	4.092319000
1	-2.084234000	-3.813978000	4.356504000
6	-3.426513000	-2.043327000	4.420225000
1	-2.987548000	-1.217982000	4.973771000
6	-3.687659000	-5.025331000	2.410947000
1	-3.606232000	-5.894097000	3.066584000
1	-4.524023000	-5.147662000	1.723098000
1	-2.764976000	-4.894772000	1.831161000
6	-5.292210000	-0.566658000	3.645081000
1	-6.287325000	-0.646907000	4.088394000
1	-4.673880000	0.162172000	4.180417000
1	-5.364241000	-0.270505000	2.594597000
6	-2.065443000	1.691703000	4.234788000
8	-2.847722000	0.925372000	4.857718000
8	-1.850048000	2.907161000	4.464883000

Cartesian coordinates of optimized geometry of CO₂ complexes of (C₆₀(CN)_n)ⁿ⁻ for n = 1 to 6 at M06L/6-31G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.

1nc				2nc			
7	-1.970475000	0.447706000	-0.189475000	6	1.385783000	2.234205000	2.350443000
1	-2.689306000	1.094437000	0.100417000	6	-0.060806000	2.211596000	2.528360000
6	-0.665353000	0.800891000	-0.011332000	6	1.970675000	2.760757000	1.209147000
7	0.118775000	-0.251408000	0.112889000	6	-0.852983000	2.638489000	1.441472000
7	-0.234636000	2.056261000	0.032633000	6	-2.054973000	1.900165000	1.087116000
1	-0.835112000	2.807665000	-0.260302000	6	-0.386078000	0.983144000	3.173913000
1	0.790835000	2.131048000	0.026314000	6	-1.540168000	0.258926000	2.806905000
6	1.678171000	-0.242337000	0.016224000	6	-2.405463000	0.762997000	1.782376000
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	6	0.175657000	-0.729069000	-3.510524000
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	6	1.159300000	3.531874000	0.137502000
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6	4.462601000	2.259356000	0.432299000	7	-5.621508000	1.499066000	-3.442321000
7	-1.322456000	6.068453000	-1.823345000	6	1.014676000	5.216156000	0.724870000
6	-1.135602000	4.966720000	-1.469887000	7	1.262714000	6.350771000	0.896708000
7	3.739084000	-4.710967000	-1.642597000	6	-1.590419000	-5.033613000	-0.674671000
6	3.076445000	-3.797436000	-1.332503000	7	-1.894770000	-6.156529000	-0.831906000
6	5.103181000	-0.510089000	-0.000592000	6	4.261176000	-2.314178000	-1.388659000
8	5.709549000	-0.057027000	0.990929000	7	5.015717000	-3.168062000	-1.664992000
8	5.469411000	-1.243294000	-0.937582000	6	5.175845000	0.209718000	-0.720376000
				8	5.858783000	0.629920000	0.237268000
				8	5.515001000	-0.037656000	-1.902240000
6c							
6	1.024973000	-1.112806000	3.098769000				
6	1.381519000	-2.221017000	2.286310000				
6	-0.293447000	-0.848492000	3.542667000				
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6	2.549615000	-2.262227000	0.075815000				
6	1.395011000	-2.940068000	-0.424632000				
6	0.149118000	1.573199000	3.307260000				
6	1.517062000	1.280699000	2.984885000				
6	-0.760346000	0.514230000	3.558336000				
6	1.959309000	-0.032329000	2.855117000				
6	2.878282000	-0.476170000	1.819233000				
6	2.084775000	2.406862000	2.079020000				
6	2.819393000	1.819089000	0.878950000				
6	3.190935000	0.466420000	0.835711000				
6	-2.537460000	1.640624000	2.257980000				
6	-1.608856000	2.711497000	1.969509000				
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6	0.790926000	3.157901000	1.666541000				
6	-1.859039000	3.167785000	0.624436000				
6	-0.794268000	3.659132000	-0.155310000				
6	0.532279000	3.522915000	0.336568000				
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6	-1.496156000	1.316505000	-2.935093000
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6	0.280391000	-0.317571000	-3.354053000
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7	-4.194516000	-3.820194000	-3.270747000
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