

Electronic supplementary information

Corannulene–Fullerene C₇₀ Noncovalent Interactions and Their Effect on the Behavior of Charge Transport and Optical Property

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Contents:

The Cartesian coordinates of geometries of complexes, including their anions and cations, optimized by using B3LYP-D3/6-31G(d) level of theory included in this work.

Cor@C₇₀-S

Atom	x	y	z
C(Fragment=1)	2.34027000	-0.44117700	-1.16020700
C(Fragment=1)	1.59635000	-0.85938100	-2.26373400
C(Fragment=1)	0.81679900	0.10017800	-3.02181500
C(Fragment=1)	-0.42293000	-0.53340000	-3.43097600
C(Fragment=1)	-1.62910300	0.20637100	-3.55636100
C(Fragment=1)	-2.83587400	-0.53169200	-3.42745100

C(Fragment=1)	-4.07309900	0.10393600	-3.01468700
C(Fragment=1)	-4.85366700	-0.85432900	-2.25573700
C(Fragment=1)	-5.59955000	-0.43559200	-1.15198600
C(Fragment=1)	-5.59876100	-1.23225700	0.06398200
C(Fragment=1)	-5.59671200	-0.32202100	1.19743700
C(Fragment=1)	-4.84796100	-0.63252500	2.33450600
C(Fragment=1)	-4.06582600	0.39432000	2.99581000
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C(Fragment=1)	-1.62049800	0.54820200	3.51888400
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C(Fragment=1)	0.82414500	0.39065500	2.99143000
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C(Fragment=1)	-1.62003200	1.92316300	2.99801700
C(Fragment=1)	-2.82664700	2.44688000	2.46192400
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C(Fragment=1)	-4.84692900	2.02307500	1.32752400
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C(Fragment=1)	-0.41443600	3.23259400	1.25831700
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C(Fragment=1)	-2.82747300	3.23370900	1.26109900
C(Fragment=1)	-4.06661700	2.96965600	0.55388900
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C(Fragment=1)	-0.42336000	-1.87634700	-2.92175000

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C(Fragment=2)	4.99203500	-2.92370900	1.44315700
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C(Fragment=2)	4.99540700	1.51868100	-2.88429900
C(Fragment=2)	4.99571600	0.18115700	-3.25428800
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H(Fragment=2)	4. 62027900	-4. 05901700	-1. 23073500
H(Fragment=2)	4. 62131200	2. 25163000	-3. 59462900
H(Fragment=2)	4. 62206900	-0. 08273000	-4. 24042500

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Atom	x	y	z
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C(Fragment=1)	1. 48417400	-0. 00008200	1. 93786700
C(Fragment=1)	1. 73651300	1. 20414000	1. 23193200
C(Fragment=1)	1. 06946400	2. 44370500	1. 58382800
C(Fragment=1)	0. 88261700	3. 22502000	0. 37490900
C(Fragment=1)	-0. 28266400	3. 97256600	0. 19524900
C(Fragment=1)	-0. 94789600	3. 97297000	-1. 09777600
C(Fragment=1)	-2. 38231600	3. 97166900	-0. 86418700
C(Fragment=1)	-3. 22011400	3. 22541700	-1. 69541500
C(Fragment=1)	-4. 30267800	2. 44462700	-1. 12756000
C(Fragment=1)	-4. 42034800	1. 20644900	-1. 87452500
C(Fragment=1)	-4. 83742900	0. 00009500	-1. 25137400
C(Fragment=1)	-4. 42040800	-1. 20627900	-1. 87452200
C(Fragment=1)	-4. 30280200	-2. 44446200	-1. 12755900
C(Fragment=1)	-3. 22029700	-3. 22531700	-1. 69541600
C(Fragment=1)	-2. 38253800	-3. 97160900	-0. 86418600
C(Fragment=1)	-0. 94811500	-3. 97299600	-1. 09777800
C(Fragment=1)	-1. 30698500	-3. 97296000	1. 22776100
C(Fragment=1)	-2. 60440600	-3. 97206900	0. 57256800
C(Fragment=1)	-3. 65365200	-3. 22503100	1. 11229900
C(Fragment=1)	-4. 51464400	-2. 44457100	0. 24437800
C(Fragment=1)	-4. 85219700	-1. 20641900	0. 92133600
C(Fragment=1)	-5. 06148300	0. 00010100	0. 20155900
C(Fragment=1)	-4. 85213200	1. 20661000	0. 92133900
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C(Fragment=1)	-1. 11745300	3. 22512900	2. 39168800
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C(Fragment=1)	-0. 25162500	1. 20659200	3. 24406000

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C(Fragment=1)	0.09321700	-2.44567700	2.57062200
C(Fragment=1)	-1.11763500	-3.22514700	2.39167800
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C(Fragment=1)	-3.44871300	-2.44514600	2.31758300
C(Fragment=1)	-4.19520600	-1.20640000	2.19782500
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C(Fragment=1)	-3.44857200	2.44525600	2.31758700
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C(Fragment=1)	-2.41841900	0.00002500	3.44872000
C(Fragment=1)	-1.66908300	-1.20647300	3.47296800
C(Fragment=1)	1.42136200	-2.44179500	-0.72040100
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C(Fragment=1)	1.92565600	-0.00008900	-0.93347400
C(Fragment=1)	1.95331700	1.20345000	-0.18478300
C(Fragment=1)	1.42150100	2.44164200	-0.72041600
C(Fragment=1)	0.79118000	2.44520200	-1.95615200
C(Fragment=1)	-0.41650300	3.22503800	-2.15085100
C(Fragment=1)	-1.29105100	2.44476800	-3.00556000
C(Fragment=1)	-2.66140900	2.44500700	-2.78258000
C(Fragment=1)	-3.40900900	1.20642000	-2.89357100
C(Fragment=1)	-2.78901100	0.00004000	-3.31562900
C(Fragment=1)	-3.40907600	-1.20630700	-2.89357200
C(Fragment=1)	-2.66154100	-2.44493500	-2.78258400
C(Fragment=1)	-1.29118600	-2.44476600	-3.00556300
C(Fragment=1)	-0.41668000	-3.22508300	-2.15084500
C(Fragment=1)	0.79104100	-2.44532100	-1.95614600
C(Fragment=1)	0.66600900	-1.20631500	-2.70281400
C(Fragment=1)	1.25627500	-0.00007100	-2.24153200
C(Fragment=1)	0.66606700	1.20620200	-2.70281900
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C(Fragment=1)	-1.33803800	0.00000000	-3.55288500
C(Fragment=1)	-0.61636000	-1.20665900	-3.34917800
C(Fragment=2)	4.53282800	-2.43671600	-2.17934800
C(Fragment=2)	4.49592300	-1.31250800	-2.99238800
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C(Fragment=2)	4.49583600	1.31074400	-2.99315000
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C(Fragment=2)	4.66888000	-2.81862900	1.63171100

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C(Fragment=2)	5.44737200	-0.00034800	-1.24974600
C(Fragment=2)	5.47771500	-1.14882800	-0.41564300
C(Fragment=2)	5.52094600	-0.70952100	0.93345600
C(Fragment=2)	5.02729000	-1.46202200	1.98594900
C(Fragment=2)	4.70980600	-0.69320400	3.17001800
C(Fragment=2)	4.70976300	0.69503800	3.16961100
C(Fragment=2)	5.02720600	1.46318400	1.98509400
C(Fragment=2)	5.52092800	0.71010200	0.93304600
H(Fragment=2)	4.14774200	-3.37298200	-2.57458600
H(Fragment=2)	4.08379300	-1.41195700	-3.99331200
H(Fragment=2)	4.08345900	1.40956600	-3.99403400
H(Fragment=2)	4.14736800	3.37138300	-2.57647300
H(Fragment=2)	4.25497700	-4.24892700	0.10676200
H(Fragment=2)	4.32537900	-3.49790700	2.40776400
H(Fragment=2)	4.32513600	3.49925600	2.40573200
H(Fragment=2)	4.25472200	4.24894000	0.10427700
H(Fragment=2)	4.36623200	-1.20968100	4.06290600
H(Fragment=2)	4.36615100	1.21202000	4.06219200

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Atom	x	y	z
C(Fragment=1)	-3.94675500	-0.02911600	1.21710400
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C(Fragment=1)	-1.21185500	0.64916100	3.40235800
C(Fragment=1)	-0.00001300	1.37983900	3.26169000
C(Fragment=1)	1.21182100	0.64914800	3.40230000
C(Fragment=1)	2.43188500	1.10517700	2.80171900
C(Fragment=1)	3.20500000	-0.05694400	2.39524600
C(Fragment=1)	3.94674500	-0.02912200	1.21710400
C(Fragment=1)	3.96049000	-1.18655400	0.33814700
C(Fragment=1)	3.95942500	-0.70353600	-1.02383100
C(Fragment=1)	3.22412600	-1.37677300	-2.00618700
C(Fragment=1)	2.44557800	-0.62347100	-2.97054100
C(Fragment=1)	1.20711800	-1.33742500	-3.22187700
C(Fragment=1)	-0.00002100	-0.65033700	-3.52083000
C(Fragment=1)	-1.20715600	-1.33743000	-3.22187800
C(Fragment=1)	-2.44562100	-0.62347800	-2.97054400
C(Fragment=1)	-3.22416800	-1.37677800	-2.00619400

C(Fragment=1)	-3.95946100	-0.70355000	-1.02383800
C(Fragment=1)	-3.96050700	-1.18656400	0.33814000
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C(Fragment=1)	-3.22391500	1.47304900	-1.93766500
C(Fragment=1)	-2.44550800	0.76689900	-2.93707500
C(Fragment=1)	-1.20682300	1.49221400	-3.15427800
C(Fragment=1)	-0.00002300	0.82002200	-3.48522000
C(Fragment=1)	1.20677400	1.49220800	-3.15427800
C(Fragment=1)	2.44545900	0.76690000	-2.93706900
C(Fragment=1)	3.22386500	1.47304800	-1.93766100
C(Fragment=1)	3.95975500	0.75263000	-0.98948200
C(Fragment=1)	3.96097100	1.17066100	0.39338400
C(Fragment=1)	3.21698900	2.29079800	0.78894900
C(Fragment=1)	2.44597700	2.26355900	2.00893100
C(Fragment=1)	1.20824500	2.97354300	1.77890100
C(Fragment=1)	-0.00000600	2.58763000	2.42121000
C(Fragment=1)	-1.20823600	2.97347500	1.77886100
C(Fragment=1)	-2.44593600	2.26349200	2.00889900
C(Fragment=1)	-3.21698200	2.29077000	0.78894300
C(Fragment=1)	-2.43979800	3.02556600	-0.19575700
C(Fragment=1)	-2.44859500	2.62545900	-1.52924600
C(Fragment=1)	-1.20664900	2.63460200	-2.28262500
C(Fragment=1)	-0.00002200	3.13503600	-1.72314900
C(Fragment=1)	1.20659800	2.63458400	-2.28262600
C(Fragment=1)	2.44852900	2.62542000	-1.52924600
C(Fragment=1)	2.43972300	3.02551000	-0.19577000
C(Fragment=1)	1.20910200	3.47026800	0.42229000
C(Fragment=1)	-0.00002000	3.56556100	-0.31606100
C(Fragment=1)	-1.20914300	3.47026600	0.42228400
C(Fragment=1)	-2.43137300	-1.23690300	2.74390800
C(Fragment=1)	-1.21154700	-0.80993300	3.36665500
C(Fragment=1)	-0.00000700	-1.53262500	3.19143000
C(Fragment=1)	1.21152500	-0.80993400	3.36663800
C(Fragment=1)	2.43134800	-1.23690000	2.74389200
C(Fragment=1)	2.44689300	-2.35662800	1.89811600
C(Fragment=1)	3.21742400	-2.32517100	0.67899800
C(Fragment=1)	2.44031100	-3.01067900	-0.34027300
C(Fragment=1)	2.44839400	-2.54718500	-1.65292300
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C(Fragment=1)	-0.00001300	-3.04587200	-1.87071200
C(Fragment=1)	-1.20672800	-2.51973900	-2.40539600
C(Fragment=1)	-2.44842200	-2.54718900	-1.65292800
C(Fragment=1)	-2.44033300	-3.01068100	-0.34027800

C(Fragment=1)	-3.21745500	-2.32518800	0.67899000
C(Fragment=1)	-2.44691500	-2.35663000	1.89811400
C(Fragment=1)	-1.20880800	-3.05437200	1.63390300
C(Fragment=1)	-0.00000600	-2.69926100	2.29401200
C(Fragment=1)	1.20878900	-3.05437000	1.63390500
C(Fragment=1)	1.20965900	-3.48532200	0.25563500
C(Fragment=1)	-0.00001100	-3.54598300	-0.48700500
C(Fragment=1)	-1.20967700	-3.48532200	0.25563400
C(Fragment=2)	-6.57460100	0.80435600	-3.12109300
C(Fragment=2)	-6.57282600	-0.58190500	-3.17087000
C(Fragment=2)	-6.93561700	-1.38779800	-2.02597900
C(Fragment=2)	-6.55274500	-2.74582200	-1.71181300
C(Fragment=2)	-6.53616800	-3.22046000	-0.40875700
C(Fragment=2)	-6.93936300	1.52689800	-1.92246800
C(Fragment=2)	-6.56041300	2.86039900	-1.51271800
C(Fragment=2)	-6.54620200	3.24069800	-0.17991800
C(Fragment=2)	-6.50315000	-1.41108500	2.95305900
C(Fragment=2)	-6.50882000	-2.50232200	2.09860300
C(Fragment=2)	-6.90318500	-2.38603000	0.71274000
C(Fragment=2)	-7.46493000	-1.16581600	0.36970000
C(Fragment=2)	-7.47915500	-0.67813200	-0.96616800
C(Fragment=2)	-7.48104600	0.74269400	-0.91513200
C(Fragment=2)	-7.46736500	1.13341200	0.45199700
C(Fragment=2)	-6.90947800	2.32747600	0.88081000
C(Fragment=2)	-6.51583300	2.34516800	2.27194600
C(Fragment=2)	-6.50669200	1.19560300	3.04559400
C(Fragment=2)	-6.88952400	-0.09078300	2.50927200
C(Fragment=2)	-7.45727700	-0.04595000	1.24583900
H(Fragment=2)	-6.17525800	1.35415300	-3.96972700
H(Fragment=2)	-6.17247700	-1.06852100	-4.05661700
H(Fragment=2)	-6.15004200	-3.37819500	-2.49896500
H(Fragment=2)	-6.12007500	-4.20703200	-0.22136500
H(Fragment=2)	-6.15998100	3.54903700	-2.25236100
H(Fragment=2)	-6.13397700	4.21314900	0.07666600
H(Fragment=2)	-6.07937500	-1.53340100	3.94665000
H(Fragment=2)	-6.08902100	-3.44012600	2.45318900
H(Fragment=2)	-6.09757900	3.25591500	2.69269700
H(Fragment=2)	-6.08220800	1.24746200	4.04495100
C(Fragment=3)	6.57276300	-0.58217000	-3.17082500
C(Fragment=3)	6.57455300	0.80408600	-3.12115600
C(Fragment=3)	6.93935300	1.52672100	-1.92260800
C(Fragment=3)	6.56042200	2.86023400	-1.51295200
C(Fragment=3)	6.54625900	3.24062400	-0.18021500
C(Fragment=3)	6.93559800	-1.38796100	-2.02588500

C(Fragment=3)	6.55273300	-2.74595400	-1.71159600
C(Fragment=3)	6.53620400	-3.22048300	-0.40849500
C(Fragment=3)	6.50685900	1.19586900	3.04546300
C(Fragment=3)	6.51597200	2.34533700	2.27171300
C(Fragment=3)	6.90956200	2.32751500	0.88057300
C(Fragment=3)	7.46743400	1.13343600	0.45186200
C(Fragment=3)	7.48106500	0.74261100	-0.91523200
C(Fragment=3)	7.47916300	-0.67821100	-0.96615000
C(Fragment=3)	7.46497800	-1.16577600	0.36976100
C(Fragment=3)	6.90324600	-2.38596000	0.71292700
C(Fragment=3)	6.50893300	-2.50212100	2.09880800
C(Fragment=3)	6.50327200	-1.41081700	2.95314100
C(Fragment=3)	6.88965100	-0.09056300	2.50923800
C(Fragment=3)	7.45735600	-0.04584000	1.24579600
H(Fragment=3)	6.17237600	-1.06886000	-4.05651400
H(Fragment=3)	6.17518100	1.35381900	-3.96981600
H(Fragment=3)	6.15996200	3.54881200	-2.25262800
H(Fragment=3)	6.13403500	4.21308900	0.07630200
H(Fragment=3)	6.15000300	-3.37839100	-2.49868200
H(Fragment=3)	6.12011500	-4.20703800	-0.22101100
H(Fragment=3)	6.08241200	1.24782600	4.04483100
H(Fragment=3)	6.09772400	3.25612500	2.69237800
H(Fragment=3)	6.08914500	-3.43989100	2.45349700
H(Fragment=3)	6.07953800	-1.53305100	3.94676300

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Atom	x	y	z
C(Fragment=1)	-0.72410400	3.97020500	1.39357100
C(Fragment=1)	-1.41712400	3.21973100	2.34670700
C(Fragment=1)	-0.69110400	2.43756700	3.32884100
C(Fragment=1)	-1.41259200	1.19911300	3.55802100
C(Fragment=1)	-0.73289700	-0.00817400	3.87240800
C(Fragment=1)	-1.41375000	-1.21374700	3.55397100
C(Fragment=1)	-0.69342600	-2.45210100	3.32063600
C(Fragment=1)	-1.42017700	-3.23026000	2.33584300
C(Fragment=1)	-0.72787900	-3.97816800	1.38017500
C(Fragment=1)	-1.17812300	-3.97534000	-0.00277000
C(Fragment=1)	-0.00273300	-3.97591700	-0.85894800
C(Fragment=1)	-0.00317900	-3.22492600	-2.03681700
C(Fragment=1)	1.16282700	-2.44416100	-2.40592000
C(Fragment=1)	0.71489200	-1.20427700	-3.01430400
C(Fragment=1)	1.45113600	0.00214200	-2.86869300
C(Fragment=1)	0.71602900	1.20974400	-3.01021600

C(Fragment=1)	1.16514600	2.44715600	-2.39767000
C(Fragment=1)	-0.00013300	3.22776900	-2.02593000
C(Fragment=1)	0.00101700	3.97483400	-0.84558200
C(Fragment=1)	-1.17437000	3.97250000	0.01061400
C(Fragment=1)	0.72919200	3.96952100	1.39258100
C(Fragment=1)	1.17757000	3.97137800	0.00901900
C(Fragment=1)	2.29853700	3.22324500	-0.35730000
C(Fragment=1)	2.28708500	2.44329000	-1.58077400
C(Fragment=1)	3.00150300	1.20295700	-1.34343200
C(Fragment=1)	2.63857700	0.00012900	-2.00199200
C(Fragment=1)	3.00032600	-1.20523000	-1.34746300
C(Fragment=1)	2.28475900	-2.44408300	-1.58898600
C(Fragment=1)	2.29550400	-3.22818400	-0.36817500
C(Fragment=1)	1.17380200	-3.97645600	-0.00437000
C(Fragment=1)	0.72542000	-3.97883700	1.37918100
C(Fragment=1)	1.41971900	-3.23160300	2.33391700
C(Fragment=1)	0.69503600	-2.45275700	3.31969000
C(Fragment=1)	1.41684400	-1.21508200	3.55205200
C(Fragment=1)	0.73755300	-0.00887200	3.87141100
C(Fragment=1)	1.41796900	1.19776700	3.55608900
C(Fragment=1)	0.69735700	2.43690500	3.32789300
C(Fragment=1)	1.42279500	3.21838800	2.34477800
C(Fragment=1)	2.58203500	2.43788300	1.95614100
C(Fragment=1)	3.00604100	2.43727000	0.63556000
C(Fragment=1)	3.44413900	1.19986300	0.01941800
C(Fragment=1)	3.53791900	-0.00495900	0.76067900
C(Fragment=1)	3.44300600	-1.20718200	0.01539000
C(Fragment=1)	3.00383100	-2.44629900	0.62736300
C(Fragment=1)	2.57966400	-2.45087000	1.94788900
C(Fragment=1)	2.57845100	-1.21386900	2.70775500
C(Fragment=1)	3.08873100	-0.00708800	2.16018300
C(Fragment=1)	2.57958300	1.19830400	2.71181100
C(Fragment=1)	-2.57762200	2.44032700	1.95963500
C(Fragment=1)	-2.57536900	1.20076100	2.71533200
C(Fragment=1)	-3.08638900	-0.00417500	2.16438700
C(Fragment=1)	-2.57651700	-1.21144200	2.71126700
C(Fragment=1)	-2.57992000	-2.44844600	1.95139800
C(Fragment=1)	-3.00582700	-2.44344500	0.63143100
C(Fragment=1)	-2.29958800	-3.22599700	-0.36505100
C(Fragment=1)	-2.28975500	-2.44190600	-1.58588400
C(Fragment=1)	-1.16896100	-2.44306400	-2.40434900
C(Fragment=1)	-0.72067800	-1.20359700	-3.01333300
C(Fragment=1)	-1.45558100	0.00351500	-2.86670900
C(Fragment=1)	-0.71953000	1.21041700	-3.00923400

C(Fragment=1)	-1.16664800	2.44825700	-2.39608300
C(Fragment=1)	-2.28747600	2.44544400	-1.57765700
C(Fragment=1)	-2.29653800	3.22542000	-0.35418200
C(Fragment=1)	-3.00353100	2.44018100	0.63965400
C(Fragment=1)	-3.44352300	1.20312700	0.02411000
C(Fragment=1)	-3.53743400	-0.00160400	0.76548000
C(Fragment=1)	-3.44466700	-1.20391700	0.02005700
C(Fragment=1)	-3.00385200	-1.20239600	-1.34339400
C(Fragment=1)	-2.64184000	0.00262400	-1.99839400
C(Fragment=1)	-3.00271500	1.20577500	-1.33932800
C(Fragment=2)	-6.00134900	3.25483400	-0.90400000
C(Fragment=2)	-5.82571100	2.82814900	-2.21315700
C(Fragment=2)	-6.12173400	1.47277600	-2.62543400
C(Fragment=2)	-5.61608900	0.70716200	-3.74436900
C(Fragment=2)	-5.61697000	-0.68113400	-3.74834800
C(Fragment=2)	-6.48748300	2.37011400	0.13282000
C(Fragment=2)	-6.31304600	2.43429300	1.56810300
C(Fragment=2)	-6.41043100	1.30765100	2.37279800
C(Fragment=2)	-6.00545500	-3.24452900	-0.92262500
C(Fragment=2)	-5.82930300	-2.81057700	-2.22931200
C(Fragment=2)	-6.12360100	-1.45249100	-2.63382600
C(Fragment=2)	-6.78122000	-0.70193900	-1.67383800
C(Fragment=2)	-6.78032000	0.71757400	-1.66977000
C(Fragment=2)	-6.95749600	1.15272800	-0.33036400
C(Fragment=2)	-7.06463200	0.00179400	0.49384000
C(Fragment=2)	-6.69898600	-0.00227600	1.82931400
C(Fragment=2)	-6.41213600	-1.31567200	2.36528400
C(Fragment=2)	-6.31618000	-2.43780500	1.55414800
C(Fragment=2)	-6.49045700	-2.36515700	0.11924700
C(Fragment=2)	-6.95890700	-1.14453000	-0.33694400
H(Fragment=2)	-5.66490800	4.25322100	-0.63670900
H(Fragment=2)	-5.35971600	3.50950900	-2.92045500
H(Fragment=2)	-5.13087500	1.22595800	-4.56745900
H(Fragment=2)	-5.13242100	-1.19582000	-4.57440400
H(Fragment=2)	-5.99603000	3.36863600	2.02372100
H(Fragment=2)	-6.16612200	1.40348000	3.42763400
H(Fragment=2)	-5.67023800	-4.24484600	-0.66106300
H(Fragment=2)	-5.36417700	-3.48846800	-2.94050700
H(Fragment=2)	-6.16802000	-1.41787500	3.41956800
H(Fragment=2)	-6.00040000	-3.37515600	2.00441400
C(Fragment=3)	6.31342400	2.43301000	1.56910200
C(Fragment=3)	6.41038700	1.30601100	2.37336500
C(Fragment=3)	6.69876400	-0.00375600	1.82943200
C(Fragment=3)	6.41155400	-1.31730400	2.36487600

C(Fragment=3)	6.31541300	-2.43909100	1.55330300
C(Fragment=3)	6.48804400	2.36933100	0.13382800
C(Fragment=3)	6.00222700	3.25454500	-0.90272500
C(Fragment=3)	5.82663200	2.82837900	-2.21205700
C(Fragment=3)	5.82883600	-2.81029100	-2.23032700
C(Fragment=3)	6.00474800	-3.24477100	-0.92378700
C(Fragment=3)	6.48990200	-2.36592700	0.11845000
C(Fragment=3)	6.95873100	-1.14525700	-0.33722000
C(Fragment=3)	7.06461600	0.00073600	0.49401700
C(Fragment=3)	6.95782000	1.15200000	-0.32976300
C(Fragment=3)	6.78072700	0.71739600	-1.66935700
C(Fragment=3)	6.12240400	1.47310100	-2.62480200
C(Fragment=3)	5.61670500	0.70803800	-3.74409100
C(Fragment=3)	5.61721600	-0.68024800	-3.74857300
C(Fragment=3)	6.12356200	-1.45214200	-2.63429300
C(Fragment=3)	6.78129800	-0.70211900	-1.67396400
H(Fragment=3)	5.99656000	3.36725200	2.02504200
H(Fragment=3)	6.16592300	1.40148400	3.42819600
H(Fragment=3)	6.16740100	-1.41986100	3.41911500
H(Fragment=3)	5.99939400	-3.37655500	2.00316700
H(Fragment=3)	5.66603600	4.25293100	-0.63511900
H(Fragment=3)	5.36087400	3.51010900	-2.91915600
H(Fragment=3)	5.36355100	-3.48776700	-2.94181400
H(Fragment=3)	5.66915900	-4.24506000	-0.66259400
H(Fragment=3)	5.13170200	1.22727100	-4.56703000
H(Fragment=3)	5.13262700	-1.19451700	-4.57486500

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Atom	x	y	z
C(Fragment=1)	-3.98855200	-4.13062500	0.90278200
C(Fragment=1)	-2.95043400	-4.60614600	1.70665600
C(Fragment=1)	-2.43703700	-3.79356000	2.79238700
C(Fragment=1)	-1.00070900	-3.98297000	2.87129300
C(Fragment=1)	-0.13545300	-2.93592600	3.28715300
C(Fragment=1)	1.20959100	-3.01541200	2.83647500
C(Fragment=1)	2.04252000	-1.83254400	2.72142500
C(Fragment=1)	2.95744400	-2.01952900	1.61180500
C(Fragment=1)	3.28305000	-0.94443400	0.78388300
C(Fragment=1)	3.34277500	-1.13143600	-0.65595900
C(Fragment=1)	2.80886000	0.06300800	-1.28626900
C(Fragment=1)	2.02787400	-0.04882400	-2.43692200
C(Fragment=1)	0.82514500	0.74970300	-2.58271000
C(Fragment=1)	-0.18567200	-0.05622400	-3.24357600

C(Fragment=1)	-1.56762400	0.10096000	-2.95256600
C(Fragment=1)	-2.39623600	-1.02464800	-3.20743400
C(Fragment=1)	-3.65506900	-1.21328300	-2.50878700
C(Fragment=1)	-3.88027600	-2.63688100	-2.34027300
C(Fragment=1)	-4.46504100	-3.12318400	-1.16873200
C(Fragment=1)	-3.92983600	-4.31827000	-0.53773200
C(Fragment=1)	-4.55968600	-2.81940100	1.16251800
C(Fragment=1)	-4.85321800	-2.19615200	-0.11770800
C(Fragment=1)	-4.64017100	-0.82653800	-0.28728200
C(Fragment=1)	-4.02356200	-0.32982000	-1.50369700
C(Fragment=1)	-3.14828300	0.77435900	-1.15853700
C(Fragment=1)	-1.95966600	1.03481100	-1.88740400
C(Fragment=1)	-0.94298000	1.74139800	-1.19524100
C(Fragment=1)	0.45243800	1.63129200	-1.57720500
C(Fragment=1)	1.26696100	1.75838000	-0.38330500
C(Fragment=1)	2.41883800	0.98723800	-0.23571100
C(Fragment=1)	2.71242900	0.36497500	1.04272200
C(Fragment=1)	1.84062100	0.54267100	2.11722600
C(Fragment=1)	1.49623700	-0.57942200	2.96878600
C(Fragment=1)	0.09875600	-0.46219500	3.34304100
C(Fragment=1)	-0.71266400	-1.60965700	3.55145600
C(Fragment=1)	-2.11156200	-1.43008200	3.37865600
C(Fragment=1)	-2.98217400	-2.54094000	3.04113400
C(Fragment=1)	-4.06527900	-2.04393200	2.21363700
C(Fragment=1)	-3.83917700	-0.62283200	2.02984000
C(Fragment=1)	-4.11589500	-0.02978400	0.80629000
C(Fragment=1)	-3.20511500	0.95877400	0.26160800
C(Fragment=1)	-2.07631200	1.40869100	0.99153400
C(Fragment=1)	-1.00071400	1.92466200	0.22545600
C(Fragment=1)	0.35781800	1.92814300	0.73272100
C(Fragment=1)	0.63954900	1.33890400	1.95706200
C(Fragment=1)	-0.42954800	0.71990400	2.71989800
C(Fragment=1)	-1.78095800	0.78226200	2.28803700
C(Fragment=1)	-2.63889700	-0.24825100	2.75597800
C(Fragment=1)	-1.81352200	-5.27851400	1.10746100
C(Fragment=1)	-0.61672600	-4.89812000	1.83378700
C(Fragment=1)	0.64217200	-4.78918200	1.18522900
C(Fragment=1)	1.59341000	-3.93036300	1.79792000
C(Fragment=1)	2.66526500	-3.31822800	1.03533100
C(Fragment=1)	2.72167000	-3.49735600	-0.34092800
C(Fragment=1)	3.07261800	-2.38587800	-1.20462200
C(Fragment=1)	2.25135400	-2.49819800	-2.39469000
C(Fragment=1)	1.73967800	-1.35535300	-2.99642600
C(Fragment=1)	0.37788100	-1.35253100	-3.49819500

C(Fragment=1)	-0.42664300	-2.52313100	-3.47082400
C(Fragment=1)	-1.83283200	-2.32033800	-3.46251900
C(Fragment=1)	-2.73920200	-3.31666100	-2.92244600
C(Fragment=1)	-2.22886800	-4.45874000	-2.32045600
C(Fragment=1)	-2.83578700	-4.97266600	-1.10789900
C(Fragment=1)	-1.75749400	-5.45760500	-0.26802500
C(Fragment=1)	-0.50253200	-5.26307200	-0.96934800
C(Fragment=1)	0.70157000	-4.97880200	-0.27135000
C(Fragment=1)	1.70781700	-4.29528700	-1.00500900
C(Fragment=1)	1.41777600	-3.67965900	-2.26988100
C(Fragment=1)	0.11382200	-3.73200300	-2.83170100
C(Fragment=1)	-0.79267900	-4.64731100	-2.23339500
C(Fragment=2)	6.63038100	-1.47842000	1.03230800
C(Fragment=2)	6.71144800	-1.59799300	-0.34791800
C(Fragment=2)	6.52294100	-0.46526600	-1.22877400
C(Fragment=2)	6.11950800	-0.42433800	-2.61798900
C(Fragment=2)	5.53168800	0.69984100	-3.18064600
C(Fragment=2)	6.35278800	-0.21354700	1.67823000
C(Fragment=2)	5.78865400	0.05957400	2.98266400
C(Fragment=2)	5.15298400	1.25839600	3.27323800
C(Fragment=2)	3.88300900	3.77909800	-1.59903300
C(Fragment=2)	4.32402100	2.96258500	-2.63103100
C(Fragment=2)	5.28529100	1.90270200	-2.41435900
C(Fragment=2)	5.86758300	1.90870300	-1.15794900
C(Fragment=2)	6.46778800	0.75804100	-0.58201400
C(Fragment=2)	6.38635900	0.88065400	0.83004900
C(Fragment=2)	5.73654000	2.10784600	1.12732600
C(Fragment=2)	5.01353100	2.31145600	2.29056300
C(Fragment=2)	4.04441700	3.38294000	2.21005900
C(Fragment=2)	3.73295400	4.00545700	1.00973000
C(Fragment=2)	4.35434600	3.62205000	-0.23979400
C(Fragment=2)	5.41600200	2.74376000	-0.10172300
H(Fragment=2)	6.67854300	-2.38278900	1.63353100
H(Fragment=2)	6.82066600	-2.59141800	-0.77556100
H(Fragment=2)	6.18401400	-1.32907700	-3.21717500
H(Fragment=2)	5.15728200	0.63260200	-4.19892900
H(Fragment=2)	5.77098100	-0.72958700	3.73004200
H(Fragment=2)	4.66076500	1.36222700	4.23687200
H(Fragment=2)	3.08601100	4.48831700	-1.80737100
H(Fragment=2)	3.85643200	3.06479700	-3.60711500
H(Fragment=2)	3.46930200	3.64675100	3.09408700
H(Fragment=2)	2.92794800	4.73531200	1.00237000
C(Fragment=3)	-5.11829200	3.00658400	2.30131100
C(Fragment=3)	-4.02626000	3.41248400	3.05554700

C(Fragment=3)	-2.97540300	4.24017900	2.50277800
C(Fragment=3)	-1.59908900	4.39944100	2.92105700
C(Fragment=3)	-0.61089500	4.83959300	2.05158300
C(Fragment=3)	-5.27366500	3.38110400	0.91195000
C(Fragment=3)	-6.02710400	2.74221200	-0.14543900
C(Fragment=3)	-5.70726900	2.91488000	-1.48499600
C(Fragment=3)	-0.48762000	5.02542400	-1.77465100
C(Fragment=3)	-0.01268000	5.17882000	-0.47982900
C(Fragment=3)	-0.89220200	5.16057700	0.66876800
C(Fragment=3)	-2.24039600	5.19350700	0.35405800
C(Fragment=3)	-3.25254000	4.75073500	1.24589000
C(Fragment=3)	-4.36618700	4.33023400	0.47242300
C(Fragment=3)	-4.04060100	4.50828800	-0.89765600
C(Fragment=3)	-4.60253900	3.74783700	-1.90932100
C(Fragment=3)	-3.82807400	3.71728300	-3.13124000
C(Fragment=3)	-2.54273300	4.23691100	-3.20276600
C(Fragment=3)	-1.89454500	4.84310600	-2.06002600
C(Fragment=3)	-2.72665500	5.04092500	-0.97090600
H(Fragment=3)	-5.82004000	2.30483900	2.74437000
H(Fragment=3)	-3.91529000	3.01324500	4.06043900
H(Fragment=3)	-1.30489700	4.07412300	3.91563200
H(Fragment=3)	0.41897900	4.83970200	2.39856600
H(Fragment=3)	-6.80136700	2.02425900	0.11234400
H(Fragment=3)	-6.24459100	2.32659600	-2.22445500
H(Fragment=3)	0.23416400	4.94136400	-2.58330400
H(Fragment=3)	1.06207200	5.20790800	-0.32595300
H(Fragment=3)	-4.21958400	3.18657500	-3.99555100
H(Fragment=3)	-1.97742000	4.09286200	-4.12021800

Anion of Cor@C₇₀-S

Atom	x	y	z
C(Fragment=1)	2.35512000	1.11100000	0.55107700
C(Fragment=1)	1.60912000	2.17209600	1.08441100
C(Fragment=1)	0.83768800	1.99192800	2.29085300
C(Fragment=1)	-0.40078900	2.72503000	2.15183100
C(Fragment=1)	-1.60951800	2.26055800	2.74082900
C(Fragment=1)	-2.81853600	2.72285200	2.15120800
C(Fragment=1)	-4.05602200	1.98815700	2.28973300
C(Fragment=1)	-4.82990600	2.16813700	1.08579300
C(Fragment=1)	-5.58428900	1.10980300	0.55440300
C(Fragment=1)	-5.58363500	0.86890000	-0.86962200
C(Fragment=1)	-5.58050200	-0.57445400	-1.08458800

C(Fragment=1)	-4.83557500	-1.11724700	-2.13876900
C(Fragment=1)	-4.05661900	-2.32135900	-1.93270900
C(Fragment=1)	-2.81622600	-2.20429500	-2.68043100
C(Fragment=1)	-1.60879300	-2.79345800	-2.21709700
C(Fragment=1)	-0.40195200	-2.20459600	-2.68248700
C(Fragment=1)	0.83956600	-2.32203500	-1.93638400
C(Fragment=1)	1.61576800	-1.11610600	-2.14272100
C(Fragment=1)	2.35270500	-0.57108600	-1.08571900
C(Fragment=1)	2.35444200	0.87055700	-0.87111700
C(Fragment=1)	2.34236500	-0.18335800	1.21933300
C(Fragment=1)	2.35945000	-1.22147100	0.20457800
C(Fragment=1)	1.61408800	-2.39558900	0.40114200
C(Fragment=1)	0.83556200	-2.94649600	-0.69362400
C(Fragment=1)	-0.39954400	-3.48992300	-0.16012000
C(Fragment=1)	-1.60823100	-3.46026300	-0.90561900
C(Fragment=1)	-2.81640600	-3.48942000	-0.15930500
C(Fragment=1)	-4.05170400	-2.94555900	-0.69135200
C(Fragment=1)	-4.83179600	-2.39619000	0.40290300
C(Fragment=1)	-5.58733900	-1.22634100	0.20729600
C(Fragment=1)	-5.56940200	-0.18658600	1.22288800
C(Fragment=1)	-4.81679400	-0.35942700	2.38461700
C(Fragment=1)	-4.04202100	0.74047000	2.93079800
C(Fragment=1)	-2.81967100	0.21210400	3.46631400
C(Fragment=1)	-1.60896100	0.95576800	3.42075900
C(Fragment=1)	-0.39755000	0.21316500	3.46730900
C(Fragment=1)	0.82467900	0.74299800	2.93205300
C(Fragment=1)	1.59864900	-0.35737700	2.38503100
C(Fragment=1)	0.82473200	-1.57292700	2.58297300
C(Fragment=1)	0.84229400	-2.57709400	1.60593500
C(Fragment=1)	-0.39970500	-3.23927000	1.25815000
C(Fragment=1)	-1.60774600	-2.97225500	1.96027100
C(Fragment=1)	-2.81561700	-3.23853800	1.25794600
C(Fragment=1)	-4.05750000	-2.57612800	1.60540500
C(Fragment=1)	-4.04051100	-1.57334400	2.58220200
C(Fragment=1)	-2.81949300	-1.22918200	3.25558500
C(Fragment=1)	-1.60797300	-1.92507600	2.99457100
C(Fragment=1)	-0.39678300	-1.22885600	3.25634800
C(Fragment=1)	0.83088700	3.02258700	0.19899400
C(Fragment=1)	-0.40062100	3.38696600	0.86826000
C(Fragment=1)	-1.61049300	3.57503500	0.14805600
C(Fragment=1)	-2.81984900	3.38482600	0.86867100
C(Fragment=1)	-4.05087700	3.01816200	0.20045000
C(Fragment=1)	-4.05973600	2.78783300	-1.17064800
C(Fragment=1)	-4.83787600	1.69871300	-1.71987000

C(Fragment=1)	-4.05736800	1.12320800	-2.79661800
C(Fragment=1)	-4.05623300	-0.25139500	-3.00129700
C(Fragment=1)	-2.81692700	-0.92854300	-3.33905900
C(Fragment=1)	-1.61022100	-0.20952100	-3.55283500
C(Fragment=1)	-0.40261200	-0.92801400	-3.34151100
C(Fragment=1)	0.83684100	-0.24984700	-3.00584500
C(Fragment=1)	0.83703300	1.12598900	-2.80103100
C(Fragment=1)	1.61622500	1.70260000	-1.72342900
C(Fragment=1)	0.83956000	2.79272100	-1.17355900
C(Fragment=1)	-0.40363400	2.89758400	-1.92021800
C(Fragment=1)	-1.61071100	3.32387000	-1.30211600
C(Fragment=1)	-2.81768800	2.89515100	-1.91854800
C(Fragment=1)	-2.81775300	1.87016300	-2.92293500
C(Fragment=1)	-1.61069600	1.24532700	-3.33685100
C(Fragment=1)	-0.40357800	1.87182100	-2.92518500
C(Fragment=2)	4.93589400	-3.13718400	-0.84640500
C(Fragment=2)	4.93482000	-2.49849700	-2.07688600
C(Fragment=2)	5.30979400	-1.10930200	-2.21767400
C(Fragment=2)	4.93163400	-0.16367600	-3.24391900
C(Fragment=2)	4.92992000	1.20396900	-3.01654400
C(Fragment=2)	5.31210100	-2.45297100	0.37049500
C(Fragment=2)	4.93340800	-2.74803600	1.73421200
C(Fragment=2)	4.93066400	-1.77466500	2.72143100
C(Fragment=2)	4.93014000	3.24288400	0.21312100
C(Fragment=2)	4.93001800	3.03635300	-1.15765800
C(Fragment=2)	5.30645100	1.76751000	-1.73947100
C(Fragment=2)	5.86103300	0.86251800	-0.84781600
C(Fragment=2)	5.86204100	-0.54023000	-1.08055500
C(Fragment=2)	5.86409800	-1.19535000	0.18125900
C(Fragment=2)	5.86270800	-0.19720100	1.19421300
C(Fragment=2)	5.30720200	-0.40596400	2.44731100
C(Fragment=2)	4.92666500	0.79988800	3.14854100
C(Fragment=2)	4.92755500	2.04012400	2.52902000
C(Fragment=2)	5.30700400	2.20226500	1.14347000
C(Fragment=2)	5.86130400	1.07446700	0.55816500
H(Fragment=2)	4.52643800	-4.14218600	-0.78396600
H(Fragment=2)	4.52495600	-3.02618000	-2.93433100
H(Fragment=2)	4.52219600	-0.53363900	-4.18053200
H(Fragment=2)	4.51916400	1.85617800	-3.78303700
H(Fragment=2)	4.52190400	-3.72602200	1.97013100
H(Fragment=2)	4.51795400	-2.02578200	3.69516400
H(Fragment=2)	4.51929000	4.17321300	0.59691200
H(Fragment=2)	4.51906000	3.81215700	-1.79863200
H(Fragment=2)	4.51206100	0.72150600	4.15025300

H(Fragment=2)	4. 51351500	2. 88862900	3. 06763200
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Anion of Cor@C₇₀-L

Atom	x	y	z
C(Fragment=1)	0. 27338800	3. 97988900	0. 18534600
C(Fragment=1)	-0. 90064900	3. 22992000	0. 37243800
C(Fragment=1)	-1. 07949100	2. 44815400	1. 57983000
C(Fragment=1)	-1. 74788000	1. 20434000	1. 23334400
C(Fragment=1)	-1. 49359900	-0. 00071800	1. 93872800
C(Fragment=1)	-1. 74735800	-1. 20583000	1. 23318300
C(Fragment=1)	-1. 07840800	-2. 44943800	1. 57958900
C(Fragment=1)	-0. 89912800	-3. 23093600	0. 37208300
C(Fragment=1)	0. 27527700	-3. 98033700	0. 18487100
C(Fragment=1)	0. 93416400	-3. 97454800	-1. 09925300
C(Fragment=1)	2. 37627300	-3. 96342500	-0. 86181000
C(Fragment=1)	3. 20867200	-3. 21109300	-1. 69297100
C(Fragment=1)	4. 29871900	-2. 43310600	-1. 12389500
C(Fragment=1)	4. 42928700	-1. 20995700	-1. 87103800
C(Fragment=1)	4. 83264700	0. 00095400	-1. 24685100
C(Fragment=1)	4. 42871700	1. 21174600	-1. 87089800
C(Fragment=1)	4. 29756400	2. 43474600	-1. 12361300
C(Fragment=1)	3. 20714800	3. 21228000	-1. 69259600
C(Fragment=1)	2. 37439300	3. 96412800	-0. 86135000
C(Fragment=1)	0. 93228900	3. 97457400	-1. 09879400
C(Fragment=1)	1. 30448900	3. 97178200	1. 21752000
C(Fragment=1)	2. 60144800	3. 98313500	0. 56991900
C(Fragment=1)	3. 65862200	3. 22818400	1. 11404700
C(Fragment=1)	4. 51806700	2. 45247600	0. 25508300
C(Fragment=1)	4. 84741800	1. 20818900	0. 92977400
C(Fragment=1)	5. 05511900	0. 00092300	0. 20782100
C(Fragment=1)	4. 84798700	-1. 20652500	0. 92963800
C(Fragment=1)	4. 51922500	-2. 45089000	0. 25480200
C(Fragment=1)	3. 66014700	-3. 22709900	1. 11366800
C(Fragment=1)	2. 60334200	-3. 98250600	0. 56945400
C(Fragment=1)	1. 30637600	-3. 97183500	1. 21705100
C(Fragment=1)	1. 11403000	-3. 22588800	2. 38483600
C(Fragment=1)	-0. 09683900	-2. 44762200	2. 56403700
C(Fragment=1)	0. 24702700	-1. 20809500	3. 23785300
C(Fragment=1)	-0. 45723100	-0. 00053800	2. 98111500
C(Fragment=1)	0. 24645900	1. 20730900	3. 23800200
C(Fragment=1)	-0. 09798900	2. 44676200	2. 56435600
C(Fragment=1)	1. 11251700	3. 22560400	2. 38521800
C(Fragment=1)	2. 20346100	2. 44638000	2. 93767600

C(Fragment=1)	3.44646300	2.44782500	2.31684500
C(Fragment=1)	4.19881900	1.20832900	2.21056000
C(Fragment=1)	3.73105000	0.00045900	2.79338400
C(Fragment=1)	4.19938500	-1.20711800	2.21041900
C(Fragment=1)	3.44761600	-2.44698900	2.31656300
C(Fragment=1)	2.20460900	-2.44620000	2.93737200
C(Fragment=1)	1.66514400	-1.20741000	3.46910000
C(Fragment=1)	2.41397000	0.00010900	3.44825100
C(Fragment=1)	1.66458500	1.20726900	3.46925300
C(Fragment=1)	-1.43928100	2.44812800	-0.71762400
C(Fragment=1)	-1.96637800	1.20314500	-0.18192700
C(Fragment=1)	-1.94064600	-0.00065200	-0.93188500
C(Fragment=1)	-1.96554200	-1.20450200	-0.18204100
C(Fragment=1)	-1.43802400	-2.44922500	-0.71788400
C(Fragment=1)	-0.80726700	-2.44131000	-1.95711200
C(Fragment=1)	0.40506600	-3.21923200	-2.15683200
C(Fragment=1)	1.27023700	-2.44462100	-3.01489200
C(Fragment=1)	2.65470600	-2.43600700	-2.78552800
C(Fragment=1)	3.39658600	-1.20974800	-2.89367300
C(Fragment=1)	2.77309100	0.00058800	-3.30376800
C(Fragment=1)	3.39600800	1.21116200	-2.89352800
C(Fragment=1)	2.65354200	2.43706200	-2.78523800
C(Fragment=1)	1.26907200	2.44503100	-3.01459500
C(Fragment=1)	0.40352500	3.21912500	-2.15642900
C(Fragment=1)	-0.80844500	2.44061800	-1.95681800
C(Fragment=1)	-0.70241100	1.21017200	-2.71280900
C(Fragment=1)	-1.27981100	-0.00042900	-2.24600600
C(Fragment=1)	-0.70181000	-1.21070800	-2.71293400
C(Fragment=1)	0.59840000	-1.20962000	-3.34513600
C(Fragment=1)	1.32106300	0.00026000	-3.54054500
C(Fragment=1)	0.59782700	1.20976700	-3.34501200
C(Fragment=2)	-4.46926800	2.42882400	-2.16547800
C(Fragment=2)	-4.41868700	1.30428900	-2.97499900
C(Fragment=2)	-4.81760900	-0.00075700	-2.49799300
C(Fragment=2)	-4.41775600	-1.30579500	-2.97430800
C(Fragment=2)	-4.46774700	-2.42999700	-2.16429500
C(Fragment=2)	-4.91451300	2.36155300	-0.79150900
C(Fragment=2)	-4.59573800	3.23908100	0.31201500
C(Fragment=2)	-4.64852400	2.80880300	1.62928600
C(Fragment=2)	-4.64800900	-2.80885600	1.63070400
C(Fragment=2)	-4.59449600	-3.23946900	0.31357900
C(Fragment=2)	-4.91310400	-2.36236200	-0.79038700
C(Fragment=2)	-5.47871600	-1.15085700	-0.42372800
C(Fragment=2)	-5.43792600	-0.00067800	-1.25819100

C(Fragment=2)	-5.47925800	1.14981700	-0.42421500
C(Fragment=2)	-5.53760000	0.71062600	0.92647100
C(Fragment=2)	-5.03194600	1.45929500	1.97837300
C(Fragment=2)	-4.70439700	0.69389400	3.15980300
C(Fragment=2)	-4.70428900	-0.69311500	3.16016700
C(Fragment=2)	-5.03161200	-1.45916100	1.97909900
C(Fragment=2)	-5.53729800	-0.71110900	0.92680000
H(Fragment=2)	-4.04221300	3.35522900	-2.53958400
H(Fragment=2)	-3.95289700	1.39165500	-3.95298800
H(Fragment=2)	-3.95184700	-1.39333600	-3.95222400
H(Fragment=2)	-4.03996300	-3.35626200	-2.53790200
H(Fragment=2)	-4.17995800	4.22155800	0.10491900
H(Fragment=2)	-4.27561900	3.47219000	2.40552100
H(Fragment=2)	-4.27668600	-3.47246600	2.40749800
H(Fragment=2)	-4.17911900	-4.22221800	0.10697500
H(Fragment=2)	-4.33599700	1.21220300	4.04176700
H(Fragment=2)	-4.33581600	-1.21091300	4.04240100

Anion of 2Cor@C₇₀-S

Atom	x	y	z
C(Fragment=1)	3.94675500	-0.02911600	-1.21710400
C(Fragment=1)	3.20503800	-0.05693800	-2.39528900
C(Fragment=1)	2.43196200	1.10520800	-2.80184300
C(Fragment=1)	1.21185500	0.64916100	-3.40235800
C(Fragment=1)	0.00001300	1.37983900	-3.26169000
C(Fragment=1)	-1.21182100	0.64914800	-3.40230000
C(Fragment=1)	-2.43188500	1.10517700	-2.80171900
C(Fragment=1)	-3.20500000	-0.05694400	-2.39524600
C(Fragment=1)	-3.94674500	-0.02912200	-1.21710400
C(Fragment=1)	-3.96049000	-1.18655400	-0.33814700
C(Fragment=1)	-3.95942500	-0.70353600	1.02383100
C(Fragment=1)	-3.22412600	-1.37677300	2.00618700
C(Fragment=1)	-2.44557800	-0.62347100	2.97054100
C(Fragment=1)	-1.20711800	-1.33742500	3.22187700
C(Fragment=1)	0.00002100	-0.65033700	3.52083000
C(Fragment=1)	1.20715600	-1.33743000	3.22187800
C(Fragment=1)	2.44562100	-0.62347800	2.97054400
C(Fragment=1)	3.22416800	-1.37677800	2.00619400
C(Fragment=1)	3.95946100	-0.70355000	1.02383800
C(Fragment=1)	3.96050700	-1.18656400	-0.33814000
C(Fragment=1)	3.96098900	1.17065000	-0.39338400
C(Fragment=1)	3.95978900	0.75263200	0.98949000
C(Fragment=1)	3.22391500	1.47304900	1.93766500

C(Fragment=1)	2.44550800	0.76689900	2.93707500
C(Fragment=1)	1.20682300	1.49221400	3.15427800
C(Fragment=1)	0.00002300	0.82002200	3.48522000
C(Fragment=1)	-1.20677400	1.49220800	3.15427800
C(Fragment=1)	-2.44545900	0.76690000	2.93706900
C(Fragment=1)	-3.22386500	1.47304800	1.93766100
C(Fragment=1)	-3.95975500	0.75263000	0.98948200
C(Fragment=1)	-3.96097100	1.17066100	-0.39338400
C(Fragment=1)	-3.21698900	2.29079800	-0.78894900
C(Fragment=1)	-2.44597700	2.26355900	-2.00893100
C(Fragment=1)	-1.20824500	2.97354300	-1.77890100
C(Fragment=1)	0.00000600	2.58763000	-2.42121000
C(Fragment=1)	1.20823600	2.97347500	-1.77886100
C(Fragment=1)	2.44593600	2.26349200	-2.00889900
C(Fragment=1)	3.21698200	2.29077000	-0.78894300
C(Fragment=1)	2.43979800	3.02556600	0.19575700
C(Fragment=1)	2.44859500	2.62545900	1.52924600
C(Fragment=1)	1.20664900	2.63460200	2.28262500
C(Fragment=1)	0.00002200	3.13503600	1.72314900
C(Fragment=1)	-1.20659800	2.63458400	2.28262600
C(Fragment=1)	-2.44852900	2.62542000	1.52924600
C(Fragment=1)	-2.43972300	3.02551000	0.19577000
C(Fragment=1)	-1.20910200	3.47026800	-0.42229000
C(Fragment=1)	0.00002000	3.56556100	0.31606100
C(Fragment=1)	1.20914300	3.47026600	-0.42228400
C(Fragment=1)	2.43137300	-1.23690300	-2.74390800
C(Fragment=1)	1.21154700	-0.80993300	-3.36665500
C(Fragment=1)	0.00000700	-1.53262500	-3.19143000
C(Fragment=1)	-1.21152500	-0.80993400	-3.36663800
C(Fragment=1)	-2.43134800	-1.23690000	-2.74389200
C(Fragment=1)	-2.44689300	-2.35662800	-1.89811600
C(Fragment=1)	-3.21742400	-2.32517100	-0.67899800
C(Fragment=1)	-2.44031100	-3.01067900	0.34027300
C(Fragment=1)	-2.44839400	-2.54718500	1.65292300
C(Fragment=1)	-1.20669900	-2.51973800	2.40539600
C(Fragment=1)	0.00001300	-3.04587200	1.87071200
C(Fragment=1)	1.20672800	-2.51973900	2.40539600
C(Fragment=1)	2.44842200	-2.54718900	1.65292800
C(Fragment=1)	2.44033300	-3.01068100	0.34027800
C(Fragment=1)	3.21745500	-2.32518800	-0.67899000
C(Fragment=1)	2.44691500	-2.35663000	-1.89811400
C(Fragment=1)	1.20880800	-3.05437200	-1.63390300
C(Fragment=1)	0.00000600	-2.69926100	-2.29401200
C(Fragment=1)	-1.20878900	-3.05437000	-1.63390500

C(Fragment=1)	-1.20965900	-3.48532200	-0.25563500
C(Fragment=1)	0.00001100	-3.54598300	0.48700500
C(Fragment=1)	1.20967700	-3.48532200	-0.25563400
C(Fragment=2)	6.57460100	0.80435600	3.12109300
C(Fragment=2)	6.57282600	-0.58190500	3.17087000
C(Fragment=2)	6.93561700	-1.38779800	2.02597900
C(Fragment=2)	6.55274500	-2.74582200	1.71181300
C(Fragment=2)	6.53616800	-3.22046000	0.40875700
C(Fragment=2)	6.93936300	1.52689800	1.92246800
C(Fragment=2)	6.56041300	2.86039900	1.51271800
C(Fragment=2)	6.54620200	3.24069800	0.17991800
C(Fragment=2)	6.50315000	-1.41108500	-2.95305900
C(Fragment=2)	6.50882000	-2.50232200	-2.09860300
C(Fragment=2)	6.90318500	-2.38603000	-0.71274000
C(Fragment=2)	7.46493000	-1.16581600	-0.36970000
C(Fragment=2)	7.47915500	-0.67813200	0.96616800
C(Fragment=2)	7.48104600	0.74269400	0.91513200
C(Fragment=2)	7.46736500	1.13341200	-0.45199700
C(Fragment=2)	6.90947800	2.32747600	-0.88081000
C(Fragment=2)	6.51583300	2.34516800	-2.27194600
C(Fragment=2)	6.50669200	1.19560300	-3.04559400
C(Fragment=2)	6.88952400	-0.09078300	-2.50927200
C(Fragment=2)	7.45727700	-0.04595000	-1.24583900
H(Fragment=2)	6.17525800	1.35415300	3.96972700
H(Fragment=2)	6.17247700	-1.06852100	4.05661700
H(Fragment=2)	6.15004200	-3.37819500	2.49896500
H(Fragment=2)	6.12007500	-4.20703200	0.22136500
H(Fragment=2)	6.15998100	3.54903700	2.25236100
H(Fragment=2)	6.13397700	4.21314900	-0.07666600
H(Fragment=2)	6.07937500	-1.53340100	-3.94665000
H(Fragment=2)	6.08902100	-3.44012600	-2.45318900
H(Fragment=2)	6.09757900	3.25591500	-2.69269700
H(Fragment=2)	6.08220800	1.24746200	-4.04495100
C(Fragment=3)	-6.57276300	-0.58217000	3.17082500
C(Fragment=3)	-6.57455300	0.80408600	3.12115600
C(Fragment=3)	-6.93935300	1.52672100	1.92260800
C(Fragment=3)	-6.56042200	2.86023400	1.51295200
C(Fragment=3)	-6.54625900	3.24062400	0.18021500
C(Fragment=3)	-6.93559800	-1.38796100	2.02588500
C(Fragment=3)	-6.55273300	-2.74595400	1.71159600
C(Fragment=3)	-6.53620400	-3.22048300	0.40849500
C(Fragment=3)	-6.50685900	1.19586900	-3.04546300
C(Fragment=3)	-6.51597200	2.34533700	-2.27171300
C(Fragment=3)	-6.90956200	2.32751500	-0.88057300

C(Fragment=3)	-7.46743400	1.13343600	-0.45186200
C(Fragment=3)	-7.48106500	0.74261100	0.91523200
C(Fragment=3)	-7.47916300	-0.67821100	0.96615000
C(Fragment=3)	-7.46497800	-1.16577600	-0.36976100
C(Fragment=3)	-6.90324600	-2.38596000	-0.71292700
C(Fragment=3)	-6.50893300	-2.50212100	-2.09880800
C(Fragment=3)	-6.50327200	-1.41081700	-2.95314100
C(Fragment=3)	-6.88965100	-0.09056300	-2.50923800
C(Fragment=3)	-7.45735600	-0.04584000	-1.24579600
H(Fragment=3)	-6.17237600	-1.06886000	4.05651400
H(Fragment=3)	-6.17518100	1.35381900	3.96981600
H(Fragment=3)	-6.15996200	3.54881200	2.25262800
H(Fragment=3)	-6.13403500	4.21308900	-0.07630200
H(Fragment=3)	-6.15000300	-3.37839100	2.49868200
H(Fragment=3)	-6.12011500	-4.20703800	0.22101100
H(Fragment=3)	-6.08241200	1.24782600	-4.04483100
H(Fragment=3)	-6.09772400	3.25612500	-2.69237800
H(Fragment=3)	-6.08914500	-3.43989100	-2.45349700
H(Fragment=3)	-6.07953800	-1.53305100	-3.94676300

Anion of 2Cor@C₇₀-L

Atom	x	y	z
C(Fragment=1)	0.73117400	-3.96957600	1.37751100
C(Fragment=1)	1.42002700	-3.21345300	2.33354900
C(Fragment=1)	0.70119700	-2.43822500	3.32094600
C(Fragment=1)	1.41694500	-1.20768200	3.54206400
C(Fragment=1)	0.73506000	0.00264100	3.84771500
C(Fragment=1)	1.41715600	1.21251100	3.54073100
C(Fragment=1)	0.70162100	2.44293300	3.31826200
C(Fragment=1)	1.42057800	3.21693800	2.32999600
C(Fragment=1)	0.73185600	3.97211600	1.37311700
C(Fragment=1)	1.18124500	3.98521400	-0.00056300
C(Fragment=1)	0.00071500	3.97380800	-0.85116000
C(Fragment=1)	0.00088000	3.22623700	-2.03337300
C(Fragment=1)	-1.16515100	2.44644700	-2.40426100
C(Fragment=1)	-0.71757700	1.20722100	-3.01478400
C(Fragment=1)	-1.45323100	-0.00088400	-2.87437800
C(Fragment=1)	-0.71778900	-1.20926900	-3.01344700
C(Fragment=1)	-1.16556800	-2.44773500	-2.40153400
C(Fragment=1)	0.00032800	-3.22732000	-2.02980000
C(Fragment=1)	0.00003100	-3.97359500	-0.84677400
C(Fragment=1)	1.18056400	-3.98426800	0.00384000
C(Fragment=1)	-0.73202600	-3.96946500	1.37721900

C(Fragment=1)	-1.18085400	-3.98405000	0.00337800
C(Fragment=1)	-2.31115500	-3.23079200	-0.36837800
C(Fragment=1)	-2.29219300	-2.44886200	-1.58846700
C(Fragment=1)	-3.01003300	-1.20524200	-1.35801400
C(Fragment=1)	-2.64512400	-0.00030100	-2.01343600
C(Fragment=1)	-3.00987600	1.20543500	-1.35938500
C(Fragment=1)	-2.29177200	2.44866800	-1.59120000
C(Fragment=1)	-2.31060600	3.23193700	-0.37196800
C(Fragment=1)	-1.18016900	3.98541100	-0.00102600
C(Fragment=1)	-0.73134900	3.97226300	1.37282300
C(Fragment=1)	-1.42058400	3.21719700	2.32944100
C(Fragment=1)	-0.70216400	2.44307200	3.31798600
C(Fragment=1)	-1.41799300	1.21274800	3.54013700
C(Fragment=1)	-0.73621900	0.00277000	3.84741100
C(Fragment=1)	-1.41819500	-1.20742700	3.54146300
C(Fragment=1)	-0.70258000	-2.43811800	3.32066500
C(Fragment=1)	-1.42113900	-3.21321900	2.33298800
C(Fragment=1)	-2.58697800	-2.43518500	1.94315600
C(Fragment=1)	-3.01654600	-2.44871800	0.61877600
C(Fragment=1)	-3.44851700	-1.20300700	0.00476900
C(Fragment=1)	-3.54268700	0.00129100	0.74895100
C(Fragment=1)	-3.44821800	1.20472700	0.00344300
C(Fragment=1)	-3.01608400	2.45104800	0.61606000
C(Fragment=1)	-2.58655200	2.43893100	1.94046600
C(Fragment=1)	-2.60249000	1.21311000	2.70392300
C(Fragment=1)	-3.09863300	0.00203400	2.15193300
C(Fragment=1)	-2.60269600	-1.20851600	2.70526000
C(Fragment=1)	2.58616900	-2.43562800	1.94420400
C(Fragment=1)	2.60179200	-1.20897700	2.70631400
C(Fragment=1)	3.09815500	0.00149800	2.15318900
C(Fragment=1)	2.60199800	1.21267100	2.70497600
C(Fragment=1)	2.58658500	2.43847400	1.94150900
C(Fragment=1)	3.01666400	2.45053900	0.61727000
C(Fragment=1)	2.31169500	3.23152300	-0.37102700
C(Fragment=1)	2.29320700	2.44824600	-1.59025900
C(Fragment=1)	1.16692600	2.44623700	-2.40378400
C(Fragment=1)	0.71939700	1.20710300	-3.01452800
C(Fragment=1)	1.45478200	-0.00113100	-2.87381700
C(Fragment=1)	0.71918500	-1.20939000	-3.01316700
C(Fragment=1)	1.16650900	-2.44793500	-2.40107400
C(Fragment=1)	2.29280100	-2.44925100	-1.58755800
C(Fragment=1)	2.31114000	-3.23118600	-0.36745600
C(Fragment=1)	3.01624900	-2.44923200	0.61997900
C(Fragment=1)	3.44863400	-1.20358200	0.00615900

C(Fragment=1)	3.54266100	0.00068900	0.75036500
C(Fragment=1)	3.44884900	1.20414300	0.00482400
C(Fragment=1)	3.01100600	1.20490300	-1.35817900
C(Fragment=1)	2.64630800	-0.00075600	-2.01237000
C(Fragment=1)	3.01076100	-1.20574900	-1.35681000
C(Fragment=2)	5.96568600	-3.23996900	-0.89766400
C(Fragment=2)	5.81398200	-2.81083700	-2.20757200
C(Fragment=2)	6.13920700	-1.46167200	-2.61307000
C(Fragment=2)	5.63412700	-0.69702000	-3.73056600
C(Fragment=2)	5.63415700	0.69011900	-3.73150500
C(Fragment=2)	6.45300200	-2.36217900	0.14246400
C(Fragment=2)	6.22828800	-2.42825500	1.56917900
C(Fragment=2)	6.31022200	-1.30426600	2.37712600
C(Fragment=2)	5.96594000	3.23697700	-0.90215000
C(Fragment=2)	5.81398600	2.80594600	-2.21140200
C(Fragment=2)	6.13929400	1.45627700	-2.61506800
C(Fragment=2)	6.80117900	0.70864100	-1.65341800
C(Fragment=2)	6.80103600	-0.71272400	-1.65241200
C(Fragment=2)	6.95486200	-1.15142600	-0.30921900
C(Fragment=2)	7.04688300	-0.00052300	0.52039900
C(Fragment=2)	6.63144400	0.00046100	1.84310200
C(Fragment=2)	6.31061600	1.30604100	2.37531700
C(Fragment=2)	6.22888800	2.42888500	1.56577700
C(Fragment=2)	6.45348400	2.36071100	0.13912500
C(Fragment=2)	6.95512000	1.14923200	-0.31085800
H(Fragment=2)	5.58649700	-4.22209600	-0.62813600
H(Fragment=2)	5.32591500	-3.47505500	-2.91627700
H(Fragment=2)	5.13492800	-1.21580500	-4.54538900
H(Fragment=2)	5.13495400	1.20781800	-4.54701400
H(Fragment=2)	5.86127700	-3.35313500	2.00551200
H(Fragment=2)	6.00388300	-1.39087700	3.41615600
H(Fragment=2)	5.58627500	4.21925200	-0.63383800
H(Fragment=2)	5.32521400	3.46889600	-2.92080800
H(Fragment=2)	6.00437700	1.39419700	3.41424600
H(Fragment=2)	5.86214200	3.35448500	2.00080700
C(Fragment=3)	-6.22796000	-2.42564800	1.57199300
C(Fragment=3)	-6.30963800	-1.30077600	2.37867700
C(Fragment=3)	-6.63127500	0.00324900	1.84326400
C(Fragment=3)	-6.30998700	1.30931100	2.37395400
C(Fragment=3)	-6.22840100	2.43123000	1.56315600
C(Fragment=3)	-6.45347900	-2.36119700	0.14534700
C(Fragment=3)	-5.96590800	-3.24001800	-0.89373800
C(Fragment=3)	-5.81457400	-2.81238900	-2.20416400
C(Fragment=3)	-5.81435600	2.80389100	-2.21436700

C(Fragment=3)	-5.96587200	3.23638900	-0.90556600
C(Fragment=3)	-6.45357400	2.36143700	0.13669600
C(Fragment=3)	-6.95582200	1.14962400	-0.31178300
C(Fragment=3)	-7.04758100	0.00079000	0.52081100
C(Fragment=3)	-6.95585600	-1.15108400	-0.30756700
C(Fragment=3)	-6.80232300	-0.71388900	-1.65131500
C(Fragment=3)	-6.14039700	-1.46386600	-2.61114400
C(Fragment=3)	-5.63528400	-0.70056100	-3.72953600
C(Fragment=3)	-5.63522100	0.68654600	-3.73205700
C(Fragment=3)	-6.14027000	1.45393400	-2.61644800
C(Fragment=3)	-6.80228200	0.70750500	-1.65391000
H(Fragment=3)	-5.86051900	-3.34998100	2.00911900
H(Fragment=3)	-6.00262500	-1.38606900	3.41761500
H(Fragment=3)	-6.00316600	1.39847000	3.41262400
H(Fragment=3)	-5.86124300	3.35724900	1.99694100
H(Fragment=3)	-5.58567400	-4.22137500	-0.62289200
H(Fragment=3)	-5.32573900	-3.47694800	-2.91202000
H(Fragment=3)	-5.32545200	3.46584000	-2.92461700
H(Fragment=3)	-5.58564800	4.21873600	-0.63829800
H(Fragment=3)	-5.13608100	-1.22036900	-4.54370300
H(Fragment=3)	-5.13597800	1.20334100	-4.54811400

Anion of 2Cor@C₇₀-SL

Atom	x	y	z
C(Fragment=1)	3.92226500	-4.14548800	-0.90964100
C(Fragment=1)	2.87481500	-4.60443000	-1.71817200
C(Fragment=1)	2.37845100	-3.77452600	-2.80536700
C(Fragment=1)	0.95030400	-3.95470200	-2.91195900
C(Fragment=1)	0.09549300	-2.89226700	-3.31061600
C(Fragment=1)	-1.25667300	-2.96044700	-2.87958600
C(Fragment=1)	-2.06457900	-1.77178500	-2.73976700
C(Fragment=1)	-2.98647400	-1.96271700	-1.62987600
C(Fragment=1)	-3.30437100	-0.88436100	-0.79665400
C(Fragment=1)	-3.36636900	-1.08192000	0.64985700
C(Fragment=1)	-2.83818600	0.10319000	1.29094100
C(Fragment=1)	-2.05964700	-0.02275800	2.45448600
C(Fragment=1)	-0.84851200	0.76307200	2.60224900
C(Fragment=1)	0.15521600	-0.04782000	3.27133100
C(Fragment=1)	1.53958700	0.09143400	2.98147500
C(Fragment=1)	2.35815700	-1.04184600	3.23611700
C(Fragment=1)	3.61205400	-1.25047300	2.53059500
C(Fragment=1)	3.82200800	-2.67633700	2.36137600
C(Fragment=1)	4.40946900	-3.16630100	1.17986300

C(Fragment=1)	3.85095100	-4.33868700	0.53786100
C(Fragment=1)	4.51253500	-2.85036400	-1.15698200
C(Fragment=1)	4.80015600	-2.23879300	0.13372000
C(Fragment=1)	4.60808800	-0.86446700	0.31086300
C(Fragment=1)	3.99451800	-0.36770200	1.52859900
C(Fragment=1)	3.12999600	0.74759300	1.18715500
C(Fragment=1)	1.94276600	1.02062800	1.91567100
C(Fragment=1)	0.93436800	1.73935800	1.22232000
C(Fragment=1)	-0.46472900	1.64547500	1.59944700
C(Fragment=1)	-1.27204600	1.78693100	0.40234500
C(Fragment=1)	-2.42928000	1.02039900	0.24565000
C(Fragment=1)	-2.72976200	0.41559600	-1.04265100
C(Fragment=1)	-1.84971400	0.59882600	-2.12144200
C(Fragment=1)	-1.51550000	-0.51329700	-2.98079000
C(Fragment=1)	-0.11040700	-0.41185700	-3.34290700
C(Fragment=1)	0.68950200	-1.56810900	-3.55686700
C(Fragment=1)	2.09081200	-1.40477900	-3.37548200
C(Fragment=1)	2.95298500	-2.52890500	-3.04717700
C(Fragment=1)	4.03230500	-2.05473500	-2.21175700
C(Fragment=1)	3.82047800	-0.63478400	-2.01272900
C(Fragment=1)	4.09630700	-0.05653700	-0.78005800
C(Fragment=1)	3.19255600	0.93793800	-0.23266300
C(Fragment=1)	2.07250700	1.40813300	-0.96435700
C(Fragment=1)	0.99855900	1.92854200	-0.19825700
C(Fragment=1)	-0.35855900	1.95257500	-0.71052600
C(Fragment=1)	-0.64143200	1.37899200	-1.94453800
C(Fragment=1)	0.42831700	0.76076900	-2.71167000
C(Fragment=1)	1.77820800	0.80071300	-2.27085100
C(Fragment=1)	2.62949500	-0.23305600	-2.74495700
C(Fragment=1)	1.73348800	-5.27362800	-1.13781500
C(Fragment=1)	0.55426000	-4.86708800	-1.85861100
C(Fragment=1)	-0.70497700	-4.73956400	-1.21003200
C(Fragment=1)	-1.65117000	-3.87359600	-1.82513100
C(Fragment=1)	-2.71829400	-3.26835700	-1.06976600
C(Fragment=1)	-2.77611400	-3.45775300	0.32183600
C(Fragment=1)	-3.10974200	-2.34381600	1.18785900
C(Fragment=1)	-2.29652700	-2.47082300	2.38863600
C(Fragment=1)	-1.78937700	-1.32613400	3.01025300
C(Fragment=1)	-0.42415800	-1.34209700	3.50630800
C(Fragment=1)	0.36784500	-2.52303600	3.47163000
C(Fragment=1)	1.77781400	-2.33470100	3.47124100
C(Fragment=1)	2.67972900	-3.34079500	2.93790700
C(Fragment=1)	2.14060200	-4.46990000	2.31756900
C(Fragment=1)	2.74334200	-4.98128300	1.09548900

C(Fragment=1)	1.66552400	-5.45850400	0.25303200
C(Fragment=1)	0.42462700	-5.25402000	0.94645100
C(Fragment=1)	-0.77225900	-4.93889900	0.24602600
C(Fragment=1)	-1.78293300	-4.25967700	0.98061000
C(Fragment=1)	-1.49248200	-3.65863600	2.27362100
C(Fragment=1)	-0.18478100	-3.72485000	2.82587500
C(Fragment=1)	0.71600800	-4.65367800	2.23867200
C(Fragment=2)	-6.59316400	-1.39848200	-1.06472400
C(Fragment=2)	-6.68512500	-1.53001100	0.31249100
C(Fragment=2)	-6.50806200	-0.40348800	1.20152100
C(Fragment=2)	-6.09548100	-0.39086500	2.58728000
C(Fragment=2)	-5.49583600	0.71839300	3.16351900
C(Fragment=2)	-6.31544300	-0.12721000	-1.69466900
C(Fragment=2)	-5.72262600	0.13957400	-2.98608100
C(Fragment=2)	-5.07091700	1.33167400	-3.26162100
C(Fragment=2)	-3.80365100	3.78115900	1.62511200
C(Fragment=2)	-4.26072400	2.96069900	2.64544000
C(Fragment=2)	-5.24802500	1.92988800	2.41414000
C(Fragment=2)	-5.84067200	1.96749400	1.16154000
C(Fragment=2)	-6.45377600	0.82949200	0.57017000
C(Fragment=2)	-6.36181400	0.96454400	-0.84187300
C(Fragment=2)	-5.69321600	2.18714500	-1.12386900
C(Fragment=2)	-4.94301400	2.37921500	-2.27345800
C(Fragment=2)	-3.94922700	3.42495100	-2.17701900
C(Fragment=2)	-3.63820700	4.03239400	-0.97010600
C(Fragment=2)	-4.28450400	3.65472700	0.26727900
C(Fragment=2)	-5.37016900	2.80677900	0.11488200
H(Fragment=2)	-6.61024300	-2.29877100	-1.67361900
H(Fragment=2)	-6.77272700	-2.52850800	0.73316100
H(Fragment=2)	-6.14407000	-1.31159200	3.16313800
H(Fragment=2)	-5.09400700	0.62617700	4.16922700
H(Fragment=2)	-5.67916800	-0.65736600	-3.72404900
H(Fragment=2)	-4.53919800	1.42521900	-4.20498900
H(Fragment=2)	-2.97670400	4.45526400	1.83471400
H(Fragment=2)	-3.77460900	3.02122900	3.61589600
H(Fragment=2)	-3.34617800	3.66542500	-3.04901000
H(Fragment=2)	-2.80866100	4.73409300	-0.94433100
C(Fragment=3)	5.14538300	2.84354400	-2.29916000
C(Fragment=3)	4.05861300	3.26610300	-3.04969100
C(Fragment=3)	3.04214100	4.13683200	-2.50213900
C(Fragment=3)	1.66492100	4.30194000	-2.91074700
C(Fragment=3)	0.69255800	4.77300400	-2.04147000
C(Fragment=3)	5.32532200	3.24434700	-0.92146900
C(Fragment=3)	6.05751200	2.57983000	0.13325000

C(Fragment=3)	5.74715600	2.76735900	1.47175100
C(Fragment=3)	0.59555800	4.99131600	1.77080500
C(Fragment=3)	0.11815700	5.14751500	0.47837300
C(Fragment=3)	0.99518500	5.11854100	-0.67040500
C(Fragment=3)	2.34721000	5.14458400	-0.36546200
C(Fragment=3)	3.34570100	4.67179200	-1.25988100
C(Fragment=3)	4.45581500	4.23321900	-0.48811800
C(Fragment=3)	4.14049100	4.42808200	0.88399900
C(Fragment=3)	4.67716700	3.64359200	1.89331000
C(Fragment=3)	3.90219800	3.61896400	3.11323600
C(Fragment=3)	2.63026300	4.16735000	3.18713100
C(Fragment=3)	2.00121200	4.79813700	2.04897300
C(Fragment=3)	2.83723500	4.99098700	0.95987100
H(Fragment=3)	5.80749800	2.09375300	-2.72362500
H(Fragment=3)	3.91072400	2.83254800	-4.03524200
H(Fragment=3)	1.35410400	3.93660700	-3.88600700
H(Fragment=3)	-0.34381000	4.75744300	-2.36808100
H(Fragment=3)	6.78616200	1.81649700	-0.12649900
H(Fragment=3)	6.24599500	2.14520900	2.21031400
H(Fragment=3)	-0.12401900	4.89241500	2.57984500
H(Fragment=3)	-0.95699300	5.16541800	0.32476400
H(Fragment=3)	4.27304700	3.05502400	3.96554000
H(Fragment=3)	2.05154900	4.01279100	4.09449300

Cation of Cor@C₇₀-S

Atom	x	y	z
C(Fragment=1)	2.36309100	1.22654000	-0.11445900
C(Fragment=1)	1.63426800	2.40742000	0.00850400
C(Fragment=1)	0.90834400	2.68679400	1.23686100
C(Fragment=1)	-0.33883800	3.33867800	0.90271500
C(Fragment=1)	-1.50899700	3.14251800	1.68284300
C(Fragment=1)	-2.74859100	3.34058100	1.02032900
C(Fragment=1)	-3.95882300	2.69234500	1.47450300
C(Fragment=1)	-4.80273200	2.41544000	0.32337700
C(Fragment=1)	-5.54940400	1.23950200	0.27318800
C(Fragment=1)	-5.61632300	0.47780400	-0.96277100
C(Fragment=1)	-5.59989500	-0.93516000	-0.62356500
C(Fragment=1)	-4.89597700	-1.83216400	-1.42725400
C(Fragment=1)	-4.08462200	-2.87406300	-0.81913800
C(Fragment=1)	-2.88729700	-3.05329100	-1.61792300

C(Fragment=1)	-1.65163400	-3.42600500	-1.02692000
C(Fragment=1)	-0.47810400	-3.05783000	-1.73594600
C(Fragment=1)	0.79187200	-2.88306100	-1.05762600
C(Fragment=1)	1.54306000	-1.84309200	-1.74218900
C(Fragment=1)	2.32234200	-0.94727800	-1.01126300
C(Fragment=1)	2.31066400	0.46564300	-1.35080300
C(Fragment=1)	2.40640800	0.28355800	0.99137400
C(Fragment=1)	2.38081800	-1.06145200	0.43613300
C(Fragment=1)	1.67683700	-2.07131900	1.08575000
C(Fragment=1)	0.86549700	-2.99821300	0.32363500
C(Fragment=1)	-0.34228200	-3.27328100	1.08010000
C(Fragment=1)	-1.58021400	-3.53644700	0.43640700
C(Fragment=1)	-2.74828000	-3.26737600	1.19675600
C(Fragment=1)	-4.02266700	-2.98798900	0.56201700
C(Fragment=1)	-4.75551700	-2.06101500	1.40049300
C(Fragment=1)	-5.52218800	-1.05106800	0.82405100
C(Fragment=1)	-5.48990800	0.29580100	1.38093500
C(Fragment=1)	-4.69543400	0.57275800	2.48941500
C(Fragment=1)	-3.91231200	1.79339300	2.53655100
C(Fragment=1)	-2.64428000	1.50022900	3.15828500
C(Fragment=1)	-1.45612400	2.18534000	2.79426500
C(Fragment=1)	-0.23872300	1.49774100	3.04183500
C(Fragment=1)	0.96363400	1.78778200	2.30036500
C(Fragment=1)	1.73181800	0.56362700	2.17502100
C(Fragment=1)	0.98038600	-0.48282800	2.84525100
C(Fragment=1)	0.95015100	-1.77513600	2.30842500
C(Fragment=1)	-0.27893800	-2.52615400	2.31490900
C(Fragment=1)	-1.45634700	-2.01936200	2.92670400
C(Fragment=1)	-2.68846900	-2.52020900	2.43125800
C(Fragment=1)	-3.91046800	-1.76611200	2.54582700
C(Fragment=1)	-3.88397700	-0.47680100	3.08161900
C(Fragment=1)	-2.63046200	0.08853800	3.50177000
C(Fragment=1)	-1.42694100	-0.66241100	3.48257000
C(Fragment=1)	-0.22349200	0.08570900	3.38472500
C(Fragment=1)	0.80697100	2.86800900	-1.08585400
C(Fragment=1)	-0.40981300	3.44028600	-0.52959400
C(Fragment=1)	-1.65007000	3.35528900	-1.21630000
C(Fragment=1)	-2.81680200	3.44166300	-0.41180100
C(Fragment=1)	-4.08288800	2.87276500	-0.84606000
C(Fragment=1)	-4.13773100	2.14536800	-2.02513400
C(Fragment=1)	-4.92377000	0.92645600	-2.08866700
C(Fragment=1)	-4.18523900	-0.00937300	-2.91197800
C(Fragment=1)	-4.17300800	-1.35885000	-2.58792300
C(Fragment=1)	-2.93795100	-2.11623700	-2.70280700

C(Fragment=1)	-1.75587100	-1.53063200	-3.22858300
C(Fragment=1)	-0.53008800	-2.12085000	-2.82147400
C(Fragment=1)	0.71332500	-1.36756200	-2.82817800
C(Fragment=1)	0.69849300	-0.01691700	-3.15269200
C(Fragment=1)	1.51582900	0.91696500	-2.40494800
C(Fragment=1)	0.74390900	2.13886300	-2.26469300
C(Fragment=1)	-0.52852800	1.95957300	-2.93851800
C(Fragment=1)	-1.71210800	2.58671400	-2.46783400
C(Fragment=1)	-2.93736900	1.96223200	-2.81962100
C(Fragment=1)	-2.96611600	0.63552300	-3.36465600
C(Fragment=1)	-1.77014100	-0.10117500	-3.57274300
C(Fragment=1)	-0.55727400	0.63220200	-3.48393800
C(Fragment=2)	4.89529500	-3.22862600	0.58843600
C(Fragment=2)	4.95686700	-3.16036800	-0.79763700
C(Fragment=2)	5.32762900	-1.94446200	-1.49208700
C(Fragment=2)	5.04559700	-1.51108000	-2.84252400
C(Fragment=2)	5.05865000	-0.16781200	-3.20863600
C(Fragment=2)	5.19370100	-2.08581800	1.42729800
C(Fragment=2)	4.78647500	-1.78080000	2.78143200
C(Fragment=2)	4.76212300	-0.47700600	3.27506600
C(Fragment=2)	4.95947600	3.05561300	-1.12188900
C(Fragment=2)	5.01150100	2.29194600	-2.28246000
C(Fragment=2)	5.35467000	0.88572700	-2.26310700
C(Fragment=2)	5.82049100	0.43250800	-1.03841000
C(Fragment=2)	5.80626100	-0.94120600	-0.66482800
C(Fragment=2)	5.73611000	-1.00979500	0.74520800
C(Fragment=2)	5.70524200	0.32317200	1.24752900
C(Fragment=2)	5.13674800	0.66096500	2.46539400
C(Fragment=2)	4.78989600	2.06097600	2.58637300
C(Fragment=2)	4.83884600	2.93004900	1.50154300
C(Fragment=2)	5.24618200	2.49412200	0.18134400
C(Fragment=2)	5.76611300	1.21221000	0.14331000
H(Fragment=2)	4.52653000	-4.14306200	1.04511300
H(Fragment=2)	4.63546400	-4.02479000	-1.37238200
H(Fragment=2)	4.72303400	-2.24145600	-3.57973600
H(Fragment=2)	4.74688500	0.09318900	-4.21642700
H(Fragment=2)	4.40733900	-2.57700300	3.41642600
H(Fragment=2)	4.36544500	-0.31315200	4.27335500
H(Fragment=2)	4.60592500	4.08058700	-1.19443700
H(Fragment=2)	4.69892900	2.75080000	-3.21659300
H(Fragment=2)	4.39576100	2.43315100	3.52810600
H(Fragment=2)	4.47930200	3.94624000	1.63901100

Cation of Cor@C₇₀-L

Atom	x	y	z
C (Fragment=1)	0.24432200	3.96130200	0.18247700
C (Fragment=1)	-0.92285100	3.22322400	0.35205700
C (Fragment=1)	-1.11999500	2.44178400	1.56325700
C (Fragment=1)	-1.76605400	1.20696500	1.21009900
C (Fragment=1)	-1.52764000	0.00590800	1.92237900
C (Fragment=1)	-1.77127900	-1.19429900	1.21022800
C (Fragment=1)	-1.13044000	-2.43177600	1.56352200
C (Fragment=1)	-0.93656100	-3.21415600	0.35237100
C (Fragment=1)	0.22739700	-3.95727100	0.18288700
C (Fragment=1)	0.90533300	-3.96294800	-1.10685100
C (Fragment=1)	2.33691800	-3.97135400	-0.85917100
C (Fragment=1)	3.18391500	-3.22752600	-1.68219700
C (Fragment=1)	4.26213700	-2.45134300	-1.10756000
C (Fragment=1)	4.38897100	-1.21237700	-1.85466300
C (Fragment=1)	4.80282800	-0.00776900	-1.22703600
C (Fragment=1)	4.39416800	1.19853700	-1.85481000
C (Fragment=1)	4.27263100	2.43809300	-1.10781600
C (Fragment=1)	3.19767200	3.21878700	-1.68250900
C (Fragment=1)	2.35387500	3.96629400	-0.85958200
C (Fragment=1)	0.92226400	3.96398900	-1.10724200
C (Fragment=1)	1.26280100	3.96207600	1.22524200
C (Fragment=1)	2.56430000	3.96601000	0.57833800
C (Fragment=1)	3.60821300	3.21802300	1.12458100
C (Fragment=1)	4.47329400	2.43827800	0.26614400
C (Fragment=1)	4.80328600	1.19779000	0.94717100
C (Fragment=1)	5.01479500	-0.00814800	0.22792500
C (Fragment=1)	4.79812800	-1.21309100	0.94729200
C (Fragment=1)	4.46285700	-2.45227300	0.26641100
C (Fragment=1)	3.59445800	-3.22822900	1.12492900
C (Fragment=1)	2.54733500	-3.97182500	0.57875700
C (Fragment=1)	1.24585500	-3.96224800	1.22566400
C (Fragment=1)	1.05452600	-3.22267900	2.39182700
C (Fragment=1)	-0.15294800	-2.43272700	2.55990200
C (Fragment=1)	0.18304700	-1.20457100	3.24380400
C (Fragment=1)	-0.51421200	0.00378900	2.98122800
C (Fragment=1)	0.18820500	1.20919900	3.24366600
C (Fragment=1)	-0.14253300	2.43868300	2.55963500
C (Fragment=1)	1.06832000	3.22346700	2.39147700
C (Fragment=1)	2.15497900	2.44630800	2.95256300
C (Fragment=1)	3.39470500	2.43813800	2.33266200
C (Fragment=1)	4.14304500	1.19965800	2.22028000
C (Fragment=1)	3.67402700	-0.00514900	2.80627400
C (Fragment=1)	4.13789500	-1.21201700	2.22041400

C(Fragment=1)	3.38425300	-2.44728100	2.33292400
C(Fragment=1)	2.14449900	-2.45010400	2.95283800
C(Fragment=1)	1.60328500	-1.20599900	3.47474400
C(Fragment=1)	2.35687000	-0.00229600	3.45748100
C(Fragment=1)	1.60846000	1.20460300	3.47464500
C(Fragment=1)	-1.45319100	2.44155200	-0.75150400
C(Fragment=1)	-1.97549800	1.20684900	-0.22941800
C(Fragment=1)	-1.94897100	0.00664600	-0.98004400
C(Fragment=1)	-1.98082300	-1.19345000	-0.22928700
C(Fragment=1)	-1.46357600	-2.43029800	-0.75125400
C(Fragment=1)	-0.81625900	-2.43302600	-1.98571600
C(Fragment=1)	0.38855200	-3.22235700	-2.16993300
C(Fragment=1)	1.27271000	-2.44887500	-3.01851900
C(Fragment=1)	2.63771300	-2.44634200	-2.77894800
C(Fragment=1)	3.39103700	-1.21058100	-2.88501600
C(Fragment=1)	2.77932900	-0.00355000	-3.31450400
C(Fragment=1)	3.39620400	1.20089300	-2.88513900
C(Fragment=1)	2.64816600	2.43984800	-2.77917100
C(Fragment=1)	1.28317500	2.44818800	-3.01874100
C(Fragment=1)	0.40233700	3.22550900	-2.17024600
C(Fragment=1)	-0.80587200	2.44136800	-1.98593300
C(Fragment=1)	-0.68410000	1.21049300	-2.73813200
C(Fragment=1)	-1.27975400	0.00514900	-2.28471900
C(Fragment=1)	-0.68924600	-1.20276100	-2.73805500
C(Fragment=1)	0.60373300	-1.20461500	-3.36549800
C(Fragment=1)	1.33087600	-0.00046800	-3.56394800
C(Fragment=1)	0.60887800	1.20677600	-3.36558700
C(Fragment=2)	-4.45775000	2.45957300	-2.18081800
C(Fragment=2)	-4.42585400	1.33309000	-2.99749200
C(Fragment=2)	-4.76413400	0.01078700	-2.50806600
C(Fragment=2)	-4.42722200	-1.30836300	-3.00685100
C(Fragment=2)	-4.46048900	-2.44068100	-2.19833300
C(Fragment=2)	-4.81337900	2.38484600	-0.77738300
C(Fragment=2)	-4.53512000	3.27165700	0.33396800
C(Fragment=2)	-4.55018000	2.83497100	1.65826700
C(Fragment=2)	-4.55230500	-2.84283600	1.63797500
C(Fragment=2)	-4.53818400	-3.27035700	0.31058200
C(Fragment=2)	-4.81603400	-2.37561000	-0.79444500
C(Fragment=2)	-5.30099600	-1.14065200	-0.40146600
C(Fragment=2)	-5.29223600	0.00650900	-1.23088700
C(Fragment=2)	-5.29999100	1.14771900	-0.39330100
C(Fragment=2)	-5.31705800	0.70336600	0.95789500
C(Fragment=2)	-4.85030400	1.46468300	2.01696000
C(Fragment=2)	-4.54572100	0.68620200	3.20236000

C(Fragment=2)	-4.54611700	-0.70517400	3.19738400
C(Fragment=2)	-4.85125800	-1.47500900	2.00642900
C(Fragment=2)	-5.31752900	-0.70583800	0.95286500
H(Fragment=2)	-4.12195000	3.40547100	-2.59643500
H(Fragment=2)	-4.06268400	1.44774700	-4.01510600
H(Fragment=2)	-4.06404100	-1.41615100	-4.02521500
H(Fragment=2)	-4.12579300	-3.38395000	-2.62075800
H(Fragment=2)	-4.22067100	4.29260800	0.13582000
H(Fragment=2)	-4.24519100	3.53499200	2.43122600
H(Fragment=2)	-4.24734900	-3.54848800	2.40580600
H(Fragment=2)	-4.22489900	-4.29024700	0.10530600
H(Fragment=2)	-4.23212100	1.19647200	4.10905000
H(Fragment=2)	-4.23277900	-1.22212000	4.10037600

Cation of 2Cor@C₇₀-S

Atom	x	y	z
C(Fragment=1)	3.95014400	0.15472800	-1.12749400
C(Fragment=1)	3.21766700	0.31654800	-2.29925400
C(Fragment=1)	2.43891100	1.52357400	-2.50586800
C(Fragment=1)	1.20482700	1.16843900	-3.15762600
C(Fragment=1)	-0.00008100	1.88132000	-2.92124000
C(Fragment=1)	-1.20495000	1.16838100	-3.15758500
C(Fragment=1)	-2.43899900	1.52346000	-2.50580500
C(Fragment=1)	-3.21768500	0.31642000	-2.29919700
C(Fragment=1)	-3.95014400	0.15457800	-1.12746400
C(Fragment=1)	-3.95663000	-1.12776000	-0.44111700
C(Fragment=1)	-3.96630100	-0.87095000	0.98871700
C(Fragment=1)	-3.22350300	-1.68789900	1.84108700
C(Fragment=1)	-2.44610900	-1.10469300	2.91402300
C(Fragment=1)	-1.20590300	-1.85030400	3.04317900
C(Fragment=1)	0.00002000	-1.21950300	3.44900200
C(Fragment=1)	1.20596700	-1.85024700	3.04315700
C(Fragment=1)	2.44614400	-1.10459000	2.91397600
C(Fragment=1)	3.22355100	-1.68775200	1.84103800
C(Fragment=1)	3.96631600	-0.87078500	0.98867300
C(Fragment=1)	3.95666400	-1.12759900	-0.44114200
C(Fragment=1)	3.95652700	1.20312800	-0.11941400
C(Fragment=1)	3.96623500	0.56856500	1.18716100
C(Fragment=1)	3.22330300	1.12399000	2.22905600
C(Fragment=1)	2.44603900	0.27191300	3.10400500
C(Fragment=1)	1.20590400	0.95455700	3.43038100
C(Fragment=1)	-0.00000600	0.23717200	3.65020200
C(Fragment=1)	-1.20594100	0.95452000	3.43040500

C(Fragment=1)	-2.44605300	0.27182200	3.10405200
C(Fragment=1)	-3.22335000	1.12388300	2.22910500
C(Fragment=1)	-3.96626600	0.56842400	1.18720700
C(Fragment=1)	-3.95656600	1.20298600	-0.11938400
C(Fragment=1)	-3.22127800	2.36816400	-0.32278100
C(Fragment=1)	-2.43554000	2.52641600	-1.53455300
C(Fragment=1)	-1.20646300	3.21046100	-1.20816700
C(Fragment=1)	-0.00009600	2.94317400	-1.90800700
C(Fragment=1)	1.20628800	3.21052900	-1.20819100
C(Fragment=1)	2.43542200	2.52653900	-1.53459500
C(Fragment=1)	3.22119400	2.36830000	-0.32281000
C(Fragment=1)	2.44827800	2.93856000	0.76047700
C(Fragment=1)	2.44298500	2.32884000	2.00648700
C(Fragment=1)	1.20596400	2.22217100	2.75758200
C(Fragment=1)	-0.00006500	2.80459200	2.28666300
C(Fragment=1)	-1.20605800	2.22213000	2.75760300
C(Fragment=1)	-2.44308200	2.32876000	2.00651300
C(Fragment=1)	-2.44840000	2.93845400	0.76049500
C(Fragment=1)	-1.20472800	3.45402900	0.21135600
C(Fragment=1)	-0.00008800	3.44390700	0.96302800
C(Fragment=1)	1.20455800	3.45409000	0.21135000
C(Fragment=1)	2.43886500	-0.78943700	-2.82537900
C(Fragment=1)	1.20479500	-0.27137000	-3.35622200
C(Fragment=1)	-0.00002900	-1.02169800	-3.32129000
C(Fragment=1)	-1.20486500	-0.27141300	-3.35618100
C(Fragment=1)	-2.43887200	-0.78952500	-2.82531600
C(Fragment=1)	-2.43544400	-2.01809400	-2.16222000
C(Fragment=1)	-3.22124100	-2.19413800	-0.95271400
C(Fragment=1)	-2.44870500	-3.03715400	-0.06458600
C(Fragment=1)	-2.44326000	-2.78773000	1.30038500
C(Fragment=1)	-1.20617600	-2.88890000	2.05247400
C(Fragment=1)	0.00004700	-3.32165800	1.44133400
C(Fragment=1)	1.20626800	-2.88884500	2.05245400
C(Fragment=1)	2.44334500	-2.78761900	1.30036000
C(Fragment=1)	2.44879700	-3.03706700	-0.06460700
C(Fragment=1)	3.22131500	-2.19402200	-0.95274300
C(Fragment=1)	2.43548800	-2.01802100	-2.16226300
C(Fragment=1)	1.20652300	-2.76512900	-2.03339800
C(Fragment=1)	-0.00000100	-2.31846800	-2.63451200
C(Fragment=1)	-1.20648200	-2.76516000	-2.03337000
C(Fragment=1)	-1.20465300	-3.38384000	-0.73239800
C(Fragment=1)	0.00004000	-3.57745900	-0.00624300
C(Fragment=1)	1.20472900	-3.38380700	-0.73240700
C(Fragment=2)	6.69734000	0.26932100	3.10494200

C(Fragment=2)	6.69870300	-1.10810200	2.91274600
C(Fragment=2)	6.96628900	-1.70479600	1.62159700
C(Fragment=2)	6.60024300	-3.00251000	1.09264200
C(Fragment=2)	6.51884400	-3.24630800	-0.27279100
C(Fragment=2)	6.96405600	1.19755400	2.02723200
C(Fragment=2)	6.59559100	2.58958400	1.87418300
C(Fragment=2)	6.51354600	3.19874700	0.62841200
C(Fragment=2)	6.30627100	-0.86759900	-3.28418900
C(Fragment=2)	6.35974400	-2.09465600	-2.63140600
C(Fragment=2)	6.79292100	-2.21742200	-1.25471800
C(Fragment=2)	7.33239900	-1.05810000	-0.72541000
C(Fragment=2)	7.41938200	-0.80940900	0.66641000
C(Fragment=2)	7.41843900	0.59932900	0.86320300
C(Fragment=2)	7.33065800	1.22037800	-0.40696100
C(Fragment=2)	6.78958600	2.47980700	-0.59806800
C(Fragment=2)	6.35627700	2.73859700	-1.95555400
C(Fragment=2)	6.30451200	1.73740400	-2.91982500
C(Fragment=2)	6.67647200	0.36898200	-2.62916900
C(Fragment=2)	7.27151100	0.19625200	-1.39047800
H(Fragment=2)	6.39798000	0.65347500	4.07654600
H(Fragment=2)	6.40042100	-1.74447100	3.74177700
H(Fragment=2)	6.29505400	-3.78948700	1.77725800
H(Fragment=2)	6.15202700	-4.21428000	-0.60383800
H(Fragment=2)	6.28911600	3.15806600	2.74826400
H(Fragment=2)	6.14472100	4.21965200	0.57594400
H(Fragment=2)	5.89028800	-0.83497300	-4.28764100
H(Fragment=2)	5.98347900	-2.97168900	-3.15141100
H(Fragment=2)	5.97813500	3.72391800	-2.21495000
H(Fragment=2)	5.88850300	1.98086800	-3.89388600
C(Fragment=3)	-6.69871200	-1.10814800	2.91273600
C(Fragment=3)	-6.69732500	0.26929300	3.10496400
C(Fragment=3)	-6.96402200	1.19755700	2.02725200
C(Fragment=3)	-6.59551600	2.58958900	1.87422000
C(Fragment=3)	-6.51344100	3.19876500	0.62844800
C(Fragment=3)	-6.96631100	-1.70481100	1.62155000
C(Fragment=3)	-6.60028300	-3.00252900	1.09255600
C(Fragment=3)	-6.51887600	-3.24628600	-0.27289900
C(Fragment=3)	-6.30438300	1.73746700	-2.91979500
C(Fragment=3)	-6.35614000	2.73864300	-1.95551300
C(Fragment=3)	-6.78948100	2.47984300	-0.59804400
C(Fragment=3)	-7.33059400	1.22043100	-0.40696500
C(Fragment=3)	-7.41841900	0.59936000	0.86320200
C(Fragment=3)	-7.41939600	-0.80938600	0.66637400
C(Fragment=3)	-7.33239800	-1.05805000	-0.72547100

C(Fragment=3)	-6.79291900	-2.21736200	-1.25480100
C(Fragment=3)	-6.35971100	-2.09457400	-2.63148200
C(Fragment=3)	-6.30620100	-0.86750700	-3.28422600
C(Fragment=3)	-6.67638600	0.36905800	-2.62917400
C(Fragment=3)	-7.27146200	0.19631900	-1.39051000
H(Fragment=3)	-6.40044100	-1.74454500	3.74174800
H(Fragment=3)	-6.39795500	0.65342600	4.07657300
H(Fragment=3)	-6.28903100	3.15804300	2.74831000
H(Fragment=3)	-6.14458800	4.21964500	0.57599200
H(Fragment=3)	-6.29511200	-3.78952200	1.77715700
H(Fragment=3)	-6.15207100	-4.21424200	-0.60397200
H(Fragment=3)	-5.88835800	1.98092900	-3.89382900
H(Fragment=3)	-5.97797300	3.72394400	-2.21487500
H(Fragment=3)	-5.98346600	-2.97159400	-3.15148900
H(Fragment=3)	-5.89021000	-0.83485700	-4.28765200

Cation of 2Cor@C₇₀-L

Atom	x	y	z
C(Fragment=1)	0.72240900	-4.00862100	1.16116700
C(Fragment=1)	1.42134000	-3.28148800	2.12282000
C(Fragment=1)	0.69649600	-2.50511500	3.11410700
C(Fragment=1)	1.41084800	-1.28192800	3.36394100
C(Fragment=1)	0.73504600	-0.07883800	3.69998400
C(Fragment=1)	1.41533600	1.12969000	3.39283100
C(Fragment=1)	0.70565300	2.36122600	3.17259000
C(Fragment=1)	1.43336100	3.15908300	2.20121800
C(Fragment=1)	0.73692700	3.91211300	1.25765400
C(Fragment=1)	1.18319100	3.93723900	-0.12674500
C(Fragment=1)	0.00654000	3.95347400	-0.97964300
C(Fragment=1)	0.00450300	3.22028700	-2.16903400
C(Fragment=1)	-1.16214900	2.44712600	-2.54826300
C(Fragment=1)	-0.71754800	1.21421100	-3.17219800
C(Fragment=1)	-1.45534000	0.00733700	-3.04446200
C(Fragment=1)	-0.72203800	-1.19873300	-3.20188200
C(Fragment=1)	-1.17116600	-2.44463900	-2.60792100
C(Fragment=1)	-0.00734300	-3.23094700	-2.24736300
C(Fragment=1)	-0.00804100	-3.99274500	-1.07598700
C(Fragment=1)	1.16864800	-4.00145800	-0.22329900
C(Fragment=1)	-0.73600900	-4.00600000	1.16202000
C(Fragment=1)	-1.18377200	-3.99715200	-0.22190000
C(Fragment=1)	-2.30455100	-3.24639400	-0.58064600
C(Fragment=1)	-2.29343200	-2.45292300	-1.79097300
C(Fragment=1)	-3.00880300	-1.21164900	-1.53610300

C(Fragment=1)	-2.64238500	-0.00101600	-2.17822200
C(Fragment=1)	-3.00424000	1.19546500	-1.50644800
C(Fragment=1)	-2.28452200	2.43989300	-1.73141100
C(Fragment=1)	-2.29225700	3.20348000	-0.50204100
C(Fragment=1)	-1.16917700	3.94163900	-0.12537100
C(Fragment=1)	-0.72141000	3.91489100	1.25847200
C(Fragment=1)	-1.41953200	3.16437300	2.20278700
C(Fragment=1)	-0.69362300	2.36377300	3.17336100
C(Fragment=1)	-1.40769100	1.13494700	3.39456800
C(Fragment=1)	-0.73149900	-0.07612500	3.70088700
C(Fragment=1)	-1.41210700	-1.27670200	3.36567800
C(Fragment=1)	-0.70240200	-2.50249000	3.11483700
C(Fragment=1)	-1.43120700	-3.27627100	2.12446200
C(Fragment=1)	-2.59223500	-2.49393600	1.74779100
C(Fragment=1)	-3.01133000	-2.46961500	0.42470300
C(Fragment=1)	-3.45210400	-1.22662700	-0.17424700
C(Fragment=1)	-3.54634400	-0.03304000	0.58236300
C(Fragment=1)	-3.44766500	1.17863100	-0.14517700
C(Fragment=1)	-3.00250900	2.40522700	0.48405200
C(Fragment=1)	-2.58359300	2.39577600	1.80719100
C(Fragment=1)	-2.57736600	1.14600400	2.54002500
C(Fragment=1)	-3.09109800	-0.05077300	1.97767000
C(Fragment=1)	-2.58165700	-1.26252400	2.51076100
C(Fragment=1)	2.58480600	-2.50341300	1.74482400
C(Fragment=1)	2.57975500	-1.27211400	2.50771600
C(Fragment=1)	3.09293800	-0.06235600	1.97404600
C(Fragment=1)	2.58409100	1.13642600	2.53690600
C(Fragment=1)	2.59412200	2.38606400	1.80423500
C(Fragment=1)	3.01154700	2.39401000	0.48055500
C(Fragment=1)	2.30303000	3.19493600	-0.50471000
C(Fragment=1)	2.29114200	2.43149900	-1.73404900
C(Fragment=1)	1.16789700	2.44284500	-2.54962100
C(Fragment=1)	0.71806200	1.21157100	-3.17304600
C(Fragment=1)	1.45156800	0.00197000	-3.04620300
C(Fragment=1)	0.71367900	-1.20137300	-3.20275600
C(Fragment=1)	1.15897200	-2.44892300	-2.60930600
C(Fragment=1)	2.28218600	-2.46142500	-1.79379400
C(Fragment=1)	2.29182400	-3.25491500	-0.58340400
C(Fragment=1)	3.00255100	-2.48068000	0.42113700
C(Fragment=1)	3.44720200	-1.23943400	-0.17822000
C(Fragment=1)	3.54664800	-0.04624300	0.57825600
C(Fragment=1)	3.45153900	1.16584100	-0.14920400
C(Fragment=1)	3.00652600	1.18433800	-1.50983600
C(Fragment=1)	2.63957400	-0.01084600	-2.18132600

C(Fragment=1)	3.00235200	-1.22273000	-1.53971300
C(Fragment=2)	6.00064200	-3.18423400	-0.79918400
C(Fragment=2)	5.90136800	-2.69102800	-2.09323300
C(Fragment=2)	6.19947500	-1.30988200	-2.41267600
C(Fragment=2)	5.76263100	-0.49037100	-3.52612900
C(Fragment=2)	5.75114500	0.89540500	-3.46046000
C(Fragment=2)	6.40388500	-2.34532000	0.31373900
C(Fragment=2)	6.14377300	-2.48601900	1.72893700
C(Fragment=2)	6.18075500	-1.39977900	2.59671700
C(Fragment=2)	5.94371800	3.32026400	-0.48756400
C(Fragment=2)	5.85284900	2.95096900	-1.82433200
C(Fragment=2)	6.17479300	1.61360900	-2.27316100
C(Fragment=2)	6.77651900	0.81769400	-1.31146900
C(Fragment=2)	6.78939300	-0.59944500	-1.37969000
C(Fragment=2)	6.88776600	-1.10111300	-0.05678200
C(Fragment=2)	6.93300000	0.00603600	0.82960900
C(Fragment=2)	6.48912500	-0.06099000	2.13911000
C(Fragment=2)	6.15599400	1.22075700	2.72141600
C(Fragment=2)	6.10004700	2.38565400	1.96159000
C(Fragment=2)	6.36365100	2.38690900	0.54081800
C(Fragment=2)	6.86718500	1.19210200	0.05325100
H(Fragment=2)	5.68332300	-4.20589800	-0.60831200
H(Fragment=2)	5.50727400	-3.34383900	-2.86755400
H(Fragment=2)	5.35181000	-0.97028000	-4.41041500
H(Fragment=2)	5.33290600	1.45028300	-4.29609800
H(Fragment=2)	5.81941100	-3.44711000	2.11846400
H(Fragment=2)	5.88855500	-1.55557900	3.63179700
H(Fragment=2)	5.60942300	4.31387600	-0.20151200
H(Fragment=2)	5.44482500	3.66745000	-2.53227700
H(Fragment=2)	5.85885900	1.27151600	3.76554200
H(Fragment=2)	5.75755300	3.29835000	2.44153100
C(Fragment=3)	-6.14553000	-2.46375200	1.75438100
C(Fragment=3)	-6.18056300	-1.36859400	2.61122800
C(Fragment=3)	-6.48763000	-0.03423700	2.14044000
C(Fragment=3)	-6.15287100	1.25306900	2.70984900
C(Fragment=3)	-6.09591300	2.41006900	1.93836500
C(Fragment=3)	-6.40625500	-2.33702700	0.33810000
C(Fragment=3)	-6.00468800	-3.18753300	-0.76662700
C(Fragment=3)	-5.90557900	-2.70736000	-2.06572600
C(Fragment=3)	-5.85000100	2.93718000	-1.85316400
C(Fragment=3)	-5.93977400	3.31994700	-0.52033400
C(Fragment=3)	-6.35986900	2.39726700	0.51761300
C(Fragment=3)	-6.86529900	1.19827200	0.04232900
C(Fragment=3)	-6.93207500	0.02014800	0.83059600

C(Fragment=3)	-6.88850100	-1.09590400	-0.04467300
C(Fragment=3)	-6.79031800	-0.60768200	-1.37257900
C(Fragment=3)	-6.20203000	-1.32925900	-2.39878400
C(Fragment=3)	-5.76448600	-0.52131400	-3.52051700
C(Fragment=3)	-5.75125300	0.86499500	-3.46860800
C(Fragment=3)	-6.17364300	1.59547900	-2.28849600
C(Fragment=3)	-6.77582500	0.81004800	-1.31865000
H(Fragment=3)	-5.82208300	-3.42121900	2.15347500
H(Fragment=3)	-5.88772300	-1.51433200	3.64759100
H(Fragment=3)	-5.85550400	1.31393300	3.75336600
H(Fragment=3)	-5.75229600	3.32721800	2.40891500
H(Fragment=3)	-5.68891200	-4.20778300	-0.56593000
H(Fragment=3)	-5.51265400	-3.36842100	-2.83362600
H(Fragment=3)	-5.44206700	3.64616700	-2.56867400
H(Fragment=3)	-5.60423300	4.31599400	-0.24436400
H(Fragment=3)	-5.35468000	-1.01055600	-4.40015000
H(Fragment=3)	-5.33245900	1.41096300	-4.30981800

Cation of 2Cor@C₇₀-SL

Atom	x	y	z
C(Fragment=1)	3.97366300	-4.06157100	-0.90265700
C(Fragment=1)	2.94019300	-4.54476800	-1.70597600
C(Fragment=1)	2.42248700	-3.73642400	-2.79747000
C(Fragment=1)	0.98797100	-3.93704100	-2.88000200
C(Fragment=1)	0.11704000	-2.89729700	-3.29938900
C(Fragment=1)	-1.22650700	-2.98215400	-2.84799800
C(Fragment=1)	-2.06272400	-1.80193600	-2.73192400
C(Fragment=1)	-2.97788800	-1.99267500	-1.61793900
C(Fragment=1)	-3.30937100	-0.91850500	-0.79208100
C(Fragment=1)	-3.37087400	-1.10531900	0.64764300
C(Fragment=1)	-2.83696500	0.08785100	1.28046600
C(Fragment=1)	-2.06636500	-0.02150900	2.43629600
C(Fragment=1)	-0.86354600	0.77850400	2.58277000
C(Fragment=1)	0.14521700	-0.01348000	3.25325200
C(Fragment=1)	1.52624900	0.15010000	2.96669600
C(Fragment=1)	2.36161700	-0.96953700	3.21914200
C(Fragment=1)	3.61141900	-1.15209000	2.51310600
C(Fragment=1)	3.85248300	-2.57502900	2.34519000
C(Fragment=1)	4.43611500	-3.04961500	1.17090200
C(Fragment=1)	3.91485500	-4.24936200	0.53730900
C(Fragment=1)	4.53094700	-2.74466700	-1.16425600
C(Fragment=1)	4.81780200	-2.11669100	0.11874300
C(Fragment=1)	4.60132100	-0.75241200	0.28801000

C(Fragment=1)	3.98192700	-0.26022400	1.50759700
C(Fragment=1)	3.09471000	0.82000000	1.16502600
C(Fragment=1)	1.90964700	1.07619300	1.89685700
C(Fragment=1)	0.89005900	1.77073700	1.19989400
C(Fragment=1)	-0.49441600	1.67231800	1.57731500
C(Fragment=1)	-1.30658600	1.79568200	0.37842400
C(Fragment=1)	-2.44532200	1.01404700	0.22855100
C(Fragment=1)	-2.73771700	0.39020400	-1.05273000
C(Fragment=1)	-1.87615600	0.57277300	-2.13270700
C(Fragment=1)	-1.53068400	-0.54659800	-2.98543400
C(Fragment=1)	-0.12949300	-0.42471600	-3.35430700
C(Fragment=1)	0.68683900	-1.56842400	-3.56274200
C(Fragment=1)	2.08384700	-1.37957000	-3.38669600
C(Fragment=1)	2.96490400	-2.48628500	-3.05184700
C(Fragment=1)	4.03972400	-1.97976700	-2.22161300
C(Fragment=1)	3.79767100	-0.55950900	-2.03870200
C(Fragment=1)	4.07299700	0.04026500	-0.81002500
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C(Fragment=1)	2.60813200	-0.18838800	-2.77188300
C(Fragment=1)	1.80926100	-5.22284000	-1.10984200
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