Electronic Supplementary Information

Photoelectron spectroscopy and computational investigations of the electronic structures and noncovalent interactions of cyclodextrin-*closo*-dodecaborate anion complexes χ-CD·$B_{12}X_{12}^{2-}$ (χ = α, β, γ; X = H, F)

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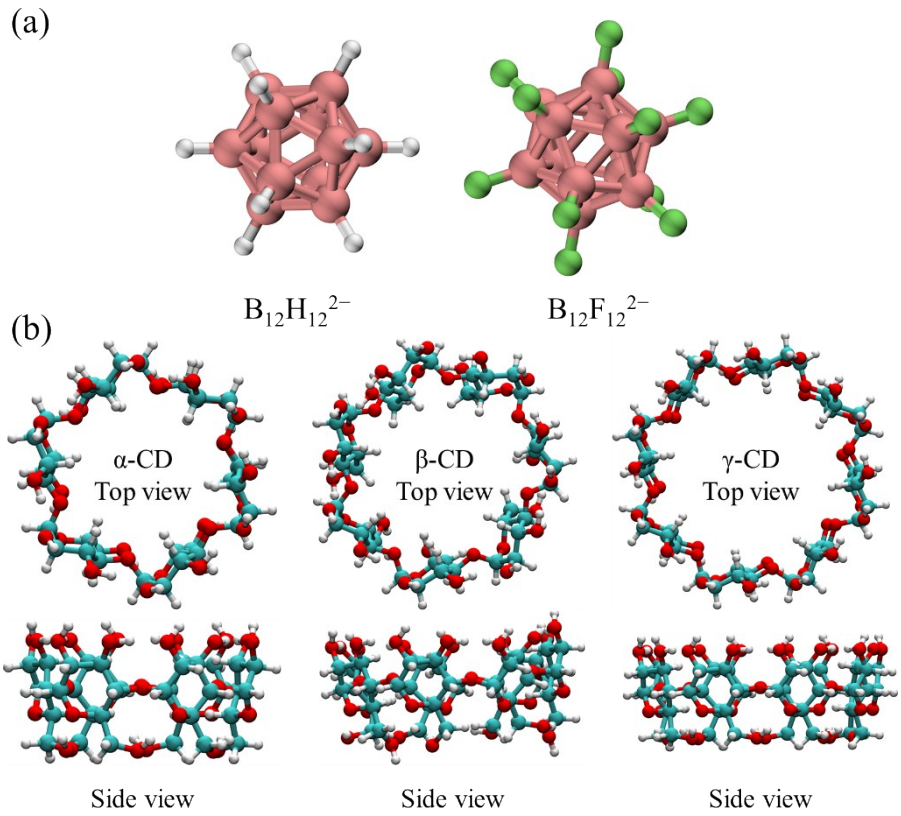


Fig. S1 (a) The optimized geometries of $B_{12}X_{12}^{2-}$ (X = H and F). The $B_{12}X_{12}^{2-}$ are shown in ball-stick model. (b) The optimized geometries of α-, β-, γ-CD, where the H, O, and C atoms are white, red, and green, respectively.

The $B_{12}H_{12}^{2-}$ and $B_{12}F_{12}^{2-}$ possess regular icosahedral structures and similar B-B bond length of 1.78 Å, while the B-F bonds (1.39 Å) in $B_{12}F_{12}^{2-}$ are longer than B-H bond (1.20 Å) in $B_{12}H_{12}^{2-}$. The C-C, C-O, C-H, and O-H bonds are 1.52, 1.42, 1.10, and 0.96 to 0.97 Å in the CDs, respectively.

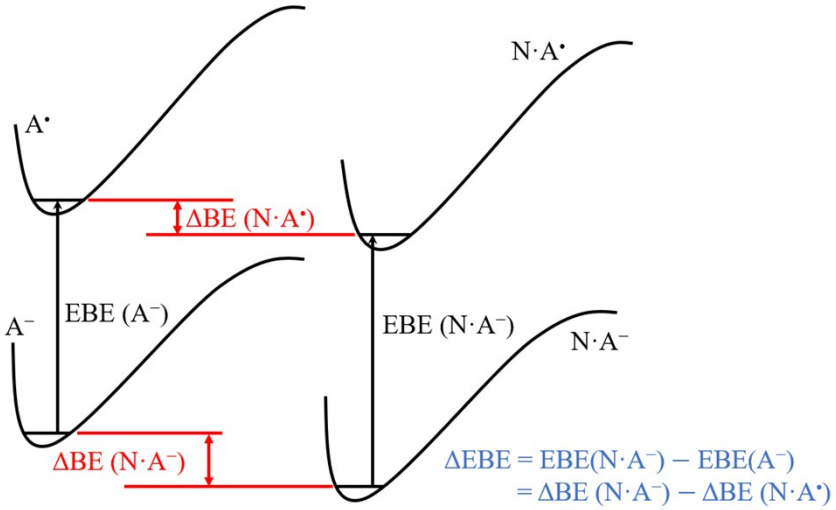
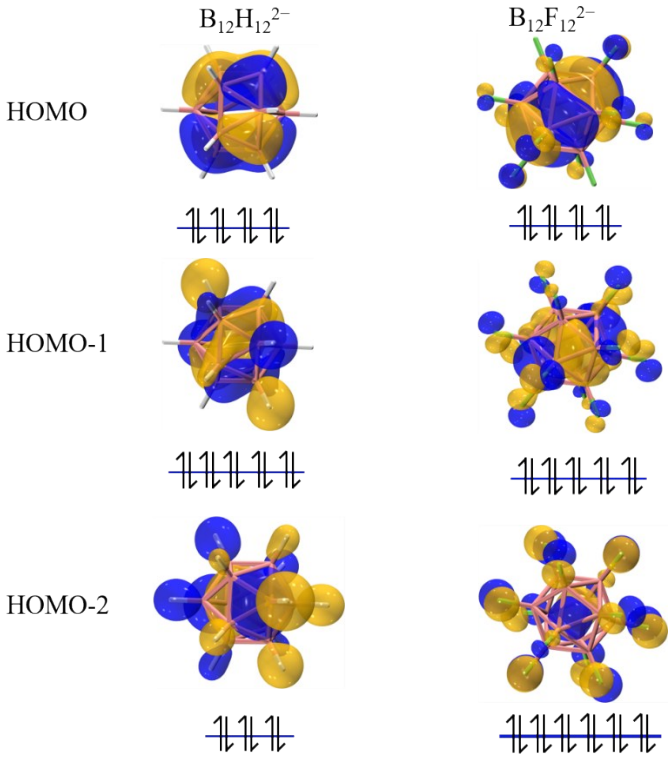


Fig. S2 Schematic of the relationship between the electron binding energy (EBE) difference and the binding energy (BE) difference of the anion A^- and neutral $A^\bullet$ guest interacting with the neutral host (N).



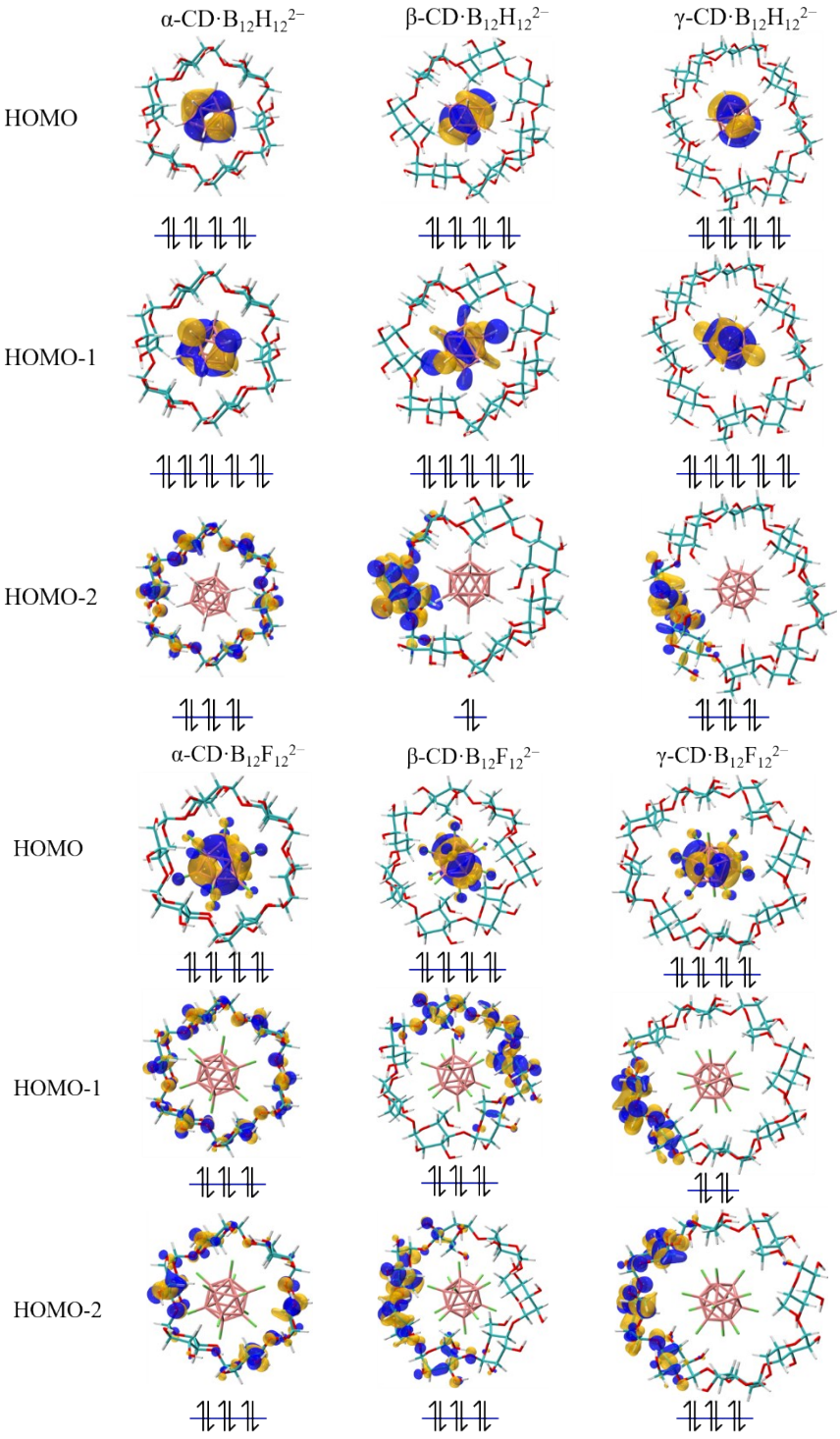


Fig. S3 Occupied molecular orbitals (MOs) calculated at the level of HF/6-311+G(d,p) for χ-CD·$B_{12}X_{12}^{2-}$ (χ = α, β, γ; X = H, F) (isovalue = 0.03). The MOs for $B_{12}X_{12}^{2-}$ are highly degenerate. The pseudo-degenerate MOs for χ-CD·$B_{12}X_{12}^{2-}$ (χ = α, β, γ; X = H, F) are grouped within 0.18

eV, and the change of shape for the MOs was also considered. The MO of the highest energy among each corresponding group is shown.

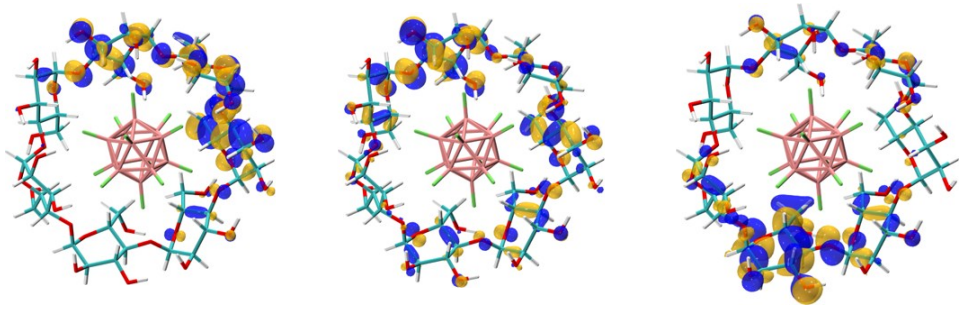


Fig. S4 The nearly degenerate HOMO-1 orbitals for β-CD·$B_{12}F_{12}^{2-}$ (isovalue = 0.03), which spread over the oxygen atoms across the whole cyclodextrin.

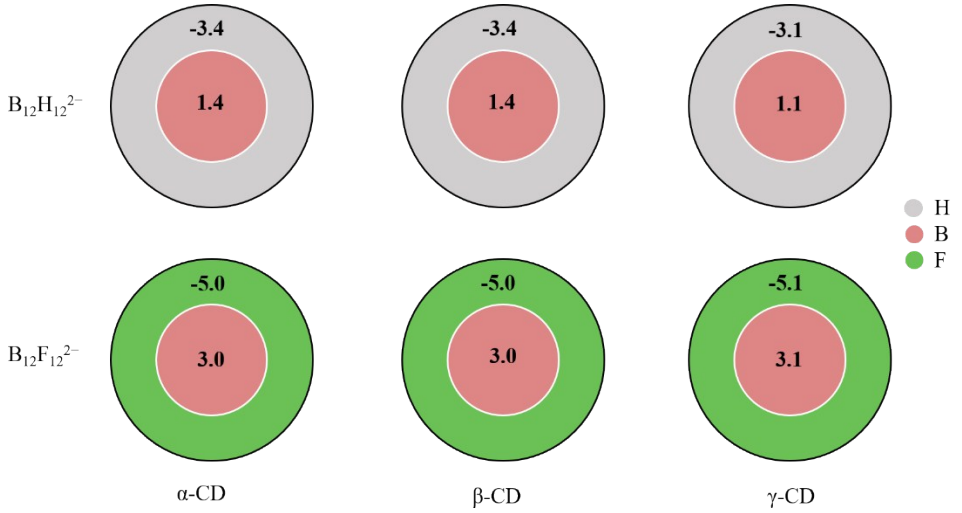


Fig. S5 The total charge distribution in χ-CD·$B_{12}X_{12}^{2-}$ using grid-based method (CHELPG). The total charges of χ-CD in χ-CD·$B_{12}X_{12}^{2-}$ is zero. Note that the inner circle represents the B_{12} unit and the outer circle the X_{12} substituents. Charges of equal atoms have been summed up.

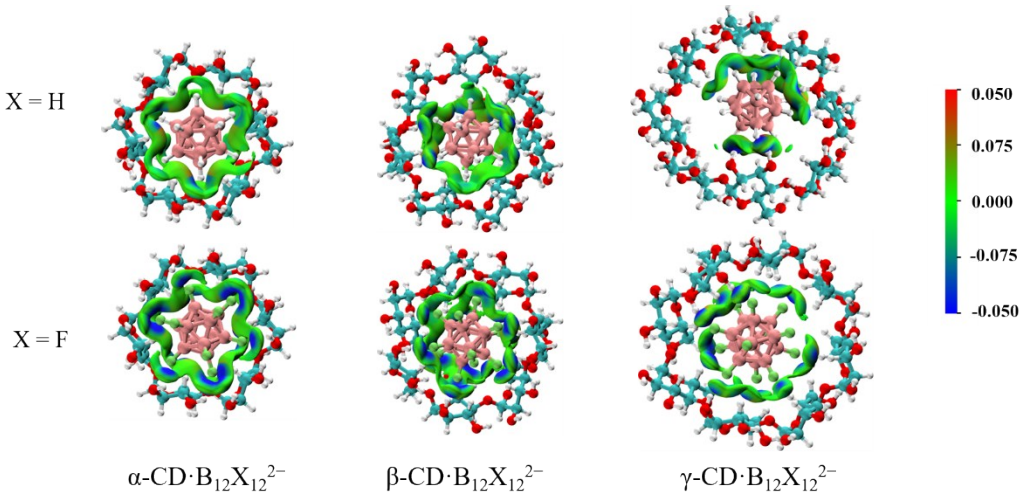


Fig. S6 The δginter = 0.005 a.u. isosurfaces colored according to a blue-green-red scheme over the range −0.05 < sign(λ2)ρ < 0.05 a.u., where the blue, green, and red isosurfaces represent the strong attractions, weak attractions, and strong repulsions, respectively. It can be nicely seen that the surfaces are interrupted in the case of γ but not for β, presumably due to the better size fit for β, and higher flexibility of the γ structure. This may explain the slightly higher stabilization observed for the β complexes.

Tab. S1 The calculated root mean square displacements (RMSDs) (in Å) of free $B_{12}X_{12}^{2-}$ *vs.* $B_{12}X_{12}^{2-}$ in χ-CD·$B_{12}X_{12}^{2-}$ (χ = α, β, γ; X = H, F) complexes and the free CDs *vs.* CDs in χ-CD·$B_{12}X_{12}^{2-}$ complexes.

	α-CD·$B_{12}H_{12}^{2-}$	β-CD·$B_{12}H_{12}^{2-}$	γ-CD·$B_{12}H_{12}^{2-}$	α-CD·$B_{12}F_{12}^{2-}$	β-CD·$B_{12}F_{12}^{2-}$	γ-CD·$B_{12}F_{12}^{2-}$
$B_{12}X_{12}^{2-}$	0.018	0.021	0.021	0.039	0.066	0.020
CDs	0.502	0.875	1.473	0.150	0.851	1.128

Tab. S2 The calculated VDEs and ADEs (in eV) for (a) $B_{12}X_{12}^{2-}$ (X = H and F) and (b) χ-CD·$B_{12}X_{12}^{2-}$ (χ = α, β, γ; X = H and F) at the level of M062X-D3/6-311+G(d,p) and PBE0-D3(BJ)/6-311+G(d,p).

(a)

eV	$B_{12}H_{12}^{2-}$		$B_{12}F_{12}^{2-}$		MAD*		
	VDE	ADE	VDE	ADE	VDE-MAD	ADE-MAD	All-MAD
M062X	1.44	1.19	2.43	2.00	0.41	0.28	0.35
PBE0	1.64	1.41	2.04	1.65	0.32	0.27	0.29
EXP.	1.15	0.93	1.90	1.70			

(b)

eV	α-CD·H		β-CD·H		γ-CD·H		α-CD·F		β-CD·F		γ-CD·F		MAD*		
	VDE	ADE	VDE	ADE	VDE	ADE	VDE	ADE	VDE	ADE	VDE	ADE	VDE-MAD	ADE-MAD	All-MAD
M062X	3.17	2.64	3.96	3.43	4.16	3.39	4.06	3.39	4.76	3.92	4.67	4.07	0.27	0.23	0.25
PBE0	3.12	2.50	3.79	3.16	3.96	3.23	3.60	2.90	4.29	3.63	4.23	3.70	0.19	0.45	0.32
EXP.	3.55	3.20	3.90	3.60	3.85	3.60	4.00	3.60	4.33	3.95	4.30	3.85			

*The mean absolute error, defined as the mean deviation between calculated values and experimental values. Note that the ADE values in this table are without ZPE corrections.

Tab. S3 (a) The experimental and calculated VDEs for χ-CD·$B_{12}X_{12}^{2-}$ (χ = α, β, γ; X = H and F). (b) The relative energy between the lowest-lying structures and corresponding isomers (in eV). (c) The index of root mean square displacements (RMSDs) (in Å) of lowest-lying χ-CD·$B_{12}X_{12}^{2-}$ (χ = α, β, γ; X = H, F). The corresponding isomers in the last column are selected as an example to represent one of the other significant low-lying isomers.

(a)

VDE/eV	EXP.	Lowest-lying	Isomer
α-CD·$B_{12}H_{12}^{2-}$	3.55	3.17	3.13
β-CD·$B_{12}H_{12}^{2-}$	3.90	3.96	3.83
γ-CD·$B_{12}H_{12}^{2-}$	3.85	4.16	4.57
α-CD·$B_{12}F_{12}^{2-}$	4.00	4.06	4.04
β-CD·$B_{12}F_{12}^{2-}$	4.33	4.76	4.80
γ-CD·$B_{12}F_{12}^{2-}$	4.30	4.67	4.56

(b)

Relative energy/eV	Lowest-lying	Isomer
α-CD·$B_{12}H_{12}^{2-}$	0	0.1186
β-CD·$B_{12}H_{12}^{2-}$	0	0.1184
γ-CD·$B_{12}H_{12}^{2-}$	0	0.3734
α-CD·$B_{12}F_{12}^{2-}$	0	0.0019
β-CD·$B_{12}F_{12}^{2-}$	0	0.1321
γ-CD·$B_{12}F_{12}^{2-}$	0	0.0344

(c)

RMSD/ Å	Lowest-lying	Isomer
α-CD·$B_{12}H_{12}^{2-}$	0	1.08
β-CD·$B_{12}H_{12}^{2-}$	0	0.86
γ-CD·$B_{12}H_{12}^{2-}$	0	1.93
α-CD·$B_{12}F_{12}^{2-}$	0	0.60
β-CD·$B_{12}F_{12}^{2-}$	0	1.69
γ-CD·$B_{12}F_{12}^{2-}$	0	1.38

Tab. S4 The calculated BEs (in eV) of singly-charged χ-CD·$B_{12}X_{12}^-$ (χ = α, β, γ; X = H and F) at the M062X-D3/6-311+G(d,p) level.

BE/eV	α-CD	β-CD	γ-CD
X = H	1.91	2.76	2.85
X = F	1.41	2.26	2.24

Tab. S5 Energy decomposition analysis (in eV) for χ-CD·$B_{12}X_{12}^{2-}$ (χ = α, β, γ; X = H and F) (a) at the SAPT0/jun-cc-pVDZ level and (b) based on force field (FF). The total interaction energies are also listed.

(a) Complexes	Electrostatic	Exchange	Dispersion	Induction	Total
α-CD·$B_{12}H_{12}^{2-}$	-2.73	2.63	-1.94	-1.33	-3.37
β-CD·$B_{12}H_{12}^{2-}$	-4.29	3.46	-2.44	-1.81	-5.08
γ-CD·$B_{12}H_{12}^{2-}$	-4.40	2.86	-1.87	-1.83	-5.24
α-CD·$B_{12}F_{12}^{2-}$	-2.83	3.04	-1.67	-1.21	-2.67
β-CD·$B_{12}F_{12}^{2-}$	-4.38	3.69	-2.07	-1.57	-4.33
γ-CD·$B_{12}F_{12}^{2-}$	-3.76	2.45	-1.58	-1.47	-4.36

(b) Complexes	Electrostatic	van der Waals	Total
α-CD·$B_{12}H_{12}^{2-}$	-1.50	-1.06	-2.56
β-CD·$B_{12}H_{12}^{2-}$	-2.65	-1.26	-3.91
γ-CD·$B_{12}H_{12}^{2-}$	-3.19	-1.05	-4.24
α-CD·$B_{12}F_{12}^{2-}$	-1.58	-0.47	-2.05
β-CD·$B_{12}F_{12}^{2-}$	-2.72	-0.56	-3.28
γ-CD·$B_{12}F_{12}^{2-}$	-2.61	-0.88	-3.49

Tab. S6 The calculated polarizability (in a.u.) of $B_{12}X_{12}^{2-}$ and χ-CD·$B_{12}X_{12}^{2-}$ (χ = α, β, γ; X = H and F) at the level of M062X-D3/6-311+G(d,p).

Polarizability/a.u.		α-CD	β-CD	γ-CD
X = H	164.61	654.23	741.09	831.49
X = F	130.98	631.63	715.75	803.58

Tab. S7 Comparison of geometry optimization and VDEs using mixed basis set (anionic $B_{12}X_{12}^{2-}$ (X= H, F) with 6-311+G(d,p) and neutral α-CD with 6-311G(d,p)) and pure 6-311G(d,p) for all atoms at the M062X-D3 level.

VDE / eV	Basis set	α-CD·$B_{12}H_{12}^{2-}$	α-CD·$B_{12}F_{12}^{2-}$
Optimization	6-311G(d,p) for α-CD / 6-311+G(d,p) for $B_{12}X_{12}^{2-}$	3.09	3.96
	6-311G(d,p) for all atoms	3.17	4.06
RMSD /Å		0.05	0.03

Cartesian coordinates for all optimized anions

$B_{12}H_{12}^{2-}$:

Atom	Coordinates (Angstroms)		
	X	Y	Z
B	-1.36961400	-0.31530600	-0.94046500
B	0.88507500	1.38613200	-0.39369000
B	1.49979800	-0.24551600	-0.74184000
B	0.10625900	-1.29713700	-1.07968600
B	-0.10626200	1.29712400	1.07968200
B	-0.88507300	-1.38613800	0.39368300
B	0.88838100	-1.34309000	0.51644500
B	1.36962000	0.31530600	0.94047900
B	0.10420400	0.38961900	-1.64219500
B	-1.49980200	0.24552400	0.74183600
B	-0.10419600	-0.38961800	1.64219900
B	-0.88839300	1.34309800	-0.51644400
H	-0.17798800	-0.66577500	2.80588400
H	-0.18152200	2.21622900	1.84484300
H	-2.56242900	0.41952300	1.26761800
H	-1.51785900	2.29481800	-0.88237100
H	-2.34014800	-0.53865700	-1.60687200
H	0.17792300	0.66575600	-2.80589000
H	1.51219500	2.36837900	-0.67262900
H	0.18155400	-2.21621300	-1.84487800
H	2.56243700	-0.41957900	-1.26757700
H	1.51789000	-2.29479800	0.88233100
H	2.34018200	0.53867700	1.60683500
H	-1.51221800	-2.36835000	0.67268400

$B_{12}F_{12}^{2-}$:

Atom	Coordinates (Angstroms)

	X	Y	Z
B	-1.34723000	0.85915600	0.56287000
B	0.75584400	-1.03488500	1.10812000
B	1.51132400	0.49160400	0.58662600
B	0.21160300	1.66218200	0.24965100
B	-0.21161100	-1.66216100	-0.24966300
B	-0.75584000	1.03490300	-1.10811500
B	1.01094100	0.80772200	-1.09343900
B	1.34723500	-0.85916600	-0.56289300
B	0.05392200	0.52338200	1.61034700
B	-1.51133500	-0.49161400	-0.58661100
F	2.74978700	0.89464800	1.06720100
F	1.83954300	1.46963500	-1.98925300
F	0.38509800	3.02422600	0.45446900
F	0.09795800	0.95225500	2.92987900
F	1.37522000	-1.88302700	2.01600200
F	2.45128900	-1.56310500	-1.02404500
F	-2.74974700	-0.89457600	-1.06738300
F	-0.38502500	-3.02423900	-0.45437100
F	-0.09814000	-0.95218400	-2.92990300
F	-1.83945800	-1.46962300	1.98935600
F	-2.45122400	1.56311300	1.02415900
F	-1.37529300	1.88287800	-2.01609900
B	-0.05390500	-0.52339100	-1.61035300
B	-1.01096400	-0.80773200	1.09343600

α-CD·$B_{12}H_{12}^{2-}$:

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	4.53318500	2.70377300	0.18485100
C	5.12125600	1.99634600	-1.03176100
C	4.65736900	0.55672400	-1.04981100
C	4.91525400	-0.13893000	0.28015800
C	4.42959000	0.69540100	1.46944100
C	4.90769200	0.20617800	2.83309400
O	4.73415800	2.67373700	-2.21010300
O	5.34749700	-0.08093800	-2.09985400
O	4.16319300	-1.34141800	0.21664700
O	4.95099000	2.03079400	1.36509000
O	4.27677200	-0.96516600	3.28468800
H	4.92143700	3.72341700	0.26919400
H	6.21551900	2.01959600	-0.93751600
H	3.57345000	0.53514700	-1.21796500
H	5.98876600	-0.35982100	0.37664500

H	3.33482300	0.70903800	1.44016000
H	6.00269400	0.09927100	2.80268400
H	4.67325200	0.98960700	3.55835900
H	4.45211500	1.99957800	-2.84276100
H	4.97170400	-0.96916400	-2.20519600
H	4.46150900	-1.69919200	2.68350000
C	-0.08249100	5.20827900	0.59120100
C	0.80794300	5.47372100	-0.62240300
C	1.68169500	4.26608500	-0.88465900
C	2.44176300	3.89444800	0.37178200
C	1.47499900	3.67168700	1.52596500
C	2.16798900	3.29060400	2.82934100
O	0.01132700	5.75293800	-1.75817700
O	2.55352800	4.62385500	-1.93571800
O	3.15285700	2.70015700	0.09744300
O	0.73514100	4.90511400	1.71027000
O	3.42634500	3.91245500	3.02675700
H	-0.66175400	6.09712400	0.86450500
H	1.44694400	6.33660400	-0.38978700
H	1.04435300	3.42150600	-1.17345900
H	3.13650800	4.69783300	0.64404000
H	0.76763700	2.87887300	1.26144500
H	1.51479100	3.56866800	3.65908700
H	2.27000400	2.20071200	2.84324100
H	0.54570800	5.48017500	-2.51661500
H	3.06514100	3.83459900	-2.17470900
H	4.08823800	3.33772900	2.62171300
C	-4.69628800	2.55151000	0.34293900
C	-4.34653400	3.46037500	-0.83111900
C	-2.85281500	3.68949200	-0.87755900
C	-2.31728700	4.18231600	0.45691500
C	-2.77884400	3.26902000	1.59636600
C	-2.49091300	3.78676600	3.00398100
O	-4.79602500	2.88893100	-2.04175600
O	-2.63499300	4.63080300	-1.90470300
O	-0.90945500	4.13099600	0.31295500
O	-4.21854300	3.15409800	1.53598500
O	-1.14343100	3.68271500	3.38828000
H	-5.78166000	2.46691700	0.46366700
H	-4.84842500	4.42381100	-0.66268800
H	-2.35046500	2.73991100	-1.10038600
H	-2.65025400	5.21585700	0.63544700
H	-2.31827500	2.28342400	1.46874700
H	-2.86402000	4.81961800	3.08293600
H	-3.06066900	3.16815600	3.70002200
H	-4.16447300	3.17143700	-2.71740500
H	-1.67752500	4.75798100	-1.99513900

H	-0.59080600	4.26430300	2.84803800
C	-4.60578800	-2.73804200	0.17456500
C	-5.12542900	-2.02907200	-1.07194700
C	-4.59712800	-0.61199400	-1.07799400
C	-4.89034500	0.11303200	0.22888700
C	-4.48225800	-0.72271300	1.44579400
C	-4.98712400	-0.20411100	2.78877200
O	-4.69662400	-2.72400400	-2.22717800
O	-5.19792800	0.04245000	-2.16871400
O	-4.11407400	1.30439900	0.17980700
O	-5.04698500	-2.04128500	1.33237500
O	-4.29982600	0.92407800	3.26671500
H	-5.00809700	-3.75245900	0.25946700
H	-6.22253600	-2.01567600	-1.03341600
H	-3.50635200	-0.65381600	-1.19222500
H	-5.96171900	0.35827000	0.27490100
H	-3.38871300	-0.77597900	1.45851300
H	-6.07106500	-0.02743100	2.71606000
H	-4.83154300	-1.00114100	3.52035400
H	-4.37611400	-2.06198900	-2.85628900
H	-4.78333500	0.91475100	-2.25448600
H	-4.43993700	1.67523900	2.67407500
C	0.08674700	-5.13590800	0.59293200
C	-0.81456400	-5.44314600	-0.60277500
C	-1.76274800	-4.29169800	-0.86063100
C	-2.49867700	-3.92104300	0.40861400
C	-1.50627900	-3.64024100	1.52758200
C	-2.17717500	-3.24330600	2.84040300
O	-0.02655700	-5.70030000	-1.74785400
O	-2.64573000	-4.72289900	-1.87674500
O	-3.22611600	-2.74068400	0.12843300
O	-0.72383600	-4.84321600	1.71994500
O	-3.44162600	-3.84654000	3.05849100
H	0.68205200	-6.01347000	0.86743400
H	-1.40708700	-6.33301600	-0.34674400
H	-1.19040300	-3.41519700	-1.18577000
H	-3.17344500	-4.72803300	0.71764400
H	-0.83277600	-2.83375200	1.21887700
H	-1.51911300	-3.53159200	3.66259800
H	-2.26272600	-2.15236900	2.85673300
H	-0.58197100	-5.45652000	-2.50027300
H	-3.19637100	-3.96428100	-2.13056100
H	-4.10138200	-3.28980900	2.62562000
C	4.74212200	-2.59057400	0.35540400
C	4.36900500	-3.46385400	-0.83779700
C	2.86677800	-3.62558500	-0.88895300
C	2.31395700	-4.13296200	0.43359400

C	2.81007500	-3.27262200	1.59943700
C	2.50726400	-3.82068500	2.99224200
O	4.83405600	-2.88084000	-2.03888100
O	2.60976600	-4.52922000	-1.93834100
O	0.90371500	-4.05106000	0.30272800
O	4.25441200	-3.20765500	1.53658800
O	1.17066400	-3.65573900	3.39196400
H	5.82862600	-2.51741800	0.47503300
H	4.83570600	-4.44799500	-0.69394800
H	2.41341300	-2.64634800	-1.09111500
H	2.62241700	-5.17902900	0.57984500
H	2.38677500	-2.26693900	1.50590800
H	2.82454700	-4.87425000	3.03633100
H	3.11603100	-3.25556400	3.70065700
H	4.18889200	-3.12302500	-2.71823800
H	1.64777500	-4.61013200	-2.03037400
H	0.58844400	-4.20746300	2.85126700
B	0.96671100	-0.34605600	-1.40572500
B	0.81861000	0.63587700	-4.11001700
B	-0.25457200	1.63199600	-3.09625900
B	-0.16244200	1.01734700	-1.43075200
B	0.19692500	-1.02791900	-4.09675600
B	-0.78066300	-0.63994600	-1.41649200
B	-1.53263700	0.58020500	-2.46983500
B	-0.93346000	0.34279100	-4.12041900
B	1.28811300	1.05310900	-2.45419600
B	0.28994200	-1.62989200	-2.43158500
B	-1.26046500	-1.06086100	-3.07488400
B	1.57493400	-0.58695000	-3.05843900
H	-2.16602000	-1.82469600	-3.28001500
H	0.32404100	-1.76046300	-5.02947200
H	0.48199900	-2.79013400	-2.21916400
H	2.68699000	-1.00093000	-3.24788700
H	1.62937000	-0.58523300	-0.43707800
H	2.18987300	1.80715400	-2.24962400
H	1.39175100	1.09147400	-5.05220400
H	-0.29596400	1.72670400	-0.47840700
H	-0.44896900	2.79746800	-3.30868900
H	-2.63258200	1.00667200	-2.28003600
H	-1.61270800	0.58727500	-5.07009100
H	-1.34236900	-1.07818800	-0.45643500

β-CD·$B_{12}H_{12}^{2-}$:

Atom	Coordinates (Angstroms)		
	X	Y	Z

C	0.46624000	5.80099300	0.62143000
C	1.41289800	6.24400100	-0.49016700
C	2.17522600	5.04560600	-1.01683700
C	2.86177000	4.32848700	0.13399000
C	1.83497800	3.93833400	1.18977100
C	2.45329100	3.22656900	2.37722400
O	0.66051900	6.86010700	-1.52033800
O	3.09234800	5.53403700	-1.98491400
O	3.47140500	3.15406400	-0.36555100
O	1.19356400	5.15290800	1.64290000
O	3.65937300	3.82576300	2.79483200
C	-4.47065700	3.94608400	0.52858300
C	-4.11661500	5.04081400	-0.47711700
C	-2.64099500	4.97881100	-0.81826300
C	-1.82416300	5.02494200	0.46016900
C	-2.23318900	3.85755300	1.35119200
C	-1.45157900	3.75863800	2.65184000
O	-4.92437600	4.88475300	-1.62769600
O	-2.35795700	6.08586400	-1.65251300
O	-0.47401100	4.95598100	0.04677900
O	-3.63001200	4.05325700	1.66365700
O	-1.13317600	5.01245200	3.22640000
C	-6.00602600	-1.04062000	0.07824200
C	-6.57838500	-0.08539700	-0.97752800
C	-5.65342300	1.11208400	-1.16027900
C	-5.23010100	1.67054500	0.19559600
C	-4.60888000	0.57661700	1.05513500
C	-4.08711400	1.03181700	2.40533900
O	-6.80866700	-0.80820600	-2.16377700
O	-6.32548800	2.10803700	-1.89789100
O	-4.32488800	2.72442800	-0.10323500
O	-5.65049900	-0.39690600	1.26618400
O	-4.90873900	1.97713200	3.06405500
C	-2.83563200	-5.16593000	-0.51380300
C	-3.21432300	-4.60676300	-1.88668700
C	-3.71876300	-3.18145700	-1.73090600
C	-4.74661000	-3.02695300	-0.61466800
C	-4.23771500	-3.67222900	0.67920700
C	-5.25549400	-3.69144200	1.80791900
O	-2.07932500	-4.66345200	-2.73844400
O	-4.28295400	-2.69732700	-2.93398900
O	-4.86961000	-1.62917600	-0.49905400
O	-3.87472100	-5.03451600	0.42277400
O	-4.78629100	-4.36305200	2.95822000
C	2.12605000	-5.27039700	1.13287600
C	1.54040900	-6.23126900	0.09163900
C	0.35813000	-5.57437200	-0.59206300

C	-0.64176700	-5.16518600	0.47403600
C	0.04531600	-4.22439000	1.45134000
C	-0.91436400	-3.66266700	2.48796300
O	2.53280300	-6.58250800	-0.85648400
O	-0.16480400	-6.50169000	-1.53030100
O	-1.71457900	-4.44455500	-0.09276800
O	1.13789600	-4.92309200	2.06948300
O	-1.89231200	-4.58094900	2.95881700
C	5.97624400	-1.70344400	0.29109200
C	6.11065000	-3.12874200	-0.23520500
C	4.74374000	-3.74561300	-0.45994500
C	3.88591100	-3.63287700	0.79313800
C	3.82113100	-2.16099200	1.19538600
C	3.03787600	-1.85182200	2.45216700
O	6.87983300	-3.14447700	-1.41374400
O	4.97006300	-5.09065100	-0.83011600
O	2.61082200	-4.14954900	0.45655700
O	5.16734700	-1.73114500	1.44530200
O	2.81153200	-0.45471900	2.56387500
C	4.82363900	3.24163500	-0.68628500
C	5.03373900	2.53109000	-2.02760800
C	4.92038800	1.02690200	-1.85041200
C	5.74306000	0.50680100	-0.66481300
C	5.31843600	1.29426800	0.58531800
C	5.97163000	1.03320900	1.94187500
O	4.10969100	3.02836500	-2.97848100
O	5.32668400	0.40668200	-3.04745600
O	5.43260400	-0.88461900	-0.68446100
O	5.61582400	2.67045400	0.31820600
O	5.06047000	1.33628600	2.98775200
H	-0.01892500	6.66178800	1.09273700
H	2.12962600	6.95844900	-0.06363500
H	1.46593400	4.34849000	-1.47852300
H	3.61089900	4.97156000	0.60965200
H	1.08137600	3.28024500	0.74279100
H	2.61495500	2.18714100	2.07587200
H	1.71808900	3.23015700	3.19323400
H	1.22399100	6.81277500	-2.30201900
H	3.42895600	4.76799800	-2.48013000
H	4.30720500	3.11033400	2.87401300
H	-5.49207900	4.07552000	0.90147500
H	-4.31601100	6.01148500	-0.00316400
H	-2.42276200	4.03107200	-1.33168400
H	-2.00862300	5.96324400	0.99704800
H	-2.11381300	2.91924000	0.79433700
H	-0.54775400	3.17586400	2.45167400
H	-2.06062600	3.19552200	3.36601900

H	-4.45877400	5.33706900	-2.33988400
H	-1.39387700	6.13953900	-1.74392400
H	-0.21307400	5.18359400	2.98813900
H	-6.75045000	-1.80177000	0.33267600
H	-7.54911500	0.28543900	-0.63521000
H	-4.74088900	0.77910600	-1.67700700
H	-6.10673000	2.07061300	0.72025800
H	-3.77797000	0.10926000	0.51623400
H	-3.07461700	1.41993100	2.25324800
H	-4.00905800	0.14464000	3.03946500
H	-5.96815400	-1.22242300	-2.41219400
H	-5.74194400	2.88045100	-1.92121300
H	-4.54387900	2.84342100	2.84404200
H	-2.61150100	-6.23426500	-0.57074900
H	-3.98923900	-5.23226000	-2.33745600
H	-2.86843800	-2.55780500	-1.43479600
H	-5.70443200	-3.47713800	-0.91783900
H	-3.35109900	-3.10533900	0.99375300
H	-6.14212200	-4.24043300	1.47701100
H	-5.53706700	-2.65844000	2.03797700
H	-1.52962600	-3.88588200	-2.54152700
H	-3.64293300	-2.08047200	-3.30967400
H	-3.95093900	-3.97068900	3.23915900
H	2.92627700	-5.75933700	1.69629300
H	1.19657700	-7.13046300	0.61968200
H	0.70913200	-4.67047800	-1.10184000
H	-1.01158600	-6.05284400	1.00658800
H	0.43912500	-3.37876000	0.88267500
H	-1.38481800	-2.77835700	2.04423600
H	-0.33933100	-3.34558300	3.35919200
H	2.04746800	-6.84966300	-1.64695700
H	-0.75381200	-6.00681300	-2.12412000
H	-2.44465000	-4.86256600	2.21708900
H	6.95609400	-1.32970500	0.60847700
H	6.60811400	-3.70824200	0.55697500
H	4.22803400	-3.19681900	-1.26009100
H	4.33370200	-4.22176200	1.60613600
H	3.38772000	-1.58851300	0.36618300
H	3.62318100	-2.14774300	3.32650100
H	2.09731300	-2.40931100	2.44846500
H	6.69594600	-3.99725900	-1.82279000
H	4.10957600	-5.51838200	-0.97003700
H	2.17209400	-0.20382800	1.87686400
H	5.13658200	4.28668100	-0.75676800
H	6.03616300	2.76677500	-2.39797000
H	3.87337600	0.78201200	-1.62049200
H	6.81832300	0.63865000	-0.85386300

H	4.23658500	1.15933900	0.70528400
H	6.81214800	1.72218800	2.04305200
H	6.32914800	0.01384800	2.05404900
H	3.29230200	2.51133300	-2.88640700
H	5.14037900	-0.53133300	-2.93331800
H	4.32874400	0.69578700	2.92978300
B	-0.33710700	0.63866200	0.11797100
B	-1.30298300	-0.63479000	-2.26012100
B	-0.08220500	-1.69339000	-1.54191900
B	0.51779400	-0.90076400	-0.07426300
B	-0.51810500	0.87512900	-2.74013800
B	1.30778500	0.60135100	-0.54404700
B	1.47229700	-0.83796100	-1.57131600
B	0.33963300	-0.67099300	-2.92860300
B	-1.19644400	-0.78817700	-0.49253100
B	0.08059900	1.66016000	-1.27038000
B	1.19508800	0.75282300	-2.30657800
B	-1.46787800	0.80079000	-1.23878100
H	2.03626100	1.27303800	-2.98113700
H	-0.88787700	1.50442700	-3.68033500
H	0.10641600	2.84351200	-1.18266700
H	-2.49825900	1.38466200	-1.13019300
H	-0.55907500	1.08822500	1.20744200
H	-2.03119200	-1.34177600	0.16186200
H	-2.22954300	-1.05095800	-2.89538100
H	0.88388800	-1.50090200	0.88920200
H	-0.14197300	-2.88389200	-1.63662400
H	2.51581200	-1.41236200	-1.69105000
H	0.57453700	-1.13849100	-3.99801000
H	2.23151900	1.02516400	0.08146000

γ-CD·$B_{12}H_{12}^{2-}$:

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	0.50760200	5.73496700	-1.08733200
C	1.22138200	4.77141100	-2.04809500
C	2.25831900	3.90024500	-1.34495100
C	3.14069000	4.79343900	-0.48511300
C	2.27385100	5.56945800	0.50240000
C	3.07652200	6.47510800	1.43014300
O	-0.41653900	5.03289500	-0.30475400
O	0.27242800	4.01723600	-2.77230300
O	3.06404600	3.24658300	-2.29958000
O	1.40664200	6.43093400	-0.25198300

O	3.73772500	5.77959400	2.45932400
H	3.67348500	5.50606700	-1.12599800
H	-0.00336200	6.50472700	-1.67090000
H	1.76299600	5.38650000	-2.77515100
H	1.76484400	3.16554600	-0.69632500
H	1.67752600	4.87843300	1.11073100
H	3.77759900	7.06805800	0.82248800
H	2.38012500	7.16603400	1.91027600
H	0.15965800	3.13791900	-2.36631000
H	2.65048100	2.40237100	-2.54879300
H	4.12217300	4.97355000	2.09755400
C	5.43936400	4.33195700	0.15113800
C	6.10871900	3.80547400	-1.12059100
C	6.01218300	2.29024400	-1.14187800
C	6.47679600	1.68737700	0.18216500
C	5.92125000	2.38286100	1.42548400
C	6.71391700	2.07094300	2.69279800
O	4.06643600	3.98687300	0.22547700
O	5.57376400	4.41478100	-2.26674800
O	6.81346300	1.79508000	-2.18883800
O	6.04309500	3.80473500	1.29353800
O	6.68202900	0.72080500	3.08377500
H	7.57660200	1.72034300	0.20230800
H	5.55422600	5.42036000	0.21379700
H	7.16597700	4.09044500	-1.06558900
H	4.95972700	2.00813500	-1.27325000
H	4.87155100	2.09814700	1.54558600
H	7.74222900	2.42859600	2.53663000
H	6.28168900	2.64994600	3.51021400
H	4.76590600	3.93049600	-2.50458700
H	6.52446200	0.88810200	-2.37244700
H	7.07278000	0.16918900	2.39486700
C	6.91609000	-0.70168400	-0.03442800
C	6.33154200	-1.63332300	-1.09958500
C	5.02099200	-2.19935400	-0.58259800
C	5.29124400	-2.92760800	0.72710100
C	5.90885300	-1.94787600	1.72608800
C	6.27630100	-2.59349500	3.05429700
O	6.02556600	0.33872100	0.19838900
O	6.14704600	-0.91767400	-2.30145700
O	4.47684100	-3.06319600	-1.56533400
O	7.12779500	-1.42095800	1.16922400
O	5.15167200	-2.89178600	3.85330200
H	5.98366200	-3.75944200	0.55959200
H	7.89534400	-0.32386900	-0.34168500
H	7.04490000	-2.45273500	-1.26019200
H	4.32931100	-1.37247500	-0.39710500

H	5.20778400	-1.12776300	1.91657900
H	6.86887700	-3.49901900	2.85600400
H	6.90029300	-1.89077300	3.61166100
H	5.34504600	-1.25549600	-2.72396900
H	3.55819900	-2.79527900	-1.73328600
H	4.38169100	-3.01602200	3.28710800
C	3.93467600	-4.75438700	1.63102100
C	3.80279600	-5.72109100	0.44301700
C	2.47143600	-5.52645300	-0.26707800
C	1.33105400	-5.51617200	0.74885200
C	1.59839600	-4.43478800	1.78630000
C	0.53620000	-4.27054400	2.86226700
O	4.05568100	-3.39882300	1.23229100
O	4.90746300	-5.62534700	-0.42207400
O	2.32010000	-6.55889700	-1.21389300
O	2.81522200	-4.79930700	2.46256900
O	-0.61234700	-3.58730600	2.41520600
H	1.27066800	-6.48758300	1.26147800
H	4.79539300	-5.03526400	2.24911100
H	3.81294900	-6.73481600	0.86063900
H	2.46096400	-4.54099500	-0.75296100
H	1.73152900	-3.47190600	1.27801400
H	0.20707000	-5.25148000	3.22018600
H	1.01112900	-3.74332700	3.69873800
H	4.74081400	-4.88212000	-1.02387000
H	1.64098700	-6.28006400	-1.84948300
H	-0.36288400	-2.90673900	1.77570400
C	-0.59514500	-6.35140400	-0.39229200
C	-1.08144400	-6.03168500	-1.80901800
C	-2.12731300	-4.93390300	-1.77674300
C	-3.16027100	-5.13202500	-0.67092100
C	-2.56481500	-5.55582200	0.66826300
C	-3.60152700	-6.12502100	1.63304500
O	0.12040800	-5.24660800	0.07274900
O	0.01648100	-5.68415500	-2.63339600
O	-2.77297200	-4.88714600	-3.03087600
O	-1.67346200	-6.65353600	0.45526000
O	-4.65594400	-5.24438600	1.95278000
H	-3.88404200	-5.89140700	-1.00423300
H	0.03514900	-7.24313000	-0.40108000
H	-1.52873300	-6.93695000	-2.23134100
H	-1.62007500	-3.98723300	-1.55732000
H	-2.03546900	-4.71293600	1.12095800
H	-3.98003800	-7.06191700	1.19881700
H	-3.09569400	-6.36957200	2.56811500
H	0.14007400	-4.72275100	-2.59692600
H	-3.09081400	-3.98185000	-3.16723500

H	-5.12346200	-5.00862500	1.14288800
C	-5.06276400	-3.71187000	-1.09863600
C	-5.10558500	-2.41237900	-1.91372100
C	-5.14410000	-1.17711700	-1.02472200
C	-6.13856700	-1.31091100	0.12536400
C	-5.92414700	-2.63988400	0.84859300
C	-6.93473500	-2.95287500	1.94480100
O	-3.82229200	-3.87490100	-0.50399300
O	-4.03410600	-2.36185300	-2.82737400
O	-5.40404400	-0.02822800	-1.80404600
O	-6.07584400	-3.70221600	-0.10058000
O	-7.04574400	-1.93579700	2.92316600
H	-7.16784100	-1.27179700	-0.25126900
H	-5.29835900	-4.56019000	-1.74625700
H	-6.03116000	-2.43624600	-2.50135300
H	-4.15322000	-1.04346600	-0.57713000
H	-4.90910900	-2.66183900	1.26620400
H	-7.92166400	-3.06601000	1.48715800
H	-6.64960300	-3.90518400	2.40295600
H	-3.30304100	-1.83278500	-2.46838200
H	-6.35555500	0.13007300	-1.77686600
H	-6.17609100	-1.54732900	3.06371100
C	-6.94461200	0.59469500	1.41425600
C	-7.46491300	1.55271200	0.34301700
C	-6.36781800	2.48301200	-0.11931200
C	-5.70210500	3.17748700	1.05305500
C	-5.33863700	2.19736200	2.17094100
C	-5.01967900	2.90247400	3.48770500
O	-5.87490300	-0.21300800	0.99323100
O	-8.01041600	0.86531600	-0.77581100
O	-6.98638000	3.40785600	-0.99913500
O	-6.46913500	1.37178500	2.47871000
O	-3.91414800	3.77160000	3.42771500
H	-6.38114200	3.94800200	1.44862300
H	-7.74865700	-0.02353000	1.81859200
H	-8.25392700	2.14667700	0.82439900
H	-5.59949200	1.90134600	-0.63847900
H	-4.49171700	1.58731500	1.84430700
H	-5.93225900	3.42248700	3.81412200
H	-4.78617000	2.14084500	4.23234700
H	-8.18260900	1.56443700	-1.42022700
H	-6.28675600	3.83699900	-1.51844400
H	-4.08465900	4.47025800	2.78586300
C	-4.50422900	5.14438900	0.30450600
C	-4.01413800	5.40641300	-1.11548400
C	-2.59435400	4.90788400	-1.25970500
C	-1.71541300	5.59555200	-0.22775300

C	-2.26976800	5.41826100	1.18670800
C	-1.62617700	6.35895900	2.20790700
O	-4.50686800	3.77875900	0.56820000
O	-4.85596800	4.77607600	-2.05972600
O	-2.20666200	5.20973400	-2.58308300
O	-3.65980500	5.80800800	1.21836600
O	-0.22606200	6.28298800	2.27817700
H	-1.67452900	6.67181000	-0.45734400
H	-5.50032300	5.57213500	0.45274600
H	-4.02575000	6.49252500	-1.27688100
H	-2.56552300	3.82600300	-1.07627500
H	-2.16640900	4.37136500	1.49008600
H	-1.96817400	7.37507100	1.96281100
H	-2.01097600	6.10151600	3.19637500
H	-4.30160700	4.60181600	-2.83216600
H	-1.39024000	4.71424100	-2.78875900
H	0.14483600	6.50681700	1.41639200
B	1.64247500	0.38378000	-1.09005900
B	1.12020700	-2.21284500	-2.19766100
B	0.85077600	-1.01586100	-3.48384700
B	1.16462800	0.58712400	-2.79280600
B	-0.06076100	-1.91410400	-0.90478000
B	-0.01307900	0.88128100	-1.50376700
B	-0.50448000	0.02347800	-2.98162800
B	-0.52866900	-1.71276600	-2.61103700
B	2.16740500	-0.78628500	-2.31485400
B	0.25590300	-0.31064400	-0.22060600
B	-1.06310000	-0.54019900	-1.39292500
B	1.60371700	-1.34797400	-0.72647000
H	-2.20552500	-0.43657200	-1.06375500
H	-0.49121700	-2.79710400	-0.23114400
H	0.04855000	-0.06732700	0.92600900
H	2.33766700	-1.83048500	0.07724300
H	2.43000900	1.10305000	-0.55064100
H	3.31726000	-0.84652500	-2.64557300
H	1.54453900	-3.30873600	-2.45015200
H	1.57935300	1.45768000	-3.50286700
H	1.06816100	-1.26087800	-4.62667000
H	-1.24686700	0.51267500	-3.77320400
H	-1.28089400	-2.46119300	-3.16160300
H	-0.43534600	1.96977100	-1.22168800

α-CD·$B_{12}F_{12}^{2-}$:

Atom	Coordinates (Angstroms)		
	X	Y	Z

C	4.45459800	2.86788300	-0.89536900
C	4.11754900	3.76256500	0.29130200
C	2.61527300	3.91389800	0.40275900
C	1.99899100	4.39823100	-0.90077400
C	2.46751800	3.53420300	-2.07699600
C	2.15024600	4.10390600	-3.45730900
O	4.66552800	3.22812800	1.47494600
O	2.38946000	4.81534400	1.46065200
O	0.59595100	4.25823000	-0.73634300
O	3.90896200	3.45729500	-2.06312900
O	0.78011300	4.15974400	-3.76411000
H	5.53667700	2.82889800	-1.05863400
H	4.55558800	4.75069700	0.09013900
H	2.17806100	2.93358100	0.61261400
H	2.26425100	5.45292500	-1.07025300
H	2.03696300	2.53291600	-1.97086400
H	2.62920100	5.09214800	-3.53348100
H	2.60966500	3.44561500	-4.19693700
H	4.02210600	3.40837100	2.17337300
H	1.43265600	4.86304000	1.62499900
H	0.31507600	4.72476600	-3.13465200
C	4.76083800	-2.43948000	-0.77138400
C	5.21390500	-1.68382100	0.47748200
C	4.60241600	-0.29900100	0.51122600
C	4.77598000	0.44556300	-0.80653600
C	4.37881600	-0.42151300	-2.00343500
C	4.77056000	0.13869600	-3.36930100
O	4.85810000	-2.41129700	1.63547800
O	5.22975100	0.38267100	1.56972500
O	3.93584900	1.59219300	-0.71223300
O	5.09692500	-1.67325100	-1.91559200
O	4.00518700	1.24165600	-3.78413000
H	5.30114800	-3.38748600	-0.87081100
H	6.30618100	-1.58317600	0.42462600
H	3.52662700	-0.40518800	0.68329400
H	5.82673200	0.75538200	-0.90224000
H	3.30037500	-0.60585200	-1.97511400
H	5.84789000	0.36665100	-3.35550300
H	4.59976500	-0.65116800	-4.10244700
H	4.53796900	-1.78188900	2.29820100
H	4.76200200	1.22219500	1.69560500
H	4.16106100	1.99658200	-3.20249700
C	0.25678600	-5.28714800	-0.90048100
C	1.20071100	-5.44625500	0.28525000
C	2.08339300	-4.22160300	0.39995100
C	2.81060600	-3.92762600	-0.90319500
C	1.82845100	-3.89789000	-2.07952900

C	2.48107700	-3.90722100	-3.45964100
O	0.46401100	-5.65787000	1.46814400
O	2.97775200	-4.48010800	1.45649800
O	3.39190300	-2.64347200	-0.73610100
O	1.03927300	-5.10667000	-2.06835500
O	3.21824100	-2.75037000	-3.76433300
H	-0.31827700	-6.20424100	-1.06566900
H	1.83723100	-6.31907000	0.08070500
H	1.45400200	-3.35277500	0.61267300
H	3.59069400	-4.68506200	-1.07424300
H	1.17794700	-3.02350200	-1.97226100
H	3.09471600	-4.81786000	-3.53699000
H	1.68143800	-3.97226100	-4.19978200
H	0.94138300	-5.19280100	2.16814600
H	3.49725300	-3.67566200	1.62314400
H	3.94024900	-2.63346900	-3.13444300
C	-4.49392600	-2.90155600	-0.77641800
C	-4.06709400	-3.67415600	0.47117000
C	-2.56182200	-3.83473200	0.50629000
C	-2.00113600	-4.35451100	-0.81138900
C	-2.55225900	-3.57466300	-2.00725800
C	-2.26100700	-4.19009900	-3.37440300
O	-4.52075400	-3.00531700	1.63034600
O	-2.28458400	-4.71987900	1.56374900
O	-0.58833500	-4.20051900	-0.71336300
O	-3.99567800	-3.57286200	-1.92107700
O	-0.92295900	-4.07588000	-3.78780400
H	-5.58492900	-2.89633000	-0.87777400
H	-4.52493500	-4.67078300	0.41552300
H	-2.11852900	-2.84915900	0.68044300
H	-2.25790500	-5.41921900	-0.90981100
H	-2.17399900	-2.54815000	-1.97559000
H	-2.60092200	-5.23754300	-3.36363300
H	-2.85973700	-3.64615900	-4.10664800
H	-3.81696800	-3.04709300	2.29425800
H	-1.32371100	-4.73299500	1.68989900
H	-0.34705400	-4.59057000	-3.20809600
C	-4.71132300	2.42329500	-0.89508300
C	-5.31725200	1.68393400	0.29183100
C	-4.69790200	0.30679500	0.40307500
C	-4.80981300	-0.46814100	-0.90092200
C	-4.29624900	0.36961600	-2.07725500
C	-4.63204000	-0.18964900	-3.45750200
O	-5.12766900	2.42609900	1.47513900
O	-5.36672700	-0.33961400	1.46027900
O	-3.98744000	-1.61357900	-0.73790100
O	-4.94969700	1.65677100	-2.06312300

O	-3.99438100	-1.40318000	-3.76609300
H	-5.21828700	3.38016300	-1.05756300
H	-6.39215700	1.56971400	0.09126000
H	-3.63036100	0.41746100	0.61391500
H	-5.85611900	-0.76522300	-1.06964600
H	-3.21370200	0.49678500	-1.97167100
H	-5.72736600	-0.27017000	-3.53238700
H	-4.29332400	0.53821200	-4.19706800
H	-4.95832900	1.77954400	2.17337100
H	-4.93044400	-1.19254500	1.62428500
H	-4.24938200	-2.08924100	-3.13679800
C	-0.26636900	5.34075300	-0.77375700
C	-1.14850400	5.35689800	0.47424600
C	-2.04293300	4.13555200	0.50845800
C	-2.77314700	3.91142700	-0.80951400
C	-1.82185600	3.99816200	-2.00513400
C	-2.50054800	4.05546500	-3.37215200
O	-0.34157200	5.41245100	1.63296700
O	-2.94837500	4.33948000	1.56547700
O	-3.34706400	2.61120800	-0.71194700
O	-1.09710600	5.24625800	-1.91829800
O	-3.07531000	2.84149500	-3.78488000
H	0.28359500	6.28309700	-0.87435400
H	-1.78100100	6.25300900	0.42005200
H	-1.41350200	3.25721300	0.68271200
H	-3.56618000	4.66684200	-0.90791500
H	-1.12313100	3.15634000	-1.97371900
H	-3.23469100	4.87624900	-3.36123800
H	-1.72955900	4.29896400	-4.10482300
H	-0.73010600	4.82406300	2.29676400
H	-3.44406300	3.51571600	1.68947400
H	-3.80865100	2.60222000	-3.20393800
B	0.90729900	0.48280100	4.04642000
B	0.03755300	1.01821100	1.35112600
B	-1.40737100	0.87414100	2.38536600
B	-0.87535100	0.53928900	4.04735000
B	0.86085200	-0.54412100	1.34873500
B	-0.03316100	-1.03261000	4.04499500
B	-1.46956800	-0.78974900	3.00430500
B	-0.90368100	-0.47584000	1.34943300
B	0.05163600	1.66298500	3.00659500
B	1.41489200	-0.88029100	3.00291800
F	-2.57434200	1.60020500	2.16156800
F	-2.67474200	-1.45374600	3.21929900
F	-1.60114400	0.99094200	5.12746700
F	0.07947200	3.03849700	3.22253300
F	0.08820300	1.80221800	0.21327600

F	-1.60678900	-0.82086300	0.20985200
F	2.59224700	-1.59272100	3.21718700
F	1.51282100	-0.97838200	0.20931500
F	-0.10047300	-3.03064900	2.15454400
F	2.67127500	1.42759900	2.15750500
F	1.66332900	0.88272900	5.12619000
F	-0.06153500	-1.88909900	5.12345500
B	-0.05667000	-1.65744300	2.38164800
B	1.46034500	0.77839100	2.38386100

β-CD·$B_{12}F_{12}^{2-}$:

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	3.73548500	4.52812200	1.06793900
C	4.84615900	4.43028700	0.02312600
C	4.84549800	3.04322100	-0.58577200
C	4.94457500	2.00105300	0.51451000
C	3.80278800	2.18666700	1.50676200
C	3.84625600	1.19515500	2.65420700
O	4.63543800	5.42163200	-0.96533400
O	5.93809500	2.97632000	-1.48946400
O	4.84467200	0.72262400	-0.08327800
O	3.90686100	3.52299200	2.04477400
O	5.15113100	1.02621000	3.15717300
C	-1.38390200	5.76752700	0.68471300
C	-0.46568600	6.42519800	-0.36339400
C	0.82033700	5.63687600	-0.57017300
C	1.41942800	5.20065600	0.75940800
C	0.37711700	4.44240700	1.56503900
C	0.88531500	3.85734900	2.87317200
O	-1.18384600	6.58604200	-1.57384800
O	1.73301700	6.43697900	-1.28177500
O	2.52349600	4.38824800	0.40447900
O	-0.67943100	5.38380800	1.84620300
O	1.81600700	4.68694600	3.54259300
C	-5.55055600	2.57088100	0.18884400
C	-5.50911400	3.79809300	-0.73134200
C	-4.08539100	4.31169500	-0.92446000
C	-3.31826300	4.32999500	0.39406400
C	-3.40333000	2.97470100	1.07915100
C	-2.62982800	2.86901100	2.38108800
O	-6.15841700	3.48436500	-1.93982700
O	-4.16297100	5.61841600	-1.45873200
O	-1.97827000	4.67554400	0.06660200

O	-4.79774300	2.75193100	1.35568000
O	-2.75642000	3.99486300	3.22630400
C	-5.37786900	-2.61811600	-0.09569600
C	-5.46711800	-2.07352500	-1.52205200
C	-5.06997900	-0.60141100	-1.56131900
C	-5.73014200	0.22721800	-0.45510900
C	-5.54152500	-0.47394500	0.89902200
C	-6.25505100	0.11981300	2.10051100
O	-4.65596700	-2.86011500	-2.37708500
O	-5.38047800	-0.02608700	-2.81171300
O	-5.07641900	1.48155500	-0.55315000
O	-6.07146400	-1.79920000	0.80505000
O	-5.82780100	-0.53943800	3.29071100
C	-1.36607200	-5.51287300	1.58956700
C	-2.44687200	-6.03751900	0.63958700
C	-3.06512600	-4.86448700	-0.09155700
C	-3.60373700	-3.86871400	0.91898100
C	-2.50716500	-3.46146200	1.89184800
C	-3.02243400	-2.52915700	2.97621500
O	-1.88300000	-6.95490900	-0.28163100
O	-4.07443100	-5.38034900	-0.94972200
O	-4.02395700	-2.69644700	0.23869300
O	-1.95181800	-4.63330100	2.51113100
O	-4.25684600	-2.94030900	3.52628200
C	3.75347100	-4.69124800	0.15230900
C	2.91427200	-5.61752500	-0.77262700
C	1.40549000	-5.66835100	-0.47234500
C	0.98130100	-5.24643200	0.93658200
C	1.85271000	-4.08301100	1.37698300
C	1.53628400	-3.45441600	2.71437100
O	3.14143400	-5.29426500	-2.12919800
O	0.95630900	-6.97595600	-0.75814700
O	-0.38455900	-4.87155200	0.82981500
O	3.18299600	-4.60834400	1.43143300
O	2.20067700	-2.20141000	2.84206600
C	6.03319000	0.02572500	-0.28710300
C	5.94135700	-0.66357900	-1.65330800
C	4.93210000	-1.79410200	-1.60346800
C	5.05685000	-2.68266500	-0.36584900
C	5.17475900	-1.83348600	0.89942400
C	5.44474800	-2.57617800	2.19600600
O	5.61291600	0.29173700	-2.64991400
O	5.06470400	-2.57000300	-2.77350500
O	3.85064100	-3.43487800	-0.43339500
O	6.25953500	-0.91592900	0.72998400
O	4.98960200	-1.82351300	3.31251300
H	3.78040600	5.48232300	1.60206800

H	5.80630200	4.59616100	0.52973800
H	3.89880500	2.89563500	-1.11546300
H	5.88803800	2.09204000	1.06357600
H	2.84261200	2.08647100	0.98612100
H	3.43909800	0.25312400	2.27768900
H	3.17365700	1.56352700	3.44060000
H	5.12142400	5.11448200	-1.73983000
H	5.83655200	2.16196600	-2.00995900
H	5.31495100	0.07253700	3.20647300
H	-2.14313900	6.48143800	1.02146600
H	-0.19858300	7.42693900	-0.01804100
H	0.58557100	4.71281000	-1.12358300
H	1.75393300	6.07255700	1.33348400
H	-0.02539000	3.62736600	0.95390200
H	1.31669700	2.87812600	2.64958600
H	0.02187800	3.69965600	3.52778000
H	-1.18182400	5.71899800	-1.99843200
H	2.57851500	5.96269600	-1.29062700
H	2.68376000	4.30383700	3.36396800
H	-6.58518500	2.39357700	0.50167100
H	-6.08208700	4.60077900	-0.25792200
H	-3.54838200	3.63443000	-1.60250000
H	-3.74840300	5.08605200	1.06272900
H	-3.04303200	2.19377000	0.40475600
H	-1.58417700	2.65774800	2.13874500
H	-3.01765800	1.99971300	2.91981900
H	-5.77973000	2.64511200	-2.23753100
H	-3.26441700	5.97051700	-1.50615800
H	-2.06044800	4.61417300	2.96884400
H	-5.84638800	-3.60335300	-0.03082500
H	-6.49584600	-2.17451700	-1.87778300
H	-3.99536800	-0.54307500	-1.37115800
H	-6.80226500	0.34919900	-0.67481100
H	-4.46634000	-0.51157600	1.10093900
H	-7.32615000	-0.07221100	2.00244600
H	-6.07297400	1.18835700	2.18669000
H	-3.73128800	-2.61712700	-2.20920000
H	-4.54281200	0.11348200	-3.26566500
H	-5.03955200	-0.08996200	3.60796200
H	-0.93147000	-6.32998700	2.17331400
H	-3.21415600	-6.53871600	1.24355200
H	-2.28381600	-4.37444700	-0.67883000
H	-4.43804500	-4.30079900	1.48317300
H	-1.71928900	-2.94648500	1.33861000
H	-3.08876000	-1.52764000	2.53770200
H	-2.27108800	-2.50339400	3.77122700
H	-2.47903200	-6.95195800	-1.04098500

H	-4.30111500	-4.68477800	-1.58744600
H	-4.95108400	-2.35213900	3.19912000
H	4.75317400	-5.11621900	0.29605700
H	3.28521100	-6.63486100	-0.62839300
H	0.91889600	-4.94181600	-1.13279800
H	1.09785100	-6.08610500	1.63331600
H	1.79910200	-3.29728700	0.61636700
H	1.90986600	-4.09139300	3.51932900
H	0.45424800	-3.33688000	2.81808000
H	2.64937500	-4.47691000	-2.28724800
H	-0.00991300	-6.96974100	-0.68069800
H	1.82791900	-1.61227200	2.17076700
H	6.88860000	0.70633500	-0.26281100
H	6.92458100	-1.07775900	-1.89787400
H	3.93226900	-1.34595100	-1.54164000
H	5.92361100	-3.35106600	-0.47653700
H	4.23698900	-1.28695900	1.00536600
H	6.52427300	-2.70237200	2.30650200
H	4.96078200	-3.55307000	2.18767200
H	4.67093200	0.20191800	-2.85481700
H	4.45163000	-3.30946900	-2.68133100
H	4.02125900	-1.91434000	3.31955500
B	0.79019200	-1.62255300	-1.66203400
B	-1.41105300	-0.04601300	-0.66400000
B	-1.39990900	0.05972700	-2.44734900
B	-0.03406300	-0.91317600	-3.06135900
B	0.08947200	0.68818000	-0.09106300
B	1.48230300	-0.17862600	-2.44918200
B	0.11454000	0.85521400	-2.95276900
B	-0.74189200	1.39139400	-1.48358400
B	-0.98581500	-1.47102900	-1.65155000
B	1.43655400	-0.29301300	-0.67792900
F	-2.57763300	0.17639500	-3.18094400
F	0.17958100	1.66573900	-4.05878000
F	-0.10841600	-1.58680000	-4.25552800
F	-1.84237200	-2.56081400	-1.79411900
F	-2.54247600	0.00977000	0.13775500
F	-1.35563500	2.62605500	-1.44841500
F	2.48537400	-0.51047800	0.20380500
F	0.17855400	1.28792100	1.15850100
F	1.82287500	2.37352000	-1.41262100
F	-0.01578800	-1.78206800	1.00407700
F	1.42494800	-2.85796700	-1.75260400
F	2.67156100	-0.22190500	-3.16682100
B	1.03595200	1.24318300	-1.47720800
B	-0.06033000	-1.08047100	-0.19794800

γ-CD·$B_{12}F_{12}^{2-}$:

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-3.30166700	6.23567500	0.61246900
C	-2.68429300	6.98963800	-0.56126100
C	-1.34355200	6.38208300	-0.90896900
C	-0.48060600	6.37136400	0.33625800
C	-1.16322700	5.59108200	1.45187300
C	-0.34658600	5.55969600	2.73678600
O	-3.57362000	4.93955100	0.18992900
O	-3.57263200	6.94090600	-1.66443300
O	-0.78485700	7.17986100	-1.93270300
O	-2.42372600	6.24407500	1.71712500
O	0.32586700	6.77701000	3.00613000
H	-0.31780700	7.39763700	0.68362900
H	-4.21470000	6.73320500	0.95233500
H	-2.52485700	8.03106700	-0.25398000
H	-1.48866200	5.34688100	-1.24564700
H	-1.34829800	4.56299800	1.12190200
H	-1.03225300	5.35108400	3.56340300
H	0.35457300	4.72596200	2.66535500
H	-3.03376400	7.13739400	-2.43973500
H	0.12713800	6.88397400	-2.08592800
H	1.23406800	6.65799900	2.70196800
C	1.92171500	6.48769800	0.21054400
C	2.81295000	6.32394000	-1.01724600
C	3.21555000	4.87137500	-1.17103200
C	3.86564300	4.42873400	0.12706200
C	2.90253500	4.61699700	1.28743400
C	3.50860200	4.13381200	2.59842100
O	0.75014600	5.77545500	-0.02743300
O	2.11623700	6.78336300	-2.16136300
O	4.09172600	4.81367800	-2.28425300
O	2.58125900	6.02144400	1.36774000
O	4.88511900	4.43505600	2.73571400
H	4.76111800	5.03323800	0.31997800
H	1.70404300	7.54432900	0.39138500
H	3.71989900	6.92328500	-0.86452300
H	2.32290800	4.25904000	-1.34470200
H	1.98468400	4.05298300	1.09809900
H	2.98598000	4.62357200	3.42334000
H	3.32537200	3.05716800	2.66839600
H	2.56239800	6.37232300	-2.91198300
H	4.20699800	3.87843800	-2.52412500

H	5.38172800	3.81806000	2.18427500
C	5.49826900	2.75809100	-0.36043300
C	5.36170400	1.62235900	-1.38277000
C	4.99752500	0.31771100	-0.69167900
C	5.90690000	0.07585900	0.50586500
C	5.84453000	1.27355100	1.44985800
C	6.72077000	1.11696600	2.68554300
O	4.20409100	3.05837900	0.07613400
O	4.39841600	1.98739800	-2.35513800
O	5.09096400	-0.75993700	-1.60501500
O	6.31369300	2.42894100	0.73921000
O	6.14357300	0.29557300	3.67261700
H	6.94106500	-0.07420700	0.17291400
H	5.95979800	3.63317300	-0.82388200
H	6.31213700	1.49118700	-1.90697600
H	3.97781700	0.39540700	-0.30126600
H	4.80677600	1.41919600	1.76874100
H	7.71242500	0.74863700	2.38109200
H	6.85570100	2.10550200	3.13165100
H	3.52085000	1.86485700	-1.95531100
H	4.19905600	-1.10688200	-1.72694000
H	5.67632100	-0.43755600	3.25523100
C	6.31398000	-2.08567200	1.58520500
C	6.64647300	-3.05598900	0.44217200
C	5.40973000	-3.84724000	0.04874200
C	4.71779900	-4.40071900	1.28499700
C	4.42259600	-3.29916500	2.29183300
C	3.70806500	-3.78131700	3.54553200
O	5.41588400	-1.07318200	1.16612400
O	7.23051400	-2.37441700	-0.64153900
O	5.79061400	-4.89507800	-0.81123900
O	5.69515400	-2.72803200	2.65892000
O	4.08820300	-5.08281200	3.96177700
H	5.35735800	-5.15340700	1.75931800
H	7.23495100	-1.63572700	1.97334300
H	7.39398400	-3.76228700	0.81838100
H	4.70071600	-3.16410600	-0.44289400
H	3.80282700	-2.52584900	1.83035400
H	3.93742800	-3.07441300	4.34658300
H	2.63398600	-3.73254500	3.34816400
H	6.51491300	-1.94106000	-1.13470400
H	5.02202100	-5.47443600	-0.91940700
H	3.37026200	-5.66519200	3.68865500
C	3.17172900	-6.27470400	1.24339000
C	2.68998000	-7.06342700	0.02736900
C	1.45858100	-6.39555600	-0.54670600
C	0.42345400	-6.23434200	0.54837700

C	0.99845600	-5.47462300	1.73144800
C	-0.02518500	-5.28748900	2.84302600
O	3.52940300	-5.00815400	0.79735000
O	3.73233700	-7.11937200	-0.92776100
O	0.99757400	-7.20962900	-1.61047100
O	2.14211500	-6.21218900	2.21115600
O	-0.85099900	-6.41499700	3.06578000
H	0.09142000	-7.22015200	0.89488500
H	4.01719700	-6.77313300	1.72573200
H	2.42049700	-8.07503000	0.35778400
H	1.73472000	-5.39711900	-0.91010000
H	1.32996600	-4.48744000	1.40476600
H	0.51245400	-5.08148900	3.77188400
H	-0.61922200	-4.40029000	2.59647200
H	3.30596600	-7.34680500	-1.76227200
H	0.27514400	-6.73796000	-2.05727100
H	-1.57878900	-6.37592800	2.43065100
C	-1.83952100	-6.20169700	-0.23473400
C	-2.36425100	-5.75095100	-1.61921500
C	-3.22909000	-4.49606200	-1.58697700
C	-4.06797900	-4.42331900	-0.32173300
C	-3.17079400	-4.62471500	0.88881100
C	-3.81565100	-4.34211000	2.23047000
O	-0.66490700	-5.49833700	0.02574900
O	-1.25936400	-5.59716600	-2.49811000
O	-4.05350900	-4.50289700	-2.72922900
O	-2.75662500	-6.00497000	0.81321100
O	-5.14848600	-4.81709700	2.32759700
H	-4.83324400	-5.20804000	-0.32619200
H	-1.63794600	-7.27632700	-0.25823200
H	-2.98195600	-6.55242800	-2.03015600
H	-2.57456200	-3.61175400	-1.57546000
H	-2.28562500	-3.98545900	0.80812000
H	-3.20505700	-4.81661700	3.00662000
H	-3.77276500	-3.26144900	2.38308900
H	-0.81481700	-4.78369600	-2.21588500
H	-4.72337800	-3.81536200	-2.59994500
H	-5.70354800	-4.02983400	2.34445100
C	-5.99533500	-3.01948200	0.05616700
C	-6.77506100	-2.27023300	-1.01904600
C	-6.28650200	-0.84263700	-1.13537300
C	-6.31370200	-0.20240600	0.23770400
C	-5.44928300	-1.01273300	1.20070400
C	-5.35467200	-0.40313700	2.58810600
O	-4.67803900	-3.14667200	-0.37120700
O	-6.63600500	-2.96071200	-2.24756700
O	-7.15559000	-0.19370900	-2.04295800

O	-6.06140200	-2.31987500	1.28133500
O	-6.57158500	0.17370300	3.03461000
H	-7.33912200	-0.19819600	0.62434900
H	-6.43924700	-4.00085500	0.23994700
H	-7.83053000	-2.24387800	-0.71732900
H	-5.25116000	-0.83776400	-1.50102600
H	-4.43635000	-1.12189100	0.79868800
H	-5.06032700	-1.19363800	3.28477700
H	-4.55206000	0.33874100	2.56497600
H	-6.92541500	-2.34124100	-2.92708100
H	-7.02044900	0.76306800	-1.96170900
H	-6.45238900	1.12821600	2.96959200
C	-6.59991500	2.15336600	0.65269100
C	-6.80087400	3.25501800	-0.38523100
C	-5.47999900	3.90959900	-0.72369000
C	-4.81475400	4.36437500	0.55880400
C	-4.62892800	3.17706300	1.49346300
C	-3.92106400	3.53876300	2.78871200
O	-5.85763900	1.12980000	0.06949300
O	-7.40652700	2.70128200	-1.54020200
O	-5.76782400	4.98971200	-1.58861300
O	-5.95002000	2.67503500	1.79069700
O	-4.32139300	4.79020600	3.31887400
H	-5.44195600	5.10801700	1.06313500
H	-7.56517900	1.77804600	1.00273900
H	-7.45739200	4.01689900	0.05482000
H	-4.82497200	3.17588500	-1.21262500
H	-4.05659600	2.39110600	0.99539900
H	-4.14157000	2.75976400	3.52330000
H	-2.84424600	3.50959200	2.59883600
H	-7.27605600	3.35385300	-2.23801600
H	-4.95398400	5.50389900	-1.71342600
H	-3.65595400	5.43172200	3.04199500
B	0.75141500	-1.34086600	1.12223500
B	0.93528900	1.04665900	-0.46676600
B	0.15867100	1.46749800	1.07443000
B	0.04666500	-0.00751000	2.06614800
B	-0.12631500	-0.09010900	-1.33684800
B	-1.01038400	-1.15007300	1.19917200
B	-1.37120900	0.58210600	1.17050300
B	-0.83302900	1.25162600	-0.39023700
B	1.47641100	0.28093200	1.04732900
B	-0.23879600	-1.57506400	-0.34673400
F	0.30006200	2.72366000	1.65488900
F	-2.47396800	1.10086700	1.83814000
F	0.11118700	0.02892800	3.43798900
F	2.72059800	0.56010800	1.59285900

F	1.77545500	1.93293500	-1.15345700
F	-1.48715900	2.33276600	-0.94903400
F	-0.40359500	-2.82503300	-0.93309800
F	-0.16353900	-0.13526900	-2.71052800
F	-2.80679700	-0.66421600	-0.83396900
F	2.40548400	-1.21792300	-1.10404500
F	1.41044600	-2.38883200	1.74885800
F	-1.82617000	-2.04198400	1.88267700
B	-1.55694500	-0.37819800	-0.31414100
B	1.29533500	-0.69064800	-0.43681800