Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information

Encapsulation of *closo*-dodecaiododododecaborate in 2-hydroxypropyl-γ-cyclodextrin prevents hemolysis

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CONTENTS

Experimental methods

General methods. $Na_2B_{12}I_{12}$ was obtained from Katchem, γ-cyclodextrin (γ-CD) was obtained from Combi-Blocks, 2-hydroxypropyl-γ-cyclodextrin (HP-γ-CD; 0.6 functionalized, average M_w = 1580 Da) was obtained from Sigma-Aldrich, phosphate-buffered saline (PBS) was obtained from Fisher Scientific. These reagents were used as received. D_2O was obtained from Cambridge Isotopes. Washed single-donor human red blood cells (RBCs) were obtained from Innovative Research. These are RBCs that have been separated from type O positive whole blood and resuspended in Alsever's Solution. Defibrinated bovine blood was obtained from HemoStat Laboratories. All manipulations were performed under ambient conditions. NMR spectra were collected using a Bruker Avance III HD 500 spectrometer equipped with a multinuclear Smart Probe. The frequencies of the ^1H and ^{11}B NMR signals are reported in ppm as chemical shifts from TMS and $BF_3{\cdot}Et_2O$, respectively. Electronic absorption spectra were recorded on VWR UV-6300PC double beam spectrophotometer.

Stability of $Na_2B_{12}I_{12}$: refluxing PBS. A 500 µL aliquot of a 10 mM solution of $Na_2B_{12}I_{12}$ in PBS (pH 7.4) was placed in an oil bath pre-heated to 100 °C. After incubating in this bath for 1 h, the sample was removed, cooled to room temperature, and spiked with 50 µL D_2O prior to acquiring a ^{11}B NMR spectrum.

Stability of $Na_2B_{12}I_{12}$: human RBCs. A 275 µL aliquot of a 20 mM solution of $Na_2B_{12}I_{12}$ in PBS (pH 7.4) was added to a 225 µL suspension of human RBCs. The mixture was allowed to stand at room temperature for 24 h. It was then spiked with 50 µL D_2O prior to acquiring a ^{11}B NMR spectrum.

Stability of $Na_2B_{12}I_{12}$: bovine serum. A 1 mL aliquot of defibrinated bovine blood was centrifuged for 15 s at 15,850 × g. A 225 µL aliquot of the serum supernatant was combined with a 275 µL aliquot of a 20 mM solution of $Na_2B_{12}I_{12}$ in PBS (pH 7.4). The mixture was allowed to stand at room temperature for 24 h. It was then spiked with 50 µL D_2O prior to acquiring a ^{11}B NMR spectrum.

Stability of $Na_2B_{12}I_{12}$: bovine blood. A 225 µL aliquot of defibrinated bovine blood was combined with a 275 µL aliquot of a 20 mM solution of $Na_2B_{12}I_{12}$ in PBS (pH 7.4). The mixture was allowed to stand at room temperature for 24 h. It was then spiked with 50 µL D_2O prior to acquiring a ^{11}B NMR spectrum.

Job plot of HP-γ-CD and $Na_2B_{12}I_{12}$. Solutions of $Na_2B_{12}I_{12}$ (20 mM) and HP-γ-CD (20 mM) were prepared in PBS (pH 7.4). Aliquots of these solutions were combined and diluted as needed with PBS to afford 500 µL solutions that varied continuously in concentration of $Na_2B_{12}I_{12}$ and HP-γ-CD from 0 to 10 mM, under the constraint that their molar concentrations summed to 10 mM. Each sample was spiked with D_2O and analyzed by ^{11}B NMR spectroscopy.

Hemolytic activity of $Na_2B_{12}I_{12}$. A 200 mM solution of $Na_2B_{12}I_{12}$ was prepared in PBS (pH 7.4). Aliquots of this solution were diluted to a target concentration of 10-100 mM by dilution with PBS to give a final volume of 250 µL. A 1 mL aliquot of a suspension of human RBCs was pelleted (15 s at 15,850 × g), the supernatant was discarded, and the cells were resuspended to a volume of 1 mL with fresh PBS. The cells were pelleted again and were washed a total of three times in this manner and resuspended in a final volume of 1 mL of PBS. A 10 µL aliquot of freshly resuspended RBCs was added to one of the 250 µL solutions of $Na_2B_{12}I_{12}$. The mixture was vortexed for 10 s and then pelleted by centrifugation at 15,850 × g for 10 s. A 200 µL aliquot of the supernatant was removed and diluted with 550 µL of PBS. The absorbance of this solution was measured from 700 to 350 nm. The subsequent samples were then

measured in turn. Three independent replicates were obtained for each concentration of hemolytic agents and the data were modeled using logistic regression. The absorbance corresponding to 100% lysis was confirmed by adding a 10 µL aliquot of freshly resuspended RBCs to 250 µL of hemolysis buffer (0.15 M NH_4Cl and 10 mM $KHCO_3$). The sample was then processed identically to the borate-treated samples.

Hemolytic activity of $Na_2B_{12}I_{12}$ in the presence of HP-γ-CD. Solutions of $Na_2B_{12}I_{12}$ (200 mM) and HP-γ-CD (200 mM) were prepared in PBS (pH 7.4). Aliquots of these stock solutions were combined, diluting with PBS, if necessary, to give 250 µL solutions that were 100 mM in $Na_2B_{12}I_{12}$ and varied in HP-γ-CD concentration from 0 to 40 mM. A 1 mL aliquot of a suspension of human RBCs was pelleted (15 s at 15,850 × g), the supernatant was discarded, and the cells were resuspended to a volume of 1 mL with fresh PBS. The cells were pelleted again and were washed a total of three times in this manner and resuspended in a final volume of 1 mL of PBS. A 10 µL aliquot of freshly resuspended RBCs was added to one of the 250 µL solutions of $Na_2B_{12}I_{12}$ with or without HP-γ-CD. The mixture was vortexed for 10 s and then pelleted by centrifugation at 15,850 × g for 10 s. A 200 µL aliquot of the supernatant was removed and diluted with 550 µL of PBS. The absorbance of this solution was measured from 700 to 350 nm. The subsequent samples were then measured in turn.

Extended exposure hemolytic activity of $Na_2B_{12}I_{12}$ in the presence of 0.5 equiv HP-γ-CD. Solutions of $Na_2B_{12}I_{12}$ (200 mM) and HP-γ-CD (200 mM) were prepared in PBS (pH 7.4). Aliquots of these stock solutions were combined and diluted with PBS to give 250 µL solutions that were 100 mM in $Na_2B_{12}I_{12}$ and 50 mM in HP-γ-CD. A 1 mL aliquot of a suspension of human RBCs was pelleted (15 s at 15,850 × g), the supernatant was discarded, and the cells were resuspended to a volume of 1 mL with fresh PBS. The cells were pelleted again and were washed a total of three times in this manner and resuspended in a final volume of 1 mL of PBS. A 10 µL aliquot of freshly resuspended RBCs was added to each of two 250 µL solutions of $Na_2B_{12}I_{12}$ and HP-γ-CD. The mixtures were vortexed and then incubated at room temperature for either 4 h or 24 h. After the prescribed time, the samples were pelleted by centrifugation at 15,850 × g for 10 s. A 200 µL aliquot of the supernatant was removed and diluted with 550 µL of PBS. The absorbance of this solution was measured from 700 to 350 nm.

Crystallography: Complex of $Na_2B_{12}I_{12}$ and γ-CD. Crystals were obtained by allowing diethyl ether to diffuse in the vapor phase into a 0.5 mL DMF solution containing $Na_2B_{12}I_{12}$ (10 mg, 5.9 µmol) and γ-CD (15 mg, 11.8 µmol). Over the course of 3 d, colorless crystals formed. Microscopic analysis of these crystals between crossed polarizers revealed them to remain perpetually extinguished regardless of orientation. A single-crystal sample was coated in Paratone oil and mounted on a MiTeGen polyimide loop and cooled to 100 K on a Rigaku Synergy-S X-ray diffractometer. Diffraction of Cu Kα radiation from a PhotonJet-S microfocus source was detected using a HyPix-6000HE hybrid photon counting detector, but reflections were only observed to a resolution of 1.5 Å and a satisfactory solution could not be obtained by direct methods, intrinsic phasing, Patterson methods, or charge flipping. The indexing of the pattern showed it to have cubic metric symmetry (consistent with the optical behavior) with a = 60.0168(13) Å. To corroborate the composition of the crystals, a portion was collected, dissolved in 550 µL of DMSO-d_6, and analyzed by ^1H and ^{11}B NMR spectroscopy. The density of these crystals was measured by isopycnic flotation: bromoform and hexanes were mixed until a ratio was achieved where 1 mg of microcrystalline $Na_2B_{12}I_{12}$/γ-CD complex would remain suspended without sinking or rising. The entire microcrystalline sample achieved isopycnic flotation at the same bromoform:hexanes ratio. The mass of 250 µL of the solvent mixture was measured to determine its density.

Crystallography: $Na_2B_{12}I_{12}\cdot 6DMF\cdot H_2O$. Crystals were obtained by allowing diethyl ether to diffuse into a DMF solution of the compound. A platy crystal was selected, mounted on a MiTeGen polyimide loop, and cooled to 100 K on a Rigaku Synergy-S X-ray diffractometer. Diffraction of Mo Kα radiation from a PhotonJet-S microfocus source was detected using a HyPix-6000HE hybrid photon counting detector. Screening, indexing, data collection, and data processing were performed with CrysAlis^{Pro}.[1] The structure was solved using SHELXT and refined using SHELXL following established strategies.[2-4] All non-H atoms were refined anisotropically. Carbon-bound H atoms were placed at calculated positions and refined with a riding model and coupled isotropic displacement parameters (1.2 × U_{eq} for DMF amide CHO groups and 1.5 × U_{eq} for methyl groups). The calculated density of these crystals was obtained by dividing the mass of the unit cell contents by the unit cell volume.

Computational experiments. All calculations were performed in the gas phase using the PM6 semi-empirical method with Gaussian 16.[5] The input geometry for the $[(\gamma\text{-CD})_2(B_{12}I_{12})]^{2-}$ complex was generated from the previously reported coordinates of $[(\gamma\text{-CD})_2(B_{12}Br_{12})]^{2-}$.[6] The input geometry for the $[(\gamma\text{-CD})(B_{12}I_{12})]^{2-}$ complex was obtained by removing one of the rings from the optimized geometry of the $[(\gamma\text{-CD})_2(B_{12}I_{12})]^{2-}$. The input geometry for the $[(HP\text{-}\gamma\text{-CD})(B_{12}I_{12})]^{2-}$ complex was generated by adding 2-hydroxypropyl groups to the O6 positions of alternating glucose units. In all cases, geometry optimizations were performed under the constraint that C_2 symmetry be maintained.

References

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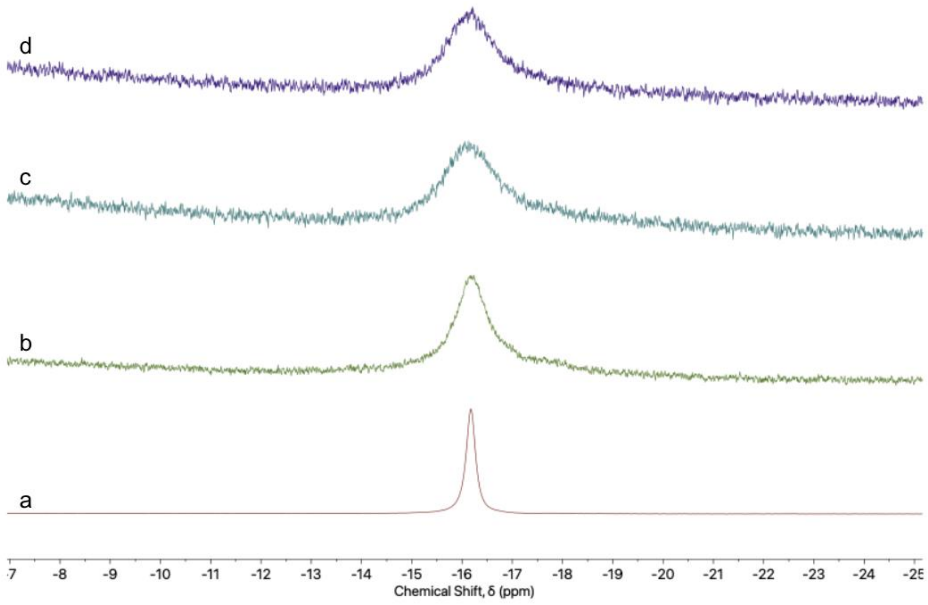

Figure S1. Stacked ^{11}B NMR spectra (160 MHz) of $Na_2B_{12}I_{12}$ in a) 10:1 PBS:D_2O after heating at 100 °C for 1 h; b) RBC suspension with 9% D_2O after incubating at room temperature for 24 h; c) defibrinated bovine blood with 9% D_2O after incubating at room temperature for 24 h; d) bovine serum with 9% D_2O after incubating at room temperature for 24 h. Spectra b-d are broadened from sample viscosity and paramagnetic impurities, but no additional signals appear.

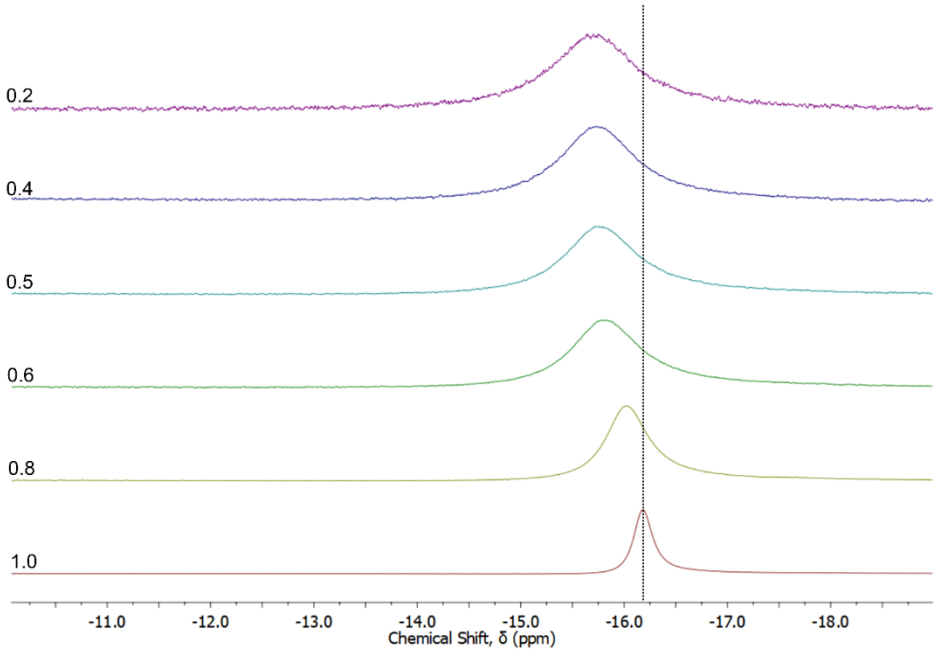

Figure S2. Stacked ^{11}B NMR spectra (10:1 PBS:D_2O, 160 MHz) of mixtures of $Na_2B_{12}I_{12}$ and HP-γ-CD with a combined concentration of 10 mM. Indicated next to each trace is the mole fraction of $Na_2B_{12}I_{12}$. Dotted line marks the position of the unperturbed $Na_2B_{12}I_{12}$.

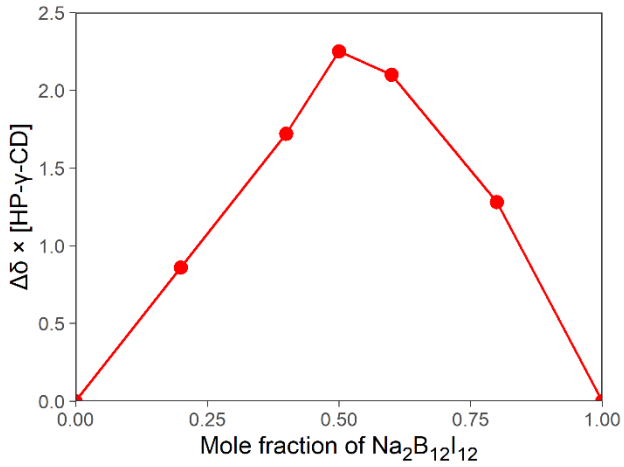

Figure S3. Job plot for the interaction of $Na_2B_{12}I_{12}$ and HP-γ-CD based on the NMR spectra in Figure S2.

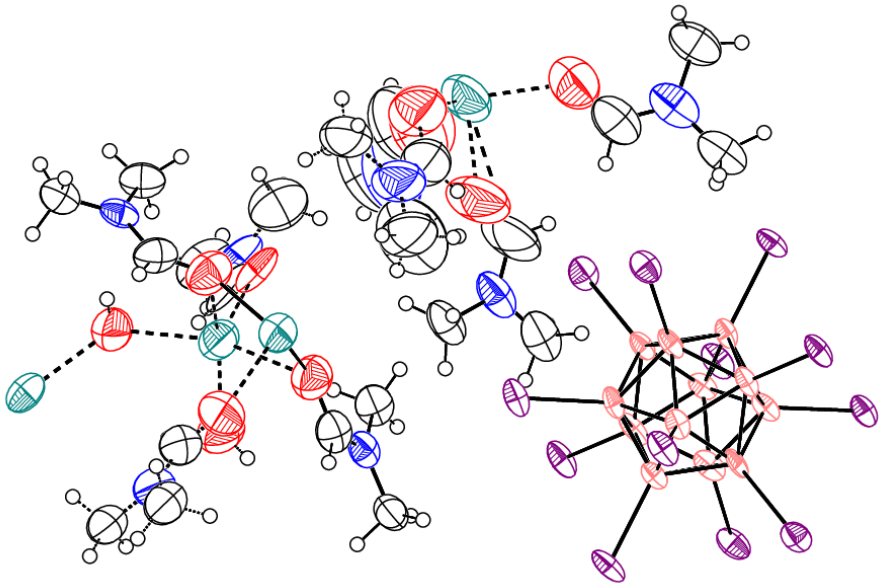

Figure S4. Thermal ellipsoid plot (50% probability level) of $Na_2B_{12}I_{12}$·6DMF·H_2O. Color code: B pink, I purple, Na teal, N blue, O red, C grey, H white spheres of arbitrary radius.

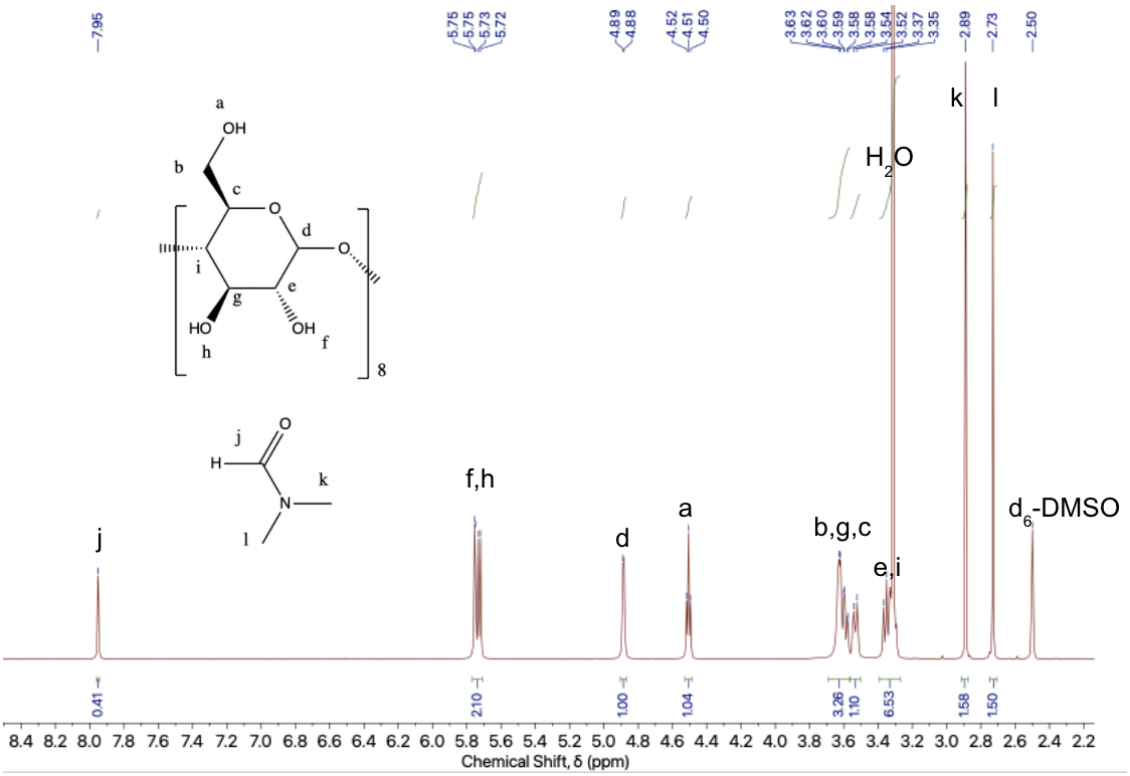

Figure S5. ^{1}H NMR spectrum (d_6-DMSO, 500 MHz) of dissolved of $Na_2B_{12}I_{12}$/γ-CD crystals.

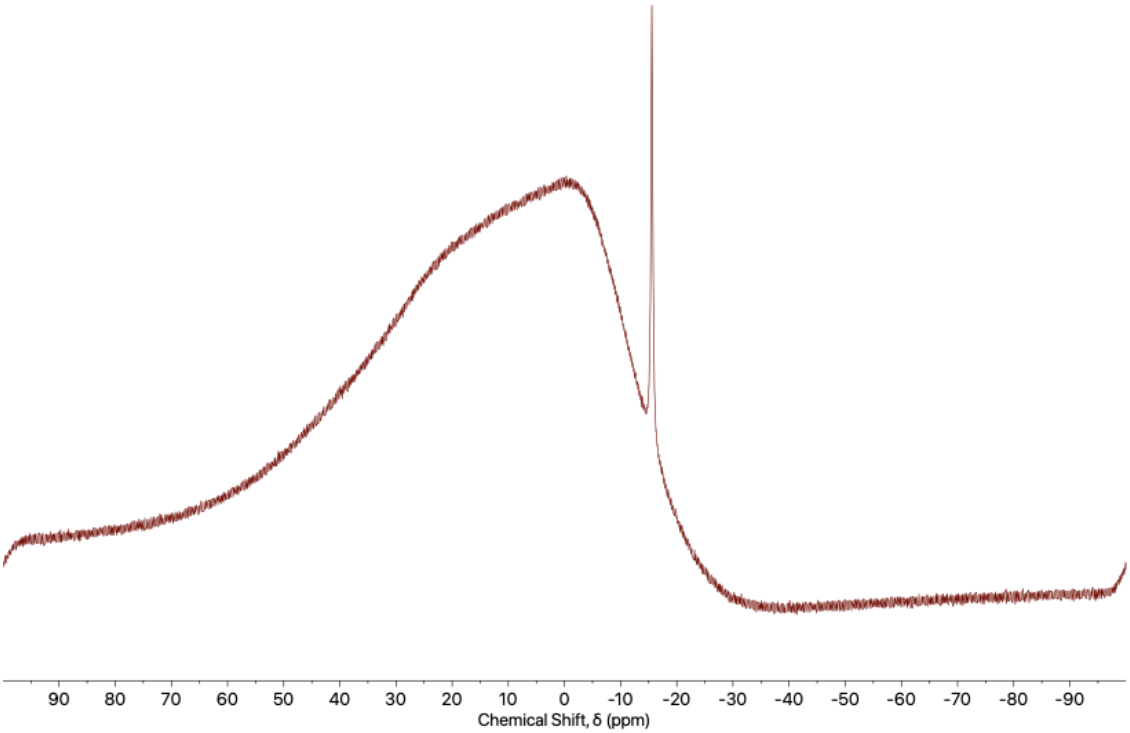

Figure S6. ^{11}B NMR spectrum (d_6-DMSO, 160 MHz) of complex of dissolved of $Na_2B_{12}I_{12}$/γ-CD crystals.

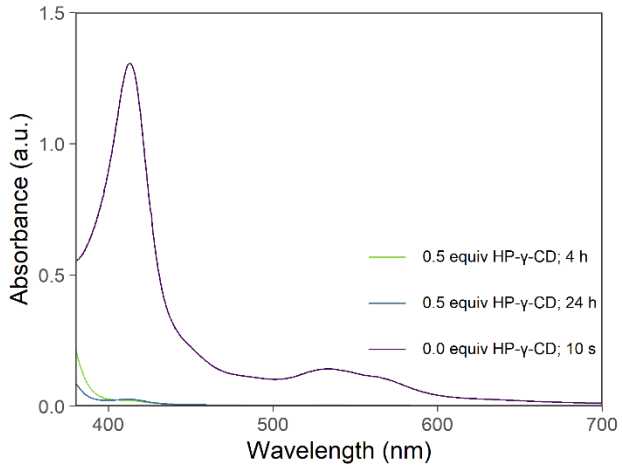

Figure S7. Hb release from RBCs suspended for extended periods (4 h or 24 h) in PBS (pH 7.4) containing 100 mM $Na_2B_{12}I_{12}$ and 50 mM HP-γ-CD. Hb release within 10 s in the absence of HP-γ-CD (reproduced from Figure 5) included for reference.

Table S1. Crystallographic details.

Compound	$Na_2[(\gamma\text{-CD})_2(B_{12}I_{12})]$ [a]	$Na_2B_{12}I_{12}\cdot 6DMF\cdot H_2O$
Empirical formula	-	$C_{18}H_{44}B_{12}I_{12}N_6Na_2O_7$
Formula weight	-	2155.09
Temperature (K)	100(2)	100(2)
Wavelength (Å)	1.54184	0.71073
Crystal system	Cubic	Orthorhombic
Space group	-	*Pbcn*
a (Å)	60.0168(13)	28.8693(6)
b (Å)		22.9629(4)
c (Å)		19.7457(3)
Volume (Å^3)	216181(8)	13089.9(4)
Z	-	8
ρ_{calc} (Mg/m^3)	-	2.187
Crystal size (mm^3)	0.18 × 0.18 × 0.14	0.22 × 0.19 × 0.04
θ range (°)	2.442 to 30.917	2.170 to 25.681
Reflections collected	27417	174695
Independent reflections	5247	12413
Parameters	-	627
Completeness (%)	99.8	99.9
R_{int}	0.0661	0.0623
R_1 (I > 2σ)	-	0.0589
R_1 (all data)	-	0.0767
wR_2 (I > 2σ)	-	0.1497
wR_2 (all data)	-	0.1659
Goodness of fit, *S*	-	1.119

[a] No solved or refined structure; data collection and unit cell parameters only. Compound name based on tentative assignment of identity.

Table S2. Cartesian coordinates (Å) of the optimized (PM6) structure of the $[(\gamma\text{-CD})_2(B_{12}I_{12})]^{2-}$ complex.

O	5.044700	2.653600	3.033900	O	5.044700	2.653600	3.033900	O	-4.450000	-2.811600	6.310500	O	-4.450000	-2.811600	6.310500
O	6.778100	1.896100	1.200700	O	6.778100	1.896100	1.200700	H	-4.989700	-2.105800	5.849400	H	-4.989700	-2.105800	5.849400
O	6.759600	-1.122400	1.262500	O	6.759600	-1.122400	1.262500	O	-3.324300	-5.327800	4.899100	O	-3.324300	-5.327800	4.899100
O	4.494700	-2.064600	2.721000	O	4.494700	-2.064600	2.721000	O	-6.414300	-5.084100	2.303700	O	-6.414300	-5.084100	2.303700
O	5.575500	0.981200	4.509100	O	5.575500	0.981200	4.509100	H	-6.533700	-5.499800	1.393400	H	-6.533700	-5.499800	1.393400
O	4.534400	-1.696700	5.826800	O	4.534400	-1.696700	5.826800	C	1.705000	-7.512700	2.545900	C	1.705000	-7.512700	2.545900
H	4.331900	-2.460500	5.219500	H	4.331900	-2.460500	5.219500	H	2.603100	-8.165300	2.579700	H	2.603100	-8.165300	2.579700
O	5.004400	-3.240500	0.497600	O	5.004400	-3.240500	0.497600	C	0.671700	-7.909700	1.467800	C	0.671700	-7.909700	1.467800
O	3.051800	-6.361200	5.507200	O	3.051800	-6.361200	5.507200	H	0.550000	-9.022900	1.453900	H	0.550000	-9.022900	1.453900
H	2.459700	-6.985900	5.002800	H	2.459700	-6.985900	5.002800	C	-0.695500	-7.229900	1.681800	C	-0.695500	-7.229900	1.681800
O	4.450000	-3.978500	4.001900	O	4.450000	-3.978500	4.001900	H	-0.703200	-6.178400	1.289500	H	-0.703200	-6.178400	1.289500
O	4.695100	-6.431200	0.978300	O	4.695100	-6.431200	0.978300	C	-1.170900	-7.263500	3.154900	C	-1.170900	-7.263500	3.154900
H	4.902800	-6.344800	0.006100	H	4.902800	-6.344800	0.006100	H	-1.630500	-8.244700	3.405600	H	-1.630500	-8.244700	3.405600
C	6.115900	1.829100	3.492300	C	6.115900	1.829100	3.492300	C	-0.053400	-6.867900	4.136800	C	-0.053400	-6.867900	4.136800
H	6.898600	2.409300	4.027500	H	6.898600	2.409300	4.027500	H	0.195500	-5.788400	4.010600	H	0.195500	-5.788400	4.010600
C	6.686800	0.997600	2.308400	C	6.686800	0.997600	2.308400	C	-0.291500	-7.268300	5.608300	C	-0.291500	-7.268300	5.608300
H	7.732900	0.683800	2.554400	H	7.732900	0.683800	2.554400	H	-0.194500	-8.366400	5.737900	H	-0.194500	-8.366400	5.737900
C	5.845600	-0.240200	1.944000	C	5.845600	-0.240200	1.944000	H	0.436100	-6.763200	6.272400	H	0.436100	-6.763200	6.272400
H	4.992300	0.026300	1.250900	H	4.992300	0.026300	1.250900	C	-3.331400	-6.403900	3.984000	C	-3.331400	-6.403900	3.984000
C	5.341600	-0.958000	3.208000	C	5.341600	-0.958000	3.208000	H	-3.248700	-7.304100	4.636300	H	-3.248700	-7.304100	4.636300
H	6.176100	-1.395100	3.804800	H	6.176100	-1.395100	3.804800	C	-4.555400	-6.401600	3.041400	C	-4.555400	-6.401600	3.041400
C	4.541900	0.038900	4.057800	C	4.541900	0.038900	4.057800	H	-5.417500	-6.940800	3.508400	H	-5.417500	-6.940800	3.508400
H	3.784300	0.615900	3.450800	H	3.784300	0.615900	3.450800	C	-5.015000	-4.993800	2.598100	C	-5.015000	-4.993800	2.598100
C	3.912500	-0.508200	5.343000	C	3.912500	-0.508200	5.343000	H	-4.445800	-4.646800	1.696200	H	-4.445800	-4.646800	1.696200
H	4.057900	0.208300	6.181500	H	4.057900	0.208300	6.181500	C	-4.910900	-3.938500	3.716700	C	-4.910900	-3.938500	3.716700
H	2.829900	-0.695300	5.182600	H	2.829900	-0.695300	5.182600	H	-5.709500	-4.065600	4.480500	H	-5.709500	-4.065600	4.480500
C	5.116300	-3.380400	2.923800	C	5.116300	-3.380400	2.923800	C	-3.268700	-3.088800	5.565600	C	-3.268700	-3.088800	5.565600
H	6.150000	-3.237500	3.322700	H	6.150000	-3.237500	3.322700	H	-2.627600	-3.618900	6.301800	H	-2.627600	-3.618900	6.301800
C	5.090000	-4.155100	1.587300	C	5.090000	-4.155100	1.587300	H	-2.785500	-2.139200	5.259600	H	-2.785500	-2.139200	5.259600
H	6.098700	-4.626700	1.430300	H	6.098700	-4.626700	1.430300	C	-3.503800	-3.986900	4.340700	C	-3.503800	-3.986900	4.340700
C	4.012200	-5.254100	1.446600	C	4.012200	-5.254100	1.446600	H	-2.714100	-3.825700	3.557100	H	-2.714100	-3.825700	3.557100
H	3.217500	-4.949900	0.704500	H	3.217500	-4.949900	0.704500	O	-5.044700	-2.653600	3.033900	O	-5.044700	-2.653600	3.033900
C	3.353100	-5.726600	2.755300	C	3.353100	-5.726600	2.755300	O	-6.778100	-1.896100	1.200700	O	-6.778100	-1.896100	1.200700
H	3.923600	-6.576400	3.199500	H	3.923600	-6.576400	3.199500	O	-6.759600	1.122400	1.262500	O	-6.759600	1.122400	1.262500
C	2.739900	-5.009000	5.187500	C	2.739900	-5.009000	5.187500	O	-4.494700	2.064600	2.721000	O	-4.494700	2.064600	2.721000
H	3.337200	-4.435800	5.934300	H	3.337200	-4.435800	5.934300	O	-5.575500	-0.981200	4.509100	O	-5.575500	-0.981200	4.509100
H	1.663000	-4.822300	5.351200	H	1.663000	-4.822300	5.351200	O	-4.534400	1.696700	5.826800	O	-4.534400	1.696700	5.826800
C	3.146200	-4.588900	3.763500	C	3.146200	-4.588900	3.763500	H	-4.331900	2.460500	5.219500	H	-4.331900	2.460500	5.219500
H	2.444900	-3.810700	3.353600	H	2.444900	-3.810700	3.353600	O	-5.004400	3.240500	0.497600	O	-5.004400	3.240500	0.497600
O	-2.012300	6.140600	2.356400	O	-2.012300	6.140600	2.356400	O	-3.051800	6.361200	5.507200	O	-3.051800	6.361200	5.507200
O	-1.170900	7.615800	0.176800	O	-1.170900	7.615800	0.176800	H	-2.459700	6.985900	5.002800	H	-2.459700	6.985900	5.002800
O	1.713300	7.981200	1.010700	O	1.713300	7.981200	1.010700	O	-4.450000	3.978500	4.001900	O	-4.450000	3.978500	4.001900
H	1.436000	8.245600	0.071700	H	1.436000	8.245600	0.071700	O	-4.695100	6.431200	0.978300	O	-4.695100	6.431200	0.978300
O	2.175600	6.220900	3.143000	O	2.175600	6.220900	3.143000	H	-4.902800	6.344800	0.006100	H	-4.902800	6.344800	0.006100
O	-1.138400	7.660800	3.851800	O	-1.138400	7.660800	3.851800	C	-6.115900	-1.829100	3.492300	C	-6.115900	-1.829100	3.492300
O	4.261300	7.192900	1.887400	O	4.261300	7.192900	1.887400	H	-6.898600	-2.409300	4.027500	H	-6.898600	-2.409300	4.027500
H	3.284000	7.105100	1.622400	H	3.284000	7.105100	1.622400	C	-6.686800	-0.997600	2.308400	C	-6.686800	-0.997600	2.308400
O	4.450000	2.811600	6.310500	O	4.450000	2.811600	6.310500	H	-7.732900	-0.683800	2.554400	H	-7.732900	-0.683800	2.554400
H	4.989700	2.105800	5.849400	H	4.989700	2.105800	5.849400	C	-5.845600	0.240200	1.944000	C	-5.845600	0.240200	1.944000
O	3.324300	5.327800	4.899100	O	3.324300	5.327800	4.899100	H	-4.992300	-0.026300	1.250900	H	-4.992300	-0.026300	1.250900
O	6.414300	5.084100	2.303700	O	6.414300	5.084100	2.303700	C	-5.341600	0.958000	3.208000	C	-5.341600	0.958000	3.208000
H	6.533700	5.499800	1.393400	H	6.533700	5.499800	1.393400	H	-6.176100	1.395100	3.804800	H	-6.176100	1.395100	3.804800
C	-1.705000	7.512700	2.545900	C	-1.705000	7.512700	2.545900	C	-4.541900	-0.038900	4.057800	C	-4.541900	-0.038900	4.057800
H	-2.603100	8.165300	2.579700	H	-2.603100	8.165300	2.579700	H	-3.784300	-0.615900	3.450800	H	-3.784300	-0.615900	3.450800
C	-0.671700	7.909700	1.467800	C	-0.671700	7.909700	1.467800	C	-3.912500	0.508200	5.343000	C	-3.912500	0.508200	5.343000
H	-0.550000	9.022900	1.453900	H	-0.550000	9.022900	1.453900	H	-4.057900	-0.208300	6.181500	H	-4.057900	-0.208300	6.181500
C	0.695500	7.229900	1.681800	C	0.695500	7.229900	1.681800	H	-2.829900	0.695300	5.182600	H	-2.829900	0.695300	5.182600
H	0.703200	6.178400	1.289500	H	0.703200	6.178400	1.289500	C	-5.116300	3.380400	2.923800	C	-5.116300	3.380400	2.923800
C	1.170900	7.263500	3.154900	C	1.170900	7.263500	3.154900	H	-6.150000	3.237500	3.322700	H	-6.150000	3.237500	3.322700
H	1.630500	8.244700	3.405600	H	1.630500	8.244700	3.405600	C	-5.090000	4.155100	1.587300	C	-5.090000	4.155100	1.587300
C	0.053400	6.867900	4.136800	C	0.053400	6.867900	4.136800	H	-6.098700	4.626700	1.430300	H	-6.098700	4.626700	1.430300
H	-0.195500	5.788400	4.010600	H	-0.195500	5.788400	4.010600	C	-4.012200	5.254100	1.446600	C	-4.012200	5.254100	1.446600
C	3.331400	6.403900	3.984000	C	3.331400	6.403900	3.984000	H	-3.217500	4.949900	0.704500	H	-3.217500	4.949900	0.704500
H	3.248700	7.304100	4.636300	H	3.248700	7.304100	4.636300	C	-3.353100	5.726600	2.755300	C	-3.353100	5.726600	2.755300
C	4.555400	6.401600	3.041400	C	4.555400	6.401600	3.041400	H	-3.923600	6.576400	3.199500	H	-3.923600	6.576400	3.199500
H	5.417500	6.940800	3.508400	H	5.417500	6.940800	3.508400	C	-2.739900	5.009000	5.187500	C	-2.739900	5.009000	5.187500
C	5.015000	4.993800	2.598100	C	5.015000	4.993800	2.598100	H	-3.337200	4.435800	5.934300	H	-3.337200	4.435800	5.934300
H	4.445800	4.646800	1.696200	H	4.445800	4.646800	1.696200	H	-1.663000	4.822300	5.351200	H	-1.663000	4.822300	5.351200
C	4.910900	3.938500	3.716700	C	4.910900	3.938500	3.716700	C	-3.146200	4.588900	3.763500	C	-3.146200	4.588900	3.763500
H	5.709500	4.065600	4.480500	H	5.709500	4.065600	4.480500	H	-2.444900	3.810700	3.353600	H	-2.444900	3.810700	3.353600
C	3.268700	3.088800	5.565600	C	3.268700	3.088800	5.565600	O	5.100100	1.929900	-1.894800	O	5.100100	1.929900	-1.894800
H	2.627600	3.618900	6.301800	H	2.627600	3.618900	6.301800	O	7.168000	0.209500	-0.972500	O	7.168000	0.209500	-0.972500
H	2.785500	2.139200	5.259600	H	2.785500	2.139200	5.259600	O	6.570200	-2.681400	-1.595000	O	6.570200	-2.681400	-1.595000
C	3.503800	3.986900	4.340700	C	3.503800	3.986900	4.340700	H	5.665500	-2.889500	-1.200700	H	5.665500	-2.889500	-1.200700
H	2.714100	3.825700	3.557100	H	2.714100	3.825700	3.557100	O	4.388400	-2.672600	-2.997500	O	4.388400	-2.672600	-2.997500
O	2.012300	-6.140600	2.356400	O	2.012300	-6.140600	2.356400	O	4.982900	-0.863500	-4.347000	O	4.982900	-0.863500	-4.347000
O	1.170900	-7.615800	0.176800	O	1.170900	-7.615800	0.176800	O	5.700600	1.952500	-5.308000	O	5.700600	1.952500	-5.308000
O	-1.713300	-7.981200	1.010700	O	-1.713300	-7.981200	1.010700	H	6.052000	2.524800	-4.569500	H	6.052000	2.524800	-4.569500
H	-1.436000	-8.245600	0.071700	H	-1.436000	-8.245600	0.071700	O	5.449000	-5.647200	-1.906100	O	5.449000	-5.647200	-1.906100
O	-2.175600	-6.220900	3.143000	O	-2.175600	-6.220900	3.143000	H	6.222300	-5.034100	-1.809000	H	6.222300	-5.034100	-1.809000
O	1.138400	-7.660800	3.851800	O	1.138400	-7.660800	3.851800	O	2.220500	-5.472200	-1.011800	O	2.220500	-5.472200	-1.011800
O	-1.614400	-6.999300	6.050000	O	-1.614400	-6.999300	6.050000	O	2.876600	-5.647400	-4.494500	O	2.876600	-5.647400	-4.494500
H	-1.823700	-6.024700	5.992600	H	-1.823700	-6.024700	5.992600	O	4.694600	-4.301500	-6.249900	O	4.694600	-4.301500	-6.249900
O	-4.261300	-7.192900	1.887400	O	-4.261300	-7.192900	1.887400	H	4.612800	-5.282000	-6.282600	H	4.612800	-5.282000	-6.282600
H	-3.284000	-7.105100	1.622400	H	-3.284000	-7.105100	1.622400	C	5.673000	0.822300	-2.684500	C	5.673000	0.822300	-2.684500

H	6.594400	1.180600	-3.205700
C	6.030800	-0.298700	-1.699700
H	5.194100	-0.505100	-0.981300
C	6.469200	-1.562100	-2.467700
H	7.514600	-1.443800	-2.846500
C	5.508700	-1.916400	-3.626000
H	5.957500	-2.572900	-4.410300
C	4.607000	0.399000	-3.699100
H	3.597900	0.242600	-3.206600
C	4.474000	1.332400	-4.909700
H	4.184100	0.750800	-5.810800
H	3.718400	2.115700	-4.701400
C	4.348300	-4.085000	-3.418300
H	5.297200	-4.332000	-3.955600
C	4.243400	-4.879800	-2.111700
H	4.145500	-4.161500	-1.239700
C	3.120200	-5.931000	-2.011000
H	3.539300	-6.879600	-1.580700
C	2.352100	-6.255200	-3.316600
H	2.322200	-7.336400	-3.572400
C	3.144200	-4.223500	-4.359500
H	2.224300	-3.718200	-3.951100
C	3.462200	-3.740400	-5.778000
H	2.648800	-3.990500	-6.484400
H	3.653600	-2.643600	-5.785300
O	-1.053400	5.683200	-3.135400
O	-0.406600	8.458900	-2.364000
H	-0.784400	8.552500	-1.446300
O	2.481200	8.310600	-1.345200
H	2.960500	7.522900	-0.941700
O	3.307000	6.102800	-2.264400
O	2.320100	6.229000	-4.358000
O	-0.249900	5.390700	-6.100300
H	-1.107800	5.398300	-5.594200
O	5.672300	6.177000	-0.182800
H	5.105700	6.785400	0.393700
O	4.796000	3.034400	0.214500
O	6.010200	3.744900	-3.040200
O	5.857000	6.087400	-4.806500
H	6.747700	5.818700	-4.487900
C	0.052400	6.499400	-3.594600
H	-0.262900	7.148900	-4.445200
C	0.509300	7.351700	-2.396100
H	0.444400	6.772500	-1.445300
C	1.916400	7.949500	-2.611100
H	1.834000	8.925500	-3.148300
C	2.904400	6.988200	-3.320700
H	3.767700	7.481800	-3.818400
C	1.116200	5.478700	-4.025700
H	1.362000	4.762000	-3.198100
C	0.769400	4.746000	-5.333800
H	1.639000	4.748400	-6.022700
H	0.447800	3.704500	-5.117400
C	4.679300	5.617700	-2.281700
H	5.367800	6.460000	-2.529600
C	4.870200	5.163600	-0.823000
H	3.864900	5.070100	-0.324800
C	5.668300	3.867900	-0.581200
H	6.587200	4.107500	0.016500
C	6.049500	3.028300	-1.811400
H	7.098400	2.654000	-1.782000
C	4.778000	4.474800	-3.303400
H	3.914000	3.769600	-3.197800
C	4.971800	4.961700	-4.746500
H	5.365200	4.148200	-5.392900
H	4.023000	5.354100	-5.175300
O	1.053400	-5.683200	-3.135400
O	0.406600	-8.458900	-2.364000
H	0.784400	-8.552500	-1.446300
O	-2.481200	-8.310600	-1.345200
H	-2.960500	-7.522900	-0.941700
O	-3.307000	-6.102800	-2.264400
O	-2.320100	-6.229000	-4.358000
O	0.249900	-5.390700	-6.100300
H	1.107800	-5.398300	-5.594200
O	-5.672300	-6.177000	-0.182800
H	-5.105700	-6.785400	0.393700
O	-4.796000	-3.034400	0.214500
O	-6.010200	-3.744900	-3.040200
O	-5.857000	-6.087400	-4.806500
H	-6.747700	-5.818700	-4.487900
C	-0.052400	-6.499400	-3.594600
H	0.262900	-7.148900	-4.445200
C	-0.509300	-7.351700	-2.396100
H	-0.444400	-6.772500	-1.445300
C	-1.916400	-7.949500	-2.611100
H	-1.834000	-8.925500	-3.148300
C	-2.904400	-6.988200	-3.320700

H	6.594400	1.180600	-3.205700
C	6.030800	-0.298700	-1.699700
H	5.194100	-0.505100	-0.981300
C	6.469200	-1.562100	-2.467700
H	7.514600	-1.443800	-2.846500
C	5.508700	-1.916400	-3.626000
H	5.957500	-2.572900	-4.410300
C	4.607000	0.399000	-3.699100
H	3.597900	0.242600	-3.206600
C	4.474000	1.332400	-4.909700
H	4.184100	0.750800	-5.810800
H	3.718400	2.115700	-4.701400
C	4.348300	-4.085000	-3.418300
H	5.297200	-4.332000	-3.955600
C	4.243400	-4.879800	-2.111700
H	4.145500	-4.161500	-1.239700
C	3.120200	-5.931000	-2.011000
H	3.539300	-6.879600	-1.580700
C	2.352100	-6.255200	-3.316600
H	2.322200	-7.336400	-3.572400
C	3.144200	-4.223500	-4.359500
H	2.224300	-3.718200	-3.951100
C	3.462200	-3.740400	-5.778000
H	2.648800	-3.990500	-6.484400
H	3.653600	-2.643600	-5.785300
O	-1.053400	5.683200	-3.135400
O	-0.406600	8.458900	-2.364000
H	-0.784400	8.552500	-1.446300
O	2.481200	8.310600	-1.345200
H	2.960500	7.522900	-0.941700
O	3.307000	6.102800	-2.264400
O	2.320100	6.229000	-4.358000
O	-0.249900	5.390700	-6.100300
H	-1.107800	5.398300	-5.594200
O	5.672300	6.177000	-0.182800
H	5.105700	6.785400	0.393700
O	4.796000	3.034400	0.214500
O	6.010200	3.744900	-3.040200
O	5.857000	6.087400	-4.806500
H	6.747700	5.818700	-4.487900
C	0.052400	6.499400	-3.594600
H	-0.262900	7.148900	-4.445200
C	0.509300	7.351700	-2.396100
H	0.444400	6.772500	-1.445300
C	1.916400	7.949500	-2.611100
H	1.834000	8.925500	-3.148300
C	2.904400	6.988200	-3.320700
H	3.767700	7.481800	-3.818400
C	1.116200	5.478700	-4.025700
H	1.362000	4.762000	-3.198100
C	0.769400	4.746000	-5.333800
H	1.639000	4.748400	-6.022700
H	0.447800	3.704500	-5.117400
C	4.679300	5.617700	-2.281700
H	5.367800	6.460000	-2.529600
C	4.870200	5.163600	-0.823000
H	3.864900	5.070100	-0.324800
C	5.668300	3.867900	-0.581200
H	6.587200	4.107500	0.016500
C	6.049500	3.028300	-1.811400
H	7.098400	2.654000	-1.782000
C	4.778000	4.474800	-3.303400
H	3.914000	3.769600	-3.197800
C	4.971800	4.961700	-4.746500
H	5.365200	4.148200	-5.392900
H	4.023000	5.354100	-5.175300
O	1.053400	-5.683200	-3.135400
O	0.406600	-8.458900	-2.364000
H	0.784400	-8.552500	-1.446300
O	-2.481200	-8.310600	-1.345200
H	-2.960500	-7.522900	-0.941700
O	-3.307000	-6.102800	-2.264400
O	-2.320100	-6.229000	-4.358000
O	0.249900	-5.390700	-6.100300
H	1.107800	-5.398300	-5.594200
O	-5.672300	-6.177000	-0.182800
H	-5.105700	-6.785400	0.393700
O	-4.796000	-3.034400	0.214500
O	-6.010200	-3.744900	-3.040200
O	-5.857000	-6.087400	-4.806500
H	-6.747700	-5.818700	-4.487900
C	-0.052400	-6.499400	-3.594600
H	0.262900	-7.148900	-4.445200
C	-0.509300	-7.351700	-2.396100
H	-0.444400	-6.772500	-1.445300
C	-1.916400	-7.949500	-2.611100
H	-1.834000	-8.925500	-3.148300
C	-2.904400	-6.988200	-3.320700

H	-3.767700	-7.481800	-3.818400
C	-1.116200	-5.478700	-4.025700
H	-1.362000	-4.762000	-3.198100
C	-0.769400	-4.746000	-5.333800
H	-1.639000	-4.748400	-6.022700
H	-0.447800	-3.704500	-5.117400
C	-4.679300	-5.617700	-2.281700
H	-5.367800	-6.460000	-2.529600
C	-4.870200	-5.163600	-0.823000
H	-3.864900	-5.070100	-0.324800
C	-5.668300	-3.867900	-0.581200
H	-6.587200	-4.107500	0.016500
C	-6.049500	-3.028300	-1.811400
H	-7.098400	-2.654000	-1.782000
C	-4.778000	-4.474800	-3.303400
H	-3.914000	-3.769600	-3.197800
C	-4.971800	-4.961700	-4.746500
H	-5.365200	-4.148200	-5.392900
H	-4.023000	-5.354100	-5.175300
O	-5.100100	-1.929900	-1.894800
O	-7.168000	-0.209500	-0.972500
O	-6.570200	2.681400	-1.595000
H	-5.665500	2.889500	-1.200700
O	-4.388400	2.672600	-2.997500
O	-4.982900	0.863500	-4.347000
O	-5.700600	-1.952500	-5.308000
H	-6.052000	-2.524800	-4.569500
O	-5.449000	5.647200	-1.906100
H	-6.222300	5.034100	-1.809000
O	-2.220500	5.472200	-1.011800
O	-2.876600	5.647400	-4.494500
O	-4.694600	4.301500	-6.249900
H	-4.612800	5.282000	-6.282600
C	-5.673000	-0.822300	-2.684500
H	-6.594400	-1.180600	-3.205700
C	-6.030800	0.298700	-1.699700
H	-5.194100	0.505100	-0.981300
C	-6.469200	1.562100	-2.467700
H	-7.514600	1.443800	-2.846500
C	-5.508700	1.916400	-3.626000
H	-5.957500	2.572900	-4.410300
C	-4.607000	-0.399000	-3.699100
H	-3.597900	-0.242600	-3.206600
C	-4.474000	-1.332400	-4.909700
H	-4.184100	-0.750800	-5.810800
H	-3.718400	-2.115700	-4.701400
C	-4.348300	4.085000	-3.418300
H	-5.297200	4.332000	-3.955600
C	-4.243400	4.879800	-2.111700
H	-4.145500	4.161500	-1.239700
C	-3.120200	5.931000	-2.011000
H	-3.539300	6.879600	-1.580700
C	-2.352100	6.255200	-3.316600
H	-2.322200	7.336400	-3.572400
C	-3.144200	4.223500	-4.359500
H	-2.224300	3.718200	-3.951100
C	-3.462200	3.740400	-5.778000
H	-2.648800	3.990500	-6.484400
H	-3.653600	2.643600	-5.785300
I	2.693700	-1.840100	-2.037600
I	3.411200	1.634800	-0.417400
I	1.064100	1.641600	2.988400
B	1.170900	-0.796000	-1.055900
B	1.559500	0.680600	-0.210300
B	0.504500	0.714500	1.186900
I	1.007000	1.622600	-3.403700
I	0.210100	3.732600	-0.114400
I	-2.611700	1.603800	1.894500
B	0.492400	0.706400	-1.584900
B	0.089700	1.630500	-0.199500
B	-1.150300	0.777700	0.661500
I	-2.693700	1.840100	-2.037600
I	-3.411200	-1.634800	-0.417400
I	-1.064100	-1.641600	2.988400
B	-1.170900	0.796000	-1.055900
B	-1.559500	-0.680600	-0.210300
B	-0.504500	-0.714500	1.186900
I	-1.007000	-1.622600	-3.403700
I	-0.210100	-3.732600	-0.114400
I	2.611700	-1.603800	1.894500
B	-0.492400	-0.706400	-1.584900
B	-0.089700	-1.630500	-0.199500
B	1.150300	-0.777700	0.661500
C	0.291500	7.268300	5.608300
H	-0.436100	6.763200	6.272400
H	0.194500	8.366400	5.737900
O	1.614400	6.999300	6.050000
H	1.823700	6.024700	5.992600

H	-3.767700	-7.481800	-3.818400
C	-1.116200	-5.478700	-4.025700
H	-1.362000	-4.762000	-3.198100
C	-0.769400	-4.746000	-5.333800
H	-1.639000	-4.748400	-6.022700
H	-0.447800	-3.704500	-5.117400
C	-4.679300	-5.617700	-2.281700
H	-5.367800	-6.460000	-2.529600
C	-4.870200	-5.163600	-0.823000
H	-3.864900	-5.070100	-0.324800
C	-5.668300	-3.867900	-0.581200
H	-6.587200	-4.107500	0.016500
C	-6.049500	-3.028300	-1.811400
H	-7.098400	-2.654000	-1.782000
C	-4.778000	-4.474800	-3.303400
H	-3.914000	-3.769600	-3.197800
C	-4.971800	-4.961700	-4.746500
H	-5.365200	-4.148200	-5.392900
H	-4.023000	-5.354100	-5.175300
O	-5.100100	-1.929900	-1.894800
O	-7.168000	-0.209500	-0.972500
O	-6.570200	2.681400	-1.595000
H	-5.665500	2.889500	-1.200700
O	-4.388400	2.672600	-2.997500
O	-4.982900	0.863500	-4.347000
O	-5.700600	-1.952500	-5.308000
H	-6.052000	-2.524800	-4.569500
O	-5.449000	5.647200	-1.906100
H	-6.222300	5.034100	-1.809000
O	-2.220500	5.472200	-1.011800
O	-2.876600	5.647400	-4.494500
O	-4.694600	4.301500	-6.249900
H	-4.612800	5.282000	-6.282600
C	-5.673000	-0.822300	-2.684500
H	-6.594400	-1.180600	-3.205700
C	-6.030800	0.298700	-1.699700
H	-5.194100	0.505100	-0.981300
C	-6.469200	1.562100	-2.467700
H	-7.514600	1.443800	-2.846500
C	-5.508700	1.916400	-3.626000
H	-5.957500	2.572900	-4.410300
C	-4.607000	-0.399000	-3.699100
H	-3.597900	-0.242600	-3.206600
C	-4.474000	-1.332400	-4.909700
H	-4.184100	-0.750800	-5.810800
H	-3.718400	-2.115700	-4.701400
C	-4.348300	4.085000	-3.418300
H	-5.297200	4.332000	-3.955600
C	-4.243400	4.879800	-2.111700
H	-4.145500	4.161500	-1.239700
C	-3.120200	5.931000	-2.011000
H	-3.539300	6.879600	-1.580700
C	-2.352100	6.255200	-3.316600
H	-2.322200	7.336400	-3.572400
C	-3.144200	4.223500	-4.359500
H	-2.224300	3.718200	-3.951100
C	-3.462200	3.740400	-5.778000
H	-2.648800	3.990500	-6.484400
H	-3.653600	2.643600	-5.785300
I	2.693700	-1.840100	-2.037600
I	3.411200	1.634800	-0.417400
I	1.064100	1.641600	2.988400
B	1.170900	-0.796000	-1.055900
B	1.559500	0.680600	-0.210300
B	0.504500	0.714500	1.186900
I	1.007000	1.622600	-3.403700
I	0.210100	3.732600	-0.114400
I	-2.611700	1.603800	1.894500
B	0.492400	0.706400	-1.584900
B	0.089700	1.630500	-0.199500
B	-1.150300	0.777700	0.661500
I	-2.693700	1.840100	-2.037600
I	-3.411200	-1.634800	-0.417400
I	-1.064100	-1.641600	2.988400
B	-1.170900	0.796000	-1.055900
B	-1.559500	-0.680600	-0.210300
B	-0.504500	-0.714500	1.186900
I	-1.007000	-1.622600	-3.403700
I	-0.210100	-3.732600	-0.114400
I	2.611700	-1.603800	1.894500
B	-0.492400	-0.706400	-1.584900
B	-0.089700	-1.630500	-0.199500
B	1.150300	-0.777700	0.661500
C	0.291500	7.268300	5.608300
H	-0.436100	6.763200	6.272400
H	0.194500	8.366400	5.737900
O	1.614400	6.999300	6.050000
H	1.823700	6.024700	5.992600

H	6.741100	1.372000	0.314000	H	6.741100	1.372000	0.314000	H	7.427700	-0.463300	-0.253100
H	6.233500	-1.903100	0.872000	H	6.233500	-1.903100	0.872000	H	1.619300	-4.695700	-1.356500
H	4.097000	-2.720400	0.501800	H	4.097000	-2.720400	0.501800	H	5.272800	2.767200	1.128500
H	-1.504700	6.649300	0.104700	H	-1.504700	6.649300	0.104700	H	-5.272800	-2.767200	1.128500
H	1.504700	-6.649300	0.104700	H	1.504700	-6.649300	0.104700	H	-7.427700	0.463300	-0.253100
H	-6.741100	-1.372000	0.314000	H	-6.741100	-1.372000	0.314000	H	-1.619300	4.695700	-1.356500
H	-6.233500	1.903100	0.872000	H	-6.233500	1.903100	0.872000				
H	-4.097000	2.720400	0.501800	H	-4.097000	2.720400	0.501800				

H	7.427700	-0.463300	-0.253100
H	1.619300	-4.695700	-1.356500
H	5.272800	2.767200	1.128500
H	-5.272800	-2.767200	1.128500
H	-7.427700	0.463300	-0.253100
H	-1.619300	4.695700	-1.356500

Table S3. Cartesian coordinates (Å) of the optimized (PM6) structure of the $[(\gamma\text{-CD})(B_{12}I_{12})]^{2-}$ complex.

O	-5.470000	-2.859300	-1.354600	O	-5.470000	-2.859300	-1.354600	C	-5.067100	-4.587600	0.260500
O	-7.501800	-2.040200	0.593300	O	-7.501800	-2.040200	0.593300	H	-5.771600	-5.269500	0.810200
O	-8.034700	0.754500	0.374000	O	-8.034700	0.754500	0.374000	C	-5.655500	-4.262100	-1.139000
H	-8.323000	0.226000	1.164400	H	-8.323000	0.226000	1.164400	H	-6.710000	-4.585300	-1.265900
O	-6.183700	1.237600	-1.834400	O	-6.183700	1.237600	-1.834400	C	-3.544100	-4.678600	-2.235200
O	-7.340800	-0.221500	-3.074900	O	-7.340800	-0.221500	-3.074900	H	-3.321900	-3.586500	-2.123400
O	-6.577300	-3.347100	-4.157200	O	-6.577300	-3.347100	-4.157200	C	-3.113700	-5.219300	-3.602600
H	-5.845900	-3.800600	-3.646300	H	-5.845900	-3.800600	-3.646300	H	-3.582000	-4.653000	-4.426400
O	-5.164800	0.944600	0.840900	O	-5.164800	0.944600	0.840900	H	-2.003200	-5.206300	-3.707800
H	-6.151700	0.836400	1.035600	H	-6.151700	0.836400	1.035600	O	-3.090900	4.343200	-0.519900
O	-3.423100	3.217400	1.568000	O	-3.423100	3.217400	1.568000	O	-3.234900	7.232400	0.219900
O	-5.364100	4.722100	-1.038800	O	-5.364100	4.722100	-1.038800	H	-2.962400	7.813300	0.964600
O	-7.946100	4.282400	-2.198000	O	-7.946100	4.282400	-2.198000	O	-0.345600	8.189900	0.100300
H	-7.796800	4.894700	-1.441700	H	-7.796800	4.894700	-1.441700	H	0.347700	7.539500	0.439500
C	-6.663800	-2.111800	-1.691500	C	-6.663800	-2.111800	-1.691500	O	0.603100	6.062000	-1.102100
H	-7.513700	-2.790800	-1.917800	H	-7.513700	-2.790800	-1.917800	O	-0.873100	6.084700	-2.857100
C	-6.920300	-1.244100	-0.441500	C	-6.920300	-1.244100	-0.441500	O	-2.784700	2.987400	-3.019200
H	-5.947300	-0.807600	-0.079300	H	-5.947300	-0.807600	-0.079300	H	-2.284200	2.480500	-2.296000
C	-7.948400	-0.144600	-0.747000	C	-7.948400	-0.144600	-0.747000	O	2.312300	6.428500	1.031800
H	-8.960300	-0.576000	-0.921400	H	-8.960300	-0.576000	-0.921400	H	2.160600	6.002000	1.912300
C	-7.495700	0.677300	-1.985200	C	-7.495700	0.677300	-1.985200	O	4.351800	4.121800	1.023600
H	-8.227500	1.436400	-2.324800	H	-8.227500	1.436400	-2.324800	O	3.843300	5.040200	-2.507200
C	-6.291200	-1.230900	-2.900400	C	-6.291200	-1.230900	-2.900400	O	2.401000	7.207600	-3.873200
H	-5.325000	-0.698800	-2.715900	H	-5.325000	-0.698800	-2.715900	H	3.364900	7.324300	-3.720200
C	-6.313900	-1.949100	-4.261100	C	-6.313900	-1.949100	-4.261100	C	-2.632800	5.506800	-1.287000
H	-7.158600	-1.574900	-4.879200	H	-7.158600	-1.574900	-4.879200	H	-3.501900	5.924200	-1.843500
H	-5.362500	-1.796000	-4.801400	H	-5.362500	-1.796000	-4.801400	C	-2.075800	6.528200	-0.275000
C	-6.077500	2.392800	-0.977900	C	-6.077500	2.392800	-0.977900	H	-1.576200	6.000200	0.578500
H	-7.045000	2.604200	-0.473200	H	-7.045000	2.604200	-0.473200	C	-1.136200	7.574100	-0.912400
C	-4.929800	2.096600	-0.001600	C	-4.929800	2.096600	-0.001600	H	-1.712500	8.416400	-1.355600
C	-4.689300	3.327700	0.897300	C	-4.689300	3.327700	0.897300	C	-0.181100	6.919100	-1.938500
H	-5.497700	3.479500	1.636200	H	-5.497700	3.479500	1.636200	H	0.409100	7.612000	-2.570300
C	-4.433500	4.569000	0.021300	C	-4.433500	4.569000	0.021300	C	-1.545400	4.952900	-2.224700
H	-4.477500	5.552400	0.542200	H	-4.477500	5.552400	0.542200	H	-0.777400	4.367300	-1.643700
C	-5.616800	3.561200	-1.879900	C	-5.616800	3.561200	-1.879900	C	-2.069800	4.149500	-3.424500
H	-4.655800	3.303500	-2.413300	H	-4.655800	3.303500	-2.413300	H	-2.802300	4.719200	-4.024400
C	-6.691700	4.040900	-2.855400	C	-6.691700	4.040900	-2.855400	H	-1.224500	3.840700	-4.070100
H	-6.377200	4.969800	-3.365300	H	-6.377200	4.969800	-3.365300	C	2.029800	6.052700	-1.275300
H	-6.933000	3.254400	-3.597200	H	-6.933000	3.254400	-3.597200	H	2.405900	7.093800	-1.376100
O	3.057600	-4.028300	-1.602200	O	3.057600	-4.028300	-1.602200	C	2.482400	5.395500	0.044500
O	2.715100	-6.505500	-0.039000	O	2.715100	-6.505500	-0.039000	H	1.824100	4.517100	0.308600
H	3.376200	-6.003000	0.535600	H	3.376200	-6.003000	0.535600	C	3.979800	5.027500	0.000600
O	-0.264400	-6.417500	0.850100	O	-0.264400	-6.417500	0.850100	H	4.584700	5.939100	0.251400
H	-0.370300	-5.460900	1.162300	H	-0.370300	-5.460900	1.162300	C	4.452100	4.470400	-1.363200
O	-1.582600	-5.113900	-0.906200	O	-1.582600	-5.113900	-0.906200	H	5.537000	4.665200	-1.542400
O	-0.150000	-5.545700	-2.691100	O	-0.150000	-5.545700	-2.691100	C	2.394200	5.178000	-2.487300
O	2.450400	-4.604300	-4.526300	O	2.450400	-4.604300	-4.526300	H	1.931300	4.159200	-2.400300
H	3.168700	-4.160800	-3.997500	H	3.168700	-4.160800	-3.997500	C	2.085200	5.808200	-3.848900
O	-3.873600	-6.505800	0.919000	O	-3.873600	-6.505800	0.919000	H	2.641600	5.295200	-4.656600
H	-3.032800	-6.797400	1.348200	H	-3.032800	-6.797400	1.348200	H	0.992700	5.783900	-4.062300
O	-5.095200	-3.404600	1.046700	O	-5.095200	-3.404600	1.046700	O	4.192100	3.032800	-1.423400
O	-4.989700	-4.883900	-2.232700	O	-4.989700	-4.883900	-2.232700	O	6.681900	2.977100	-0.022900
O	-3.452400	-6.605900	-3.739000	O	-3.452400	-6.605900	-3.739000	O	8.244700	0.541800	-0.275400
H	-4.412600	-6.725200	-3.554400	H	-4.412600	-6.725200	-3.554400	H	8.072700	1.006500	0.579100
C	2.048600	-5.099900	-1.831600	C	2.048600	-5.099900	-1.831600	O	6.239800	-0.874400	-1.451700
H	2.539300	-5.909400	-2.423800	H	2.539300	-5.909400	-2.423800	O	6.167600	0.502400	-3.288800
C	1.664900	-5.606800	-0.429600	C	1.664900	-5.606800	-0.429600	O	4.330100	2.824100	-4.524100
H	1.592600	-4.752400	0.304600	H	1.592600	-4.752400	0.304600	H	4.002400	3.451500	-3.825000
C	0.384700	-6.461700	-0.410900	C	0.384700	-6.461700	-0.410900	O	7.083700	-3.069600	0.354900
H	0.663300	-7.543500	-0.508500	H	0.663300	-7.543500	-0.508500	H	7.408600	-2.200800	0.688100
C	-0.650300	-6.091200	-1.503000	C	-0.650300	-6.091200	-1.503000	O	4.377100	-4.473600	0.684100
H	-1.243300	-6.964300	-1.864400	H	-1.243300	-6.964300	-1.864400	O	4.958400	-3.992600	-2.909000
C	0.874100	-4.501600	-2.604100	C	0.874100	-4.501600	-2.604100	O	7.181500	-3.006100	-4.407600
H	0.407600	-3.616000	-2.075400	H	0.407600	-3.616000	-2.075400	H	7.087200	-3.963500	-4.198400
C	1.164200	-4.171100	-4.075800	C	1.164200	-4.171100	-4.075800	C	5.370600	2.327000	-1.969200
H	0.467200	-4.721200	-4.741600	H	0.467200	-4.721200	-4.741600	H	5.942100	3.046200	-2.601900
H	1.074500	-3.080900	-4.247600	H	1.074500	-3.080900	-4.247600	C	6.200000	1.851700	-0.757600
C	-2.993300	-5.499400	-1.061900	C	-2.993300	-5.499400	-1.061900	H	5.592100	1.186300	-0.082600
H	-3.043100	-6.593900	-1.288300	H	-3.043100	-6.593900	-1.288300	C	7.455900	1.143700	-1.306000
C	-3.663200	-5.222100	0.295500	C	-3.663200	-5.222100	0.295500	H	8.125500	1.859500	-1.837100
H	-2.998800	-4.598900	0.969000	H	-2.998800	-4.598900	0.969000	C	7.021100	-0.004600	-2.255400

C	-5.067100	-4.587600	0.260500
H	-5.771600	-5.269500	0.810200
C	-5.655500	-4.262100	-1.139000
H	-6.710000	-4.585300	-1.265900
C	-3.544100	-4.678600	-2.235200
H	-3.321900	-3.586500	-2.123400
C	-3.113700	-5.219300	-3.602600
H	-3.582000	-4.653000	-4.426400
H	-2.003200	-5.206300	-3.707800
O	-3.090900	4.343200	-0.519900
O	-3.234900	7.232400	0.219900
H	-2.962400	7.813300	0.964600
O	-0.345600	8.189900	0.100300
H	0.347700	7.539500	0.439500
O	0.603100	6.062000	-1.102100
O	-0.873100	6.084700	-2.857100
O	-2.784700	2.987400	-3.019200
H	-2.284200	2.480500	-2.296000
O	2.312300	6.428500	1.031800
H	2.160600	6.002000	1.912300
O	4.351800	4.121800	1.023600
O	3.843300	5.040200	-2.507200
O	2.401000	7.207600	-3.873200
H	3.364900	7.324300	-3.720200
C	-2.632800	5.506800	-1.287000
H	-3.501900	5.924200	-1.843500
C	-2.075800	6.528200	-0.275000
H	-1.576200	6.000200	0.578500
C	-1.136200	7.574100	-0.912400
H	-1.712500	8.416400	-1.355600
C	-0.181100	6.919100	-1.938500
H	0.409100	7.612000	-2.570300
C	-1.545400	4.952900	-2.224700
H	-0.777400	4.367300	-1.643700
C	-2.069800	4.149500	-3.424500
H	-2.802300	4.719200	-4.024400
H	-1.224500	3.840700	-4.070100
C	2.029800	6.052700	-1.275300
H	2.405900	7.093800	-1.376100
C	2.482400	5.395500	0.044500
H	1.824100	4.517100	0.308600
C	3.979800	5.027500	0.000600
H	4.584700	5.939100	0.251400
C	4.452100	4.470400	-1.363200
H	5.537000	4.665200	-1.542400
C	2.394200	5.178000	-2.487300
H	1.931300	4.159200	-2.400300
C	2.085200	5.808200	-3.848900
H	2.641600	5.295200	-4.656600
H	0.992700	5.783900	-4.062300
O	4.192100	3.032800	-1.423400
O	6.681900	2.977100	-0.022900
O	8.244700	0.541800	-0.275400
H	8.072700	1.006500	0.579100
O	6.239800	-0.874400	-1.451700
O	6.167600	0.502400	-3.288800
O	4.330100	2.824100	-4.524100
H	4.002400	3.451500	-3.825000
O	7.083700	-3.069600	0.354900
H	7.408600	-2.200800	0.688100
O	4.377100	-4.473600	0.684100
O	4.958400	-3.992600	-2.909000
O	7.181500	-3.006100	-4.407600
H	7.087200	-3.963500	-4.198400
C	5.370600	2.327000	-1.969200
H	5.942100	3.046200	-2.601900
C	6.200000	1.851700	-0.757600
H	5.592100	1.186300	-0.082600
C	7.455900	1.143700	-1.306000
H	8.125500	1.859500	-1.837100
C	7.021100	-0.004600	-2.255400

H	7.843800	-0.502200	-2.801300	H	7.843800	-0.502200	-2.801300	H	3.693800	-3.707400	0.799600	H	3.693800	-3.707400	0.799600
C	4.928400	1.122700	-2.813000	C	4.928400	1.122700	-2.813000	I	1.564100	-0.295900	4.951000	I	1.564100	-0.295900	4.951000
H	4.380500	0.355700	-2.197400	H	4.380500	0.355700	-2.197400	I	1.894300	-3.326600	2.575000	I	1.894300	-3.326600	2.575000
C	4.158600	1.470900	-4.093600	C	4.158600	1.470900	-4.093600	I	4.041500	-0.059500	1.906900	I	4.041500	-0.059500	1.906900
H	4.549600	0.886300	-4.951200	H	4.549600	0.886300	-4.951200	I	-1.715400	1.544800	4.067900	I	-1.715400	1.544800	4.067900
H	3.075200	1.273600	-3.955000	H	3.075200	1.273600	-3.955000	I	2.389100	-2.091300	-0.994000	I	2.389100	-2.091300	-0.994000
C	6.279100	-2.290100	-1.751000	C	6.279100	-2.290100	-1.751000	I	1.727700	3.020000	2.854900	I	1.727700	3.020000	2.854900
H	7.317200	-2.597600	-2.014300	H	7.317200	-2.597600	-2.014300	I	-0.830900	0.111000	-2.118600	I	-0.830900	0.111000	-2.118600
C	5.861600	-2.862400	-0.378900	C	5.861600	-2.862400	-0.378900	I	-1.650500	-2.360100	3.674200	I	-1.650500	-2.360100	3.674200
H	5.208500	-2.125200	0.174300	H	5.208500	-2.125200	0.174300	I	-1.603400	2.973900	0.515800	I	-1.603400	2.973900	0.515800
C	5.217200	-4.255100	-0.434800	C	5.217200	-4.255100	-0.434800	I	-1.094300	-3.231800	-0.073900	I	-1.094300	-3.231800	-0.073900
H	6.016400	-5.033000	-0.304500	H	6.016400	-5.033000	-0.304500	I	2.434700	1.975700	-0.838500	I	2.434700	1.975700	-0.838500
C	4.416800	-4.549100	-1.726200	C	4.416800	-4.549100	-1.726200	I	-3.397400	-0.218100	1.021500	I	-3.397400	-0.218100	1.021500
H	4.382700	-5.639500	-1.963100	H	4.382700	-5.639500	-1.963100	B	1.050000	-1.531500	1.885800	B	1.050000	-1.531500	1.885800
C	5.295400	-2.577800	-2.895100	C	5.295400	-2.577800	-2.895100	B	0.861400	-0.202200	2.990400	B	0.861400	-0.202200	2.990400
H	4.354000	-1.983700	-2.770300	H	4.354000	-1.983700	-2.770300	B	1.957100	-0.083000	1.645400	B	1.957100	-0.083000	1.645400
C	5.899800	-2.374300	-4.291400	C	5.899800	-2.374300	-4.291400	B	0.932800	1.254800	2.044500	B	0.932800	1.254800	2.044500
H	5.229300	-2.776600	-5.073200	H	5.229300	-2.776600	-5.073200	B	-0.286500	-1.515000	0.788300	B	-0.286500	-1.515000	0.788300
H	6.115200	-1.299800	-4.484300	H	6.115200	-1.299800	-4.484300	B	1.251700	-0.886300	0.283500	B	1.251700	-0.886300	0.283500
H	-6.761900	-2.594700	1.019200	H	-6.761900	-2.594700	1.019200	B	-0.523800	-1.092900	2.453300	B	-0.523800	-1.092900	2.453300
H	-3.379400	2.333400	2.146600	H	-3.379400	2.333400	2.146600	B	-0.406400	1.312500	0.935900	B	-0.406400	1.312500	0.935900
H	-3.984200	1.818100	-0.566200	H	-3.984200	1.818100	-0.566200	B	-0.211500	-0.044300	-0.120000	B	-0.211500	-0.044300	-0.120000
H	-4.382100	-2.732900	0.752900	H	-4.382100	-2.732900	0.752900	B	1.177500	0.839100	0.389800	B	1.177500	0.839100	0.389800
H	3.722300	3.300100	1.054400	H	3.722300	3.300100	1.054400	B	-0.597600	0.639600	2.539600	B	-0.597600	0.639600	2.539600
H	5.938200	3.318700	0.584100	H	5.938200	3.318700	0.584100	B	-1.312700	-0.183600	1.203300	B	-1.312700	-0.183600	1.203300

Table S4. Cartesian coordinates (Å) of the optimized (PM6) structure of the $[(HP\text{-}\gamma\text{-}CD)(B_{12}I_{12})]^{2-}$ complex.

O	-4.742300	-4.095800	-1.283100	O	-4.742300	-4.095800	-1.283100	H	-3.746400	-4.030100	0.789800	H	-3.746400	-4.030100	0.789800
O	-6.929500	-3.964000	0.633000	O	-6.929500	-3.964000	0.633000	O	-3.488500	-5.515500	-2.512500	O	-3.488500	-5.515500	-2.512500
H	-6.090800	-4.442200	0.943500	H	-6.090800	-4.442200	0.943500	O	-1.879300	-5.364800	-4.628500	O	-1.879300	-5.364800	-4.628500
O	-8.068500	-1.337600	0.549400	O	-8.068500	-1.337600	0.549400	C	3.341700	-4.471200	-1.616000	C	3.341700	-4.471200	-1.616000
H	-8.198600	-1.946900	1.322200	H	-8.198600	-1.946900	1.322200	H	4.033400	-5.122400	-2.203400	H	4.033400	-5.122400	-2.203400
O	-6.324300	-0.422400	-1.602100	O	-6.324300	-0.422400	-1.602100	C	2.983300	-5.137700	-0.272700	C	2.983300	-5.137700	-0.272700
O	-7.228600	-1.981100	-2.939900	O	-7.228600	-1.981100	-2.939900	H	2.646700	-4.375500	0.485700	H	2.646700	-4.375500	0.485700
O	-5.585500	-4.833700	-4.130600	O	-5.585500	-4.833700	-4.130600	C	1.953600	-6.273700	-0.428000	C	1.953600	-6.273700	-0.428000
H	-4.602100	-4.895800	-3.915700	H	-4.602100	-4.895800	-3.915700	H	2.493300	-7.240200	-0.603600	H	2.493300	-7.240200	-0.603600
O	-5.186700	-0.513200	1.021600	O	-5.186700	-0.513200	1.021600	C	0.917400	-6.041900	-1.555500	C	0.917400	-6.041900	-1.555500
H	-6.109400	-0.888700	1.182300	H	-6.109400	-0.888700	1.182300	H	0.507200	-6.988500	-1.990300	H	0.507200	-6.988500	-1.990300
O	-4.065800	2.099600	1.821800	O	-4.065800	2.099600	1.821800	C	2.117200	-4.100600	-2.452200	C	2.117200	-4.100600	-2.452200
O	-6.289000	3.160600	-0.778800	O	-6.289000	3.160600	-0.778800	H	1.417900	-3.392600	-1.911700	H	1.417900	-3.392600	-1.911700
O	-8.729800	1.856400	-2.077300	O	-8.729800	1.856400	-2.077300	C	2.429200	-3.594200	-3.867500	C	2.429200	-3.594200	-3.867500
C	-6.094800	-3.727600	-1.638800	C	-6.094800	-3.727600	-1.638800	H	1.874000	-4.186600	-4.623600	H	1.874000	-4.186600	-4.623600
H	-6.711300	-4.622700	-1.863700	H	-6.711300	-4.622700	-1.863700	H	2.165900	-2.521600	-3.955200	H	2.165900	-2.521600	-3.955200
C	-6.552000	-3.000900	-0.355600	C	-6.552000	-3.000900	-0.355600	C	-1.510500	-5.823900	-1.313600	C	-1.510500	-5.823900	-1.313600
H	-5.705400	-2.371400	0.042400	H	-5.705400	-2.371400	0.042400	H	-1.356300	-6.807200	-1.827900	H	-1.356300	-6.807200	-1.827900
C	-7.798800	-2.145100	-0.612200	C	-7.798800	-2.145100	-0.612200	C	-2.251500	-6.044700	0.018700	C	-2.251500	-6.044700	0.018700
H	-8.695000	-2.773200	-0.813000	H	-8.695000	-2.773200	-0.813000	H	-1.840000	-5.384600	0.838000	H	-1.840000	-5.384600	0.838000
C	-7.523700	-1.184900	-1.803200	C	-7.523700	-1.184900	-1.803200	C	-3.785500	-5.878500	-0.036700	C	-3.785500	-5.878500	-0.036700
H	-8.379700	-0.541900	-2.094600	H	-8.379700	-0.541900	-2.094600	H	-4.260600	-6.827200	0.324800	H	-4.260600	-6.827200	0.324800
C	-5.997300	-2.771300	-2.844100	C	-5.997300	-2.771300	-2.844100	C	-4.393400	-5.476400	-1.414200	C	-4.393400	-5.476400	-1.414200
H	-5.142200	-2.066100	-2.709700	H	-5.142200	-2.066100	-2.709700	H	-5.237000	-6.112600	-1.749100	H	-5.237000	-6.112600	-1.749100
C	-5.988200	-3.471300	-4.217900	C	-5.988200	-3.471300	-4.217900	C	-2.237900	-4.819200	-2.217800	C	-2.237900	-4.819200	-2.217800
H	-7.018200	-3.527300	-4.628100	H	-7.018200	-3.527300	-4.628100	H	-2.463100	-3.860400	-1.670200	H	-2.463100	-3.860400	-1.670200
H	-5.338300	-2.932000	-4.929200	H	-5.338300	-2.932000	-4.929200	C	-1.567100	-4.473500	-3.547100	C	-1.567100	-4.473500	-3.547100
C	-6.453700	0.727300	-0.743400	C	-6.453700	0.727300	-0.743400	H	-1.963000	-3.514700	-3.942200	H	-1.963000	-3.514700	-3.942200
H	-7.439400	0.715900	-0.213000	H	-7.439400	0.715900	-0.213000	H	-0.466900	-4.392300	-3.403400	H	-0.466900	-4.392300	-3.403400
C	-5.251400	0.684500	0.210500	C	-5.251400	0.684500	0.210500	O	-3.988000	3.304200	-0.252700	O	-3.988000	3.304200	-0.252700
C	-5.313700	1.919100	1.135800	C	-5.313700	1.919100	1.135800	O	-4.807200	6.059100	0.522200	O	-4.807200	6.059100	0.522200
H	-6.143300	1.862300	1.864300	H	-6.143300	1.862300	1.864300	H	-4.674600	6.685700	1.267400	H	-4.674600	6.685700	1.267400
C	-5.349000	3.203000	0.282500	C	-5.349000	3.203000	0.282500	O	-2.273900	7.731500	0.351600	O	-2.273900	7.731500	0.351600
H	-5.615300	4.139800	0.822500	H	-5.615300	4.139800	0.822500	H	-1.425100	7.292700	0.677800	H	-1.425100	7.292700	0.677800
C	-6.287700	1.979700	-1.632300	C	-6.287700	1.979700	-1.632300	O	-0.799900	5.935100	-0.850300	O	-0.799900	5.935100	-0.850300
H	-5.294600	1.958100	-2.171100	H	-5.294600	1.958100	-2.171100	O	-2.247100	5.532400	-2.586200	O	-2.247100	5.532400	-2.586200
C	-7.437600	2.197400	-2.617000	C	-7.437600	2.197400	-2.617000	O	-3.372300	2.070100	-2.709100	O	-3.372300	2.070100	-2.709100
H	-7.445800	3.236100	-2.990200	H	-7.445800	3.236100	-2.990200	H	-2.782600	1.694600	-1.971800	H	-2.782600	1.694600	-1.971800
H	-7.357600	1.481700	-3.461900	H	-7.357600	1.481700	-3.461900	O	0.830600	6.815000	1.209900	O	0.830600	6.815000	1.209900
O	4.074600	-3.223400	-1.271000	O	4.074600	-3.223400	-1.271000	H	0.898500	6.432900	2.118100	H	0.898500	6.432900	2.118100
O	4.184600	-5.784200	0.177600	O	4.184600	-5.784200	0.177600	O	3.319300	5.023900	1.238000	O	3.319300	5.023900	1.238000
H	4.661800	-5.175500	0.825400	H	4.661800	-5.175500	0.825400	O	2.564000	5.612700	-2.321500	O	2.564000	5.612700	-2.321500
O	1.238500	-6.525600	0.774400	O	1.238500	-6.525600	0.774400	O	0.686400	7.482100	-3.527200	O	0.686400	7.482100	-3.527200
H	0.917100	-5.659700	1.182900	H	0.917100	-5.659700	1.182900	C	-3.810500	4.547600	-1.011400	C	-3.810500	4.547600	-1.011400
O	-0.195900	-5.270700	-0.976400	O	-0.195900	-5.270700	-0.976400	H	-4.748300	4.748200	-1.576000	H	-4.748300	4.748200	-1.576000
O	1.374600	-5.344200	-2.683200	O	1.374600	-5.344200	-2.683200	C	-3.516300	5.670400	0.003600	C	-3.516300	5.670400	0.003600
O	3.793100	-3.767500	-4.260600	O	3.793100	-3.767500	-4.260600	H	-2.885500	5.284300	0.845900	H	-2.885500	5.284300	0.845900
H	4.395600	-3.258700	-3.651100	H	4.395600	-3.258700	-3.651100	C	-2.885300	6.918400	-0.648000	C	-2.885300	6.918400	-0.648000
O	-2.048300	-7.422300	0.393300	O	-2.048300	-7.422300	0.393300	H	-3.664200	7.576800	-1.093400	H	-3.664200	7.576800	-1.093400
H	-1.129700	-7.519800	0.754600	H	-1.129700	-7.519800	0.754600	C	-1.799900	6.530900	-1.679800	C	-1.799900	6.530900	-1.679800
O	-4.202400	-4.924100	0.935500	O	-4.202400	-4.924100	0.935500	H	-1.440600	7.361900	-2.322700	H	-1.440600	7.361900	-2.322700

C	-2.612100	4.275300	-1.939600
H	-1.722400	3.913400	-1.350500
C	-2.912700	3.350100	-3.128900
H	-3.732500	3.735400	-3.761600
H	-2.001100	3.217200	-3.743500
C	0.581600	6.283500	-1.067200
H	0.682700	7.382200	-1.207300
C	1.206200	5.801700	0.256200
H	0.766600	4.813300	0.579500
C	2.745400	5.770900	0.179300
H	3.140400	6.804200	0.369400
C	3.300900	5.264800	-1.172100
H	4.314900	5.680800	-1.393400
C	1.116600	5.490600	-2.273200
H	0.856000	4.402700	-2.179900
C	0.676500	6.036300	-3.636300
H	1.404900	5.763200	-4.423600
H	-0.338800	5.669400	-3.889300
O	3.368500	3.800700	-1.150100
O	5.823100	4.563900	0.026300
H	5.149400	4.741100	0.758100
O	7.851000	2.309500	0.098300
H	7.426000	1.539000	0.579600
O	6.407600	0.513000	-0.944100
O	5.816000	1.619500	-2.873400
O	3.403600	3.266000	-4.182200
H	2.978900	3.876200	-3.522200
O	7.336200	-1.225500	1.169800
H	6.952100	-1.358700	2.070000
O	5.315200	-3.470300	1.149300
O	6.061700	-2.838900	-2.398700
O	8.608300	-1.531000	-3.227400
C	4.666500	3.332200	-1.679900
H	5.024400	4.085000	-2.421100
C	5.624500	3.236700	-0.469200
H	5.201000	2.580700	0.335300
C	6.998600	2.740000	-0.963800
H	7.576000	3.561700	-1.443400
C	6.825000	1.502700	-1.890800
H	7.734600	1.236200	-2.467900
C	4.486900	1.968700	-2.359500
H	4.187400	1.159700	-1.634200
C	3.593100	1.969400	-3.606300
H	4.073600	1.399900	-4.427000
H	2.598900	1.533300	-3.367200
C	6.861500	-0.851100	-1.096900
H	7.983900	-0.872100	-1.080900
C	6.305700	-1.473200	0.190500
H	5.359300	-0.942100	0.519700
C	6.119600	-2.994900	0.083600
H	7.101300	-3.508600	0.250600
C	5.521500	-3.461400	-1.258000
H	5.718300	-4.544200	-1.456900
C	6.290100	-1.406400	-2.410200
H	5.301700	-0.922700	-2.624500
C	7.244100	-1.248500	-3.611300
H	7.024100	-2.037900	-4.361900
H	7.139000	-0.248900	-4.067100
I	1.581900	-0.034400	5.262200
I	2.667700	-2.890800	2.897800
I	3.964100	0.840900	2.260700
I	-2.045900	0.907400	4.334200
I	2.943100	-1.502700	-0.687100
I	0.936200	3.243500	3.137500
I	-0.724300	-0.208600	-1.848600

C	-2.612100	4.275300	-1.939600
H	-1.722400	3.913400	-1.350500
C	-2.912700	3.350100	-3.128900
H	-3.732500	3.735400	-3.761600
H	-2.001100	3.217200	-3.743500
C	0.581600	6.283500	-1.067200
H	0.682700	7.382200	-1.207300
C	1.206200	5.801700	0.256200
H	0.766600	4.813300	0.579500
C	2.745400	5.770900	0.179300
H	3.140400	6.804200	0.369400
C	3.300900	5.264800	-1.172100
H	4.314900	5.680800	-1.393400
C	1.116600	5.490600	-2.273200
H	0.856000	4.402700	-2.179900
C	0.676500	6.036300	-3.636300
H	1.404900	5.763200	-4.423600
H	-0.338800	5.669400	-3.889300
O	3.368500	3.800700	-1.150100
O	5.823100	4.563900	0.026300
H	5.149400	4.741100	0.758100
O	7.851000	2.309500	0.098300
H	7.426000	1.539000	0.579600
O	6.407600	0.513000	-0.944100
O	5.816000	1.619500	-2.873400
O	3.403600	3.266000	-4.182200
H	2.978900	3.876200	-3.522200
O	7.336200	-1.225500	1.169800
H	6.952100	-1.358700	2.070000
O	5.315200	-3.470300	1.149300
O	6.061700	-2.838900	-2.398700
O	8.608300	-1.531000	-3.227400
C	4.666500	3.332200	-1.679900
H	5.024400	4.085000	-2.421100
C	5.624500	3.236700	-0.469200
H	5.201000	2.580700	0.335300
C	6.998600	2.740000	-0.963800
H	7.576000	3.561700	-1.443400
C	6.825000	1.502700	-1.890800
H	7.734600	1.236200	-2.467900
C	4.486900	1.968700	-2.359500
H	4.187400	1.159700	-1.634200
C	3.593100	1.969400	-3.606300
H	4.073600	1.399900	-4.427000
H	2.598900	1.533300	-3.367200
C	6.861500	-0.851100	-1.096900
H	7.983900	-0.872100	-1.080900
C	6.305700	-1.473200	0.190500
H	5.359300	-0.942100	0.519700
C	6.119600	-2.994900	0.083600
H	7.101300	-3.508600	0.250600
C	5.521500	-3.461400	-1.258000
H	5.718300	-4.544200	-1.456900
C	6.290100	-1.406400	-2.410200
H	5.301700	-0.922700	-2.624500
C	7.244100	-1.248500	-3.611300
H	7.024100	-2.037900	-4.361900
H	7.139000	-0.248900	-4.067100
I	1.581900	-0.034400	5.262200
I	2.667700	-2.890800	2.897800
I	3.964100	0.840900	2.260700
I	-2.045900	0.907400	4.334200
I	2.943100	-1.502700	-0.687100
I	0.936200	3.243500	3.137500
I	-0.724300	-0.208600	-1.848600

I	-0.992300	-2.841700	3.926300
I	-2.236900	2.348900	0.791400
I	-0.147300	-3.488000	0.142500
I	1.896600	2.425300	-0.502300
I	-3.183000	-1.203300	1.215400
B	1.441700	-1.339200	2.187800
B	0.903700	-0.111100	3.291600
B	1.956200	0.290300	1.965400
B	0.619600	1.323000	2.353600
B	0.166300	-1.656100	1.071800
B	1.504700	-0.657900	0.587400
B	-0.203500	-1.321600	2.730100
B	-0.672100	1.037600	1.221700
B	-0.121800	-0.215800	0.164200
B	0.984800	0.989200	0.702200
B	-0.714000	0.332800	2.817700
B	-1.179300	-0.638600	1.466000
C	-9.258300	2.832700	-1.144900
C	-10.279700	2.035800	-0.310200
H	-9.752900	3.624700	-1.733100
H	-8.441500	3.270900	-0.541300
C	-9.653700	1.360500	0.898200
H	-10.826400	1.310600	-0.958800
H	-10.388400	0.765400	1.451000
H	-8.847500	0.665600	0.575800
H	-9.203600	2.070900	1.597800
O	-11.327700	2.937800	0.092600
H	-11.017400	3.545600	0.788300
C	-1.082700	-6.560300	-4.720900
C	-1.894700	-7.723400	-4.127900
H	-0.104300	-6.445000	-4.211500
H	-0.918700	-6.660800	-5.807800
C	-2.284700	-8.787200	-5.145600
H	-2.789300	-7.322800	-3.584400
H	-2.887100	-9.580100	-4.691500
H	-2.879100	-8.349800	-5.957800
H	-1.399200	-9.257600	-5.589400
O	-0.991000	-8.301300	-3.147600
H	-1.417000	-9.041700	-2.677700
C	9.571500	-0.473000	-3.406700
C	10.051400	-0.025700	-2.009700
H	9.163100	0.379600	-3.977500
H	10.372000	-0.957000	-3.993600
C	11.546700	-0.214300	-1.791800
H	9.451500	-0.555000	-1.218800
H	11.838400	0.116600	-0.787600
H	11.839600	-1.264200	-1.896900
H	12.127800	0.384400	-2.503300
O	9.758400	1.384800	-1.962800
H	9.507000	1.671800	-1.042700
C	-0.190800	8.163400	-4.452100
C	-0.488800	9.488700	-3.729700
H	-1.118800	7.586200	-4.628500
H	0.359000	8.296900	-5.397200
C	-0.510800	10.689700	-4.667400
H	0.227600	9.632500	-2.886300
H	-0.748400	11.611700	-4.125800
H	0.455400	10.832600	-5.163200
H	-1.279100	10.569300	-5.442200
O	-1.817300	9.301900	-3.188300
H	-1.955400	9.863000	-2.401900
H	-3.811800	1.236000	2.377800
H	-4.273500	0.658600	-0.364500
H	2.927900	4.072100	1.284300
H	4.418500	-2.945700	1.193500

I	-0.992300	-2.841700	3.926300
I	-2.236900	2.348900	0.791400
I	-0.147300	-3.488000	0.142500
I	1.896600	2.425300	-0.502300
I	-3.183000	-1.203300	1.215400
B	1.441700	-1.339200	2.187800
B	0.903700	-0.111100	3.291600
B	1.956200	0.290300	1.965400
B	0.619600	1.323000	2.353600
B	0.166300	-1.656100	1.071800
B	1.504700	-0.657900	0.587400
B	-0.203500	-1.321600	2.730100
B	-0.672100	1.037600	1.221700
B	-0.121800	-0.215800	0.164200
B	0.984800	0.989200	0.702200
B	-0.714000	0.332800	2.817700
B	-1.179300	-0.638600	1.466000
C	-9.258300	2.832700	-1.144900
C	-10.279700	2.035800	-0.310200
H	-9.752900	3.624700	-1.733100
H	-8.441500	3.270900	-0.541300
C	-9.653700	1.360500	0.898200
H	-10.826400	1.310600	-0.958800
H	-10.388400	0.765400	1.451000
H	-8.847500	0.665600	0.575800
H	-9.203600	2.070900	1.597800
O	-11.327700	2.937800	0.092600
H	-11.017400	3.545600	0.788300
C	-1.082700	-6.560300	-4.720900
C	-1.894700	-7.723400	-4.127900
H	-0.104300	-6.445000	-4.211500
H	-0.918700	-6.660800	-5.807800
C	-2.284700	-8.787200	-5.145600
H	-2.789300	-7.322800	-3.584400
H	-2.887100	-9.580100	-4.691500
H	-2.879100	-8.349800	-5.957800
H	-1.399200	-9.257600	-5.589400
O	-0.991000	-8.301300	-3.147600
H	-1.417000	-9.041700	-2.677700
C	9.571500	-0.473000	-3.406700
C	10.051400	-0.025700	-2.009700
H	9.163100	0.379600	-3.977500
H	10.372000	-0.957000	-3.993600
C	11.546700	-0.214300	-1.791800
H	9.451500	-0.555000	-1.218800
H	11.838400	0.116600	-0.787600
H	11.839600	-1.264200	-1.896900
H	12.127800	0.384400	-2.503300
O	9.758400	1.384800	-1.962800
H	9.507000	1.671800	-1.042700
C	-0.190800	8.163400	-4.452100
C	-0.488800	9.488700	-3.729700
H	-1.118800	7.586200	-4.628500
H	0.359000	8.296900	-5.397200
C	-0.510800	10.689700	-4.667400
H	0.227600	9.632500	-2.886300
H	-0.748400	11.611700	-4.125800
H	0.455400	10.832600	-5.163200
H	-1.279100	10.569300	-5.442200
O	-1.817300	9.301900	-3.188300
H	-1.955400	9.863000	-2.401900
H	-3.811800	1.236000	2.377800
H	-4.273500	0.658600	-0.364500
H	2.927900	4.072100	1.284300
H	4.418500	-2.945700	1.193500