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

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ABSTRACT $Na_2B_{12}I_{12}$ has many of the properties desired by an X-ray contrast agent but is lethal at the concentrations needed for medical imaging. We demonstrate here that PBS solutions with > 50 mM $Na_2B_{12}I_{12}$ induce hemolysis, consistent with the previously reported superchaotropic nature of the anion. The presence of < 1 equiv of 2-hydroxypropyl-γ-cyclodextrin prevents hemolysis and suggests a strategy for exploiting $B_{12}I_{12}^{2-}$ as an X-ray contrast agent.

Although recent developments in magnetic resonance and nuclear imaging are driving advancement in medical diagnosis, X-ray imaging remains the most common form of medical imaging, allowing for rapid, non-invasive diagnosis.[1] X-ray tubes used in medical imaging typically contain a tungsten anode and, when operated between 50 and 150 kV, emit radiation with wavelengths ranging from 50 to 9 nm.[2] Radiographic contrast depends on the differences in the extent to which the imaged materials absorb the X-rays used (i.e., radiopacity), which in turn generally scales with the atomic numbers of the elements in those materials. As a result, Ca-containing bone material contrasts well with soft tissues that predominantly contain C, H, N, and O. Contrast between soft tissues can be obtained by introducing an X-ray contrast agent (XCA) of greater or lesser radiopacity.[3] An example of the former is the use of suspended $BaSO_4$ to image the gastrointestinal tract and an example of the latter is the injection of air into a joint to visualize the articular space. In many cases, e.g., when blockage or pressure is a concern, a soluble XCA is used. The most common soluble XCAs feature iodoarene rings functionalized with water-solubilizing groups. Although these iodinated species are generally well tolerated, some individuals reportedly suffer from contrast-induced nephropathy or disruption of thyroid function.[4-5]

The similarities between arenes and *closo*-boranes have led to the investigation of the latter as a motif in drug design.[6] In particular, the icosahedral *closo*-dodecaborate scaffold, which occupies a volume approximately the same as that of an adamantyl group and roughly 50% larger than that of the sphere described by a rotating phenyl ring,[7] provides a rigid and biostable icosahedral framework upon which to construct functional molecules.[8] In the context of XCA design, it is noteworthy that modern iodine-containing XCAs feature 1,3,5-triiodophenyl groups (Fig. 1).[3] Although periodinated rings would afford greater contrast, they severely impair

solubility. In contrast, the periodinated $B_{12}I_{12}^{2-}$ forms salts that are highly water-soluble. For example, $Na_2B_{12}I_{12}$ is 90% iodine by mass and can be prepared as solutions with > 200 mM concentration (>300 mg iodine mL^{-1}).

Given the high iodine content and water solubility of $Na_2B_{12}I_{12}$, it is unsurprising that in the same year that the synthesis of this salt was first reported,[9] it was investigated as an intravascular XCA.[10] This study found $Na_2B_{12}I_{12}$ to be toxic to mice and cats and the investigators concluded that further development of the compound for this application would be inappropriate and, indeed, no further reports appeared.[‡] The origin of the toxicity of $Na_2B_{12}I_{12}$ remained unexplained and seemed unlikely to stem from its chemical reactivity. Indeed, part of the original interest in using $B_{12}I_{12}^{2-}$ salts for biological applications stemmed from the stability of the B—B and B—I bonds and the distinct *lack* of reactivity of the cluster: earlier reports describe the $B_{12}I_{12}^{2-}$ ion being unchanged after treatment with $Cl_{2\,(g)}$, heating to 85 °C in 5 M NaOH, or heating to 150 °C in neat H_2SO_4.[9] We confirmed the inertness of the cluster under biologically relevant conditions by demonstrating a lack of any new ^{11}B NMR signals after refluxing $Na_2B_{12}I_{12}$ in phosphate-buffered saline (PBS, pH 7.4) for 1 h. There was also an absence of new signals after 24 h incubation at room temperature with a suspension of human red blood cells (RBCs), bovine serum, or defibrinated bovine blood (Fig. S1).

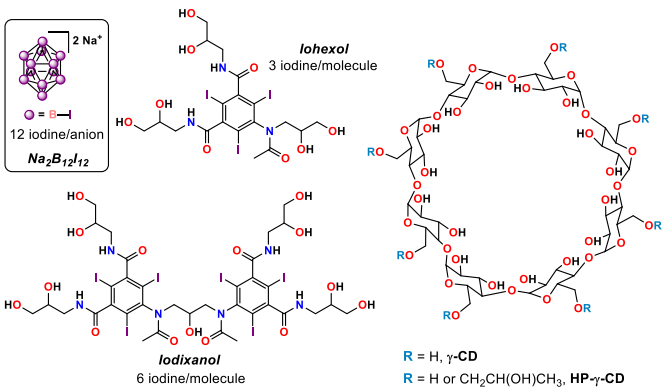

Fig. 1 Chemical structures of $Na_2B_{12}I_{12}$, two examples of commercially used iodinated XCAs (iohexol and iodixanol), γ-cyclodextrin (γ-CD), and 2-hydroxypropyl-γ-cyclodextrin (HP-γ-CD).

Insight into the biological effects of $B_{12}I_{12}^{2-}$ can be gleaned from more recent physical inorganic studies of the $B_{12}X_{12}^{2-}$ anions, where X = F, Cl, Br, or I. In aqueous solution, these ions are readily encapsulated in an appropriately sized supramolecular host molecule (e.g., cucurbituril, cyclodextrin, calixarene).[11-12] Interestingly, the process is not governed by the entropy-driven hydrophobic effect but rather the enthalpy-driven chaotropic effect. In fact, because $B_{12}X_{12}^{2-}$ ions exhibit a chaotropism that far outstrips that of the classical Hofmeister series chaotropes, they are termed *superchaotropes*.[13] One manifestation of this chaotropism is the ability of $B_{12}X_{12}^{2-}$ ions to enhance the release of cargo from liposomes.[14-16] We reasoned that, at the high concentrations needed to function as an XCA, the superchaotropic activity of $B_{12}I_{12}^{2-}$ was disrupting the integrity of cell membranes. We observed that exposure of human RBCs to 100 mM $Na_2B_{12}I_{12}$ resulted in rapid hemolysis, as judged by clarification of the suspension. The dose dependence of this hemolytic effect was explored by suspending RBCs in a PBS solution of $Na_2B_{12}I_{12}$ for 10 s, followed by rapid centrifugation to pellet the cells, and removal of the supernatant. The extent of hemolysis was determined by measuring the absorbance of the hemoglobin (Hb) in the supernatant (Fig. 2).

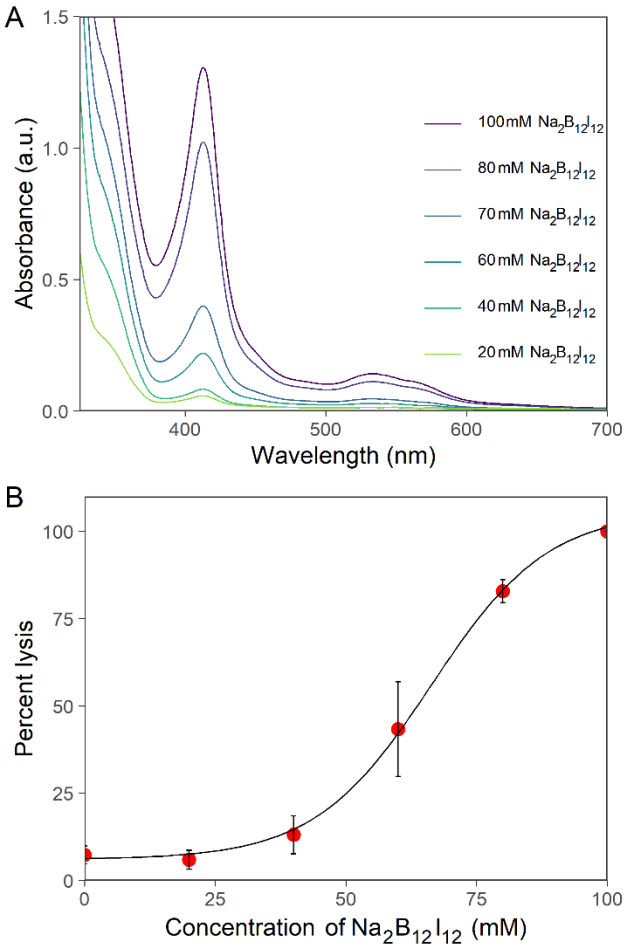

Fig. 2 A) Hb release from RBCs suspended in PBS (pH 7.4) containing increasing concentrations of $Na_2B_{12}I_{12}$. B) Proportion of RBCs lysed by $Na_2B_{12}I_{12}$ on the basis of the absorption of the supernatant at 413 nm (Soret band) after pelleting. Error bars reflect ± SEM for three independent replicates and the fitted curve was obtained by logistic regression (IC_{50} = 66.33 mM).

If this hemolytic activity does indeed stem from the chaotropic activity of the borate anions, we hypothesized that encapsulation within a supramolecular host, which is driven by the same chaotropism, would prevent them from damaging cells. The interaction of $B_{12}I_{12}^{2-}$ with the most common biologically produced cyclodextrins (i.e., α-, β-, and γ-CD) has been previously explored by isothermal calorimetry and it interacts most strongly with γ-CD (Fig. 1; K_a = 6.7 x 10^4 L mol$^-$

[1]).[13] Single-crystal X-ray diffraction studies of $B_{12}Br_{12}^{2-}$/γ-CD show the perbrominated cluster to form a 2:1 complex with the cyclic oligosaccharide in the solid state.[13] We succeeded in growing crystals from a 2:1 mixture of γ-CD and $Na_2B_{12}I_{12}$ by allowing diethyl ether to diffuse into a DMF solution of the two species. ^{1}H and ^{11}B NMR spectra of solutions prepared from isolated crystals suggest that they contained both γ-CD and $B_{12}I_{12}^{2-}$, along with 4 equiv of DMF with respect to γ-CD (Fig. S5, S6). To confirm that the sample was not a mixture of γ-CD crystals and $Na_2B_{12}I_{12}$ crystals, isopycnic flotation density measurements were performed. The crystals all exhibited the same isopycnic point in a mixture of bromoform and hexanes. The measured density (ρ_{exp} = 1.6 g mL^{-1}) was greater than the calculated density of γ-CD (1.41 g mL^{-1} for the tetradecahydrate)[17] and below the calculated density of $Na_2B_{12}I_{12}\cdot 6DMF\cdot H_2O$ (2.19 g mL^{-1}, see ESI). This result is consistent with the present crystals containing both substances. Unfortunately, the crystals did not diffract beyond 1.5 Å (Fig. 3A), and no solution could be obtained by direct methods, Patterson methods, intrinsic phasing, or charge flipping.

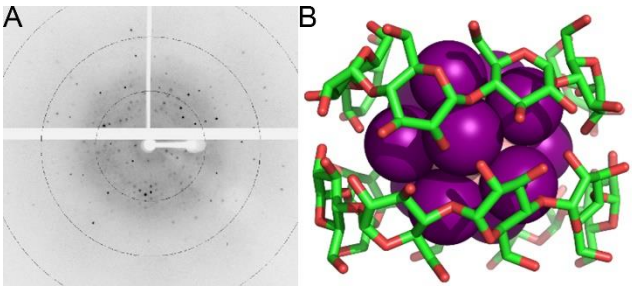

Fig. 3 A) X-ray diffraction (Cu Kα) from a crystal containing γ-CD, $Na_2B_{12}I_{12}$, and DMF showing clean, but low-resolution reflections. Circles are drawn at resolution levels of 3.66, 2.15, and 1.71 Å. B) Semi-empirically (PM6) optimized structure of a putative $[(\gamma\text{-CD})_2(B_{12}I_{12})]^{2-}$ complex based on cumulative crystallographic data and previous work with $B_{12}Br_{12}^{2-}$.[13] $B_{12}I_{12}^{2-}$ is shown as spheres and γ-CD as sticks. Color code: I purple, B pink, C green, O red.

Nevertheless, the diffraction pattern was indexed and exhibited cubic metric symmetry (a = 60.0168(13) Å), which was consistent with the fact that the crystals were perpetually extinguished when viewed between crossed polarizers. The volume of the unit cell (216,181 Å^3) is consistent with the composition (γ-CD)$_2$·$Na_2B_{12}I_{12}$·8DMF and Z = 48, if the non-H atoms have the chemically reasonable average volume of 19 Å^3;[18] the number of DMF molecules is consistent with the NMR data obtained from the crystals. The systematic absences and enantiomeric purity of the γ-CD narrow the possible space groups to F23 and F432. With Z = 48, the complex would reside on a general position in the former and on a 2-fold axis in the latter. In summary, although the structure could not be solved, the aggregate crystallographic data suggest that the crystals may contain a 2:1 complex of the type observed for $B_{12}Br_{12}^{2-}$.[13] A semi-empirical (PM6) geometry optimization confirms that such a host-guest complex is a minimum on the potential energy surface of this supramolecular system (Fig. 3B). We stress that the structure depicted in Fig. 3B is a theoretically optimized structure that, although consistent with the data collected from the crystals, was not obtained by refinement of a full crystal structure against the observed structure factors.

Although the X-ray diffraction data support the interaction of γ-CD with $B_{12}I_{12}^{2-}$, and suggest that they may form a 2:1 complex in the solid state, gas-phase experiments and solution-phase thermodynamic measurements indicate that the 1:1 complex predominates in solution.[13,19-20] To appropriately avoid deviation from ideal-solution behavior, the prior thermodynamic measurements were performed on relatively dilute solutions (< 0.5 mM).[11,13,21-22] Although $Na_2B_{12}I_{12}$ and γ-CD are both highly water-soluble, we have observed that PBS solutions containing > 6 mM of each species form an insoluble gel. Addition of PBS to dilute the mixture below this concentration produces fluid solutions. Unfortunately, as depicted in Fig. 2, $Na_2B_{12}I_{12}$ alone does not induce hemolysis at concentrations below 6 mM. Although the chaotropism-driven

complexation of $B_{12}I_{12}^{2-}$ by γ-CD may well prevent the physical interaction with cells that leads to hemolysis, the low solubility of the complex prevents us from investigating this effect.

We turned, therefore, to the more water-soluble 2-hydroxypropyl-γ-CD (HP-γ-CD).[§] Semi-empirical (PM6) geometry optimization calculations predicted that the hydroxypropyl groups would not significantly perturb the host-guest interaction, as compared to unfunctionalized γ-CD (Fig. 4). ^{11}B NMR spectroscopic experiments show that addition of HP-γ-CD to solutions of $Na_2B_{12}I_{12}$ produces a shift in the resonance for the cluster (Fig. S2). The method of continuous variation permitted the stoichiometry of the complexation between HP-γ-CD and $B_{12}I_{12}^{2-}$ to be determined, confirming that the two form a 1:1 complex in PBS (Fig. S3). Although the ^{11}B resonance broadens in addition to shifting downfield as the molar fraction of HP-γ-CD is increased, the sharp nature of the Job plot speaks to the strength of the interaction. Further detailed studies are needed to quantify the thermodynamic parameters characterizing the binding interaction.

As intended, the complex formed upon combination of $Na_2B_{12}I_{12}$ and HP-γ-CD is significantly more soluble than the complex with unfunctionalized γ-CD; no precipitation is observed upon combination of equivalent volumes of 200 mM $Na_2B_{12}I_{12}$ and 200 mM HP-γ-CD (affording a 100 mM solution of the complex).

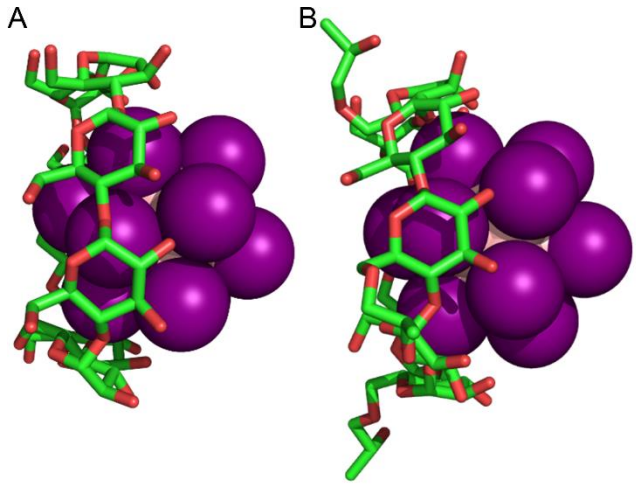

Fig. 4 Semi-empirically (PM6) optimized structures of (A) $[(\gamma\text{-CD})(B_{12}I_{12})]^{2-}$ and (B) $[(\text{HP-}\gamma\text{-CD})(B_{12}I_{12})]^{2-}$ highlighting that the 2-hydroxypropyl groups in the latter do not impact the binding of $B_{12}I_{12}^{2-}$. Note that the HP-γ-CD used in this work featured an average of between four and five 2-hydroxypropyl groups. The calculations were performed with four HP groups on alternating glucose units. $B_{12}I_{12}^{2-}$ is shown as spheres and γ-CD as sticks. Color code: I purple, B pink, C green, O red.

We next performed the Hb-release hemolysis assay by suspending RBCs in solutions that featured a consistent concentration of $Na_2B_{12}I_{12}$ (100 mM) but a systematic increase in the concentration of HP-γ-CD. As was also demonstrated in Fig. 2, these experiments confirm that in the absence of cyclodextrin, 100 mM $Na_2B_{12}I_{12}$ results in complete hemolysis. Strikingly, the presence of even small amounts of HP-γ-CD results in a drastic decrease in hemolysis (Fig. 5).

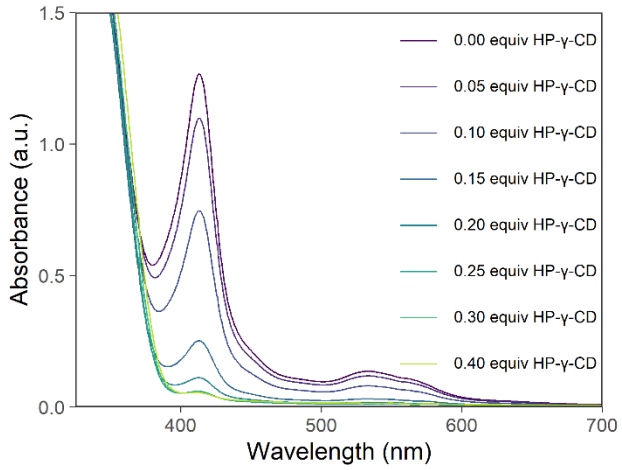

Fig. 5 Hb release from RBCs suspended in PBS (pH 7.4) containing 100 mM $Na_2B_{12}I_{12}$ with addition of increasing amounts of HP-γ-CD.

This attenuation of hemolysis increases with increasing HP-γ-CD concentration until it falls to near-baseline levels upon the addition of 0.4 equiv (Fig. 5). This protection was also

maintained over periods reflective of the time over which an XCA would remain in circulation:[23] RBC incubation with 100 mM $Na_2B_{12}I_{12}$ and 50 mM HP-γ-CD (0.5 equiv) for either 4 h or 24 h resulted in no hemolysis (Fig. S7).

These results show that $Na_2B_{12}I_{12}$ induces rapid hemolysis at the concentrations used in medical imaging. This disruption of cell structure may be the origin of the previously reported toxicity of $Na_2B_{12}I_{12}$ and likely arises from the superchaotropic nature of the $B_{12}I_{12}^{2-}$ anions. This hypothesis is corroborated by the ability of γ-CD, which binds to $B_{12}I_{12}^{2-}$ because of its superchaotropic nature, to inhibit hemolysis. X-ray crystallography suggests that, in the solid state, $B_{12}I_{12}^{2-}$ may interact with γ-CD in the same manner as previously reported for $B_{12}Br_{12}^{2-}$: formation of a 2:1 γ-CD:borate complex. Prior solution-phase data support the formation of a 1:1 complex in solution. Unfortunately, the complex formed upon addition of $Na_2B_{12}I_{12}$ to γ-CD exhibits water solubility that is too low to observe any hemolysis-protective effect. The derivatized cyclic oligosaccharide HP-γ-CD forms a 1:1 complex with $B_{12}I_{12}^{2-}$ that is much more water-soluble. The protective effect of HP-γ-CD can be observed in hemolysis assays, where it can prevent cell destruction when added at substoichiometric levels. The 100 mM solutions of $Na_2B_{12}I_{12}$ with 0.4 equiv of HP-γ-CD feature an iodine concentration of 153 mg iodine mL^{-1}; further studies are underway to determine whether concentrations reaching those used in medical imaging (e.g., 300 mg iodine mL^{-1}) can be achieved with this strategy.

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There are no conflicts to declare.

NOTES

‡ The chemistry of other iodoboranes and iodocarboranes has been explored,[24-28] and potential XCA applications were mentioned as motivations for this work but, to the best of our knowledge, none of these compounds have been subsequently explored as imaging agents.

§ In the work presented here, HP-γ-CD refers to a material in which 60% of O6-positions of the γ-CDs are functionalized with 2-hydroxypropyl groups and the average M_W is ≈ 1580 Da.

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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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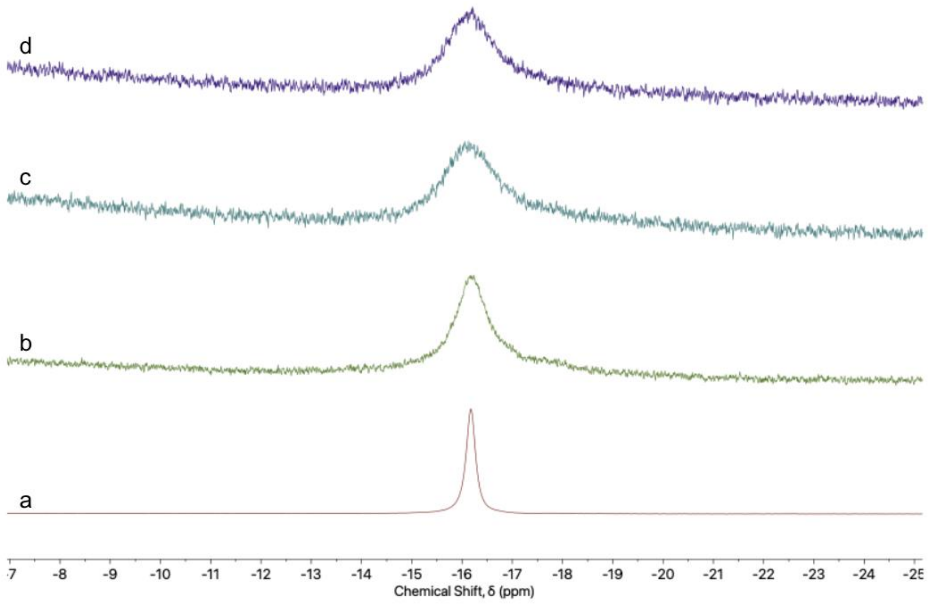

Figure S1. Stacked ^{11}B NMR spectra (160 MHz) of $Na_2B_{12}I_{12}$ in a) 10:1 PBS:D_2O after heating at 100 °C for 1 h; b) RBC suspension with 9% D_2O after incubating at room temperature for 24 h; c) defibrinated bovine blood with 9% D_2O after incubating at room temperature for 24 h; d) bovine serum 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.

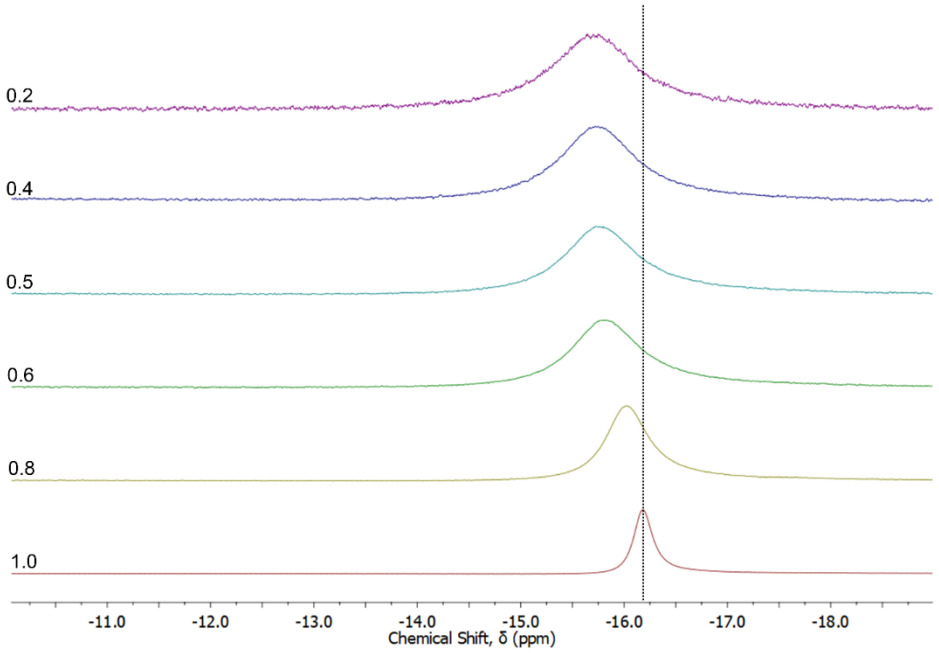

Figure S2. Stacked ^{11}B NMR spectra (10:1 PBS:D_2O, 160 MHz) of mixtures of $Na_2B_{12}I_{12}$ and HP-γ-CD with a combined concentration of 10 mM. Indicated next to each trace is the mole fraction of $Na_2B_{12}I_{12}$. Dotted line marks the position of the unperturbed $Na_2B_{12}I_{12}$.

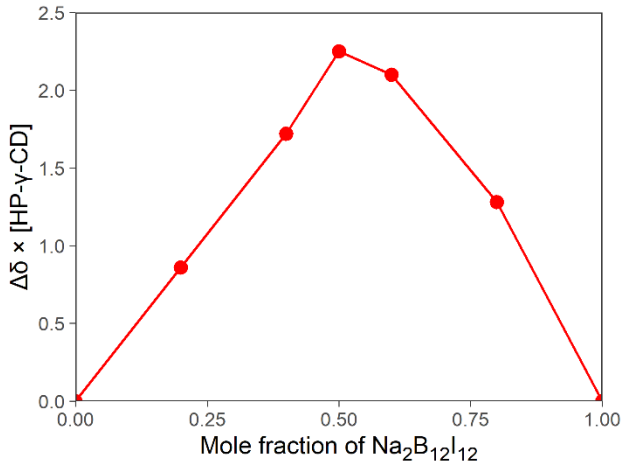

Figure S3. Job plot for the interaction of $Na_2B_{12}I_{12}$ and HP-γ-CD based on the NMR spectra in Figure S2.

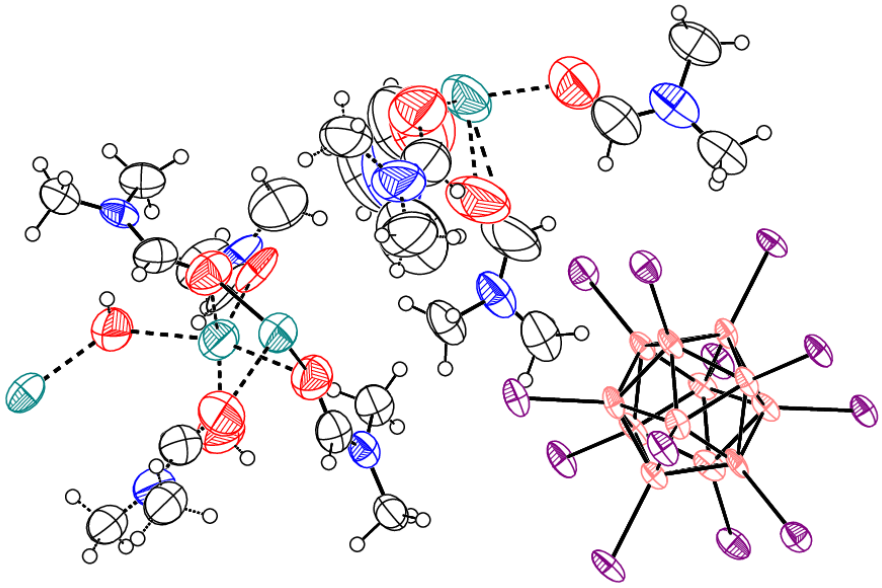

Figure S4. Thermal ellipsoid plot (50% probability level) of $Na_2B_{12}I_{12}$·6DMF·H_2O. Color code: B pink, I purple, Na teal, N blue, O red, C grey, H white spheres of arbitrary radius.

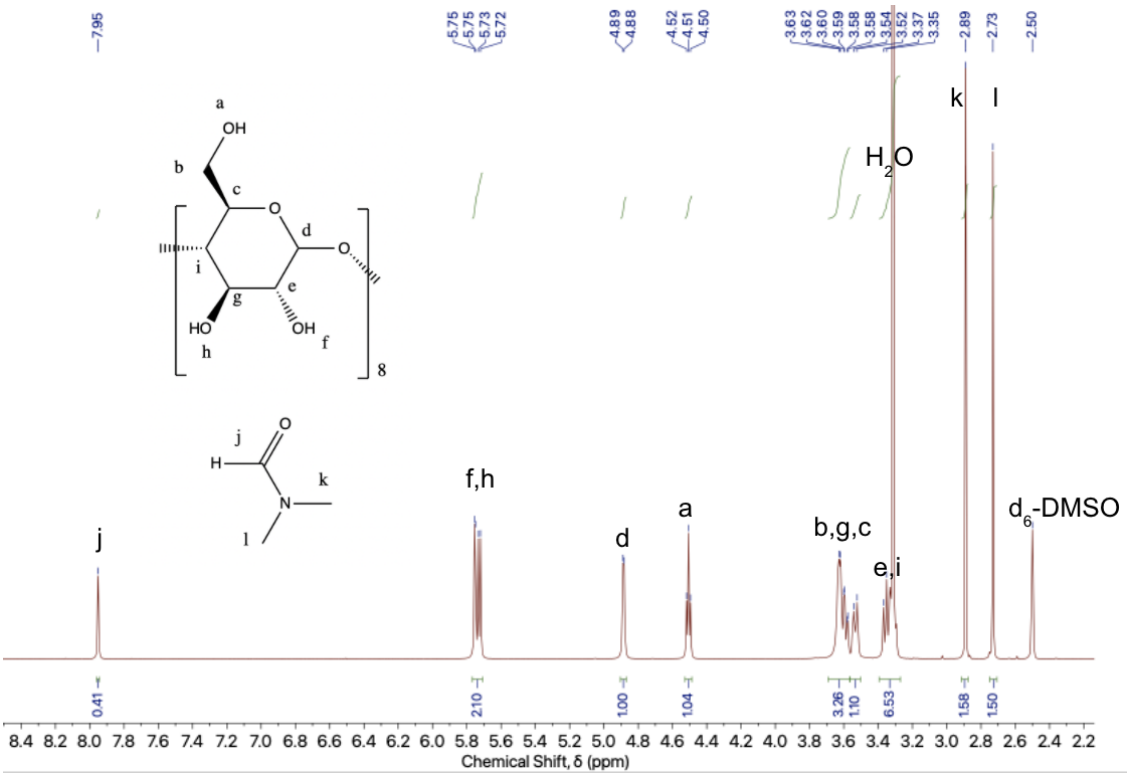

Figure S5. ^{1}H NMR spectrum (d_6-DMSO, 500 MHz) of dissolved of $Na_2B_{12}I_{12}$/γ-CD crystals.

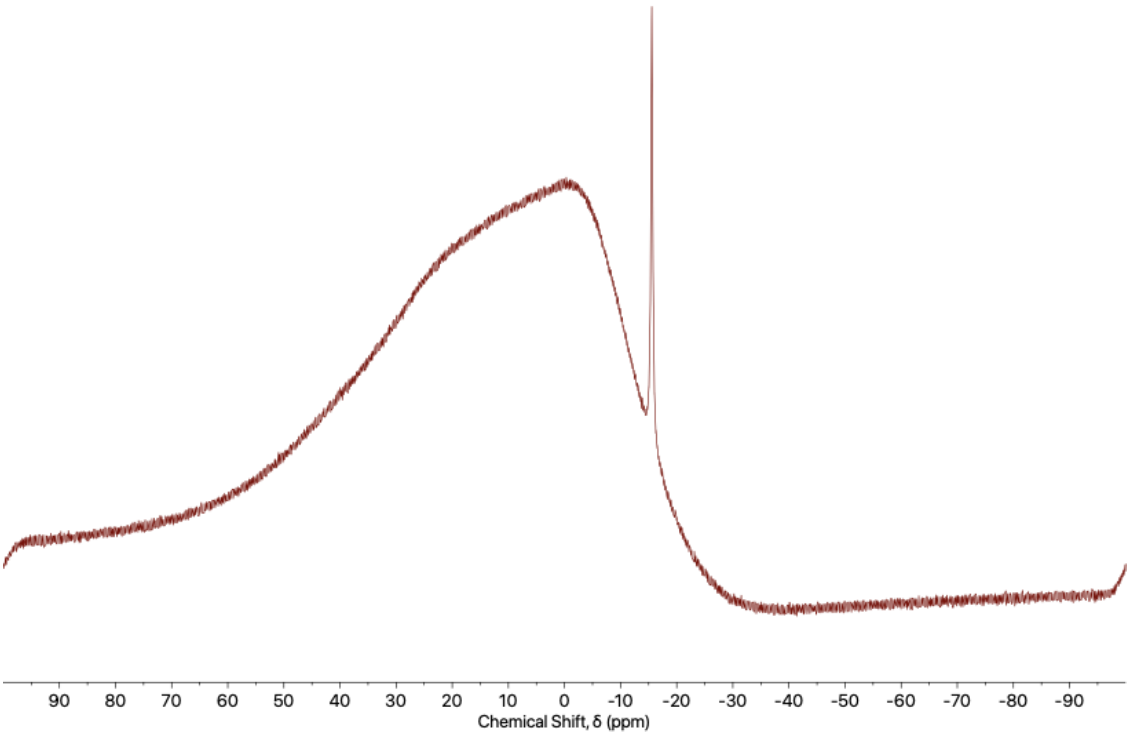

Figure S6. ^{11}B NMR spectrum (d_6-DMSO, 160 MHz) of complex of dissolved of $Na_2B_{12}I_{12}$/γ-CD crystals.

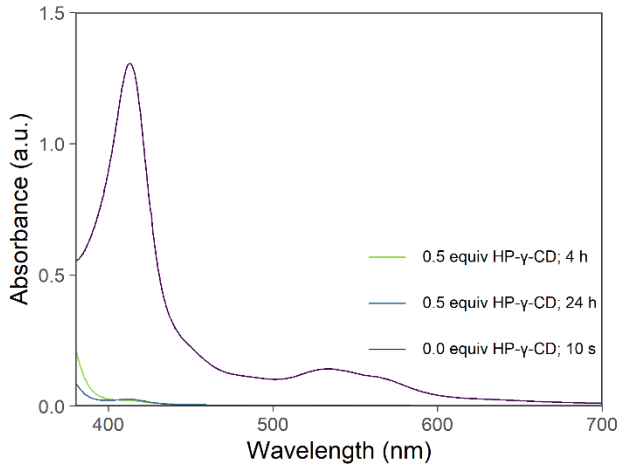

Figure S7. Hb release from RBCs suspended for extended periods (4 h or 24 h) in PBS (pH 7.4) containing 100 mM $Na_2B_{12}I_{12}$ and 50 mM HP-γ-CD. Hb release within 10 s in the absence of HP-γ-CD (reproduced from Figure 5) included for reference.

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