

Pi-Extended Hypervalent Iodine Macrocycles and Their Supramolecular Assembly with Buckminster Fullerene

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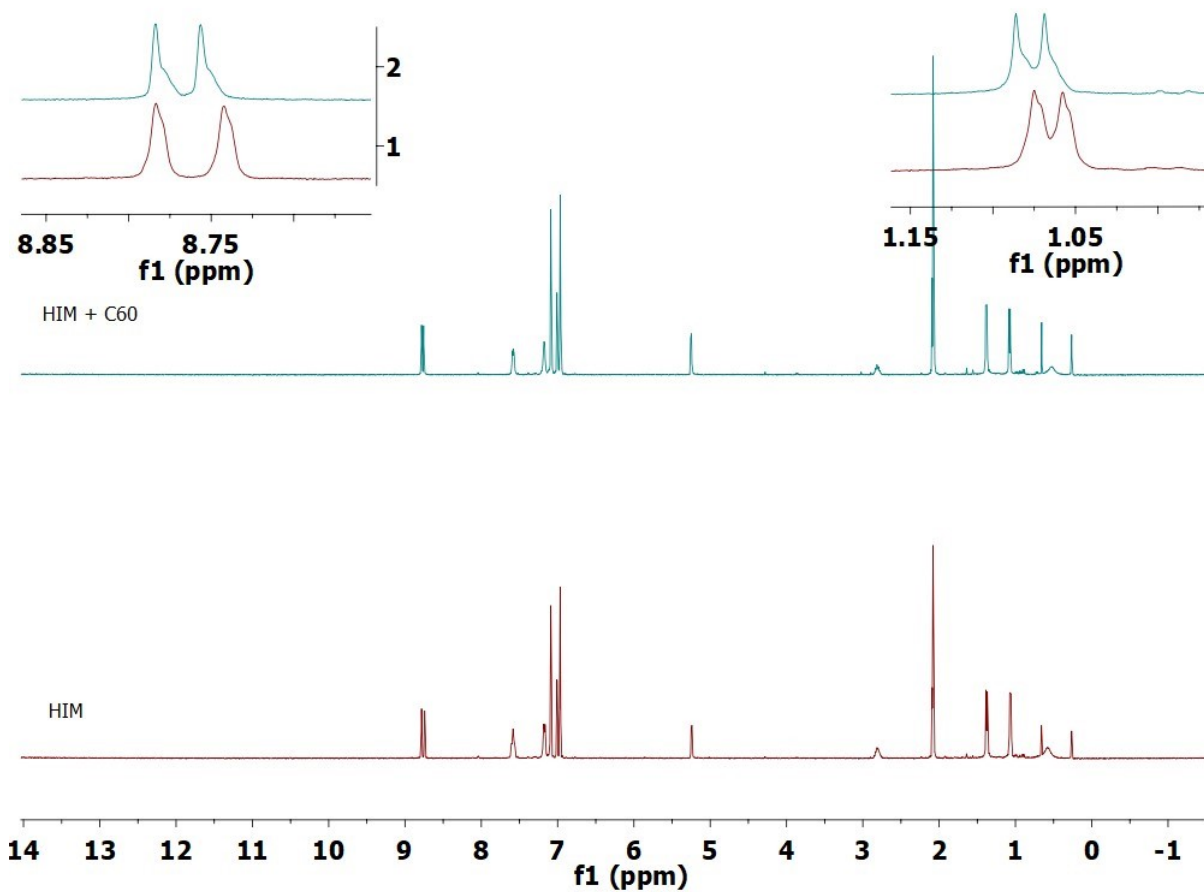
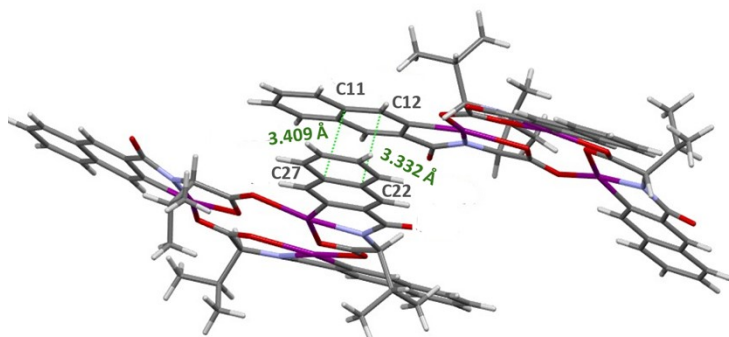


Figure SI1: ^1H NMR (400 MHz, 298 K) of HIM **6** before and after the addition of C₆₀ in deuterated toluene. The aromatic doublet at 8.74 ppm shifts to 8.76 ppm. Similar shifting was also noticed for methyl signal within the aliphatic region, where the signal originally detected at 1.06 ppm shifted to 1.07 ppm.

1.HIM and C₆₀ NMR study

2.HIM/C₆₀ co-crystal information



Carbon atoms	Pi-Pi stacking distance (Å)
C11-C27	3.409
C12-C22	3.332

Table S11. Pi-Pi stacking distances between Naphthalene HIM-Naphthalene HIM

Figure S12: Crystal structure showing π - π interactions between naphthalene- naphthalene pairs. The π - π distance between C11-C27 and C12-C22 are 3.409Å and 3.332Å.

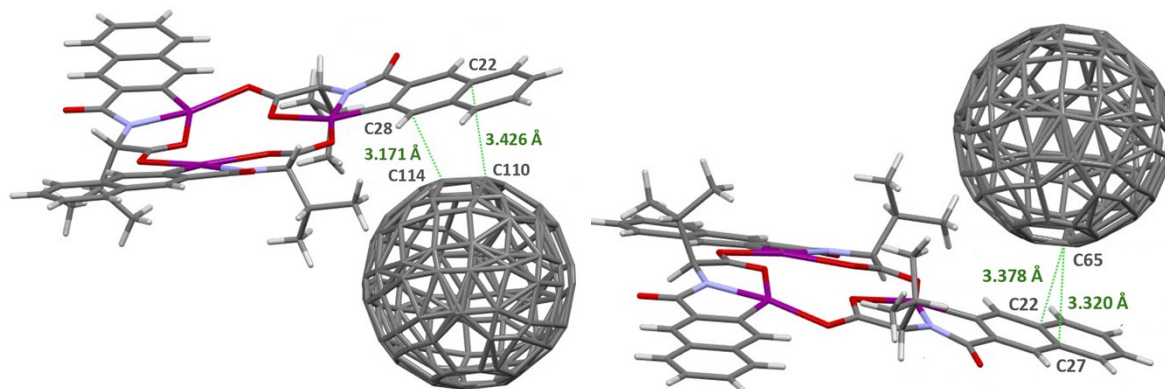


Figure S13: Crystal structure showing π - π interactions between naphthalene-fullerene pairs. Left) The π - π distance between C28-C114 and C22-C110 are 3.171Å and 3.426Å respectively. Right) The π - π distance between C22-C65 and C27-C65 are 3.378Å and 3.320Å respectively.

3. Assignment of protons in Val-HIM 6b (Naphthalene system)

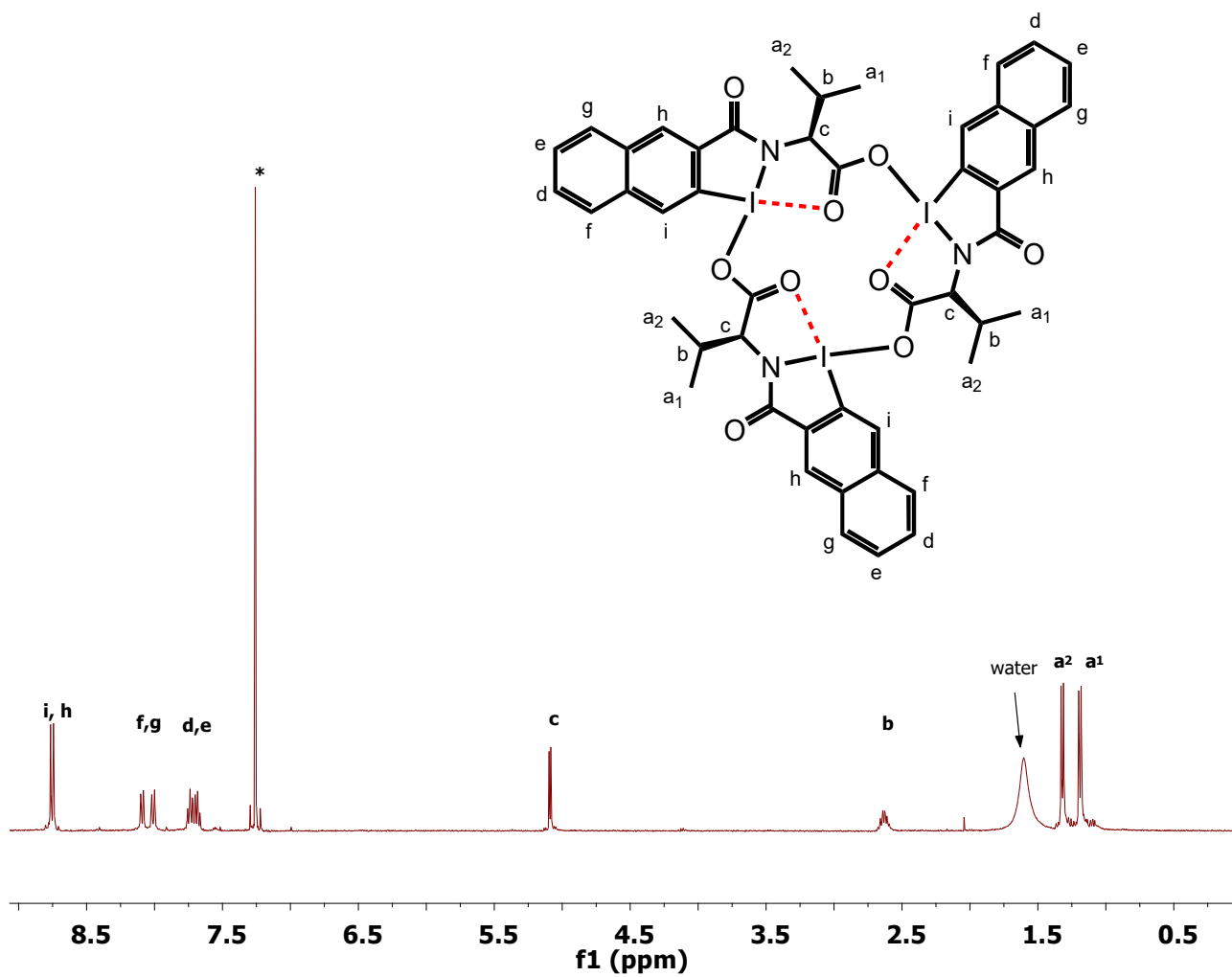


Figure S14: ¹H NMR (400 MHz, 298 K) spectra of **6b** in CDCl₃. * Denoted solvent CDCl₃ peak

Assignment of protons in Val-HIM 6c (Anthraquinone system)

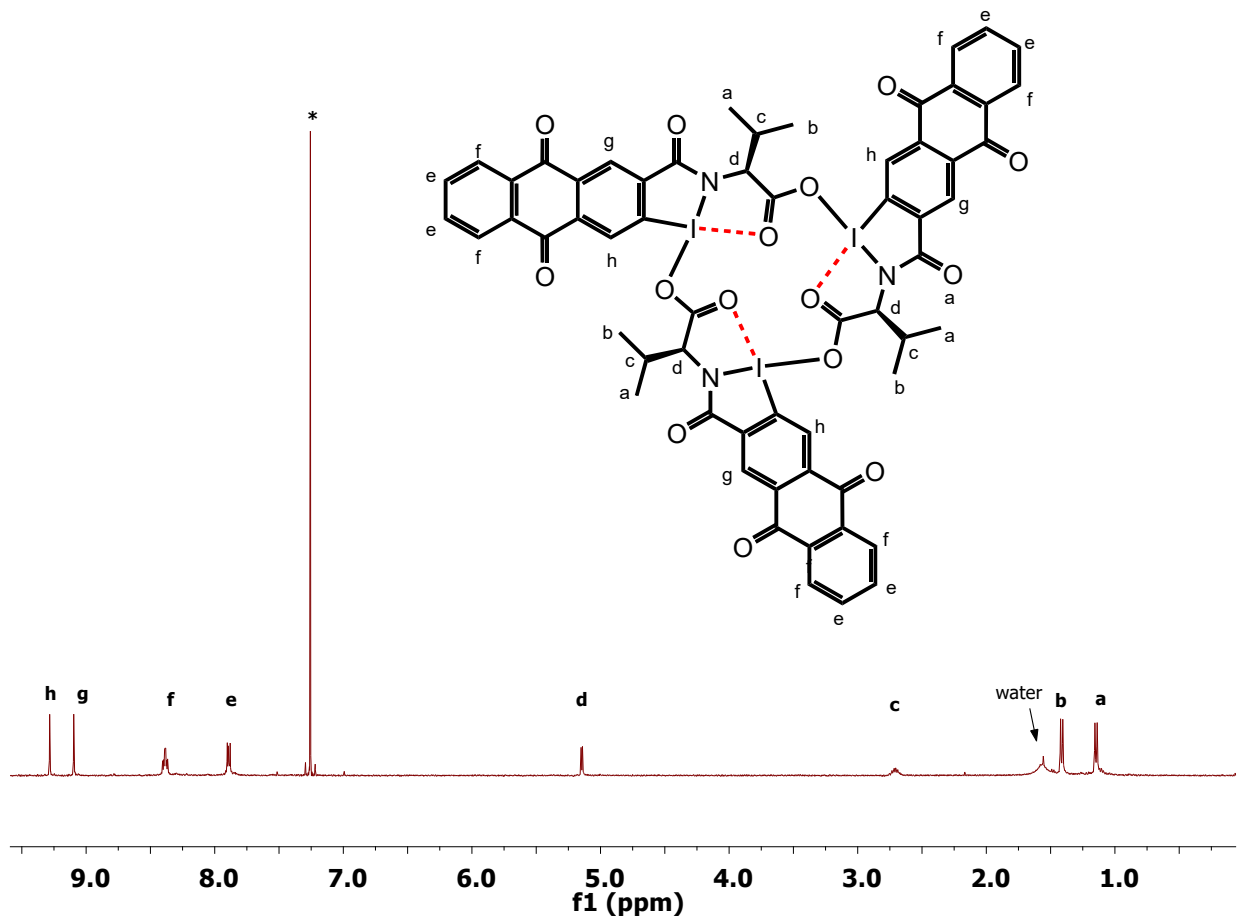


Figure S15: ¹H NMR (400 MHz, 298 K) spectra of 6c in CDCl₃. *Residual CHCl₃ peak from the NMR

4.NMR Titrations

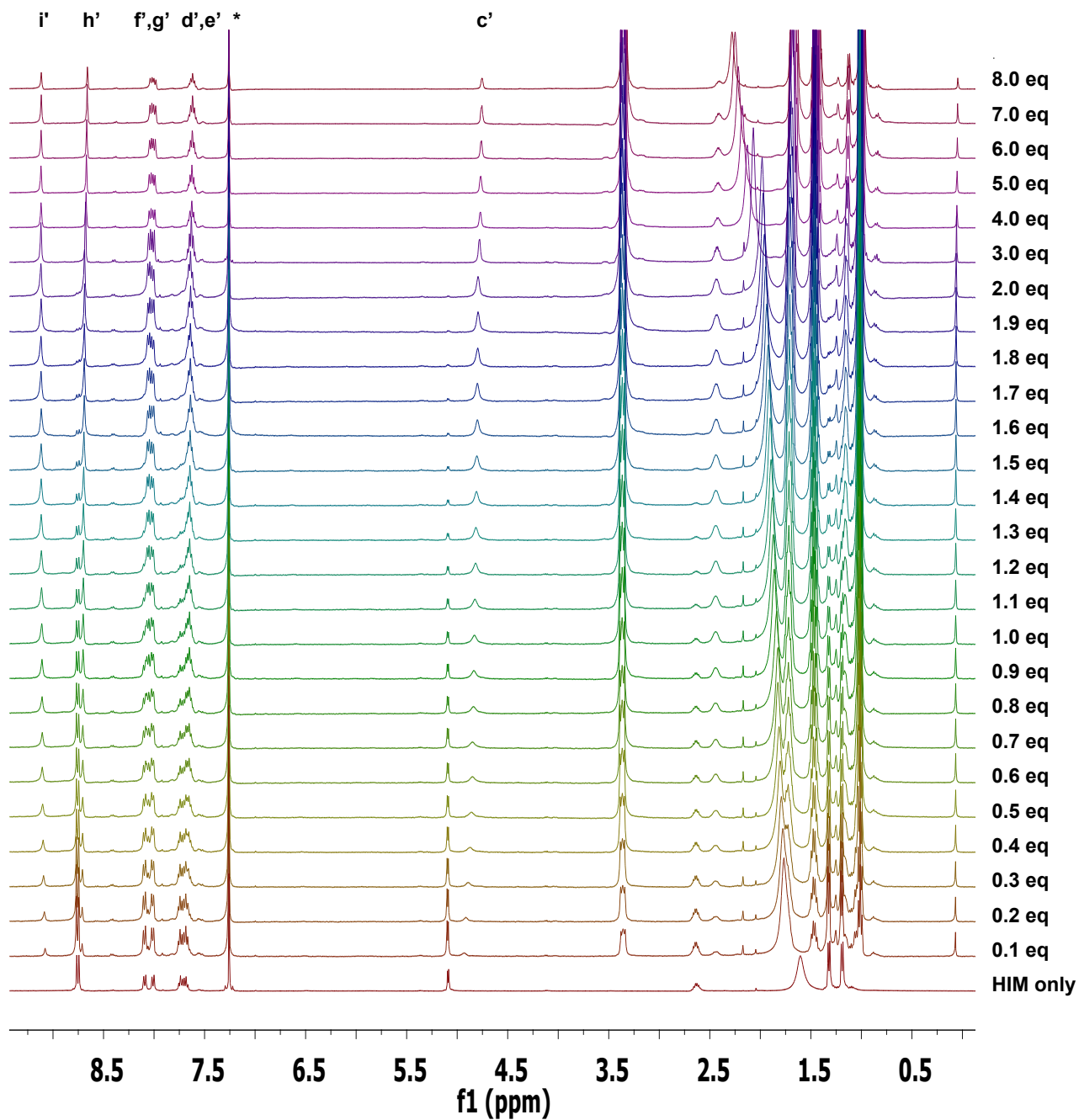


Figure SI6: ^1H NMR (400 MHz, 298 K) titration of **6b** with TBA(Cl) at an incremental equivalency (0 to 8 equivalents TBA(Cl) in CDCl_3 . *Residual CHCl_3 peak from the NMR solvent.

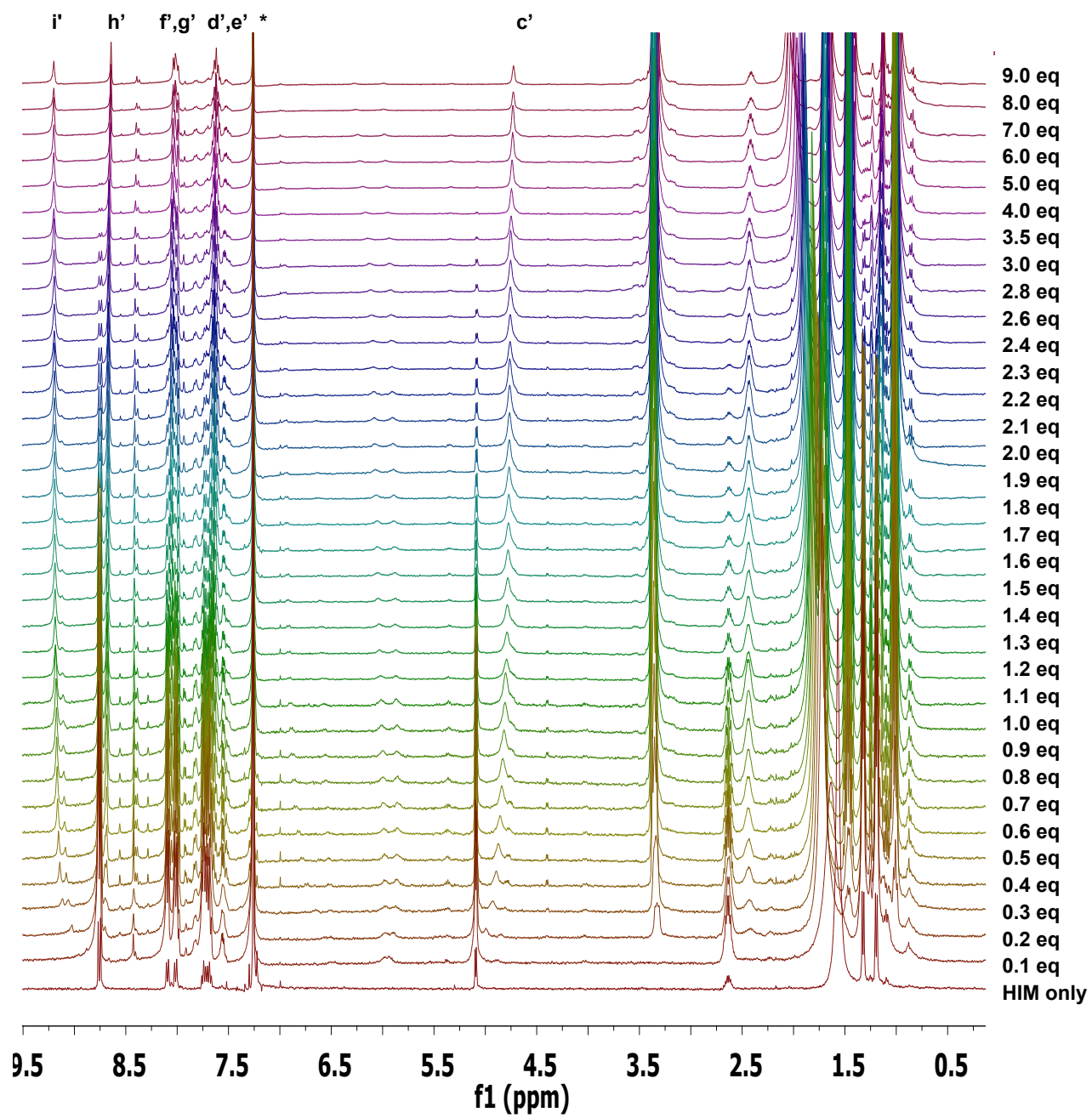
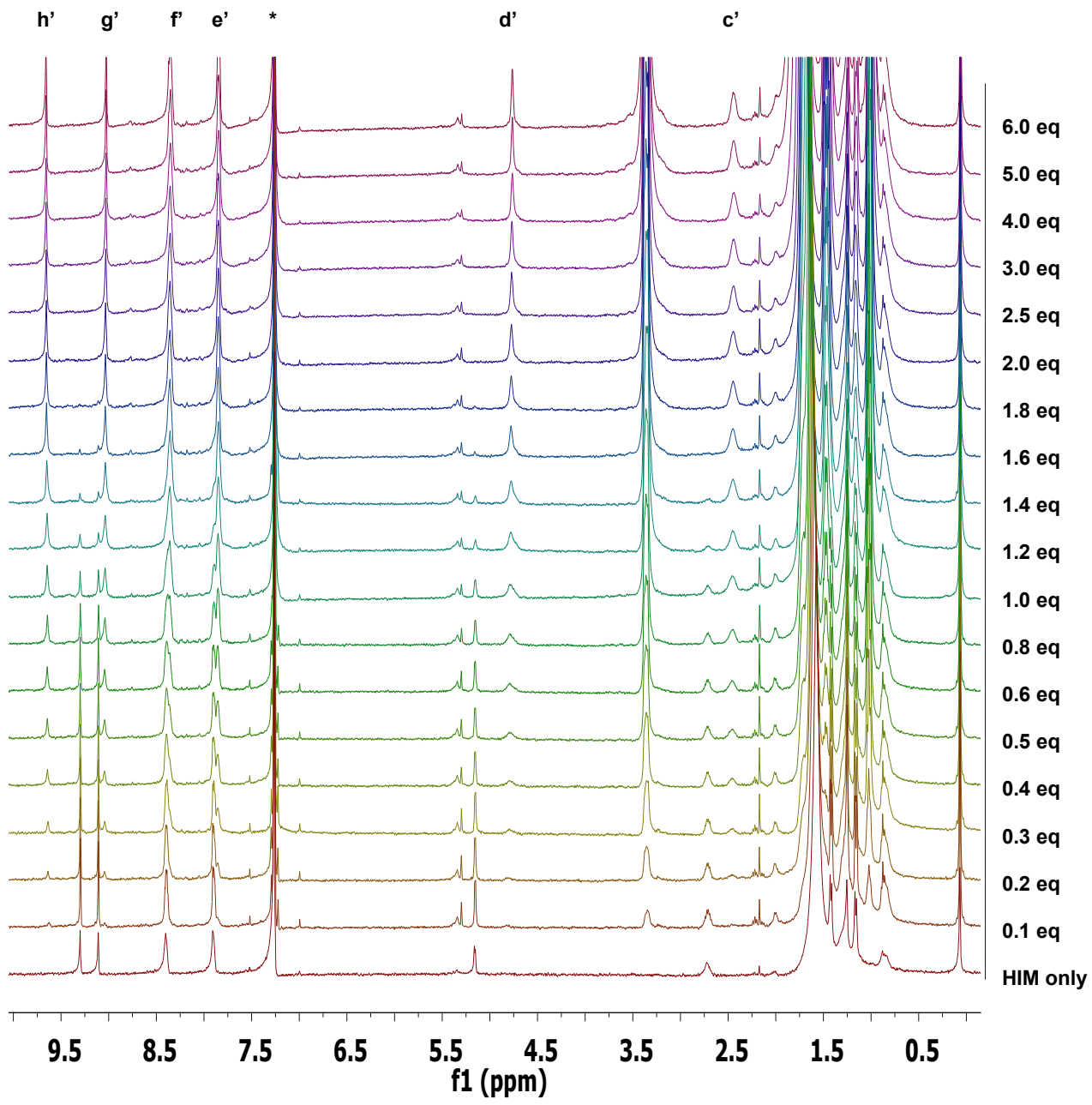


Figure SI7: ¹H NMR (400 MHz, 298 K) titration of **6b** with TBA(Br) at an incremental equivalency (0 to 9 equivalents TBA(Br) in CDCl₃). *Residual CHCl₃ peak from the NMR solvent.



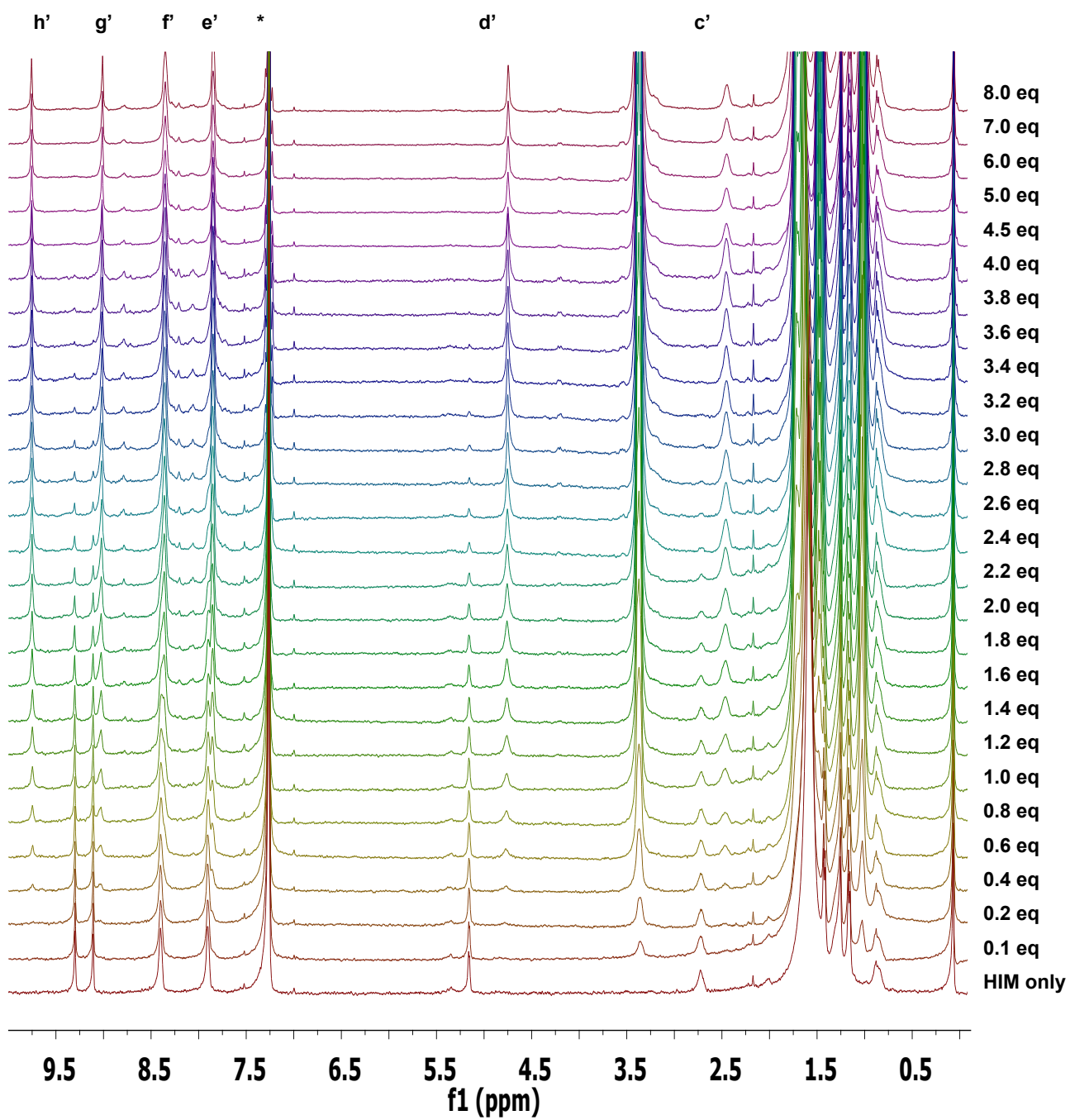
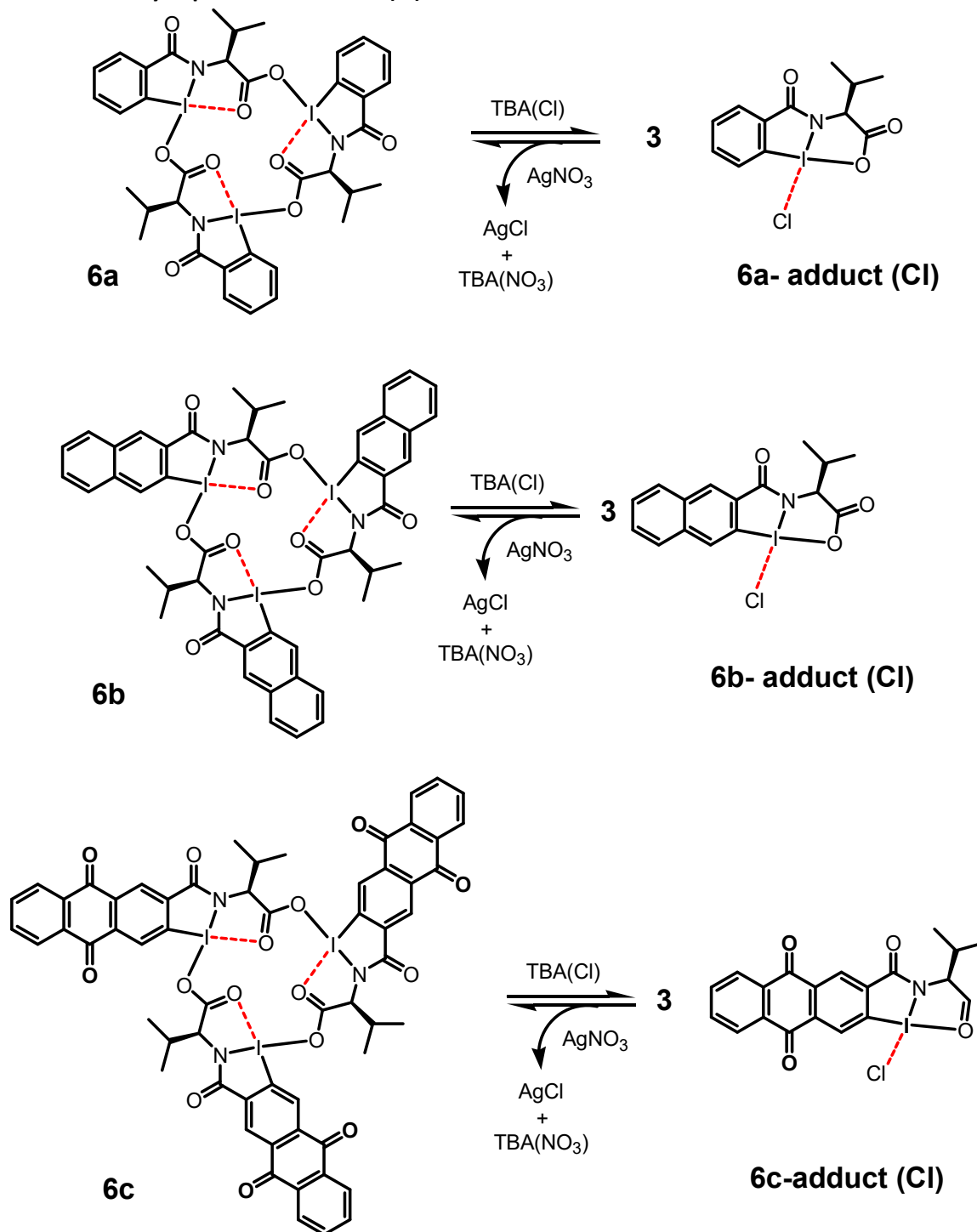


Figure S19: ^1H NMR titration of **6c** with TBA(Br) at an incremental equivalency (0 to 8 equivalents TBA(Br) in CDCl_3 . * Residual CHCl_3 peak from the NMR solvent.

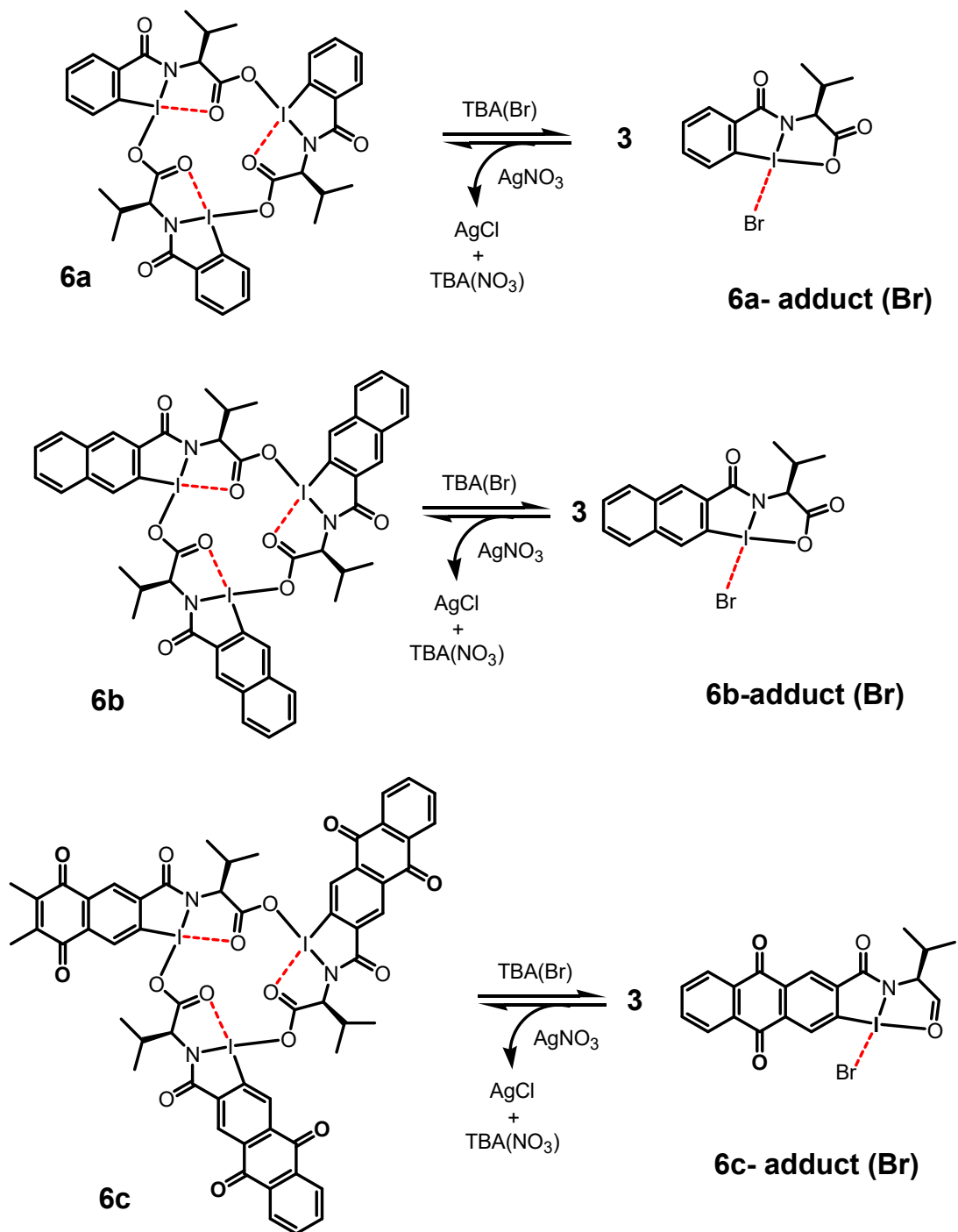
5. Reversibility Experiment

a. Reversibility Experiment with TBA(Cl)



Scheme SI1: Scheme of HIM **6a-6c** disassembly by addition of chloride anion. The HIM can reform when AgNO₃ is added to coordinate the chloride anion.

b. Reversibility Experiment with TBA(Br)



Scheme S12: Scheme of HIM **6a-6c** disassembly by addition of bromide anion. The HIM can reform when AgNO₃ is added to coordinate the chloride anion.

6.Binding Experiments

The association between the HIM **6b-6c** and different anions was analyzed utilizing ^1H NMR spectrometry in deuterated chloroform. From the ^1H NMR study, the data was used to determine the binding constant between the HIM and anion in Bindfit (<http://app.supramolecular.org/bindfit/>). Three different HIMs (**6a-c**) were compared for their binding affinity with Cl^- and Br^- . Tetrabutylammonium salts were used for the experiment.

In case of HIM **6b**, an incremental equivalent addition of salt to the HIM was performed for this experiment. Stock solution (A) of HIM was prepared at a concentration of 4.3 mM (12.9 mM in monomer) which was kept constant throughout the process. A portion of HIM stock was used to prepare salt stock (B) at an equivalence of 20 to 40 times. 0.5 mL of stock A was taken to the NMR tube and the spectra ^1H NMR spectrum was recorded.

For chloride anion: Stock solution B (with TBA(Cl)) was added stepwise in a 0.1 equivalence (versus the HIM) until a 1:2 equivalence of HIM to salt was added. After each stepwise addition of stock B to the NMR tube of stock A, ^1H NMR was recorded. After 2 equivalence of stock B was added to the NMR tube the increment rate increased to 1 equivalence for each addition till the last addition.

For bromide anion: Stock solution B (with TBA(Br)) was added stepwise in a 0.1 equivalence (versus the HIM) increase until a 1:2.4 equivalence of HIM to salt was added. After each stepwise addition of stock B to the NMR tube of stock A, ^1H NMR was recorded. The incremental rate increased to 0.2 equivalency from 2.4 to 3.0 equivalence and 0.5 equivalence from 3.0 to 4 equivalence. After 4 equivalence of stock B was added to the NMR tube the increment rate kept 1 equivalence for each addition till the last addition.

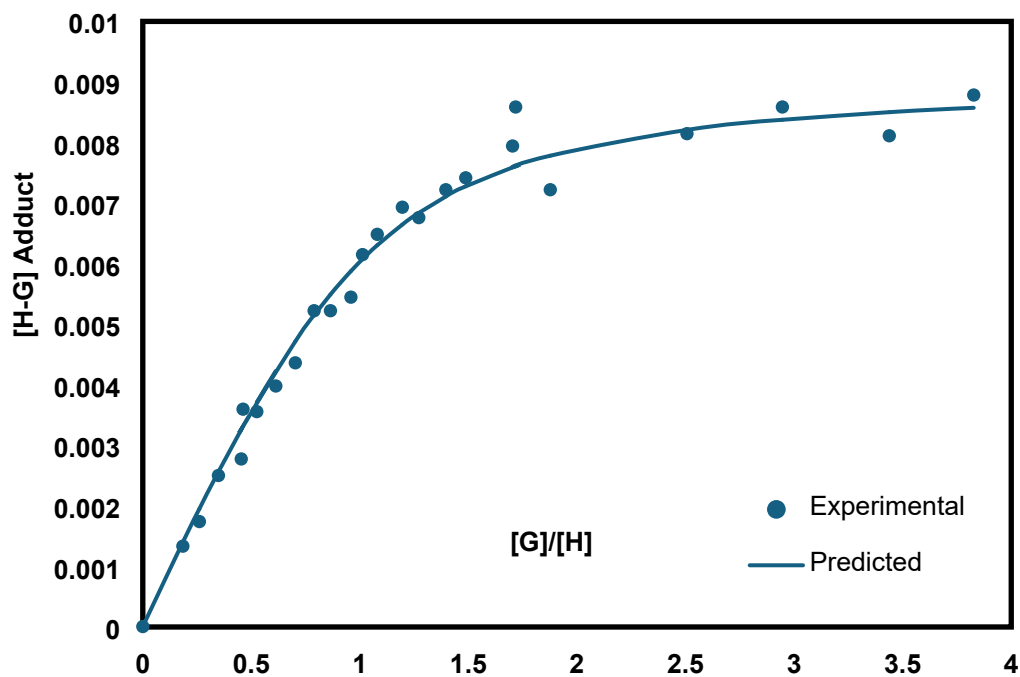


Figure SI10: Binding Isotherm of HIM 6b with TBA(Cl).

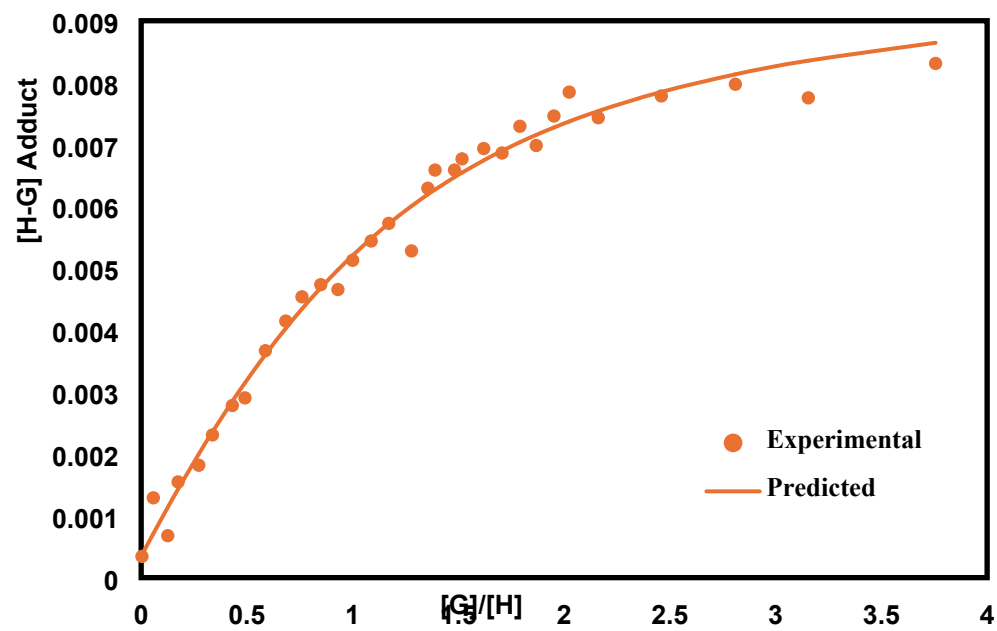


Figure SI11: Binding Isotherm of HIM 6b with TBA(Br).

In case of **6c**, an incremental equivalent addition of salt to the HIM was performed for this experiment. Stock solution (A) of HIM was prepared at a concentration of 4.3 mM (12.9 mM in monomer) which was kept constant throughout the process. A portion of HIM stock was used to prepare salt stock (B) at an equivalence of 20 to 40 times. 0.5 mL of stock A was taken to the NMR tube and the spectra ^1H NMR spectrum was recorded.

For chloride anion: Then stock B (with TBA-Cl) was added stepwise in a 0.1 equivalence (verses the HIM) increase until a 0.6 equivalence of HIM to salt was added. After each stepwise addition of stock B to the NMR tube of stock A, ^1H NMR was recorded. The incremental rate increased to 0.2 equivalency from 0.6 to 2.0 equivalence and added 0.5 equivalence from 2.0 to 3 equivalence. After 3 equivalence of stock B was added to the NMR tube the increment rate kept 1 equivalence for each addition till the last addition.

For bromide anion: Initially 0.1 equivalence of stock B (with TBA-Br) was added and then stock B (with TBA-Br) was added stepwise in a 0.2 equivalence (verses the HIM) increase until a 1:4 equivalence of HIM to salt was added. After each stepwise addition of stock B to the NMR tube of stock A, ^1H NMR was recorded. The incremental rate increased to 0.5 equivalency from 4.0 to 5.0 equivalence. After 5.0 equivalence of stock B was added to the NMR tube the increment rate kept 1 equivalence for each addition till the last addition.

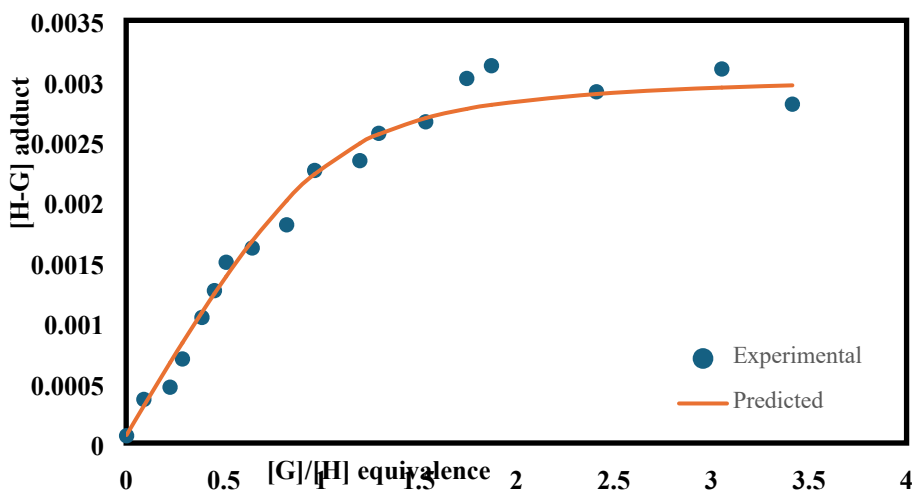


Figure SI12: Binding Isotherm of **6c** with TBA(Cl)

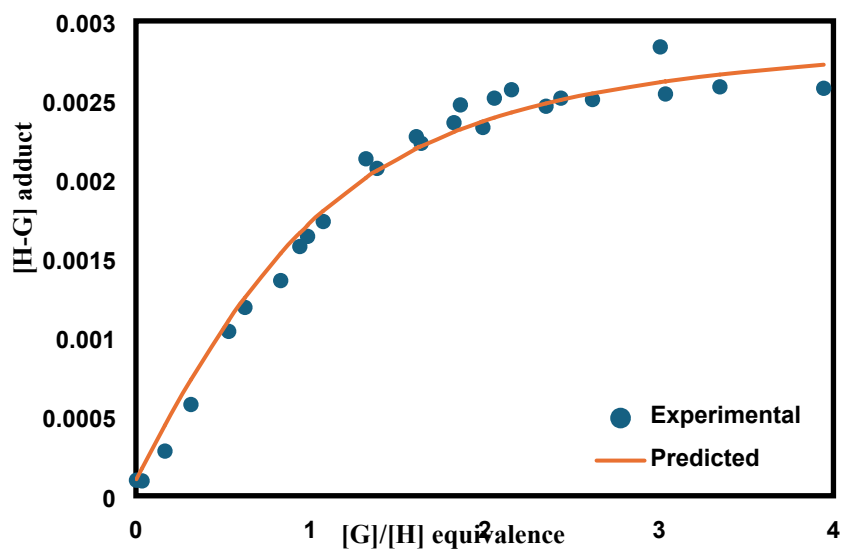


Figure SI13: Binding Isotherm of **6c** with TBA(Br)

7. Fluorescence Spectra

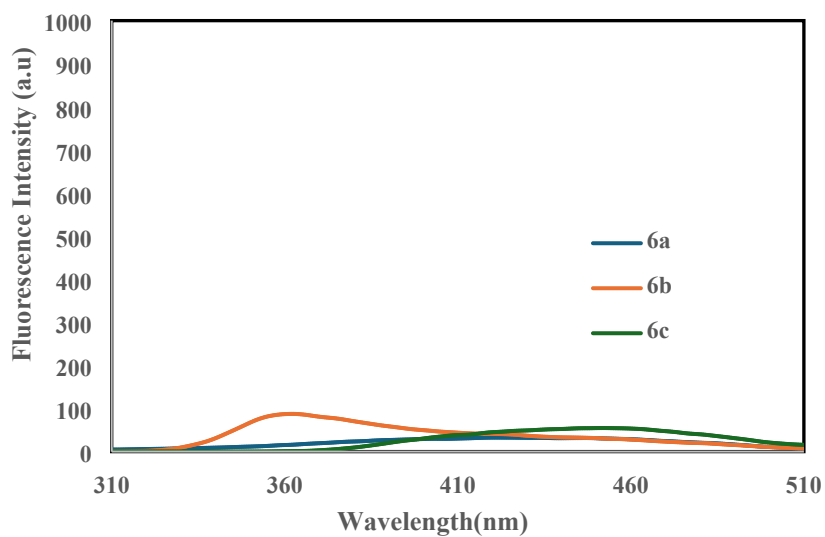
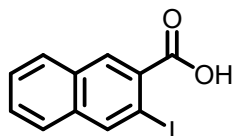


Figure SI14: Emission spectra of HIM **6a-6c** in chloroform. Excitation at 275 nm.

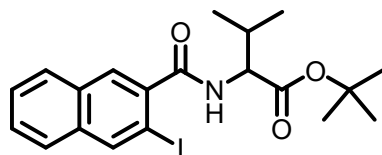
8. Experimental Section

Unless otherwise noted, all reagents were used as received and all reactions were carried out under an argon atmosphere. Column chromatography was performed on a CombiFlash® Rf system with Redisep normal phase silica columns (Teledyne ISCO Inc., Lincoln, NE). NMR were recorded on a Varian 400 MHz NMR station at room temperature, unless otherwise noted. High resolution mass spectra were obtained from the University of Illinois Mass Spectrometry Services.

Compound 3a, 4a, and 6a were previously prepared. (J. Org. Chem., 2024, 89, 7437-7445.)



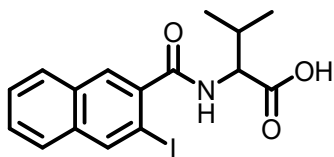
3-Iodo-2-naphthoic acid. To an ice-cold stirred suspension of commercially available 3-amino-2-naphthoic acid (1.0 g, 5.34 mmol) in 40 mL of a 1:1 mixture of 37% aqueous HCl (20 mL) and H₂O (20 mL) was slowly added an aqueous solution of NaNO₂ (737 mg, 10.7 mmol, in 10 mL of distilled water). The resulting orange solution was stirred at 0 °C for 2 h, after which time an aqueous solution of KI (5.30 g, 32.0 mmol, in 10 mL of distilled water) was added dropwise. The mixture was stirred at 0 °C for 30 min, then at room temperature for 1 h, and finally heated at 60 °C for 1 h. EtOAc (20 mL) was then poured into the mixture and heating was maintained for an additional 30 min. Powdered Na₂S₂O₃ was added until complete de-colorization of the solution. The solid was removed by filtration. The reaction mixture was then extracted with EtOAc (4 x 25 mL). The organic layers were combined, washed with brine (100 mL), dried over MgSO₄, filtered, and evaporated to dryness. The resulting brown oily residue was purified by column chromatography (Hexane/EtOAc, 1:1) to yield 1.2 g (75%) as a beige solid. ¹H NMR (400 MHz, DMSO) δ 8.63 (s, 1H), 8.36 (s, 1H), 8.04 (d, *J* = 7.6 Hz, 1H), 7.93 (d, *J* = 7.8 Hz, 1H), 7.67 – 7.58 (m, 2H). ¹³C{¹H} NMR (400 MHz, DMSO) δ 168.1, 139.7, 135.0, 133.1, 131.2, 130.2, 128.6, 127.4, 126.6, 89.6. HRMS (TOF MS ES+) *m/z*: [M + H]⁺ Calcd for C₁₁H₈IO₂ 298.9569; found 298.9565.



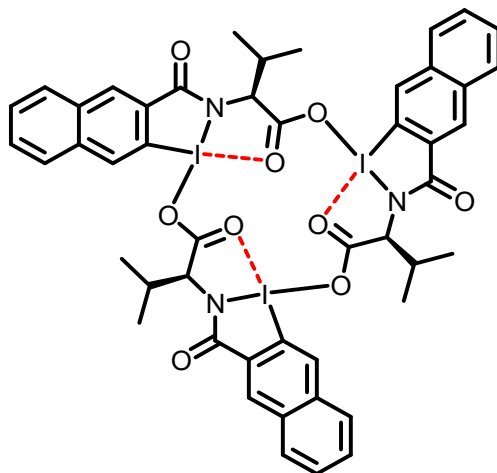
2-[(3-Iodo-9,10-dioxo-9,10-dihydro-anthracene-2-carbonyl)-amino]-3-methyl-butanoic acid tert-butyl ester.

To a solution of 3-Iodo-2-naphthoic acid (22.4 mg, 0.075 mmol) dissolved in DMF (5 ml) was added EDC.HCl (15.3 mg, 0.08 mmol) and HOBt (12.3 mg, 0.08 mmol) at 0°C. The reaction mixture was sonicated to make the solution homogeneous, and argon bubbled through the solution for 15 min. The L- valine tertiary-butyl ester hydrochloride (17.3 mg, 0.083 mmol) was added followed by diisopropylamine (24.8 mg, 0.024 mmol). The mixture was stirred overnight allowing the ice to melt to set the reaction at room temperature. After the completion of the reaction, the solution was poured into water (25 ml) and the precipitate was filtered, washed with water, and dried under vacuum to yield 20 mg (67%) of pure colorless powder. Melting point 88-90°C; ¹H NMR (400 MHz, CDCl₃) δ 8.42 (s, 1H), 7.92 (s, 1H), 7.84 (dd, *J* = 6.4, 3.2 Hz, 1H), 7.74 (dd, *J* = 5.6, 3.6 Hz, 1H), 7.56 – 7.53 (m, 2H), 6.42 (d, *J* = 8.6 Hz, 1H), 4.72 (dd, *J* = 8.7, 4.4 Hz, 1H), 2.47 – 2.17 (m, 1H), 1.52

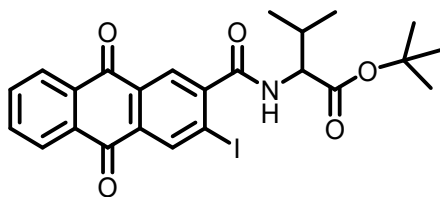
(s, 9H), 1.12 (d, $J = 6.9$ Hz, 3H), 1.03 (d, $J = 6.9$ Hz, 3H). $^{13}\text{C}\{^1\text{H}\}$ NMR (400 MHz, CDCl_3) δ 170.9, 169.0, 139.7, 138.4, 135.1, 131.9, 128.3, 128.0, 127.7, 127.4, 126.8, 88.7, 82.4, 58.1, 31.8, 28.2, 19.3, 18.1. HRMS (TOF MS ES+) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{20}\text{H}_{25}\text{INO}_3$ 454.0879; found 454.0872.



2-[(3-iodo-naphthalen-2-yl)amino]-3-methyl-butanoic acid To a 50 ml round bottom flask was added 2-[(3-iodo-naphthalen-2-yl)amino]-3-methyl-butanoic acid tert-butyl ester (924 mg, 2.04 mmol) and 30 mL dichloromethane. After the system was cooled at 0°C , TFA (5.11 g, 44.9 mmol) was added dropwise. The reaction was allowed to warm slowly to room temperature and kept stirring for 12 h. The solvent, by-product and extra TFA was removed *in vacuo* by co-evaporation with DCM and hexane multiple times to give 627 mg (77%) as a colorless solid. Melting point $178\text{--}180^\circ\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 8.40 (s, 1H), 7.91 (s, 1H), 7.85 – 7.81 (m, 1H), 7.75 – 7.71 (m, 1H), 7.58 – 7.51 (m, 2H), 6.44 (d, $J = 8.9$ Hz, 1H), 4.87 (dd, $J = 8.6, 4.6$ Hz, 1H), 2.56 – 2.19 (m, 1H), 1.16 (d, $J = 6.9$ Hz, 3H), 1.06 (d, $J = 6.9$ Hz, 3H). $^{13}\text{C}\{^1\text{H}\}$ NMR (400 MHz, CDCl_3) δ 175.8, 169.7, 139.7, 137.9, 135.1, 131.8, 128.4, 128.2, 128.0, 127.5, 126.8, 88.3, 57.8, 31.4, 19.4, 18.0. HRMS (TOF MS ES+) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{17}\text{INO}_3$ 398.0253; found 398.0247.

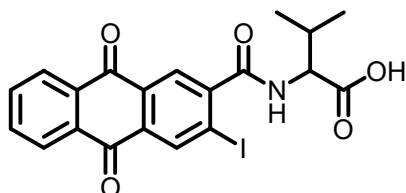


Valine HIM in Naphthalene system 2-[(3-iodo-naphthalen-2-yl)amino]-3-methyl-butanoic acid (100 mg, 0.25mmol) and 77% mCPBA (130 mg, 0.75 mmol) were dissolved in chloroform (6 ml) in a 10 mL round bottom flask. The reaction was kept stirring at room temperature for 8 h. The reaction mixture was concentrated by vacuum at room temperature. The residue was suspended in 10 mL diethyl ether, and then was filtrated and wash with diethyl ether (2×10 ml) to give 81 mg (82%) as a colorless solid. Melting point $135\text{--}136^\circ\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 8.77 (s, 1H), 8.75 (s, 1H), 8.09 (d, $J = 8.0$ Hz, 1H), 8.01 (d, $J = 8.0$ Hz, 1H), 7.76 – 7.66 (m, 2H), 5.09 (d, $J = 5.1$ Hz, 1H), 2.68 – 2.60 (m, 1H), 1.32 (d, $J = 6.9$ Hz, 3H), 1.19 (d, $J = 6.9$ Hz, 3H). $^{13}\text{C}\{^1\text{H}\}$ NMR (400 MHz, CDCl_3) δ 179.1, 167.3, 136.9, 133.3, 131.7, 130.5, 129.5, 129.4, 129.0, 128.5, 128.4, 113.9, 63.6, 33.2, 20.3, 18.0. HRMS (TOF MS ES+) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{48}\text{H}_{43}\text{I}_3\text{N}_3\text{O}_9$ 1186.0133; found 1186.0127.

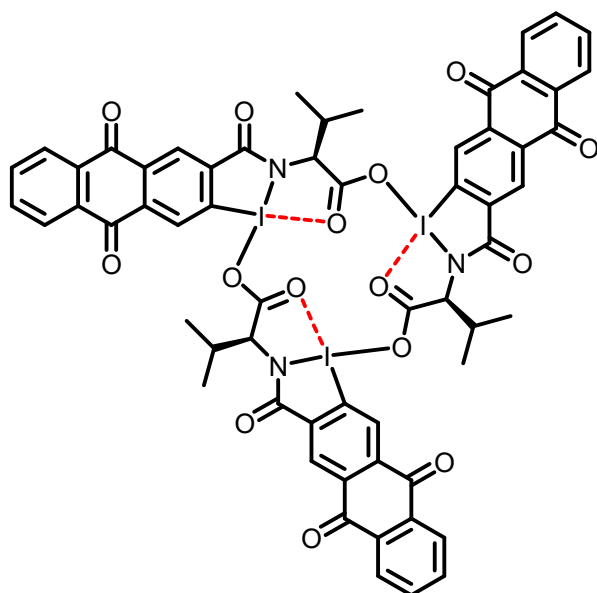


2-[(3-iodo-9,10-dioxo-9,10-dihydro-anthracene-2-carbonyl)-amino]-3-methyl-butyl tert-butyl ester.

To a solution of 3-iodo-anthraquinone-2-carboxylic acid (28.4 mg, 0.075 mmol) dissolved in DMF (5 ml) was added EDC.HCl (15.3 mg, 0.08 mmol) and HOBT (12.3 mg, 0.08 mmol) at 0°C. The reaction mixture was sonicated to make the solution homogeneous, and argon bubbled through the solution for 15 min. The L-valine tertiary-butyl ester hydrochloride (17.30 mg, 0.083 mmol) was added followed by diisopropylamine (24.8 mg, 0.024 mmol). The mixture was stirred overnight allowing the ice to melt to set the reaction at room temperature. After the completion of the reaction, the solution was poured into water (25 ml) and the precipitate was filtered, washed with enough water, and dried under vacuum to yield 22 mg (55%) of pure yellow powder. Melting point > 290°C; ¹H NMR (400 MHz, CDCl₃) δ 8.41 (s, 1H), 7.91 (s, 1H), 7.82 (dd, *J* = 8.3, 4.1 Hz, 1H), 7.74 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.57 – 7.50 (m, 2H), 6.44 (d, *J* = 8.6 Hz, 1H), 4.71 (dd, *J* = 8.7, 4.4 Hz, 1H), 2.42 – 2.29 (m, 1H), 1.52 (s, 9H), 1.12 (d, *J* = 6.9 Hz, 3H), 1.03 (d, *J* = 6.9 Hz, 3H). ¹³C{¹H} NMR (400 MHz, CDCl₃) δ 182.1, 181.5, 170.5, 167.8, 147.4, 139.0, 134.8, 134.8, 133.8, 133.3, 133.0, 132.9, 127.6, 127.6, 126.5, 100.5, 82.8, 58.3, 31.9, 28.3, 19.2, 18.1. HRMS (TOF MS ES-) *m/z*: [M - H]⁺ Calcd for C₂₄H₂₃INO₅ 532.0621; found 532.0613.



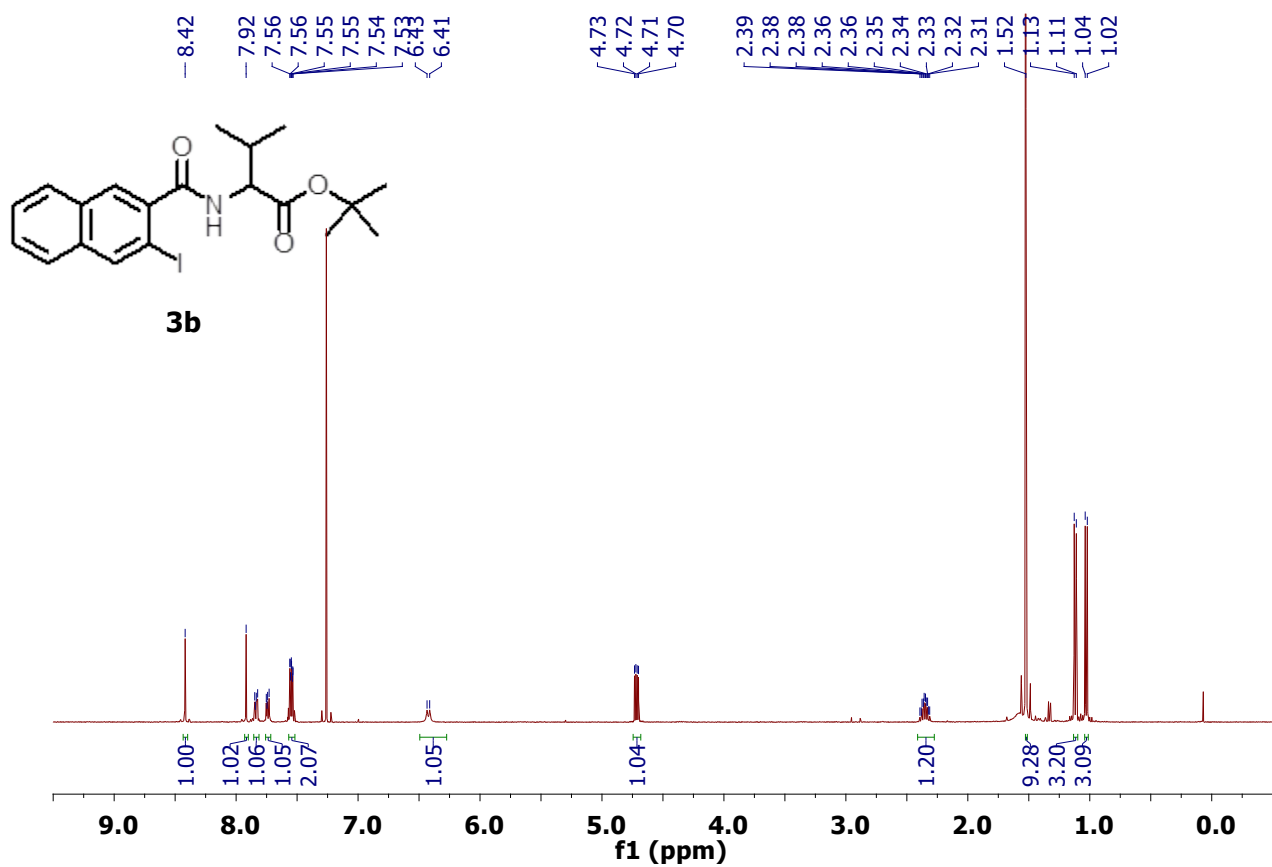
2-[(3-iodo-9,10-dioxo-9,10-dihydro-anthracene-2-carbonyl)-amino]-3-methyl-butyl acid To a 50 mL round bottom flask was added 2-[(3-iodo-9,10-dioxo-9,10-dihydro-anthracene-2-carbonyl)-amino]-3-methyl-butyl tert-butyl ester (26.7 mg, 0.05 mmol) and dry dichloromethane (5 ml). After the system was cooled at 0°C, TFA (125 mg, 1.1 mmol) was added dropwise. The reaction was warmed slowly to room temperature and stirred for 12 h. Excess TFA was removed by co-evaporation with DCM and hexane three times and the product was dried under high vacuum to obtain 22 mg (92%) of pure yellow solid. Melting point > 290°C; ¹H NMR (400 MHz, DMSO) δ 12.79 (s, 1H), 8.98 (d, *J* = 8.5 Hz, 1H), 8.58 (s, 1H), 8.27 – 8.21 (m, 2H), 8.00 – 7.95 (m, 2H), 7.93 (s, 1H), 4.37 (dd, *J* = 8.4, 5.9 Hz, 1H), 2.24 – 2.18 (m, 1H), 1.03 (d, *J* = 6.8 Hz, 3H), 0.98 (d, *J* = 6.8 Hz, 3H). ¹³C{¹H} NMR (400 MHz, DMSO₃) δ 182.0, 181.1, 172.5, 168.1, 147.9, 137.2, 134.9, 133.2, 133.0, 132.8, 132.1, 126.9, 126.9, 125.6, 102.0, 57.8, 29.7, 19.4, 18.2. (Note: One carbon peak is merged at 134.9 ppm.) HRMS (TOF MS ES-) *m/z*: [M - H]⁺ Calcd for C₂₀H₁₅INO₅ 475.9995; found 475.9991.



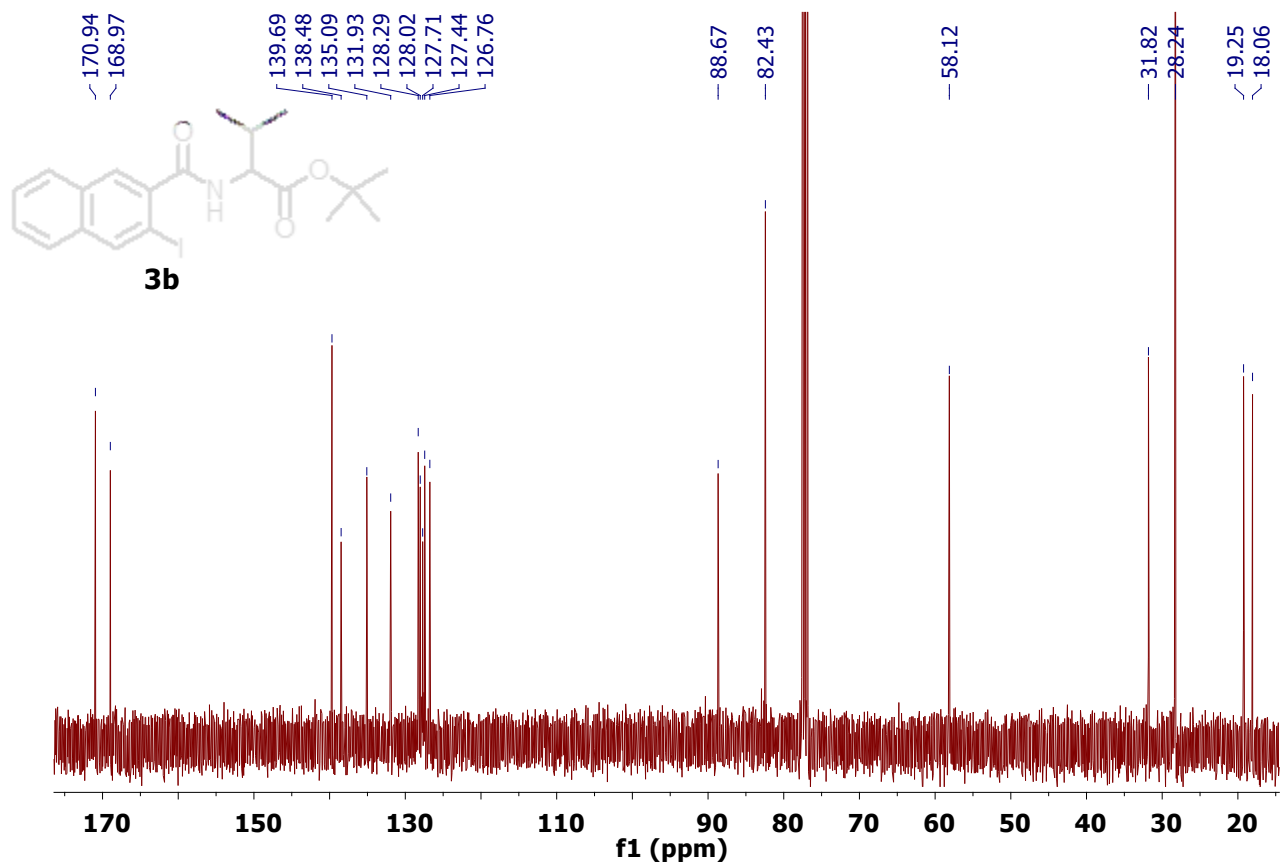
Valine HIM in Anthraquinone system 2-[(3-Iodo-9,10-dioxo-9,10-dihydro-anthracene-2-carbonyl)-amino]-3-methyl-butyrlic acid (120 mg, 0.25 mmol) and 77% mCPBA (130 mg, 0.75 mmol) were dissolved in chloroform (6 ml) in a 10 ml round bottom flask. The reaction was kept stirring at room temperature for 8 h. The reaction mixture was concentrated by vacuum at room temperature. The residue was suspended in 5 ml diethyl ether followed by sonication. The precipitate formed was filtered and wash with diethyl ether (2 × 5 ml) to give 75 mg (63%) of the product as a yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 9.29 (s, 1H), 9.10 (s, 1H), 8.41 – 8.37 (m, 2H), 7.91 – 7.88 (m, 2H), 5.15 (d, J = 4.3 Hz, 1H), 2.74 – 2.69 (m, 1H), 1.42 (d, J = 6.9 Hz, 3H), 1.15 (d, J = 6.9 Hz, 3H). Too insoluble for ^{13}C NMR characterization. HRMS (TOF MS ES+) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{60}\text{H}_{43}\text{I}_3\text{N}_3\text{O}_{15}$ 1425.9828; found 1425.9819.

9. NMR Spectra

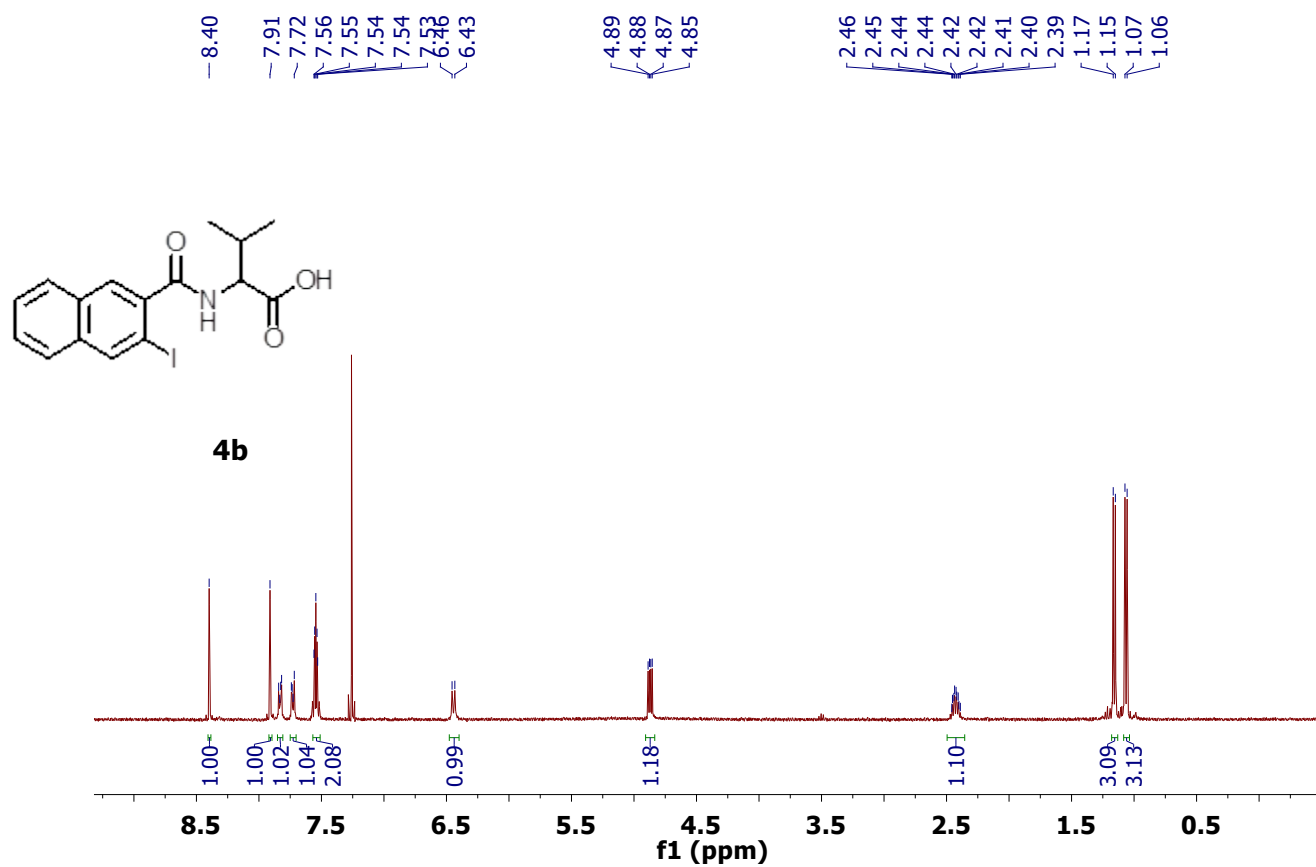
^1H NMR- **3b** (400 MHz, CDCl_3)



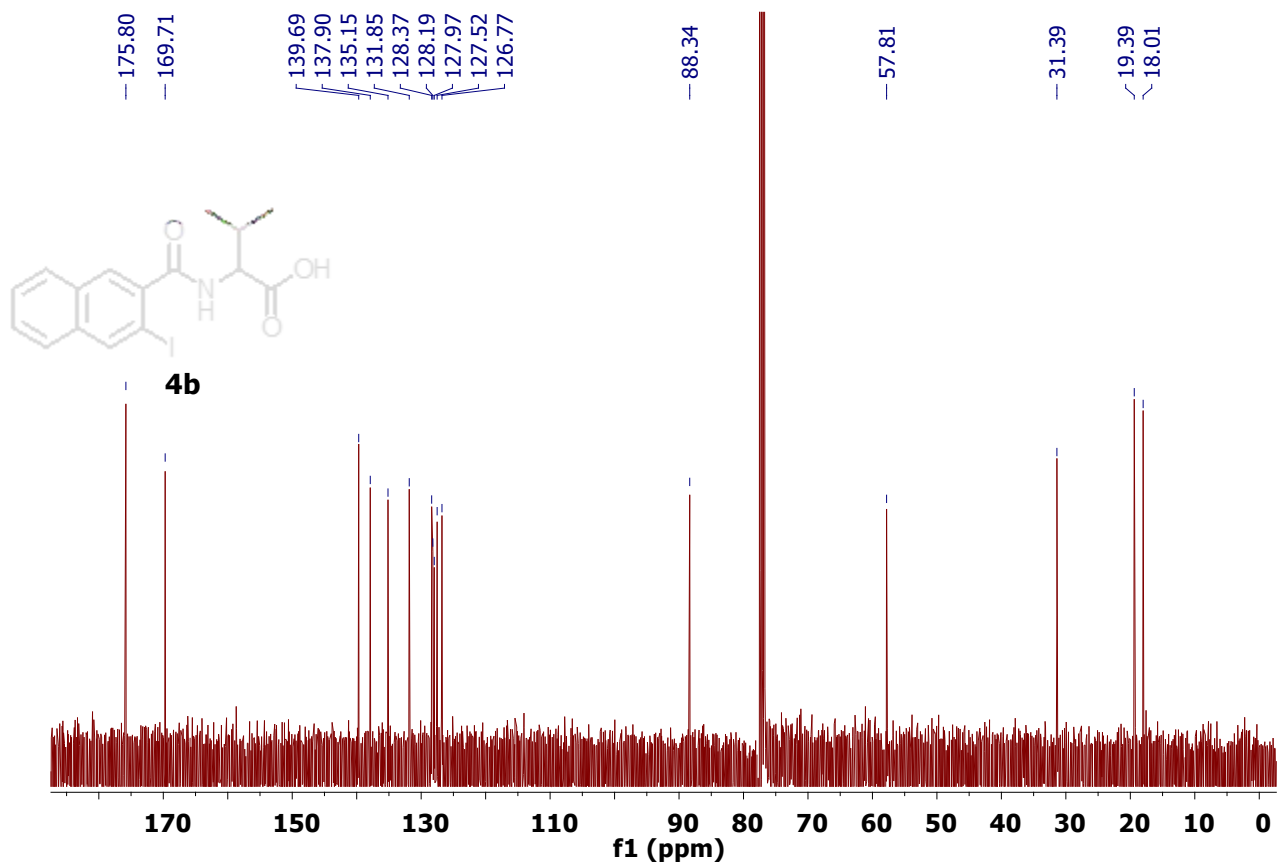
$^{13}\text{C}\{^1\text{H}\}$ NMR- **3b** (400 MHz, CDCl_3)



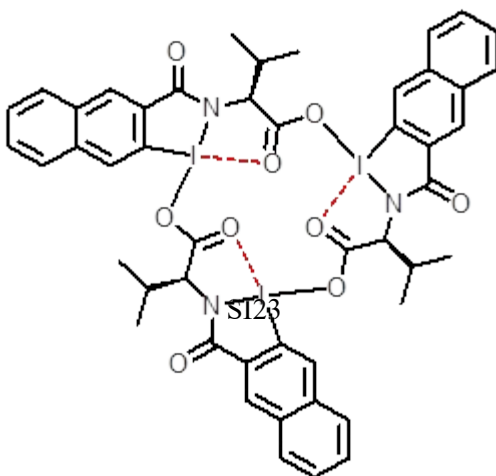
¹H NMR- **4b** (400 MHz, CDCl₃)

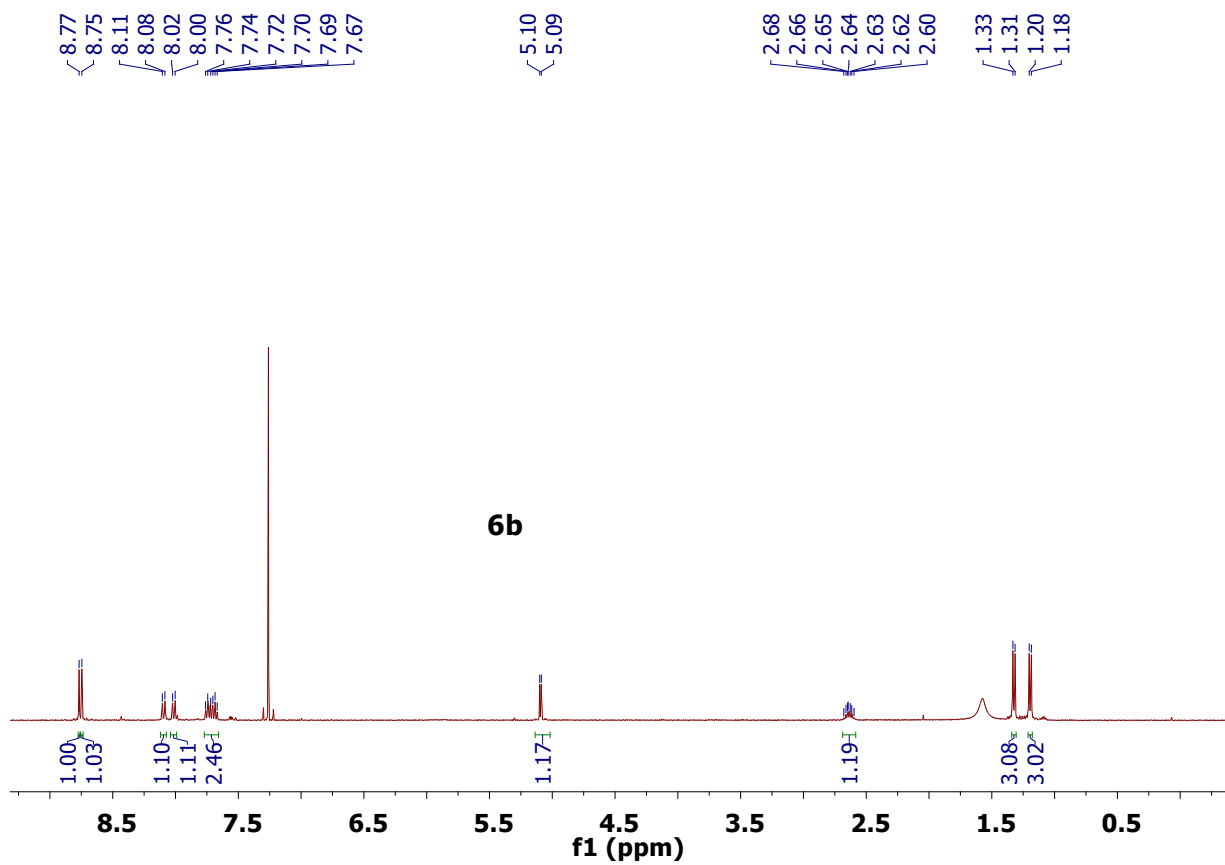


$^{13}\text{C}\{^1\text{H}\}$ NMR- **4b** (400 MHz, CDCl_3)

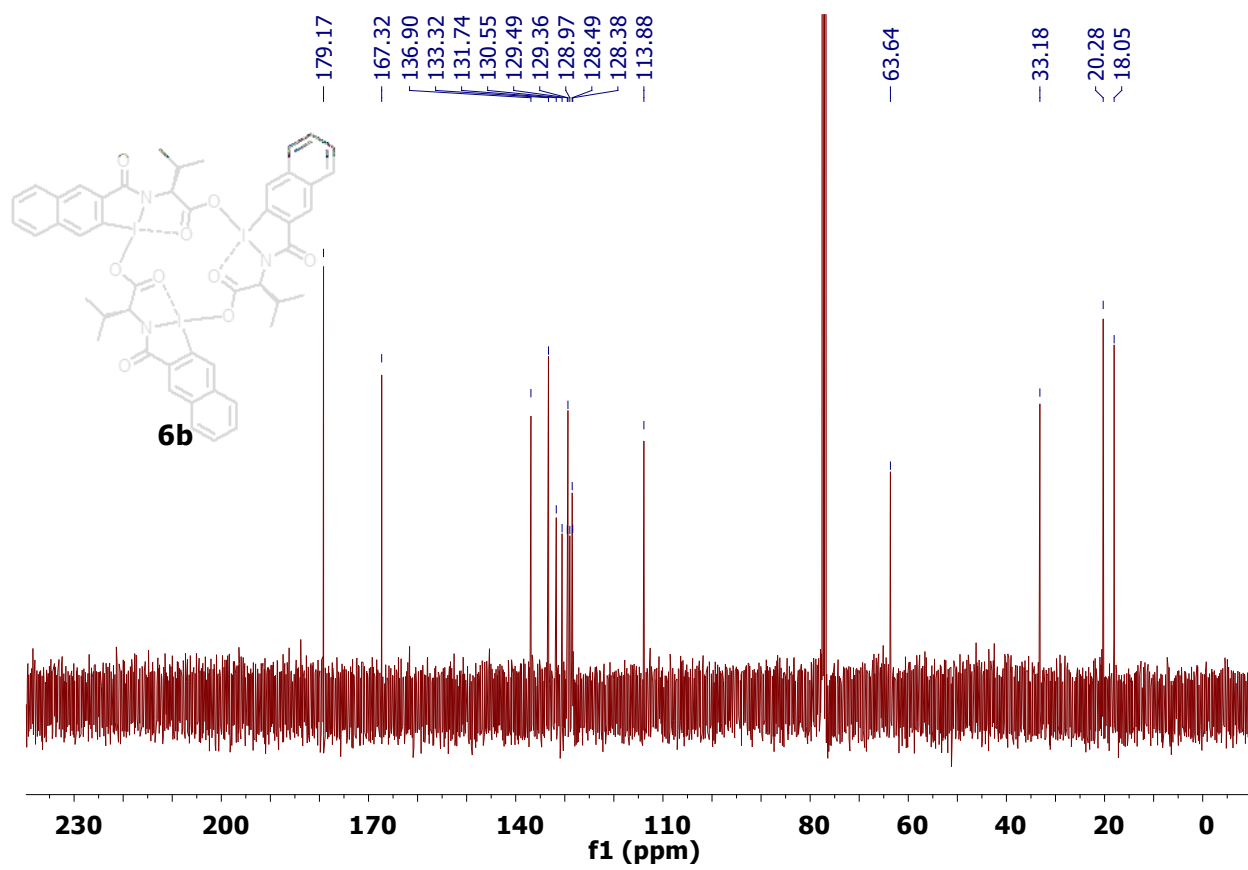


^1H NMR- **6b** (400 MHz, CDCl_3)

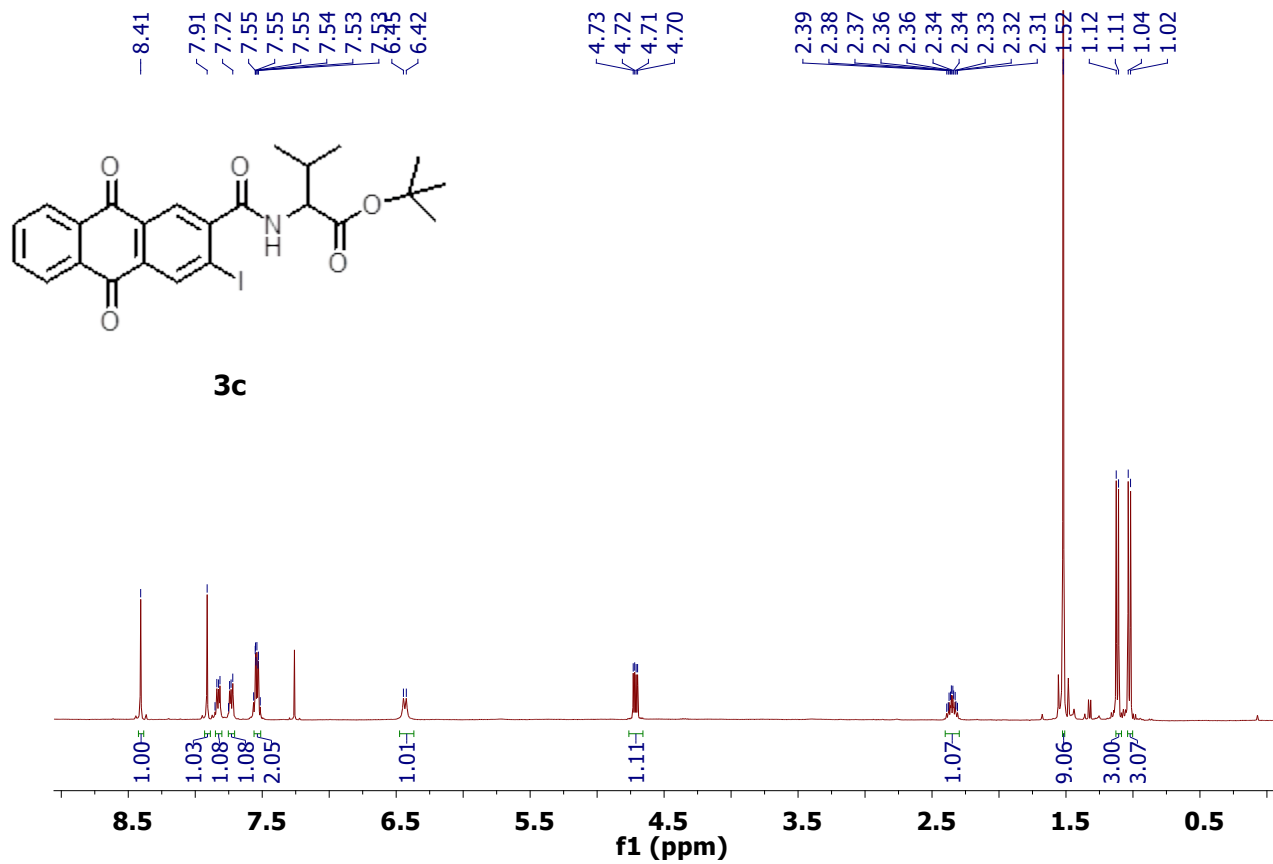




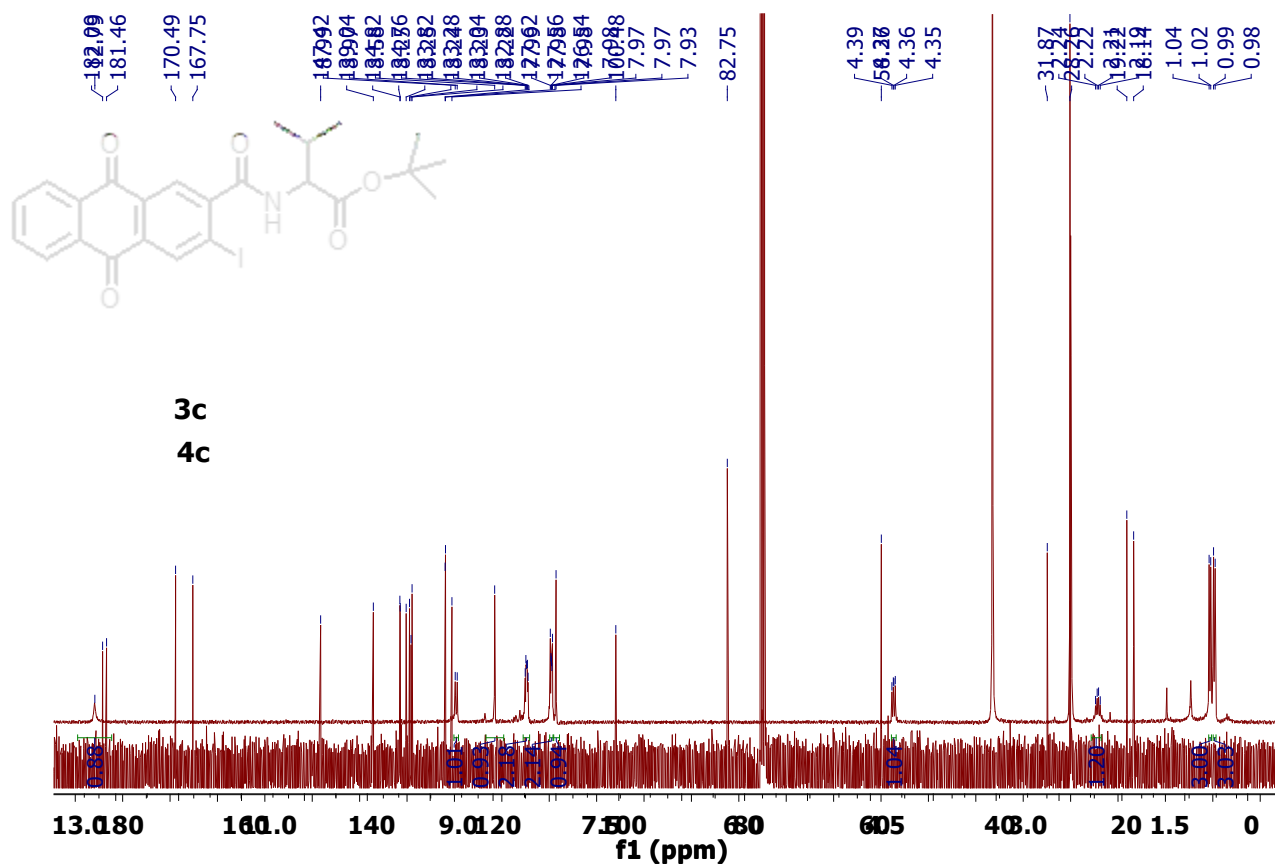
$^{13}\text{C}\{^1\text{H}\}$ NMR- **6b** (400 MHz, CDCl_3)



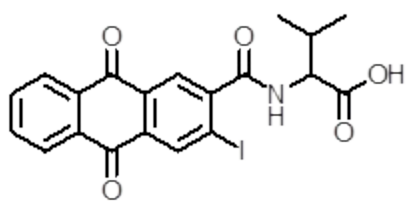
^1H NMR- **3c** (400 MHz, CDCl_3)

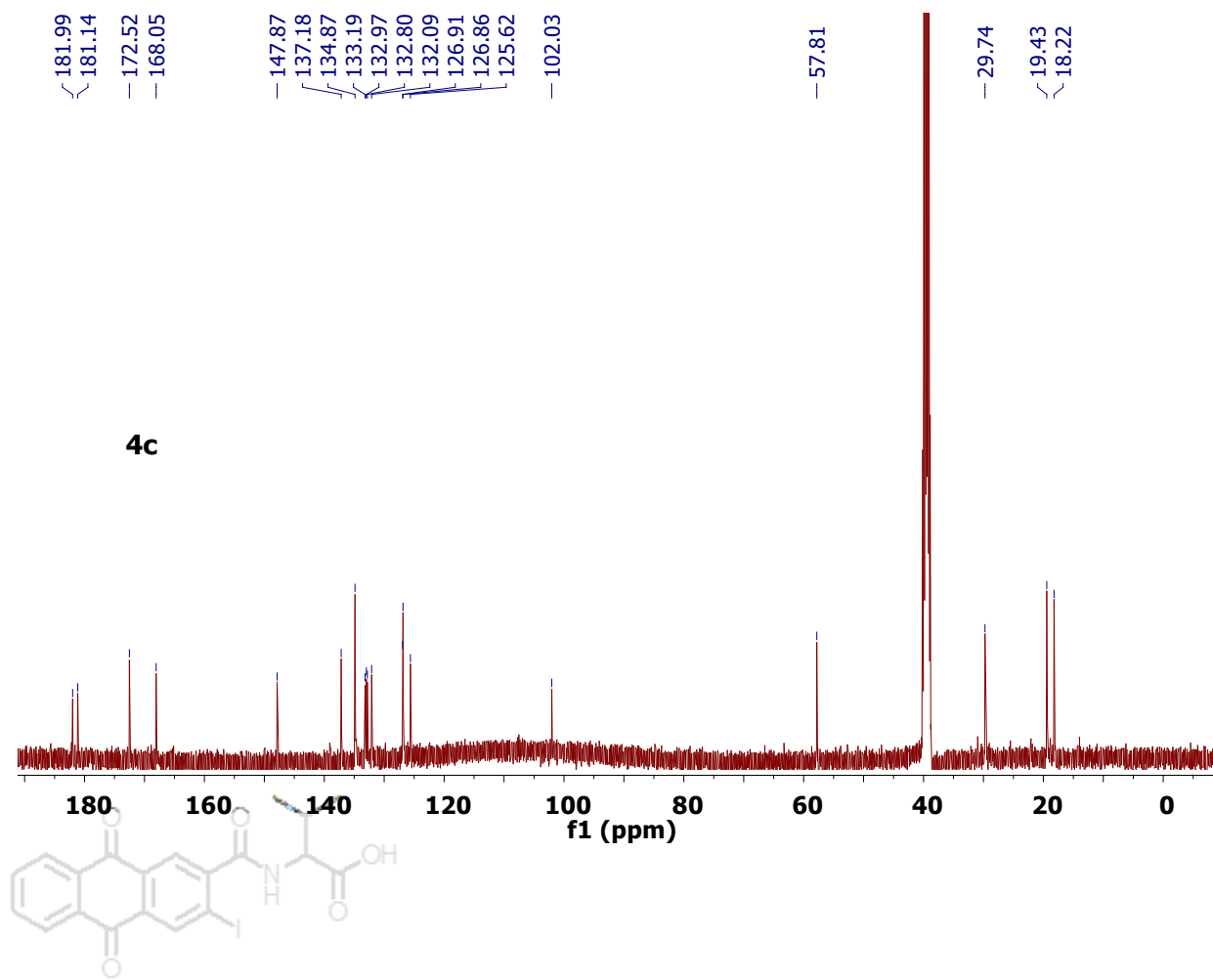


$^{13}\text{C}\{^1\text{H}\}$ NMR- **3c** (400 MHz, CDCl_3)



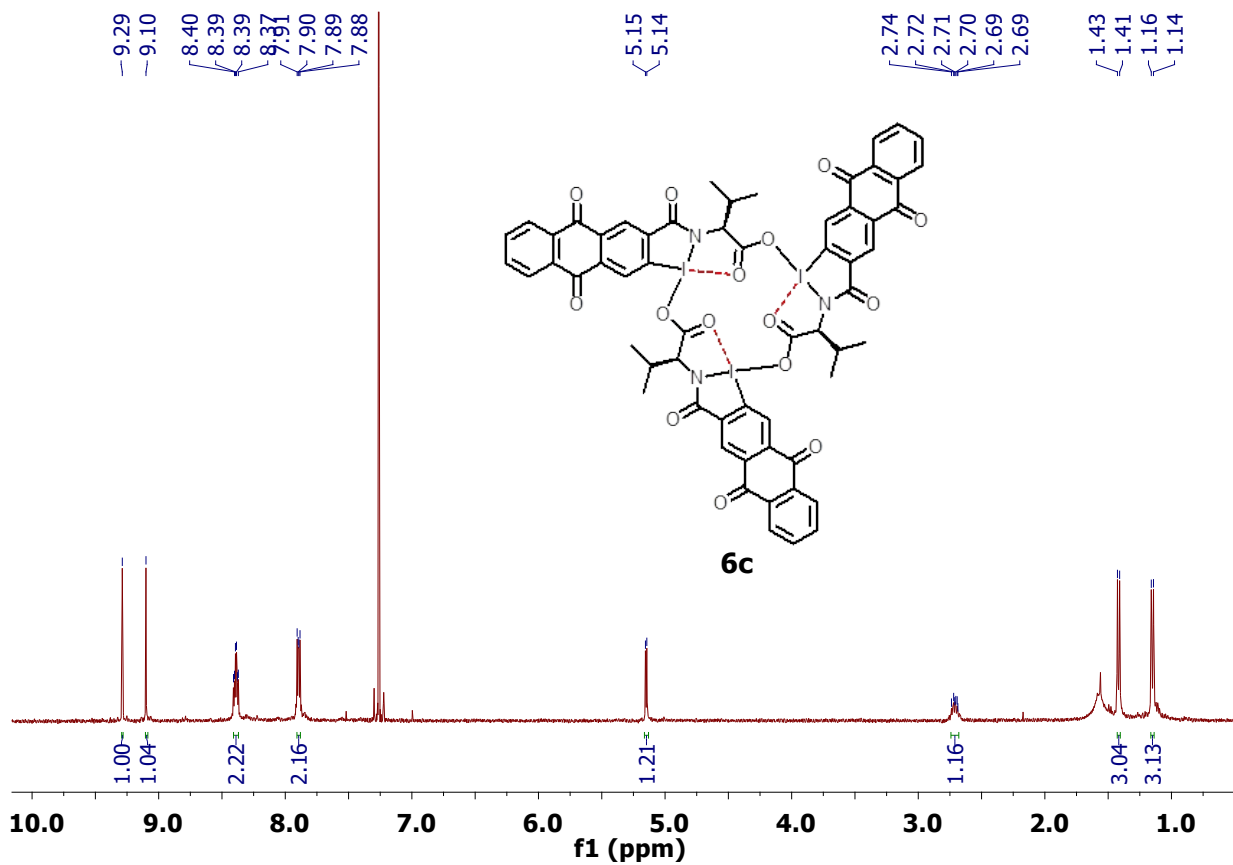
^1H NMR- **4c** (400 MHz, CDCl_3)





$^{13}\text{C}\{^1\text{H}\}$ NMR- **4c** (400 MHz, CDCl_3)

¹H NMR- **6c** (400 MHz, CDCl₃)



9. Crystallographic Information

Intensity data were collected on a Bruker D8 Venture kappa diffractometer equipped with a Photon II CPAD detector. An μs microfocus Mo source ($\lambda = 0.71073 \text{ \AA}$) coupled with a multi-layer mirror monochromator provided the incident beam. The sample was mounted on a 0.3 mm nylon loop with the minimal amount of Paratone-N oil. Data was collected at 100 K using a cold stream of $\text{N}_2(\text{g})$ provided by an Oxford Cryostream 700 LT device. Preliminary unit cell constants were determined with a set of 24 narrow frame scans. Data was collected as a series of ϕ and/or ω scans with typical scan width of 0.5° and counting time of 10-30 seconds/frame at a crystal to detector distance of ~ 3.7 cm. The collection, cell refinement, and integration of intensity data was carried out with the APEX3 software.¹ Final cell constants were determined by global refinement of reflections from the complete data set. A multi-scan absorption correction was performed with SADABS.² The structure was phased with intrinsic methods using SHELXT3 and refined with the full-matrix least-squares program SHELXL.⁴

(1) Bruker (2018). APEX3. Bruker AXS, Inc., Madison, Wisconsin, USA.

(2) Krause, L., Herbst-Irmer, R., Sheldrick, G. M. and Stalke, D. J. *Appl. Cryst.*, 2015, 48, 3-10.

(3) Sheldrick, G. M. *Acta Cryst.* 2015, A71, 3-8.

(4) Sheldrick, G. M. *Acta Cryst.* 2015, C71, 3-8. SI39

Valine HIM in Naphthalene system

CCDC # 2388281

The structure was confirmed by obtaining a single crystal that was solved using X-ray diffraction. The single crystal of valine HIM in naphthalene system, **6b** suitable for X-ray crystallography was obtained using chloroform and diethyl ether by vapor diffusion method. The single crystal was run at 100K using a wavelength of 0.71073 Å. From the analysis of single crystal data set, analogous to the previously reported single crystal structure of valine HIM and Phenylalanine HIM, valine HIM in naphthalene system is also a distorted planar macrocyclic system consisting of the amino acids carbonyl oxygen facing inside the ring. All three isopropyl groups are located above the plane.

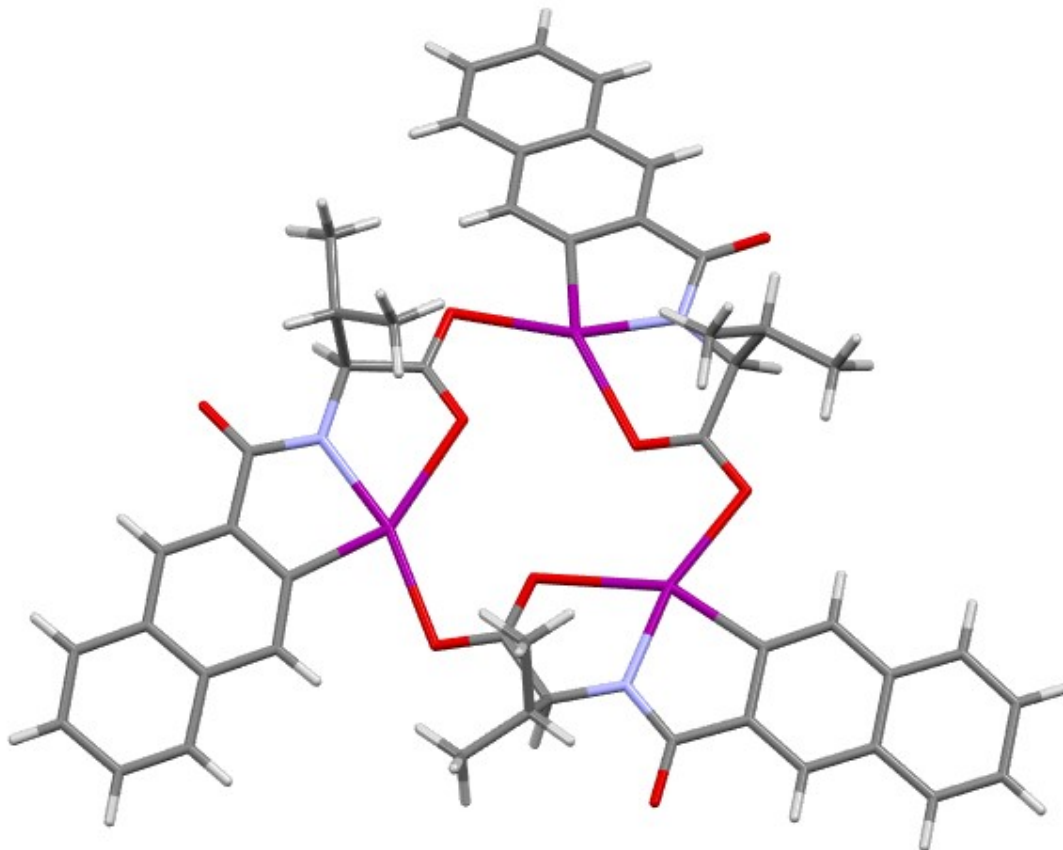


Figure S115: Perspective view of crystallographically independent molecules of Valine HIM in Naphthalene system. Solvent is removed for clarity. Nitrogen, oxygen and iodine atoms are denoted by light blue, red and purple color respectively. Hydrogens atoms are omitted. (Capped sticks style)

Adduct (HIM monomer 7b)

CCDC # 2388282

From the X-ray analysis, we observed one adduct per tetraethylammonium cation. The iodine atom is covalently bonded to chlorine atom with quite a long bond length of 2.73 Å. The perspective view of crystallographically independent molecules of adduct is shown in the figure below.

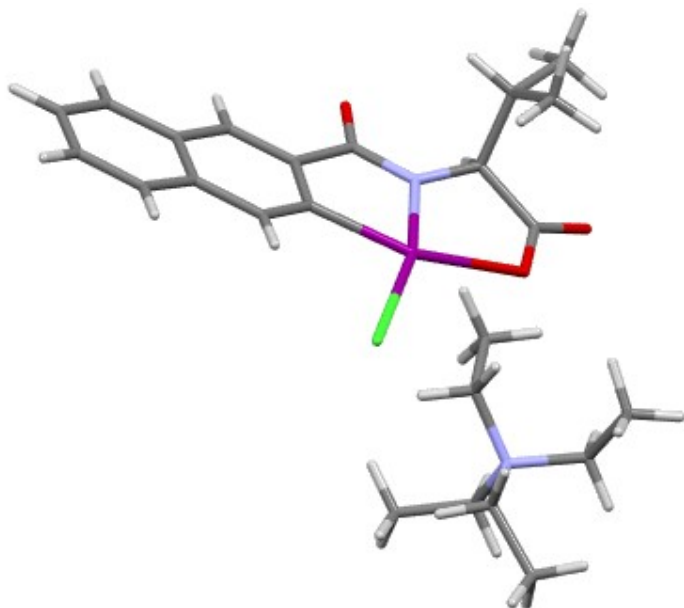


Figure S116: Perspective view of crystallographically independent molecules of HIM monomer **7b**. Solvents are removed for clarity. Nitrogen, oxygen, iodine and chlorine atoms are denoted by light blue, red, pink and green color respectively. Hydrogens atoms are omitted. (Capped sticks style)

Valine HIM in Naphthalene system 6b/C60

CCDC # 2388283

The structure was confirmed by obtaining a single crystal that was solved using X-ray diffraction. The single crystal of Valine HIM in Naphthalene system **6b**/C₆₀ suitable for X-ray crystallography was obtained using chloroform/1,2-dichlorobenzene, and diethyl ether by vapor diffusion method. The single crystal was run at 100K using a wavelength of 0.71073 Å. From the analysis of single crystal data set, we observed that valine HIM in naphthalene system is also a distorted planar macrocyclic system consisting of the amino acids carbonyl oxygen facing inside the ring. All three isopropyl groups are located above the plane. Three fullerenes are co-crystallized with every two macrocycles.

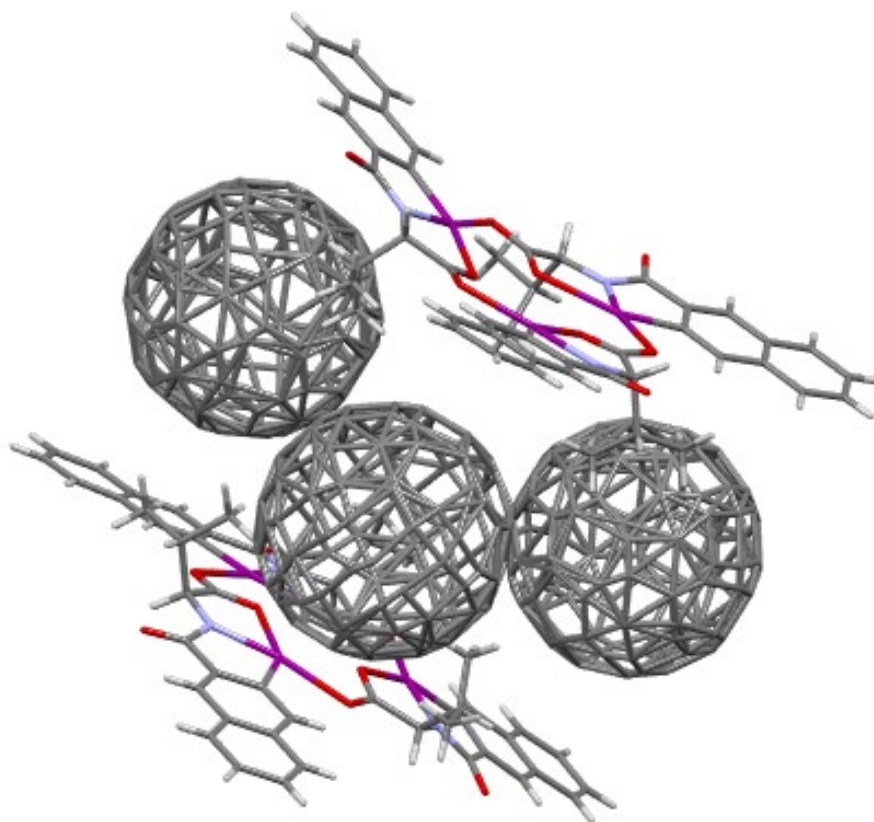


Figure SI17: Perspective view of crystallographically independent molecules of Valine HIM in Naphthalene system. Solvent is removed for clarity. Nitrogen, oxygen and iodine atoms are denoted by light blue, red and purple color respectively. Hydrogens atoms are omitted. (Capped sticks style)

University of Illinois, Department of Chemistry
George L. Clark X- R Facility and 3M Materials Laboratory

Structure report for compound **Valine HIM in Naphthalene System**

Identification code	CCDC 2388281
Empirical formula	C _{50.64} H _{46.93} Cl _{3.36} I ₃ N ₃ O _{9.38}
Principal Investigator:	Professor Dr. Kyle N Plunkett

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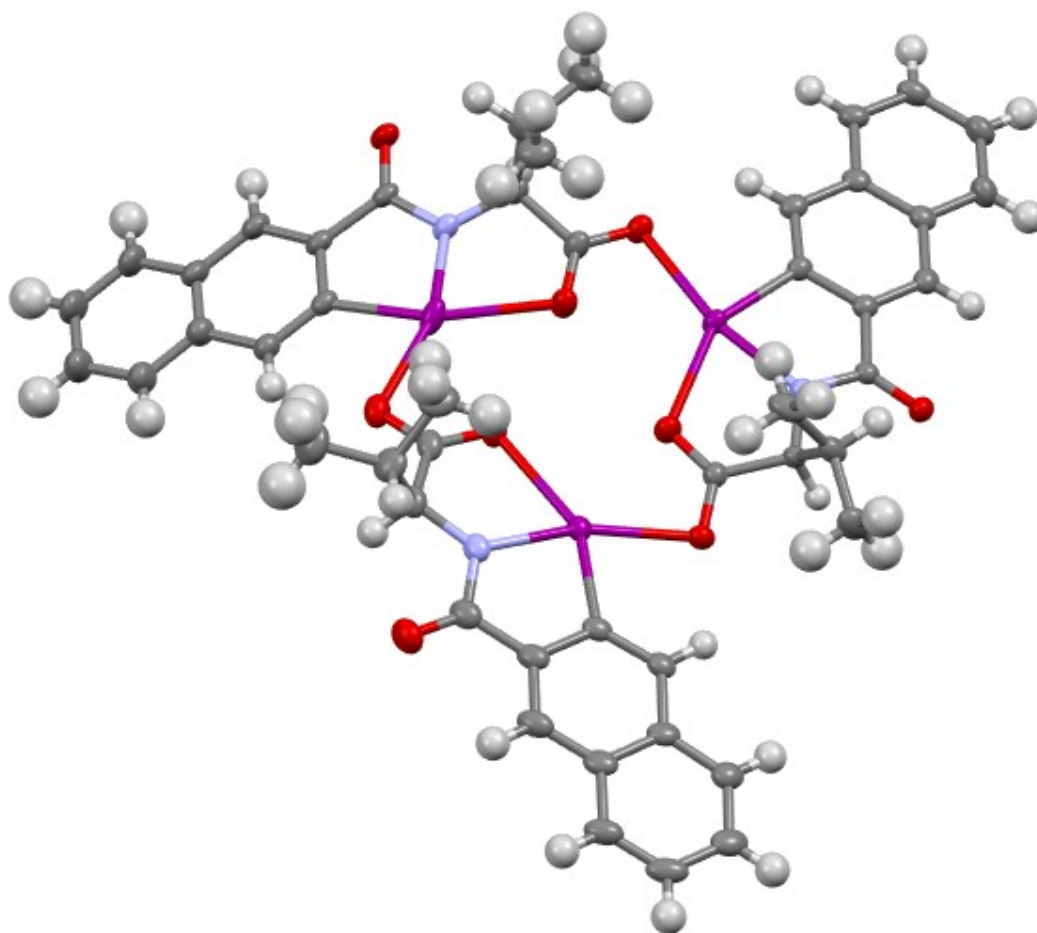


Figure SI18: Perspective view of crystallographically independent molecules of Valine HIM in Naphthalene system. Solvent is removed for clarity. Nitrogen, oxygen, and iodine atoms are denoted by light blue, red and purple color respectively. Hydrogens atoms are omitted. (Ellipsoid style)

Table 1. Crystal data and structure refinement for 4468ds.

Identification code	CCDC 2388281	
Empirical formula	C50.64 H46.93 Cl3.36 I3 N3 O9.38	
Formula weight	1347.33	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁	
Unit cell dimensions	a = 14.7131(3) Å	a = 90°.
	b = 22.8611(4) Å	b = 96.0622(4)°.
	c = 15.1145(3) Å	g = 90°.
Volume	5055.45(17) Å ³	
Z	4	
Density (calculated)	1.770 Mg/m ³	
Absorption coefficient	2.092 mm ⁻¹	
F(000)	2652	
Crystal size	0.259 x 0.184 x 0.100 mm ³	
Theta range for data collection	2.228 to 28.339°.	
Index ranges	-19<=h<=19, -30<=k<=30, -19<=l<=20	
Reflections collected	181866	
Independent reflections	25204 [R(int) = 0.0356]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6633	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	25204 / 1013 / 1553	
Goodness-of-fit on F ²	1.066	
Final R indices [I>2sigma(I)]	R1 = 0.0233, wR2 = 0.0588	
R indices (all data)	R1 = 0.0244, wR2 = 0.0597	
Absolute structure parameter	-0.027(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.132 and -1.524 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4468ds. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1)	6685(1)	3596(1)	942(1)	21(1)
I(2)	8151(1)	5401(1)	2749(1)	20(1)
I(3)	5965(1)	5766(1)	-191(1)	20(1)
I(4)	8751(1)	4462(1)	9886(1)	23(1)
I(5)	7797(1)	6508(1)	8411(1)	23(1)
I(6)	6520(1)	4560(1)	6931(1)	33(1)
O(1)	5726(2)	2752(2)	-1398(2)	28(1)
O(2)	5481(2)	4934(2)	-1014(2)	25(1)
O(3)	6171(3)	4560(2)	236(2)	30(1)
O(4)	9928(3)	4414(2)	4485(3)	39(1)
O(5)	7569(2)	3489(2)	2337(2)	28(1)
O(6)	7442(3)	4447(2)	2140(3)	37(1)
O(7)	6086(3)	7588(2)	-200(2)	30(1)
O(8)	7846(2)	6339(2)	2173(2)	25(1)
O(9)	6976(3)	5758(2)	1270(3)	36(1)
O(10)	10246(2)	5098(2)	12182(2)	27(1)
O(11)	8550(2)	6420(2)	9864(2)	26(1)
O(12)	8410(3)	5500(2)	9391(2)	30(1)
O(13)	6564(3)	7659(2)	6529(3)	42(1)
O(14)	6128(2)	5486(2)	6329(2)	32(1)
O(15)	7168(3)	5667(2)	7459(3)	32(1)
N(1)	5959(3)	3440(2)	-305(3)	23(1)
N(2)	8716(3)	4689(2)	3501(3)	25(1)
N(3)	6229(3)	6630(2)	244(3)	22(1)
N(4)	9432(3)	5045(2)	10812(3)	22(1)
N(5)	7155(3)	6829(2)	7202(3)	28(1)
C(1)	6805(3)	2679(2)	871(3)	22(1)
C(2)	7196(3)	2326(2)	1531(3)	24(1)
C(3)	7195(3)	1708(2)	1371(3)	25(1)
C(4)	7585(3)	1311(2)	2027(3)	28(1)
C(5)	7553(4)	723(2)	1881(4)	32(1)

C(6)	7136(3)	495(2)	1077(4)	28(1)
C(7)	6772(3)	861(2)	415(3)	26(1)
C(8)	6798(3)	1483(2)	537(3)	24(1)
C(9)	6415(3)	1872(2)	-124(3)	24(1)
C(10)	6422(3)	2467(2)	43(3)	22(1)
C(11)	6011(3)	2891(2)	-629(3)	23(1)
C(12)	5499(3)	3895(2)	-879(3)	21(1)
C(13)	5749(3)	4500(2)	-517(3)	22(1)
C(14)	4443(3)	3798(2)	-972(3)	24(1)
C(15)	4026(3)	3987(2)	-142(4)	31(1)
C(16)	3990(3)	4082(2)	-1818(3)	30(1)
C(17)	9159(3)	5828(2)	3604(3)	23(1)
C(18)	9280(3)	6421(2)	3659(3)	25(1)
C(19)	9989(4)	6638(2)	4290(3)	28(1)
C(20)	10118(4)	7248(2)	4415(4)	36(1)
C(21)	10800(5)	7451(3)	5028(4)	46(2)
C(22)	11367(5)	7060(3)	5540(4)	48(2)
C(23)	11261(4)	6473(3)	5440(4)	40(1)
C(24)	10556(4)	6242(2)	4812(3)	32(1)
C(25)	10409(3)	5637(2)	4712(3)	29(1)
C(26)	9718(3)	5427(2)	4117(3)	27(1)
C(27)	9489(3)	4792(2)	4055(3)	28(1)
C(28)	8271(3)	4118(2)	3488(3)	25(1)
C(29)	7732(3)	4019(2)	2590(3)	24(1)
C(30)	7640(5)	4071(3)	4257(4)	48(2)
C(31)	7220(20)	3468(6)	4278(18)	43(4)
C(32)	6936(9)	4534(5)	4245(8)	70(4)
C(31A)	7250(50)	3497(13)	4410(50)	42(7)
C(32A)	7730(30)	4507(13)	4900(20)	86(7)
C(33)	5328(3)	6229(2)	-1290(3)	21(1)
C(34)	4880(3)	5980(2)	-2029(3)	22(1)
C(35)	4542(3)	6359(2)	-2741(3)	24(1)
C(36)	4081(4)	6131(3)	-3538(4)	33(1)
C(37)	3821(4)	6493(3)	-4249(4)	41(1)
C(38)	3991(4)	7101(3)	-4188(4)	41(1)
C(39)	4404(4)	7336(3)	-3420(4)	34(1)

C(40)	4699(3)	6972(2)	-2674(3)	26(1)
C(41)	5146(3)	7200(2)	-1876(3)	27(1)
C(42)	5450(3)	6839(2)	-1185(3)	21(1)
C(43)	5945(3)	7065(2)	-345(3)	22(1)
C(44)	6772(3)	6791(2)	1084(3)	23(1)
C(45)	7228(3)	6253(2)	1519(3)	24(1)
C(46)	6178(4)	7093(2)	1723(3)	36(1)
C(47)	5598(5)	6663(4)	2187(4)	57(2)
C(48)	6742(6)	7489(3)	2388(5)	66(2)
C(49)	9317(3)	3869(2)	10852(3)	23(1)
C(50)	9218(3)	3270(2)	10822(3)	26(1)
C(51)	9607(3)	2938(2)	11562(3)	24(1)
C(52)	9518(3)	2316(2)	11572(4)	28(1)
C(53)	9868(4)	2003(2)	12303(4)	31(1)
C(54)	10326(4)	2285(2)	13055(4)	34(1)
C(55)	10422(4)	2883(2)	13058(4)	33(1)
C(56)	10070(3)	3224(2)	12310(3)	25(1)
C(57)	10160(3)	3839(2)	12309(3)	25(1)
C(58)	9787(3)	4161(2)	11589(3)	22(1)
C(59)	9859(3)	4809(2)	11567(3)	21(1)
C(60)	9417(3)	5690(2)	10719(3)	22(1)
C(61)	8732(3)	5869(2)	9938(3)	24(1)
C(62)	10371(3)	5934(2)	10580(4)	30(1)
C(63)	10596(4)	5858(2)	9627(4)	38(1)
C(64)	10469(4)	6571(2)	10874(5)	42(1)
C(65)	7905(3)	7414(2)	8649(3)	25(1)
C(66)	8313(3)	7669(2)	9405(4)	26(1)
C(67)	8292(3)	8287(2)	9474(4)	29(1)
C(68)	8685(3)	8583(2)	10246(4)	32(1)
C(69)	8656(4)	9182(3)	10309(4)	37(1)
C(70)	8246(4)	9514(3)	9598(4)	38(1)
C(71)	7862(4)	9247(2)	8832(4)	37(1)
C(72)	7869(3)	8624(2)	8760(4)	31(1)
C(73)	7444(4)	8341(2)	7995(4)	36(1)
C(74)	7455(4)	7735(2)	7935(4)	30(1)
C(75)	7008(4)	7418(3)	7151(4)	33(1)

C(76)	6714(3)	6461(3)	6482(3)	31(1)
C(77)	6663(3)	5835(2)	6794(3)	28(1)
C(78)	7253(4)	6491(3)	5644(3)	38(1)
C(79)	6644(5)	6337(4)	4808(4)	56(2)
C(80)	8112(4)	6110(3)	5755(5)	45(1)
O(16)	5975(6)	2827(3)	6529(6)	33(2)
O(17)	8115(9)	3616(8)	9114(9)	28(2)
O(18)	7559(7)	4364(5)	8302(8)	31(2)
N(6)	6567(6)	3694(4)	7100(7)	26(2)
C(81)	5360(6)	4339(4)	6030(7)	26(2)
C(82)	4765(6)	4704(4)	5562(6)	29(1)
C(83)	3956(3)	4457(3)	5089(5)	36(1)
C(84)	3305(5)	4822(2)	4642(5)	47(2)
C(85)	2500(4)	4587(3)	4223(5)	53(2)
C(86)	2347(4)	3987(3)	4252(5)	54(2)
C(87)	2998(4)	3623(2)	4699(5)	45(2)
C(88)	3803(4)	3858(2)	5118(4)	36(1)
C(89)	4470(6)	3488(4)	5584(6)	32(1)
C(90)	5239(6)	3734(4)	6043(6)	27(1)
C(91)	5951(6)	3360(4)	6564(6)	24(1)
C(92)	7285(7)	3401(4)	7673(7)	27(2)
C(93)	7679(7)	3831(5)	8410(7)	28(2)
C(94)	8082(7)	3171(5)	7160(8)	32(2)
C(95)	8663(9)	2722(5)	7720(9)	44(3)
C(96)	8686(13)	3661(7)	6874(11)	47(3)
O(16A)	6300(9)	2684(5)	6569(9)	31(2)
O(17A)	8303(15)	3587(12)	9124(12)	27(2)
O(18A)	7829(9)	4304(7)	8193(10)	25(3)
N(6A)	6795(8)	3582(5)	7111(10)	24(2)
C(81A)	5436(9)	4158(6)	6146(11)	26(2)
C(82A)	4725(7)	4485(6)	5802(9)	30(2)
C(83A)	3909(7)	4190(5)	5451(9)	34(2)
C(84A)	3124(7)	4504(6)	5165(10)	42(2)
C(85A)	2311(9)	4222(6)	4903(11)	48(2)
C(86A)	2274(9)	3610(6)	4899(11)	47(2)
C(87A)	3045(8)	3290(5)	5183(10)	41(2)

C(88A)	3867(7)	3583(5)	5456(9)	35(2)
C(89A)	4651(8)	3255(6)	5790(9)	31(2)
C(90A)	5423(8)	3552(6)	6149(10)	27(2)
C(91A)	6218(10)	3213(5)	6601(10)	26(2)
C(92A)	7559(9)	3324(6)	7663(10)	26(2)
C(93A)	7902(12)	3776(7)	8388(11)	27(2)
C(94A)	8358(10)	3125(7)	7130(11)	31(2)
C(95A)	9062(12)	2769(8)	7710(13)	40(3)
C(96A)	8768(16)	3628(9)	6657(12)	32(3)
CI(1)	4384(2)	5110(2)	1678(2)	63(1)
CI(2)	5622(3)	5209(2)	3322(2)	73(1)
CI(3)	4964(3)	4057(1)	2689(3)	74(1)
C(98)	5280(2)	4771(1)	2374(2)	68(3)
CI(1A)	5223(3)	4875(2)	1958(3)	61(1)
CI(2A)	4830(3)	5334(2)	3664(3)	63(1)
CI(3A)	4465(3)	4112(2)	3221(3)	65(1)
C(98A)	4487(12)	4838(6)	2777(10)	65(2)
CI(4)	4021(3)	6220(2)	3487(3)	71(1)
CI(5)	2192(4)	6580(4)	3649(4)	104(2)
CI(6)	2690(4)	6210(3)	1940(4)	90(2)
C(99)	3169(10)	6595(7)	2985(8)	75(3)
CI(4A)	2392(6)	6531(3)	3250(4)	102(2)
CI(5A)	2308(3)	5285(2)	3415(3)	69(1)
CI(6A)	2643(3)	5833(2)	1746(2)	52(1)
C(99A)	2060(12)	5897(6)	2756(9)	66(3)
C(100)	-361(7)	5271(4)	7518(7)	84(3)
C(101)	234(7)	4989(4)	6874(5)	76(3)
O(19)	619(5)	4468(3)	7262(4)	73(2)
C(102)	1191(6)	4168(4)	6712(6)	80(2)
C(103)	1562(8)	3620(4)	7193(9)	110(5)
CI(7)	2154(7)	4628(4)	6311(6)	67(2)
CI(8)	1281(8)	3636(5)	6939(9)	83(3)
CI(9)	434(8)	4790(5)	7062(8)	74(3)
C(104)	1137(16)	4344(9)	6410(20)	75(3)

Table 3. Bond lengths [Å] and angles [°] for 4468ds.

I(1)-N(1)	2.097(4)
I(1)-C(1)	2.107(5)
I(1)-O(5)	2.370(3)
I(2)-C(17)	2.102(4)
I(2)-N(2)	2.104(4)
I(2)-O(8)	2.340(3)
I(3)-C(33)	2.105(4)
I(3)-N(3)	2.107(4)
I(3)-O(2)	2.341(3)
I(4)-C(49)	2.098(5)
I(4)-N(4)	2.109(4)
I(4)-O(17A)	2.37(3)
I(4)-O(17)	2.397(17)
I(5)-N(5)	2.098(4)
I(5)-C(65)	2.104(5)
I(5)-O(11)	2.363(3)
I(6)-N(6)	1.996(9)
I(6)-C(81A)	2.097(12)
I(6)-C(81)	2.130(8)
I(6)-N(6A)	2.282(13)
I(6)-O(14)	2.353(4)
I(6)-O(18)	2.482(12)
O(1)-C(11)	1.235(6)
O(2)-C(13)	1.282(6)
O(3)-C(13)	1.246(6)
O(4)-C(27)	1.223(6)
O(5)-C(29)	1.285(6)
O(6)-C(29)	1.242(6)
O(7)-C(43)	1.230(6)
O(8)-C(45)	1.286(6)
O(9)-C(45)	1.235(6)
O(10)-C(59)	1.229(6)
O(11)-C(61)	1.290(6)
O(12)-C(61)	1.239(6)

O(13)-C(75)	1.217(7)
O(14)-C(77)	1.278(6)
O(15)-C(77)	1.245(6)
N(1)-C(11)	1.353(6)
N(1)-C(12)	1.473(6)
N(2)-C(27)	1.360(6)
N(2)-C(28)	1.459(6)
N(3)-C(43)	1.369(6)
N(3)-C(44)	1.473(6)
N(4)-C(59)	1.354(6)
N(4)-C(60)	1.480(6)
N(5)-C(75)	1.365(7)
N(5)-C(76)	1.472(7)
C(1)-C(2)	1.363(7)
C(1)-C(10)	1.403(7)
C(2)-C(3)	1.433(7)
C(2)-H(2)	0.9500
C(3)-C(4)	1.419(7)
C(3)-C(8)	1.427(7)
C(4)-C(5)	1.363(7)
C(4)-H(4)	0.9500
C(5)-C(6)	1.403(8)
C(5)-H(5)	0.9500
C(6)-C(7)	1.369(7)
C(6)-H(6)	0.9500
C(7)-C(8)	1.435(7)
C(7)-H(7)	0.9500
C(8)-C(9)	1.409(7)
C(9)-C(10)	1.385(6)
C(9)-H(9)	0.9500
C(10)-C(11)	1.485(6)
C(12)-C(13)	1.516(6)
C(12)-C(14)	1.561(6)
C(12)-H(12)	1.0000
C(14)-C(15)	1.517(7)
C(14)-C(16)	1.523(7)

C(14)-H(14)	1.0000
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(18)	1.368(7)
C(17)-C(26)	1.408(7)
C(18)-C(19)	1.425(6)
C(18)-H(18)	0.9500
C(19)-C(24)	1.414(8)
C(19)-C(20)	1.416(7)
C(20)-C(21)	1.373(8)
C(20)-H(20)	0.9500
C(21)-C(22)	1.400(9)
C(21)-H(21)	0.9500
C(22)-C(23)	1.357(9)
C(22)-H(22)	0.9500
C(23)-C(24)	1.431(7)
C(23)-H(23)	0.9500
C(24)-C(25)	1.407(8)
C(25)-C(26)	1.370(7)
C(25)-H(25)	0.9500
C(26)-C(27)	1.493(7)
C(28)-C(29)	1.516(6)
C(28)-C(30)	1.566(8)
C(28)-H(28)	1.0000
C(30)-C(32A)	1.39(2)
C(30)-C(31A)	1.46(2)
C(30)-C(32)	1.480(13)
C(30)-C(31)	1.517(11)
C(30)-H(30A)	1.0000
C(30)-H(30B)	0.9(3)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800

C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(31A)-H(31D)	0.9800
C(31A)-H(31E)	0.9800
C(31A)-H(31F)	0.9800
C(32A)-H(32D)	0.9800
C(32A)-H(32E)	0.9800
C(32A)-H(32F)	0.9800
C(33)-C(34)	1.361(6)
C(33)-C(42)	1.412(6)
C(34)-C(35)	1.429(6)
C(34)-H(34)	0.9500
C(35)-C(36)	1.417(7)
C(35)-C(40)	1.422(7)
C(36)-C(37)	1.378(8)
C(36)-H(36)	0.9500
C(37)-C(38)	1.414(9)
C(37)-H(37)	0.9500
C(38)-C(39)	1.364(8)
C(38)-H(38)	0.9500
C(39)-C(40)	1.431(7)
C(39)-H(39)	0.9500
C(40)-C(41)	1.412(7)
C(41)-C(42)	1.369(7)
C(41)-H(41)	0.9500
C(42)-C(43)	1.488(7)
C(44)-C(45)	1.518(6)
C(44)-C(46)	1.534(7)
C(44)-H(44)	1.0000
C(46)-C(47)	1.520(9)
C(46)-C(48)	1.531(9)
C(46)-H(46)	1.0000
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800

C(47)-H(47C)	0.9800
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-C(50)	1.378(7)
C(49)-C(58)	1.414(7)
C(50)-C(51)	1.422(7)
C(50)-H(50)	0.9500
C(51)-C(56)	1.417(7)
C(51)-C(52)	1.428(7)
C(52)-C(53)	1.371(7)
C(52)-H(52)	0.9500
C(53)-C(54)	1.415(8)
C(53)-H(53)	0.9500
C(54)-C(55)	1.373(8)
C(54)-H(54)	0.9500
C(55)-C(56)	1.425(7)
C(55)-H(55)	0.9500
C(56)-C(57)	1.412(7)
C(57)-C(58)	1.378(7)
C(57)-H(57)	0.9500
C(58)-C(59)	1.487(6)
C(60)-C(61)	1.526(6)
C(60)-C(62)	1.546(7)
C(60)-H(60)	1.0000
C(62)-C(63)	1.521(8)
C(62)-C(64)	1.524(7)
C(62)-H(62)	1.0000
C(63)-H(63A)	0.9800
C(63)-H(63B)	0.9800
C(63)-H(63C)	0.9800
C(64)-H(64A)	0.9800
C(64)-H(64B)	0.9800
C(64)-H(64C)	0.9800
C(65)-C(66)	1.364(7)
C(65)-C(74)	1.412(7)

C(66)-C(67)	1.418(7)
C(66)-H(66)	0.9500
C(67)-C(72)	1.416(8)
C(67)-C(68)	1.417(8)
C(68)-C(69)	1.374(8)
C(68)-H(68)	0.9500
C(69)-C(70)	1.399(9)
C(69)-H(69)	0.9500
C(70)-C(71)	1.377(9)
C(70)-H(70)	0.9500
C(71)-C(72)	1.428(8)
C(71)-H(71)	0.9500
C(72)-C(73)	1.412(9)
C(73)-C(74)	1.389(8)
C(73)-H(73)	0.9500
C(74)-C(75)	1.482(8)
C(76)-C(77)	1.512(8)
C(76)-C(78)	1.565(7)
C(76)-H(76)	1.0000
C(78)-C(79)	1.511(9)
C(78)-C(80)	1.531(9)
C(78)-H(78)	1.0000
C(79)-H(79A)	0.9800
C(79)-H(79B)	0.9800
C(79)-H(79C)	0.9800
C(80)-H(80A)	0.9800
C(80)-H(80B)	0.9800
C(80)-H(80C)	0.9800
O(16)-C(91)	1.220(10)
O(17)-C(93)	1.281(9)
O(18)-C(93)	1.240(9)
N(6)-C(91)	1.379(8)
N(6)-C(92)	1.457(11)
C(81)-C(82)	1.354(12)
C(81)-C(90)	1.395(12)
C(82)-C(83)	1.437(8)

C(82)-H(82)	0.9500
C(83)-C(84)	1.3900
C(83)-C(88)	1.3900
C(84)-C(85)	1.3900
C(84)-H(84)	0.9500
C(85)-C(86)	1.3900
C(85)-H(85)	0.9500
C(86)-C(87)	1.3900
C(86)-H(86)	0.9500
C(87)-C(88)	1.3900
C(87)-H(87)	0.9500
C(88)-C(89)	1.425(11)
C(89)-C(90)	1.383(9)
C(89)-H(89)	0.9500
C(90)-C(91)	1.507(13)
C(92)-C(93)	1.550(9)
C(92)-C(94)	1.564(12)
C(92)-H(92)	1.0000
C(94)-C(96)	1.521(12)
C(94)-C(95)	1.531(12)
C(94)-H(94)	1.0000
C(95)-H(95A)	0.9800
C(95)-H(95B)	0.9800
C(95)-H(95C)	0.9800
C(96)-H(96A)	0.9800
C(96)-H(96B)	0.9800
C(96)-H(96C)	0.9800
O(16A)-C(91A)	1.216(13)
O(17A)-C(93A)	1.278(11)
O(18A)-C(93A)	1.245(11)
N(6A)-C(91A)	1.375(11)
N(6A)-C(92A)	1.452(13)
C(81A)-C(82A)	1.345(14)
C(81A)-C(90A)	1.386(14)
C(82A)-C(83A)	1.428(11)
C(82A)-H(82A)	0.9500

C(83A)-C(84A)	1.390(11)
C(83A)-C(88A)	1.390(11)
C(84A)-C(85A)	1.380(11)
C(84A)-H(84A)	0.9500
C(85A)-C(86A)	1.399(12)
C(85A)-H(85A)	0.9500
C(86A)-C(87A)	1.381(12)
C(86A)-H(86A)	0.9500
C(87A)-C(88A)	1.406(11)
C(87A)-H(87A)	0.9500
C(88A)-C(89A)	1.422(14)
C(89A)-C(90A)	1.385(11)
C(89A)-H(89A)	0.9500
C(90A)-C(91A)	1.506(15)
C(92A)-C(93A)	1.552(11)
C(92A)-C(94A)	1.560(14)
C(92A)-H(92A)	1.0000
C(94A)-C(96A)	1.514(13)
C(94A)-C(95A)	1.521(14)
C(94A)-H(94A)	1.0000
C(95A)-H(95D)	0.9800
C(95A)-H(95E)	0.9800
C(95A)-H(95F)	0.9800
C(96A)-H(96D)	0.9800
C(96A)-H(96E)	0.9800
C(96A)-H(96F)	0.9800
CI(1)-C(98)	1.7762
CI(2)-C(98)	1.7762
CI(3)-C(98)	1.7761
C(98)-H(98)	1.0000
CI(1A)-C(98A)	1.732(15)
CI(2A)-C(98A)	1.789(14)
CI(3A)-C(98A)	1.791(15)
C(98A)-H(98A)	1.0000
CI(4)-C(99)	1.638(13)
CI(5)-C(99)	1.839(13)

Cl(6)-C(99)	1.877(16)
C(99)-H(99)	1.0000
Cl(4A)-C(99A)	1.678(15)
Cl(5A)-C(99A)	1.734(14)
Cl(6A)-C(99A)	1.834(14)
C(99A)-H(99A)	1.0000
C(100)-C(101)	1.5202
C(100)-H(10A)	0.9800
C(100)-H(10B)	0.9800
C(100)-H(10C)	0.9800
C(101)-O(19)	1.4205
C(101)-H(10D)	0.9900
C(101)-H(10E)	0.9900
O(19)-C(102)	1.4204
C(102)-C(103)	1.5202
C(102)-H(10F)	0.9900
C(102)-H(10G)	0.9900
C(103)-H(10H)	0.9800
C(103)-H(10I)	0.9800
C(103)-H(10J)	0.9800
Cl(7)-C(104)	1.65(2)
Cl(8)-C(104)	1.80(2)
Cl(9)-C(104)	1.81(2)
C(104)-H(104)	1.0000
N(1)-I(1)-C(1)	79.81(17)
N(1)-I(1)-O(5)	164.16(13)
C(1)-I(1)-O(5)	84.37(15)
C(17)-I(2)-N(2)	79.30(17)
C(17)-I(2)-O(8)	84.18(15)
N(2)-I(2)-O(8)	163.48(14)
C(33)-I(3)-N(3)	79.97(17)
C(33)-I(3)-O(2)	84.49(15)
N(3)-I(3)-O(2)	164.46(13)
C(49)-I(4)-N(4)	79.62(16)
C(49)-I(4)-O(17A)	82.2(4)

N(4)-I(4)-O(17A)	161.1(4)
C(49)-I(4)-O(17)	85.7(3)
N(4)-I(4)-O(17)	165.3(3)
N(5)-I(5)-C(65)	79.87(19)
N(5)-I(5)-O(11)	164.44(15)
C(65)-I(5)-O(11)	84.57(17)
N(6)-I(6)-C(81)	82.0(3)
C(81A)-I(6)-N(6A)	75.7(4)
N(6)-I(6)-O(14)	161.0(3)
C(81A)-I(6)-O(14)	92.0(4)
C(81)-I(6)-O(14)	79.6(3)
N(6A)-I(6)-O(14)	163.8(4)
N(6)-I(6)-O(18)	72.8(3)
C(81)-I(6)-O(18)	150.8(4)
O(14)-I(6)-O(18)	126.1(3)
C(13)-O(2)-I(3)	105.1(3)
C(29)-O(5)-I(1)	103.6(3)
C(45)-O(8)-I(2)	103.7(3)
C(61)-O(11)-I(5)	103.7(3)
C(77)-O(14)-I(6)	103.7(3)
C(11)-N(1)-C(12)	118.9(4)
C(11)-N(1)-I(1)	116.1(3)
C(12)-N(1)-I(1)	124.6(3)
C(27)-N(2)-C(28)	120.4(4)
C(27)-N(2)-I(2)	117.2(3)
C(28)-N(2)-I(2)	122.3(3)
C(43)-N(3)-C(44)	118.7(4)
C(43)-N(3)-I(3)	116.4(3)
C(44)-N(3)-I(3)	124.6(3)
C(59)-N(4)-C(60)	118.5(4)
C(59)-N(4)-I(4)	116.9(3)
C(60)-N(4)-I(4)	124.4(3)
C(75)-N(5)-C(76)	117.9(4)
C(75)-N(5)-I(5)	116.7(4)
C(76)-N(5)-I(5)	124.5(3)
C(2)-C(1)-C(10)	123.2(4)

C(2)-C(1)-I(1)	125.7(4)
C(10)-C(1)-I(1)	111.1(3)
C(1)-C(2)-C(3)	117.9(5)
C(1)-C(2)-H(2)	121.1
C(3)-C(2)-H(2)	121.1
C(4)-C(3)-C(8)	119.0(4)
C(4)-C(3)-C(2)	121.2(5)
C(8)-C(3)-C(2)	119.8(4)
C(5)-C(4)-C(3)	120.8(5)
C(5)-C(4)-H(4)	119.6
C(3)-C(4)-H(4)	119.6
C(4)-C(5)-C(6)	120.9(5)
C(4)-C(5)-H(5)	119.6
C(6)-C(5)-H(5)	119.6
C(7)-C(6)-C(5)	120.5(5)
C(7)-C(6)-H(6)	119.8
C(5)-C(6)-H(6)	119.8
C(6)-C(7)-C(8)	120.6(5)
C(6)-C(7)-H(7)	119.7
C(8)-C(7)-H(7)	119.7
C(9)-C(8)-C(3)	119.6(4)
C(9)-C(8)-C(7)	122.1(5)
C(3)-C(8)-C(7)	118.2(4)
C(10)-C(9)-C(8)	119.8(5)
C(10)-C(9)-H(9)	120.1
C(8)-C(9)-H(9)	120.1
C(9)-C(10)-C(1)	119.7(4)
C(9)-C(10)-C(11)	121.4(4)
C(1)-C(10)-C(11)	118.8(4)
O(1)-C(11)-N(1)	123.6(4)
O(1)-C(11)-C(10)	123.3(4)
N(1)-C(11)-C(10)	113.0(4)
N(1)-C(12)-C(13)	110.7(4)
N(1)-C(12)-C(14)	110.1(4)
C(13)-C(12)-C(14)	111.4(4)
N(1)-C(12)-H(12)	108.2

C(13)-C(12)-H(12)	108.2
C(14)-C(12)-H(12)	108.2
O(3)-C(13)-O(2)	122.8(4)
O(3)-C(13)-C(12)	120.5(4)
O(2)-C(13)-C(12)	116.6(4)
C(15)-C(14)-C(16)	113.2(4)
C(15)-C(14)-C(12)	111.7(4)
C(16)-C(14)-C(12)	111.0(4)
C(15)-C(14)-H(14)	106.8
C(16)-C(14)-H(14)	106.8
C(12)-C(14)-H(14)	106.8
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(18)-C(17)-C(26)	123.1(4)
C(18)-C(17)-I(2)	125.2(3)
C(26)-C(17)-I(2)	111.7(3)
C(17)-C(18)-C(19)	117.8(4)
C(17)-C(18)-H(18)	121.1
C(19)-C(18)-H(18)	121.1
C(24)-C(19)-C(20)	119.5(5)
C(24)-C(19)-C(18)	119.8(5)
C(20)-C(19)-C(18)	120.7(5)
C(21)-C(20)-C(19)	120.1(5)
C(21)-C(20)-H(20)	119.9
C(19)-C(20)-H(20)	119.9
C(20)-C(21)-C(22)	120.4(6)

C(20)-C(21)-H(21)	119.8
C(22)-C(21)-H(21)	119.8
C(23)-C(22)-C(21)	121.1(5)
C(23)-C(22)-H(22)	119.5
C(21)-C(22)-H(22)	119.5
C(22)-C(23)-C(24)	120.3(6)
C(22)-C(23)-H(23)	119.9
C(24)-C(23)-H(23)	119.9
C(25)-C(24)-C(19)	119.7(5)
C(25)-C(24)-C(23)	121.7(5)
C(19)-C(24)-C(23)	118.6(5)
C(26)-C(25)-C(24)	120.6(5)
C(26)-C(25)-H(25)	119.7
C(24)-C(25)-H(25)	119.7
C(25)-C(26)-C(17)	118.9(5)
C(25)-C(26)-C(27)	121.9(5)
C(17)-C(26)-C(27)	119.0(4)
O(4)-C(27)-N(2)	124.5(5)
O(4)-C(27)-C(26)	123.4(5)
N(2)-C(27)-C(26)	112.0(4)
N(2)-C(28)-C(29)	109.8(4)
N(2)-C(28)-C(30)	110.6(4)
C(29)-C(28)-C(30)	111.1(5)
N(2)-C(28)-H(28)	108.5
C(29)-C(28)-H(28)	108.5
C(30)-C(28)-H(28)	108.5
O(6)-C(29)-O(5)	122.6(4)
O(6)-C(29)-C(28)	119.3(4)
O(5)-C(29)-C(28)	118.1(4)
C(32A)-C(30)-C(31A)	123(3)
C(32)-C(30)-C(31)	111.2(14)
C(32A)-C(30)-C(28)	116.7(13)
C(31A)-C(30)-C(28)	117(2)
C(32)-C(30)-C(28)	114.3(6)
C(31)-C(30)-C(28)	110.9(11)
C(32)-C(30)-H(30A)	106.7

C(31)-C(30)-H(30A)	106.7
C(28)-C(30)-H(30A)	106.7
C(32A)-C(30)-H(30B)	108(10)
C(31A)-C(30)-H(30B)	98(10)
C(28)-C(30)-H(30B)	80(10)
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(30)-C(31A)-H(31D)	109.5
C(30)-C(31A)-H(31E)	109.5
H(31D)-C(31A)-H(31E)	109.5
C(30)-C(31A)-H(31F)	109.5
H(31D)-C(31A)-H(31F)	109.5
H(31E)-C(31A)-H(31F)	109.5
C(30)-C(32A)-H(32D)	109.5
C(30)-C(32A)-H(32E)	109.5
H(32D)-C(32A)-H(32E)	109.5
C(30)-C(32A)-H(32F)	109.5
H(32D)-C(32A)-H(32F)	109.5
H(32E)-C(32A)-H(32F)	109.5
C(34)-C(33)-C(42)	123.4(4)
C(34)-C(33)-I(3)	125.0(3)
C(42)-C(33)-I(3)	111.6(3)
C(33)-C(34)-C(35)	117.7(4)
C(33)-C(34)-H(34)	121.2
C(35)-C(34)-H(34)	121.2
C(36)-C(35)-C(40)	118.8(5)

C(36)-C(35)-C(34)	121.0(5)
C(40)-C(35)-C(34)	120.2(4)
C(37)-C(36)-C(35)	120.7(5)
C(37)-C(36)-H(36)	119.6
C(35)-C(36)-H(36)	119.6
C(36)-C(37)-C(38)	120.5(5)
C(36)-C(37)-H(37)	119.7
C(38)-C(37)-H(37)	119.7
C(39)-C(38)-C(37)	120.1(5)
C(39)-C(38)-H(38)	119.9
C(37)-C(38)-H(38)	119.9
C(38)-C(39)-C(40)	120.8(5)
C(38)-C(39)-H(39)	119.6
C(40)-C(39)-H(39)	119.6
C(41)-C(40)-C(35)	118.9(4)
C(41)-C(40)-C(39)	122.2(5)
C(35)-C(40)-C(39)	119.0(5)
C(42)-C(41)-C(40)	120.9(5)
C(42)-C(41)-H(41)	119.5
C(40)-C(41)-H(41)	119.5
C(41)-C(42)-C(33)	118.9(5)
C(41)-C(42)-C(43)	122.2(4)
C(33)-C(42)-C(43)	118.9(4)
O(7)-C(43)-N(3)	123.7(4)
O(7)-C(43)-C(42)	123.2(4)
N(3)-C(43)-C(42)	113.1(4)
N(3)-C(44)-C(45)	110.2(4)
N(3)-C(44)-C(46)	111.2(4)
C(45)-C(44)-C(46)	110.3(4)
N(3)-C(44)-H(44)	108.4
C(45)-C(44)-H(44)	108.4
C(46)-C(44)-H(44)	108.4
O(9)-C(45)-O(8)	122.7(4)
O(9)-C(45)-C(44)	120.4(4)
O(8)-C(45)-C(44)	116.9(4)
C(47)-C(46)-C(48)	111.8(6)

C(47)-C(46)-C(44)	112.7(5)
C(48)-C(46)-C(44)	111.9(6)
C(47)-C(46)-H(46)	106.6
C(48)-C(46)-H(46)	106.6
C(44)-C(46)-H(46)	106.6
C(46)-C(47)-H(47A)	109.5
C(46)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(46)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(46)-C(48)-H(48A)	109.5
C(46)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(46)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(50)-C(49)-C(58)	122.4(5)
C(50)-C(49)-I(4)	125.8(4)
C(58)-C(49)-I(4)	111.7(3)
C(49)-C(50)-C(51)	118.2(5)
C(49)-C(50)-H(50)	120.9
C(51)-C(50)-H(50)	120.9
C(56)-C(51)-C(50)	120.0(4)
C(56)-C(51)-C(52)	119.2(5)
C(50)-C(51)-C(52)	120.7(5)
C(53)-C(52)-C(51)	120.1(5)
C(53)-C(52)-H(52)	120.0
C(51)-C(52)-H(52)	120.0
C(52)-C(53)-C(54)	121.0(5)
C(52)-C(53)-H(53)	119.5
C(54)-C(53)-H(53)	119.5
C(55)-C(54)-C(53)	119.8(5)
C(55)-C(54)-H(54)	120.1
C(53)-C(54)-H(54)	120.1
C(54)-C(55)-C(56)	120.9(5)

C(54)-C(55)-H(55)	119.6
C(56)-C(55)-H(55)	119.6
C(57)-C(56)-C(51)	119.7(5)
C(57)-C(56)-C(55)	121.3(5)
C(51)-C(56)-C(55)	118.9(5)
C(58)-C(57)-C(56)	120.2(5)
C(58)-C(57)-H(57)	119.9
C(56)-C(57)-H(57)	119.9
C(57)-C(58)-C(49)	119.4(5)
C(57)-C(58)-C(59)	121.8(5)
C(49)-C(58)-C(59)	118.8(4)
O(10)-C(59)-N(4)	124.0(4)
O(10)-C(59)-C(58)	123.1(4)
N(4)-C(59)-C(58)	112.9(4)
N(4)-C(60)-C(61)	110.1(4)
N(4)-C(60)-C(62)	111.6(4)
C(61)-C(60)-C(62)	109.4(4)
N(4)-C(60)-H(60)	108.5
C(61)-C(60)-H(60)	108.5
C(62)-C(60)-H(60)	108.5
O(12)-C(61)-O(11)	123.1(4)
O(12)-C(61)-C(60)	120.5(4)
O(11)-C(61)-C(60)	116.3(4)
C(63)-C(62)-C(64)	111.3(5)
C(63)-C(62)-C(60)	112.3(4)
C(64)-C(62)-C(60)	111.4(4)
C(63)-C(62)-H(62)	107.2
C(64)-C(62)-H(62)	107.2
C(60)-C(62)-H(62)	107.2
C(62)-C(63)-H(63A)	109.5
C(62)-C(63)-H(63B)	109.5
H(63A)-C(63)-H(63B)	109.5
C(62)-C(63)-H(63C)	109.5
H(63A)-C(63)-H(63C)	109.5
H(63B)-C(63)-H(63C)	109.5
C(62)-C(64)-H(64A)	109.5

C(62)-C(64)-H(64B)	109.5
H(64A)-C(64)-H(64B)	109.5
C(62)-C(64)-H(64C)	109.5
H(64A)-C(64)-H(64C)	109.5
H(64B)-C(64)-H(64C)	109.5
C(66)-C(65)-C(74)	123.2(5)
C(66)-C(65)-I(5)	125.7(4)
C(74)-C(65)-I(5)	111.1(4)
C(65)-C(66)-C(67)	118.5(5)
C(65)-C(66)-H(66)	120.7
C(67)-C(66)-H(66)	120.7
C(72)-C(67)-C(68)	118.5(5)
C(72)-C(67)-C(66)	119.8(5)
C(68)-C(67)-C(66)	121.7(5)
C(69)-C(68)-C(67)	121.3(6)
C(69)-C(68)-H(68)	119.4
C(67)-C(68)-H(68)	119.4
C(68)-C(69)-C(70)	120.1(6)
C(68)-C(69)-H(69)	119.9
C(70)-C(69)-H(69)	119.9
C(71)-C(70)-C(69)	120.7(5)
C(71)-C(70)-H(70)	119.7
C(69)-C(70)-H(70)	119.7
C(70)-C(71)-C(72)	120.1(6)
C(70)-C(71)-H(71)	120.0
C(72)-C(71)-H(71)	120.0
C(73)-C(72)-C(67)	119.8(5)
C(73)-C(72)-C(71)	120.9(5)
C(67)-C(72)-C(71)	119.3(5)
C(74)-C(73)-C(72)	120.2(5)
C(74)-C(73)-H(73)	119.9
C(72)-C(73)-H(73)	119.9
C(73)-C(74)-C(65)	118.5(5)
C(73)-C(74)-C(75)	122.1(5)
C(65)-C(74)-C(75)	119.4(5)
O(13)-C(75)-N(5)	123.9(6)

O(13)-C(75)-C(74)	123.7(5)
N(5)-C(75)-C(74)	112.4(5)
N(5)-C(76)-C(77)	110.1(4)
N(5)-C(76)-C(78)	110.6(4)
C(77)-C(76)-C(78)	109.9(5)
N(5)-C(76)-H(76)	108.7
C(77)-C(76)-H(76)	108.7
C(78)-C(76)-H(76)	108.7
O(15)-C(77)-O(14)	122.1(5)
O(15)-C(77)-C(76)	119.9(5)
O(14)-C(77)-C(76)	117.8(4)
C(79)-C(78)-C(80)	111.6(6)
C(79)-C(78)-C(76)	111.1(5)
C(80)-C(78)-C(76)	111.7(5)
C(79)-C(78)-H(78)	107.4
C(80)-C(78)-H(78)	107.4
C(76)-C(78)-H(78)	107.4
C(78)-C(79)-H(79A)	109.5
C(78)-C(79)-H(79B)	109.5
H(79A)-C(79)-H(79B)	109.5
C(78)-C(79)-H(79C)	109.5
H(79A)-C(79)-H(79C)	109.5
H(79B)-C(79)-H(79C)	109.5
C(78)-C(80)-H(80A)	109.5
C(78)-C(80)-H(80B)	109.5
H(80A)-C(80)-H(80B)	109.5
C(78)-C(80)-H(80C)	109.5
H(80A)-C(80)-H(80C)	109.5
H(80B)-C(80)-H(80C)	109.5
C(93)-O(17)-I(4)	103.3(8)
C(93)-O(18)-I(6)	110.7(7)
C(91)-N(6)-C(92)	119.1(8)
C(91)-N(6)-I(6)	117.5(6)
C(92)-N(6)-I(6)	123.0(5)
C(82)-C(81)-C(90)	122.9(8)
C(82)-C(81)-I(6)	128.2(7)

C(90)-C(81)-I(6)	108.7(6)
C(81)-C(82)-C(83)	118.2(8)
C(81)-C(82)-H(82)	120.9
C(83)-C(82)-H(82)	120.9
C(84)-C(83)-C(88)	120.0
C(84)-C(83)-C(82)	119.9(5)
C(88)-C(83)-C(82)	120.0(6)
C(83)-C(84)-C(85)	120.0
C(83)-C(84)-H(84)	120.0
C(85)-C(84)-H(84)	120.0
C(86)-C(85)-C(84)	120.0
C(86)-C(85)-H(85)	120.0
C(84)-C(85)-H(85)	120.0
C(85)-C(86)-C(87)	120.0
C(85)-C(86)-H(86)	120.0
C(87)-C(86)-H(86)	120.0
C(88)-C(87)-C(86)	120.0
C(88)-C(87)-H(87)	120.0
C(86)-C(87)-H(87)	120.0
C(87)-C(88)-C(83)	120.0
C(87)-C(88)-C(89)	120.3(5)
C(83)-C(88)-C(89)	119.7(5)
C(90)-C(89)-C(88)	119.4(8)
C(90)-C(89)-H(89)	120.3
C(88)-C(89)-H(89)	120.3
C(89)-C(90)-C(81)	119.6(9)
C(89)-C(90)-C(91)	121.3(8)
C(81)-C(90)-C(91)	119.1(6)
O(16)-C(91)-N(6)	123.9(9)
O(16)-C(91)-C(90)	124.3(7)
N(6)-C(91)-C(90)	111.8(7)
N(6)-C(92)-C(93)	109.2(7)
N(6)-C(92)-C(94)	113.3(7)
C(93)-C(92)-C(94)	109.0(7)
N(6)-C(92)-H(92)	108.4
C(93)-C(92)-H(92)	108.4

C(94)-C(92)-H(92)	108.4
O(18)-C(93)-O(17)	122.6(9)
O(18)-C(93)-C(92)	119.4(8)
O(17)-C(93)-C(92)	118.0(9)
C(96)-C(94)-C(95)	110.0(10)
C(96)-C(94)-C(92)	112.6(8)
C(95)-C(94)-C(92)	110.9(8)
C(96)-C(94)-H(94)	107.8
C(95)-C(94)-H(94)	107.8
C(92)-C(94)-H(94)	107.8
C(94)-C(95)-H(95A)	109.5
C(94)-C(95)-H(95B)	109.5
H(95A)-C(95)-H(95B)	109.5
C(94)-C(95)-H(95C)	109.5
H(95A)-C(95)-H(95C)	109.5
H(95B)-C(95)-H(95C)	109.5
C(94)-C(96)-H(96A)	109.5
C(94)-C(96)-H(96B)	109.5
H(96A)-C(96)-H(96B)	109.5
C(94)-C(96)-H(96C)	109.5
H(96A)-C(96)-H(96C)	109.5
H(96B)-C(96)-H(96C)	109.5
C(93A)-O(17A)-I(4)	102.6(12)
C(91A)-N(6A)-C(92A)	117.8(10)
C(91A)-N(6A)-I(6)	116.4(8)
C(92A)-N(6A)-I(6)	125.7(8)
C(82A)-C(81A)-C(90A)	123.2(11)
C(82A)-C(81A)-I(6)	119.3(9)
C(90A)-C(81A)-I(6)	116.5(8)
C(81A)-C(82A)-C(83A)	118.0(12)
C(81A)-C(82A)-H(82A)	121.0
C(83A)-C(82A)-H(82A)	121.0
C(84A)-C(83A)-C(88A)	118.8(9)
C(84A)-C(83A)-C(82A)	120.7(10)
C(88A)-C(83A)-C(82A)	120.3(10)
C(85A)-C(84A)-C(83A)	120.9(11)

C(85A)-C(84A)-H(84A)	119.5
C(83A)-C(84A)-H(84A)	119.5
C(84A)-C(85A)-C(86A)	120.1(11)
C(84A)-C(85A)-H(85A)	119.9
C(86A)-C(85A)-H(85A)	119.9
C(87A)-C(86A)-C(85A)	119.9(11)
C(87A)-C(86A)-H(86A)	120.0
C(85A)-C(86A)-H(86A)	120.0
C(86A)-C(87A)-C(88A)	119.4(11)
C(86A)-C(87A)-H(87A)	120.3
C(88A)-C(87A)-H(87A)	120.3
C(83A)-C(88A)-C(87A)	120.8(9)
C(83A)-C(88A)-C(89A)	119.6(9)
C(87A)-C(88A)-C(89A)	119.5(10)
C(90A)-C(89A)-C(88A)	118.8(11)
C(90A)-C(89A)-H(89A)	120.6
C(88A)-C(89A)-H(89A)	120.6
C(89A)-C(90A)-C(81A)	120.0(12)
C(89A)-C(90A)-C(91A)	119.4(11)
C(81A)-C(90A)-C(91A)	120.4(9)
O(16A)-C(91A)-N(6A)	125.1(12)
O(16A)-C(91A)-C(90A)	124.7(10)
N(6A)-C(91A)-C(90A)	110.0(10)
N(6A)-C(92A)-C(93A)	108.0(10)
N(6A)-C(92A)-C(94A)	113.7(10)
C(93A)-C(92A)-C(94A)	110.6(10)
N(6A)-C(92A)-H(92A)	108.1
C(93A)-C(92A)-H(92A)	108.1
C(94A)-C(92A)-H(92A)	108.1
O(18A)-C(93A)-O(17A)	123.7(12)
O(18A)-C(93A)-C(92A)	117.7(11)
O(17A)-C(93A)-C(92A)	118.4(12)
C(96A)-C(94A)-C(95A)	113.4(13)
C(96A)-C(94A)-C(92A)	112.4(11)
C(95A)-C(94A)-C(92A)	111.3(11)
C(96A)-C(94A)-H(94A)	106.4

C(95A)-C(94A)-H(94A)	106.4
C(92A)-C(94A)-H(94A)	106.4
C(94A)-C(95A)-H(95D)	109.5
C(94A)-C(95A)-H(95E)	109.5
H(95D)-C(95A)-H(95E)	109.5
C(94A)-C(95A)-H(95F)	109.5
H(95D)-C(95A)-H(95F)	109.5
H(95E)-C(95A)-H(95F)	109.5
C(94A)-C(96A)-H(96D)	109.5
C(94A)-C(96A)-H(96E)	109.5
H(96D)-C(96A)-H(96E)	109.5
C(94A)-C(96A)-H(96F)	109.5
H(96D)-C(96A)-H(96F)	109.5
H(96E)-C(96A)-H(96F)	109.5
CI(3)-C(98)-CI(1)	111.2
CI(3)-C(98)-CI(2)	111.2
CI(1)-C(98)-CI(2)	111.2
CI(3)-C(98)-H(98)	107.7
CI(1)-C(98)-H(98)	107.7
CI(2)-C(98)-H(98)	107.7
CI(1A)-C(98A)-CI(2A)	110.9(8)
CI(1A)-C(98A)-CI(3A)	110.5(9)
CI(2A)-C(98A)-CI(3A)	108.8(8)
CI(1A)-C(98A)-H(98A)	108.9
CI(2A)-C(98A)-H(98A)	108.9
CI(3A)-C(98A)-H(98A)	108.9
CI(4)-C(99)-CI(5)	110.0(7)
CI(4)-C(99)-CI(6)	110.2(9)
CI(5)-C(99)-CI(6)	101.9(9)
CI(4)-C(99)-H(99)	111.5
CI(5)-C(99)-H(99)	111.5
CI(6)-C(99)-H(99)	111.5
CI(4A)-C(99A)-CI(5A)	114.1(9)
CI(4A)-C(99A)-CI(6A)	107.5(9)
CI(5A)-C(99A)-CI(6A)	109.0(8)
CI(4A)-C(99A)-H(99A)	108.7

Cl(5A)-C(99A)-H(99A)	108.7
Cl(6A)-C(99A)-H(99A)	108.7
C(101)-C(100)-H(10A)	109.5
C(101)-C(100)-H(10B)	109.5
H(10A)-C(100)-H(10B)	109.5
C(101)-C(100)-H(10C)	109.5
H(10A)-C(100)-H(10C)	109.5
H(10B)-C(100)-H(10C)	109.5
O(19)-C(101)-C(100)	108.8
O(19)-C(101)-H(10D)	109.9
C(100)-C(101)-H(10D)	109.9
O(19)-C(101)-H(10E)	109.9
C(100)-C(101)-H(10E)	109.9
H(10D)-C(101)-H(10E)	108.3
C(102)-O(19)-C(101)	113.5
O(19)-C(102)-C(103)	108.8
O(19)-C(102)-H(10F)	109.9
C(103)-C(102)-H(10F)	109.9
O(19)-C(102)-H(10G)	109.9
C(103)-C(102)-H(10G)	109.9
H(10F)-C(102)-H(10G)	108.3
C(102)-C(103)-H(10H)	109.5
C(102)-C(103)-H(10I)	109.5
H(10H)-C(103)-H(10I)	109.5
C(102)-C(103)-H(10J)	109.5
H(10H)-C(103)-H(10J)	109.5
H(10I)-C(103)-H(10J)	109.5
Cl(7)-C(104)-Cl(8)	109.2(15)
Cl(7)-C(104)-Cl(9)	113.8(15)
Cl(8)-C(104)-Cl(9)	108.3(14)
Cl(7)-C(104)-H(104)	108.5
Cl(8)-C(104)-H(104)	108.5
Cl(9)-C(104)-H(104)	108.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4468ds. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + \dots + 2hka^*b^*U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
I(1)	21(1)	18(1)	22(1)	1(1)	-1(1)	-2(1)
I(2)	18(1)	21(1)	19(1)	-2(1)	-1(1)	2(1)
I(3)	18(1)	17(1)	24(1)	1(1)	-1(1)	0(1)
I(4)	27(1)	20(1)	21(1)	-1(1)	2(1)	-5(1)
I(5)	19(1)	25(1)	25(1)	2(1)	5(1)	-1(1)
I(6)	34(1)	43(1)	21(1)	1(1)	1(1)	-20(1)
O(1)	31(2)	24(2)	28(2)	-3(1)	-4(1)	-3(1)
O(2)	25(2)	21(2)	26(2)	4(1)	-4(1)	-3(1)
O(3)	35(2)	21(2)	31(2)	2(1)	-10(2)	-1(2)
O(4)	40(2)	33(2)	40(2)	2(2)	-18(2)	4(2)
O(5)	35(2)	23(2)	24(2)	2(1)	-7(1)	-3(1)
O(6)	44(2)	21(2)	40(2)	0(2)	-19(2)	0(2)
O(7)	39(2)	20(2)	30(2)	1(1)	2(2)	1(1)
O(8)	26(2)	23(2)	26(2)	-3(1)	-4(1)	1(1)
O(9)	45(2)	16(2)	41(2)	0(2)	-20(2)	3(2)
O(10)	26(2)	25(2)	28(2)	-5(1)	-2(1)	-1(1)
O(11)	26(2)	20(2)	31(2)	0(1)	2(1)	0(1)
O(12)	34(2)	22(2)	32(2)	-1(1)	-2(2)	-4(1)
O(13)	45(2)	44(2)	37(2)	11(2)	2(2)	6(2)
O(14)	25(2)	44(2)	28(2)	1(2)	2(1)	-4(2)
O(15)	29(2)	36(2)	30(2)	4(2)	-2(2)	-7(2)
N(1)	24(2)	19(2)	23(2)	1(1)	-7(2)	0(1)
N(2)	24(2)	25(2)	23(2)	3(2)	-5(2)	0(2)
N(3)	23(2)	16(2)	27(2)	-3(2)	-1(2)	1(1)
N(4)	24(2)	20(2)	23(2)	-3(1)	2(2)	-1(1)
N(5)	28(2)	34(2)	23(2)	3(2)	6(2)	3(2)
C(1)	22(2)	20(2)	26(2)	1(2)	4(2)	-1(2)
C(2)	24(2)	23(2)	25(2)	2(2)	3(2)	-1(2)
C(3)	18(2)	23(2)	34(2)	2(2)	4(2)	-2(2)
C(4)	27(2)	26(2)	31(2)	5(2)	4(2)	3(2)
C(5)	28(2)	30(3)	41(3)	13(2)	10(2)	6(2)

C(6)	26(2)	19(2)	41(3)	3(2)	11(2)	2(2)
C(7)	21(2)	22(2)	36(2)	1(2)	7(2)	1(2)
C(8)	19(2)	21(2)	33(2)	1(2)	8(2)	1(2)
C(9)	21(2)	21(2)	31(2)	-2(2)	5(2)	-2(2)
C(10)	20(2)	19(2)	27(2)	1(2)	1(2)	-3(2)
C(11)	20(2)	21(2)	28(2)	-1(2)	2(2)	-3(2)
C(12)	21(2)	19(2)	22(2)	3(2)	-3(2)	-2(2)
C(13)	20(2)	20(2)	27(2)	-1(2)	-1(2)	-3(2)
C(14)	22(2)	19(2)	31(2)	0(2)	0(2)	-3(2)
C(15)	24(2)	35(3)	35(3)	4(2)	6(2)	1(2)
C(16)	29(2)	28(2)	32(3)	2(2)	-6(2)	-2(2)
C(17)	20(2)	29(2)	18(2)	-3(2)	-2(2)	-2(2)
C(18)	25(2)	31(2)	20(2)	-1(2)	1(2)	-2(2)
C(19)	32(2)	30(3)	22(2)	0(2)	2(2)	-9(2)
C(20)	45(3)	31(3)	31(3)	4(2)	-6(2)	-11(2)
C(21)	62(4)	39(3)	33(3)	0(2)	-11(3)	-21(3)
C(22)	53(4)	47(4)	38(3)	3(3)	-18(3)	-23(3)
C(23)	38(3)	47(3)	32(3)	4(2)	-12(2)	-14(3)
C(24)	31(2)	39(3)	24(2)	-2(2)	-2(2)	-8(2)
C(25)	24(2)	33(3)	28(2)	3(2)	-5(2)	-1(2)
C(26)	25(2)	30(2)	24(2)	-1(2)	0(2)	1(2)
C(27)	28(2)	33(3)	22(2)	1(2)	-5(2)	-2(2)
C(28)	28(2)	23(2)	22(2)	2(2)	-3(2)	-2(2)
C(29)	23(2)	25(2)	24(2)	-2(2)	-2(2)	2(2)
C(30)	69(4)	42(3)	38(3)	-10(3)	20(3)	-21(3)
C(31)	56(6)	36(5)	39(9)	4(4)	13(6)	-15(4)
C(32)	97(8)	51(6)	74(7)	-4(5)	62(6)	-5(6)
C(31A)	48(10)	42(10)	35(13)	4(9)	5(10)	0(9)
C(32A)	106(13)	78(12)	84(12)	-5(11)	57(11)	-7(12)
C(33)	16(2)	23(2)	23(2)	3(2)	4(2)	2(2)
C(34)	16(2)	23(2)	27(2)	2(2)	3(2)	2(2)
C(35)	19(2)	27(2)	27(2)	1(2)	1(2)	5(2)
C(36)	27(2)	34(3)	36(3)	-3(2)	-5(2)	5(2)
C(37)	37(3)	47(3)	35(3)	1(3)	-13(2)	8(3)
C(38)	38(3)	44(3)	38(3)	7(2)	-9(2)	12(2)
C(39)	31(3)	33(3)	37(3)	6(2)	-5(2)	9(2)

C(40)	22(2)	31(2)	25(2)	2(2)	2(2)	7(2)
C(41)	24(2)	27(2)	29(2)	3(2)	5(2)	6(2)
C(42)	17(2)	22(2)	25(2)	2(2)	4(2)	4(2)
C(43)	19(2)	20(2)	27(2)	2(2)	3(2)	2(2)
C(44)	26(2)	19(2)	24(2)	0(2)	-1(2)	4(2)
C(45)	21(2)	23(2)	25(2)	-1(2)	-2(2)	4(2)
C(46)	49(3)	36(3)	23(2)	1(2)	2(2)	24(2)
C(47)	45(3)	93(6)	36(3)	27(3)	21(3)	33(4)
C(48)	102(6)	46(4)	44(4)	-19(3)	-18(4)	34(4)
C(49)	21(2)	22(2)	25(2)	-2(2)	5(2)	-3(2)
C(50)	23(2)	26(2)	29(2)	-5(2)	9(2)	-3(2)
C(51)	21(2)	24(2)	29(2)	0(2)	11(2)	2(2)
C(52)	27(2)	23(2)	35(3)	-1(2)	11(2)	1(2)
C(53)	28(2)	22(2)	46(3)	6(2)	10(2)	2(2)
C(54)	32(3)	30(3)	38(3)	8(2)	2(2)	4(2)
C(55)	30(3)	32(3)	36(3)	4(2)	-3(2)	0(2)
C(56)	19(2)	25(2)	31(2)	1(2)	5(2)	2(2)
C(57)	20(2)	28(2)	28(2)	-2(2)	4(2)	0(2)
C(58)	18(2)	22(2)	28(2)	-2(2)	5(2)	-2(2)
C(59)	19(2)	20(2)	24(2)	0(2)	4(2)	1(2)
C(60)	23(2)	18(2)	24(2)	-1(2)	1(2)	1(2)
C(61)	21(2)	25(2)	24(2)	-1(2)	2(2)	-2(2)
C(62)	22(2)	22(2)	44(3)	2(2)	-1(2)	-2(2)
C(63)	33(3)	32(3)	52(3)	10(2)	20(2)	6(2)
C(64)	37(3)	27(3)	60(4)	-1(2)	-5(3)	-7(2)
C(65)	19(2)	23(2)	34(2)	2(2)	11(2)	1(2)
C(66)	20(2)	26(2)	32(3)	3(2)	8(2)	2(2)
C(67)	24(2)	25(2)	40(3)	-2(2)	15(2)	2(2)
C(68)	24(2)	32(3)	43(3)	-4(2)	9(2)	0(2)
C(69)	26(2)	34(3)	54(3)	-8(2)	16(2)	-1(2)
C(70)	38(3)	24(2)	58(3)	1(2)	28(3)	0(2)
C(71)	39(3)	26(3)	49(3)	5(2)	22(3)	4(2)
C(72)	30(2)	29(2)	38(3)	2(2)	18(2)	4(2)
C(73)	39(3)	30(3)	40(3)	9(2)	18(2)	8(2)
C(74)	31(2)	28(2)	32(3)	4(2)	14(2)	5(2)
C(75)	33(3)	34(3)	32(3)	7(2)	12(2)	4(2)

C(76)	28(2)	41(3)	25(2)	3(2)	5(2)	0(2)
C(77)	21(2)	41(3)	23(2)	1(2)	6(2)	-1(2)
C(78)	45(3)	46(3)	26(2)	2(2)	13(2)	-5(3)
C(79)	64(4)	72(5)	33(3)	4(3)	5(3)	-5(4)
C(80)	39(3)	48(3)	51(4)	-9(3)	25(3)	-6(3)
O(16)	45(5)	22(4)	30(3)	-6(3)	-3(4)	-2(3)
O(17)	33(5)	24(3)	26(3)	0(2)	2(3)	-7(4)
O(18)	39(5)	24(3)	29(4)	3(3)	-3(3)	-5(3)
N(6)	31(3)	23(3)	23(2)	-3(2)	3(3)	-7(3)
C(81)	27(3)	26(3)	24(3)	-8(3)	5(2)	-6(3)
C(82)	29(3)	28(3)	29(3)	-6(3)	1(3)	-4(3)
C(83)	33(3)	32(3)	41(3)	-8(3)	-4(3)	-1(3)
C(84)	42(4)	41(4)	55(4)	-11(3)	-14(3)	2(3)
C(85)	46(3)	45(4)	62(4)	-14(3)	-21(3)	3(3)
C(86)	45(3)	48(4)	63(4)	-21(3)	-20(3)	-1(3)
C(87)	41(3)	42(3)	49(3)	-17(3)	-13(3)	-3(3)
C(88)	35(3)	33(3)	39(3)	-16(2)	-4(3)	0(3)
C(89)	33(3)	29(3)	32(3)	-12(3)	1(3)	-5(3)
C(90)	31(3)	26(3)	25(2)	-9(2)	4(2)	-5(2)
C(91)	30(3)	23(3)	21(2)	-7(3)	5(3)	-6(3)
C(92)	36(4)	22(3)	24(2)	3(2)	3(3)	-5(3)
C(93)	34(4)	24(3)	24(2)	1(2)	1(3)	-7(3)
C(94)	41(4)	25(3)	29(3)	4(3)	6(3)	2(3)
C(95)	55(6)	39(5)	39(5)	1(4)	5(6)	14(5)
C(96)	51(6)	43(5)	50(7)	-1(6)	22(5)	1(5)
O(16A)	40(6)	23(5)	28(4)	-5(4)	-3(5)	0(4)
O(17A)	34(6)	24(4)	24(3)	-1(3)	1(4)	-7(4)
O(18A)	34(6)	22(5)	19(4)	-8(3)	4(4)	-7(5)
N(6A)	32(4)	20(3)	21(3)	-1(3)	2(3)	-8(3)
C(81A)	27(3)	27(4)	24(3)	-9(3)	4(3)	-4(3)
C(82A)	29(3)	30(3)	30(3)	-8(3)	3(3)	-2(3)
C(83A)	31(3)	35(3)	35(3)	-11(3)	-1(3)	-3(3)
C(84A)	38(3)	39(3)	47(3)	-11(3)	-8(3)	1(3)
C(85A)	41(3)	47(4)	54(4)	-14(3)	-13(3)	0(3)
C(86A)	40(4)	47(4)	51(4)	-17(4)	-9(4)	-3(4)
C(87A)	39(4)	40(4)	42(4)	-16(3)	-6(4)	-5(4)

C(88A)	33(3)	35(3)	36(3)	-16(3)	-3(3)	-5(3)
C(89A)	31(4)	32(4)	30(4)	-11(3)	4(3)	-6(3)
C(90A)	30(3)	26(3)	25(3)	-8(3)	5(3)	-7(3)
C(91A)	33(4)	24(4)	23(3)	-4(3)	4(3)	-7(3)
C(92A)	35(4)	22(3)	23(3)	1(3)	2(3)	-5(3)
C(93A)	35(4)	22(3)	24(3)	-1(3)	3(3)	-6(3)
C(94A)	41(5)	26(3)	27(3)	0(3)	7(4)	-1(4)
C(95A)	46(7)	39(6)	37(6)	9(5)	9(7)	7(7)
C(96A)	43(6)	32(6)	23(6)	-6(5)	11(5)	1(5)
CI(1)	60(2)	72(2)	54(2)	1(2)	-3(2)	2(2)
CI(2)	68(2)	71(2)	77(3)	-21(2)	-4(2)	-11(2)
CI(3)	71(3)	56(2)	96(3)	5(2)	8(2)	-2(2)
C(98)	69(5)	65(5)	69(5)	-5(5)	-3(5)	0(5)
CI(1A)	69(2)	58(2)	58(2)	-2(2)	18(2)	3(2)
CI(2A)	62(2)	59(2)	65(2)	-12(2)	-4(2)	-1(2)
CI(3A)	75(3)	58(2)	61(2)	-6(2)	7(2)	-19(2)
C(98A)	66(5)	62(5)	66(5)	-6(4)	1(4)	-8(4)
CI(4)	65(2)	88(3)	65(2)	20(2)	22(2)	21(2)
CI(5)	93(3)	149(5)	76(3)	48(4)	41(3)	60(3)
CI(6)	81(3)	108(4)	84(3)	18(3)	20(3)	16(3)
C(99)	94(6)	88(6)	53(5)	35(5)	49(5)	48(6)
CI(4A)	157(6)	77(3)	71(4)	-20(3)	9(4)	27(4)
CI(5A)	57(2)	90(3)	61(2)	20(2)	13(2)	9(2)
CI(6A)	52(2)	65(3)	42(2)	-4(2)	11(1)	1(2)
C(99A)	70(6)	69(6)	57(6)	11(5)	7(5)	21(6)
C(100)	111(8)	59(6)	78(7)	-5(5)	-7(6)	-4(6)
C(101)	99(6)	68(6)	61(5)	18(5)	5(5)	-26(5)
O(19)	90(4)	64(4)	65(4)	-1(3)	5(3)	-15(4)
C(102)	86(5)	75(5)	76(5)	-10(4)	-5(4)	-8(4)
C(103)	100(9)	105(8)	118(10)	-16(8)	-27(8)	7(8)
CI(7)	80(5)	70(5)	52(4)	-13(4)	10(4)	-4(4)
CI(8)	77(6)	59(4)	101(6)	5(5)	-41(5)	9(4)
CI(9)	90(5)	48(5)	86(5)	2(4)	22(4)	-34(4)
C(104)	86(5)	64(5)	72(5)	-3(5)	-3(5)	-11(5)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4468ds.

	x	y	z	U(eq)
H(2)	7461	2484	2080	29
H(4)	7872	1458	2576	34
H(5)	7816	465	2329	39
H(6)	7108	83	991	34
H(7)	6498	701	-129	31
H(9)	6154	1726	-682	29
H(12)	5713	3861	-1483	25
H(14)	4340	3367	-1036	29
H(15A)	4116	4408	-53	46
H(15B)	4323	3775	374	46
H(15C)	3371	3898	-210	46
H(16A)	4241	3913	-2336	45
H(16B)	4107	4504	-1798	45
H(16C)	3329	4012	-1864	45
H(18)	8904	6679	3290	30
H(20)	9732	7516	4075	43
H(21)	10888	7861	5104	55
H(22)	11833	7207	5964	57
H(23)	11657	6214	5789	48
H(25)	10793	5370	5059	35
H(28)	8755	3811	3580	30
H(30A)	8045	4117	4827	58
H(30B)	7210(190)	4200(120)	3790(190)	58
H(31A)	7695	3170	4286	65
H(31B)	6898	3429	4814	65
H(31C)	6777	3414	3749	65
H(32A)	7229	4919	4232	106
H(32B)	6496	4488	3716	106
H(32C)	6617	4503	4780	106
H(31D)	7254	3257	3877	63

H(31E)	7620	3305	4909	63
H(31F)	6624	3544	4561	63
H(32D)	8004	4855	4654	129
H(32E)	7126	4607	5071	129
H(32F)	8122	4368	5419	129
H(34)	4795	5568	-2071	26
H(36)	3951	5725	-3583	39
H(37)	3525	6333	-4783	49
H(38)	3816	7347	-4685	49
H(39)	4497	7747	-3378	41
H(41)	5238	7610	-1818	32
H(44)	7260	7071	945	28
H(46)	5744	7353	1352	43
H(47A)	5287	6396	1747	85
H(47B)	5142	6879	2486	85
H(47C)	5990	6438	2628	85
H(48A)	7056	7786	2064	99
H(48B)	7196	7253	2752	99
H(48C)	6338	7681	2773	99
H(50)	8899	3084	10320	31
H(52)	9216	2119	11071	33
H(53)	9801	1589	12305	38
H(54)	10567	2062	13557	40
H(55)	10727	3071	13565	40
H(57)	10479	4031	12805	30
H(60)	9220	5863	11276	26
H(62)	10830	5703	10970	36
H(63A)	10186	6102	9230	57
H(63B)	10518	5447	9453	57
H(63C)	11231	5976	9586	57
H(64A)	11101	6699	10845	63
H(64B)	10314	6608	11487	63
H(64C)	10055	6815	10481	63
H(66)	8604	7438	9874	31
H(68)	8973	8362	10729	39
H(69)	8915	9371	10835	45

H(70)	8233	9928	9645	46
H(71)	7592	9477	8351	44
H(73)	7150	8566	7519	43
H(76)	6079	6608	6315	37
H(78)	7456	6905	5582	46
H(79A)	6992	6372	4292	84
H(79B)	6122	6605	4738	84
H(79C)	6425	5935	4851	84
H(80A)	7936	5696	5733	67
H(80B)	8461	6195	6329	67
H(80C)	8490	6194	5273	67
H(82)	4879	5113	5547	35
H(84)	3410	5231	4622	57
H(85)	2055	4836	3918	63
H(86)	1797	3827	3966	64
H(87)	2893	3213	4719	54
H(89)	4386	3076	5581	38
H(92)	7009	3061	7964	32
H(94)	7803	2968	6611	38
H(95A)	9097	2539	7355	66
H(95B)	8264	2421	7932	66
H(95C)	8999	2918	8230	66
H(96A)	9130	3500	6500	70
H(96B)	9011	3844	7402	70
H(96C)	8307	3954	6537	70
H(82A)	4764	4900	5792	35
H(84A)	3147	4919	5150	51
H(85A)	1777	4443	4724	58
H(86A)	1718	3416	4702	56
H(87A)	3021	2874	5192	49
H(89A)	4644	2839	5766	37
H(92A)	7330	2973	7965	32
H(94A)	8083	2854	6655	37
H(95D)	9491	2589	7337	61
H(95E)	8753	2463	8019	61
H(95F)	9398	3027	8149	61

H(96D)	9233	3479	6297	48
H(96E)	9049	3907	7097	48
H(96F)	8286	3826	6270	48
H(98)	5817	4732	2025	82
H(98A)	3857	4944	2511	78
H(99)	3355	7005	2860	90
H(99A)	1386	5912	2582	79
H(10A)	-722	5587	7216	126
H(10B)	28	5432	8027	126
H(10C)	-772	4977	7728	126
H(10D)	-139	4898	6306	92
H(10E)	727	5262	6746	92
H(10F)	1703	4424	6581	96
H(10G)	837	4060	6141	96
H(10H)	1056	3397	7398	166
H(10I)	1992	3731	7705	166
H(10J)	1878	3379	6786	166
H(104)	808	4290	5806	90

Table 6. Torsion angles [°] for 4468ds.

C(10)-C(1)-C(2)-C(3)	-1.3(7)
I(1)-C(1)-C(2)-C(3)	178.4(3)
C(1)-C(2)-C(3)-C(4)	-179.7(4)
C(1)-C(2)-C(3)-C(8)	0.4(7)
C(8)-C(3)-C(4)-C(5)	-2.4(7)
C(2)-C(3)-C(4)-C(5)	177.7(5)
C(3)-C(4)-C(5)-C(6)	0.2(8)
C(4)-C(5)-C(6)-C(7)	1.4(8)
C(5)-C(6)-C(7)-C(8)	-0.8(7)
C(4)-C(3)-C(8)-C(9)	-179.5(4)
C(2)-C(3)-C(8)-C(9)	0.5(6)
C(4)-C(3)-C(8)-C(7)	2.9(6)
C(2)-C(3)-C(8)-C(7)	-177.2(4)
C(6)-C(7)-C(8)-C(9)	-178.9(4)
C(6)-C(7)-C(8)-C(3)	-1.3(7)
C(3)-C(8)-C(9)-C(10)	-0.5(7)
C(7)-C(8)-C(9)-C(10)	177.0(4)
C(8)-C(9)-C(10)-C(1)	-0.3(7)
C(8)-C(9)-C(10)-C(11)	-178.9(4)
C(2)-C(1)-C(10)-C(9)	1.3(7)
I(1)-C(1)-C(10)-C(9)	-178.5(4)
C(2)-C(1)-C(10)-C(11)	179.9(4)
I(1)-C(1)-C(10)-C(11)	0.1(5)
C(12)-N(1)-C(11)-O(1)	3.2(7)
I(1)-N(1)-C(11)-O(1)	-169.9(4)
C(12)-N(1)-C(11)-C(10)	-175.2(4)
I(1)-N(1)-C(11)-C(10)	11.7(5)
C(9)-C(10)-C(11)-O(1)	-7.6(7)
C(1)-C(10)-C(11)-O(1)	173.8(5)
C(9)-C(10)-C(11)-N(1)	170.8(4)
C(1)-C(10)-C(11)-N(1)	-7.8(6)
C(11)-N(1)-C(12)-C(13)	-163.3(4)
I(1)-N(1)-C(12)-C(13)	9.2(5)
C(11)-N(1)-C(12)-C(14)	73.2(5)

I(1)-N(1)-C(12)-C(14)	-114.3(4)
I(3)-O(2)-C(13)-O(3)	0.2(5)
I(3)-O(2)-C(13)-C(12)	178.2(3)
N(1)-C(12)-C(13)-O(3)	-10.2(6)
C(14)-C(12)-C(13)-O(3)	112.6(5)
N(1)-C(12)-C(13)-O(2)	171.8(4)
C(14)-C(12)-C(13)-O(2)	-65.4(5)
N(1)-C(12)-C(14)-C(15)	75.9(5)
C(13)-C(12)-C(14)-C(15)	-47.2(5)
N(1)-C(12)-C(14)-C(16)	-156.7(4)
C(13)-C(12)-C(14)-C(16)	80.2(5)
C(26)-C(17)-C(18)-C(19)	-2.1(7)
I(2)-C(17)-C(18)-C(19)	178.9(3)
C(17)-C(18)-C(19)-C(24)	1.9(7)
C(17)-C(18)-C(19)-C(20)	-176.5(5)
C(24)-C(19)-C(20)-C(21)	1.3(9)
C(18)-C(19)-C(20)-C(21)	179.7(6)
C(19)-C(20)-C(21)-C(22)	-0.7(10)
C(20)-C(21)-C(22)-C(23)	0.4(11)
C(21)-C(22)-C(23)-C(24)	-0.7(11)
C(20)-C(19)-C(24)-C(25)	177.8(5)
C(18)-C(19)-C(24)-C(25)	-0.6(8)
C(20)-C(19)-C(24)-C(23)	-1.5(8)
C(18)-C(19)-C(24)-C(23)	-179.9(5)
C(22)-C(23)-C(24)-C(25)	-178.0(6)
C(22)-C(23)-C(24)-C(19)	1.3(9)
C(19)-C(24)-C(25)-C(26)	-0.5(8)
C(23)-C(24)-C(25)-C(26)	178.8(5)
C(24)-C(25)-C(26)-C(17)	0.4(7)
C(24)-C(25)-C(26)-C(27)	-174.1(5)
C(18)-C(17)-C(26)-C(25)	1.0(7)
I(2)-C(17)-C(26)-C(25)	-179.8(4)
C(18)-C(17)-C(26)-C(27)	175.6(5)
I(2)-C(17)-C(26)-C(27)	-5.2(5)
C(28)-N(2)-C(27)-O(4)	9.7(8)
I(2)-N(2)-C(27)-O(4)	-174.6(4)

C(28)-N(2)-C(27)-C(26)	-167.4(4)
I(2)-N(2)-C(27)-C(26)	8.2(6)
C(25)-C(26)-C(27)-O(4)	-4.5(8)
C(17)-C(26)-C(27)-O(4)	-179.0(5)
C(25)-C(26)-C(27)-N(2)	172.6(5)
C(17)-C(26)-C(27)-N(2)	-1.8(6)
C(27)-N(2)-C(28)-C(29)	-154.3(4)
I(2)-N(2)-C(28)-C(29)	30.3(5)
C(27)-N(2)-C(28)-C(30)	82.8(6)
I(2)-N(2)-C(28)-C(30)	-92.6(5)
I(1)-O(5)-C(29)-O(6)	0.5(6)
I(1)-O(5)-C(29)-C(28)	178.2(3)
N(2)-C(28)-C(29)-O(6)	-26.4(6)
C(30)-C(28)-C(29)-O(6)	96.2(6)
N(2)-C(28)-C(29)-O(5)	155.8(4)
C(30)-C(28)-C(29)-O(5)	-81.6(6)
N(2)-C(28)-C(30)-C(32A)	-11(2)
C(29)-C(28)-C(30)-C(32A)	-134(2)
N(2)-C(28)-C(30)-C(31A)	-171(4)
C(29)-C(28)-C(30)-C(31A)	67(4)
N(2)-C(28)-C(30)-C(32)	56.4(9)
C(29)-C(28)-C(30)-C(32)	-65.7(8)
N(2)-C(28)-C(30)-C(31)	-177.0(15)
C(29)-C(28)-C(30)-C(31)	60.9(15)
C(42)-C(33)-C(34)-C(35)	1.8(7)
I(3)-C(33)-C(34)-C(35)	-175.7(3)
C(33)-C(34)-C(35)-C(36)	179.0(4)
C(33)-C(34)-C(35)-C(40)	1.7(7)
C(40)-C(35)-C(36)-C(37)	2.5(8)
C(34)-C(35)-C(36)-C(37)	-174.8(5)
C(35)-C(36)-C(37)-C(38)	-1.4(9)
C(36)-C(37)-C(38)-C(39)	-0.9(9)
C(37)-C(38)-C(39)-C(40)	2.0(9)
C(36)-C(35)-C(40)-C(41)	179.2(4)
C(34)-C(35)-C(40)-C(41)	-3.5(7)
C(36)-C(35)-C(40)-C(39)	-1.3(7)

C(34)-C(35)-C(40)-C(39)	176.0(4)
C(38)-C(39)-C(40)-C(41)	178.6(5)
C(38)-C(39)-C(40)-C(35)	-0.9(8)
C(35)-C(40)-C(41)-C(42)	1.9(7)
C(39)-C(40)-C(41)-C(42)	-177.7(5)
C(40)-C(41)-C(42)-C(33)	1.5(7)
C(40)-C(41)-C(42)-C(43)	178.4(4)
C(34)-C(33)-C(42)-C(41)	-3.5(7)
I(3)-C(33)-C(42)-C(41)	174.3(3)
C(34)-C(33)-C(42)-C(43)	179.5(4)
I(3)-C(33)-C(42)-C(43)	-2.7(5)
C(44)-N(3)-C(43)-O(7)	-3.1(7)
I(3)-N(3)-C(43)-O(7)	-176.8(4)
C(44)-N(3)-C(43)-C(42)	176.7(4)
I(3)-N(3)-C(43)-C(42)	3.0(5)
C(41)-C(42)-C(43)-O(7)	2.8(7)
C(33)-C(42)-C(43)-O(7)	179.6(4)
C(41)-C(42)-C(43)-N(3)	-177.0(4)
C(33)-C(42)-C(43)-N(3)	-0.1(6)
C(43)-N(3)-C(44)-C(45)	-164.8(4)
I(3)-N(3)-C(44)-C(45)	8.4(5)
C(43)-N(3)-C(44)-C(46)	72.6(5)
I(3)-N(3)-C(44)-C(46)	-114.2(4)
I(2)-O(8)-C(45)-O(9)	-5.9(6)
I(2)-O(8)-C(45)-C(44)	171.0(3)
N(3)-C(44)-C(45)-O(9)	-14.7(6)
C(46)-C(44)-C(45)-O(9)	108.4(6)
N(3)-C(44)-C(45)-O(8)	168.3(4)
C(46)-C(44)-C(45)-O(8)	-68.6(6)
N(3)-C(44)-C(46)-C(47)	77.7(5)
C(45)-C(44)-C(46)-C(47)	-44.8(6)
N(3)-C(44)-C(46)-C(48)	-155.3(5)
C(45)-C(44)-C(46)-C(48)	82.2(6)
C(58)-C(49)-C(50)-C(51)	-0.1(7)
I(4)-C(49)-C(50)-C(51)	-176.4(3)
C(49)-C(50)-C(51)-C(56)	0.8(7)

C(49)-C(50)-C(51)-C(52)	179.4(4)
C(56)-C(51)-C(52)-C(53)	0.9(7)
C(50)-C(51)-C(52)-C(53)	-177.7(4)
C(51)-C(52)-C(53)-C(54)	-0.5(8)
C(52)-C(53)-C(54)-C(55)	0.2(8)
C(53)-C(54)-C(55)-C(56)	-0.4(8)
C(50)-C(51)-C(56)-C(57)	-1.3(7)
C(52)-C(51)-C(56)-C(57)	-179.8(4)
C(50)-C(51)-C(56)-C(55)	177.5(4)
C(52)-C(51)-C(56)-C(55)	-1.0(7)
C(54)-C(55)-C(56)-C(57)	179.6(5)
C(54)-C(55)-C(56)-C(51)	0.8(8)
C(51)-C(56)-C(57)-C(58)	1.0(7)
C(55)-C(56)-C(57)-C(58)	-177.8(5)
C(56)-C(57)-C(58)-C(49)	-0.3(7)
C(56)-C(57)-C(58)-C(59)	179.4(4)
C(50)-C(49)-C(58)-C(57)	-0.2(7)
I(4)-C(49)-C(58)-C(57)	176.6(3)
C(50)-C(49)-C(58)-C(59)	-179.8(4)
I(4)-C(49)-C(58)-C(59)	-3.1(5)
C(60)-N(4)-C(59)-O(10)	-0.7(7)
I(4)-N(4)-C(59)-O(10)	-176.5(4)
C(60)-N(4)-C(59)-C(58)	177.4(4)
I(4)-N(4)-C(59)-C(58)	1.7(5)
C(57)-C(58)-C(59)-O(10)	-0.5(8)
C(49)-C(58)-C(59)-O(10)	179.2(4)
C(57)-C(58)-C(59)-N(4)	-178.6(4)
C(49)-C(58)-C(59)-N(4)	1.0(6)
C(59)-N(4)-C(60)-C(61)	-167.1(4)
I(4)-N(4)-C(60)-C(61)	8.3(5)
C(59)-N(4)-C(60)-C(62)	71.1(5)
I(4)-N(4)-C(60)-C(62)	-113.4(4)
I(5)-O(11)-C(61)-O(12)	-10.8(5)
I(5)-O(11)-C(61)-C(60)	165.9(3)
N(4)-C(60)-C(61)-O(12)	-13.2(6)
C(62)-C(60)-C(61)-O(12)	109.8(5)

N(4)-C(60)-C(61)-O(11)	170.0(4)
C(62)-C(60)-C(61)-O(11)	-67.0(5)
N(4)-C(60)-C(62)-C(63)	78.8(5)
C(61)-C(60)-C(62)-C(63)	-43.3(5)
N(4)-C(60)-C(62)-C(64)	-155.6(4)
C(61)-C(60)-C(62)-C(64)	82.3(5)
C(74)-C(65)-C(66)-C(67)	-0.7(7)
I(5)-C(65)-C(66)-C(67)	-177.3(3)
C(65)-C(66)-C(67)-C(72)	-1.1(7)
C(65)-C(66)-C(67)-C(68)	178.7(4)
C(72)-C(67)-C(68)-C(69)	0.2(7)
C(66)-C(67)-C(68)-C(69)	-179.6(5)
C(67)-C(68)-C(69)-C(70)	-0.9(8)
C(68)-C(69)-C(70)-C(71)	0.4(8)
C(69)-C(70)-C(71)-C(72)	0.8(8)
C(68)-C(67)-C(72)-C(73)	-177.8(5)
C(66)-C(67)-C(72)-C(73)	2.0(7)
C(68)-C(67)-C(72)-C(71)	1.0(7)
C(66)-C(67)-C(72)-C(71)	-179.2(4)
C(70)-C(71)-C(72)-C(73)	177.3(5)
C(70)-C(71)-C(72)-C(67)	-1.5(8)
C(67)-C(72)-C(73)-C(74)	-1.1(8)
C(71)-C(72)-C(73)-C(74)	-179.9(5)
C(72)-C(73)-C(74)-C(65)	-0.6(8)
C(72)-C(73)-C(74)-C(75)	179.2(5)
C(66)-C(65)-C(74)-C(73)	1.6(7)
I(5)-C(65)-C(74)-C(73)	178.6(4)
C(66)-C(65)-C(74)-C(75)	-178.2(5)
I(5)-C(65)-C(74)-C(75)	-1.2(6)
C(76)-N(5)-C(75)-O(13)	-3.0(8)
I(5)-N(5)-C(75)-O(13)	-172.4(4)
C(76)-N(5)-C(75)-C(74)	177.4(4)
I(5)-N(5)-C(75)-C(74)	8.1(6)
C(73)-C(74)-C(75)-O(13)	-3.8(8)
C(65)-C(74)-C(75)-O(13)	176.0(5)
C(73)-C(74)-C(75)-N(5)	175.7(5)

C(65)-C(74)-C(75)-N(5)	-4.5(7)
C(75)-N(5)-C(76)-C(77)	-159.7(4)
I(5)-N(5)-C(76)-C(77)	8.8(5)
C(75)-N(5)-C(76)-C(78)	78.6(6)
I(5)-N(5)-C(76)-C(78)	-112.9(4)
I(6)-O(14)-C(77)-O(15)	-6.8(5)
I(6)-O(14)-C(77)-C(76)	169.3(3)
N(5)-C(76)-C(77)-O(15)	-18.9(6)
C(78)-C(76)-C(77)-O(15)	103.2(5)
N(5)-C(76)-C(77)-O(14)	164.9(4)
C(78)-C(76)-C(77)-O(14)	-73.0(6)
N(5)-C(76)-C(78)-C(79)	-156.5(5)
C(77)-C(76)-C(78)-C(79)	81.7(6)
N(5)-C(76)-C(78)-C(80)	78.1(6)
C(77)-C(76)-C(78)-C(80)	-43.7(6)
C(90)-C(81)-C(82)-C(83)	2.6(15)
I(6)-C(81)-C(82)-C(83)	-171.3(7)
C(81)-C(82)-C(83)-C(84)	176.4(8)
C(81)-C(82)-C(83)-C(88)	-0.2(11)
C(88)-C(83)-C(84)-C(85)	0.0
C(82)-C(83)-C(84)-C(85)	-176.6(7)
C(83)-C(84)-C(85)-C(86)	0.0
C(84)-C(85)-C(86)-C(87)	0.0
C(85)-C(86)-C(87)-C(88)	0.0
C(86)-C(87)-C(88)-C(83)	0.0
C(86)-C(87)-C(88)-C(89)	179.4(8)
C(84)-C(83)-C(88)-C(87)	0.0
C(82)-C(83)-C(88)-C(87)	176.6(7)
C(84)-C(83)-C(88)-C(89)	-179.4(8)
C(82)-C(83)-C(88)-C(89)	-2.8(9)
C(87)-C(88)-C(89)-C(90)	-176.0(7)
C(83)-C(88)-C(89)-C(90)	3.4(11)
C(88)-C(89)-C(90)-C(81)	-1.1(14)
C(88)-C(89)-C(90)-C(91)	178.5(8)
C(82)-C(81)-C(90)-C(89)	-2.0(16)
I(6)-C(81)-C(90)-C(89)	173.0(8)

C(82)-C(81)-C(90)-C(91)	178.4(10)
I(6)-C(81)-C(90)-C(91)	-6.6(11)
C(92)-N(6)-C(91)-O(16)	-1.0(15)
I(6)-N(6)-C(91)-O(16)	171.3(9)
C(92)-N(6)-C(91)-C(90)	178.0(8)
I(6)-N(6)-C(91)-C(90)	-9.7(11)
C(89)-C(90)-C(91)-O(16)	10.3(15)
C(81)-C(90)-C(91)-O(16)	-170.1(10)
C(89)-C(90)-C(91)-N(6)	-168.7(9)
C(81)-C(90)-C(91)-N(6)	10.8(13)
C(91)-N(6)-C(92)-C(93)	-161.9(9)
I(6)-N(6)-C(92)-C(93)	26.3(11)
C(91)-N(6)-C(92)-C(94)	76.4(11)
I(6)-N(6)-C(92)-C(94)	-95.5(9)
I(6)-O(18)-C(93)-O(17)	-172.9(9)
I(6)-O(18)-C(93)-C(92)	6.6(11)
I(4)-O(17)-C(93)-O(18)	-9.0(13)
I(4)-O(17)-C(93)-C(92)	171.5(8)
N(6)-C(92)-C(93)-O(18)	-19.5(13)
C(94)-C(92)-C(93)-O(18)	104.8(11)
N(6)-C(92)-C(93)-O(17)	160.1(10)
C(94)-C(92)-C(93)-O(17)	-75.7(11)
N(6)-C(92)-C(94)-C(96)	72.9(12)
C(93)-C(92)-C(94)-C(96)	-48.9(12)
N(6)-C(92)-C(94)-C(95)	-163.5(9)
C(93)-C(92)-C(94)-C(95)	74.7(10)
C(90A)-C(81A)-C(82A)-C(83A)	2(2)
I(6)-C(81A)-C(82A)-C(83A)	-165.6(11)
C(81A)-C(82A)-C(83A)-C(84A)	173.8(15)
C(81A)-C(82A)-C(83A)-C(88A)	-1(2)
C(88A)-C(83A)-C(84A)-C(85A)	1(2)
C(82A)-C(83A)-C(84A)-C(85A)	-174.0(15)
C(83A)-C(84A)-C(85A)-C(86A)	-2(3)
C(84A)-C(85A)-C(86A)-C(87A)	2(3)
C(85A)-C(86A)-C(87A)-C(88A)	-1(2)
C(84A)-C(83A)-C(88A)-C(87A)	0(2)

C(82A)-C(83A)-C(88A)-C(87A)	174.6(13)
C(84A)-C(83A)-C(88A)-C(89A)	-176.8(14)
C(82A)-C(83A)-C(88A)-C(89A)	-2(2)
C(86A)-C(87A)-C(88A)-C(83A)	1(2)
C(86A)-C(87A)-C(88A)-C(89A)	176.9(14)
C(83A)-C(88A)-C(89A)-C(90A)	4(2)
C(87A)-C(88A)-C(89A)-C(90A)	-172.8(14)
C(88A)-C(89A)-C(90A)-C(81A)	-3(2)
C(88A)-C(89A)-C(90A)-C(91A)	172.9(13)
C(82A)-C(81A)-C(90A)-C(89A)	0(2)
I(6)-C(81A)-C(90A)-C(89A)	167.8(11)
C(82A)-C(81A)-C(90A)-C(91A)	-175.8(15)
I(6)-C(81A)-C(90A)-C(91A)	-7.6(19)
C(92A)-N(6A)-C(91A)-O(16A)	-1(2)
I(6)-N(6A)-C(91A)-O(16A)	175.0(14)
C(92A)-N(6A)-C(91A)-C(90A)	174.5(12)
I(6)-N(6A)-C(91A)-C(90A)	-9.9(16)
C(89A)-C(90A)-C(91A)-O(16A)	11(2)
C(81A)-C(90A)-C(91A)-O(16A)	-173.2(16)
C(89A)-C(90A)-C(91A)-N(6A)	-163.8(13)
C(81A)-C(90A)-C(91A)-N(6A)	11.7(19)
C(91A)-N(6A)-C(92A)-C(93A)	-161.3(13)
I(6)-N(6A)-C(92A)-C(93A)	23.6(15)
C(91A)-N(6A)-C(92A)-C(94A)	75.6(16)
I(6)-N(6A)-C(92A)-C(94A)	-99.5(12)
I(4)-O(17A)-C(93A)-O(18A)	1(2)
I(4)-O(17A)-C(93A)-C(92A)	175.9(12)
N(6A)-C(92A)-C(93A)-O(18A)	-31.6(18)
C(94A)-C(92A)-C(93A)-O(18A)	93.3(15)
N(6A)-C(92A)-C(93A)-O(17A)	153.4(15)
C(94A)-C(92A)-C(93A)-O(17A)	-81.6(17)
N(6A)-C(92A)-C(94A)-C(96A)	60.9(16)
C(93A)-C(92A)-C(94A)-C(96A)	-60.8(15)
N(6A)-C(92A)-C(94A)-C(95A)	-170.6(13)
C(93A)-C(92A)-C(94A)-C(95A)	67.7(15)
C(100)-C(101)-O(19)-C(102)	-180.0

C(101)-O(19)-C(102)-C(103)

180.0

Symmetry transformations used to generate equivalent atoms:

**University of Illinois, Department of Chemistry
George L. Clark X- R Facility and 3M Materials Laboratory**

Structure report for compound **Valine HIM adduct in Naphthalene System 7b**

Identification code	CCDC 2388282
Empirical formula	C ₂₄ H ₃₅ Cl I N ₂ O _{3.50}
Principal Investigator:	Professor Dr. Kyle N Plunkett

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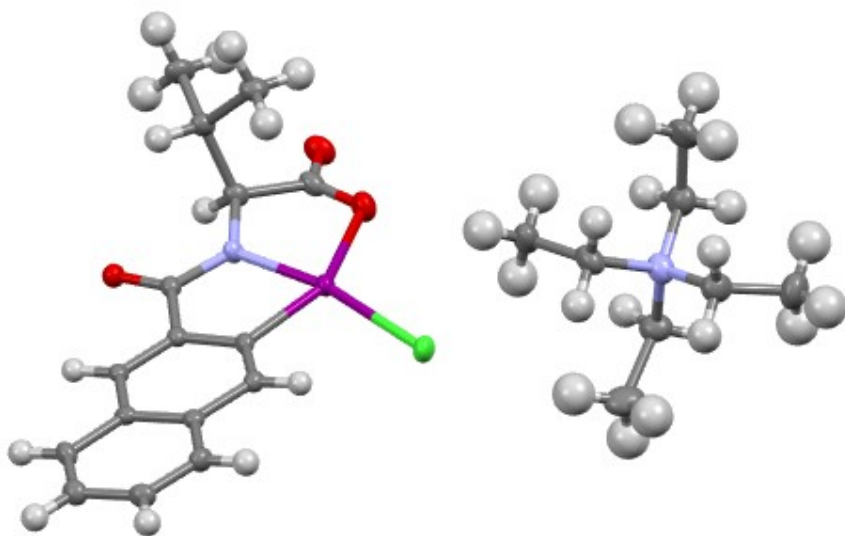


Figure SI19: Perspective view of crystallographically independent molecules of adduct. Solvents are removed for clarity. Nitrogen, oxygen, iodine and chlorine atoms are denoted by light blue, red, pink and green color respectively. Hydrogens atoms are omitted. (Ellipsoid style)

Table 1. Crystal data and structure refinement for 4536ds.

Identification code	CCDC 2388282	
Empirical formula	C ₂₄ H ₃₅ Cl I N ₂ O _{3.50}	
Formula weight	569.89	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁	
Unit cell dimensions	a = 22.5400(5) Å	a = 90°.
	b = 12.1496(3) Å	b = 94.3703(6)°.
	c = 26.9010(6) Å	g = 90°.
Volume	7345.5(3) Å ³	
Z	12	
Density (calculated)	1.546 Mg/m ³	
Absorption coefficient	1.447 mm ⁻¹	
F(000)	3492	
Crystal size	0.213 x 0.086 x 0.051 mm ³	
Theta range for data collection	2.025 to 28.329°.	
Index ranges	-30<=h<=30, -16<=k<=16, -35<=l<=35	
Reflections collected	256976	
Independent reflections	36572 [R(int) = 0.0713]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6786	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	36572 / 890 / 2014	
Goodness-of-fit on F ²	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0338, wR2 = 0.0609	
R indices (all data)	R1 = 0.0465, wR2 = 0.0671	
Absolute structure parameter	-0.030(5)	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.288 and -0.823 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4536ds. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I11	3333(1)	5464(1)	9517(1)	20(1)
Cl11	4280(1)	6539(1)	9163(1)	30(1)
O11	2966(2)	2477(3)	10392(2)	33(1)
O21	1548(1)	5508(4)	9818(1)	23(1)
O31	3474(2)	3770(3)	10012(2)	29(1)
N11	2506(2)	4953(4)	9735(2)	20(1)
C11	1959(2)	8436(4)	9007(2)	19(1)
C21	1548(2)	9290(4)	8871(2)	22(1)
C31	1703(2)	10134(4)	8571(2)	23(1)
C41	2277(2)	10177(4)	8391(2)	24(1)
C51	2682(2)	9367(5)	8517(2)	24(1)
C61	2537(2)	8476(4)	8825(2)	20(1)
C71	2955(2)	7630(5)	8957(2)	22(1)
C81	2786(2)	6788(4)	9251(2)	19(1)
C91	2210(2)	6710(4)	9425(2)	18(1)
C101	1810(2)	7526(4)	9304(2)	20(1)
C111	2052(2)	5684(4)	9684(2)	20(1)
C121	2405(2)	3845(4)	9926(2)	21(1)
C131	2994(2)	3315(5)	10135(2)	25(1)
C141	2086(2)	3124(4)	9512(2)	22(1)
C151	2508(3)	2752(5)	9126(2)	27(1)
C161	1767(3)	2145(5)	9725(2)	30(1)
I12	5053(1)	5444(1)	7764(1)	19(1)
Cl12	5986(1)	6559(1)	7376(1)	27(1)
O12	4746(2)	2483(3)	8677(2)	29(1)
O22	3306(1)	5498(4)	8158(1)	22(1)
O32	5225(2)	3758(3)	8258(2)	27(1)
N12	4244(2)	4930(3)	8018(2)	19(1)
C12	3646(2)	8398(4)	7310(2)	18(1)
C22	3225(2)	9256(4)	7194(2)	22(1)
C32	3356(2)	10098(4)	6885(2)	22(1)

C42	3907(2)	10134(4)	6673(2)	24(1)
C52	4324(2)	9329(4)	6777(2)	23(1)
C62	4210(2)	8441(4)	7099(2)	20(1)
C72	4635(2)	7604(4)	7215(2)	21(1)
C82	4493(2)	6769(4)	7517(2)	17(1)
C92	3934(2)	6681(4)	7720(2)	19(1)
C102	3519(2)	7499(4)	7618(2)	19(1)
C112	3791(2)	5668(4)	7995(2)	17(1)
C122	4157(2)	3840(4)	8228(2)	19(1)
C132	4757(2)	3310(4)	8407(2)	22(1)
C142	3807(2)	3101(4)	7839(2)	20(1)
C152	4198(3)	2695(5)	7439(2)	28(1)
C162	3500(3)	2137(5)	8083(2)	29(1)
I13	8194(1)	5452(1)	4250(1)	18(1)
CI13	9087(1)	6622(1)	3884(1)	26(1)
O13	7947(2)	2459(3)	5169(2)	35(1)
O23	6446(1)	5368(4)	4639(1)	22(1)
O33	8398(2)	3709(3)	4721(2)	28(1)
N13	7393(2)	4853(3)	4489(2)	17(1)
C13	6735(2)	8316(4)	3796(2)	17(1)
C23	6303(2)	9148(4)	3680(2)	20(1)
C33	6421(2)	10007(4)	3378(2)	22(1)
C43	6979(2)	10084(4)	3171(2)	23(1)
C53	7403(2)	9305(4)	3273(2)	21(1)
C63	7297(2)	8401(4)	3590(2)	18(1)
C73	7742(2)	7590(4)	3709(2)	18(1)
C83	7611(2)	6731(4)	4008(2)	16(1)
C93	7051(2)	6606(4)	4199(2)	16(1)
C103	6621(2)	7395(4)	4100(2)	18(1)
C113	6930(2)	5571(5)	4471(2)	19(1)
C123	7337(2)	3763(4)	4711(2)	20(1)
C133	7942(2)	3270(5)	4890(2)	25(1)
C143	6990(2)	3000(4)	4330(2)	23(1)
C153	7366(3)	2684(5)	3903(2)	28(1)
C163	6742(3)	1970(5)	4569(2)	34(1)
I14	6680(1)	5381(1)	5974(1)	18(1)

CI14	7544(1)	6492(1)	5549(1)	23(1)
O14	6449(2)	2351(3)	6877(2)	31(1)
O24	4963(1)	5362(3)	6434(1)	22(1)
O34	6894(2)	3657(3)	6449(2)	31(1)
N14	5895(2)	4830(4)	6264(2)	21(1)
C14	5212(2)	8255(4)	5547(2)	19(1)
C24	4780(2)	9095(4)	5442(2)	21(1)
C34	4890(2)	9937(4)	5124(2)	24(1)
C44	5426(2)	9987(4)	4890(2)	22(1)
C54	5855(2)	9187(4)	4982(2)	19(1)
C64	5760(2)	8309(4)	5314(2)	18(1)
C74	6207(2)	7492(4)	5421(2)	17(1)
C84	6086(2)	6663(4)	5741(2)	16(1)
C94	5544(2)	6565(4)	5962(2)	18(1)
C104	5115(2)	7362(4)	5867(2)	19(1)
C114	5434(2)	5556(5)	6249(2)	19(1)
C124	5832(2)	3734(4)	6474(2)	21(1)
C134	6439(3)	3197(5)	6617(2)	25(1)
C144	5447(2)	3019(4)	6097(2)	22(1)
C154	5134(3)	2091(5)	6353(2)	28(1)
C164	5811(3)	2575(5)	5681(2)	28(1)
I15	1530(1)	5530(1)	1146(1)	18(1)
CI15	2482(1)	6690(1)	862(1)	28(1)
O15	1162(2)	2571(3)	2043(2)	31(1)
O25	-278(1)	5458(4)	1350(1)	22(1)
O35	1672(2)	3795(3)	1622(2)	30(1)
N15	694(2)	4950(3)	1312(2)	19(1)
C15	134(2)	8403(4)	554(2)	17(1)
C25	-283(2)	9234(4)	397(2)	21(1)
C35	-117(2)	10097(4)	111(2)	24(1)
C45	472(2)	10183(4)	-29(2)	23(1)
C55	887(2)	9400(4)	119(2)	23(1)
C65	729(2)	8494(4)	412(2)	18(1)
C75	1156(2)	7674(4)	571(2)	18(1)
C85	981(2)	6822(4)	852(2)	17(1)
C95	390(2)	6691(4)	981(2)	17(1)

C105	-25(2)	7479(4)	838(2)	17(1)
C115	231(2)	5662(4)	1240(2)	18(1)
C125	610(2)	3848(4)	1518(2)	22(1)
C135	1193(3)	3372(5)	1751(2)	24(1)
C145	314(2)	3100(4)	1101(2)	23(1)
C155	23(3)	2083(5)	1305(2)	30(1)
C165	760(3)	2778(5)	722(2)	26(1)
I16	9781(1)	5626(1)	2653(1)	18(1)
CI16	10706(1)	6775(1)	2370(1)	26(1)
O16	9419(2)	2621(3)	3531(2)	38(1)
O26	7983(1)	5550(3)	2904(1)	22(1)
O36	9921(2)	3879(3)	3132(2)	31(1)
N16	8944(2)	5024(3)	2826(2)	18(1)
C16	8365(2)	8493(4)	2097(2)	18(1)
C26	7948(2)	9330(4)	1961(2)	20(1)
C36	8100(2)	10189(4)	1672(2)	21(1)
C46	8675(2)	10258(4)	1499(2)	21(1)
C56	9091(2)	9471(4)	1627(2)	20(1)
C66	8950(2)	8571(4)	1931(2)	18(1)
C76	9384(2)	7750(4)	2077(2)	18(1)
C86	9217(2)	6897(4)	2364(2)	16(1)
C96	8638(2)	6775(4)	2516(2)	17(1)
C106	8219(2)	7571(4)	2388(2)	18(1)
C116	8485(2)	5737(4)	2775(2)	18(1)
C126	8858(2)	3928(4)	3034(2)	23(1)
C136	9444(3)	3434(5)	3258(2)	27(1)
C146	8547(3)	3178(4)	2623(2)	24(1)
C156	8288(3)	2140(5)	2834(2)	34(1)
C166	8972(3)	2899(5)	2221(2)	27(1)
N17	4237(3)	4503(8)	1550(4)	31(1)
C17	4186(4)	5044(6)	2055(3)	35(2)
C27	4021(8)	6300(14)	2026(6)	45(4)
C37	4304(4)	3289(7)	1640(3)	37(2)
C47	4314(5)	2587(7)	1183(4)	42(2)
C57	3694(3)	4746(6)	1198(3)	34(2)
C67	3104(4)	4309(8)	1391(4)	38(2)

C77	4767(3)	4955(7)	1303(3)	34(2)
C87	5373(5)	4686(15)	1565(5)	45(3)
N1A8	4202(11)	4580(30)	1573(14)	34(3)
C1A8	4125(14)	5840(20)	1558(10)	39(3)
C2A8	4140(40)	6310(50)	2120(20)	45(8)
C3A8	4252(14)	4170(20)	1053(10)	38(3)
C4A8	4310(30)	2920(30)	1029(18)	52(8)
C5A8	3687(11)	4050(20)	1819(10)	35(3)
C6A8	3083(15)	3950(40)	1510(20)	53(8)
C7A8	4757(11)	4320(30)	1907(10)	36(3)
C8A8	5359(15)	4540(60)	1710(20)	37(8)
N19	2789(2)	4311(4)	3304(2)	21(1)
C19	2660(3)	4795(5)	2794(2)	29(1)
C29	2020(3)	5166(6)	2674(2)	42(2)
C39	2370(3)	3367(5)	3386(2)	27(1)
C49	2374(3)	2451(5)	3005(2)	32(1)
C59	3417(2)	3864(5)	3360(2)	27(1)
C69	3903(3)	4723(5)	3385(2)	33(1)
C79	2696(2)	5215(4)	3681(2)	24(1)
C89	2865(3)	4920(5)	4222(2)	32(1)
N110	9723(2)	4550(4)	6548(2)	21(1)
C110	9625(3)	3393(5)	6358(2)	32(1)
C210	9516(3)	3291(5)	5792(2)	32(1)
C310	9242(2)	5315(6)	6348(2)	33(1)
C410	8617(3)	5022(6)	6496(3)	49(2)
C510	9757(3)	4486(5)	7107(2)	33(1)
C610	9869(3)	5585(5)	7369(2)	36(1)
C710	10304(3)	5027(5)	6375(2)	35(1)
C810	10866(3)	4448(6)	6596(3)	56(2)
N111	935(2)	4332(3)	4647(2)	18(1)
C111	1144(2)	5345(5)	4379(2)	22(1)
C211	884(2)	5488(5)	3842(2)	28(1)
C311	259(2)	4245(5)	4606(2)	25(1)
C411	-66(2)	5234(5)	4800(2)	30(1)
C511	1176(3)	3305(4)	4413(2)	25(1)
C611	990(3)	2240(5)	4644(2)	30(1)

C711	1153(2)	4432(4)	5190(2)	22(1)
C811	1824(3)	4435(6)	5293(2)	34(1)
N112	6006(7)	4502(13)	9820(5)	27(2)
C112	5988(6)	5017(9)	10331(4)	34(2)
C212	5850(18)	6210(20)	10352(10)	37(5)
C312	6497(5)	5036(10)	9548(4)	34(2)
C412	7127(9)	4760(20)	9761(8)	37(4)
C512	5437(4)	4687(9)	9504(4)	30(2)
C612	4883(9)	4190(20)	9702(7)	39(4)
C712	6119(5)	3276(9)	9883(4)	33(2)
C812	6103(11)	2616(15)	9415(7)	40(4)
N1A13	5988(9)	4570(15)	9845(6)	28(2)
C1A13	5497(5)	4037(11)	10124(5)	32(2)
C2A13	4883(10)	4120(30)	9893(7)	39(5)
C3A13	5891(6)	5808(10)	9819(5)	34(2)
C4A13	5780(20)	6400(30)	10300(13)	51(7)
C5A13	5962(6)	4144(11)	9321(5)	33(2)
C6A13	6056(12)	2908(16)	9273(8)	39(5)
C7A13	6570(5)	4283(12)	10132(5)	35(2)
C8A13	7127(12)	4600(30)	9913(10)	46(6)
N114	7705(9)	4495(16)	8104(8)	23(2)
C114	7652(10)	5733(17)	8036(9)	34(3)
C214	7581(13)	6370(20)	8512(11)	49(5)
C314	8220(10)	4140(20)	8456(11)	26(3)
C414	8827(13)	4490(40)	8321(17)	33(6)
C514	7151(10)	4030(30)	8314(11)	27(3)
C614	6580(11)	4130(30)	7974(11)	34(5)
C714	7757(9)	4017(18)	7592(7)	26(3)
C814	7788(12)	2772(19)	7572(9)	39(5)
N1A15	7749(10)	4619(18)	8148(8)	24(2)
C1A15	7688(11)	5866(17)	8195(9)	31(3)
C2A15	7631(16)	6330(20)	8713(11)	54(6)
C3A15	8305(11)	4250(30)	8451(11)	26(4)
C4A15	8884(13)	4620(40)	8262(19)	31(5)
C5A15	7229(11)	4060(30)	8362(12)	30(4)
C6A15	6614(13)	4300(30)	8105(12)	41(6)

C7A15	7783(11)	4390(20)	7603(8)	31(3)
C8A15	7814(13)	3160(20)	7484(10)	39(5)
O(1)	7965(2)	2498(4)	6209(2)	38(1)
O(2)	1000(2)	2836(4)	3083(2)	32(1)
O(3)	750(2)	7047(4)	5480(2)	39(1)

Table 3. Bond lengths [Å] and angles [°] for 4536ds.

I11-N11	2.090(4)
I11-C81	2.118(5)
I11-O31	2.458(4)
I11-Cl11	2.7351(15)
O11-C131	1.235(7)
O21-C111	1.237(6)
O31-C131	1.282(7)
N11-C111	1.354(6)
N11-C121	1.465(6)
C11-C21	1.419(7)
C11-C101	1.420(7)
C11-C61	1.427(7)
C21-C31	1.367(7)
C21-H21	0.9500
C31-C41	1.416(7)
C31-H31	0.9500
C41-C51	1.368(7)
C41-H41	0.9500
C51-C61	1.418(8)
C51-H51	0.9500
C61-C71	1.420(7)
C71-C81	1.366(7)
C71-H71	0.9500
C81-C91	1.415(7)
C91-C101	1.363(7)
C91-C111	1.486(7)
C101-H101	0.9500
C121-C131	1.542(7)
C121-C141	1.551(7)
C121-H121	1.0000
C141-C161	1.523(7)
C141-C151	1.530(7)
C141-H141	1.0000
C151-H15A1	0.9800

C151-H15B1	0.9800
C151-H15C1	0.9800
C161-H16A1	0.9800
C161-H16B1	0.9800
C161-H16C1	0.9800
I12-N12	2.090(4)
I12-C82	2.120(5)
I12-O32	2.458(4)
I12-C112	2.7704(13)
O12-C132	1.240(6)
O22-C112	1.225(5)
O32-C132	1.278(6)
N12-C112	1.358(6)
N12-C122	1.459(6)
C12-C102	1.413(7)
C12-C22	1.428(7)
C12-C62	1.431(7)
C22-C32	1.365(7)
C22-H22	0.9500
C32-C42	1.407(7)
C32-H32	0.9500
C42-C52	1.370(7)
C42-H42	0.9500
C52-C62	1.420(7)
C52-H52	0.9500
C62-C72	1.416(7)
C72-C82	1.355(7)
C72-H72	0.9500
C82-C92	1.412(7)
C92-C102	1.379(7)
C92-C112	1.485(7)
C102-H102	0.9500
C122-C132	1.542(7)
C122-C142	1.550(7)
C122-H122	1.0000
C142-C152	1.522(7)

C142-C162	1.534(7)
C142-H142	1.0000
C152-H15A2	0.9800
C152-H15B2	0.9800
C152-H15C2	0.9800
C162-H16A2	0.9800
C162-H16B2	0.9800
C162-H16C2	0.9800
I13-N13	2.091(4)
I13-C83	2.107(5)
I13-CI13	2.7096(14)
O13-C133	1.238(7)
O23-C113	1.239(5)
O33-C133	1.274(7)
N13-C113	1.358(6)
N13-C123	1.463(6)
C13-C103	1.421(7)
C13-C23	1.422(7)
C13-C63	1.427(7)
C23-C33	1.362(7)
C23-H23	0.9500
C33-C43	1.417(7)
C33-H33	0.9500
C43-C53	1.358(7)
C43-H43	0.9500
C53-C63	1.421(7)
C53-H53	0.9500
C63-C73	1.426(7)
C73-C83	1.364(7)
C73-H73	0.9500
C83-C93	1.407(7)
C93-C103	1.375(7)
C93-C113	1.489(7)
C103-H103	0.9500
C123-C133	1.532(7)
C123-C143	1.549(7)

C123-H123	1.0000
C143-C153	1.527(7)
C143-C163	1.532(8)
C143-H143	1.0000
C153-H15A3	0.9800
C153-H15B3	0.9800
C153-H15C3	0.9800
C163-H16A3	0.9800
C163-H16B3	0.9800
C163-H16C3	0.9800
I14-N14	2.098(4)
I14-C84	2.117(5)
I14-O34	2.482(4)
I14-C114	2.6945(13)
O14-C134	1.242(7)
O24-C114	1.227(5)
O34-C134	1.281(7)
N14-C114	1.361(6)
N14-C124	1.457(6)
C14-C104	1.412(7)
C14-C24	1.424(7)
C14-C64	1.428(7)
C24-C34	1.367(7)
C24-H24	0.9500
C34-C44	1.407(7)
C34-H34	0.9500
C44-C54	1.380(7)
C44-H44	0.9500
C54-C64	1.418(7)
C54-H54	0.9500
C64-C74	1.428(7)
C74-C84	1.366(7)
C74-H74	0.9500
C84-C94	1.405(7)
C94-C104	1.378(7)
C94-C114	1.481(7)

C104-H104	0.9500
C124-C134	1.537(7)
C124-C144	1.550(7)
C124-H124	1.0000
C144-C154	1.523(7)
C144-C164	1.535(7)
C144-H144	1.0000
C154-H15A4	0.9800
C154-H15B4	0.9800
C154-H15C4	0.9800
C164-H16A4	0.9800
C164-H16B4	0.9800
C164-H16C4	0.9800
I15-N15	2.093(4)
I15-C85	2.115(5)
I15-O35	2.474(4)
I15-Cl15	2.7230(14)
O15-C135	1.256(7)
O25-C115	1.232(5)
O35-C135	1.268(7)
N15-C115	1.358(6)
N15-C125	1.466(6)
C15-C105	1.419(7)
C15-C25	1.420(7)
C15-C65	1.428(7)
C25-C35	1.368(7)
C25-H25	0.9500
C35-C45	1.412(7)
C35-H35	0.9500
C45-C55	1.372(7)
C45-H45	0.9500
C55-C65	1.415(7)
C55-H55	0.9500
C65-C75	1.428(7)
C75-C85	1.358(7)
C75-H75	0.9500

C85-C95	1.410(7)
C95-C105	1.373(7)
C95-C115	1.489(7)
C105-H105	0.9500
C125-C135	1.527(7)
C125-C145	1.555(7)
C125-H125	1.0000
C145-C155	1.520(7)
C145-C165	1.535(7)
C145-H145	1.0000
C155-H15A5	0.9800
C155-H15B5	0.9800
C155-H15C5	0.9800
C165-H16A5	0.9800
C165-H16B5	0.9800
C165-H16C5	0.9800
I16-N16	2.108(4)
I16-C86	2.111(5)
I16-CI16	2.6677(14)
O16-C136	1.236(7)
O26-C116	1.228(6)
O36-C136	1.272(7)
N16-C116	1.350(6)
N16-C126	1.462(6)
C16-C26	1.415(7)
C16-C106	1.419(7)
C16-C66	1.426(7)
C26-C36	1.360(7)
C26-H26	0.9500
C36-C46	1.414(7)
C36-H36	0.9500
C46-C56	1.364(7)
C46-H46	0.9500
C56-C66	1.416(7)
C56-H56	0.9500
C66-C76	1.432(7)

C76-C86	1.363(7)
C76-H76	0.9500
C86-C96	1.405(7)
C96-C106	1.377(7)
C96-C116	1.493(7)
C106-H106	0.9500
C126-C136	1.531(8)
C126-C146	1.557(8)
C126-H126	1.0000
C146-C156	1.519(8)
C146-C166	1.536(7)
C146-H146	1.0000
C156-H15A6	0.9800
C156-H15B6	0.9800
C156-H15C6	0.9800
C166-H16A6	0.9800
C166-H16B6	0.9800
C166-H16C6	0.9800
N17-C37	1.501(13)
N17-C77	1.515(12)
N17-C57	1.518(12)
N17-C17	1.521(12)
C17-C27	1.571(18)
C17-H1A7	0.9900
C17-H1B7	0.9900
C27-H2A7	0.9800
C27-H2B7	0.9800
C27-H2C7	0.9800
C37-C47	1.497(12)
C37-H3A7	0.9900
C37-H3B7	0.9900
C47-H4A7	0.9800
C47-H4B7	0.9800
C47-H4C7	0.9800
C57-C67	1.556(11)
C57-H5A7	0.9900

C57-H5B7	0.9900
C67-H6A7	0.9800
C67-H6B7	0.9800
C67-H6C7	0.9800
C77-C87	1.524(12)
C77-H7A7	0.9900
C77-H7B7	0.9900
C87-H8A7	0.9800
C87-H8B7	0.9800
C87-H8C7	0.9800
N1A8-C3A8	1.50(3)
N1A8-C7A8	1.52(3)
N1A8-C5A8	1.52(3)
N1A8-C1A8	1.53(3)
C1A8-C2A8	1.61(3)
C1A8-H1C8	0.9900
C1A8-H1D8	0.9900
C2A8-H2D8	0.9800
C2A8-H2E8	0.9800
C2A8-H2F8	0.9800
C3A8-C4A8	1.52(3)
C3A8-H3C8	0.9900
C3A8-H3D8	0.9900
C4A8-H4D8	0.9800
C4A8-H4E8	0.9800
C4A8-H4F8	0.9800
C5A8-C6A8	1.54(3)
C5A8-H5C8	0.9900
C5A8-H5D8	0.9900
C6A8-H6D8	0.9800
C6A8-H6E8	0.9800
C6A8-H6F8	0.9800
C7A8-C8A8	1.52(3)
C7A8-H7C8	0.9900
C7A8-H7D8	0.9900
C8A8-H8D8	0.9800

C8A8-H8E8	0.9800
C8A8-H8F8	0.9800
N19-C19	1.499(7)
N19-C39	1.513(7)
N19-C59	1.514(7)
N19-C79	1.521(7)
C19-C29	1.523(8)
C19-H1A9	0.9900
C19-H1B9	0.9900
C29-H2A9	0.9800
C29-H2B9	0.9800
C29-H2C9	0.9800
C39-C49	1.514(8)
C39-H3A9	0.9900
C39-H3B9	0.9900
C49-H4A9	0.9800
C49-H4B9	0.9800
C49-H4C9	0.9800
C59-C69	1.511(8)
C59-H5A9	0.9900
C59-H5B9	0.9900
C69-H6A9	0.9800
C69-H6B9	0.9800
C69-H6C9	0.9800
C79-C89	1.519(7)
C79-H7A9	0.9900
C79-H7B9	0.9900
C89-H8A9	0.9800
C89-H8B9	0.9800
C89-H8C9	0.9800
N110-C310	1.496(7)
N110-C510	1.503(7)
N110-C110	1.506(7)
N110-C710	1.537(7)
C110-C210	1.529(8)
C110-H1A10	0.9900

C110-H1B10	0.9900
C210-H2A10	0.9800
C210-H2B10	0.9800
C210-H2C10	0.9800
C310-C410	1.536(9)
C310-H3A10	0.9900
C310-H3B10	0.9900
C410-H4A10	0.9800
C410-H4B10	0.9800
C410-H4C10	0.9800
C510-C610	1.522(8)
C510-H5A10	0.9900
C510-H5B10	0.9900
C610-H6A10	0.9800
C610-H6B10	0.9800
C610-H6C10	0.9800
C710-C810	1.529(9)
C710-H7A10	0.9900
C710-H7B10	0.9900
C810-H8A10	0.9800
C810-H8B10	0.9800
C810-H8C10	0.9800
N111-C711	1.510(6)
N111-C511	1.516(6)
N111-C111	1.520(7)
N111-C311	1.523(6)
C111-C211	1.526(6)
C111-H1A11	0.9900
C111-H1B11	0.9900
C211-H2A11	0.9800
C211-H2B11	0.9800
C211-H2C11	0.9800
C311-C411	1.520(8)
C311-H3A11	0.9900
C311-H3B11	0.9900
C411-H4A11	0.9800

C411-H4B11	0.9800
C411-H4C11	0.9800
C511-C611	1.508(7)
C511-H5A11	0.9900
C511-H5B11	0.9900
C611-H6A11	0.9800
C611-H6B11	0.9800
C611-H6C11	0.9800
C711-C811	1.516(7)
C711-H7A11	0.9900
C711-H7B11	0.9900
C811-H8A11	0.9800
C811-H8B11	0.9800
C811-H8C11	0.9800
N112-C512	1.500(17)
N112-C112	1.514(17)
N112-C712	1.518(17)
N112-C312	1.519(17)
C112-C212	1.48(2)
C112-H1A12	0.9900
C112-H1B12	0.9900
C212-H2A12	0.9800
C212-H2B12	0.9800
C212-H2C12	0.9800
C312-C412	1.53(2)
C312-H3A12	0.9900
C312-H3B12	0.9900
C412-H4A12	0.9800
C412-H4B12	0.9800
C412-H4C12	0.9800
C512-C612	1.52(2)
C512-H5A12	0.9900
C512-H5B12	0.9900
C612-H6A12	0.9800
C612-H6B12	0.9800
C612-H6C12	0.9800

C712-C812	1.49(2)
C712-H7A12	0.9900
C712-H7B12	0.9900
C812-H8A12	0.9800
C812-H8B12	0.9800
C812-H8C12	0.9800
N1A13-C5A13	1.499(19)
N1A13-C7A13	1.512(19)
N1A13-C3A13	1.520(19)
N1A13-C1A13	1.53(2)
C1A13-C2A13	1.48(2)
C1A13-H1C13	0.9900
C1A13-H1D13	0.9900
C2A13-H2D13	0.9800
C2A13-H2E13	0.9800
C2A13-H2F13	0.9800
C3A13-C4A13	1.52(3)
C3A13-H3C13	0.9900
C3A13-H3D13	0.9900
C4A13-H4D13	0.9800
C4A13-H4E13	0.9800
C4A13-H4F13	0.9800
C5A13-C6A13	1.52(2)
C5A13-H5C13	0.9900
C5A13-H5D13	0.9900
C6A13-H6D13	0.9800
C6A13-H6E13	0.9800
C6A13-H6F13	0.9800
C7A13-C8A13	1.48(3)
C7A13-H7C13	0.9900
C7A13-H7D13	0.9900
C8A13-H8D13	0.9800
C8A13-H8E13	0.9800
C8A13-H8F13	0.9800
N114-C314	1.506(15)
N114-C714	1.510(15)

N114-C114	1.518(15)
N114-C514	1.520(14)
C114-C214	1.516(17)
C114-H1A14	0.9900
C114-H1B14	0.9900
C214-H2A14	0.9800
C214-H2B14	0.9800
C214-H2C14	0.9800
C314-C414	1.504(17)
C314-H3A14	0.9900
C314-H3B14	0.9900
C414-H4A14	0.9800
C414-H4B14	0.9800
C414-H4C14	0.9800
C514-C614	1.527(16)
C514-H5A14	0.9900
C514-H5B14	0.9900
C614-H6A14	0.9800
C614-H6B14	0.9800
C614-H6C14	0.9800
C714-C814	1.516(16)
C714-H7A14	0.9900
C714-H7B14	0.9900
C814-H8A14	0.9800
C814-H8B14	0.9800
C814-H8C14	0.9800
N1A15-C7A15	1.499(16)
N1A15-C5A15	1.508(16)
N1A15-C3A15	1.508(15)
N1A15-C1A15	1.528(16)
C1A15-C2A15	1.514(18)
C1A15-H1C15	0.9900
C1A15-H1D15	0.9900
C2A15-H2D15	0.9800
C2A15-H2E15	0.9800
C2A15-H2F15	0.9800

C3A15-C4A15	1.505(18)
C3A15-H3C15	0.9900
C3A15-H3D15	0.9900
C4A15-H4D15	0.9800
C4A15-H4E15	0.9800
C4A15-H4F15	0.9800
C5A15-C6A15	1.528(18)
C5A15-H5C15	0.9900
C5A15-H5D15	0.9900
C6A15-H6D15	0.9800
C6A15-H6E15	0.9800
C6A15-H6F15	0.9800
C7A15-C8A15	1.536(18)
C7A15-H7C15	0.9900
C7A15-H7D15	0.9900
C8A15-H8D15	0.9800
C8A15-H8E15	0.9800
C8A15-H8F15	0.9800
O(1)-H(1E)	0.87(5)
O(1)-H(1F)	0.86(5)
O(2)-H(2G)	0.72(8)
O(2)-H(2H)	0.97(7)
O(3)-H(3E)	0.77(8)
O(3)-H(3F)	0.77(8)
N11-I11-C81	79.17(19)
N11-I11-O31	71.40(15)
C81-I11-O31	150.10(17)
N11-I11-Cl11	167.40(12)
C81-I11-Cl11	88.26(15)
O31-I11-Cl11	121.01(10)
C131-O31-I11	115.1(3)
C111-N11-C121	120.1(4)
C111-N11-I11	117.4(3)
C121-N11-I11	122.5(3)
C21-C11-C101	122.4(5)

C21-C11-C61	118.9(5)
C101-C11-C61	118.7(5)
C31-C21-C11	120.6(5)
C31-C21-H21	119.7
C11-C21-H21	119.7
C21-C31-C41	120.7(5)
C21-C31-H31	119.6
C41-C31-H31	119.6
C51-C41-C31	119.9(5)
C51-C41-H41	120.0
C31-C41-H41	120.0
C41-C51-C61	121.0(5)
C41-C51-H51	119.5
C61-C51-H51	119.5
C51-C61-C71	121.3(5)
C51-C61-C11	118.9(5)
C71-C61-C11	119.8(5)
C81-C71-C61	118.5(5)
C81-C71-H71	120.7
C61-C71-H71	120.7
C71-C81-C91	123.0(5)
C71-C81-I11	125.7(4)
C91-C81-I11	111.3(4)
C101-C91-C81	118.6(5)
C101-C91-C111	123.0(5)
C81-C91-C111	118.0(4)
C91-C101-C11	121.3(5)
C91-C101-H101	119.3
C11-C101-H101	119.3
O21-C111-N11	124.2(5)
O21-C111-C91	122.7(5)
N11-C111-C91	113.1(4)
N11-C121-C131	111.1(4)
N11-C121-C141	110.0(4)
C131-C121-C141	111.4(4)
N11-C121-H121	108.1

C131-C121-H121	108.1
C141-C121-H121	108.1
O11-C131-O31	125.5(5)
O11-C131-C121	117.9(5)
O31-C131-C121	116.5(5)
C161-C141-C151	111.1(4)
C161-C141-C121	112.2(5)
C151-C141-C121	112.1(4)
C161-C141-H141	107.0
C151-C141-H141	107.0
C121-C141-H141	107.0
C141-C151-H15A1	109.5
C141-C151-H15B1	109.5
H15A1-C151-H15B1	109.5
C141-C151-H15C1	109.5
H15A1-C151-H15C1	109.5
H15B1-C151-H15C1	109.5
C141-C161-H16A1	109.5
C141-C161-H16B1	109.5
H16A1-C161-H16B1	109.5
C141-C161-H16C1	109.5
H16A1-C161-H16C1	109.5
H16B1-C161-H16C1	109.5
N12-I12-C82	79.40(18)
N12-I12-O32	71.30(14)
C82-I12-O32	150.20(16)
N12-I12-Cl12	167.12(12)
C82-I12-Cl12	87.84(14)
O32-I12-Cl12	121.20(9)
C132-O32-I12	115.1(3)
C112-N12-C122	119.6(4)
C112-N12-I12	117.4(3)
C122-N12-I12	123.0(3)
C102-C12-C22	122.1(5)
C102-C12-C62	119.1(5)
C22-C12-C62	118.8(5)

C32-C22-C12	120.7(5)
C32-C22-H22	119.7
C12-C22-H22	119.7
C22-C32-C42	120.6(5)
C22-C32-H32	119.7
C42-C32-H32	119.7
C52-C42-C32	120.6(5)
C52-C42-H42	119.7
C32-C42-H42	119.7
C42-C52-C62	120.9(5)
C42-C52-H52	119.6
C62-C52-H52	119.6
C72-C62-C52	121.9(5)
C72-C62-C12	119.5(5)
C52-C62-C12	118.6(5)
C82-C72-C62	118.9(5)
C82-C72-H72	120.6
C62-C72-H72	120.6
C72-C82-C92	123.1(5)
C72-C82-I12	126.4(4)
C92-C82-I12	110.4(3)
C102-C92-C82	118.7(5)
C102-C92-C112	121.7(5)
C82-C92-C112	119.3(4)
C92-C102-C12	120.5(5)
C92-C102-H102	119.7
C12-C102-H102	119.7
O22-C112-N12	124.2(5)
O22-C112-C92	123.5(5)
N12-C112-C92	112.2(4)
N12-C122-C132	111.1(4)
N12-C122-C142	109.9(4)
C132-C122-C142	111.0(4)
N12-C122-H122	108.2
C132-C122-H122	108.2
C142-C122-H122	108.2

O12-C132-O32	125.6(5)
O12-C132-C122	117.7(5)
O32-C132-C122	116.7(5)
C152-C142-C162	111.1(5)
C152-C142-C122	111.8(4)
C162-C142-C122	112.1(4)
C152-C142-H142	107.2
C162-C142-H142	107.2
C122-C142-H142	107.2
C142-C152-H15A2	109.5
C142-C152-H15B2	109.5
H15A2-C152-H15B2	109.5
C142-C152-H15C2	109.5
H15A2-C152-H15C2	109.5
H15B2-C152-H15C2	109.5
C142-C162-H16A2	109.5
C142-C162-H16B2	109.5
H16A2-C162-H16B2	109.5
C142-C162-H16C2	109.5
H16A2-C162-H16C2	109.5
H16B2-C162-H16C2	109.5
N13-I13-C83	79.53(18)
N13-I13-Cl13	167.42(12)
C83-I13-Cl13	87.94(14)
C113-N13-C123	120.4(4)
C113-N13-I13	116.4(3)
C123-N13-I13	123.0(3)
C103-C13-C23	122.4(5)
C103-C13-C63	119.1(5)
C23-C13-C63	118.5(5)
C33-C23-C13	120.9(5)
C33-C23-H23	119.6
C13-C23-H23	119.6
C23-C33-C43	120.4(5)
C23-C33-H33	119.8
C43-C33-H33	119.8

C53-C43-C33	120.4(5)
C53-C43-H43	119.8
C33-C43-H43	119.8
C43-C53-C63	120.8(5)
C43-C53-H53	119.6
C63-C53-H53	119.6
C53-C63-C73	121.5(5)
C53-C63-C13	119.0(5)
C73-C63-C13	119.6(5)
C83-C73-C63	118.7(5)
C83-C73-H73	120.6
C63-C73-H73	120.6
C73-C83-C93	122.7(5)
C73-C83-I13	126.0(4)
C93-C83-I13	111.3(3)
C103-C93-C83	119.5(5)
C103-C93-C113	122.2(4)
C83-C93-C113	118.2(4)
C93-C103-C13	120.4(5)
C93-C103-H103	119.8
C13-C103-H103	119.8
O23-C113-N13	123.8(5)
O23-C113-C93	123.0(5)
N13-C113-C93	113.0(4)
N13-C123-C133	112.4(4)
N13-C123-C143	109.0(4)
C133-C123-C143	111.5(4)
N13-C123-H123	107.9
C133-C123-H123	107.9
C143-C123-H123	107.9
O13-C133-O33	125.4(5)
O13-C133-C123	118.0(5)
O33-C133-C123	116.6(5)
C153-C143-C163	110.5(5)
C153-C143-C123	111.5(4)
C163-C143-C123	113.2(5)

C153-C143-H143	107.1
C163-C143-H143	107.1
C123-C143-H143	107.1
C143-C153-H15A3	109.5
C143-C153-H15B3	109.5
H15A3-C153-H15B3	109.5
C143-C153-H15C3	109.5
H15A3-C153-H15C3	109.5
H15B3-C153-H15C3	109.5
C143-C163-H16A3	109.5
C143-C163-H16B3	109.5
H16A3-C163-H16B3	109.5
C143-C163-H16C3	109.5
H16A3-C163-H16C3	109.5
H16B3-C163-H16C3	109.5
N14-I14-C84	79.18(18)
N14-I14-O34	71.08(15)
C84-I14-O34	150.12(16)
N14-I14-Cl14	167.20(12)
C84-I14-Cl14	88.09(14)
O34-I14-Cl14	121.54(10)
C134-O34-I14	114.9(3)
C114-N14-C124	120.5(4)
C114-N14-I14	116.5(3)
C124-N14-I14	123.0(3)
C104-C14-C24	122.4(5)
C104-C14-C64	118.9(5)
C24-C14-C64	118.7(5)
C34-C24-C14	120.5(5)
C34-C24-H24	119.7
C14-C24-H24	119.7
C24-C34-C44	120.9(5)
C24-C34-H34	119.5
C44-C34-H34	119.5
C54-C44-C34	120.3(5)
C54-C44-H44	119.9

C34-C44-H44	119.9
C44-C54-C64	120.3(5)
C44-C54-H54	119.8
C64-C54-H54	119.8
C54-C64-C14	119.2(5)
C54-C64-C74	120.8(5)
C14-C64-C74	120.0(5)
C84-C74-C64	118.0(5)
C84-C74-H74	121.0
C64-C74-H74	121.0
C74-C84-C94	123.4(5)
C74-C84-I14	125.3(4)
C94-C84-I14	111.3(3)
C104-C94-C84	118.9(5)
C104-C94-C114	122.4(4)
C84-C94-C114	118.5(4)
C94-C104-C14	120.9(5)
C94-C104-H104	119.6
C14-C104-H104	119.6
O24-C114-N14	123.1(5)
O24-C114-C94	123.6(5)
N14-C114-C94	113.2(4)
N14-C124-C134	112.0(4)
N14-C124-C144	108.9(4)
C134-C124-C144	111.6(4)
N14-C124-H124	108.0
C134-C124-H124	108.0
C144-C124-H124	108.0
O14-C134-O34	125.3(5)
O14-C134-C124	118.1(5)
O34-C134-C124	116.6(5)
C154-C144-C164	111.1(4)
C154-C144-C124	112.0(4)
C164-C144-C124	111.8(4)
C154-C144-H144	107.2
C164-C144-H144	107.2

C124-C144-H144	107.2
C144-C154-H15A4	109.5
C144-C154-H15B4	109.5
H15A4-C154-H15B4	109.5
C144-C154-H15C4	109.5
H15A4-C154-H15C4	109.5
H15B4-C154-H15C4	109.5
C144-C164-H16A4	109.5
C144-C164-H16B4	109.5
H16A4-C164-H16B4	109.5
C144-C164-H16C4	109.5
H16A4-C164-H16C4	109.5
H16B4-C164-H16C4	109.5
N15-I15-C85	79.53(18)
N15-I15-O35	71.67(15)
C85-I15-O35	150.98(16)
N15-I15-Cl15	167.30(12)
C85-I15-Cl15	87.84(14)
O35-I15-Cl15	120.85(10)
C135-O35-I15	114.0(3)
C115-N15-C125	121.0(4)
C115-N15-I15	116.8(3)
C125-N15-I15	122.2(3)
C105-C15-C25	122.3(5)
C105-C15-C65	119.1(5)
C25-C15-C65	118.6(5)
C35-C25-C15	120.6(5)
C35-C25-H25	119.7
C15-C25-H25	119.7
C25-C35-C45	120.6(5)
C25-C35-H35	119.7
C45-C35-H35	119.7
C55-C45-C35	120.3(5)
C55-C45-H45	119.8
C35-C45-H45	119.8
C45-C55-C65	120.4(5)

C45-C55-H55	119.8
C65-C55-H55	119.8
C55-C65-C15	119.4(5)
C55-C65-C75	121.2(5)
C15-C65-C75	119.4(5)
C85-C75-C65	118.8(5)
C85-C75-H75	120.6
C65-C75-H75	120.6
C75-C85-C95	122.8(5)
C75-C85-I15	126.0(4)
C95-C85-I15	111.2(4)
C105-C95-C85	119.3(5)
C105-C95-C115	122.2(4)
C85-C95-C115	118.4(4)
C95-C105-C15	120.5(5)
C95-C105-H105	119.7
C15-C105-H105	119.7
O25-C115-N15	123.9(5)
O25-C115-C95	122.9(5)
N15-C115-C95	113.1(4)
N15-C125-C135	111.6(4)
N15-C125-C145	108.8(4)
C135-C125-C145	112.5(4)
N15-C125-H125	107.9
C135-C125-H125	107.9
C145-C125-H125	107.9
O15-C135-O35	125.0(5)
O15-C135-C125	117.6(5)
O35-C135-C125	117.4(5)
C155-C145-C165	110.8(5)
C155-C145-C125	112.8(5)
C165-C145-C125	111.2(5)
C155-C145-H145	107.2
C165-C145-H145	107.2
C125-C145-H145	107.2
C145-C155-H15A5	109.5

C145-C155-H15B5	109.5
H15A5-C155-H15B5	109.5
C145-C155-H15C5	109.5
H15A5-C155-H15C5	109.5
H15B5-C155-H15C5	109.5
C145-C165-H16A5	109.5
C145-C165-H16B5	109.5
H16A5-C165-H16B5	109.5
C145-C165-H16C5	109.5
H16A5-C165-H16C5	109.5
H16B5-C165-H16C5	109.5
N16-I16-C86	79.07(18)
N16-I16-Cl16	167.50(12)
C86-I16-Cl16	88.49(14)
C116-N16-C126	120.1(4)
C116-N16-I16	116.6(3)
C126-N16-I16	123.1(3)
C26-C16-C106	122.1(5)
C26-C16-C66	118.9(5)
C106-C16-C66	119.0(5)
C36-C26-C16	120.5(5)
C36-C26-H26	119.7
C16-C26-H26	119.7
C26-C36-C46	120.7(5)
C26-C36-H36	119.6
C46-C36-H36	119.6
C56-C46-C36	120.3(5)
C56-C46-H46	119.8
C36-C46-H46	119.8
C46-C56-C66	120.4(5)
C46-C56-H56	119.8
C66-C56-H56	119.8
C56-C66-C16	119.1(5)
C56-C66-C76	121.2(5)
C16-C66-C76	119.8(5)
C86-C76-C66	118.2(5)

C86-C76-H76	120.9
C66-C76-H76	120.9
C76-C86-C96	123.3(5)
C76-C86-I16	125.4(4)
C96-C86-I16	111.3(4)
C106-C96-C86	119.2(5)
C106-C96-C116	122.1(4)
C86-C96-C116	118.5(4)
C96-C106-C16	120.6(5)
C96-C106-H106	119.7
C16-C106-H106	119.7
O26-C116-N16	124.5(5)
O26-C116-C96	122.6(5)
N16-C116-C96	112.8(4)
N16-C126-C136	111.9(5)
N16-C126-C146	109.1(4)
C136-C126-C146	112.2(4)
N16-C126-H126	107.8
C136-C126-H126	107.8
C146-C126-H126	107.8
O16-C136-O36	125.1(6)
O16-C136-C126	118.1(5)
O36-C136-C126	116.8(5)
C156-C146-C166	111.1(5)
C156-C146-C126	112.7(5)
C166-C146-C126	111.0(5)
C156-C146-H146	107.3
C166-C146-H146	107.3
C126-C146-H146	107.3
C146-C156-H15A6	109.5
C146-C156-H15B6	109.5
H15A6-C156-H15B6	109.5
C146-C156-H15C6	109.5
H15A6-C156-H15C6	109.5
H15B6-C156-H15C6	109.5
C146-C166-H16A6	109.5

C146-C166-H16B6	109.5
H16A6-C166-H16B6	109.5
C146-C166-H16C6	109.5
H16A6-C166-H16C6	109.5
H16B6-C166-H16C6	109.5
C37-N17-C77	110.7(7)
C37-N17-C57	111.0(6)
C77-N17-C57	106.3(9)
C37-N17-C17	107.1(9)
C77-N17-C17	110.6(7)
C57-N17-C17	111.2(7)
N17-C17-C27	114.1(9)
N17-C17-H1A7	108.7
C27-C17-H1A7	108.7
N17-C17-H1B7	108.7
C27-C17-H1B7	108.7
H1A7-C17-H1B7	107.6
C17-C27-H2A7	109.5
C17-C27-H2B7	109.5
H2A7-C27-H2B7	109.5
C17-C27-H2C7	109.5
H2A7-C27-H2C7	109.5
H2B7-C27-H2C7	109.5
C47-C37-N17	115.8(8)
C47-C37-H3A7	108.3
N17-C37-H3A7	108.3
C47-C37-H3B7	108.3
N17-C37-H3B7	108.3
H3A7-C37-H3B7	107.4
C37-C47-H4A7	109.5
C37-C47-H4B7	109.5
H4A7-C47-H4B7	109.5
C37-C47-H4C7	109.5
H4A7-C47-H4C7	109.5
H4B7-C47-H4C7	109.5
N17-C57-C67	113.1(7)

N17-C57-H5A7	109.0
C67-C57-H5A7	109.0
N17-C57-H5B7	109.0
C67-C57-H5B7	109.0
H5A7-C57-H5B7	107.8
C57-C67-H6A7	109.5
C57-C67-H6B7	109.5
H6A7-C67-H6B7	109.5
C57-C67-H6C7	109.5
H6A7-C67-H6C7	109.5
H6B7-C67-H6C7	109.5
N17-C77-C87	115.3(8)
N17-C77-H7A7	108.4
C87-C77-H7A7	108.4
N17-C77-H7B7	108.4
C87-C77-H7B7	108.4
H7A7-C77-H7B7	107.5
C77-C87-H8A7	109.5
C77-C87-H8B7	109.5
H8A7-C87-H8B7	109.5
C77-C87-H8C7	109.5
H8A7-C87-H8C7	109.5
H8B7-C87-H8C7	109.5
C3A8-N1A8-C7A8	111(2)
C3A8-N1A8-C5A8	112(2)
C7A8-N1A8-C5A8	106(3)
C3A8-N1A8-C1A8	109(3)
C7A8-N1A8-C1A8	108(2)
C5A8-N1A8-C1A8	110(2)
N1A8-C1A8-C2A8	110(3)
N1A8-C1A8-H1C8	109.7
C2A8-C1A8-H1C8	109.7
N1A8-C1A8-H1D8	109.7
C2A8-C1A8-H1D8	109.7
H1C8-C1A8-H1D8	108.2
C1A8-C2A8-H2D8	109.5

C1A8-C2A8-H2E8	109.5
H2D8-C2A8-H2E8	109.5
C1A8-C2A8-H2F8	109.5
H2D8-C2A8-H2F8	109.5
H2E8-C2A8-H2F8	109.5
N1A8-C3A8-C4A8	113(3)
N1A8-C3A8-H3C8	109.0
C4A8-C3A8-H3C8	109.0
N1A8-C3A8-H3D8	109.0
C4A8-C3A8-H3D8	109.0
H3C8-C3A8-H3D8	107.8
C3A8-C4A8-H4D8	109.5
C3A8-C4A8-H4E8	109.5
H4D8-C4A8-H4E8	109.5
C3A8-C4A8-H4F8	109.5
H4D8-C4A8-H4F8	109.5
H4E8-C4A8-H4F8	109.5
N1A8-C5A8-C6A8	118(3)
N1A8-C5A8-H5C8	107.8
C6A8-C5A8-H5C8	107.8
N1A8-C5A8-H5D8	107.8
C6A8-C5A8-H5D8	107.8
H5C8-C5A8-H5D8	107.1
C5A8-C6A8-H6D8	109.5
C5A8-C6A8-H6E8	109.5
H6D8-C6A8-H6E8	109.5
C5A8-C6A8-H6F8	109.5
H6D8-C6A8-H6F8	109.5
H6E8-C6A8-H6F8	109.5
C8A8-C7A8-N1A8	118(3)
C8A8-C7A8-H7C8	107.7
N1A8-C7A8-H7C8	107.7
C8A8-C7A8-H7D8	107.7
N1A8-C7A8-H7D8	107.7
H7C8-C7A8-H7D8	107.1
C7A8-C8A8-H8D8	109.5

C7A8-C8A8-H8E8	109.5
H8D8-C8A8-H8E8	109.5
C7A8-C8A8-H8F8	109.5
H8D8-C8A8-H8F8	109.5
H8E8-C8A8-H8F8	109.5
C19-N19-C39	110.6(4)
C19-N19-C59	110.2(4)
C39-N19-C59	107.6(4)
C19-N19-C79	107.5(4)
C39-N19-C79	109.3(4)
C59-N19-C79	111.6(4)
N19-C19-C29	115.1(5)
N19-C19-H1A9	108.5
C29-C19-H1A9	108.5
N19-C19-H1B9	108.5
C29-C19-H1B9	108.5
H1A9-C19-H1B9	107.5
C19-C29-H2A9	109.5
C19-C29-H2B9	109.5
H2A9-C29-H2B9	109.5
C19-C29-H2C9	109.5
H2A9-C29-H2C9	109.5
H2B9-C29-H2C9	109.5
N19-C39-C49	115.0(5)
N19-C39-H3A9	108.5
C49-C39-H3A9	108.5
N19-C39-H3B9	108.5
C49-C39-H3B9	108.5
H3A9-C39-H3B9	107.5
C39-C49-H4A9	109.5
C39-C49-H4B9	109.5
H4A9-C49-H4B9	109.5
C39-C49-H4C9	109.5
H4A9-C49-H4C9	109.5
H4B9-C49-H4C9	109.5
C69-C59-N19	115.2(5)

C69-C59-H5A9	108.5
N19-C59-H5A9	108.5
C69-C59-H5B9	108.5
N19-C59-H5B9	108.5
H5A9-C59-H5B9	107.5
C59-C69-H6A9	109.5
C59-C69-H6B9	109.5
H6A9-C69-H6B9	109.5
C59-C69-H6C9	109.5
H6A9-C69-H6C9	109.5
H6B9-C69-H6C9	109.5
C89-C79-N19	115.6(4)
C89-C79-H7A9	108.4
N19-C79-H7A9	108.4
C89-C79-H7B9	108.4
N19-C79-H7B9	108.4
H7A9-C79-H7B9	107.4
C79-C89-H8A9	109.5
C79-C89-H8B9	109.5
H8A9-C89-H8B9	109.5
C79-C89-H8C9	109.5
H8A9-C89-H8C9	109.5
H8B9-C89-H8C9	109.5
C310-N110-C510	111.9(4)
C310-N110-C110	112.0(4)
C510-N110-C110	106.6(4)
C310-N110-C710	105.6(4)
C510-N110-C710	110.0(4)
C110-N110-C710	110.8(4)
N110-C110-C210	114.9(5)
N110-C110-H1A10	108.5
C210-C110-H1A10	108.5
N110-C110-H1B10	108.5
C210-C110-H1B10	108.5
H1A10-C110-H1B10	107.5
C110-C210-H2A10	109.5

C110-C210-H2B10	109.5
H2A10-C210-H2B10	109.5
C110-C210-H2C10	109.5
H2A10-C210-H2C10	109.5
H2B10-C210-H2C10	109.5
N110-C310-C410	114.6(5)
N110-C310-H3A10	108.6
C410-C310-H3A10	108.6
N110-C310-H3B10	108.6
C410-C310-H3B10	108.6
H3A10-C310-H3B10	107.6
C310-C410-H4A10	109.5
C310-C410-H4B10	109.5
H4A10-C410-H4B10	109.5
C310-C410-H4C10	109.5
H4A10-C410-H4C10	109.5
H4B10-C410-H4C10	109.5
N110-C510-C610	114.3(5)
N110-C510-H5A10	108.7
C610-C510-H5A10	108.7
N110-C510-H5B10	108.7
C610-C510-H5B10	108.7
H5A10-C510-H5B10	107.6
C510-C610-H6A10	109.5
C510-C610-H6B10	109.5
H6A10-C610-H6B10	109.5
C510-C610-H6C10	109.5
H6A10-C610-H6C10	109.5
H6B10-C610-H6C10	109.5
C810-C710-N110	114.2(5)
C810-C710-H7A10	108.7
N110-C710-H7A10	108.7
C810-C710-H7B10	108.7
N110-C710-H7B10	108.7
H7A10-C710-H7B10	107.6
C710-C810-H8A10	109.5

C710-C810-H8B10	109.5
H8A10-C810-H8B10	109.5
C710-C810-H8C10	109.5
H8A10-C810-H8C10	109.5
H8B10-C810-H8C10	109.5
C711-N111-C511	111.5(4)
C711-N111-C111	107.7(4)
C511-N111-C111	109.6(4)
C711-N111-C311	109.0(4)
C511-N111-C311	107.6(4)
C111-N111-C311	111.5(4)
N111-C111-C211	115.5(4)
N111-C111-H1A11	108.4
C211-C111-H1A11	108.4
N111-C111-H1B11	108.4
C211-C111-H1B11	108.4
H1A11-C111-H1B11	107.5
C111-C211-H2A11	109.5
C111-C211-H2B11	109.5
H2A11-C211-H2B11	109.5
C111-C211-H2C11	109.5
H2A11-C211-H2C11	109.5
H2B11-C211-H2C11	109.5
C411-C311-N111	115.2(4)
C411-C311-H3A11	108.5
N111-C311-H3A11	108.5
C411-C311-H3B11	108.5
N111-C311-H3B11	108.5
H3A11-C311-H3B11	107.5
C311-C411-H4A11	109.5
C311-C411-H4B11	109.5
H4A11-C411-H4B11	109.5
C311-C411-H4C11	109.5
H4A11-C411-H4C11	109.5
H4B11-C411-H4C11	109.5
C611-C511-N111	114.6(4)

C611-C511-H5A11	108.6
N111-C511-H5A11	108.6
C611-C511-H5B11	108.6
N111-C511-H5B11	108.6
H5A11-C511-H5B11	107.6
C511-C611-H6A11	109.5
C511-C611-H6B11	109.5
H6A11-C611-H6B11	109.5
C511-C611-H6C11	109.5
H6A11-C611-H6C11	109.5
H6B11-C611-H6C11	109.5
N111-C711-C811	115.1(5)
N111-C711-H7A11	108.5
C811-C711-H7A11	108.5
N111-C711-H7B11	108.5
C811-C711-H7B11	108.5
H7A11-C711-H7B11	107.5
C711-C811-H8A11	109.5
C711-C811-H8B11	109.5
H8A11-C811-H8B11	109.5
C711-C811-H8C11	109.5
H8A11-C811-H8C11	109.5
H8B11-C811-H8C11	109.5
C512-N112-C112	111.8(12)
C512-N112-C712	109.9(12)
C112-N112-C712	108.6(10)
C512-N112-C312	106.7(10)
C112-N112-C312	109.4(12)
C712-N112-C312	110.4(12)
C212-C112-N112	117.3(14)
C212-C112-H1A12	108.0
N112-C112-H1A12	108.0
C212-C112-H1B12	108.0
N112-C112-H1B12	108.0
H1A12-C112-H1B12	107.2
C112-C212-H2A12	109.5

C112-C212-H2B12	109.5
H2A12-C212-H2B12	109.5
C112-C212-H2C12	109.5
H2A12-C212-H2C12	109.5
H2B12-C212-H2C12	109.5
N112-C312-C412	114.7(11)
N112-C312-H3A12	108.6
C412-C312-H3A12	108.6
N112-C312-H3B12	108.6
C412-C312-H3B12	108.6
H3A12-C312-H3B12	107.6
C312-C412-H4A12	109.5
C312-C412-H4B12	109.5
H4A12-C412-H4B12	109.5
C312-C412-H4C12	109.5
H4A12-C412-H4C12	109.5
H4B12-C412-H4C12	109.5
N112-C512-C612	115.5(11)
N112-C512-H5A12	108.4
C612-C512-H5A12	108.4
N112-C512-H5B12	108.4
C612-C512-H5B12	108.4
H5A12-C512-H5B12	107.5
C512-C612-H6A12	109.5
C512-C612-H6B12	109.5
H6A12-C612-H6B12	109.5
C512-C612-H6C12	109.5
H6A12-C612-H6C12	109.5
H6B12-C612-H6C12	109.5
C812-C712-N112	116.1(11)
C812-C712-H7A12	108.3
N112-C712-H7A12	108.3
C812-C712-H7B12	108.3
N112-C712-H7B12	108.3
H7A12-C712-H7B12	107.4
C712-C812-H8A12	109.5

C712-C812-H8B12	109.5
H8A12-C812-H8B12	109.5
C712-C812-H8C12	109.5
H8A12-C812-H8C12	109.5
H8B12-C812-H8C12	109.5
C5A13-N1A13-C7A13	111.7(14)
C5A13-N1A13-C3A13	107.6(12)
C7A13-N1A13-C3A13	111.6(14)
C5A13-N1A13-C1A13	109.8(14)
C7A13-N1A13-C1A13	106.4(12)
C3A13-N1A13-C1A13	109.7(14)
C2A13-C1A13-N1A13	116.9(13)
C2A13-C1A13-H1C13	108.1
N1A13-C1A13-H1C13	108.1
C2A13-C1A13-H1D13	108.1
N1A13-C1A13-H1D13	108.1
H1C13-C1A13-H1D13	107.3
C1A13-C2A13-H2D13	109.5
C1A13-C2A13-H2E13	109.5
H2D13-C2A13-H2E13	109.5
C1A13-C2A13-H2F13	109.5
H2D13-C2A13-H2F13	109.5
H2E13-C2A13-H2F13	109.5
C4A13-C3A13-N1A13	117.5(17)
C4A13-C3A13-H3C13	107.9
N1A13-C3A13-H3C13	107.9
C4A13-C3A13-H3D13	107.9
N1A13-C3A13-H3D13	107.9
H3C13-C3A13-H3D13	107.2
C3A13-C4A13-H4D13	109.5
C3A13-C4A13-H4E13	109.5
H4D13-C4A13-H4E13	109.5
C3A13-C4A13-H4F13	109.5
H4D13-C4A13-H4F13	109.5
H4E13-C4A13-H4F13	109.5
N1A13-C5A13-C6A13	115.1(13)

N1A13-C5A13-H5C13	108.5
C6A13-C5A13-H5C13	108.5
N1A13-C5A13-H5D13	108.5
C6A13-C5A13-H5D13	108.5
H5C13-C5A13-H5D13	107.5
C5A13-C6A13-H6D13	109.5
C5A13-C6A13-H6E13	109.5
H6D13-C6A13-H6E13	109.5
C5A13-C6A13-H6F13	109.5
H6D13-C6A13-H6F13	109.5
H6E13-C6A13-H6F13	109.5
C8A13-C7A13-N1A13	117.7(14)
C8A13-C7A13-H7C13	107.9
N1A13-C7A13-H7C13	107.9
C8A13-C7A13-H7D13	107.9
N1A13-C7A13-H7D13	107.9
H7C13-C7A13-H7D13	107.2
C7A13-C8A13-H8D13	109.5
C7A13-C8A13-H8E13	109.5
H8D13-C8A13-H8E13	109.5
C7A13-C8A13-H8F13	109.5
H8D13-C8A13-H8F13	109.5
H8E13-C8A13-H8F13	109.5
C314-N114-C714	110.7(15)
C314-N114-C114	114.3(14)
C714-N114-C114	106.4(12)
C314-N114-C514	105.9(13)
C714-N114-C514	108.5(14)
C114-N114-C514	110.9(15)
C214-C114-N114	114.8(14)
C214-C114-H1A14	108.6
N114-C114-H1A14	108.6
C214-C114-H1B14	108.6
N114-C114-H1B14	108.6
H1A14-C114-H1B14	107.5
C114-C214-H2A14	109.5

C114-C214-H2B14	109.5
H2A14-C214-H2B14	109.5
C114-C214-H2C14	109.5
H2A14-C214-H2C14	109.5
H2B14-C214-H2C14	109.5
C414-C314-N114	116.0(18)
C414-C314-H3A14	108.3
N114-C314-H3A14	108.3
C414-C314-H3B14	108.3
N114-C314-H3B14	108.3
H3A14-C314-H3B14	107.4
C314-C414-H4A14	109.5
C314-C414-H4B14	109.5
H4A14-C414-H4B14	109.5
C314-C414-H4C14	109.5
H4A14-C414-H4C14	109.5
H4B14-C414-H4C14	109.5
N114-C514-C614	115.1(16)
N114-C514-H5A14	108.5
C614-C514-H5A14	108.5
N114-C514-H5B14	108.5
C614-C514-H5B14	108.5
H5A14-C514-H5B14	107.5
C514-C614-H6A14	109.5
C514-C614-H6B14	109.5
H6A14-C614-H6B14	109.5
C514-C614-H6C14	109.5
H6A14-C614-H6C14	109.5
H6B14-C614-H6C14	109.5
N114-C714-C814	115.1(13)
N114-C714-H7A14	108.5
C814-C714-H7A14	108.5
N114-C714-H7B14	108.5
C814-C714-H7B14	108.5
H7A14-C714-H7B14	107.5
C714-C814-H8A14	109.5

C714-C814-H8B14	109.5
H8A14-C814-H8B14	109.5
C714-C814-H8C14	109.5
H8A14-C814-H8C14	109.5
H8B14-C814-H8C14	109.5
C7A15-N1A15-C5A15	112.9(16)
C7A15-N1A15-C3A15	111.8(16)
C5A15-N1A15-C3A15	107.4(15)
C7A15-N1A15-C1A15	106.1(14)
C5A15-N1A15-C1A15	109.9(16)
C3A15-N1A15-C1A15	108.8(16)
C2A15-C1A15-N1A15	117.2(16)
C2A15-C1A15-H1C15	108.0
N1A15-C1A15-H1C15	108.0
C2A15-C1A15-H1D15	108.0
N1A15-C1A15-H1D15	108.0
H1C15-C1A15-H1D15	107.2
C1A15-C2A15-H2D15	109.5
C1A15-C2A15-H2E15	109.5
H2D15-C2A15-H2E15	109.5
C1A15-C2A15-H2F15	109.5
H2D15-C2A15-H2F15	109.5
H2E15-C2A15-H2F15	109.5
C4A15-C3A15-N1A15	115.9(19)
C4A15-C3A15-H3C15	108.3
N1A15-C3A15-H3C15	108.3
C4A15-C3A15-H3D15	108.3
N1A15-C3A15-H3D15	108.3
H3C15-C3A15-H3D15	107.4
C3A15-C4A15-H4D15	109.5
C3A15-C4A15-H4E15	109.5
H4D15-C4A15-H4E15	109.5
C3A15-C4A15-H4F15	109.5
H4D15-C4A15-H4F15	109.5
H4E15-C4A15-H4F15	109.5
N1A15-C5A15-C6A15	116.4(19)

N1A15-C5A15-H5C15	108.2
C6A15-C5A15-H5C15	108.2
N1A15-C5A15-H5D15	108.2
C6A15-C5A15-H5D15	108.2
H5C15-C5A15-H5D15	107.4
C5A15-C6A15-H6D15	109.5
C5A15-C6A15-H6E15	109.5
H6D15-C6A15-H6E15	109.5
C5A15-C6A15-H6F15	109.5
H6D15-C6A15-H6F15	109.5
H6E15-C6A15-H6F15	109.5
N1A15-C7A15-C8A15	113.1(15)
N1A15-C7A15-H7C15	109.0
C8A15-C7A15-H7C15	109.0
N1A15-C7A15-H7D15	109.0
C8A15-C7A15-H7D15	109.0
H7C15-C7A15-H7D15	107.8
C7A15-C8A15-H8D15	109.5
C7A15-C8A15-H8E15	109.5
H8D15-C8A15-H8E15	109.5
C7A15-C8A15-H8F15	109.5
H8D15-C8A15-H8F15	109.5
H8E15-C8A15-H8F15	109.5
H(1E)-O(1)-H(1F)	104(7)
H(2G)-O(2)-H(2H)	90(7)
H(3E)-O(3)-H(3F)	104(8)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4536ds. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^*2U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
I11	15(1)	21(1)	24(1)	-2(1)	1(1)	0(1)
Cl11	19(1)	34(1)	38(1)	0(1)	2(1)	-3(1)
O11	32(2)	30(2)	36(2)	13(2)	0(2)	3(2)
O21	20(2)	22(2)	28(2)	-1(2)	5(1)	-2(2)
O31	23(2)	28(2)	36(2)	1(2)	-1(2)	4(2)
N11	18(2)	19(2)	25(2)	0(2)	7(2)	-1(2)
C11	19(3)	15(2)	22(3)	-6(2)	4(2)	0(2)
C21	21(3)	22(3)	22(3)	-6(2)	3(2)	0(2)
C31	26(3)	20(3)	24(3)	-1(2)	1(2)	2(2)
C41	30(3)	22(3)	20(3)	1(2)	3(2)	-2(2)
C51	22(3)	27(3)	24(3)	-2(2)	2(2)	-4(2)
C61	24(3)	20(3)	17(3)	-3(2)	0(2)	-2(2)
C71	17(2)	28(3)	22(3)	-4(2)	1(2)	-1(2)
C81	17(2)	16(2)	24(3)	-5(2)	-3(2)	4(2)
C91	17(2)	18(3)	20(3)	-4(2)	2(2)	-1(2)
C101	18(3)	20(3)	24(3)	-6(2)	4(2)	1(2)
C111	23(2)	19(3)	19(2)	-3(2)	0(2)	0(2)
C121	23(3)	19(3)	21(3)	1(2)	8(2)	1(2)
C131	22(3)	30(3)	22(3)	-1(2)	2(2)	4(2)
C141	21(3)	18(3)	26(3)	-1(2)	5(2)	-2(2)
C151	27(3)	26(3)	27(3)	-4(2)	6(2)	-1(2)
C161	29(3)	23(3)	38(3)	-3(2)	10(3)	-3(2)
I12	14(1)	18(1)	24(1)	2(1)	3(1)	0(1)
Cl12	18(1)	27(1)	36(1)	8(1)	6(1)	-1(1)
O12	27(2)	31(2)	30(2)	13(2)	0(2)	2(2)
O22	18(2)	22(2)	26(2)	1(2)	6(1)	-1(2)
O32	18(2)	27(2)	36(2)	8(2)	3(2)	1(2)
N12	15(2)	19(2)	25(2)	2(2)	6(2)	1(2)
C12	14(2)	16(2)	26(3)	-2(2)	4(2)	-1(2)
C22	19(3)	19(3)	27(3)	-2(2)	6(2)	1(2)
C32	18(2)	23(3)	26(3)	1(2)	0(2)	3(2)

C42	23(3)	22(3)	26(3)	6(2)	3(2)	0(2)
C52	18(3)	26(3)	25(3)	3(2)	5(2)	-2(2)
C62	19(3)	19(3)	20(3)	-1(2)	2(2)	0(2)
C72	17(2)	24(3)	22(3)	0(2)	2(2)	-1(2)
C82	13(2)	13(2)	24(3)	2(2)	1(2)	5(2)
C92	16(2)	18(3)	21(3)	-3(2)	2(2)	-1(2)
C102	14(2)	21(3)	22(3)	-1(2)	2(2)	0(2)
C112	17(2)	18(3)	16(2)	-3(2)	-2(2)	2(2)
C122	17(2)	21(3)	18(3)	4(2)	1(2)	-2(2)
C132	20(3)	24(3)	23(3)	1(2)	3(2)	-1(2)
C142	19(3)	18(3)	22(3)	1(2)	1(2)	0(2)
C152	35(3)	22(3)	26(3)	-2(2)	4(2)	0(2)
C162	27(3)	21(3)	40(4)	2(2)	5(3)	-5(2)
I13	15(1)	18(1)	20(1)	-1(1)	1(1)	1(1)
Cl13	16(1)	32(1)	29(1)	5(1)	2(1)	-2(1)
O13	41(3)	30(2)	33(2)	9(2)	3(2)	6(2)
O23	17(2)	22(2)	27(2)	-2(2)	4(1)	-2(2)
O33	25(2)	25(2)	35(2)	3(2)	1(2)	6(2)
N13	16(2)	16(2)	21(2)	0(2)	6(2)	-2(2)
C13	19(2)	16(2)	15(2)	-2(2)	0(2)	1(2)
C23	19(3)	19(3)	21(3)	-4(2)	2(2)	2(2)
C33	25(3)	21(3)	19(3)	-4(2)	-1(2)	6(2)
C43	30(3)	19(3)	19(3)	0(2)	0(2)	0(2)
C53	20(3)	23(3)	20(3)	-2(2)	2(2)	-5(2)
C63	19(3)	16(2)	18(3)	-1(2)	0(2)	-1(2)
C73	16(2)	17(2)	20(3)	-2(2)	1(2)	0(2)
C83	16(2)	15(2)	18(2)	-3(2)	0(2)	2(2)
C93	18(2)	18(2)	13(2)	-4(2)	1(2)	-1(2)
C103	17(2)	18(2)	19(3)	-3(2)	1(2)	-1(2)
C113	20(2)	17(3)	19(2)	-6(2)	2(2)	0(2)
C123	22(3)	20(3)	19(3)	-1(2)	7(2)	1(2)
C133	27(3)	23(3)	24(3)	-1(2)	2(2)	6(2)
C143	21(3)	23(3)	26(3)	-2(2)	4(2)	-2(2)
C153	34(3)	27(3)	22(3)	-3(2)	7(2)	-2(2)
C163	41(4)	29(3)	34(3)	1(3)	16(3)	-4(3)
I14	16(1)	16(1)	22(1)	0(1)	2(1)	1(1)

Cl14	16(1)	24(1)	28(1)	0(1)	3(1)	-2(1)
O14	34(2)	27(2)	31(2)	9(2)	2(2)	0(2)
O24	20(2)	19(2)	28(2)	-1(2)	7(1)	-1(2)
O34	24(2)	29(2)	40(2)	8(2)	5(2)	3(2)
N14	21(2)	17(2)	26(2)	1(2)	7(2)	-1(2)
C14	17(2)	17(2)	23(3)	-4(2)	2(2)	0(2)
C24	19(3)	22(3)	23(3)	-4(2)	2(2)	1(2)
C34	21(3)	22(3)	28(3)	-1(2)	-3(2)	4(2)
C44	23(3)	19(2)	24(3)	2(2)	1(2)	3(2)
C54	18(2)	19(3)	21(3)	-1(2)	1(2)	-3(2)
C64	15(2)	18(2)	20(3)	-2(2)	1(2)	-1(2)
C74	15(2)	18(2)	20(3)	-4(2)	4(2)	-2(2)
C84	14(2)	15(2)	18(2)	-2(2)	-3(2)	2(2)
C94	17(2)	16(2)	22(3)	-3(2)	3(2)	-2(2)
C104	17(2)	17(2)	24(3)	-4(2)	4(2)	-1(2)
C114	21(2)	18(3)	18(2)	-3(2)	8(2)	0(2)
C124	24(3)	18(3)	21(3)	1(2)	5(2)	0(2)
C134	27(3)	22(3)	26(3)	-2(2)	2(2)	2(2)
C144	25(3)	17(3)	24(3)	0(2)	4(2)	3(2)
C154	25(3)	20(3)	40(3)	0(2)	7(3)	-1(2)
C164	32(3)	23(3)	28(3)	-4(2)	5(2)	-3(2)
I15	14(1)	19(1)	22(1)	-1(1)	1(1)	1(1)
Cl15	16(1)	28(1)	39(1)	-2(1)	3(1)	-2(1)
O15	39(2)	27(2)	27(2)	7(2)	5(2)	6(2)
O25	18(2)	22(2)	25(2)	-1(2)	4(1)	-1(2)
O35	24(2)	31(2)	35(2)	4(2)	3(2)	5(2)
N15	16(2)	18(2)	24(2)	2(2)	6(2)	0(2)
C15	20(3)	15(2)	17(2)	-2(2)	-1(2)	-1(2)
C25	19(3)	22(3)	20(3)	0(2)	1(2)	5(2)
C35	25(3)	24(3)	22(3)	1(2)	0(2)	3(2)
C45	29(3)	19(3)	21(3)	3(2)	1(2)	1(2)
C55	20(3)	23(3)	26(3)	-1(2)	4(2)	-3(2)
C65	19(3)	17(2)	18(3)	-4(2)	1(2)	0(2)
C75	16(2)	20(3)	18(3)	-2(2)	2(2)	-1(2)
C85	15(2)	18(2)	18(3)	-2(2)	-1(2)	1(2)
C95	16(2)	18(2)	18(2)	-4(2)	2(2)	1(2)

C105	16(2)	16(2)	20(3)	-5(2)	2(2)	1(2)
C115	17(2)	19(3)	19(2)	-3(2)	1(2)	1(2)
C125	25(3)	19(3)	23(3)	2(2)	6(2)	0(2)
C135	28(3)	23(3)	23(3)	0(2)	3(2)	7(2)
C145	24(3)	19(3)	28(3)	0(2)	5(2)	-1(2)
C155	33(3)	21(3)	38(3)	0(2)	11(3)	-7(2)
C165	33(3)	24(3)	24(3)	-3(2)	6(2)	-2(2)
I16	16(1)	17(1)	22(1)	0(1)	0(1)	3(1)
CI16	16(1)	25(1)	36(1)	0(1)	1(1)	1(1)
O16	57(3)	24(2)	34(2)	12(2)	9(2)	14(2)
O26	19(2)	19(2)	28(2)	-3(2)	7(1)	-3(2)
O36	27(2)	24(2)	40(2)	6(2)	-2(2)	4(2)
N16	18(2)	13(2)	25(2)	1(2)	5(2)	1(2)
C16	19(2)	16(2)	18(2)	-4(2)	1(2)	-3(2)
C26	18(2)	18(2)	23(3)	-4(2)	1(2)	1(2)
C36	22(2)	20(3)	21(2)	0(2)	-3(2)	4(2)
C46	25(2)	16(3)	20(2)	3(2)	-1(2)	-1(2)
C56	19(3)	19(3)	21(3)	2(2)	2(2)	-2(2)
C66	19(2)	17(2)	16(2)	-2(2)	-2(2)	-1(2)
C76	15(2)	20(3)	20(3)	-4(2)	3(2)	-1(2)
C86	14(2)	14(2)	21(3)	-5(2)	0(2)	4(2)
C96	15(2)	16(2)	20(3)	1(2)	1(2)	1(2)
C106	15(2)	19(3)	21(3)	-3(2)	4(2)	-2(2)
C116	19(2)	17(3)	17(2)	-3(2)	2(2)	0(2)
C126	29(3)	15(3)	25(3)	3(2)	8(2)	2(2)
C136	36(3)	22(3)	22(3)	-5(2)	4(2)	6(2)
C146	27(3)	17(3)	30(3)	-3(2)	8(2)	2(2)
C156	49(4)	21(3)	34(3)	-5(2)	15(3)	-7(3)
C166	37(3)	21(3)	24(3)	0(2)	4(2)	2(2)
N17	31(3)	34(3)	28(3)	2(3)	3(2)	5(3)
C17	42(4)	33(4)	30(4)	-3(3)	3(3)	-2(3)
C27	61(9)	44(6)	31(6)	-10(5)	7(5)	-9(6)
C37	35(4)	35(4)	39(4)	4(3)	-5(3)	2(3)
C47	42(5)	25(4)	58(6)	3(4)	-4(5)	10(4)
C57	36(4)	33(4)	34(4)	-3(3)	1(3)	11(3)
C67	27(4)	28(5)	60(7)	2(4)	0(4)	3(4)

C77	34(4)	34(4)	36(4)	0(3)	10(3)	-4(3)
C87	29(5)	52(8)	55(9)	1(7)	2(4)	-6(4)
N1A8	34(5)	35(5)	34(5)	1(5)	2(5)	5(5)
C1A8	40(6)	38(6)	40(6)	4(6)	4(6)	3(6)
C2A8	48(16)	45(14)	43(16)	20(13)	9(14)	0(14)
C3A8	37(6)	39(6)	38(6)	0(6)	4(6)	7(6)
C4A8	47(14)	46(15)	63(15)	-9(14)	-2(15)	9(14)
C5A8	35(6)	34(6)	35(6)	0(6)	2(6)	4(6)
C6A8	44(14)	48(16)	65(16)	-2(14)	-2(13)	23(13)
C7A8	33(6)	38(6)	35(6)	2(6)	-4(6)	3(6)
C8A8	24(13)	48(15)	39(16)	16(14)	8(12)	-9(12)
N19	18(2)	22(2)	24(2)	3(2)	2(2)	3(2)
C19	36(3)	29(3)	22(3)	4(2)	3(2)	0(2)
C29	39(3)	54(5)	30(3)	5(3)	-8(3)	9(3)
C39	23(3)	28(3)	31(3)	1(2)	4(2)	-3(2)
C49	28(3)	26(3)	43(4)	-7(3)	3(3)	-5(2)
C59	21(3)	25(3)	34(3)	0(2)	3(2)	3(2)
C69	22(3)	29(3)	47(4)	-4(3)	2(3)	-1(2)
C79	20(2)	21(3)	30(3)	-3(2)	4(2)	1(2)
C89	31(3)	38(3)	27(3)	-4(3)	0(2)	3(3)
N110	25(2)	17(2)	20(2)	2(2)	3(2)	0(2)
C110	35(3)	21(3)	42(4)	0(3)	3(3)	-2(2)
C210	38(3)	25(3)	33(3)	-10(2)	3(3)	-3(3)
C310	34(3)	30(3)	34(3)	0(3)	-1(2)	6(3)
C410	34(4)	60(5)	52(4)	-2(3)	3(3)	14(3)
C510	39(4)	32(3)	27(3)	7(3)	1(3)	1(3)
C610	48(3)	34(4)	28(3)	-12(3)	7(2)	-5(3)
C710	32(3)	34(3)	41(4)	-5(3)	9(3)	-11(3)
C810	26(3)	53(5)	86(6)	-30(4)	-2(4)	7(3)
N111	19(2)	16(2)	20(2)	1(2)	4(2)	-1(2)
C111	21(2)	21(3)	24(2)	0(2)	-2(2)	-3(2)
C211	34(3)	26(3)	24(2)	1(3)	0(2)	0(3)
C311	22(3)	25(3)	27(3)	1(2)	0(2)	-3(2)
C411	25(3)	30(3)	36(3)	3(2)	2(2)	6(2)
C511	30(3)	17(3)	30(3)	-4(2)	8(2)	3(2)
C611	29(3)	21(3)	40(3)	-1(2)	13(3)	1(2)

C711	25(3)	21(3)	20(3)	1(2)	0(2)	0(2)
C811	25(3)	46(4)	30(3)	5(3)	-2(2)	3(3)
N112	27(4)	28(4)	27(4)	6(4)	1(4)	1(4)
C112	38(5)	33(5)	31(5)	-3(4)	8(4)	-1(4)
C212	45(10)	27(9)	40(8)	-10(7)	10(8)	15(7)
C312	32(4)	33(4)	37(5)	-2(4)	6(4)	1(4)
C412	24(6)	34(9)	51(12)	3(9)	-7(7)	-3(5)
C512	27(4)	27(4)	35(5)	2(4)	0(4)	5(4)
C612	28(6)	36(8)	52(11)	4(9)	7(8)	5(5)
C712	30(4)	33(5)	35(5)	1(4)	-5(4)	2(4)
C812	35(7)	33(8)	51(11)	0(7)	-2(9)	9(7)
N1A13	28(4)	27(4)	29(4)	5(4)	2(4)	2(4)
C1A13	33(5)	29(5)	33(5)	3(4)	4(4)	-3(4)
C2A13	31(8)	45(9)	40(11)	6(10)	9(8)	-7(7)
C3A13	34(5)	26(5)	43(5)	7(4)	5(4)	3(4)
C4A13	52(13)	27(11)	75(12)	-3(10)	9(11)	5(10)
C5A13	30(5)	40(5)	31(5)	-1(4)	5(4)	1(4)
C6A13	26(8)	55(12)	38(10)	-16(9)	9(9)	3(9)
C7A13	31(5)	37(5)	37(5)	3(4)	-5(4)	3(4)
C8A13	39(9)	53(12)	44(13)	11(10)	-4(8)	0(8)
N114	24(4)	19(4)	27(4)	7(4)	0(4)	-5(4)
C114	38(5)	24(6)	39(7)	3(6)	5(6)	-2(5)
C214	55(9)	33(8)	60(13)	-17(10)	4(11)	-11(7)
C314	17(6)	31(6)	30(5)	7(5)	4(5)	-13(5)
C414	25(8)	43(13)	33(10)	9(8)	11(7)	-10(8)
C514	15(6)	31(5)	34(6)	8(5)	5(5)	-8(5)
C614	19(7)	42(10)	43(12)	5(8)	2(7)	9(7)
C714	30(5)	22(7)	25(5)	1(6)	2(4)	-7(6)
C814	37(8)	31(10)	47(10)	-12(8)	-2(7)	11(9)
N1A15	25(4)	21(5)	26(4)	6(4)	6(4)	-4(4)
C1A15	36(6)	23(6)	35(8)	1(6)	9(7)	-4(5)
C2A15	69(11)	42(9)	55(13)	-10(10)	23(12)	0(8)
C3A15	20(7)	29(7)	27(5)	7(5)	0(5)	-2(6)
C4A15	17(8)	36(12)	40(13)	11(9)	2(8)	-9(7)
C5A15	24(7)	30(6)	35(6)	7(6)	1(6)	3(6)
C6A15	30(8)	42(11)	49(14)	9(10)	-9(9)	-4(7)

C7A15	35(6)	27(8)	31(5)	1(6)	0(5)	-2(7)
C8A15	36(8)	37(11)	44(9)	-10(9)	-4(7)	6(10)
O(1)	36(3)	38(3)	42(3)	5(2)	5(2)	11(2)
O(2)	24(2)	35(3)	37(3)	2(2)	-2(2)	6(2)
O(3)	41(3)	35(3)	41(3)	-12(2)	15(2)	-14(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4536ds.

	x	y	z	U(eq)
H21	1162	9274	8990	26
H31	1423	10699	8482	28
H41	2380	10768	8183	29
H51	3067	9401	8395	29
H71	3343	7649	8842	27
H101	1423	7485	9420	25
H121	2138	3910	10205	25
H141	1774	3594	9334	26
H15A1	2279	2395	8846	40
H15B1	2798	2229	9280	40
H15C1	2717	3392	9004	40
H16A1	1572	1714	9452	45
H16B1	1468	2411	9943	45
H16C1	2057	1682	9918	45
H22	2850	9241	7333	26
H32	3072	10665	6812	27
H42	3991	10721	6456	28
H52	4694	9365	6631	27
H72	5013	7628	7082	25
H102	3144	7459	7757	22
H122	3915	3923	8522	23
H142	3487	3566	7668	24
H15A2	3950	2331	7173	42
H15B2	4491	2171	7587	42
H15C2	4404	3321	7301	42
H16A2	3282	1694	7825	44
H16B2	3221	2422	8314	44
H16C2	3800	1677	8266	44
H23	5926	9105	3816	24
H33	6128	10557	3305	26

H43	7057	10685	2959	27
H53	7775	9366	3132	25
H73	8123	7645	3582	21
H103	6245	7323	4235	22
H123	7098	3842	5007	24
H143	6642	3430	4181	28
H15A3	7117	2296	3645	41
H15B3	7692	2202	4030	41
H15C3	7531	3350	3761	41
H16A3	6506	1545	4315	51
H16B3	6488	2189	4832	51
H16C3	7071	1518	4712	51
H24	4413	9069	5593	25
H34	4599	10496	5061	29
H44	5493	10574	4668	27
H54	6216	9225	4822	23
H74	6576	7524	5274	21
H104	4749	7310	6019	23
H124	5616	3807	6783	25
H144	5131	3508	5936	26
H15A4	4918	1630	6101	42
H15B4	4853	2403	6575	42
H15C4	5429	1643	6547	42
H16A4	5548	2171	5438	42
H16B4	6121	2079	5825	42
H16C4	5996	3190	5515	42
H25	-680	9190	491	25
H35	-402	10642	6	28
H45	581	10786	-227	27
H55	1283	9468	25	27
H75	1555	7724	483	22
H105	-422	7406	930	21
H125	328	3914	1786	26
H145	-7	3541	918	28
H15A5	-168	1656	1028	45
H15B5	-276	2308	1530	45

H15C5	327	1630	1487	45
H16A5	556	2351	452	40
H16B5	1079	2334	888	40
H16C5	930	3445	585	40
H26	7558	9291	2072	24
H36	7816	10748	1586	25
H46	8773	10856	1293	25
H56	9478	9527	1511	24
H76	9778	7798	1976	22
H106	7828	7502	2495	22
H126	8585	4002	3308	27
H146	8209	3607	2458	29
H15A6	8075	1722	2565	52
H15B6	8011	2340	3083	52
H15C6	8609	1687	2992	52
H16A6	8752	2516	1944	40
H16B6	9293	2425	2364	40
H16C6	9142	3580	2097	40
H1A7	4570	4960	2256	42
H1B7	3879	4651	2231	42
H2A7	4302	6687	1826	68
H2B7	4042	6611	2363	68
H2C7	3617	6385	1869	68
H3A7	4678	3163	1849	44
H3B7	3972	3039	1832	44
H4A7	3935	2662	982	63
H4B7	4373	1816	1282	63
H4C7	4640	2824	987	63
H5A7	3749	4408	870	41
H5B7	3661	5552	1149	41
H6A7	2774	4448	1141	58
H6B7	3029	4687	1702	58
H6C7	3139	3516	1453	58
H7A7	4727	5765	1280	41
H7B7	4755	4665	958	41
H8A7	5439	3889	1556	68

H8B7	5384	4932	1912	68
H8C7	5684	5063	1396	68
H1C8	3743	6027	1372	47
H1D8	4451	6173	1383	47
H2D8	4231	7096	2116	68
H2E8	4437	5917	2330	68
H2F8	3744	6204	2245	68
H3C8	4604	4505	916	46
H3D8	3896	4397	841	46
H4D8	4298	2688	680	78
H4E8	3979	2580	1189	78
H4F8	4688	2695	1203	78
H5C8	3622	4470	2125	42
H5D8	3814	3298	1925	42
H6D8	3149	3898	1157	79
H6E8	2841	4601	1569	79
H6F8	2875	3289	1615	79
H7C8	4737	4740	2220	43
H7D8	4741	3527	1995	43
H8D8	5602	3868	1741	56
H8E8	5560	5131	1903	56
H8F8	5304	4753	1358	56
H1A9	2760	4240	2544	35
H1B9	2926	5435	2760	35
H2A9	1984	5516	2345	63
H2B9	1910	5694	2926	63
H2C9	1755	4527	2673	63
H3A9	1960	3661	3385	33
H3B9	2475	3051	3721	33
H4A9	2222	2730	2678	48
H4B9	2121	1845	3104	48
H4C9	2782	2184	2986	48
H5A9	3462	3413	3667	32
H5B9	3475	3371	3074	32
H6A9	4291	4361	3374	49
H6B9	3895	5138	3697	49

H6C9	3840	5226	3102	49
H7A9	2932	5865	3594	28
H7B9	2272	5432	3650	28
H8A9	2649	4256	4310	48
H8B9	2760	5529	4438	48
H8C9	3294	4783	4268	48
H1A10	9279	3077	6513	39
H1B10	9978	2945	6468	39
H2A10	9812	3730	5631	48
H2B10	9116	3561	5687	48
H2C10	9551	2518	5695	48
H3A10	9237	5323	5980	39
H3B10	9341	6069	6467	39
H4A10	8320	5445	6290	73
H4B10	8586	5200	6848	73
H4C10	8545	4233	6443	73
H5A10	10080	3971	7220	39
H5B10	9379	4176	7210	39
H6A10	10247	5892	7277	55
H6B10	9887	5475	7731	55
H6C10	9545	6095	7269	55
H7A10	10292	4979	6007	42
H7B10	10328	5815	6467	42
H8A10	10840	3660	6520	83
H8B10	10904	4551	6959	83
H8C10	11215	4761	6452	83
H1A11	1583	5314	4379	26
H1B11	1043	6005	4571	26
H2A11	1059	6141	3697	42
H2B11	452	5579	3838	42
H2C11	975	4836	3647	42
H3A11	121	4132	4251	30
H3B11	144	3584	4792	30
H4A11	-3	5874	4589	45
H4B11	87	5391	5143	45
H4C11	-493	5073	4793	45

H5A11	1042	3298	4054	30
H5B11	1616	3344	4441	30
H6A11	565	2113	4555	44
H6B11	1061	2284	5007	44
H6C11	1221	1632	4518	44
H7A11	988	3812	5375	27
H7B11	993	5121	5323	27
H8A11	1988	3744	5175	51
H8B11	1924	4508	5653	51
H8C11	1993	5056	5119	51
H1A12	5688	4616	10511	40
H1B12	6379	4894	10515	40
H2A12	6128	6620	10160	55
H2B12	5888	6456	10699	55
H2C12	5442	6337	10210	55
H3A12	6445	5844	9556	41
H3B12	6454	4803	9194	41
H4A12	7217	3992	9686	55
H4B12	7156	4868	10123	55
H4C12	7412	5244	9611	55
H5A12	5483	4380	9168	36
H5B12	5374	5489	9465	36
H6A12	4539	4329	9466	58
H6B12	4816	4518	10025	58
H6C12	4938	3391	9742	58
H7A12	6515	3177	10064	40
H7B12	5820	2973	10096	40
H8A12	5698	2624	9253	60
H8B12	6220	1856	9495	60
H8C12	6379	2934	9190	60
H1C13	5594	3246	10169	38
H1D13	5506	4371	10461	38
H2D13	4776	4898	9848	58
H2E13	4608	3769	10110	58
H2F13	4858	3751	9568	58
H3C13	6245	6143	9682	41

H3D13	5547	5952	9576	41
H4D13	5827	7196	10253	77
H4E13	6072	6150	10566	77
H4F13	5379	6242	10391	77
H5C13	6270	4528	9142	40
H5D13	5570	4336	9153	40
H6D13	5736	2516	9426	59
H6E13	6440	2703	9444	59
H6F13	6052	2709	8920	59
H7C13	6571	4627	10466	42
H7D13	6579	3475	10182	42
H8D13	7173	4168	9612	69
H8E13	7466	4470	10155	69
H8F13	7110	5388	9826	69
H1A14	8012	6003	7886	40
H1B14	7306	5889	7798	40
H2A14	7638	7160	8450	74
H2B14	7878	6122	8773	74
H2C14	7181	6252	8621	74
H3A14	8159	4431	8792	31
H3B14	8214	3324	8479	31
H4A14	8901	4185	7993	50
H4B14	9129	4206	8571	50
H4C14	8848	5290	8310	50
H5A14	7091	4404	8633	32
H5B14	7221	3237	8390	32
H6A14	6531	4894	7861	52
H6B14	6239	3915	8157	52
H6C14	6604	3647	7684	52
H7A14	8118	4321	7456	31
H7B14	7410	4264	7372	31
H8A14	7793	2533	7224	58
H8B14	7439	2458	7717	58
H8C14	8151	2519	7761	58
H1C15	8039	6210	8060	37
H1D15	7334	6100	7981	37

H2D15	7675	7128	8706	82
H2E15	7943	6010	8944	82
H2F15	7240	6137	8823	82
H3C15	8286	4530	8795	31
H3D15	8305	3440	8466	31
H4D15	8981	4153	7984	46
H4E15	9201	4569	8531	46
H4F15	8847	5388	8148	46
H5C15	7225	4270	8717	36
H5D15	7296	3252	8352	36
H6D15	6607	4083	7753	61
H6E15	6529	5086	8128	61
H6F15	6313	3879	8268	61
H7C15	8139	4759	7488	37
H7D15	7429	4710	7416	37
H8D15	7932	3059	7143	59
H8E15	7423	2821	7512	59
H8F15	8108	2801	7719	59
H(1E)	7950(40)	2450(70)	5887(19)	58
H(1F)	7620(30)	2750(60)	6270(30)	58
H(2G)	710(30)	3070(70)	3070(30)	49
H(2H)	990(30)	2790(60)	2720(30)	49
H(3E)	760(40)	7240(70)	5750(30)	58
H(3F)	970(40)	7440(70)	5360(30)	58

Table 6. Torsion angles [°] for 4536ds.

C101-C11-C21-C31	-177.9(5)
C61-C11-C21-C31	0.1(8)
C11-C21-C31-C41	-0.2(8)
C21-C31-C41-C51	0.0(8)
C31-C41-C51-C61	0.2(8)
C41-C51-C61-C71	179.8(5)
C41-C51-C61-C11	-0.2(8)
C21-C11-C61-C51	0.1(7)
C101-C11-C61-C51	178.2(5)
C21-C11-C61-C71	-180.0(5)
C101-C11-C61-C71	-1.9(7)
C51-C61-C71-C81	-179.3(5)
C11-C61-C71-C81	0.7(8)
C61-C71-C81-C91	1.1(8)
C61-C71-C81-I11	-177.9(4)
C71-C81-C91-C101	-1.7(8)
I11-C81-C91-C101	177.4(4)
C71-C81-C91-C111	171.8(5)
I11-C81-C91-C111	-9.0(6)
C81-C91-C101-C11	0.5(8)
C111-C91-C101-C11	-172.8(5)
C21-C11-C101-C91	179.3(5)
C61-C11-C101-C91	1.3(8)
C121-N11-C111-O21	4.5(7)
I11-N11-C111-O21	-176.7(4)
C121-N11-C111-C91	-172.5(4)
I11-N11-C111-C91	6.3(5)
C101-C91-C111-O21	-1.6(8)
C81-C91-C111-O21	-174.9(5)
C101-C91-C111-N11	175.4(5)
C81-C91-C111-N11	2.1(7)
C111-N11-C121-C131	-158.9(4)
I11-N11-C121-C131	22.4(6)
C111-N11-C121-C141	77.3(6)

I11-N11-C121-C141	-101.4(4)
I11-O31-C131-O11	-178.3(5)
I11-O31-C131-C121	4.1(6)
N11-C121-C131-O11	166.6(5)
C141-C121-C131-O11	-70.4(6)
N11-C121-C131-O31	-15.6(7)
C141-C121-C131-O31	107.5(5)
N11-C121-C141-C161	-158.6(4)
C131-C121-C141-C161	77.7(6)
N11-C121-C141-C151	75.5(5)
C131-C121-C141-C151	-48.1(6)
C102-C12-C22-C32	-178.3(5)
C62-C12-C22-C32	0.5(8)
C12-C22-C32-C42	0.3(8)
C22-C32-C42-C52	-0.6(8)
C32-C42-C52-C62	0.1(8)
C42-C52-C62-C72	-179.6(5)
C42-C52-C62-C12	0.7(8)
C102-C12-C62-C72	-1.8(8)
C22-C12-C62-C72	179.3(5)
C102-C12-C62-C52	177.9(5)
C22-C12-C62-C52	-1.0(8)
C52-C62-C72-C82	-178.7(5)
C12-C62-C72-C82	1.0(8)
C62-C72-C82-C92	1.0(8)
C62-C72-C82-I12	-178.1(4)
C72-C82-C92-C102	-2.1(8)
I12-C82-C92-C102	177.1(4)
C72-C82-C92-C112	172.3(5)
I12-C82-C92-C112	-8.4(6)
C82-C92-C102-C12	1.2(8)
C112-C92-C102-C12	-173.1(5)
C22-C12-C102-C92	179.5(5)
C62-C12-C102-C92	0.7(8)
C122-N12-C112-O22	2.7(7)
I12-N12-C112-O22	-175.5(4)

C122-N12-C112-C92	-173.5(4)
I12-N12-C112-C92	8.3(5)
C102-C92-C112-O22	-1.5(8)
C82-C92-C112-O22	-175.8(5)
C102-C92-C112-N12	174.8(5)
C82-C92-C112-N12	0.5(7)
C112-N12-C122-C132	-157.9(4)
I12-N12-C122-C132	20.2(6)
C112-N12-C122-C142	78.8(6)
I12-N12-C122-C142	-103.1(4)
I12-O32-C132-O12	-177.0(4)
I12-O32-C132-C122	4.0(6)
N12-C122-C132-O12	166.7(5)
C142-C122-C132-O12	-70.7(6)
N12-C122-C132-O32	-14.2(7)
C142-C122-C132-O32	108.4(5)
N12-C122-C142-C152	76.2(5)
C132-C122-C142-C152	-47.1(6)
N12-C122-C142-C162	-158.3(4)
C132-C122-C142-C162	78.4(5)
C103-C13-C23-C33	-178.3(5)
C63-C13-C23-C33	0.3(7)
C13-C23-C33-C43	0.1(8)
C23-C33-C43-C53	-0.2(8)
C33-C43-C53-C63	-0.1(8)
C43-C53-C63-C73	-178.7(5)
C43-C53-C63-C13	0.6(8)
C103-C13-C63-C53	178.1(5)
C23-C13-C63-C53	-0.6(7)
C103-C13-C63-C73	-2.7(7)
C23-C13-C63-C73	178.6(5)
C53-C63-C73-C83	-179.0(5)
C13-C63-C73-C83	1.8(7)
C63-C73-C83-C93	0.9(7)
C63-C73-C83-I13	-178.6(4)
C73-C83-C93-C103	-2.6(7)

I13-C83-C93-C103	177.0(4)
C73-C83-C93-C113	172.7(4)
I13-C83-C93-C113	-7.7(5)
C83-C93-C103-C13	1.6(7)
C113-C93-C103-C13	-173.5(4)
C23-C13-C103-C93	179.6(5)
C63-C13-C103-C93	1.0(7)
C123-N13-C113-O23	0.5(7)
I13-N13-C113-O23	-173.6(4)
C123-N13-C113-C93	-175.8(4)
I13-N13-C113-C93	10.1(5)
C103-C93-C113-O23	-2.5(7)
C83-C93-C113-O23	-177.6(4)
C103-C93-C113-N13	173.9(4)
C83-C93-C113-N13	-1.3(6)
C113-N13-C123-C133	-156.6(4)
I13-N13-C123-C133	17.1(6)
C113-N13-C123-C143	79.3(5)
I13-N13-C123-C143	-107.0(4)
N13-C123-C133-O13	166.1(5)
C143-C123-C133-O13	-71.1(6)
N13-C123-C133-O33	-16.5(7)
C143-C123-C133-O33	106.2(5)
N13-C123-C143-C153	72.2(6)
C133-C123-C143-C153	-52.5(6)
N13-C123-C143-C163	-162.4(4)
C133-C123-C143-C163	72.9(6)
C104-C14-C24-C34	-179.1(5)
C64-C14-C24-C34	-0.2(8)
C14-C24-C34-C44	0.8(8)
C24-C34-C44-C54	-0.6(8)
C34-C44-C54-C64	-0.2(8)
C44-C54-C64-C14	0.8(8)
C44-C54-C64-C74	-178.4(5)
C104-C14-C64-C54	178.3(5)
C24-C14-C64-C54	-0.6(7)

C104-C14-C64-C74	-2.4(7)
C24-C14-C64-C74	178.6(5)
C54-C64-C74-C84	-179.5(5)
C14-C64-C74-C84	1.2(7)
C64-C74-C84-C94	1.2(7)
C64-C74-C84-I14	-178.3(4)
C74-C84-C94-C104	-2.3(8)
I14-C84-C94-C104	177.2(4)
C74-C84-C94-C114	172.1(5)
I14-C84-C94-C114	-8.4(6)
C84-C94-C104-C14	1.0(8)
C114-C94-C104-C14	-173.2(5)
C24-C14-C104-C94	-179.8(5)
C64-C14-C104-C94	1.3(8)
C124-N14-C114-O24	4.3(7)
I14-N14-C114-O24	-175.4(4)
C124-N14-C114-C94	-171.9(4)
I14-N14-C114-C94	8.4(5)
C104-C94-C114-O24	-1.7(8)
C84-C94-C114-O24	-175.9(5)
C104-C94-C114-N14	174.5(5)
C84-C94-C114-N14	0.3(7)
C114-N14-C124-C134	-160.7(4)
I14-N14-C124-C134	18.9(6)
C114-N14-C124-C144	75.3(6)
I14-N14-C124-C144	-105.1(4)
I14-O34-C134-O14	-177.5(5)
I14-O34-C134-C124	3.7(6)
N14-C124-C134-O14	167.8(5)
C144-C124-C134-O14	-69.8(6)
N14-C124-C134-O34	-13.3(7)
C144-C124-C134-O34	109.1(5)
N14-C124-C144-C154	-154.6(4)
C134-C124-C144-C154	81.2(6)
N14-C124-C144-C164	79.9(5)
C134-C124-C144-C164	-44.3(6)

C105-C15-C25-C35	-178.1(5)
C65-C15-C25-C35	0.7(8)
C15-C25-C35-C45	-0.6(8)
C25-C35-C45-C55	0.0(8)
C35-C45-C55-C65	0.4(8)
C45-C55-C65-C15	-0.3(8)
C45-C55-C65-C75	-179.8(5)
C105-C15-C65-C55	178.6(5)
C25-C15-C65-C55	-0.2(7)
C105-C15-C65-C75	-1.9(7)
C25-C15-C65-C75	179.2(5)
C55-C65-C75-C85	179.9(5)
C15-C65-C75-C85	0.5(7)
C65-C75-C85-C95	2.0(8)
C65-C75-C85-I15	-178.5(4)
C75-C85-C95-C105	-3.0(8)
I15-C85-C95-C105	177.5(4)
C75-C85-C95-C115	173.1(5)
I15-C85-C95-C115	-6.5(5)
C85-C95-C105-C15	1.4(7)
C115-C95-C105-C15	-174.5(4)
C25-C15-C105-C95	179.7(5)
C65-C15-C105-C95	1.0(7)
C125-N15-C115-O25	1.8(7)
I15-N15-C115-O25	-175.5(4)
C125-N15-C115-C95	-174.1(4)
I15-N15-C115-C95	8.6(5)
C105-C95-C115-O25	-1.2(8)
C85-C95-C115-O25	-177.1(5)
C105-C95-C115-N15	174.8(5)
C85-C95-C115-N15	-1.2(6)
C115-N15-C125-C135	-158.0(5)
I15-N15-C125-C135	19.2(6)
C115-N15-C125-C145	77.3(6)
I15-N15-C125-C145	-105.5(4)
I15-O35-C135-O15	-171.1(4)

I15-O35-C135-C125	11.3(6)
N15-C125-C135-O15	163.0(5)
C145-C125-C135-O15	-74.4(6)
N15-C125-C135-O35	-19.2(7)
C145-C125-C135-O35	103.4(6)
N15-C125-C145-C155	-161.0(4)
C135-C125-C145-C155	74.8(6)
N15-C125-C145-C165	73.9(5)
C135-C125-C145-C165	-50.3(6)
C106-C16-C26-C36	-178.4(5)
C66-C16-C26-C36	0.5(7)
C16-C26-C36-C46	0.6(8)
C26-C36-C46-C56	-1.1(8)
C36-C46-C56-C66	0.5(8)
C46-C56-C66-C16	0.6(7)
C46-C56-C66-C76	-178.7(5)
C26-C16-C66-C56	-1.1(7)
C106-C16-C66-C56	177.9(5)
C26-C16-C66-C76	178.2(5)
C106-C16-C66-C76	-2.8(7)
C56-C66-C76-C86	-179.1(5)
C16-C66-C76-C86	1.6(7)
C66-C76-C86-C96	1.1(8)
C66-C76-C86-I16	-177.1(3)
C76-C86-C96-C106	-2.5(8)
I16-C86-C96-C106	175.9(4)
C76-C86-C96-C116	172.3(5)
I16-C86-C96-C116	-9.2(6)
C86-C96-C106-C16	1.2(7)
C116-C96-C106-C16	-173.5(4)
C26-C16-C106-C96	-179.7(5)
C66-C16-C106-C96	1.4(7)
C126-N16-C116-O26	2.0(8)
I16-N16-C116-O26	-172.8(4)
C126-N16-C116-C96	-175.0(4)
I16-N16-C116-C96	10.3(5)

C106-C96-C116-O26	-2.7(8)
C86-C96-C116-O26	-177.4(5)
C106-C96-C116-N16	174.3(5)
C86-C96-C116-N16	-0.4(6)
C116-N16-C126-C136	-156.6(5)
I16-N16-C126-C136	17.8(6)
C116-N16-C126-C146	78.7(6)
I16-N16-C126-C146	-106.9(4)
N16-C126-C136-O16	165.8(5)
C146-C126-C136-O16	-71.3(6)
N16-C126-C136-O36	-16.5(7)
C146-C126-C136-O36	106.5(6)
N16-C126-C146-C156	-164.1(5)
C136-C126-C146-C156	71.3(6)
N16-C126-C146-C166	70.6(6)
C136-C126-C146-C166	-54.0(6)
C37-N17-C17-C27	-171.7(10)
C77-N17-C17-C27	67.6(12)
C57-N17-C17-C27	-50.3(12)
C77-N17-C37-C47	-64.0(10)
C57-N17-C37-C47	53.9(11)
C17-N17-C37-C47	175.4(8)
C37-N17-C57-C67	58.2(10)
C77-N17-C57-C67	178.7(7)
C17-N17-C57-C67	-60.9(10)
C37-N17-C77-C87	-52.7(12)
C57-N17-C77-C87	-173.3(10)
C17-N17-C77-C87	65.9(12)
C3A8-N1A8-C1A8-C2A8	-174(4)
C7A8-N1A8-C1A8-C2A8	-53(4)
C5A8-N1A8-C1A8-C2A8	62(4)
C7A8-N1A8-C3A8-C4A8	62(4)
C5A8-N1A8-C3A8-C4A8	-56(4)
C1A8-N1A8-C3A8-C4A8	-178(3)
C3A8-N1A8-C5A8-C6A8	-45(4)
C7A8-N1A8-C5A8-C6A8	-167(3)

C1A8-N1A8-C5A8-C6A8	76(4)
C3A8-N1A8-C7A8-C8A8	46(5)
C5A8-N1A8-C7A8-C8A8	168(4)
C1A8-N1A8-C7A8-C8A8	-74(5)
C39-N19-C19-C29	55.1(6)
C59-N19-C19-C29	174.0(5)
C79-N19-C19-C29	-64.2(6)
C19-N19-C39-C49	56.4(6)
C59-N19-C39-C49	-64.0(6)
C79-N19-C39-C49	174.6(5)
C19-N19-C59-C69	70.2(6)
C39-N19-C59-C69	-169.1(5)
C79-N19-C59-C69	-49.1(7)
C19-N19-C79-C89	-174.1(5)
C39-N19-C79-C89	65.8(6)
C59-N19-C79-C89	-53.2(6)
C310-N110-C110-C210	51.6(7)
C510-N110-C110-C210	174.3(5)
C710-N110-C110-C210	-66.0(6)
C510-N110-C310-C410	-57.9(7)
C110-N110-C310-C410	61.8(6)
C710-N110-C310-C410	-177.6(5)
C310-N110-C510-C610	-58.4(7)
C110-N110-C510-C610	178.8(5)
C710-N110-C510-C610	58.6(6)
C310-N110-C710-C810	172.6(5)
C510-N110-C710-C810	51.7(7)
C110-N110-C710-C810	-66.0(6)
C711-N111-C111-C211	-170.6(4)
C511-N111-C111-C211	68.0(5)
C311-N111-C111-C211	-51.0(6)
C711-N111-C311-C411	61.8(6)
C511-N111-C311-C411	-177.2(4)
C111-N111-C311-C411	-57.0(6)
C711-N111-C511-C611	61.8(6)
C111-N111-C511-C611	-179.1(5)

C311-N111-C511-C611	-57.7(6)
C511-N111-C711-C811	56.8(6)
C111-N111-C711-C811	-63.4(6)
C311-N111-C711-C811	175.4(5)
C512-N112-C112-C212	-56(2)
C712-N112-C112-C212	-177(2)
C312-N112-C112-C212	62(2)
C512-N112-C312-C412	-169.4(15)
C112-N112-C312-C412	69.5(17)
C712-N112-C312-C412	-50.0(18)
C112-N112-C512-C612	-62.0(17)
C712-N112-C512-C612	58.7(17)
C312-N112-C512-C612	178.4(13)
C512-N112-C712-C812	52.6(18)
C112-N112-C712-C812	175.2(15)
C312-N112-C712-C812	-64.8(18)
C5A13-N1A13-C1A13-C2A13	-54(2)
C7A13-N1A13-C1A13-C2A13	-175.1(17)
C3A13-N1A13-C1A13-C2A13	64(2)
C5A13-N1A13-C3A13-C4A13	169(2)
C7A13-N1A13-C3A13-C4A13	-68(3)
C1A13-N1A13-C3A13-C4A13	49(3)
C7A13-N1A13-C5A13-C6A13	57(2)
C3A13-N1A13-C5A13-C6A13	179.5(16)
C1A13-N1A13-C5A13-C6A13	-61.1(19)
C5A13-N1A13-C7A13-C8A13	54(2)
C3A13-N1A13-C7A13-C8A13	-67(2)
C1A13-N1A13-C7A13-C8A13	174(2)
C314-N114-C114-C214	-59(2)
C714-N114-C114-C214	178.7(18)
C514-N114-C114-C214	61(2)
C714-N114-C314-C414	61(3)
C114-N114-C314-C414	-59(3)
C514-N114-C314-C414	179(3)
C314-N114-C514-C614	-171(2)
C714-N114-C514-C614	-52(3)

C114-N114-C514-C614	65(3)
C314-N114-C714-C814	58(2)
C114-N114-C714-C814	-177.5(17)
C514-N114-C714-C814	-58(2)
C7A15-N1A15-C1A15-C2A15	179(2)
C5A15-N1A15-C1A15-C2A15	57(2)
C3A15-N1A15-C1A15-C2A15	-61(2)
C7A15-N1A15-C3A15-C4A15	49(3)
C5A15-N1A15-C3A15-C4A15	173(3)
C1A15-N1A15-C3A15-C4A15	-68(3)
C7A15-N1A15-C5A15-C6A15	-56(3)
C3A15-N1A15-C5A15-C6A15	-179(3)
C1A15-N1A15-C5A15-C6A15	63(3)
C5A15-N1A15-C7A15-C8A15	-57(2)
C3A15-N1A15-C7A15-C8A15	64(2)
C1A15-N1A15-C7A15-C8A15	-177.1(19)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 4536ds [\AA and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
O(1)-H(1E)...O13	0.87(5)	1.93(5)	2.795(6)	175(8)
O(1)-H(1F)...O34	0.86(5)	2.06(5)	2.909(6)	168(8)
O(2)-H(2H)...O15	0.97(7)	1.92(7)	2.869(6)	166(7)

Symmetry transformations used to generate equivalent atoms:

**University of Illinois, Department of Chemistry
George L. Clark X- R Facility and 3M Materials Laboratory**

Structure report for compound **Valine HIM in Naphthalene System 6b/C60**

Identification code	CCDC 2388283
Empirical formula	C284 H97 Cl12 I6 N6 O19
Principal Investigator:	Professor Dr. Kyle N Plunkett

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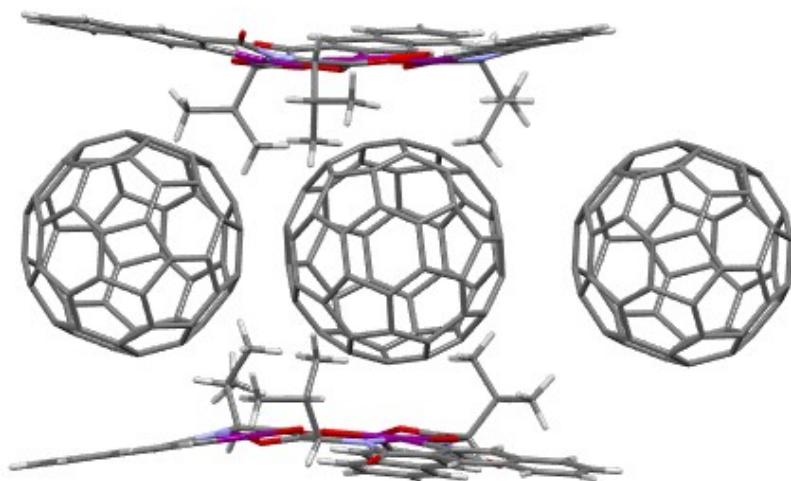


Figure SI20: Perspective view of crystallographically independent molecules of Valine HIM in Naphthalene system. Solvent is removed for clarity. Nitrogen, oxygen and iodine atoms are denoted by light blue, red and purple color respectively. Hydrogens atoms are omitted. (Capped sticks style)

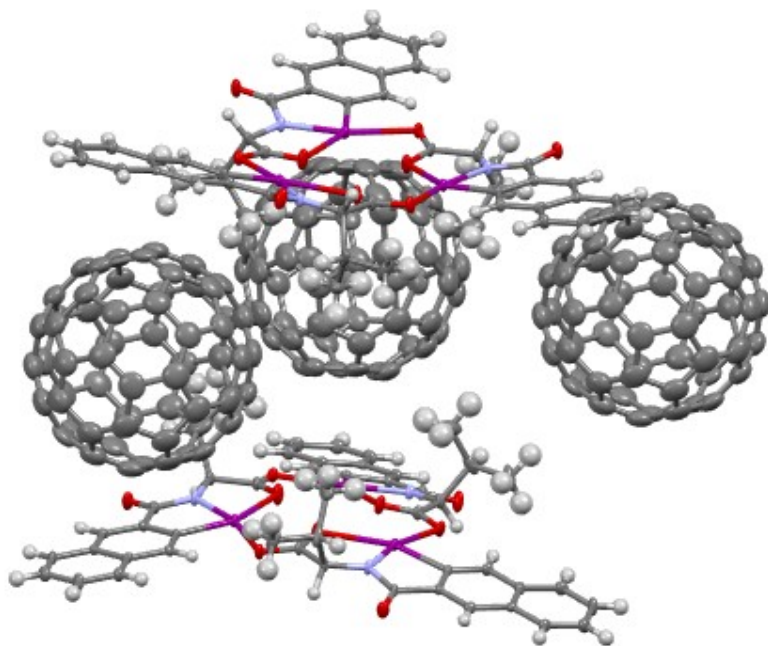


Figure SI21: Perspective view of crystallographically independent molecules of Valine HIM in Naphthalene system. Solvent is removed for clarity. Nitrogen, oxygen and iodine atoms are denoted by light blue, red and purple color respectively. Hydrogens atoms are omitted. (Ellipsoid style)

Table 1. Crystal data and structure refinement for 19949ds_sq.

Identification code	CCDC 2388283	
Empirical formula	C ₂₈₄ H ₉₇ Cl ₁₂ I ₆ N ₆ O ₁₉	
Formula weight	5083.47	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	I2	
Unit cell dimensions	a = 18.9051(5) Å	a = 90°.
	b = 18.3265(4) Å	b = 95.6366(4)°.
	c = 27.6546(9) Å	g = 90°.
Volume	9535.0(5) Å ³	
Z	2	
Density (calculated)	1.771 Mg/m ³	
Absorption coefficient	1.229 mm ⁻¹	
F(000)	5034	
Crystal size	0.187 x 0.137 x 0.050 mm ³	
Theta range for data collection	2.373 to 28.329°.	
Index ranges	-25<=h<=25, -24<=k<=24, -36<=l<=36	
Reflections collected	182786	
Independent reflections	23780 [R(int) = 0.0439]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.7079	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	23780 / 3457 / 1783	
Goodness-of-fit on F ²	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0483, wR2 = 0.1327	
R indices (all data)	R1 = 0.0497, wR2 = 0.1340	
Absolute structure parameter	0.000(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.014 and -1.510 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 19949ds_sq. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1)	6844(1)	5120(1)	3146(1)	14(1)
I(2)	7409(1)	2420(1)	3725(1)	14(1)
I(3)	8436(1)	4653(1)	4786(1)	13(1)
Cl(1)	9922(1)	3754(2)	6948(1)	36(1)
Cl(2)	10807(2)	3548(2)	7854(1)	39(1)
Cl(3)	10504(1)	5004(1)	7494(1)	38(1)
O(1)	8133(3)	5832(3)	4504(2)	18(1)
O(2)	7515(4)	5109(4)	3979(2)	28(1)
O(3)	7082(3)	7378(3)	3106(2)	24(1)
O(4)	6491(3)	4095(3)	2671(2)	18(1)
O(5)	6949(4)	3614(3)	3370(2)	24(1)
O(6)	6613(3)	1348(3)	2454(2)	23(1)
O(7)	8135(3)	2282(3)	4453(2)	20(1)
O(8)	7927(3)	3476(3)	4433(2)	23(1)
O(9)	9879(4)	3453(3)	5709(3)	28(1)
N(1)	7041(4)	6203(3)	3383(2)	16(1)
N(2)	6820(4)	2224(3)	3047(2)	16(1)
N(3)	8917(3)	3765(4)	5185(2)	16(1)
C(1)	7701(4)	5727(4)	4125(3)	17(1)
C(2)	7386(4)	6394(4)	3862(3)	15(1)
C(3)	6920(4)	6735(4)	3044(3)	17(1)
C(4)	6535(4)	6454(4)	2578(3)	14(1)
C(5)	6289(4)	6911(4)	2208(3)	16(1)
C(6)	5909(4)	6631(4)	1782(3)	14(1)
C(7)	5644(4)	7090(4)	1391(3)	19(1)
C(8)	5279(4)	6801(5)	981(3)	23(2)
C(9)	5166(5)	6038(5)	944(3)	24(2)
C(10)	5408(4)	5575(4)	1321(3)	19(2)
C(11)	5790(4)	5867(4)	1742(3)	16(1)
C(12)	6048(4)	5395(4)	2129(3)	14(1)
C(13)	6408(4)	5702(4)	2536(3)	12(1)

C(14)	6859(5)	6780(5)	4175(3)	29(2)
C(15)	7243(6)	7232(5)	4586(3)	34(2)
C(16)	6353(6)	6240(8)	4373(4)	40(2)
C(17)	6654(4)	3546(4)	2951(3)	16(1)
C(18)	6464(4)	2792(4)	2739(3)	16(1)
C(19)	6857(4)	1533(4)	2864(3)	14(1)
C(20)	7223(4)	1011(4)	3224(3)	13(1)
C(21)	7254(4)	272(4)	3125(3)	15(1)
C(22)	7619(4)	-200(4)	3469(3)	15(1)
C(23)	7665(4)	-964(4)	3377(3)	19(1)
C(24)	8032(5)	-1404(4)	3706(3)	24(2)
C(25)	8370(5)	-1115(5)	4144(3)	25(2)
C(26)	8336(4)	-380(5)	4247(3)	22(2)
C(27)	7960(4)	97(4)	3907(3)	17(1)
C(28)	7919(4)	853(4)	4007(3)	17(1)
C(29)	7552(4)	1289(4)	3666(3)	13(1)
C(30)	5647(5)	2684(5)	2694(4)	28(2)
C(31)	5263(6)	3156(5)	2288(4)	35(2)
C(32)	5332(6)	2814(7)	3164(4)	41(2)
C(33)	8231(4)	2923(4)	4622(3)	17(1)
C(34)	8726(4)	2994(4)	5089(3)	18(1)
C(35)	9490(4)	3931(4)	5500(3)	18(1)
C(36)	9601(4)	4723(4)	5571(2)	14(1)
C(37)	10102(4)	4995(4)	5918(3)	17(1)
C(38)	10196(4)	5758(4)	5971(3)	14(1)
C(39)	10695(4)	6056(5)	6338(3)	19(2)
C(40)	10775(4)	6796(5)	6385(3)	23(2)
C(41)	10381(4)	7274(5)	6059(3)	22(2)
C(42)	9893(4)	7002(5)	5697(3)	20(2)
C(43)	9788(4)	6246(4)	5648(3)	15(1)
C(44)	9262(4)	5957(4)	5292(3)	14(1)
C(45)	9171(4)	5211(4)	5271(2)	13(1)
C(46)	8399(6)	2653(5)	5526(3)	28(2)
C(47)	7670(7)	2952(7)	5578(5)	47(3)
C(48)	8382(6)	1818(6)	5503(4)	39(3)
C(49)	10171(6)	4102(6)	7534(4)	36(2)

C(115)	5957(3)	4479(3)	6491(2)	71(3)
C(116)	6608(3)	4389(3)	6257(2)	73(3)
C(117)	5501(3)	5037(3)	6354(2)	70(3)
C(118)	6763(3)	4862(3)	5900(2)	72(3)
C(119)	7485(3)	5130(3)	5888(2)	61(3)
C(120)	7164(3)	4154(2)	6624(2)	69(3)
C(121)	7843(3)	4406(3)	6613(2)	67(3)
C(122)	8008(3)	4909(3)	6234(2)	68(3)
C(123)	5315(2)	5282(4)	7200(2)	70(3)
C(124)	5800(3)	4689(3)	7346(2)	68(3)
C(125)	5170(2)	5451(4)	6719(2)	65(3)
C(126)	6111(3)	4300(3)	7002(2)	69(3)
C(127)	6857(3)	4099(2)	7085(2)	72(3)
C(128)	6215(3)	4902(3)	7794(2)	69(3)
C(129)	6917(3)	4713(3)	7872(2)	70(3)
C(130)	7247(3)	4299(3)	7506(2)	72(3)
C(131)	5239(2)	6755(4)	6902(2)	74(3)
C(132)	5394(3)	6575(4)	7414(2)	68(3)
C(133)	5131(2)	6210(4)	6566(2)	74(3)
C(134)	5430(3)	5862(4)	7558(2)	71(3)
C(135)	5987(3)	5627(4)	7925(2)	70(3)
C(136)	5911(3)	7099(3)	7627(2)	75(3)
C(137)	6434(3)	6878(4)	7973(2)	67(3)
C(138)	6473(3)	6119(4)	8126(2)	72(3)
C(139)	5835(3)	6861(4)	6009(2)	68(3)
C(140)	5950(3)	7441(3)	6367(2)	75(3)
C(141)	5438(3)	6265(4)	6105(2)	73(3)
C(142)	5661(3)	7389(3)	6800(2)	67(3)
C(143)	6076(3)	7602(3)	7248(2)	72(3)
C(144)	6671(3)	7709(3)	6355(2)	70(3)
C(145)	7062(4)	7909(2)	6776(2)	74(3)
C(146)	6755(4)	7854(2)	7237(2)	71(3)
C(147)	6278(3)	5455(4)	5755(2)	74(3)
C(148)	6700(3)	6090(4)	5652(1)	66(3)
C(149)	5666(3)	5540(4)	5974(2)	74(3)
C(150)	6485(3)	6771(4)	5776(2)	69(3)

C(151)	7002(3)	7295(3)	5989(2)	69(3)
C(152)	7446(3)	5889(4)	5735(2)	68(3)
C(153)	7932(3)	6381(4)	5936(2)	65(3)
C(154)	7704(3)	7106(3)	6067(2)	68(3)
C(155)	7962(3)	7528(3)	7370(2)	73(3)
C(156)	7807(3)	7708(3)	6859(2)	68(3)
C(157)	8119(3)	7319(3)	6515(2)	68(3)
C(158)	8418(3)	6971(3)	7507(2)	73(3)
C(159)	7641(3)	6553(4)	8106(2)	74(3)
C(160)	7155(4)	7146(3)	7961(2)	76(3)
C(161)	7311(4)	7619(3)	7604(2)	79(3)
C(162)	8252(3)	6468(4)	7887(2)	71(3)
C(163)	8084(3)	5146(4)	7852(2)	65(3)
C(164)	7434(3)	5237(4)	8085(2)	68(3)
C(165)	7219(3)	5918(4)	8209(1)	68(3)
C(166)	8481(3)	5743(4)	7756(2)	69(3)
C(167)	8679(2)	5253(4)	6959(2)	70(3)
C(168)	8258(3)	4619(3)	7061(2)	65(3)
C(169)	7969(3)	4567(3)	7494(2)	72(3)
C(170)	8788(2)	5798(4)	7295(2)	70(3)
C(171)	8604(2)	6726(3)	6661(2)	66(3)
C(172)	8488(3)	6146(4)	6303(2)	62(3)
C(173)	8525(3)	5433(4)	6447(2)	64(3)
C(174)	8749(2)	6557(4)	7142(2)	65(3)
C(215)	5954(5)	4979(5)	7708(3)	70(3)
C(216)	6431(5)	4434(5)	7540(4)	67(3)
C(217)	5423(4)	5266(6)	7393(4)	69(3)
C(218)	6350(5)	4208(4)	7066(4)	66(3)
C(219)	6971(6)	4104(4)	6803(4)	68(3)
C(220)	7138(6)	4569(5)	7779(3)	73(3)
C(221)	7722(5)	4471(5)	7531(4)	71(3)
C(222)	7635(5)	4231(4)	7028(4)	72(3)
C(223)	5658(5)	6487(6)	7726(3)	71(3)
C(224)	6222(5)	6182(6)	8060(3)	69(3)
C(225)	5271(4)	6043(6)	7402(4)	69(3)
C(226)	6366(5)	5451(6)	8052(3)	68(3)

C(227)	7098(6)	5198(6)	8096(3)	71(4)
C(228)	6802(6)	6706(6)	8113(3)	74(3)
C(229)	7491(6)	6467(6)	8155(3)	75(4)
C(230)	7643(5)	5690(6)	8146(3)	72(4)
C(231)	5308(4)	6953(6)	6760(4)	71(3)
C(232)	5720(5)	7425(5)	7103(4)	70(3)
C(233)	5090(3)	6283(6)	6905(4)	64(3)
C(234)	5889(5)	7199(5)	7572(4)	73(3)
C(235)	6596(6)	7334(5)	7811(3)	74(3)
C(236)	6246(5)	7800(4)	6845(4)	72(3)
C(237)	6911(6)	7927(4)	7071(4)	69(3)
C(238)	7091(6)	7687(4)	7568(4)	75(4)
C(239)	5387(4)	5733(6)	6145(3)	72(3)
C(240)	5618(5)	6445(6)	5991(3)	72(3)
C(241)	5131(3)	5654(6)	6588(4)	69(3)
C(242)	5580(4)	7036(5)	6289(4)	73(3)
C(243)	6159(5)	7560(5)	6342(4)	73(4)
C(244)	6238(5)	6340(6)	5728(3)	72(3)
C(245)	6784(5)	6833(6)	5778(3)	71(3)
C(246)	6743(5)	7462(5)	6094(3)	72(3)
C(247)	5786(5)	4513(5)	6732(4)	67(4)
C(248)	6058(5)	4597(5)	6261(4)	72(4)
C(249)	5337(4)	5026(5)	6890(4)	67(3)
C(250)	5864(5)	5188(6)	5977(3)	75(3)
C(251)	6391(5)	5564(6)	5719(3)	74(4)
C(252)	6790(6)	4344(4)	6305(4)	73(4)
C(253)	7285(5)	4697(5)	6062(3)	71(3)
C(254)	7079(5)	5325(6)	5760(3)	72(3)
C(255)	7927(5)	7052(5)	6165(3)	66(3)
C(256)	7516(5)	6580(6)	5821(3)	67(3)
C(257)	7659(5)	5849(6)	5813(3)	66(3)
C(258)	8458(4)	6765(5)	6480(4)	64(3)
C(259)	8095(5)	7518(5)	7142(4)	67(4)
C(260)	7531(5)	7823(4)	6807(4)	66(3)
C(261)	7450(5)	7597(4)	6334(4)	66(3)
C(262)	8544(4)	7005(5)	6983(4)	66(3)

C(263)	8494(4)	6298(6)	7728(3)	73(3)
C(264)	8017(5)	6843(6)	7896(3)	76(3)
C(265)	7823(5)	7434(5)	7612(4)	75(4)
C(266)	8750(4)	6376(6)	7285(4)	69(3)
C(267)	8573(4)	5078(5)	7114(4)	70(3)
C(268)	8302(5)	4994(5)	7584(3)	72(3)
C(269)	8263(5)	5586(6)	7882(3)	72(4)
C(270)	8791(3)	5748(6)	6969(4)	65(4)
C(271)	8223(5)	5544(6)	6148(3)	65(3)
C(272)	7992(5)	4832(5)	6302(4)	70(3)
C(273)	8162(5)	4606(5)	6770(4)	68(3)
C(274)	8610(4)	5988(6)	6471(4)	65(3)
C(55)	6568(4)	9240(5)	4942(4)	97(6)
C(56)	6538(4)	9298(5)	5464(4)	102(6)
C(57)	6704(4)	9845(5)	4677(4)	91(5)
C(58)	6645(4)	9958(5)	5690(4)	91(6)
C(59)	6200(5)	10178(5)	6064(3)	99(6)
C(60)	5979(5)	8817(4)	5598(4)	103(6)
C(61)	5560(6)	9024(4)	5950(3)	91(6)
C(62)	5674(6)	9725(5)	6190(3)	87(5)
C(63)	5798(5)	9483(5)	4030(3)	68(5)
C(64)	5654(5)	8840(4)	4312(4)	92(5)
C(65)	6307(5)	9970(5)	4207(4)	80(5)
C(66)	6027(5)	8722(4)	4754(4)	110(6)
C(67)	5663(5)	8461(3)	5159(4)	91(6)
C(68)	4893(5)	8704(4)	4248(4)	88(5)
C(69)	4551(5)	8458(3)	4629(4)	99(6)
C(70)	4947(6)	8332(3)	5099(4)	103(6)
C(71)	5545(6)	10995(5)	3932(3)	89(6)
C(72)	5004(6)	10477(5)	3744(3)	81(5)
C(73)	6176(5)	10749(5)	4157(4)	92(6)
C(74)	5127(6)	9744(5)	3792(3)	71(5)
C(75)	4568(5)	9263(5)	3926(3)	90(5)
C(76)	4314(6)	10774(5)	3828(3)	87(6)
C(77)	3788(5)	10321(5)	3954(3)	101(6)
C(78)	3918(5)	9542(5)	4005(3)	87(5)

C(79)	6157(5)	11686(4)	4784(4)	110(6)
C(80)	5486(6)	11947(4)	4545(4)	99(6)
C(81)	6492(4)	11105(5)	4596(4)	87(5)
C(82)	5189(6)	11612(4)	4132(3)	101(6)
C(83)	4428(6)	11476(4)	4068(3)	88(5)
C(84)	5041(6)	12167(3)	4919(4)	101(6)
C(85)	4325(5)	12039(3)	4859(4)	86(5)
C(86)	4009(5)	11683(4)	4420(4)	95(6)
C(87)	6790(4)	10601(5)	5408(4)	92(5)
C(88)	6434(4)	11219(5)	5608(4)	77(5)
C(89)	6818(4)	10546(5)	4917(4)	88(5)
C(90)	6127(5)	11745(4)	5306(4)	89(5)
C(91)	5437(5)	12042(3)	5389(4)	100(6)
C(92)	6070(5)	10957(5)	6013(3)	79(5)
C(93)	5420(5)	11237(5)	6092(3)	80(5)
C(94)	5094(5)	11796(4)	5771(4)	86(5)
C(95)	3420(4)	11260(5)	5076(4)	100(6)
C(96)	3961(5)	11778(4)	5264(4)	109(6)
C(97)	4334(5)	11660(4)	5706(4)	84(5)
C(98)	3284(4)	10655(5)	5341(4)	96(6)
C(99)	3198(4)	9898(5)	4610(4)	96(6)
C(100)	3343(4)	10541(5)	4328(4)	91(6)
C(101)	3450(4)	11201(5)	4554(4)	97(6)
C(102)	3170(4)	9953(5)	5101(4)	101(6)
C(103)	3831(5)	8813(4)	5234(4)	108(6)
C(104)	3861(5)	8755(4)	4713(4)	89(6)
C(105)	3554(4)	9281(5)	4410(4)	86(5)
C(106)	3496(4)	9394(5)	5422(4)	96(6)
C(107)	4443(6)	9505(5)	6086(3)	90(6)
C(108)	4799(6)	8887(4)	5886(3)	103(6)
C(109)	4502(6)	8552(4)	5473(4)	100(6)
C(110)	3812(5)	9750(5)	5861(3)	98(6)
C(111)	4190(5)	11017(5)	5988(3)	67(5)
C(112)	4861(6)	10755(5)	6226(3)	64(5)
C(113)	4984(6)	10023(5)	6274(3)	76(5)
C(114)	3681(5)	10529(5)	5811(4)	86(5)

O(10)	5136(6)	3929(6)	5145(4)	44(3)
C(51)	4163(9)	3921(12)	5620(6)	41(5)
C(52)	4436(7)	4185(10)	5168(6)	42(5)
C(53)	5394(8)	4089(11)	4691(5)	56(6)
C(54)	6177(8)	3944(13)	4733(8)	62(7)
Cl(4)	8236(3)	8510(3)	5396(1)	71(1)
Cl(5)	8576(2)	9971(2)	5739(2)	64(1)
Cl(6)	9184(2)	8736(2)	6268(1)	65(1)
C(50)	8415(7)	9061(7)	5907(5)	50(3)

Table 3. Bond lengths [Å] and angles [°] for 19949ds_sq.

I(1)-C(13)	2.094(7)
I(1)-N(1)	2.110(6)
I(1)-O(4)	2.352(5)
I(2)-C(29)	2.097(7)
I(2)-N(2)	2.116(6)
I(2)-O(7)	2.335(6)
I(3)-C(45)	2.099(7)
I(3)-N(3)	2.120(6)
I(3)-O(1)	2.348(6)
Cl(1)-C(49)	1.762(12)
Cl(2)-C(49)	1.748(11)
Cl(3)-C(49)	1.776(12)
O(1)-C(1)	1.279(9)
O(2)-C(1)	1.242(10)
O(3)-C(3)	1.227(10)
O(4)-C(17)	1.289(9)
O(5)-C(17)	1.244(10)
O(6)-C(19)	1.227(9)
O(7)-C(33)	1.271(9)
O(8)-C(33)	1.254(10)
O(9)-C(35)	1.248(10)
N(1)-C(3)	1.356(10)
N(1)-C(2)	1.461(9)
N(2)-C(19)	1.368(9)
N(2)-C(18)	1.464(9)
N(3)-C(35)	1.358(10)
N(3)-C(34)	1.475(10)
C(1)-C(2)	1.515(10)
C(2)-C(14)	1.555(11)
C(2)-H(2)	1.0000
C(3)-C(4)	1.506(11)
C(4)-C(5)	1.368(10)
C(4)-C(13)	1.402(10)
C(5)-C(6)	1.413(10)

C(5)-H(5)	0.9500
C(6)-C(11)	1.422(10)
C(6)-C(7)	1.423(10)
C(7)-C(8)	1.374(12)
C(7)-H(7)	0.9500
C(8)-C(9)	1.417(12)
C(8)-H(8)	0.9500
C(9)-C(10)	1.386(11)
C(9)-H(9)	0.9500
C(10)-C(11)	1.414(11)
C(10)-H(10)	0.9500
C(11)-C(12)	1.424(10)
C(12)-C(13)	1.377(10)
C(12)-H(12)	0.9500
C(14)-C(16)	1.515(16)
C(14)-C(15)	1.531(13)
C(14)-H(14)	1.0000
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(18)	1.529(10)
C(18)-C(30)	1.551(12)
C(18)-H(18)	1.0000
C(19)-C(20)	1.500(10)
C(20)-C(21)	1.385(10)
C(20)-C(29)	1.413(10)
C(21)-C(22)	1.416(10)
C(21)-H(21)	0.9500
C(22)-C(27)	1.422(10)
C(22)-C(23)	1.426(10)
C(23)-C(24)	1.355(11)
C(23)-H(23)	0.9500
C(24)-C(25)	1.415(12)

C(24)-H(24)	0.9500
C(25)-C(26)	1.379(12)
C(25)-H(25)	0.9500
C(26)-C(27)	1.422(11)
C(26)-H(26)	0.9500
C(27)-C(28)	1.417(11)
C(28)-C(29)	1.370(10)
C(28)-H(28)	0.9500
C(30)-C(32)	1.500(16)
C(30)-C(31)	1.541(12)
C(30)-H(30)	1.0000
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(34)	1.523(10)
C(34)-C(46)	1.544(11)
C(34)-H(34)	1.0000
C(35)-C(36)	1.477(10)
C(36)-C(37)	1.375(10)
C(36)-C(45)	1.422(10)
C(37)-C(38)	1.415(10)
C(37)-H(37)	0.9500
C(38)-C(39)	1.424(10)
C(38)-C(43)	1.436(11)
C(39)-C(40)	1.370(12)
C(39)-H(39)	0.9500
C(40)-C(41)	1.415(12)
C(40)-H(40)	0.9500
C(41)-C(42)	1.386(11)
C(41)-H(41)	0.9500
C(42)-C(43)	1.404(11)
C(42)-H(42)	0.9500
C(43)-C(44)	1.430(10)

C(44)-C(45)	1.378(10)
C(44)-H(44)	0.9500
C(46)-C(47)	1.504(17)
C(46)-C(48)	1.532(14)
C(46)-H(46)	1.0000
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-H(49)	1.0000
C(115)-C(117)	1.3671
C(115)-C(126)	1.4532
C(115)-C(116)	1.4533
C(116)-C(118)	1.3672
C(116)-C(120)	1.4533
C(117)-C(125)	1.4533
C(117)-C(149)	1.4533
C(118)-C(147)	1.4533
C(118)-C(119)	1.4533
C(119)-C(122)	1.3671
C(119)-C(152)	1.4533
C(120)-C(121)	1.3670
C(120)-C(127)	1.4533
C(121)-C(122)	1.4532
C(121)-C(168)	1.4534
C(122)-C(173)	1.4534
C(123)-C(125)	1.3671
C(123)-C(124)	1.4533
C(123)-C(134)	1.4534
C(124)-C(126)	1.3671
C(124)-C(128)	1.4532
C(125)-C(133)	1.4533
C(126)-C(127)	1.4533
C(127)-C(130)	1.3670

C(128)-C(129)	1.3671
C(128)-C(135)	1.4532
C(129)-C(130)	1.4532
C(129)-C(164)	1.4533
C(130)-C(169)	1.4533
C(131)-C(133)	1.3671
C(131)-C(132)	1.4533
C(131)-C(142)	1.4533
C(132)-C(134)	1.3672
C(132)-C(136)	1.4533
C(133)-C(141)	1.4533
C(134)-C(135)	1.4533
C(135)-C(138)	1.3671
C(136)-C(137)	1.3670
C(136)-C(143)	1.4533
C(137)-C(160)	1.4533
C(137)-C(138)	1.4534
C(138)-C(165)	1.4533
C(139)-C(141)	1.3671
C(139)-C(150)	1.4533
C(139)-C(140)	1.4534
C(140)-C(142)	1.3670
C(140)-C(144)	1.4533
C(141)-C(149)	1.4534
C(142)-C(143)	1.4533
C(143)-C(146)	1.3671
C(144)-C(145)	1.3671
C(144)-C(151)	1.4533
C(145)-C(146)	1.4532
C(145)-C(156)	1.4533
C(146)-C(161)	1.4533
C(147)-C(149)	1.3671
C(147)-C(148)	1.4533
C(148)-C(150)	1.3671
C(148)-C(152)	1.4533
C(150)-C(151)	1.4532

C(151)-C(154)	1.3671
C(152)-C(153)	1.3671
C(153)-C(154)	1.4532
C(153)-C(172)	1.4533
C(154)-C(157)	1.4534
C(155)-C(158)	1.3671
C(155)-C(161)	1.4532
C(155)-C(156)	1.4533
C(156)-C(157)	1.3671
C(157)-C(171)	1.4533
C(158)-C(174)	1.4534
C(158)-C(162)	1.4534
C(159)-C(162)	1.3670
C(159)-C(165)	1.4533
C(159)-C(160)	1.4534
C(160)-C(161)	1.3672
C(162)-C(166)	1.4533
C(163)-C(166)	1.3671
C(163)-C(169)	1.4532
C(163)-C(164)	1.4533
C(164)-C(165)	1.3671
C(166)-C(170)	1.4534
C(167)-C(170)	1.3670
C(167)-C(173)	1.4533
C(167)-C(168)	1.4534
C(168)-C(169)	1.3670
C(170)-C(174)	1.4533
C(171)-C(174)	1.3670
C(171)-C(172)	1.4533
C(172)-C(173)	1.3671
C(215)-C(217)	1.3671
C(215)-C(226)	1.4533
C(215)-C(216)	1.4533
C(216)-C(218)	1.3671
C(216)-C(220)	1.4534
C(217)-C(249)	1.4533

C(217)-C(225)	1.4534
C(218)-C(247)	1.4533
C(218)-C(219)	1.4534
C(219)-C(222)	1.3670
C(219)-C(252)	1.4532
C(220)-C(221)	1.3671
C(220)-C(227)	1.4532
C(221)-C(268)	1.4533
C(221)-C(222)	1.4534
C(222)-C(273)	1.4533
C(223)-C(225)	1.3670
C(223)-C(234)	1.4532
C(223)-C(224)	1.4533
C(224)-C(226)	1.3670
C(224)-C(228)	1.4534
C(225)-C(233)	1.4533
C(226)-C(227)	1.4534
C(227)-C(230)	1.3670
C(228)-C(229)	1.3671
C(228)-C(235)	1.4533
C(229)-C(230)	1.4533
C(229)-C(264)	1.4533
C(230)-C(269)	1.4533
C(231)-C(233)	1.3671
C(231)-C(232)	1.4532
C(231)-C(242)	1.4533
C(232)-C(234)	1.3671
C(232)-C(236)	1.4534
C(233)-C(241)	1.4533
C(234)-C(235)	1.4534
C(235)-C(238)	1.3670
C(236)-C(237)	1.3671
C(236)-C(243)	1.4533
C(237)-C(238)	1.4532
C(237)-C(260)	1.4534
C(238)-C(265)	1.4532

C(239)-C(241)	1.3670
C(239)-C(250)	1.4533
C(239)-C(240)	1.4534
C(240)-C(242)	1.3671
C(240)-C(244)	1.4532
C(241)-C(249)	1.4533
C(242)-C(243)	1.4533
C(243)-C(246)	1.3670
C(244)-C(245)	1.3671
C(244)-C(251)	1.4533
C(245)-C(256)	1.4533
C(245)-C(246)	1.4533
C(246)-C(261)	1.4533
C(247)-C(249)	1.3670
C(247)-C(248)	1.4533
C(248)-C(250)	1.3669
C(248)-C(252)	1.4534
C(250)-C(251)	1.4534
C(251)-C(254)	1.3671
C(252)-C(253)	1.3671
C(253)-C(272)	1.4533
C(253)-C(254)	1.4533
C(254)-C(257)	1.4533
C(255)-C(258)	1.3671
C(255)-C(256)	1.4533
C(255)-C(261)	1.4533
C(256)-C(257)	1.3671
C(257)-C(271)	1.4533
C(258)-C(274)	1.4532
C(258)-C(262)	1.4533
C(259)-C(262)	1.3670
C(259)-C(265)	1.4533
C(259)-C(260)	1.4533
C(260)-C(261)	1.3670
C(262)-C(266)	1.4533
C(263)-C(266)	1.3671

C(263)-C(269)	1.4532
C(263)-C(264)	1.4533
C(264)-C(265)	1.3671
C(266)-C(270)	1.4532
C(267)-C(270)	1.3670
C(267)-C(268)	1.4533
C(267)-C(273)	1.4533
C(268)-C(269)	1.3671
C(270)-C(274)	1.4534
C(271)-C(274)	1.3671
C(271)-C(272)	1.4533
C(272)-C(273)	1.3670
C(55)-C(57)	1.3671
C(55)-C(56)	1.4533
C(55)-C(66)	1.4534
C(56)-C(58)	1.3671
C(56)-C(60)	1.4533
C(57)-C(89)	1.4532
C(57)-C(65)	1.4533
C(58)-C(87)	1.4532
C(58)-C(59)	1.4533
C(59)-C(62)	1.3672
C(59)-C(92)	1.4533
C(60)-C(61)	1.3671
C(60)-C(67)	1.4533
C(61)-C(108)	1.4532
C(61)-C(62)	1.4533
C(62)-C(113)	1.4532
C(63)-C(65)	1.3670
C(63)-C(74)	1.4534
C(63)-C(64)	1.4534
C(64)-C(66)	1.3671
C(64)-C(68)	1.4534
C(65)-C(73)	1.4534
C(66)-C(67)	1.4532
C(67)-C(70)	1.3670

C(68)-C(69)	1.3670
C(68)-C(75)	1.4533
C(69)-C(70)	1.4533
C(69)-C(104)	1.4533
C(70)-C(109)	1.4536
C(71)-C(73)	1.3671
C(71)-C(72)	1.4533
C(71)-C(82)	1.4533
C(72)-C(74)	1.3669
C(72)-C(76)	1.4533
C(73)-C(81)	1.4534
C(74)-C(75)	1.4533
C(75)-C(78)	1.3671
C(76)-C(77)	1.3671
C(76)-C(83)	1.4533
C(77)-C(78)	1.4532
C(77)-C(100)	1.4532
C(78)-C(105)	1.4533
C(79)-C(81)	1.3672
C(79)-C(80)	1.4531
C(79)-C(90)	1.4533
C(80)-C(82)	1.3672
C(80)-C(84)	1.4533
C(81)-C(89)	1.4535
C(82)-C(83)	1.4534
C(83)-C(86)	1.3670
C(84)-C(85)	1.3670
C(84)-C(91)	1.4533
C(85)-C(86)	1.4533
C(85)-C(96)	1.4533
C(86)-C(101)	1.4535
C(87)-C(89)	1.3670
C(87)-C(88)	1.4535
C(88)-C(90)	1.3670
C(88)-C(92)	1.4534
C(90)-C(91)	1.4532

C(91)-C(94)	1.3671
C(92)-C(93)	1.3671
C(93)-C(94)	1.4533
C(93)-C(112)	1.4534
C(94)-C(97)	1.4532
C(95)-C(98)	1.3671
C(95)-C(96)	1.4533
C(95)-C(101)	1.4535
C(96)-C(97)	1.3671
C(97)-C(111)	1.4534
C(98)-C(114)	1.4532
C(98)-C(102)	1.4533
C(99)-C(102)	1.3670
C(99)-C(100)	1.4533
C(99)-C(105)	1.4534
C(100)-C(101)	1.3671
C(102)-C(106)	1.4534
C(103)-C(106)	1.3670
C(103)-C(109)	1.4532
C(103)-C(104)	1.4532
C(104)-C(105)	1.3670
C(106)-C(110)	1.4534
C(107)-C(110)	1.3670
C(107)-C(108)	1.4533
C(107)-C(113)	1.4534
C(108)-C(109)	1.3671
C(110)-C(114)	1.4534
C(111)-C(114)	1.3671
C(111)-C(112)	1.4533
C(112)-C(113)	1.3670
O(10)-C(52)	1.4117
O(10)-C(53)	1.4204
C(51)-C(52)	1.4806
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800

C(52)-H(52)	0.9500
C(53)-C(54)	1.4977
C(53)-H(53A)	0.9900
C(53)-H(53B)	0.9900
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
Cl(4)-C(50)	1.744(15)
Cl(5)-C(50)	1.765(13)
Cl(6)-C(50)	1.782(14)
C(50)-H(50)	1.0000

C(13)-I(1)-N(1)	79.3(3)
C(13)-I(1)-O(4)	83.6(2)
N(1)-I(1)-O(4)	162.9(2)
C(29)-I(2)-N(2)	79.9(3)
C(29)-I(2)-O(7)	83.7(2)
N(2)-I(2)-O(7)	163.6(2)
C(45)-I(3)-N(3)	79.6(3)
C(45)-I(3)-O(1)	83.6(2)
N(3)-I(3)-O(1)	163.2(2)
C(1)-O(1)-I(3)	104.4(5)
C(17)-O(4)-I(1)	104.5(5)
C(33)-O(7)-I(2)	105.6(5)
C(3)-N(1)-C(2)	119.0(6)
C(3)-N(1)-I(1)	116.7(5)
C(2)-N(1)-I(1)	123.8(5)
C(19)-N(2)-C(18)	118.7(6)
C(19)-N(2)-I(2)	116.3(5)
C(18)-N(2)-I(2)	124.5(5)
C(35)-N(3)-C(34)	119.7(6)
C(35)-N(3)-I(3)	115.9(5)
C(34)-N(3)-I(3)	123.9(5)
O(2)-C(1)-O(1)	122.8(7)
O(2)-C(1)-C(2)	119.6(7)
O(1)-C(1)-C(2)	117.5(7)

N(1)-C(2)-C(1)	111.2(6)
N(1)-C(2)-C(14)	111.2(6)
C(1)-C(2)-C(14)	110.0(6)
N(1)-C(2)-H(2)	108.1
C(1)-C(2)-H(2)	108.1
C(14)-C(2)-H(2)	108.1
O(3)-C(3)-N(1)	124.8(7)
O(3)-C(3)-C(4)	122.8(7)
N(1)-C(3)-C(4)	112.3(6)
C(5)-C(4)-C(13)	119.9(7)
C(5)-C(4)-C(3)	122.1(7)
C(13)-C(4)-C(3)	118.0(6)
C(4)-C(5)-C(6)	120.5(7)
C(4)-C(5)-H(5)	119.7
C(6)-C(5)-H(5)	119.7
C(5)-C(6)-C(11)	119.1(7)
C(5)-C(6)-C(7)	122.1(7)
C(11)-C(6)-C(7)	118.8(7)
C(8)-C(7)-C(6)	120.7(7)
C(8)-C(7)-H(7)	119.7
C(6)-C(7)-H(7)	119.7
C(7)-C(8)-C(9)	120.0(7)
C(7)-C(8)-H(8)	120.0
C(9)-C(8)-H(8)	120.0
C(10)-C(9)-C(8)	120.9(8)
C(10)-C(9)-H(9)	119.5
C(8)-C(9)-H(9)	119.5
C(9)-C(10)-C(11)	119.5(7)
C(9)-C(10)-H(10)	120.2
C(11)-C(10)-H(10)	120.2
C(10)-C(11)-C(6)	120.1(7)
C(10)-C(11)-C(12)	119.9(7)
C(6)-C(11)-C(12)	120.0(7)
C(13)-C(12)-C(11)	118.1(7)
C(13)-C(12)-H(12)	121.0
C(11)-C(12)-H(12)	121.0

C(12)-C(13)-C(4)	122.4(7)
C(12)-C(13)-I(1)	125.0(5)
C(4)-C(13)-I(1)	112.6(5)
C(16)-C(14)-C(15)	110.9(8)
C(16)-C(14)-C(2)	111.5(8)
C(15)-C(14)-C(2)	112.1(8)
C(16)-C(14)-H(14)	107.3
C(15)-C(14)-H(14)	107.3
C(2)-C(14)-H(14)	107.3
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
O(5)-C(17)-O(4)	122.8(7)
O(5)-C(17)-C(18)	120.9(7)
O(4)-C(17)-C(18)	116.3(6)
N(2)-C(18)-C(17)	110.1(6)
N(2)-C(18)-C(30)	110.7(6)
C(17)-C(18)-C(30)	109.9(6)
N(2)-C(18)-H(18)	108.7
C(17)-C(18)-H(18)	108.7
C(30)-C(18)-H(18)	108.7
O(6)-C(19)-N(2)	124.7(7)
O(6)-C(19)-C(20)	122.8(7)
N(2)-C(19)-C(20)	112.5(6)
C(21)-C(20)-C(29)	120.0(7)
C(21)-C(20)-C(19)	121.3(7)
C(29)-C(20)-C(19)	118.7(6)

C(20)-C(21)-C(22)	119.5(7)
C(20)-C(21)-H(21)	120.2
C(22)-C(21)-H(21)	120.2
C(21)-C(22)-C(27)	119.3(7)
C(21)-C(22)-C(23)	120.9(7)
C(27)-C(22)-C(23)	119.8(7)
C(24)-C(23)-C(22)	120.1(7)
C(24)-C(23)-H(23)	120.0
C(22)-C(23)-H(23)	120.0
C(23)-C(24)-C(25)	120.6(7)
C(23)-C(24)-H(24)	119.7
C(25)-C(24)-H(24)	119.7
C(26)-C(25)-C(24)	121.1(7)
C(26)-C(25)-H(25)	119.4
C(24)-C(25)-H(25)	119.4
C(25)-C(26)-C(27)	119.5(7)
C(25)-C(26)-H(26)	120.2
C(27)-C(26)-H(26)	120.2
C(28)-C(27)-C(22)	120.8(7)
C(28)-C(27)-C(26)	120.3(7)
C(22)-C(27)-C(26)	118.9(7)
C(29)-C(28)-C(27)	118.1(7)
C(29)-C(28)-H(28)	121.0
C(27)-C(28)-H(28)	121.0
C(28)-C(29)-C(20)	122.3(7)
C(28)-C(29)-I(2)	125.7(5)
C(20)-C(29)-I(2)	112.0(5)
C(32)-C(30)-C(31)	110.1(8)
C(32)-C(30)-C(18)	112.8(8)
C(31)-C(30)-C(18)	112.4(8)
C(32)-C(30)-H(30)	107.1
C(31)-C(30)-H(30)	107.1
C(18)-C(30)-H(30)	107.1
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5

C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
O(8)-C(33)-O(7)	123.4(7)
O(8)-C(33)-C(34)	120.1(7)
O(7)-C(33)-C(34)	116.5(7)
N(3)-C(34)-C(33)	110.7(6)
N(3)-C(34)-C(46)	110.9(6)
C(33)-C(34)-C(46)	111.5(7)
N(3)-C(34)-H(34)	107.9
C(33)-C(34)-H(34)	107.9
C(46)-C(34)-H(34)	107.9
O(9)-C(35)-N(3)	122.5(7)
O(9)-C(35)-C(36)	123.9(7)
N(3)-C(35)-C(36)	113.5(6)
C(37)-C(36)-C(45)	119.7(7)
C(37)-C(36)-C(35)	121.9(7)
C(45)-C(36)-C(35)	118.4(6)
C(36)-C(37)-C(38)	120.1(7)
C(36)-C(37)-H(37)	119.9
C(38)-C(37)-H(37)	119.9
C(37)-C(38)-C(39)	121.4(7)
C(37)-C(38)-C(43)	119.8(7)
C(39)-C(38)-C(43)	118.9(7)
C(40)-C(39)-C(38)	120.4(7)
C(40)-C(39)-H(39)	119.8
C(38)-C(39)-H(39)	119.8
C(39)-C(40)-C(41)	120.5(7)
C(39)-C(40)-H(40)	119.8
C(41)-C(40)-H(40)	119.8

C(42)-C(41)-C(40)	120.5(8)
C(42)-C(41)-H(41)	119.7
C(40)-C(41)-H(41)	119.7
C(41)-C(42)-C(43)	120.2(8)
C(41)-C(42)-H(42)	119.9
C(43)-C(42)-H(42)	119.9
C(42)-C(43)-C(44)	120.9(7)
C(42)-C(43)-C(38)	119.5(7)
C(44)-C(43)-C(38)	119.6(7)
C(45)-C(44)-C(43)	118.1(7)
C(45)-C(44)-H(44)	120.9
C(43)-C(44)-H(44)	120.9
C(44)-C(45)-C(36)	122.5(6)
C(44)-C(45)-I(3)	125.6(5)
C(36)-C(45)-I(3)	111.8(5)
C(47)-C(46)-C(48)	110.7(9)
C(47)-C(46)-C(34)	111.7(8)
C(48)-C(46)-C(34)	112.4(8)
C(47)-C(46)-H(46)	107.2
C(48)-C(46)-H(46)	107.2
C(34)-C(46)-H(46)	107.2
C(46)-C(47)-H(47A)	109.5
C(46)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(46)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(46)-C(48)-H(48A)	109.5
C(46)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(46)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
Cl(2)-C(49)-Cl(1)	111.3(6)
Cl(2)-C(49)-Cl(3)	110.0(6)
Cl(1)-C(49)-Cl(3)	110.1(6)

CI(2)-C(49)-H(49)	108.4
CI(1)-C(49)-H(49)	108.4
CI(3)-C(49)-H(49)	108.4
C(117)-C(115)-C(126)	120.0
C(117)-C(115)-C(116)	120.0
C(126)-C(115)-C(116)	108.0
C(118)-C(116)-C(115)	120.0
C(118)-C(116)-C(120)	120.0
C(115)-C(116)-C(120)	108.0
C(115)-C(117)-C(125)	120.0
C(115)-C(117)-C(149)	120.0
C(125)-C(117)-C(149)	108.0
C(116)-C(118)-C(147)	120.0
C(116)-C(118)-C(119)	120.0
C(147)-C(118)-C(119)	108.0
C(122)-C(119)-C(152)	120.0
C(122)-C(119)-C(118)	120.0
C(152)-C(119)-C(118)	108.0
C(121)-C(120)-C(127)	120.0
C(121)-C(120)-C(116)	120.0
C(127)-C(120)-C(116)	108.0
C(120)-C(121)-C(122)	120.0
C(120)-C(121)-C(168)	120.0
C(122)-C(121)-C(168)	108.0
C(119)-C(122)-C(121)	120.0
C(119)-C(122)-C(173)	120.0
C(121)-C(122)-C(173)	108.0
C(125)-C(123)-C(124)	120.0
C(125)-C(123)-C(134)	120.0
C(124)-C(123)-C(134)	108.0
C(126)-C(124)-C(128)	120.0
C(126)-C(124)-C(123)	120.0
C(128)-C(124)-C(123)	108.0
C(123)-C(125)-C(117)	120.0
C(123)-C(125)-C(133)	120.0
C(117)-C(125)-C(133)	108.0

C(124)-C(126)-C(115)	120.0
C(124)-C(126)-C(127)	120.0
C(115)-C(126)-C(127)	108.0
C(130)-C(127)-C(120)	120.0
C(130)-C(127)-C(126)	120.0
C(120)-C(127)-C(126)	108.0
C(129)-C(128)-C(135)	120.0
C(129)-C(128)-C(124)	120.0
C(135)-C(128)-C(124)	108.0
C(128)-C(129)-C(130)	120.0
C(128)-C(129)-C(164)	120.0
C(130)-C(129)-C(164)	108.0
C(127)-C(130)-C(129)	120.0
C(127)-C(130)-C(169)	120.0
C(129)-C(130)-C(169)	108.0
C(133)-C(131)-C(132)	120.0
C(133)-C(131)-C(142)	120.0
C(132)-C(131)-C(142)	108.0
C(134)-C(132)-C(136)	120.0
C(134)-C(132)-C(131)	120.0
C(136)-C(132)-C(131)	108.0
C(131)-C(133)-C(125)	120.0
C(131)-C(133)-C(141)	120.0
C(125)-C(133)-C(141)	108.0
C(132)-C(134)-C(135)	120.0
C(132)-C(134)-C(123)	120.0
C(135)-C(134)-C(123)	108.0
C(138)-C(135)-C(128)	120.0
C(138)-C(135)-C(134)	120.0
C(128)-C(135)-C(134)	108.0
C(137)-C(136)-C(132)	120.0
C(137)-C(136)-C(143)	120.0
C(132)-C(136)-C(143)	108.0
C(136)-C(137)-C(160)	120.0
C(136)-C(137)-C(138)	120.0
C(160)-C(137)-C(138)	108.0

C(135)-C(138)-C(165)	120.0
C(135)-C(138)-C(137)	120.0
C(165)-C(138)-C(137)	108.0
C(141)-C(139)-C(150)	120.0
C(141)-C(139)-C(140)	120.0
C(150)-C(139)-C(140)	108.0
C(142)-C(140)-C(144)	120.0
C(142)-C(140)-C(139)	120.0
C(144)-C(140)-C(139)	108.0
C(139)-C(141)-C(133)	120.0
C(139)-C(141)-C(149)	120.0
C(133)-C(141)-C(149)	108.0
C(140)-C(142)-C(143)	120.0
C(140)-C(142)-C(131)	120.0
C(143)-C(142)-C(131)	108.0
C(146)-C(143)-C(136)	120.0
C(146)-C(143)-C(142)	120.0
C(136)-C(143)-C(142)	108.0
C(145)-C(144)-C(151)	120.0
C(145)-C(144)-C(140)	120.0
C(151)-C(144)-C(140)	108.0
C(144)-C(145)-C(146)	120.0
C(144)-C(145)-C(156)	120.0
C(146)-C(145)-C(156)	108.0
C(143)-C(146)-C(145)	120.0
C(143)-C(146)-C(161)	120.0
C(145)-C(146)-C(161)	108.0
C(149)-C(147)-C(118)	120.0
C(149)-C(147)-C(148)	120.0
C(118)-C(147)-C(148)	108.0
C(150)-C(148)-C(152)	120.0
C(150)-C(148)-C(147)	120.0
C(152)-C(148)-C(147)	108.0
C(147)-C(149)-C(117)	120.0
C(147)-C(149)-C(141)	120.0
C(117)-C(149)-C(141)	108.0

C(148)-C(150)-C(151)	120.0
C(148)-C(150)-C(139)	120.0
C(151)-C(150)-C(139)	108.0
C(154)-C(151)-C(150)	120.0
C(154)-C(151)-C(144)	120.0
C(150)-C(151)-C(144)	108.0
C(153)-C(152)-C(119)	120.0
C(153)-C(152)-C(148)	120.0
C(119)-C(152)-C(148)	108.0
C(152)-C(153)-C(154)	120.0
C(152)-C(153)-C(172)	120.0
C(154)-C(153)-C(172)	108.0
C(151)-C(154)-C(153)	120.0
C(151)-C(154)-C(157)	120.0
C(153)-C(154)-C(157)	108.0
C(158)-C(155)-C(161)	120.0
C(158)-C(155)-C(156)	120.0
C(161)-C(155)-C(156)	108.0
C(157)-C(156)-C(145)	120.0
C(157)-C(156)-C(155)	120.0
C(145)-C(156)-C(155)	108.0
C(156)-C(157)-C(171)	120.0
C(156)-C(157)-C(154)	120.0
C(171)-C(157)-C(154)	108.0
C(155)-C(158)-C(174)	120.0
C(155)-C(158)-C(162)	120.0
C(174)-C(158)-C(162)	108.0
C(162)-C(159)-C(165)	120.0
C(162)-C(159)-C(160)	120.0
C(165)-C(159)-C(160)	108.0
C(161)-C(160)-C(137)	120.0
C(161)-C(160)-C(159)	120.0
C(137)-C(160)-C(159)	108.0
C(160)-C(161)-C(155)	120.0
C(160)-C(161)-C(146)	120.0
C(155)-C(161)-C(146)	108.0

C(159)-C(162)-C(166)	120.0
C(159)-C(162)-C(158)	120.0
C(166)-C(162)-C(158)	108.0
C(166)-C(163)-C(169)	120.0
C(166)-C(163)-C(164)	120.0
C(169)-C(163)-C(164)	108.0
C(165)-C(164)-C(129)	120.0
C(165)-C(164)-C(163)	120.0
C(129)-C(164)-C(163)	108.0
C(164)-C(165)-C(138)	120.0
C(164)-C(165)-C(159)	120.0
C(138)-C(165)-C(159)	108.0
C(163)-C(166)-C(162)	120.0
C(163)-C(166)-C(170)	120.0
C(162)-C(166)-C(170)	108.0
C(170)-C(167)-C(173)	120.0
C(170)-C(167)-C(168)	120.0
C(173)-C(167)-C(168)	108.0
C(169)-C(168)-C(121)	120.0
C(169)-C(168)-C(167)	120.0
C(121)-C(168)-C(167)	108.0
C(168)-C(169)-C(163)	120.0
C(168)-C(169)-C(130)	120.0
C(163)-C(169)-C(130)	108.0
C(167)-C(170)-C(174)	120.0
C(167)-C(170)-C(166)	120.0
C(174)-C(170)-C(166)	108.0
C(174)-C(171)-C(172)	120.0
C(174)-C(171)-C(157)	120.0
C(172)-C(171)-C(157)	108.0
C(173)-C(172)-C(171)	120.0
C(173)-C(172)-C(153)	120.0
C(171)-C(172)-C(153)	108.0
C(172)-C(173)-C(167)	120.0
C(172)-C(173)-C(122)	120.0
C(167)-C(173)-C(122)	108.0

C(171)-C(174)-C(170)	120.0
C(171)-C(174)-C(158)	120.0
C(170)-C(174)-C(158)	108.0
C(217)-C(215)-C(226)	120.0
C(217)-C(215)-C(216)	120.0
C(226)-C(215)-C(216)	108.0
C(218)-C(216)-C(215)	120.0
C(218)-C(216)-C(220)	120.0
C(215)-C(216)-C(220)	108.0
C(215)-C(217)-C(249)	120.0
C(215)-C(217)-C(225)	120.0
C(249)-C(217)-C(225)	108.0
C(216)-C(218)-C(247)	120.0
C(216)-C(218)-C(219)	120.0
C(247)-C(218)-C(219)	108.0
C(222)-C(219)-C(252)	120.0
C(222)-C(219)-C(218)	120.0
C(252)-C(219)-C(218)	108.0
C(221)-C(220)-C(227)	120.0
C(221)-C(220)-C(216)	120.0
C(227)-C(220)-C(216)	108.0
C(220)-C(221)-C(268)	120.0
C(220)-C(221)-C(222)	120.0
C(268)-C(221)-C(222)	108.0
C(219)-C(222)-C(273)	120.0
C(219)-C(222)-C(221)	120.0
C(273)-C(222)-C(221)	108.0
C(225)-C(223)-C(234)	120.0
C(225)-C(223)-C(224)	120.0
C(234)-C(223)-C(224)	108.0
C(226)-C(224)-C(223)	120.0
C(226)-C(224)-C(228)	120.0
C(223)-C(224)-C(228)	108.0
C(223)-C(225)-C(233)	120.0
C(223)-C(225)-C(217)	120.0
C(233)-C(225)-C(217)	108.0

C(224)-C(226)-C(215)	120.0
C(224)-C(226)-C(227)	120.0
C(215)-C(226)-C(227)	108.0
C(230)-C(227)-C(220)	120.0
C(230)-C(227)-C(226)	120.0
C(220)-C(227)-C(226)	108.0
C(229)-C(228)-C(235)	120.0
C(229)-C(228)-C(224)	120.0
C(235)-C(228)-C(224)	108.0
C(228)-C(229)-C(230)	120.0
C(228)-C(229)-C(264)	120.0
C(230)-C(229)-C(264)	108.0
C(227)-C(230)-C(229)	120.0
C(227)-C(230)-C(269)	120.0
C(229)-C(230)-C(269)	108.0
C(233)-C(231)-C(232)	120.0
C(233)-C(231)-C(242)	120.0
C(232)-C(231)-C(242)	108.0
C(234)-C(232)-C(231)	120.0
C(234)-C(232)-C(236)	120.0
C(231)-C(232)-C(236)	108.0
C(231)-C(233)-C(225)	120.0
C(231)-C(233)-C(241)	120.0
C(225)-C(233)-C(241)	108.0
C(232)-C(234)-C(223)	120.0
C(232)-C(234)-C(235)	120.0
C(223)-C(234)-C(235)	108.0
C(238)-C(235)-C(228)	120.0
C(238)-C(235)-C(234)	120.0
C(228)-C(235)-C(234)	108.0
C(237)-C(236)-C(243)	120.0
C(237)-C(236)-C(232)	120.0
C(243)-C(236)-C(232)	108.0
C(236)-C(237)-C(238)	120.0
C(236)-C(237)-C(260)	120.0
C(238)-C(237)-C(260)	108.0

C(235)-C(238)-C(237)	120.0
C(235)-C(238)-C(265)	120.0
C(237)-C(238)-C(265)	108.0
C(241)-C(239)-C(250)	120.0
C(241)-C(239)-C(240)	120.0
C(250)-C(239)-C(240)	108.0
C(242)-C(240)-C(244)	120.0
C(242)-C(240)-C(239)	120.0
C(244)-C(240)-C(239)	108.0
C(239)-C(241)-C(249)	120.0
C(239)-C(241)-C(233)	120.0
C(249)-C(241)-C(233)	108.0
C(240)-C(242)-C(243)	120.0
C(240)-C(242)-C(231)	120.0
C(243)-C(242)-C(231)	108.0
C(246)-C(243)-C(242)	120.0
C(246)-C(243)-C(236)	120.0
C(242)-C(243)-C(236)	108.0
C(245)-C(244)-C(240)	120.0
C(245)-C(244)-C(251)	120.0
C(240)-C(244)-C(251)	108.0
C(244)-C(245)-C(256)	120.0
C(244)-C(245)-C(246)	120.0
C(256)-C(245)-C(246)	108.0
C(243)-C(246)-C(261)	120.0
C(243)-C(246)-C(245)	120.0
C(261)-C(246)-C(245)	108.0
C(249)-C(247)-C(218)	120.0
C(249)-C(247)-C(248)	120.0
C(218)-C(247)-C(248)	108.0
C(250)-C(248)-C(247)	120.0
C(250)-C(248)-C(252)	120.0
C(247)-C(248)-C(252)	108.0
C(247)-C(249)-C(217)	120.0
C(247)-C(249)-C(241)	120.0
C(217)-C(249)-C(241)	108.0

C(248)-C(250)-C(239)	120.0
C(248)-C(250)-C(251)	120.0
C(239)-C(250)-C(251)	108.0
C(254)-C(251)-C(244)	120.0
C(254)-C(251)-C(250)	120.0
C(244)-C(251)-C(250)	108.0
C(253)-C(252)-C(219)	120.0
C(253)-C(252)-C(248)	120.0
C(219)-C(252)-C(248)	108.0
C(252)-C(253)-C(272)	120.0
C(252)-C(253)-C(254)	120.0
C(272)-C(253)-C(254)	108.0
C(251)-C(254)-C(257)	120.0
C(251)-C(254)-C(253)	120.0
C(257)-C(254)-C(253)	108.0
C(258)-C(255)-C(256)	120.0
C(258)-C(255)-C(261)	120.0
C(256)-C(255)-C(261)	108.0
C(257)-C(256)-C(255)	120.0
C(257)-C(256)-C(245)	120.0
C(255)-C(256)-C(245)	108.0
C(256)-C(257)-C(254)	120.0
C(256)-C(257)-C(271)	120.0
C(254)-C(257)-C(271)	108.0
C(255)-C(258)-C(274)	120.0
C(255)-C(258)-C(262)	120.0
C(274)-C(258)-C(262)	108.0
C(262)-C(259)-C(265)	120.0
C(262)-C(259)-C(260)	120.0
C(265)-C(259)-C(260)	108.0
C(261)-C(260)-C(259)	120.0
C(261)-C(260)-C(237)	120.0
C(259)-C(260)-C(237)	108.0
C(260)-C(261)-C(255)	120.0
C(260)-C(261)-C(246)	120.0
C(255)-C(261)-C(246)	108.0

C(259)-C(262)-C(266)	120.0
C(259)-C(262)-C(258)	120.0
C(266)-C(262)-C(258)	108.0
C(266)-C(263)-C(269)	120.0
C(266)-C(263)-C(264)	120.0
C(269)-C(263)-C(264)	108.0
C(265)-C(264)-C(263)	120.0
C(265)-C(264)-C(229)	120.0
C(263)-C(264)-C(229)	108.0
C(264)-C(265)-C(238)	120.0
C(264)-C(265)-C(259)	120.0
C(238)-C(265)-C(259)	108.0
C(263)-C(266)-C(270)	120.0
C(263)-C(266)-C(262)	120.0
C(270)-C(266)-C(262)	108.0
C(270)-C(267)-C(268)	120.0
C(270)-C(267)-C(273)	120.0
C(268)-C(267)-C(273)	108.0
C(269)-C(268)-C(267)	120.0
C(269)-C(268)-C(221)	120.0
C(267)-C(268)-C(221)	108.0
C(268)-C(269)-C(263)	120.0
C(268)-C(269)-C(230)	120.0
C(263)-C(269)-C(230)	108.0
C(267)-C(270)-C(266)	120.0
C(267)-C(270)-C(274)	120.0
C(266)-C(270)-C(274)	108.0
C(274)-C(271)-C(272)	120.0
C(274)-C(271)-C(257)	120.0
C(272)-C(271)-C(257)	108.0
C(273)-C(272)-C(271)	120.0
C(273)-C(272)-C(253)	120.0
C(271)-C(272)-C(253)	108.0
C(272)-C(273)-C(267)	120.0
C(272)-C(273)-C(222)	120.0
C(267)-C(273)-C(222)	108.0

C(271)-C(274)-C(258)	120.0
C(271)-C(274)-C(270)	120.0
C(258)-C(274)-C(270)	108.0
C(57)-C(55)-C(56)	120.0
C(57)-C(55)-C(66)	120.0
C(56)-C(55)-C(66)	108.0
C(58)-C(56)-C(55)	120.0
C(58)-C(56)-C(60)	120.0
C(55)-C(56)-C(60)	108.0
C(55)-C(57)-C(89)	120.0
C(55)-C(57)-C(65)	120.0
C(89)-C(57)-C(65)	108.0
C(56)-C(58)-C(87)	120.0
C(56)-C(58)-C(59)	120.0
C(87)-C(58)-C(59)	108.0
C(62)-C(59)-C(58)	120.0
C(62)-C(59)-C(92)	120.0
C(58)-C(59)-C(92)	108.0
C(61)-C(60)-C(56)	120.0
C(61)-C(60)-C(67)	120.0
C(56)-C(60)-C(67)	108.0
C(60)-C(61)-C(108)	120.0
C(60)-C(61)-C(62)	120.0
C(108)-C(61)-C(62)	108.0
C(59)-C(62)-C(113)	120.0
C(59)-C(62)-C(61)	120.0
C(113)-C(62)-C(61)	108.0
C(65)-C(63)-C(74)	120.0
C(65)-C(63)-C(64)	120.0
C(74)-C(63)-C(64)	108.0
C(66)-C(64)-C(68)	120.0
C(66)-C(64)-C(63)	120.0
C(68)-C(64)-C(63)	108.0
C(63)-C(65)-C(57)	120.0
C(63)-C(65)-C(73)	120.0
C(57)-C(65)-C(73)	108.0

C(64)-C(66)-C(67)	120.0
C(64)-C(66)-C(55)	120.0
C(67)-C(66)-C(55)	108.0
C(70)-C(67)-C(66)	120.0
C(70)-C(67)-C(60)	120.0
C(66)-C(67)-C(60)	108.0
C(69)-C(68)-C(75)	120.0
C(69)-C(68)-C(64)	120.0
C(75)-C(68)-C(64)	108.0
C(68)-C(69)-C(70)	120.0
C(68)-C(69)-C(104)	120.0
C(70)-C(69)-C(104)	108.0
C(67)-C(70)-C(69)	120.0
C(67)-C(70)-C(109)	120.0
C(69)-C(70)-C(109)	108.0
C(73)-C(71)-C(72)	120.0
C(73)-C(71)-C(82)	120.0
C(72)-C(71)-C(82)	108.0
C(74)-C(72)-C(76)	120.0
C(74)-C(72)-C(71)	120.0
C(76)-C(72)-C(71)	108.0
C(71)-C(73)-C(65)	120.0
C(71)-C(73)-C(81)	120.0
C(65)-C(73)-C(81)	108.0
C(72)-C(74)-C(75)	120.0
C(72)-C(74)-C(63)	120.0
C(75)-C(74)-C(63)	108.0
C(78)-C(75)-C(68)	120.0
C(78)-C(75)-C(74)	120.0
C(68)-C(75)-C(74)	108.0
C(77)-C(76)-C(83)	120.0
C(77)-C(76)-C(72)	120.0
C(83)-C(76)-C(72)	108.0
C(76)-C(77)-C(78)	120.0
C(76)-C(77)-C(100)	120.0
C(78)-C(77)-C(100)	108.0

C(75)-C(78)-C(77)	120.0
C(75)-C(78)-C(105)	120.0
C(77)-C(78)-C(105)	108.0
C(81)-C(79)-C(80)	120.0
C(81)-C(79)-C(90)	120.0
C(80)-C(79)-C(90)	108.0
C(82)-C(80)-C(79)	120.0
C(82)-C(80)-C(84)	120.0
C(79)-C(80)-C(84)	108.0
C(79)-C(81)-C(73)	120.0
C(79)-C(81)-C(89)	120.0
C(73)-C(81)-C(89)	108.0
C(80)-C(82)-C(71)	120.0
C(80)-C(82)-C(83)	120.0
C(71)-C(82)-C(83)	108.0
C(86)-C(83)-C(76)	120.0
C(86)-C(83)-C(82)	120.0
C(76)-C(83)-C(82)	108.0
C(85)-C(84)-C(91)	120.0
C(85)-C(84)-C(80)	120.0
C(91)-C(84)-C(80)	108.0
C(84)-C(85)-C(86)	120.0
C(84)-C(85)-C(96)	120.0
C(86)-C(85)-C(96)	108.0
C(83)-C(86)-C(85)	120.0
C(83)-C(86)-C(101)	120.0
C(85)-C(86)-C(101)	108.0
C(89)-C(87)-C(58)	120.0
C(89)-C(87)-C(88)	120.0
C(58)-C(87)-C(88)	108.0
C(90)-C(88)-C(92)	120.0
C(90)-C(88)-C(87)	120.0
C(92)-C(88)-C(87)	108.0
C(87)-C(89)-C(57)	120.0
C(87)-C(89)-C(81)	120.0
C(57)-C(89)-C(81)	108.0

C(88)-C(90)-C(91)	120.0
C(88)-C(90)-C(79)	120.0
C(91)-C(90)-C(79)	108.0
C(94)-C(91)-C(90)	120.0
C(94)-C(91)-C(84)	120.0
C(90)-C(91)-C(84)	108.0
C(93)-C(92)-C(59)	120.0
C(93)-C(92)-C(88)	120.0
C(59)-C(92)-C(88)	108.0
C(92)-C(93)-C(94)	120.0
C(92)-C(93)-C(112)	120.0
C(94)-C(93)-C(112)	108.0
C(91)-C(94)-C(97)	120.0
C(91)-C(94)-C(93)	120.0
C(97)-C(94)-C(93)	108.0
C(98)-C(95)-C(96)	120.0
C(98)-C(95)-C(101)	120.0
C(96)-C(95)-C(101)	108.0
C(97)-C(96)-C(95)	120.0
C(97)-C(96)-C(85)	120.0
C(95)-C(96)-C(85)	108.0
C(96)-C(97)-C(94)	120.0
C(96)-C(97)-C(111)	120.0
C(94)-C(97)-C(111)	108.0
C(95)-C(98)-C(114)	120.0
C(95)-C(98)-C(102)	120.0
C(114)-C(98)-C(102)	108.0
C(102)-C(99)-C(100)	120.0
C(102)-C(99)-C(105)	120.0
C(100)-C(99)-C(105)	108.0
C(101)-C(100)-C(77)	120.0
C(101)-C(100)-C(99)	120.0
C(77)-C(100)-C(99)	108.0
C(100)-C(101)-C(86)	120.0
C(100)-C(101)-C(95)	120.0
C(86)-C(101)-C(95)	108.0

C(99)-C(102)-C(98)	120.0
C(99)-C(102)-C(106)	120.0
C(98)-C(102)-C(106)	108.0
C(106)-C(103)-C(109)	120.0
C(106)-C(103)-C(104)	120.0
C(109)-C(103)-C(104)	108.0
C(105)-C(104)-C(103)	120.0
C(105)-C(104)-C(69)	120.0
C(103)-C(104)-C(69)	108.0
C(104)-C(105)-C(78)	120.0
C(104)-C(105)-C(99)	120.0
C(78)-C(105)-C(99)	108.0
C(103)-C(106)-C(110)	120.0
C(103)-C(106)-C(102)	120.0
C(110)-C(106)-C(102)	108.0
C(110)-C(107)-C(108)	120.0
C(110)-C(107)-C(113)	120.0
C(108)-C(107)-C(113)	108.0
C(109)-C(108)-C(61)	120.0
C(109)-C(108)-C(107)	120.0
C(61)-C(108)-C(107)	108.0
C(108)-C(109)-C(103)	120.0
C(108)-C(109)-C(70)	120.0
C(103)-C(109)-C(70)	108.0
C(107)-C(110)-C(114)	120.0
C(107)-C(110)-C(106)	120.0
C(114)-C(110)-C(106)	108.0
C(114)-C(111)-C(112)	120.0
C(114)-C(111)-C(97)	120.0
C(112)-C(111)-C(97)	108.0
C(113)-C(112)-C(111)	120.0
C(113)-C(112)-C(93)	120.0
C(111)-C(112)-C(93)	108.0
C(112)-C(113)-C(62)	120.0
C(112)-C(113)-C(107)	120.0
C(62)-C(113)-C(107)	108.0

C(111)-C(114)-C(98)	120.0
C(111)-C(114)-C(110)	120.0
C(98)-C(114)-C(110)	108.0
C(52)-O(10)-C(53)	112.0
C(52)-C(51)-H(51A)	109.5
C(52)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(52)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
O(10)-C(52)-C(51)	109.6
O(10)-C(52)-H(52)	125.2
C(51)-C(52)-H(52)	125.2
O(10)-C(53)-C(54)	108.5
O(10)-C(53)-H(53A)	110.0
C(54)-C(53)-H(53A)	110.0
O(10)-C(53)-H(53B)	110.0
C(54)-C(53)-H(53B)	110.0
H(53A)-C(53)-H(53B)	108.4
C(53)-C(54)-H(54A)	109.5
C(53)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(53)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
Cl(4)-C(50)-Cl(5)	111.0(7)
Cl(4)-C(50)-Cl(6)	110.1(8)
Cl(5)-C(50)-Cl(6)	108.1(7)
Cl(4)-C(50)-H(50)	109.2
Cl(5)-C(50)-H(50)	109.2
Cl(6)-C(50)-H(50)	109.2

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 19949ds_sq. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
I(1)	18(1)	10(1)	15(1)	1(1)	-2(1)	0(1)
I(2)	18(1)	9(1)	13(1)	-1(1)	-1(1)	1(1)
I(3)	13(1)	12(1)	14(1)	-1(1)	-2(1)	0(1)
Cl(1)	37(1)	35(1)	37(1)	-1(1)	1(1)	-3(1)
Cl(2)	47(1)	36(1)	33(1)	0(1)	2(1)	6(1)
Cl(3)	37(1)	27(1)	48(1)	-1(1)	-1(1)	1(1)
O(1)	21(3)	14(2)	17(3)	-2(2)	-5(2)	1(2)
O(2)	41(3)	14(3)	25(3)	1(3)	-17(3)	-2(3)
O(3)	39(3)	12(2)	20(3)	-2(2)	-7(2)	0(3)
O(4)	30(3)	8(2)	17(3)	1(2)	-3(2)	0(2)
O(5)	39(3)	12(3)	18(3)	-1(2)	-11(2)	0(2)
O(6)	32(3)	17(3)	16(3)	-3(2)	-8(2)	1(2)
O(7)	31(3)	9(3)	19(3)	-2(2)	-5(2)	4(2)
O(8)	31(3)	10(2)	24(3)	-3(2)	-13(2)	2(2)
O(9)	31(3)	16(3)	33(3)	4(2)	-17(3)	-1(2)
N(1)	21(3)	9(3)	18(3)	-1(2)	-5(2)	1(2)
N(2)	21(3)	11(3)	15(3)	-1(2)	-6(2)	3(2)
N(3)	17(3)	13(3)	17(3)	0(2)	-5(2)	0(2)
C(1)	20(3)	13(3)	16(3)	3(3)	-2(3)	2(3)
C(2)	22(3)	12(3)	11(3)	0(2)	-4(3)	0(3)
C(3)	21(4)	15(3)	15(3)	2(3)	0(3)	1(3)
C(4)	19(3)	10(3)	14(3)	1(2)	4(3)	-1(3)
C(5)	19(3)	15(3)	16(3)	-1(3)	5(3)	2(3)
C(6)	17(3)	14(3)	12(3)	3(2)	2(3)	4(3)
C(7)	23(4)	14(3)	20(4)	5(3)	2(3)	5(3)
C(8)	22(4)	26(4)	21(4)	6(3)	-3(3)	3(3)
C(9)	28(4)	21(4)	21(4)	3(3)	-12(3)	2(3)
C(10)	24(4)	13(3)	21(4)	1(3)	0(3)	1(3)
C(11)	15(3)	13(3)	18(3)	-3(3)	-1(3)	2(3)
C(12)	17(3)	11(3)	14(3)	2(2)	2(3)	-1(2)
C(13)	15(3)	8(3)	14(3)	4(2)	0(2)	2(2)

C(14)	36(5)	32(5)	17(4)	-3(3)	-4(3)	17(4)
C(15)	61(7)	21(4)	21(4)	-4(3)	8(4)	5(4)
C(16)	31(5)	66(8)	24(4)	-3(5)	3(4)	-2(5)
C(17)	20(3)	8(3)	17(3)	1(3)	-3(3)	-1(3)
C(18)	23(4)	9(3)	17(3)	2(3)	-5(3)	0(3)
C(19)	19(3)	8(3)	16(3)	2(2)	-1(3)	2(2)
C(20)	13(3)	16(3)	11(3)	1(2)	0(2)	2(3)
C(21)	15(3)	13(3)	17(3)	-3(2)	2(2)	-3(2)
C(22)	15(3)	13(3)	17(3)	1(3)	4(3)	2(2)
C(23)	23(4)	12(3)	21(4)	-2(3)	3(3)	-1(3)
C(24)	33(4)	15(4)	23(4)	1(3)	4(3)	2(3)
C(25)	34(4)	15(4)	24(4)	5(3)	-8(3)	2(3)
C(26)	28(4)	19(4)	19(3)	-3(3)	1(3)	-1(3)
C(27)	19(3)	12(3)	21(3)	2(3)	4(3)	-1(3)
C(28)	20(3)	14(3)	16(3)	-2(3)	-1(3)	1(3)
C(29)	13(3)	10(3)	16(3)	0(2)	3(2)	-1(2)
C(30)	23(4)	13(3)	45(5)	5(3)	-14(4)	0(3)
C(31)	38(5)	24(4)	38(5)	-6(4)	-23(4)	10(4)
C(32)	28(5)	44(6)	52(6)	19(5)	9(4)	13(4)
C(33)	22(3)	13(3)	15(3)	-2(3)	-6(3)	0(3)
C(34)	24(4)	13(3)	15(3)	1(3)	-5(3)	-2(3)
C(35)	18(3)	15(3)	20(4)	2(3)	-3(3)	1(3)
C(36)	15(3)	13(3)	14(3)	2(3)	-1(2)	-1(3)
C(37)	15(3)	19(4)	15(3)	1(3)	-1(2)	0(3)
C(38)	12(3)	18(3)	15(3)	-4(3)	5(2)	-5(3)
C(39)	16(3)	25(4)	16(3)	2(3)	-3(3)	-4(3)
C(40)	21(4)	25(4)	23(4)	-4(3)	-1(3)	-4(3)
C(41)	24(4)	19(4)	24(4)	-8(3)	-2(3)	-5(3)
C(42)	19(3)	24(4)	17(3)	-1(3)	-2(3)	-3(3)
C(43)	11(3)	16(3)	17(3)	-5(3)	1(2)	-2(3)
C(44)	12(3)	15(3)	15(3)	-1(3)	-1(2)	-5(3)
C(45)	16(3)	10(3)	12(3)	-1(2)	-2(2)	-2(2)
C(46)	46(5)	23(4)	13(3)	0(3)	-4(3)	-17(4)
C(47)	56(7)	41(6)	49(6)	-15(5)	29(6)	-17(5)
C(48)	46(6)	27(5)	39(5)	18(4)	-19(4)	-15(4)
C(49)	38(5)	35(5)	36(5)	4(4)	5(4)	7(4)

C(115)	69(6)	64(6)	81(6)	-12(5)	9(5)	-22(5)
C(116)	80(6)	59(6)	80(6)	-26(6)	4(6)	-8(6)
C(117)	57(5)	76(6)	76(6)	-3(5)	-1(5)	-22(5)
C(118)	75(6)	76(6)	63(6)	-21(5)	3(5)	-5(5)
C(119)	66(6)	72(6)	50(5)	-17(5)	26(5)	15(5)
C(120)	77(6)	48(6)	83(6)	-13(6)	8(6)	8(6)
C(121)	73(6)	56(6)	74(6)	-9(5)	13(6)	23(5)
C(122)	70(6)	69(6)	70(6)	-12(6)	24(6)	22(6)
C(123)	51(5)	83(6)	78(6)	14(6)	21(5)	-19(5)
C(124)	63(5)	69(6)	74(6)	17(5)	18(5)	-26(5)
C(125)	39(5)	80(6)	76(6)	11(6)	7(5)	-19(5)
C(126)	69(6)	56(6)	82(6)	3(5)	12(6)	-23(5)
C(127)	79(6)	50(6)	84(6)	12(6)	0(6)	-6(6)
C(128)	70(6)	75(6)	65(5)	29(5)	19(5)	-11(5)
C(129)	76(6)	71(6)	63(5)	31(5)	7(5)	-2(5)
C(130)	81(6)	56(5)	79(6)	24(5)	-1(5)	3(5)
C(131)	54(6)	83(6)	88(6)	6(6)	13(6)	21(6)
C(132)	53(5)	78(6)	78(6)	-2(6)	33(5)	22(5)
C(133)	50(5)	86(6)	83(6)	11(6)	0(5)	6(5)
C(134)	55(6)	90(6)	73(6)	12(6)	36(5)	-2(6)
C(135)	68(6)	86(6)	62(6)	13(6)	34(5)	-2(6)
C(136)	76(6)	73(6)	80(6)	-18(6)	32(6)	27(6)
C(137)	75(6)	73(6)	57(6)	-21(5)	28(5)	17(6)
C(138)	78(6)	88(6)	53(6)	2(6)	24(6)	8(6)
C(139)	64(6)	75(6)	62(6)	20(6)	-12(5)	17(6)
C(140)	74(6)	67(6)	85(6)	24(6)	3(6)	21(6)
C(141)	56(6)	89(6)	71(6)	16(6)	-11(5)	3(6)
C(142)	61(6)	60(6)	81(6)	9(6)	9(6)	35(5)
C(143)	78(6)	55(6)	83(6)	-12(5)	17(6)	27(5)
C(144)	80(6)	53(6)	79(6)	27(5)	8(6)	11(6)
C(145)	86(6)	47(6)	88(6)	5(6)	9(6)	-2(6)
C(146)	81(6)	44(5)	89(6)	-16(6)	14(6)	12(5)
C(147)	75(6)	88(6)	56(6)	-8(6)	-3(6)	-7(6)
C(148)	70(6)	83(6)	45(5)	4(5)	7(5)	4(5)
C(149)	63(6)	89(6)	66(6)	-3(6)	-13(5)	-5(6)
C(150)	71(6)	80(6)	54(5)	26(5)	-3(5)	0(6)

C(151)	78(6)	68(6)	62(6)	32(5)	12(5)	-1(6)
C(152)	72(6)	83(6)	50(6)	1(6)	22(6)	10(6)
C(153)	64(5)	79(6)	58(5)	13(5)	29(5)	-1(5)
C(154)	72(6)	71(6)	63(5)	24(5)	21(5)	-8(5)
C(155)	76(6)	63(6)	80(6)	-18(5)	12(6)	-23(5)
C(156)	74(6)	53(6)	79(6)	1(5)	15(6)	-19(5)
C(157)	69(6)	64(5)	73(6)	15(5)	20(5)	-22(5)
C(158)	64(6)	78(6)	74(6)	-10(5)	-3(5)	-25(5)
C(159)	78(6)	86(6)	55(6)	-13(6)	-4(6)	-7(6)
C(160)	85(6)	74(6)	69(6)	-28(5)	4(5)	-3(5)
C(161)	88(7)	63(6)	87(6)	-29(6)	14(6)	-5(6)
C(162)	61(6)	85(6)	63(6)	-7(6)	-11(5)	-5(6)
C(163)	65(6)	70(6)	55(6)	20(6)	-21(5)	18(6)
C(164)	74(6)	77(6)	50(6)	30(6)	-9(6)	-2(6)
C(165)	75(6)	84(6)	45(5)	6(5)	8(5)	1(6)
C(166)	53(6)	85(6)	65(6)	16(6)	-18(6)	2(6)
C(167)	53(5)	80(6)	77(6)	10(6)	8(5)	18(6)
C(168)	61(6)	60(6)	73(6)	11(6)	-2(5)	24(5)
C(169)	72(6)	63(6)	78(6)	22(6)	-5(6)	18(6)
C(170)	48(5)	84(6)	76(6)	12(6)	-4(6)	4(6)
C(171)	55(5)	75(6)	72(6)	14(5)	21(5)	-20(5)
C(172)	52(6)	80(6)	61(6)	10(6)	33(5)	-4(6)
C(173)	50(5)	76(6)	70(6)	1(5)	24(5)	15(5)
C(174)	45(5)	80(6)	71(6)	6(6)	4(5)	-20(5)
C(215)	67(6)	77(6)	70(6)	22(5)	27(5)	-12(6)
C(216)	71(6)	57(6)	73(6)	24(5)	11(6)	-11(6)
C(217)	56(6)	80(6)	76(6)	16(6)	27(5)	-15(5)
C(218)	66(6)	52(6)	78(6)	9(6)	8(6)	-14(6)
C(219)	74(6)	51(5)	80(6)	-2(6)	8(6)	0(6)
C(220)	79(6)	69(6)	68(6)	30(6)	2(6)	1(6)
C(221)	71(6)	64(6)	76(6)	27(6)	-5(6)	14(6)
C(222)	74(6)	55(6)	85(6)	9(6)	2(6)	14(6)
C(223)	67(6)	83(6)	68(6)	0(6)	35(5)	15(6)
C(224)	73(7)	84(7)	53(6)	0(6)	30(6)	8(6)
C(225)	50(6)	82(7)	81(6)	9(6)	33(6)	7(6)
C(226)	72(6)	81(6)	53(6)	21(6)	21(6)	-2(6)

C(227)	79(7)	79(6)	54(6)	27(6)	5(6)	-1(6)
C(228)	83(6)	83(6)	59(6)	-14(6)	13(6)	6(6)
C(229)	79(7)	86(7)	58(6)	-11(6)	-5(6)	-5(6)
C(230)	75(7)	84(7)	52(6)	13(6)	-11(6)	1(6)
C(231)	54(6)	74(6)	84(6)	12(6)	9(6)	25(6)
C(232)	62(6)	66(6)	85(6)	-4(6)	20(6)	32(6)
C(233)	38(6)	77(7)	80(7)	4(6)	17(6)	12(6)
C(234)	74(6)	73(6)	78(6)	-16(6)	30(6)	27(6)
C(235)	83(6)	67(6)	75(6)	-23(6)	19(6)	12(6)
C(236)	75(6)	54(6)	87(6)	6(6)	11(6)	21(6)
C(237)	80(6)	47(6)	83(6)	-10(6)	17(6)	4(6)
C(238)	84(7)	60(6)	83(7)	-27(6)	14(6)	-4(6)
C(239)	53(6)	85(6)	76(6)	1(6)	-9(6)	-5(6)
C(240)	60(6)	85(6)	67(6)	15(6)	-10(6)	4(6)
C(241)	46(6)	80(6)	81(6)	6(6)	2(6)	-8(6)
C(242)	61(6)	77(6)	80(6)	14(6)	-3(6)	18(6)
C(243)	73(6)	61(6)	83(6)	28(6)	1(6)	18(6)
C(244)	68(6)	87(6)	57(6)	10(6)	-8(6)	2(6)
C(245)	75(6)	79(6)	57(6)	23(6)	6(6)	4(6)
C(246)	79(6)	67(6)	71(6)	28(6)	7(6)	7(6)
C(247)	62(6)	61(6)	77(7)	-1(6)	11(6)	-20(6)
C(248)	74(6)	66(6)	75(7)	-14(6)	0(6)	-16(6)
C(249)	53(6)	70(6)	80(6)	5(6)	12(6)	-22(5)
C(250)	69(6)	82(6)	72(6)	-10(6)	-6(6)	-11(6)
C(251)	75(6)	88(7)	56(6)	-7(6)	-3(6)	-4(6)
C(252)	79(7)	59(6)	80(6)	-22(6)	8(6)	-6(6)
C(253)	76(6)	66(6)	72(6)	-19(6)	14(6)	10(6)
C(254)	78(6)	82(6)	57(6)	-12(6)	10(6)	6(6)
C(255)	66(6)	72(6)	66(6)	19(5)	25(5)	-10(5)
C(256)	71(6)	78(6)	52(6)	18(5)	19(5)	1(6)
C(257)	71(6)	82(6)	50(6)	0(6)	25(6)	9(6)
C(258)	56(6)	73(6)	68(6)	14(6)	25(5)	-15(5)
C(259)	68(6)	58(6)	75(7)	-5(6)	11(6)	-25(6)
C(260)	72(6)	49(6)	79(6)	4(5)	14(6)	-10(6)
C(261)	75(6)	55(6)	71(6)	23(5)	18(6)	-11(5)
C(262)	59(6)	67(6)	75(6)	1(6)	10(6)	-25(5)

C(263)	57(6)	85(6)	72(6)	0(6)	-13(6)	-8(6)
C(264)	77(6)	81(6)	70(6)	-14(6)	-5(6)	-15(6)
C(265)	80(7)	66(6)	77(7)	-20(6)	-1(6)	-17(6)
C(266)	52(5)	80(6)	73(6)	3(6)	-5(5)	-10(6)
C(267)	55(6)	75(6)	79(6)	12(6)	4(6)	18(6)
C(268)	62(6)	77(6)	74(6)	17(6)	-10(6)	15(6)
C(269)	64(6)	84(7)	61(6)	16(6)	-20(6)	5(6)
C(270)	43(6)	78(7)	73(6)	6(6)	8(6)	5(6)
C(271)	63(6)	79(6)	60(6)	0(6)	30(5)	11(6)
C(272)	70(6)	70(6)	73(6)	-12(6)	21(6)	21(6)
C(273)	60(6)	66(6)	78(6)	-2(6)	11(6)	24(6)
C(274)	53(6)	78(6)	70(6)	9(6)	29(6)	2(6)
C(55)	56(9)	98(11)	137(11)	-8(10)	12(10)	47(9)
C(56)	67(10)	104(11)	130(11)	16(11)	-17(10)	40(10)
C(57)	43(9)	113(11)	120(11)	-31(10)	28(9)	9(9)
C(58)	52(9)	112(11)	100(11)	4(10)	-40(9)	21(9)
C(59)	91(10)	120(11)	76(10)	1(10)	-41(9)	4(10)
C(60)	95(11)	92(11)	118(11)	27(10)	-10(10)	40(10)
C(61)	108(11)	89(10)	75(10)	42(10)	-3(10)	40(10)
C(62)	95(10)	108(11)	55(9)	22(10)	-16(9)	25(10)
C(63)	67(9)	85(10)	59(9)	-48(8)	43(8)	2(9)
C(64)	105(10)	82(10)	93(10)	-50(9)	31(9)	31(9)
C(65)	61(9)	102(11)	88(10)	-26(9)	57(8)	-7(9)
C(66)	100(11)	95(10)	137(11)	-23(10)	11(10)	48(10)
C(67)	85(11)	68(10)	122(12)	1(10)	12(10)	45(9)
C(68)	106(11)	74(10)	85(10)	-54(9)	11(10)	-6(10)
C(69)	111(11)	72(10)	109(11)	-29(10)	-17(10)	-19(10)
C(70)	114(11)	74(10)	119(12)	-5(10)	0(11)	0(11)
C(71)	105(11)	97(11)	70(10)	25(10)	40(10)	3(10)
C(72)	98(11)	106(11)	42(9)	11(9)	18(9)	21(10)
C(73)	81(10)	108(11)	96(11)	4(10)	48(9)	-22(10)
C(74)	84(10)	96(10)	35(8)	-31(9)	16(8)	2(9)
C(75)	100(11)	94(11)	71(10)	-42(9)	-9(9)	-7(10)
C(76)	95(11)	110(11)	53(10)	18(10)	-13(9)	28(10)
C(77)	99(11)	115(11)	81(10)	0(10)	-42(10)	8(10)
C(78)	80(10)	102(11)	71(10)	-28(10)	-34(9)	-22(10)

C(79)	103(11)	97(11)	131(11)	16(10)	10(10)	-43(10)
C(80)	113(11)	71(10)	115(11)	30(10)	22(10)	-25(10)
C(81)	57(9)	99(11)	113(11)	9(10)	42(9)	-47(9)
C(82)	116(11)	90(11)	100(11)	35(10)	25(10)	1(10)
C(83)	101(11)	82(10)	78(10)	45(9)	5(10)	44(10)
C(84)	121(11)	58(9)	122(12)	12(10)	3(10)	-6(10)
C(85)	98(11)	42(9)	120(11)	15(9)	14(10)	33(9)
C(86)	97(11)	73(10)	111(11)	35(10)	-2(10)	39(10)
C(87)	37(8)	116(11)	118(11)	-3(10)	-23(9)	-22(9)
C(88)	45(9)	98(11)	83(10)	-22(9)	-22(8)	-40(9)
C(89)	28(8)	114(11)	126(11)	-15(10)	21(9)	-22(9)
C(90)	83(10)	75(10)	104(11)	-10(10)	-13(10)	-57(9)
C(91)	113(11)	69(10)	112(11)	-13(10)	-15(10)	-23(10)
C(92)	66(9)	101(11)	65(10)	-30(9)	-21(9)	-22(9)
C(93)	89(10)	85(10)	62(9)	-41(9)	-4(9)	-12(9)
C(94)	109(11)	67(10)	81(10)	-38(9)	8(10)	-12(10)
C(95)	78(10)	92(11)	131(11)	-8(10)	16(10)	36(10)
C(96)	114(11)	83(10)	129(11)	-20(10)	9(10)	31(10)
C(97)	109(11)	71(10)	76(10)	-35(9)	27(9)	24(10)
C(98)	70(10)	110(11)	113(11)	-32(10)	29(10)	11(10)
C(99)	57(10)	107(11)	119(11)	-2(10)	-21(10)	-19(10)
C(100)	65(10)	99(11)	102(11)	0(10)	-32(10)	20(10)
C(101)	75(10)	91(11)	121(11)	11(10)	-11(10)	36(10)
C(102)	64(10)	114(11)	126(11)	-17(11)	12(10)	-18(10)
C(103)	109(11)	96(11)	119(11)	-2(10)	11(11)	-39(10)
C(104)	90(10)	73(10)	97(11)	-20(9)	-20(10)	-53(9)
C(105)	65(10)	92(11)	94(11)	-26(10)	-26(9)	-44(9)
C(106)	82(10)	104(11)	108(11)	-3(10)	34(10)	-36(10)
C(107)	115(11)	102(11)	58(10)	18(10)	37(10)	4(10)
C(108)	127(11)	97(11)	86(11)	23(10)	9(10)	6(11)
C(109)	118(11)	79(10)	101(11)	7(10)	10(11)	-19(10)
C(110)	101(11)	116(11)	83(10)	-2(10)	43(10)	-20(10)
C(111)	76(10)	80(10)	52(9)	-43(8)	34(8)	3(9)
C(112)	80(10)	85(10)	30(8)	-26(8)	23(8)	7(9)
C(113)	99(10)	97(11)	33(8)	12(9)	16(9)	23(10)
C(114)	79(10)	106(11)	82(10)	-28(10)	47(9)	-4(10)

O(10)	41(8)	47(8)	42(8)	7(6)	-6(6)	2(6)
C(51)	39(10)	53(13)	33(10)	-13(9)	4(8)	-4(9)
C(52)	33(9)	54(10)	37(10)	16(8)	-3(8)	11(8)
C(53)	53(12)	57(11)	56(12)	3(10)	-7(10)	-1(10)
C(54)	52(14)	49(14)	83(18)	-11(13)	4(14)	-11(12)
Cl(4)	88(3)	77(3)	45(2)	-2(2)	3(2)	-26(2)
Cl(5)	61(2)	49(2)	82(3)	7(2)	-1(2)	-3(2)
Cl(6)	70(2)	68(2)	55(2)	4(2)	-3(2)	18(2)
C(50)	55(7)	41(6)	53(7)	12(5)	1(6)	-4(6)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 19949ds_sq.

	x	y	z	U(eq)
H(2)	7783	6741	3816	18
H(5)	6374	7421	2237	19
H(7)	5721	7602	1413	23
H(8)	5103	7112	722	28
H(9)	4920	5840	658	29
H(10)	5318	5066	1297	23
H(12)	5973	4882	2108	17
H(14)	6567	7125	3958	35
H(15A)	7461	7661	4449	51
H(15B)	7614	6935	4763	51
H(15C)	6902	7391	4809	51
H(16A)	6009	6504	4551	60
H(16B)	6622	5898	4592	60
H(16C)	6100	5970	4103	60
H(18)	6632	2759	2408	20
H(21)	7031	83	2828	18
H(23)	7437	-1164	3086	23
H(24)	8063	-1912	3642	28
H(25)	8625	-1432	4370	30
H(26)	8563	-194	4543	26
H(28)	8140	1052	4301	20
H(30)	5553	2163	2603	34
H(31A)	5467	3061	1982	52
H(31B)	5322	3673	2373	52
H(31C)	4756	3034	2251	52
H(32A)	5341	3338	3237	61
H(32B)	5609	2550	3426	61
H(32C)	4840	2640	3135	61
H(34)	9173	2722	5042	21
H(37)	10386	4670	6123	20

H(39)	10974	5739	6552	23
H(40)	11096	6990	6638	28
H(41)	10453	7786	6088	27
H(42)	9628	7327	5482	24
H(44)	8984	6271	5076	17
H(46)	8710	2792	5825	33
H(47A)	7692	3486	5596	71
H(47B)	7498	2760	5876	71
H(47C)	7344	2806	5297	71
H(48A)	8029	1661	5240	58
H(48B)	8254	1624	5813	58
H(48C)	8852	1635	5442	58
H(49)	9740	4118	7716	44
H(51A)	3648	3997	5600	62
H(51B)	4392	4191	5898	62
H(51C)	4267	3400	5661	62
H(52)	4180	4482	4929	51
H(53A)	5300	4607	4605	67
H(53B)	5149	3780	4433	67
H(54A)	6281	3572	4495	92
H(54B)	6333	3768	5061	92
H(54C)	6431	4395	4670	92
H(50)	8000	9050	6105	60

Table 6. Torsion angles [°] for 19949ds_sq.

I(3)-O(1)-C(1)-O(2)	0.9(10)
I(3)-O(1)-C(1)-C(2)	178.4(6)
C(3)-N(1)-C(2)-C(1)	-160.6(7)
I(1)-N(1)-C(2)-C(1)	10.4(9)
C(3)-N(1)-C(2)-C(14)	76.5(9)
I(1)-N(1)-C(2)-C(14)	-112.5(7)
O(2)-C(1)-C(2)-N(1)	-15.7(11)
O(1)-C(1)-C(2)-N(1)	166.8(7)
O(2)-C(1)-C(2)-C(14)	107.9(9)
O(1)-C(1)-C(2)-C(14)	-69.6(9)
C(2)-N(1)-C(3)-O(3)	0.4(12)
I(1)-N(1)-C(3)-O(3)	-171.3(7)
C(2)-N(1)-C(3)-C(4)	-177.7(6)
I(1)-N(1)-C(3)-C(4)	10.6(8)
O(3)-C(3)-C(4)-C(5)	-5.6(12)
N(1)-C(3)-C(4)-C(5)	172.5(7)
O(3)-C(3)-C(4)-C(13)	176.7(8)
N(1)-C(3)-C(4)-C(13)	-5.2(10)
C(13)-C(4)-C(5)-C(6)	-0.2(11)
C(3)-C(4)-C(5)-C(6)	-177.9(7)
C(4)-C(5)-C(6)-C(11)	-0.4(11)
C(4)-C(5)-C(6)-C(7)	179.9(7)
C(5)-C(6)-C(7)-C(8)	179.8(7)
C(11)-C(6)-C(7)-C(8)	0.1(12)
C(6)-C(7)-C(8)-C(9)	-0.3(13)
C(7)-C(8)-C(9)-C(10)	1.1(14)
C(8)-C(9)-C(10)-C(11)	-1.7(13)
C(9)-C(10)-C(11)-C(6)	1.5(12)
C(9)-C(10)-C(11)-C(12)	-179.4(8)
C(5)-C(6)-C(11)-C(10)	179.6(7)
C(7)-C(6)-C(11)-C(10)	-0.7(11)
C(5)-C(6)-C(11)-C(12)	0.5(11)
C(7)-C(6)-C(11)-C(12)	-179.8(7)
C(10)-C(11)-C(12)-C(13)	-179.0(7)

C(6)-C(11)-C(12)-C(13)	0.1(11)
C(11)-C(12)-C(13)-C(4)	-0.8(11)
C(11)-C(12)-C(13)-I(1)	-179.3(5)
C(5)-C(4)-C(13)-C(12)	0.8(11)
C(3)-C(4)-C(13)-C(12)	178.6(7)
C(5)-C(4)-C(13)-I(1)	179.5(5)
C(3)-C(4)-C(13)-I(1)	-2.7(9)
N(1)-C(2)-C(14)-C(16)	76.4(9)
C(1)-C(2)-C(14)-C(16)	-47.2(9)
N(1)-C(2)-C(14)-C(15)	-158.6(7)
C(1)-C(2)-C(14)-C(15)	77.8(9)
I(1)-O(4)-C(17)-O(5)	-1.6(10)
I(1)-O(4)-C(17)-C(18)	178.5(5)
C(19)-N(2)-C(18)-C(17)	-164.7(7)
I(2)-N(2)-C(18)-C(17)	6.6(9)
C(19)-N(2)-C(18)-C(30)	73.6(9)
I(2)-N(2)-C(18)-C(30)	-115.1(7)
O(5)-C(17)-C(18)-N(2)	-13.0(11)
O(4)-C(17)-C(18)-N(2)	167.0(7)
O(5)-C(17)-C(18)-C(30)	109.2(9)
O(4)-C(17)-C(18)-C(30)	-70.8(9)
C(18)-N(2)-C(19)-O(6)	0.2(12)
I(2)-N(2)-C(19)-O(6)	-171.8(6)
C(18)-N(2)-C(19)-C(20)	-178.9(6)
I(2)-N(2)-C(19)-C(20)	9.1(8)
O(6)-C(19)-C(20)-C(21)	-5.4(12)
N(2)-C(19)-C(20)-C(21)	173.7(7)
O(6)-C(19)-C(20)-C(29)	173.4(7)
N(2)-C(19)-C(20)-C(29)	-7.4(10)
C(29)-C(20)-C(21)-C(22)	-0.3(11)
C(19)-C(20)-C(21)-C(22)	178.5(7)
C(20)-C(21)-C(22)-C(27)	-1.3(11)
C(20)-C(21)-C(22)-C(23)	-179.6(7)
C(21)-C(22)-C(23)-C(24)	178.3(8)
C(27)-C(22)-C(23)-C(24)	0.0(11)
C(22)-C(23)-C(24)-C(25)	0.4(13)

C(23)-C(24)-C(25)-C(26)	-0.1(14)
C(24)-C(25)-C(26)-C(27)	-0.5(14)
C(21)-C(22)-C(27)-C(28)	2.0(11)
C(23)-C(22)-C(27)-C(28)	-179.7(7)
C(21)-C(22)-C(27)-C(26)	-178.9(7)
C(23)-C(22)-C(27)-C(26)	-0.6(11)
C(25)-C(26)-C(27)-C(28)	179.9(8)
C(25)-C(26)-C(27)-C(22)	0.9(12)
C(22)-C(27)-C(28)-C(29)	-1.1(11)
C(26)-C(27)-C(28)-C(29)	179.8(7)
C(27)-C(28)-C(29)-C(20)	-0.5(11)
C(27)-C(28)-C(29)-I(2)	179.8(5)
C(21)-C(20)-C(29)-C(28)	1.2(11)
C(19)-C(20)-C(29)-C(28)	-177.6(7)
C(21)-C(20)-C(29)-I(2)	-179.1(5)
C(19)-C(20)-C(29)-I(2)	2.1(8)
N(2)-C(18)-C(30)-C(32)	67.7(9)
C(17)-C(18)-C(30)-C(32)	-54.1(9)
N(2)-C(18)-C(30)-C(31)	-167.2(7)
C(17)-C(18)-C(30)-C(31)	71.0(9)
I(2)-O(7)-C(33)-O(8)	5.3(10)
I(2)-O(7)-C(33)-C(34)	-176.7(6)
C(35)-N(3)-C(34)-C(33)	-162.3(7)
I(3)-N(3)-C(34)-C(33)	8.7(9)
C(35)-N(3)-C(34)-C(46)	73.3(9)
I(3)-N(3)-C(34)-C(46)	-115.6(7)
O(8)-C(33)-C(34)-N(3)	-14.6(11)
O(7)-C(33)-C(34)-N(3)	167.3(7)
O(8)-C(33)-C(34)-C(46)	109.4(9)
O(7)-C(33)-C(34)-C(46)	-68.7(10)
C(34)-N(3)-C(35)-O(9)	1.5(12)
I(3)-N(3)-C(35)-O(9)	-170.2(7)
C(34)-N(3)-C(35)-C(36)	-178.3(7)
I(3)-N(3)-C(35)-C(36)	10.0(9)
O(9)-C(35)-C(36)-C(37)	-7.6(13)
N(3)-C(35)-C(36)-C(37)	172.2(7)

O(9)-C(35)-C(36)-C(45)	172.9(8)
N(3)-C(35)-C(36)-C(45)	-7.3(10)
C(45)-C(36)-C(37)-C(38)	-1.1(11)
C(35)-C(36)-C(37)-C(38)	179.5(7)
C(36)-C(37)-C(38)-C(39)	178.0(7)
C(36)-C(37)-C(38)-C(43)	-2.6(11)
C(37)-C(38)-C(39)-C(40)	-179.7(7)
C(43)-C(38)-C(39)-C(40)	0.9(11)
C(38)-C(39)-C(40)-C(41)	-2.2(13)
C(39)-C(40)-C(41)-C(42)	2.1(13)
C(40)-C(41)-C(42)-C(43)	-0.6(12)
C(41)-C(42)-C(43)-C(44)	177.0(7)
C(41)-C(42)-C(43)-C(38)	-0.6(12)
C(37)-C(38)-C(43)-C(42)	-178.9(7)
C(39)-C(38)-C(43)-C(42)	0.5(11)
C(37)-C(38)-C(43)-C(44)	3.4(10)
C(39)-C(38)-C(43)-C(44)	-177.2(7)
C(42)-C(43)-C(44)-C(45)	-178.1(7)
C(38)-C(43)-C(44)-C(45)	-0.5(10)
C(43)-C(44)-C(45)-C(36)	-3.3(11)
C(43)-C(44)-C(45)-I(3)	179.8(5)
C(37)-C(36)-C(45)-C(44)	4.2(11)
C(35)-C(36)-C(45)-C(44)	-176.3(7)
C(37)-C(36)-C(45)-I(3)	-178.5(5)
C(35)-C(36)-C(45)-I(3)	1.0(8)
N(3)-C(34)-C(46)-C(47)	70.5(9)
C(33)-C(34)-C(46)-C(47)	-53.3(9)
N(3)-C(34)-C(46)-C(48)	-164.3(7)
C(33)-C(34)-C(46)-C(48)	71.8(10)
C(117)-C(115)-C(116)-C(118)	0.0
C(126)-C(115)-C(116)-C(118)	-142.6
C(117)-C(115)-C(116)-C(120)	142.6
C(126)-C(115)-C(116)-C(120)	0.0
C(126)-C(115)-C(117)-C(125)	0.0
C(116)-C(115)-C(117)-C(125)	-138.2
C(126)-C(115)-C(117)-C(149)	138.2

C(116)-C(115)-C(117)-C(149)	0.0
C(115)-C(116)-C(118)-C(147)	0.0
C(120)-C(116)-C(118)-C(147)	-138.2
C(115)-C(116)-C(118)-C(119)	138.2
C(120)-C(116)-C(118)-C(119)	0.0
C(116)-C(118)-C(119)-C(122)	0.0
C(147)-C(118)-C(119)-C(122)	142.6
C(116)-C(118)-C(119)-C(152)	-142.6
C(147)-C(118)-C(119)-C(152)	0.0
C(118)-C(116)-C(120)-C(121)	0.0
C(115)-C(116)-C(120)-C(121)	-142.6
C(118)-C(116)-C(120)-C(127)	142.6
C(115)-C(116)-C(120)-C(127)	0.0
C(127)-C(120)-C(121)-C(122)	-138.2
C(116)-C(120)-C(121)-C(122)	0.0
C(127)-C(120)-C(121)-C(168)	0.0
C(116)-C(120)-C(121)-C(168)	138.2
C(152)-C(119)-C(122)-C(121)	138.2
C(118)-C(119)-C(122)-C(121)	0.0
C(152)-C(119)-C(122)-C(173)	0.0
C(118)-C(119)-C(122)-C(173)	-138.2
C(120)-C(121)-C(122)-C(119)	0.0
C(168)-C(121)-C(122)-C(119)	-142.6
C(120)-C(121)-C(122)-C(173)	142.6
C(168)-C(121)-C(122)-C(173)	0.0
C(125)-C(123)-C(124)-C(126)	0.0
C(134)-C(123)-C(124)-C(126)	-142.6
C(125)-C(123)-C(124)-C(128)	142.6
C(134)-C(123)-C(124)-C(128)	0.0
C(124)-C(123)-C(125)-C(117)	0.0
C(134)-C(123)-C(125)-C(117)	138.2
C(124)-C(123)-C(125)-C(133)	-138.2
C(134)-C(123)-C(125)-C(133)	0.0
C(115)-C(117)-C(125)-C(123)	0.0
C(149)-C(117)-C(125)-C(123)	-142.6
C(115)-C(117)-C(125)-C(133)	142.6

C(149)-C(117)-C(125)-C(133)	0.0
C(128)-C(124)-C(126)-C(115)	-138.2
C(123)-C(124)-C(126)-C(115)	0.0
C(128)-C(124)-C(126)-C(127)	0.0
C(123)-C(124)-C(126)-C(127)	138.2
C(117)-C(115)-C(126)-C(124)	0.0
C(116)-C(115)-C(126)-C(124)	142.6
C(117)-C(115)-C(126)-C(127)	-142.6
C(116)-C(115)-C(126)-C(127)	0.0
C(121)-C(120)-C(127)-C(130)	0.0
C(116)-C(120)-C(127)-C(130)	-142.6
C(121)-C(120)-C(127)-C(126)	142.6
C(116)-C(120)-C(127)-C(126)	0.0
C(124)-C(126)-C(127)-C(130)	0.0
C(115)-C(126)-C(127)-C(130)	142.6
C(124)-C(126)-C(127)-C(120)	-142.6
C(115)-C(126)-C(127)-C(120)	0.0
C(126)-C(124)-C(128)-C(129)	0.0
C(123)-C(124)-C(128)-C(129)	-142.6
C(126)-C(124)-C(128)-C(135)	142.6
C(123)-C(124)-C(128)-C(135)	0.0
C(135)-C(128)-C(129)-C(130)	-138.2
C(124)-C(128)-C(129)-C(130)	0.0
C(135)-C(128)-C(129)-C(164)	0.0
C(124)-C(128)-C(129)-C(164)	138.2
C(120)-C(127)-C(130)-C(129)	138.2
C(126)-C(127)-C(130)-C(129)	0.0
C(120)-C(127)-C(130)-C(169)	0.0
C(126)-C(127)-C(130)-C(169)	-138.2
C(128)-C(129)-C(130)-C(127)	0.0
C(164)-C(129)-C(130)-C(127)	-142.6
C(128)-C(129)-C(130)-C(169)	142.6
C(164)-C(129)-C(130)-C(169)	0.0
C(133)-C(131)-C(132)-C(134)	0.0
C(142)-C(131)-C(132)-C(134)	-142.6
C(133)-C(131)-C(132)-C(136)	142.6

C(142)-C(131)-C(132)-C(136)	0.0
C(132)-C(131)-C(133)-C(125)	0.0
C(142)-C(131)-C(133)-C(125)	138.2
C(132)-C(131)-C(133)-C(141)	-138.2
C(142)-C(131)-C(133)-C(141)	0.0
C(123)-C(125)-C(133)-C(131)	0.0
C(117)-C(125)-C(133)-C(131)	-142.6
C(123)-C(125)-C(133)-C(141)	142.6
C(117)-C(125)-C(133)-C(141)	0.0
C(136)-C(132)-C(134)-C(135)	0.0
C(131)-C(132)-C(134)-C(135)	138.2
C(136)-C(132)-C(134)-C(123)	-138.2
C(131)-C(132)-C(134)-C(123)	0.0
C(125)-C(123)-C(134)-C(132)	0.0
C(124)-C(123)-C(134)-C(132)	142.6
C(125)-C(123)-C(134)-C(135)	-142.6
C(124)-C(123)-C(134)-C(135)	0.0
C(129)-C(128)-C(135)-C(138)	0.0
C(124)-C(128)-C(135)-C(138)	-142.6
C(129)-C(128)-C(135)-C(134)	142.6
C(124)-C(128)-C(135)-C(134)	0.0
C(132)-C(134)-C(135)-C(138)	0.0
C(123)-C(134)-C(135)-C(138)	142.6
C(132)-C(134)-C(135)-C(128)	-142.6
C(123)-C(134)-C(135)-C(128)	0.0
C(134)-C(132)-C(136)-C(137)	0.0
C(131)-C(132)-C(136)-C(137)	-142.6
C(134)-C(132)-C(136)-C(143)	142.6
C(131)-C(132)-C(136)-C(143)	0.0
C(132)-C(136)-C(137)-C(160)	138.2
C(143)-C(136)-C(137)-C(160)	0.0
C(132)-C(136)-C(137)-C(138)	0.0
C(143)-C(136)-C(137)-C(138)	-138.2
C(128)-C(135)-C(138)-C(165)	0.0
C(134)-C(135)-C(138)-C(165)	-138.2
C(128)-C(135)-C(138)-C(137)	138.2

C(134)-C(135)-C(138)-C(137)	0.0
C(136)-C(137)-C(138)-C(135)	0.0
C(160)-C(137)-C(138)-C(135)	-142.6
C(136)-C(137)-C(138)-C(165)	142.6
C(160)-C(137)-C(138)-C(165)	0.0
C(141)-C(139)-C(140)-C(142)	0.0
C(150)-C(139)-C(140)-C(142)	-142.6
C(141)-C(139)-C(140)-C(144)	142.6
C(150)-C(139)-C(140)-C(144)	0.0
C(150)-C(139)-C(141)-C(133)	138.2
C(140)-C(139)-C(141)-C(133)	0.0
C(150)-C(139)-C(141)-C(149)	0.0
C(140)-C(139)-C(141)-C(149)	-138.2
C(131)-C(133)-C(141)-C(139)	0.0
C(125)-C(133)-C(141)-C(139)	-142.6
C(131)-C(133)-C(141)-C(149)	142.6
C(125)-C(133)-C(141)-C(149)	0.0
C(144)-C(140)-C(142)-C(143)	0.0
C(139)-C(140)-C(142)-C(143)	138.2
C(144)-C(140)-C(142)-C(131)	-138.2
C(139)-C(140)-C(142)-C(131)	0.0
C(133)-C(131)-C(142)-C(140)	0.0
C(132)-C(131)-C(142)-C(140)	142.6
C(133)-C(131)-C(142)-C(143)	-142.6
C(132)-C(131)-C(142)-C(143)	0.0
C(137)-C(136)-C(143)-C(146)	0.0
C(132)-C(136)-C(143)-C(146)	-142.6
C(137)-C(136)-C(143)-C(142)	142.6
C(132)-C(136)-C(143)-C(142)	0.0
C(140)-C(142)-C(143)-C(146)	0.0
C(131)-C(142)-C(143)-C(146)	142.6
C(140)-C(142)-C(143)-C(136)	-142.6
C(131)-C(142)-C(143)-C(136)	0.0
C(142)-C(140)-C(144)-C(145)	0.0
C(139)-C(140)-C(144)-C(145)	-142.6
C(142)-C(140)-C(144)-C(151)	142.6

C(139)-C(140)-C(144)-C(151)	0.0
C(151)-C(144)-C(145)-C(146)	-138.2
C(140)-C(144)-C(145)-C(146)	0.0
C(151)-C(144)-C(145)-C(156)	0.0
C(140)-C(144)-C(145)-C(156)	138.2
C(136)-C(143)-C(146)-C(145)	138.2
C(142)-C(143)-C(146)-C(145)	0.0
C(136)-C(143)-C(146)-C(161)	0.0
C(142)-C(143)-C(146)-C(161)	-138.2
C(144)-C(145)-C(146)-C(143)	0.0
C(156)-C(145)-C(146)-C(143)	-142.6
C(144)-C(145)-C(146)-C(161)	142.6
C(156)-C(145)-C(146)-C(161)	0.0
C(116)-C(118)-C(147)-C(149)	0.0
C(119)-C(118)-C(147)-C(149)	-142.6
C(116)-C(118)-C(147)-C(148)	142.6
C(119)-C(118)-C(147)-C(148)	0.0
C(149)-C(147)-C(148)-C(150)	0.0
C(118)-C(147)-C(148)-C(150)	-142.6
C(149)-C(147)-C(148)-C(152)	142.6
C(118)-C(147)-C(148)-C(152)	0.0
C(118)-C(147)-C(149)-C(117)	0.0
C(148)-C(147)-C(149)-C(117)	-138.2
C(118)-C(147)-C(149)-C(141)	138.2
C(148)-C(147)-C(149)-C(141)	0.0
C(115)-C(117)-C(149)-C(147)	0.0
C(125)-C(117)-C(149)-C(147)	142.6
C(115)-C(117)-C(149)-C(141)	-142.6
C(125)-C(117)-C(149)-C(141)	0.0
C(139)-C(141)-C(149)-C(147)	0.0
C(133)-C(141)-C(149)-C(147)	-142.6
C(139)-C(141)-C(149)-C(117)	142.6
C(133)-C(141)-C(149)-C(117)	0.0
C(152)-C(148)-C(150)-C(151)	0.0
C(147)-C(148)-C(150)-C(151)	138.2
C(152)-C(148)-C(150)-C(139)	-138.2

C(147)-C(148)-C(150)-C(139)	0.0
C(141)-C(139)-C(150)-C(148)	0.0
C(140)-C(139)-C(150)-C(148)	142.6
C(141)-C(139)-C(150)-C(151)	-142.6
C(140)-C(139)-C(150)-C(151)	0.0
C(148)-C(150)-C(151)-C(154)	0.0
C(139)-C(150)-C(151)-C(154)	142.6
C(148)-C(150)-C(151)-C(144)	-142.6
C(139)-C(150)-C(151)-C(144)	0.0
C(145)-C(144)-C(151)-C(154)	0.0
C(140)-C(144)-C(151)-C(154)	-142.6
C(145)-C(144)-C(151)-C(150)	142.6
C(140)-C(144)-C(151)-C(150)	0.0
C(122)-C(119)-C(152)-C(153)	0.0
C(118)-C(119)-C(152)-C(153)	142.6
C(122)-C(119)-C(152)-C(148)	-142.6
C(118)-C(119)-C(152)-C(148)	0.0
C(150)-C(148)-C(152)-C(153)	0.0
C(147)-C(148)-C(152)-C(153)	-142.6
C(150)-C(148)-C(152)-C(119)	142.6
C(147)-C(148)-C(152)-C(119)	0.0
C(119)-C(152)-C(153)-C(154)	-138.2
C(148)-C(152)-C(153)-C(154)	0.0
C(119)-C(152)-C(153)-C(172)	0.0
C(148)-C(152)-C(153)-C(172)	138.2
C(150)-C(151)-C(154)-C(153)	0.0
C(144)-C(151)-C(154)-C(153)	138.2
C(150)-C(151)-C(154)-C(157)	-138.2
C(144)-C(151)-C(154)-C(157)	0.0
C(152)-C(153)-C(154)-C(151)	0.0
C(172)-C(153)-C(154)-C(151)	-142.6
C(152)-C(153)-C(154)-C(157)	142.6
C(172)-C(153)-C(154)-C(157)	0.0
C(144)-C(145)-C(156)-C(157)	0.0
C(146)-C(145)-C(156)-C(157)	142.6
C(144)-C(145)-C(156)-C(155)	-142.6

C(146)-C(145)-C(156)-C(155)	0.0
C(158)-C(155)-C(156)-C(157)	0.0
C(161)-C(155)-C(156)-C(157)	-142.6
C(158)-C(155)-C(156)-C(145)	142.6
C(161)-C(155)-C(156)-C(145)	0.0
C(145)-C(156)-C(157)-C(171)	-138.2
C(155)-C(156)-C(157)-C(171)	0.0
C(145)-C(156)-C(157)-C(154)	0.0
C(155)-C(156)-C(157)-C(154)	138.2
C(151)-C(154)-C(157)-C(156)	0.0
C(153)-C(154)-C(157)-C(156)	-142.6
C(151)-C(154)-C(157)-C(171)	142.6
C(153)-C(154)-C(157)-C(171)	0.0
C(161)-C(155)-C(158)-C(174)	138.2
C(156)-C(155)-C(158)-C(174)	0.0
C(161)-C(155)-C(158)-C(162)	0.0
C(156)-C(155)-C(158)-C(162)	-138.2
C(136)-C(137)-C(160)-C(161)	0.0
C(138)-C(137)-C(160)-C(161)	142.6
C(136)-C(137)-C(160)-C(159)	-142.6
C(138)-C(137)-C(160)-C(159)	0.0
C(162)-C(159)-C(160)-C(161)	0.0
C(165)-C(159)-C(160)-C(161)	-142.6
C(162)-C(159)-C(160)-C(137)	142.6
C(165)-C(159)-C(160)-C(137)	0.0
C(137)-C(160)-C(161)-C(155)	-138.2
C(159)-C(160)-C(161)-C(155)	0.0
C(137)-C(160)-C(161)-C(146)	0.0
C(159)-C(160)-C(161)-C(146)	138.2
C(158)-C(155)-C(161)-C(160)	0.0
C(156)-C(155)-C(161)-C(160)	142.6
C(158)-C(155)-C(161)-C(146)	-142.6
C(156)-C(155)-C(161)-C(146)	0.0
C(143)-C(146)-C(161)-C(160)	0.0
C(145)-C(146)-C(161)-C(160)	-142.6
C(143)-C(146)-C(161)-C(155)	142.6

C(145)-C(146)-C(161)-C(155)	0.0
C(165)-C(159)-C(162)-C(166)	0.0
C(160)-C(159)-C(162)-C(166)	-138.2
C(165)-C(159)-C(162)-C(158)	138.2
C(160)-C(159)-C(162)-C(158)	0.0
C(155)-C(158)-C(162)-C(159)	0.0
C(174)-C(158)-C(162)-C(159)	-142.6
C(155)-C(158)-C(162)-C(166)	142.6
C(174)-C(158)-C(162)-C(166)	0.0
C(128)-C(129)-C(164)-C(165)	0.0
C(130)-C(129)-C(164)-C(165)	142.6
C(128)-C(129)-C(164)-C(163)	-142.6
C(130)-C(129)-C(164)-C(163)	0.0
C(166)-C(163)-C(164)-C(165)	0.0
C(169)-C(163)-C(164)-C(165)	-142.6
C(166)-C(163)-C(164)-C(129)	142.6
C(169)-C(163)-C(164)-C(129)	0.0
C(129)-C(164)-C(165)-C(138)	0.0
C(163)-C(164)-C(165)-C(138)	138.2
C(129)-C(164)-C(165)-C(159)	-138.2
C(163)-C(164)-C(165)-C(159)	0.0
C(135)-C(138)-C(165)-C(164)	0.0
C(137)-C(138)-C(165)-C(164)	-142.6
C(135)-C(138)-C(165)-C(159)	142.6
C(137)-C(138)-C(165)-C(159)	0.0
C(162)-C(159)-C(165)-C(164)	0.0
C(160)-C(159)-C(165)-C(164)	142.6
C(162)-C(159)-C(165)-C(138)	-142.6
C(160)-C(159)-C(165)-C(138)	0.0
C(169)-C(163)-C(166)-C(162)	138.2
C(164)-C(163)-C(166)-C(162)	0.0
C(169)-C(163)-C(166)-C(170)	0.0
C(164)-C(163)-C(166)-C(170)	-138.2
C(159)-C(162)-C(166)-C(163)	0.0
C(158)-C(162)-C(166)-C(163)	-142.6
C(159)-C(162)-C(166)-C(170)	142.6

C(158)-C(162)-C(166)-C(170)	0.0
C(120)-C(121)-C(168)-C(169)	0.0
C(122)-C(121)-C(168)-C(169)	142.6
C(120)-C(121)-C(168)-C(167)	-142.6
C(122)-C(121)-C(168)-C(167)	0.0
C(170)-C(167)-C(168)-C(169)	0.0
C(173)-C(167)-C(168)-C(169)	-142.6
C(170)-C(167)-C(168)-C(121)	142.6
C(173)-C(167)-C(168)-C(121)	0.0
C(121)-C(168)-C(169)-C(163)	-138.2
C(167)-C(168)-C(169)-C(163)	0.0
C(121)-C(168)-C(169)-C(130)	0.0
C(167)-C(168)-C(169)-C(130)	138.2
C(166)-C(163)-C(169)-C(168)	0.0
C(164)-C(163)-C(169)-C(168)	142.6
C(166)-C(163)-C(169)-C(130)	-142.6
C(164)-C(163)-C(169)-C(130)	0.0
C(127)-C(130)-C(169)-C(168)	0.0
C(129)-C(130)-C(169)-C(168)	-142.6
C(127)-C(130)-C(169)-C(163)	142.6
C(129)-C(130)-C(169)-C(163)	0.0
C(173)-C(167)-C(170)-C(174)	0.0
C(168)-C(167)-C(170)-C(174)	-138.2
C(173)-C(167)-C(170)-C(166)	138.2
C(168)-C(167)-C(170)-C(166)	0.0
C(163)-C(166)-C(170)-C(167)	0.0
C(162)-C(166)-C(170)-C(167)	-142.6
C(163)-C(166)-C(170)-C(174)	142.6
C(162)-C(166)-C(170)-C(174)	0.0
C(156)-C(157)-C(171)-C(174)	0.0
C(154)-C(157)-C(171)-C(174)	-142.6
C(156)-C(157)-C(171)-C(172)	142.6
C(154)-C(157)-C(171)-C(172)	0.0
C(174)-C(171)-C(172)-C(173)	0.0
C(157)-C(171)-C(172)-C(173)	-142.6
C(174)-C(171)-C(172)-C(153)	142.6

C(157)-C(171)-C(172)-C(153)	0.0
C(152)-C(153)-C(172)-C(173)	0.0
C(154)-C(153)-C(172)-C(173)	142.6
C(152)-C(153)-C(172)-C(171)	-142.6
C(154)-C(153)-C(172)-C(171)	0.0
C(171)-C(172)-C(173)-C(167)	0.0
C(153)-C(172)-C(173)-C(167)	-138.2
C(171)-C(172)-C(173)-C(122)	138.2
C(153)-C(172)-C(173)-C(122)	0.0
C(170)-C(167)-C(173)-C(172)	0.0
C(168)-C(167)-C(173)-C(172)	142.6
C(170)-C(167)-C(173)-C(122)	-142.6
C(168)-C(167)-C(173)-C(122)	0.0
C(119)-C(122)-C(173)-C(172)	0.0
C(121)-C(122)-C(173)-C(172)	-142.6
C(119)-C(122)-C(173)-C(167)	142.6
C(121)-C(122)-C(173)-C(167)	0.0
C(172)-C(171)-C(174)-C(170)	0.0
C(157)-C(171)-C(174)-C(170)	138.2
C(172)-C(171)-C(174)-C(158)	-138.2
C(157)-C(171)-C(174)-C(158)	0.0
C(167)-C(170)-C(174)-C(171)	0.0
C(166)-C(170)-C(174)-C(171)	-142.6
C(167)-C(170)-C(174)-C(158)	142.6
C(166)-C(170)-C(174)-C(158)	0.0
C(155)-C(158)-C(174)-C(171)	0.0
C(162)-C(158)-C(174)-C(171)	142.6
C(155)-C(158)-C(174)-C(170)	-142.6
C(162)-C(158)-C(174)-C(170)	0.0
C(217)-C(215)-C(216)-C(218)	0.0
C(226)-C(215)-C(216)-C(218)	-142.6
C(217)-C(215)-C(216)-C(220)	142.6
C(226)-C(215)-C(216)-C(220)	0.0
C(226)-C(215)-C(217)-C(249)	138.2
C(216)-C(215)-C(217)-C(249)	0.0
C(226)-C(215)-C(217)-C(225)	0.0

C(216)-C(215)-C(217)-C(225)	-138.2
C(215)-C(216)-C(218)-C(247)	0.0
C(220)-C(216)-C(218)-C(247)	-138.2
C(215)-C(216)-C(218)-C(219)	138.2
C(220)-C(216)-C(218)-C(219)	0.0
C(216)-C(218)-C(219)-C(222)	0.0
C(247)-C(218)-C(219)-C(222)	142.6
C(216)-C(218)-C(219)-C(252)	-142.6
C(247)-C(218)-C(219)-C(252)	0.0
C(218)-C(216)-C(220)-C(221)	0.0
C(215)-C(216)-C(220)-C(221)	-142.6
C(218)-C(216)-C(220)-C(227)	142.6
C(215)-C(216)-C(220)-C(227)	0.0
C(227)-C(220)-C(221)-C(268)	0.0
C(216)-C(220)-C(221)-C(268)	138.2
C(227)-C(220)-C(221)-C(222)	-138.2
C(216)-C(220)-C(221)-C(222)	0.0
C(252)-C(219)-C(222)-C(273)	0.0
C(218)-C(219)-C(222)-C(273)	-138.2
C(252)-C(219)-C(222)-C(221)	138.2
C(218)-C(219)-C(222)-C(221)	0.0
C(220)-C(221)-C(222)-C(219)	0.0
C(268)-C(221)-C(222)-C(219)	-142.6
C(220)-C(221)-C(222)-C(273)	142.6
C(268)-C(221)-C(222)-C(273)	0.0
C(225)-C(223)-C(224)-C(226)	0.0
C(234)-C(223)-C(224)-C(226)	-142.6
C(225)-C(223)-C(224)-C(228)	142.6
C(234)-C(223)-C(224)-C(228)	0.0
C(234)-C(223)-C(225)-C(233)	0.0
C(224)-C(223)-C(225)-C(233)	-138.2
C(234)-C(223)-C(225)-C(217)	138.2
C(224)-C(223)-C(225)-C(217)	0.0
C(215)-C(217)-C(225)-C(223)	0.0
C(249)-C(217)-C(225)-C(223)	-142.6
C(215)-C(217)-C(225)-C(233)	142.6

C(249)-C(217)-C(225)-C(233)	0.0
C(223)-C(224)-C(226)-C(215)	0.0
C(228)-C(224)-C(226)-C(215)	-138.2
C(223)-C(224)-C(226)-C(227)	138.2
C(228)-C(224)-C(226)-C(227)	0.0
C(217)-C(215)-C(226)-C(224)	0.0
C(216)-C(215)-C(226)-C(224)	142.6
C(217)-C(215)-C(226)-C(227)	-142.6
C(216)-C(215)-C(226)-C(227)	0.0
C(221)-C(220)-C(227)-C(230)	0.0
C(216)-C(220)-C(227)-C(230)	-142.6
C(221)-C(220)-C(227)-C(226)	142.6
C(216)-C(220)-C(227)-C(226)	0.0
C(224)-C(226)-C(227)-C(230)	0.0
C(215)-C(226)-C(227)-C(230)	142.6
C(224)-C(226)-C(227)-C(220)	-142.6
C(215)-C(226)-C(227)-C(220)	0.0
C(226)-C(224)-C(228)-C(229)	0.0
C(223)-C(224)-C(228)-C(229)	-142.6
C(226)-C(224)-C(228)-C(235)	142.6
C(223)-C(224)-C(228)-C(235)	0.0
C(235)-C(228)-C(229)-C(230)	-138.2
C(224)-C(228)-C(229)-C(230)	0.0
C(235)-C(228)-C(229)-C(264)	0.0
C(224)-C(228)-C(229)-C(264)	138.2
C(220)-C(227)-C(230)-C(229)	138.2
C(226)-C(227)-C(230)-C(229)	0.0
C(220)-C(227)-C(230)-C(269)	0.0
C(226)-C(227)-C(230)-C(269)	-138.2
C(228)-C(229)-C(230)-C(227)	0.0
C(264)-C(229)-C(230)-C(227)	-142.6
C(228)-C(229)-C(230)-C(269)	142.6
C(264)-C(229)-C(230)-C(269)	0.0
C(233)-C(231)-C(232)-C(234)	0.0
C(242)-C(231)-C(232)-C(234)	-142.6
C(233)-C(231)-C(232)-C(236)	142.6

C(242)-C(231)-C(232)-C(236)	0.0
C(232)-C(231)-C(233)-C(225)	0.0
C(242)-C(231)-C(233)-C(225)	138.2
C(232)-C(231)-C(233)-C(241)	-138.2
C(242)-C(231)-C(233)-C(241)	0.0
C(223)-C(225)-C(233)-C(231)	0.0
C(217)-C(225)-C(233)-C(231)	-142.6
C(223)-C(225)-C(233)-C(241)	142.6
C(217)-C(225)-C(233)-C(241)	0.0
C(231)-C(232)-C(234)-C(223)	0.0
C(236)-C(232)-C(234)-C(223)	-138.2
C(231)-C(232)-C(234)-C(235)	138.2
C(236)-C(232)-C(234)-C(235)	0.0
C(225)-C(223)-C(234)-C(232)	0.0
C(224)-C(223)-C(234)-C(232)	142.6
C(225)-C(223)-C(234)-C(235)	-142.6
C(224)-C(223)-C(234)-C(235)	0.0
C(229)-C(228)-C(235)-C(238)	0.0
C(224)-C(228)-C(235)-C(238)	-142.6
C(229)-C(228)-C(235)-C(234)	142.6
C(224)-C(228)-C(235)-C(234)	0.0
C(232)-C(234)-C(235)-C(238)	0.0
C(223)-C(234)-C(235)-C(238)	142.6
C(232)-C(234)-C(235)-C(228)	-142.6
C(223)-C(234)-C(235)-C(228)	0.0
C(234)-C(232)-C(236)-C(237)	0.0
C(231)-C(232)-C(236)-C(237)	-142.6
C(234)-C(232)-C(236)-C(243)	142.6
C(231)-C(232)-C(236)-C(243)	0.0
C(243)-C(236)-C(237)-C(238)	-138.2
C(232)-C(236)-C(237)-C(238)	0.0
C(243)-C(236)-C(237)-C(260)	0.0
C(232)-C(236)-C(237)-C(260)	138.2
C(228)-C(235)-C(238)-C(237)	138.2
C(234)-C(235)-C(238)-C(237)	0.0
C(228)-C(235)-C(238)-C(265)	0.0

C(234)-C(235)-C(238)-C(265)	-138.2
C(236)-C(237)-C(238)-C(235)	0.0
C(260)-C(237)-C(238)-C(235)	-142.6
C(236)-C(237)-C(238)-C(265)	142.6
C(260)-C(237)-C(238)-C(265)	0.0
C(241)-C(239)-C(240)-C(242)	0.0
C(250)-C(239)-C(240)-C(242)	-142.6
C(241)-C(239)-C(240)-C(244)	142.6
C(250)-C(239)-C(240)-C(244)	0.0
C(250)-C(239)-C(241)-C(249)	0.0
C(240)-C(239)-C(241)-C(249)	-138.2
C(250)-C(239)-C(241)-C(233)	138.2
C(240)-C(239)-C(241)-C(233)	0.0
C(231)-C(233)-C(241)-C(239)	0.0
C(225)-C(233)-C(241)-C(239)	-142.6
C(231)-C(233)-C(241)-C(249)	142.6
C(225)-C(233)-C(241)-C(249)	0.0
C(244)-C(240)-C(242)-C(243)	0.0
C(239)-C(240)-C(242)-C(243)	138.2
C(244)-C(240)-C(242)-C(231)	-138.2
C(239)-C(240)-C(242)-C(231)	0.0
C(233)-C(231)-C(242)-C(240)	0.0
C(232)-C(231)-C(242)-C(240)	142.6
C(233)-C(231)-C(242)-C(243)	-142.6
C(232)-C(231)-C(242)-C(243)	0.0
C(240)-C(242)-C(243)-C(246)	0.0
C(231)-C(242)-C(243)-C(246)	142.6
C(240)-C(242)-C(243)-C(236)	-142.6
C(231)-C(242)-C(243)-C(236)	0.0
C(237)-C(236)-C(243)-C(246)	0.0
C(232)-C(236)-C(243)-C(246)	-142.6
C(237)-C(236)-C(243)-C(242)	142.6
C(232)-C(236)-C(243)-C(242)	0.0
C(242)-C(240)-C(244)-C(245)	0.0
C(239)-C(240)-C(244)-C(245)	-142.6
C(242)-C(240)-C(244)-C(251)	142.6

C(239)-C(240)-C(244)-C(251)	0.0
C(240)-C(244)-C(245)-C(256)	138.2
C(251)-C(244)-C(245)-C(256)	0.0
C(240)-C(244)-C(245)-C(246)	0.0
C(251)-C(244)-C(245)-C(246)	-138.2
C(242)-C(243)-C(246)-C(261)	-138.2
C(236)-C(243)-C(246)-C(261)	0.0
C(242)-C(243)-C(246)-C(245)	0.0
C(236)-C(243)-C(246)-C(245)	138.2
C(244)-C(245)-C(246)-C(243)	0.0
C(256)-C(245)-C(246)-C(243)	-142.6
C(244)-C(245)-C(246)-C(261)	142.6
C(256)-C(245)-C(246)-C(261)	0.0
C(216)-C(218)-C(247)-C(249)	0.0
C(219)-C(218)-C(247)-C(249)	-142.6
C(216)-C(218)-C(247)-C(248)	142.6
C(219)-C(218)-C(247)-C(248)	0.0
C(249)-C(247)-C(248)-C(250)	0.0
C(218)-C(247)-C(248)-C(250)	-142.6
C(249)-C(247)-C(248)-C(252)	142.6
C(218)-C(247)-C(248)-C(252)	0.0
C(218)-C(247)-C(249)-C(217)	0.0
C(248)-C(247)-C(249)-C(217)	-138.2
C(218)-C(247)-C(249)-C(241)	138.2
C(248)-C(247)-C(249)-C(241)	0.0
C(215)-C(217)-C(249)-C(247)	0.0
C(225)-C(217)-C(249)-C(247)	142.6
C(215)-C(217)-C(249)-C(241)	-142.6
C(225)-C(217)-C(249)-C(241)	0.0
C(239)-C(241)-C(249)-C(247)	0.0
C(233)-C(241)-C(249)-C(247)	-142.6
C(239)-C(241)-C(249)-C(217)	142.6
C(233)-C(241)-C(249)-C(217)	0.0
C(247)-C(248)-C(250)-C(239)	0.0
C(252)-C(248)-C(250)-C(239)	-138.2
C(247)-C(248)-C(250)-C(251)	138.2

C(252)-C(248)-C(250)-C(251)	0.0
C(241)-C(239)-C(250)-C(248)	0.0
C(240)-C(239)-C(250)-C(248)	142.6
C(241)-C(239)-C(250)-C(251)	-142.6
C(240)-C(239)-C(250)-C(251)	0.0
C(245)-C(244)-C(251)-C(254)	0.0
C(240)-C(244)-C(251)-C(254)	-142.6
C(245)-C(244)-C(251)-C(250)	142.6
C(240)-C(244)-C(251)-C(250)	0.0
C(248)-C(250)-C(251)-C(254)	0.0
C(239)-C(250)-C(251)-C(254)	142.6
C(248)-C(250)-C(251)-C(244)	-142.6
C(239)-C(250)-C(251)-C(244)	0.0
C(222)-C(219)-C(252)-C(253)	0.0
C(218)-C(219)-C(252)-C(253)	142.6
C(222)-C(219)-C(252)-C(248)	-142.6
C(218)-C(219)-C(252)-C(248)	0.0
C(250)-C(248)-C(252)-C(253)	0.0
C(247)-C(248)-C(252)-C(253)	-142.6
C(250)-C(248)-C(252)-C(219)	142.6
C(247)-C(248)-C(252)-C(219)	0.0
C(219)-C(252)-C(253)-C(272)	0.0
C(248)-C(252)-C(253)-C(272)	138.2
C(219)-C(252)-C(253)-C(254)	-138.2
C(248)-C(252)-C(253)-C(254)	0.0
C(244)-C(251)-C(254)-C(257)	0.0
C(250)-C(251)-C(254)-C(257)	-138.2
C(244)-C(251)-C(254)-C(253)	138.2
C(250)-C(251)-C(254)-C(253)	0.0
C(252)-C(253)-C(254)-C(251)	0.0
C(272)-C(253)-C(254)-C(251)	-142.6
C(252)-C(253)-C(254)-C(257)	142.6
C(272)-C(253)-C(254)-C(257)	0.0
C(258)-C(255)-C(256)-C(257)	0.0
C(261)-C(255)-C(256)-C(257)	-142.6
C(258)-C(255)-C(256)-C(245)	142.6

C(261)-C(255)-C(256)-C(245)	0.0
C(244)-C(245)-C(256)-C(257)	0.0
C(246)-C(245)-C(256)-C(257)	142.6
C(244)-C(245)-C(256)-C(255)	-142.6
C(246)-C(245)-C(256)-C(255)	0.0
C(255)-C(256)-C(257)-C(254)	138.2
C(245)-C(256)-C(257)-C(254)	0.0
C(255)-C(256)-C(257)-C(271)	0.0
C(245)-C(256)-C(257)-C(271)	-138.2
C(251)-C(254)-C(257)-C(256)	0.0
C(253)-C(254)-C(257)-C(256)	-142.6
C(251)-C(254)-C(257)-C(271)	142.6
C(253)-C(254)-C(257)-C(271)	0.0
C(256)-C(255)-C(258)-C(274)	0.0
C(261)-C(255)-C(258)-C(274)	138.2
C(256)-C(255)-C(258)-C(262)	-138.2
C(261)-C(255)-C(258)-C(262)	0.0
C(262)-C(259)-C(260)-C(261)	0.0
C(265)-C(259)-C(260)-C(261)	-142.6
C(262)-C(259)-C(260)-C(237)	142.6
C(265)-C(259)-C(260)-C(237)	0.0
C(236)-C(237)-C(260)-C(261)	0.0
C(238)-C(237)-C(260)-C(261)	142.6
C(236)-C(237)-C(260)-C(259)	-142.6
C(238)-C(237)-C(260)-C(259)	0.0
C(259)-C(260)-C(261)-C(255)	0.0
C(237)-C(260)-C(261)-C(255)	-138.2
C(259)-C(260)-C(261)-C(246)	138.2
C(237)-C(260)-C(261)-C(246)	0.0
C(258)-C(255)-C(261)-C(260)	0.0
C(256)-C(255)-C(261)-C(260)	142.6
C(258)-C(255)-C(261)-C(246)	-142.6
C(256)-C(255)-C(261)-C(246)	0.0
C(243)-C(246)-C(261)-C(260)	0.0
C(245)-C(246)-C(261)-C(260)	-142.6
C(243)-C(246)-C(261)-C(255)	142.6

C(245)-C(246)-C(261)-C(255)	0.0
C(265)-C(259)-C(262)-C(266)	0.0
C(260)-C(259)-C(262)-C(266)	-138.2
C(265)-C(259)-C(262)-C(258)	138.2
C(260)-C(259)-C(262)-C(258)	0.0
C(255)-C(258)-C(262)-C(259)	0.0
C(274)-C(258)-C(262)-C(259)	-142.6
C(255)-C(258)-C(262)-C(266)	142.6
C(274)-C(258)-C(262)-C(266)	0.0
C(266)-C(263)-C(264)-C(265)	0.0
C(269)-C(263)-C(264)-C(265)	-142.6
C(266)-C(263)-C(264)-C(229)	142.6
C(269)-C(263)-C(264)-C(229)	0.0
C(228)-C(229)-C(264)-C(265)	0.0
C(230)-C(229)-C(264)-C(265)	142.6
C(228)-C(229)-C(264)-C(263)	-142.6
C(230)-C(229)-C(264)-C(263)	0.0
C(263)-C(264)-C(265)-C(238)	138.2
C(229)-C(264)-C(265)-C(238)	0.0
C(263)-C(264)-C(265)-C(259)	0.0
C(229)-C(264)-C(265)-C(259)	-138.2
C(235)-C(238)-C(265)-C(264)	0.0
C(237)-C(238)-C(265)-C(264)	-142.6
C(235)-C(238)-C(265)-C(259)	142.6
C(237)-C(238)-C(265)-C(259)	0.0
C(262)-C(259)-C(265)-C(264)	0.0
C(260)-C(259)-C(265)-C(264)	142.6
C(262)-C(259)-C(265)-C(238)	-142.6
C(260)-C(259)-C(265)-C(238)	0.0
C(269)-C(263)-C(266)-C(270)	0.0
C(264)-C(263)-C(266)-C(270)	-138.2
C(269)-C(263)-C(266)-C(262)	138.2
C(264)-C(263)-C(266)-C(262)	0.0
C(259)-C(262)-C(266)-C(263)	0.0
C(258)-C(262)-C(266)-C(263)	-142.6
C(259)-C(262)-C(266)-C(270)	142.6

C(258)-C(262)-C(266)-C(270)	0.0
C(270)-C(267)-C(268)-C(269)	0.0
C(273)-C(267)-C(268)-C(269)	-142.6
C(270)-C(267)-C(268)-C(221)	142.6
C(273)-C(267)-C(268)-C(221)	0.0
C(220)-C(221)-C(268)-C(269)	0.0
C(222)-C(221)-C(268)-C(269)	142.6
C(220)-C(221)-C(268)-C(267)	-142.6
C(222)-C(221)-C(268)-C(267)	0.0
C(267)-C(268)-C(269)-C(263)	0.0
C(221)-C(268)-C(269)-C(263)	-138.2
C(267)-C(268)-C(269)-C(230)	138.2
C(221)-C(268)-C(269)-C(230)	0.0
C(266)-C(263)-C(269)-C(268)	0.0
C(264)-C(263)-C(269)-C(268)	142.6
C(266)-C(263)-C(269)-C(230)	-142.6
C(264)-C(263)-C(269)-C(230)	0.0
C(227)-C(230)-C(269)-C(268)	0.0
C(229)-C(230)-C(269)-C(268)	-142.6
C(227)-C(230)-C(269)-C(263)	142.6
C(229)-C(230)-C(269)-C(263)	0.0
C(268)-C(267)-C(270)-C(266)	0.0
C(273)-C(267)-C(270)-C(266)	138.2
C(268)-C(267)-C(270)-C(274)	-138.2
C(273)-C(267)-C(270)-C(274)	0.0
C(263)-C(266)-C(270)-C(267)	0.0
C(262)-C(266)-C(270)-C(267)	-142.6
C(263)-C(266)-C(270)-C(274)	142.6
C(262)-C(266)-C(270)-C(274)	0.0
C(256)-C(257)-C(271)-C(274)	0.0
C(254)-C(257)-C(271)-C(274)	-142.6
C(256)-C(257)-C(271)-C(272)	142.6
C(254)-C(257)-C(271)-C(272)	0.0
C(274)-C(271)-C(272)-C(273)	0.0
C(257)-C(271)-C(272)-C(273)	-142.6
C(274)-C(271)-C(272)-C(253)	142.6

C(257)-C(271)-C(272)-C(253)	0.0
C(252)-C(253)-C(272)-C(273)	0.0
C(254)-C(253)-C(272)-C(273)	142.6
C(252)-C(253)-C(272)-C(271)	-142.6
C(254)-C(253)-C(272)-C(271)	0.0
C(271)-C(272)-C(273)-C(267)	0.0
C(253)-C(272)-C(273)-C(267)	-138.2
C(271)-C(272)-C(273)-C(222)	138.2
C(253)-C(272)-C(273)-C(222)	0.0
C(270)-C(267)-C(273)-C(272)	0.0
C(268)-C(267)-C(273)-C(272)	142.6
C(270)-C(267)-C(273)-C(222)	-142.6
C(268)-C(267)-C(273)-C(222)	0.0
C(219)-C(222)-C(273)-C(272)	0.0
C(221)-C(222)-C(273)-C(272)	-142.6
C(219)-C(222)-C(273)-C(267)	142.6
C(221)-C(222)-C(273)-C(267)	0.0
C(272)-C(271)-C(274)-C(258)	-138.2
C(257)-C(271)-C(274)-C(258)	0.0
C(272)-C(271)-C(274)-C(270)	0.0
C(257)-C(271)-C(274)-C(270)	138.2
C(255)-C(258)-C(274)-C(271)	0.0
C(262)-C(258)-C(274)-C(271)	142.6
C(255)-C(258)-C(274)-C(270)	-142.6
C(262)-C(258)-C(274)-C(270)	0.0
C(267)-C(270)-C(274)-C(271)	0.0
C(266)-C(270)-C(274)-C(271)	-142.6
C(267)-C(270)-C(274)-C(258)	142.6
C(266)-C(270)-C(274)-C(258)	0.0
C(57)-C(55)-C(56)-C(58)	0.0
C(66)-C(55)-C(56)-C(58)	-142.6
C(57)-C(55)-C(56)-C(60)	142.6
C(66)-C(55)-C(56)-C(60)	0.0
C(56)-C(55)-C(57)-C(89)	0.0
C(66)-C(55)-C(57)-C(89)	138.2
C(56)-C(55)-C(57)-C(65)	-138.2

C(66)-C(55)-C(57)-C(65)	0.0
C(55)-C(56)-C(58)-C(87)	0.0
C(60)-C(56)-C(58)-C(87)	-138.2
C(55)-C(56)-C(58)-C(59)	138.2
C(60)-C(56)-C(58)-C(59)	0.0
C(56)-C(58)-C(59)-C(62)	0.0
C(87)-C(58)-C(59)-C(62)	142.6
C(56)-C(58)-C(59)-C(92)	-142.6
C(87)-C(58)-C(59)-C(92)	0.0
C(58)-C(56)-C(60)-C(61)	0.0
C(55)-C(56)-C(60)-C(61)	-142.6
C(58)-C(56)-C(60)-C(67)	142.6
C(55)-C(56)-C(60)-C(67)	0.0
C(56)-C(60)-C(61)-C(108)	138.2
C(67)-C(60)-C(61)-C(108)	0.0
C(56)-C(60)-C(61)-C(62)	0.0
C(67)-C(60)-C(61)-C(62)	-138.2
C(58)-C(59)-C(62)-C(113)	-138.2
C(92)-C(59)-C(62)-C(113)	0.0
C(58)-C(59)-C(62)-C(61)	0.0
C(92)-C(59)-C(62)-C(61)	138.2
C(60)-C(61)-C(62)-C(59)	0.0
C(108)-C(61)-C(62)-C(59)	-142.6
C(60)-C(61)-C(62)-C(113)	142.6
C(108)-C(61)-C(62)-C(113)	0.0
C(65)-C(63)-C(64)-C(66)	0.0
C(74)-C(63)-C(64)-C(66)	-142.6
C(65)-C(63)-C(64)-C(68)	142.6
C(74)-C(63)-C(64)-C(68)	0.0
C(74)-C(63)-C(65)-C(57)	138.2
C(64)-C(63)-C(65)-C(57)	0.0
C(74)-C(63)-C(65)-C(73)	0.0
C(64)-C(63)-C(65)-C(73)	-138.2
C(55)-C(57)-C(65)-C(63)	0.0
C(89)-C(57)-C(65)-C(63)	-142.6
C(55)-C(57)-C(65)-C(73)	142.6

C(89)-C(57)-C(65)-C(73)	0.0
C(68)-C(64)-C(66)-C(67)	0.0
C(63)-C(64)-C(66)-C(67)	138.2
C(68)-C(64)-C(66)-C(55)	-138.2
C(63)-C(64)-C(66)-C(55)	0.0
C(57)-C(55)-C(66)-C(64)	0.0
C(56)-C(55)-C(66)-C(64)	142.6
C(57)-C(55)-C(66)-C(67)	-142.6
C(56)-C(55)-C(66)-C(67)	0.0
C(64)-C(66)-C(67)-C(70)	0.0
C(55)-C(66)-C(67)-C(70)	142.6
C(64)-C(66)-C(67)-C(60)	-142.6
C(55)-C(66)-C(67)-C(60)	0.0
C(61)-C(60)-C(67)-C(70)	0.0
C(56)-C(60)-C(67)-C(70)	-142.6
C(61)-C(60)-C(67)-C(66)	142.6
C(56)-C(60)-C(67)-C(66)	0.0
C(66)-C(64)-C(68)-C(69)	0.0
C(63)-C(64)-C(68)-C(69)	-142.6
C(66)-C(64)-C(68)-C(75)	142.6
C(63)-C(64)-C(68)-C(75)	0.0
C(75)-C(68)-C(69)-C(70)	-138.2
C(64)-C(68)-C(69)-C(70)	0.0
C(75)-C(68)-C(69)-C(104)	0.0
C(64)-C(68)-C(69)-C(104)	138.2
C(66)-C(67)-C(70)-C(69)	0.0
C(60)-C(67)-C(70)-C(69)	138.2
C(66)-C(67)-C(70)-C(109)	-138.2
C(60)-C(67)-C(70)-C(109)	0.0
C(68)-C(69)-C(70)-C(67)	0.0
C(104)-C(69)-C(70)-C(67)	-142.6
C(68)-C(69)-C(70)-C(109)	142.6
C(104)-C(69)-C(70)-C(109)	0.0
C(73)-C(71)-C(72)-C(74)	0.0
C(82)-C(71)-C(72)-C(74)	-142.6
C(73)-C(71)-C(72)-C(76)	142.6

C(82)-C(71)-C(72)-C(76)	0.0
C(72)-C(71)-C(73)-C(65)	0.0
C(82)-C(71)-C(73)-C(65)	138.2
C(72)-C(71)-C(73)-C(81)	-138.2
C(82)-C(71)-C(73)-C(81)	0.0
C(63)-C(65)-C(73)-C(71)	0.0
C(57)-C(65)-C(73)-C(71)	-142.6
C(63)-C(65)-C(73)-C(81)	142.6
C(57)-C(65)-C(73)-C(81)	0.0
C(76)-C(72)-C(74)-C(75)	0.0
C(71)-C(72)-C(74)-C(75)	138.2
C(76)-C(72)-C(74)-C(63)	-138.2
C(71)-C(72)-C(74)-C(63)	0.0
C(65)-C(63)-C(74)-C(72)	0.0
C(64)-C(63)-C(74)-C(72)	142.6
C(65)-C(63)-C(74)-C(75)	-142.6
C(64)-C(63)-C(74)-C(75)	0.0
C(69)-C(68)-C(75)-C(78)	0.0
C(64)-C(68)-C(75)-C(78)	-142.6
C(69)-C(68)-C(75)-C(74)	142.6
C(64)-C(68)-C(75)-C(74)	0.0
C(72)-C(74)-C(75)-C(78)	0.0
C(63)-C(74)-C(75)-C(78)	142.6
C(72)-C(74)-C(75)-C(68)	-142.6
C(63)-C(74)-C(75)-C(68)	0.0
C(74)-C(72)-C(76)-C(77)	0.0
C(71)-C(72)-C(76)-C(77)	-142.6
C(74)-C(72)-C(76)-C(83)	142.6
C(71)-C(72)-C(76)-C(83)	0.0
C(83)-C(76)-C(77)-C(78)	-138.2
C(72)-C(76)-C(77)-C(78)	0.0
C(83)-C(76)-C(77)-C(100)	0.0
C(72)-C(76)-C(77)-C(100)	138.2
C(68)-C(75)-C(78)-C(77)	138.2
C(74)-C(75)-C(78)-C(77)	0.0
C(68)-C(75)-C(78)-C(105)	0.0

C(74)-C(75)-C(78)-C(105)	-138.2
C(76)-C(77)-C(78)-C(75)	0.0
C(100)-C(77)-C(78)-C(75)	-142.6
C(76)-C(77)-C(78)-C(105)	142.6
C(100)-C(77)-C(78)-C(105)	0.0
C(81)-C(79)-C(80)-C(82)	0.0
C(90)-C(79)-C(80)-C(82)	-142.6
C(81)-C(79)-C(80)-C(84)	142.6
C(90)-C(79)-C(80)-C(84)	0.0
C(80)-C(79)-C(81)-C(73)	0.0
C(90)-C(79)-C(81)-C(73)	138.2
C(80)-C(79)-C(81)-C(89)	-138.2
C(90)-C(79)-C(81)-C(89)	0.0
C(71)-C(73)-C(81)-C(79)	0.0
C(65)-C(73)-C(81)-C(79)	-142.6
C(71)-C(73)-C(81)-C(89)	142.6
C(65)-C(73)-C(81)-C(89)	0.0
C(79)-C(80)-C(82)-C(71)	0.0
C(84)-C(80)-C(82)-C(71)	-138.2
C(79)-C(80)-C(82)-C(83)	138.2
C(84)-C(80)-C(82)-C(83)	0.0
C(73)-C(71)-C(82)-C(80)	0.0
C(72)-C(71)-C(82)-C(80)	142.6
C(73)-C(71)-C(82)-C(83)	-142.6
C(72)-C(71)-C(82)-C(83)	0.0
C(77)-C(76)-C(83)-C(86)	0.0
C(72)-C(76)-C(83)-C(86)	-142.6
C(77)-C(76)-C(83)-C(82)	142.6
C(72)-C(76)-C(83)-C(82)	0.0
C(80)-C(82)-C(83)-C(86)	0.0
C(71)-C(82)-C(83)-C(86)	142.6
C(80)-C(82)-C(83)-C(76)	-142.6
C(71)-C(82)-C(83)-C(76)	0.0
C(82)-C(80)-C(84)-C(85)	0.0
C(79)-C(80)-C(84)-C(85)	-142.6
C(82)-C(80)-C(84)-C(91)	142.6

C(79)-C(80)-C(84)-C(91)	0.0
C(91)-C(84)-C(85)-C(86)	-138.2
C(80)-C(84)-C(85)-C(86)	0.0
C(91)-C(84)-C(85)-C(96)	0.0
C(80)-C(84)-C(85)-C(96)	138.2
C(76)-C(83)-C(86)-C(85)	138.2
C(82)-C(83)-C(86)-C(85)	0.0
C(76)-C(83)-C(86)-C(101)	0.0
C(82)-C(83)-C(86)-C(101)	-138.2
C(84)-C(85)-C(86)-C(83)	0.0
C(96)-C(85)-C(86)-C(83)	-142.6
C(84)-C(85)-C(86)-C(101)	142.6
C(96)-C(85)-C(86)-C(101)	0.0
C(56)-C(58)-C(87)-C(89)	0.0
C(59)-C(58)-C(87)-C(89)	-142.6
C(56)-C(58)-C(87)-C(88)	142.6
C(59)-C(58)-C(87)-C(88)	0.0
C(89)-C(87)-C(88)-C(90)	0.0
C(58)-C(87)-C(88)-C(90)	-142.6
C(89)-C(87)-C(88)-C(92)	142.6
C(58)-C(87)-C(88)-C(92)	0.0
C(58)-C(87)-C(89)-C(57)	0.0
C(88)-C(87)-C(89)-C(57)	-138.2
C(58)-C(87)-C(89)-C(81)	138.2
C(88)-C(87)-C(89)-C(81)	0.0
C(55)-C(57)-C(89)-C(87)	0.0
C(65)-C(57)-C(89)-C(87)	142.6
C(55)-C(57)-C(89)-C(81)	-142.6
C(65)-C(57)-C(89)-C(81)	0.0
C(79)-C(81)-C(89)-C(87)	0.0
C(73)-C(81)-C(89)-C(87)	-142.6
C(79)-C(81)-C(89)-C(57)	142.6
C(73)-C(81)-C(89)-C(57)	0.0
C(92)-C(88)-C(90)-C(91)	0.0
C(87)-C(88)-C(90)-C(91)	138.2
C(92)-C(88)-C(90)-C(79)	-138.2

C(87)-C(88)-C(90)-C(79)	0.0
C(81)-C(79)-C(90)-C(88)	0.0
C(80)-C(79)-C(90)-C(88)	142.6
C(81)-C(79)-C(90)-C(91)	-142.6
C(80)-C(79)-C(90)-C(91)	0.0
C(88)-C(90)-C(91)-C(94)	0.0
C(79)-C(90)-C(91)-C(94)	142.6
C(88)-C(90)-C(91)-C(84)	-142.6
C(79)-C(90)-C(91)-C(84)	0.0
C(85)-C(84)-C(91)-C(94)	0.0
C(80)-C(84)-C(91)-C(94)	-142.6
C(85)-C(84)-C(91)-C(90)	142.6
C(80)-C(84)-C(91)-C(90)	0.0
C(62)-C(59)-C(92)-C(93)	0.0
C(58)-C(59)-C(92)-C(93)	142.6
C(62)-C(59)-C(92)-C(88)	-142.6
C(58)-C(59)-C(92)-C(88)	0.0
C(90)-C(88)-C(92)-C(93)	0.0
C(87)-C(88)-C(92)-C(93)	-142.6
C(90)-C(88)-C(92)-C(59)	142.6
C(87)-C(88)-C(92)-C(59)	0.0
C(59)-C(92)-C(93)-C(94)	-138.2
C(88)-C(92)-C(93)-C(94)	0.0
C(59)-C(92)-C(93)-C(112)	0.0
C(88)-C(92)-C(93)-C(112)	138.2
C(90)-C(91)-C(94)-C(97)	-138.2
C(84)-C(91)-C(94)-C(97)	0.0
C(90)-C(91)-C(94)-C(93)	0.0
C(84)-C(91)-C(94)-C(93)	138.2
C(92)-C(93)-C(94)-C(91)	0.0
C(112)-C(93)-C(94)-C(91)	-142.6
C(92)-C(93)-C(94)-C(97)	142.6
C(112)-C(93)-C(94)-C(97)	0.0
C(98)-C(95)-C(96)-C(97)	0.0
C(101)-C(95)-C(96)-C(97)	-142.6
C(98)-C(95)-C(96)-C(85)	142.6

C(101)-C(95)-C(96)-C(85)	0.0
C(84)-C(85)-C(96)-C(97)	0.0
C(86)-C(85)-C(96)-C(97)	142.6
C(84)-C(85)-C(96)-C(95)	-142.6
C(86)-C(85)-C(96)-C(95)	0.0
C(95)-C(96)-C(97)-C(94)	138.2
C(85)-C(96)-C(97)-C(94)	0.0
C(95)-C(96)-C(97)-C(111)	0.0
C(85)-C(96)-C(97)-C(111)	-138.2
C(91)-C(94)-C(97)-C(96)	0.0
C(93)-C(94)-C(97)-C(96)	-142.6
C(91)-C(94)-C(97)-C(111)	142.6
C(93)-C(94)-C(97)-C(111)	0.0
C(96)-C(95)-C(98)-C(114)	0.0
C(101)-C(95)-C(98)-C(114)	138.2
C(96)-C(95)-C(98)-C(102)	-138.2
C(101)-C(95)-C(98)-C(102)	0.0
C(76)-C(77)-C(100)-C(101)	0.0
C(78)-C(77)-C(100)-C(101)	142.6
C(76)-C(77)-C(100)-C(99)	-142.6
C(78)-C(77)-C(100)-C(99)	0.0
C(102)-C(99)-C(100)-C(101)	0.0
C(105)-C(99)-C(100)-C(101)	-142.6
C(102)-C(99)-C(100)-C(77)	142.6
C(105)-C(99)-C(100)-C(77)	0.0
C(77)-C(100)-C(101)-C(86)	0.0
C(99)-C(100)-C(101)-C(86)	138.2
C(77)-C(100)-C(101)-C(95)	-138.2
C(99)-C(100)-C(101)-C(95)	0.0
C(83)-C(86)-C(101)-C(100)	0.0
C(85)-C(86)-C(101)-C(100)	-142.6
C(83)-C(86)-C(101)-C(95)	142.6
C(85)-C(86)-C(101)-C(95)	0.0
C(98)-C(95)-C(101)-C(100)	0.0
C(96)-C(95)-C(101)-C(100)	142.6
C(98)-C(95)-C(101)-C(86)	-142.6

C(96)-C(95)-C(101)-C(86)	0.0
C(100)-C(99)-C(102)-C(98)	0.0
C(105)-C(99)-C(102)-C(98)	138.2
C(100)-C(99)-C(102)-C(106)	-138.2
C(105)-C(99)-C(102)-C(106)	0.0
C(95)-C(98)-C(102)-C(99)	0.0
C(114)-C(98)-C(102)-C(99)	-142.6
C(95)-C(98)-C(102)-C(106)	142.6
C(114)-C(98)-C(102)-C(106)	0.0
C(106)-C(103)-C(104)-C(105)	0.0
C(109)-C(103)-C(104)-C(105)	-142.6
C(106)-C(103)-C(104)-C(69)	142.6
C(109)-C(103)-C(104)-C(69)	0.0
C(68)-C(69)-C(104)-C(105)	0.0
C(70)-C(69)-C(104)-C(105)	142.6
C(68)-C(69)-C(104)-C(103)	-142.6
C(70)-C(69)-C(104)-C(103)	0.0
C(103)-C(104)-C(105)-C(78)	138.2
C(69)-C(104)-C(105)-C(78)	0.0
C(103)-C(104)-C(105)-C(99)	0.0
C(69)-C(104)-C(105)-C(99)	-138.2
C(75)-C(78)-C(105)-C(104)	0.0
C(77)-C(78)-C(105)-C(104)	-142.6
C(75)-C(78)-C(105)-C(99)	142.6
C(77)-C(78)-C(105)-C(99)	0.0
C(102)-C(99)-C(105)-C(104)	0.0
C(100)-C(99)-C(105)-C(104)	142.6
C(102)-C(99)-C(105)-C(78)	-142.6
C(100)-C(99)-C(105)-C(78)	0.0
C(109)-C(103)-C(106)-C(110)	0.0
C(104)-C(103)-C(106)-C(110)	-138.2
C(109)-C(103)-C(106)-C(102)	138.2
C(104)-C(103)-C(106)-C(102)	0.0
C(99)-C(102)-C(106)-C(103)	0.0
C(98)-C(102)-C(106)-C(103)	-142.6
C(99)-C(102)-C(106)-C(110)	142.6

C(98)-C(102)-C(106)-C(110)	0.0
C(60)-C(61)-C(108)-C(109)	0.0
C(62)-C(61)-C(108)-C(109)	142.6
C(60)-C(61)-C(108)-C(107)	-142.6
C(62)-C(61)-C(108)-C(107)	0.0
C(110)-C(107)-C(108)-C(109)	0.0
C(113)-C(107)-C(108)-C(109)	-142.6
C(110)-C(107)-C(108)-C(61)	142.6
C(113)-C(107)-C(108)-C(61)	0.0
C(61)-C(108)-C(109)-C(103)	-138.2
C(107)-C(108)-C(109)-C(103)	0.0
C(61)-C(108)-C(109)-C(70)	0.0
C(107)-C(108)-C(109)-C(70)	138.2
C(106)-C(103)-C(109)-C(108)	0.0
C(104)-C(103)-C(109)-C(108)	142.6
C(106)-C(103)-C(109)-C(70)	-142.6
C(104)-C(103)-C(109)-C(70)	0.0
C(67)-C(70)-C(109)-C(108)	0.0
C(69)-C(70)-C(109)-C(108)	-142.6
C(67)-C(70)-C(109)-C(103)	142.6
C(69)-C(70)-C(109)-C(103)	0.0
C(108)-C(107)-C(110)-C(114)	-138.2
C(113)-C(107)-C(110)-C(114)	0.0
C(108)-C(107)-C(110)-C(106)	0.0
C(113)-C(107)-C(110)-C(106)	138.2
C(103)-C(106)-C(110)-C(107)	0.0
C(102)-C(106)-C(110)-C(107)	-142.6
C(103)-C(106)-C(110)-C(114)	142.6
C(102)-C(106)-C(110)-C(114)	0.0
C(96)-C(97)-C(111)-C(114)	0.0
C(94)-C(97)-C(111)-C(114)	-142.6
C(96)-C(97)-C(111)-C(112)	142.6
C(94)-C(97)-C(111)-C(112)	0.0
C(114)-C(111)-C(112)-C(113)	0.0
C(97)-C(111)-C(112)-C(113)	-142.6
C(114)-C(111)-C(112)-C(93)	142.6

C(97)-C(111)-C(112)-C(93)	0.0
C(92)-C(93)-C(112)-C(113)	0.0
C(94)-C(93)-C(112)-C(113)	142.6
C(92)-C(93)-C(112)-C(111)	-142.6
C(94)-C(93)-C(112)-C(111)	0.0
C(111)-C(112)-C(113)-C(62)	138.2
C(93)-C(112)-C(113)-C(62)	0.0
C(111)-C(112)-C(113)-C(107)	0.0
C(93)-C(112)-C(113)-C(107)	-138.2
C(59)-C(62)-C(113)-C(112)	0.0
C(61)-C(62)-C(113)-C(112)	-142.6
C(59)-C(62)-C(113)-C(107)	142.6
C(61)-C(62)-C(113)-C(107)	0.0
C(110)-C(107)-C(113)-C(112)	0.0
C(108)-C(107)-C(113)-C(112)	142.6
C(110)-C(107)-C(113)-C(62)	-142.6
C(108)-C(107)-C(113)-C(62)	0.0
C(112)-C(111)-C(114)-C(98)	-138.2
C(97)-C(111)-C(114)-C(98)	0.0
C(112)-C(111)-C(114)-C(110)	0.0
C(97)-C(111)-C(114)-C(110)	138.2
C(95)-C(98)-C(114)-C(111)	0.0
C(102)-C(98)-C(114)-C(111)	142.6
C(95)-C(98)-C(114)-C(110)	-142.6
C(102)-C(98)-C(114)-C(110)	0.0
C(107)-C(110)-C(114)-C(111)	0.0
C(106)-C(110)-C(114)-C(111)	-142.6
C(107)-C(110)-C(114)-C(98)	142.6
C(106)-C(110)-C(114)-C(98)	0.0
C(53)-O(10)-C(52)-C(51)	172.7
C(52)-O(10)-C(53)-C(54)	168.3

Symmetry transformations used to generate equivalent atoms:

10.DFT calculations

DFT Calculations were performed on 11 systems using Gaussian16W software. Geometry optimization and frequency calculations were performed on the systems mentioned in the table below. All calculations were in the ground state using B3LYP method and 6-31G(d,p) basis set for all atoms except iodine, which were handled with LanL2DZ basis set. The systems were optimized in chloroform solvent using the PCM solvent model. For each optimized structure, 0 imaginary frequencies were found, indicating the structure optimization had reached a minimum. For the purpose of calculating binding energy, an energy calculation was performed on a Cl atom and a Br atom using the same method and 6-31G(d,p) basis set in chloroform solvent by PCM model. We note that the DFT calculations were performed using a smaller basis set, which may result in a high basis set superposition error. Additionally, dispersion interactions were not included in the calculations. We are currently exploring various methods and basis sets to estimate the accuracy of these results and will report our findings in future work.

The relative binding energies in Table 2 in manuscript are calculated based on the binding energies shown in table below.

HIM monomer + TBA(X)	Binding Energy (kJ/mol)	I-X Bond Length	Charge I (e ⁻)	Charge X (e ⁻)
6a Monomer			1.085	
6a- Cl	-74.4	2.91	1.073	-0.707
6a- Br	685.6	3.01	1.044	-0.655
6b Monomer			1.082	
6b- Cl	-73.8	2.91	1.074	-0.706
6b- Br	685.8	3.01	1.044	-0.653
6c Monomer			1.118	
6c-Cl	-78.4	2.88	1.102	-0.689
6c-Br	680.8	2.98	1.073	-0.635

Table SI2: Geometry optimization and frequency calculations table.

HIM monomer 6a-Cl

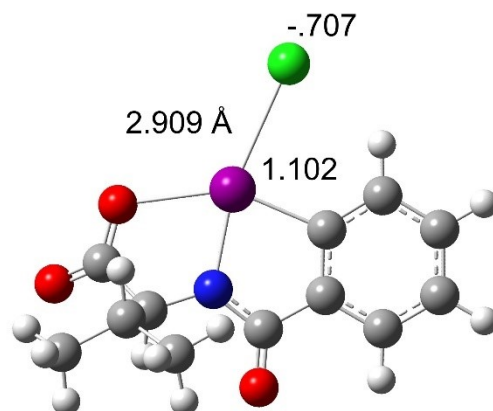


Figure SI22. DFT energy minimized structures of **6a**-chloride using B3LYP/6-31G(d,p) functional. Nitrogen, oxygen and iodine atoms are denoted by blue, red and purple color respectively. I-Cl bond distance is 2.909 Å. The charges on the I atom and oxygen atom are 1.102 eV and -0.707 eV respectively.

Coordinates for DFT Calculated Structure of HIM monomer 6a-Cl

Job Type: geometry optimization and frequency calculation

Method: Ground state, Default spin, DFT, B3LYP

Basis Set: 6-31G(d,p) for all atoms excluding Iodine, LanL2DZ for Iodine

Solvent: Chloroform using PCM solvent model

Total Energy: -1216.607637 Hartree

Number of Imaginary Frequencies: 0

Center Number	Atomic Number	X	Y	Z
1	6	2.00175	-2.929049	-0.425939
2	6	1.215278	-1.775467	-0.328993
3	6	1.827554	-0.567134	-0.010325
4	6	3.193123	-0.456925	0.208571
5	6	3.964882	-1.620165	0.113023
6	6	3.37434	-2.848743	-0.204244
7	1	1.513692	-3.866786	-0.670824
8	1	3.63701	0.504652	0.443015
9	1	5.035408	-1.561397	0.286867

10	1	3.988359	-3.741289	-0.277336
11	6	-0.264013	-1.82417	-0.520971
12	8	-0.871496	-2.866787	-0.793522
13	53	0.425455	1.080082	-0.025284
14	7	-0.861642	-0.618924	-0.325495
15	6	-2.65173	0.986253	-0.92266
16	8	-1.838284	1.923797	-0.599026
17	6	-2.949917	-0.546413	1.075148
18	6	-2.443968	-1.764578	1.860078
19	6	-4.483044	-0.580749	0.968633
20	1	-2.663756	0.358147	1.630896
21	1	-1.364885	-1.721349	2.03062
22	1	-2.933433	-1.805441	2.839619
23	1	-2.663628	-2.695656	1.328603
24	1	-4.869184	0.268912	0.402746
25	1	-4.811842	-1.496337	0.461511
26	1	-4.933285	-0.574155	1.967262
27	1	-2.717176	-1.173342	-1.012066
28	8	-3.694297	1.112088	-1.579209
29	6	-2.303011	-0.413961	-0.342109
30	17	2.624132	2.899178	0.537671

HIM monomer 6a-Br

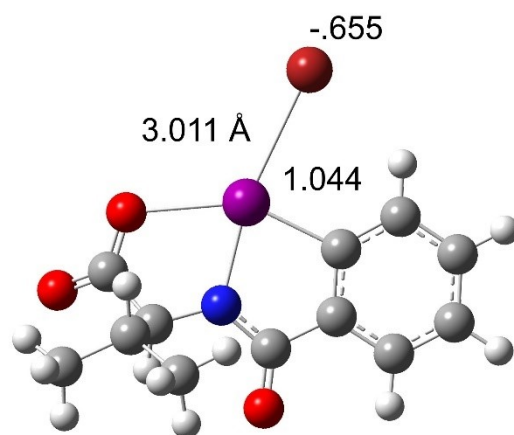


Figure S123. DFT energy minimized structures of **6a**-bromide using B3LYP/6-31G(d,p) functional. Nitrogen, oxygen and iodine atoms are denoted by blue, red and purple color respectively. I-Cl bond distance is 3.011 Å. The charges on the I atom and oxygen atom are 1.044 eV and -0.655 eV respectively.

Coordinates for DFT Calculated Structure of HIM monomer 6a-Br

Job Type: geometry optimization and frequency calculation

Method: Ground state, Default spin, DFT, B3LYP

Basis Set: 6-31G(d,p) for all atoms excluding Iodine, LanL2DZ for Iodine

Solvent: Chloroform using PCM solvent model

Total Energy: -3327.822223 Hartree

Number of Imaginary Frequencies: 0

Center Number	Atomic Number	X	Y	Z
1	6	-0.694926	3.60332	-0.365841
2	6	-0.298486	2.262534	-0.302327
3	6	-1.260283	1.287698	-0.053676
4	6	-2.601841	1.592259	0.126076
5	6	-2.981219	2.93752	0.063517
6	6	-2.034329	3.938026	-0.182655
7	1	0.063672	4.355481	-0.556367
8	1	-3.326115	0.804697	0.306331
9	1	-4.025115	3.200973	0.207206
10	1	-2.345043	4.977348	-0.231187
11	6	1.133858	1.869325	-0.461561
12	8	2.032385	2.692603	-0.679987
13	53	-0.425859	-0.710041	-0.105264
14	7	1.334437	0.536649	-0.303058
15	6	2.572516	-1.514154	-0.947171
16	8	1.513147	-2.179736	-0.667937
17	6	3.275772	-0.209156	1.111102
18	6	3.145455	1.079697	1.934476
19	6	4.75002	-0.635306	1.019923
20	1	2.719637	-1.002085	1.631779
21	1	2.10021	1.356889	2.095491
22	1	3.608015	0.941853	2.918319
23	1	3.642122	1.917788	1.436049
24	1	4.87392	-1.544944	0.42937
25	1	5.348521	0.153129	0.546785
26	1	5.158602	-0.806192	2.021954
27	1	3.284436	0.527597	-0.951828
28	8	3.544907	-1.919765	-1.599752
29	6	2.646334	-0.093434	-0.315655
30	35	-3.157547	-1.898905	0.333447

HIM monomer 6b-Cl

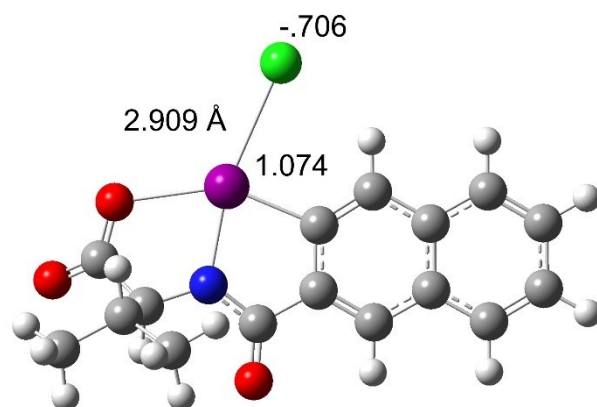


Figure SI24: DFT energy minimized structures of **6b**-chloride using B3LYP/6-31G(d,p) functional. Nitrogen, oxygen and iodine atoms are denoted by blue, red and purple color respectively. I-Cl bond distance is 2.909 Å. The charges on the I atom and oxygen atom are 1.074 eV and -0.706 eV respectively.

Coordinates for DFT Calculated Structure of HIM monomer 6b-Cl

Job Type: geometry optimization and frequency calculation

Method: Ground state, Default spin, DFT, B3LYP

Basis Set: 6-31G(d,p) for all atoms excluding iodine, LanL2DZ for Iodine

Solvent: Chloroform using PCM solvent model

Total Energy: -1370.251804 Hartree

Number of Imaginary Frequencies: 0

Center Number	Atomic Number	X	Y	Z
1	6	-0.386726	-1.683882	-0.505847
2	8	-0.603533	-2.874786	-0.762132
3	53	-0.738221	1.293118	-0.04813
4	7	-1.35994	-0.755029	-0.31075
5	6	-3.599206	0.12624	-0.904528
6	8	-3.155127	1.291602	-0.604191
7	6	-3.335647	-1.395553	1.108184
8	6	-2.43386	-2.357109	1.894591
9	6	-4.762416	-1.959949	1.015152
10	1	-3.37683	-0.443565	1.656949
11	1	-1.43702	-1.939367	2.059411
12	1	-2.874656	-2.561388	2.876797
13	1	-2.316525	-3.308502	1.366651
14	1	-5.420678	-1.304163	0.442584

15	1	-4.75564	-2.939458	0.521078
16	1	-5.182841	-2.096663	2.01743
17	1	-2.91423	-1.922112	-0.976428
18	8	-4.628429	-0.124853	-1.545972
19	6	-2.783563	-1.060102	-0.315525
20	6	0.988059	-1.13036	-0.332025
21	6	1.14941	0.237333	-0.023749
22	6	2.105044	-1.934718	-0.4268
23	6	2.373062	0.811212	0.18202
24	6	3.400716	-1.400608	-0.217749
25	1	1.9701	-2.986503	-0.660861
26	6	3.53715	-0.005506	0.094531
27	1	2.459093	1.870955	0.401623
28	6	4.57205	-2.203128	-0.306375
29	6	4.837172	0.528761	0.305601
30	6	5.817068	-1.654494	-0.096687
31	1	4.465448	-3.25833	-0.542855
32	6	5.950363	-0.276794	0.211785
33	1	4.936574	1.584577	0.541125
34	1	6.704785	-2.276104	-0.167231
35	1	6.938945	0.142563	0.374243
36	17	0.704319	3.764957	0.471679

HIM monomer 6b-Br

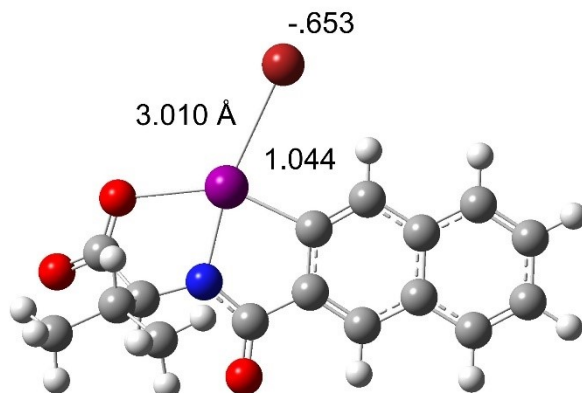


Figure SI25. DFT energy minimized structures of **6b**-bromide using B3LYP/6-31G(d,p) functional. Nitrogen, oxygen and iodine atoms are denoted by blue, red and purple color respectively. I-Cl bond distance is 3.010 Å. The charges on the I atom and oxygen atom are 1.044 eV and -0.653 eV respectively.

Coordinates for DFT Calculated Structure of HIM monomer 6b-Br

Job Type: geometry optimization and frequency calculation

Method: Ground state, Default spin, DFT, B3LYP

Basis Set: 6-31G(d,p) for all atoms excluding iodine, LanL2DZ for iodine

Solvent: Chloroform using PCM solvent model

Total Energy: -3481.46653 Hartree

Number of Imaginary Frequencies: 0

Center Number	Atomic Number	X	Y	Z
1	6	-0.53406	-2.002197	-0.462761
2	8	-0.799969	-3.194707	-0.66397
3	53	-0.744123	1.014018	-0.13006
4	7	-1.461906	-1.024447	-0.307839
5	6	-3.663741	-0.076575	-0.941044
6	8	-3.179622	1.08468	-0.695589
7	6	-3.451402	-1.488067	1.156144
8	6	-2.594463	-2.453597	1.986526
9	6	-4.908443	-1.97507	1.106615
10	1	-3.433881	-0.50654	1.651369
11	1	-1.574958	-2.082037	2.12022
12	1	-3.034688	-2.5817	2.981833
13	1	-2.532987	-3.436811	1.509766
14	1	-5.537043	-1.312491	0.509094
15	1	-4.963267	-2.976411	0.661587
16	1	-5.323046	-2.038138	2.118684

17	1	-3.074378	-2.154997	-0.895594
18	8	-4.698178	-0.323813	-1.577567
19	6	-2.897096	-1.262672	-0.287917
20	6	0.865726	-1.501616	-0.318134
21	6	1.09416	-0.13107	-0.068296
22	6	1.942893	-2.361344	-0.38165
23	6	2.345511	0.389667	0.111258
24	6	3.263827	-1.883572	-0.196757
25	1	1.755104	-3.413869	-0.571824
26	6	3.468635	-0.485345	0.057498
27	1	2.487812	1.451726	0.28758
28	6	4.394188	-2.745504	-0.252166
29	6	4.793559	-0.00705	0.24695
30	6	5.664939	-2.250377	-0.064841
31	1	4.235462	-3.803052	-0.444847
32	6	5.865855	-0.869395	0.18717
33	1	4.945111	1.051352	0.439484
34	1	6.521072	-2.91708	-0.109242
35	1	6.873997	-0.492724	0.333238
36	35	0.795691	3.563839	0.305205

HIM monomer 6c-Cl

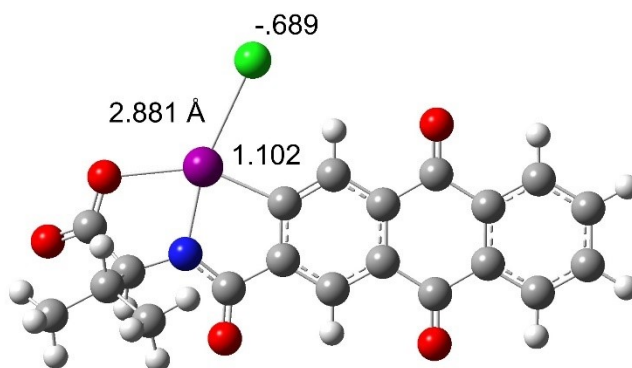


Figure SI26: DFT energy minimized structures of **6c**-chloride using B3LYP/6-31G(d,p) functional. Nitrogen, oxygen and iodine atoms are denoted by blue, red and purple color respectively. I-Cl bond distance is 2.881 Å. The charges on the I atom and oxygen atom are 1.102 eV and -0.689 eV respectively.

Coordinates for DFT Calculated Structure of HIM monomer 6C-Cl

Job Type: geometry optimization and frequency calculation

Method: Ground state, Default spin, DFT, B3LYP

Basis Set: 6-31G(d,p) for all atoms excluding Iodine, LanL2DZ for Iodine

Solvent: Chloroform using PCM solvent model

Total Energy: -1673.13186 Hartree

Number of Imaginary Frequencies: 0

Center Number	Atomic Number	X	Y	Z
1	6	-1.338783	-1.653972	-0.453534
2	8	-1.432273	-2.86718	-0.669955
3	53	-1.960455	1.294174	-0.100014
4	7	-2.389032	-0.815385	-0.271326
5	6	-4.703937	-0.157525	-0.852236
6	8	-4.35319	1.052197	-0.59898
7	6	-4.281134	-1.596851	1.191409
8	6	-3.278103	-2.434489	1.996659
9	6	-5.641897	-2.309369	1.130134
10	1	-4.416843	-0.637602	1.711359
11	1	-2.329814	-1.909768	2.141041
12	1	-3.689247	-2.654079	2.988197
13	1	-3.064852	-3.383873	1.496092
14	1	-6.368269	-1.747344	0.540417
15	1	-5.534685	-3.300505	0.672318
16	1	-6.040621	-2.451909	2.140331
17	1	-3.839276	-2.138532	-0.885926
18	8	-5.722801	-0.511694	-1.457498
19	6	-3.778073	-1.250908	-0.248858
20	6	7.373056	0.289337	0.247932
21	6	6.175359	0.995828	0.32813
22	6	4.954064	0.334758	0.150769
23	6	4.941436	-1.050655	-0.108917
24	6	6.150213	-1.752746	-0.187288
25	6	7.360517	-1.08667	-0.01013
26	6	3.689005	1.117821	0.241483
27	6	3.661846	-1.78803	-0.302952
28	6	2.393904	-1.006386	-0.21614
29	6	2.405185	0.381996	0.039382
30	6	1.203302	1.100717	0.109105
31	1	1.219463	2.169983	0.292253
32	6	0.015409	0.410896	-0.064434
33	6	-0.020006	-0.960893	-0.31473
34	6	1.178381	-1.669708	-0.391764
35	1	8.31716	0.807451	0.385793
36	1	6.161851	2.061853	0.526827

37	1	6.117324	-2.81802	-0.387956
38	1	8.294904	-1.636065	-0.072499

HIM monomer 6c-Br

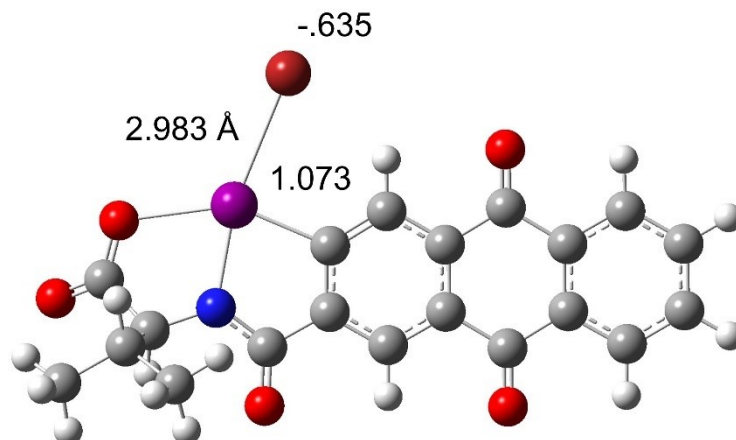


Figure SI27: DFT energy minimized structures of **6c**-bromide using B3LYP/6-31G(d,p) functional. Nitrogen, oxygen and iodine atoms are denoted by blue, red and purple color respectively. I-Cl bond distance is 2.983 Å. The charges on the I atom and oxygen atom are 1.073 eV and -0.635 eV respectively.

Coordinates for DFT Calculated Structure of HIM monomer 6c-Br

Job Type: geometry optimization and frequency calculation

Method: Ground state, Default spin, DFT, B3LYP

Basis Set: 6-31G(d,p) for all atoms excluding Iodine, LanL2DZ for Iodine

Solvent: Chloroform using PCM solvent model

Total Energy: -3784.346757 Hartree

Number of Imaginary Frequencies: 0

Center Number	Atomic Number	X	Y	Z
1	6	-1.242669	-1.968214	-0.430173
2	8	-1.3005	-3.188762	-0.622685
3	53	-1.92831	0.983466	-0.137531
4	7	-2.311125	-1.152729	-0.268636
5	6	-4.641045	-0.559872	-0.87398
6	8	-4.328445	0.662836	-0.639188
7	6	-4.194288	-1.955773	1.193924
8	6	-3.173003	-2.745811	2.023983

9	6	-5.531052	-2.712462	1.133657
10	1	-4.365281	-0.991983	1.694748
11	1	-2.243773	-2.18767	2.167106
12	1	-3.586583	-2.96076	3.015609
13	1	-2.92387	-3.696439	1.54274
14	1	-6.268688	-2.184019	0.527154
15	1	-5.387811	-3.707588	0.69465
16	1	-5.935026	-2.849922	2.142568
17	1	-3.726343	-2.519364	-0.871044
18	8	-5.646589	-0.954563	-1.478503
19	6	-3.689115	-1.619914	-0.248449
20	6	7.426129	0.17932	0.216686
21	6	6.214065	0.862926	0.276669
22	6	5.00661	0.171379	0.122214
23	6	5.022585	-1.221495	-0.093586
24	6	6.245615	-1.90041	-0.152094
25	6	7.441998	-1.204073	0.00195
26	6	3.725382	0.930124	0.190301
27	6	3.75834	-1.991397	-0.261485
28	6	2.474711	-1.233505	-0.200563
29	6	2.457463	0.161427	0.014938
30	6	1.240822	0.856153	0.066922
31	1	1.236939	1.930197	0.222204
32	6	0.06675	0.138763	-0.086921

Coordinates for DFT Calculated Structure of HIM 6a monomer (without anions)

Job Type: geometry optimization and frequency calculation

Method: Ground state, Default spin, DFT, B3LYP

Basis Set: 6-31G(d,p) for all atoms excluding Iodine, LanL2DZ for Iodine

Solvent: Chloroform using PCM solvent model

Total Energy: -756.233551 Hartree

Number of Imaginary Frequencies: 0

Center Number	Atomic Number	X	Y	Z
1	6	-2.918791	1.872623	-0.546238
2	6	-1.842108	0.998179	-0.361833
3	6	-2.081044	-0.276683	0.138391
4	6	-3.354537	-0.72738	0.45515
5	6	-4.423117	0.157264	0.270904

6	6	-4.206455	1.447382	-0.227244
7	1	-2.724585	2.867638	-0.932389
8	1	-3.528384	-1.728887	0.835132
9	1	-5.429406	-0.166603	0.518027
10	1	-5.047354	2.119234	-0.365631
11	6	-0.440398	1.40349	-0.652849
12	8	-0.116459	2.502989	-1.098367
13	53	-0.283887	-1.462033	0.214794
14	7	0.483951	0.443287	-0.325036
15	6	2.58315	-0.789037	-0.753325
16	8	1.964837	-1.824922	-0.279782
17	6	2.582111	1.13689	0.8925
18	6	1.777338	2.278749	1.528515
19	6	4.024971	1.588418	0.614253
20	1	2.612377	0.30478	1.610564
21	1	0.772225	1.961027	1.818757
22	1	2.288478	2.625583	2.432574
23	1	1.681082	3.126045	0.843528
24	1	4.619185	0.79514	0.158007
25	1	4.032697	2.449602	-0.064547
26	1	4.506682	1.896166	1.547889
27	1	2.119453	1.247673	-1.25872
28	8	3.649967	-0.817245	-1.360355
29	6	1.927071	0.576904	-0.415552

Coordinates for DFT Calculated Structure of HIM monomer 6b (without anions)

Job Type: geometry optimization and frequency calculation

Method: Ground state, Default spin, DFT, B3LYP

Basis Set: 6-31G(d,p) for all atoms excluding Iodine, LanL2DZ for Iodine

Solvent: Chloroform using PCM solvent model

Total Energy: -909.87796 Hartree

Number of Imaginary Frequencies: 0

Center Number	Atomic Number	X	Y	Z
1	6	0.264034	1.306073	-0.618858
2	8	0.471283	2.449472	-1.022532
3	53	0.736473	-1.560341	0.136314
4	7	1.286712	0.450416	-0.290411
5	6	3.52189	-0.515507	-0.738144
6	8	3.020265	-1.635414	-0.32254

7	6	3.281269	1.340806	0.969267
8	6	2.334751	2.345521	1.640402
9	6	4.654281	1.983956	0.716793
10	1	3.416526	0.493442	1.656609
11	1	1.378919	1.889702	1.912456
12	1	2.795125	2.723343	2.55923
13	1	2.130878	3.196736	0.984379
14	1	5.344575	1.291464	0.232721
15	1	4.551477	2.865179	0.072248
16	1	5.0926	2.313793	1.664232
17	1	2.824652	1.467778	-1.181992
18	8	4.596702	-0.393493	-1.319221
19	6	2.705093	0.751101	-0.363363
20	6	-1.086999	0.736334	-0.373627
21	6	-1.187964	-0.591774	0.088621
22	6	-2.234793	1.482585	-0.545398
23	6	-2.385321	-1.187968	0.374009
24	6	-3.504469	0.92131	-0.261254
25	1	-2.150008	2.506766	-0.895762
26	6	-3.584099	-0.434496	0.208635
27	1	-2.451524	-2.215555	0.72031
28	6	-4.706124	1.664044	-0.426209
29	6	-4.859495	-0.990723	0.493407
30	6	-5.926691	1.095143	-0.141893
31	1	-4.64212	2.688745	-0.780849
32	6	-6.003123	-0.242573	0.321192
33	1	-4.918814	-2.01572	0.848156
34	1	-6.838502	1.669867	-0.271556
35	1	-6.973254	-0.677904	0.540883

Coordinates for DFT Calculated Structure of HIM monomer 6c (without anions)

Job Type: geometry optimization and frequency calculation

Method: Ground state, Default spin, DFT, B3LYP

Basis Set: 6-31G(d,p) for all atoms excluding Iodine, LanL2DZ for Iodine

Solvent: Chloroform using PCM solvent model

Total Energy: -1212.756261 Hartree

Number of Imaginary Frequencies: 0

Center Number	Atomic Number	X	Y	Z
1	6	1.409603	1.341434	-0.505864
2	8	1.564532	2.526225	-0.790765
3	53	1.983617	-1.566437	-0.018819
4	7	2.457147	0.49272	-0.260411
5	6	4.724134	-0.349294	-0.755232
6	8	4.250914	-1.520936	-0.454716
7	6	4.391657	1.307447	1.134305
8	6	3.420898	2.251473	1.857173
9	6	5.774838	1.964141	0.998426
10	1	4.49773	0.39864	1.743902
11	1	2.454194	1.778914	2.050703
12	1	3.845933	2.540835	2.82371
13	1	3.244935	3.160837	1.275298
14	1	6.489499	1.312637	0.493451
15	1	5.702734	2.89568	0.424656
16	1	6.166698	2.213198	1.989694
17	1	3.977051	1.650185	-1.003037
18	8	5.798697	-0.145299	-1.309266
19	6	3.8659	0.847383	-0.267286
20	6	-7.323296	-0.464712	0.294718
21	6	-6.131858	-1.17729	0.408301
22	6	-4.905174	-0.535264	0.1999
23	6	-4.880308	0.837516	-0.125704
24	6	-6.083073	1.54471	-0.237108
25	6	-7.298778	0.897191	-0.028153
26	6	-3.649878	-1.320596	0.327685
27	6	-3.597349	1.555811	-0.355414
28	6	-2.331576	0.769347	-0.230892
29	6	-2.357985	-0.602346	0.093044
30	6	-1.164405	-1.328945	0.201279
31	1	-1.218415	-2.384402	0.445847
32	6	0.028258	-0.660182	-0.00739
33	6	0.077276	0.69454	-0.329349
34	6	-1.110785	1.415062	-0.441531
35	1	-8.271631	-0.967364	0.456933
36	1	-6.129103	-2.232665	0.657573
37	1	-6.042932	2.59891	-0.488038
38	1	-8.228262	1.450927	-0.116338
39	1	-1.086907	2.470564	-0.687715
40	8	-3.567557	2.749129	-0.637766
41	8	-3.656816	-2.514036	0.613539

DFT Calculated Energy of Chlorine

Job Type: energy

Method: Ground state, Default spin, DFT, B3LYP

Basis Set: 6-31G(d,p)

Solvent: Chloroform using PCM solvent model

Total Energy: -460.34574 Hartree

DFT Calculated Energy of Bromine

Job Type: energy

Method: Ground state, Default spin, DFT, B3LYP

Basis Set: 6-31G(d,p)

Solvent: Chloroform using PCM solvent model

Total Energy: -2571.849795 Hartree

