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Structure of the Active Nanocomplex of Antiviral and Anti-Infectious Iodine-Containing Drug FS-1

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Abstract: Chromatographic analysis shows that the ionic nanostructured complex of the FS-1 drug contains nanocomplexes of α-dextrin with a size of ~40–48 Å. Based on good agreement between the UV spectra of the model structures and the experimental spectrum of the FS-1 drug, the structure of the active FS-1 nanocomplex is proposed. The structure of the active centers of the drug in the dextrin ring was calculated using the quantum-chemical approach DFT/B3PW91. The active centers, i.e., a complex of molecular iodine with lithium halide (I), a binuclear complex of magnesium and lithium containing molecular iodine, triiodide (II), and triiodide (III), are located inside the dextrin helix. The polypeptide outside the dextrin helix forms a hydrogen bond with dextrin in Complex I and coordinates the molecular iodine in Complex II. It is revealed that the active centers of the FS-1drug can be segregated from the dextrin helix and form complexes with DNA nucleotide triplets. The active centers of the FS-1 drug are only segregated on specific sections of DNA. The formation of a complex between the DNA nucleotide and the active center of FS-1 is a key stage in the mechanisms of anti-HIV, anti-coronavirus (Complex I) and antibacterial action (Complex II).

Keywords: iodine-containing drug; α-dextrin; DFT method; DNA nucleotide triplets

Citation: Yuldasheva, G.A.-R.; Kurmanaliyeva, A.; Ilin, A. Structure of the Active Nanocomplex of Antiviral and Anti-Infectious Iodine-Containing Drug FS-1. *Quantum Rep.* **2021**, *3*, 746–812. https://doi.org/10.3390/quantum3040047

Academic Editors: Richard Dronskowski, Elena Besley and Andrei L. Tchougréeff

Received: 29 September 2021
Accepted: 30 November 2021
Published: 13 December 2021

1. Introduction

Molecular iodine has a broad spectrum of antimicrobial and antiviral effects. There are several groups of iodine preparations: (1) containing elemental iodine, (2) inorganic iodides, (3) organic substances—hormones, (4) organic substances eliminating iodine, (5) organic substances that firmly bind iodine.

However, currently, all known molecular iodine containing medications are practically not used for parenteral administration, due to their high toxicity.

A distinctive feature of the FS-1 drug is that its active substance includes not only an iodine-containing polymer complex (a molecular iodine complex with low molecular weight α-dextrins and peptides) but also potassium, lithium and magnesium halides. In the composition of the FS-1 drug, molecular iodine is in such an active form that, when administered parenterally, it minimizes toxic effects in the human body [1].

The use of the antimicrobial properties of iodine in the composition of iodine/polymer complexes began in the second half of the 20th century. Compounds of mobile equilibrium systems of iodine and its salts aqueous solutions with starch, amylase, amylopectin, and polyvinyl alcohol have been well studied. The advantages of such high-polymer iodine complexes as compared to the sulfonamides and antibiotics have been established—a wide spectrum of antimicrobial action both in vivo and in vitro, exclusion of the emergence of new resistant forms of microorganisms, low toxicity in combination with a high chemotherapeutic index and the effectiveness of short-term treatment [2,3].

For the latest three decades, new nanoparticles are being researched for the purpose of developing new drug delivery systems. Macromolecules, such as proteins and nucleic acids, demonstrate low stability in biological matrix. Their efficient delivery to target

sites is widely limited in vivo, as these molecules are unlikely to be able to cross various biological barrier, whereas polysaccharides are able to overcome cellular barriers for the delivery of pharmaceutical molecules into cells [4].

Dextrin is an unbranched polysaccharide that exhibits high water solubility and is widely used in food and medicine [5]. The presence of hydroxyl groups makes it possible for dextrin to interact with protein. A hydrogen bond is formed between the OH group of the glucose ring and the oxygen atom of the peptide amido group.

Important tasks that can be achieved with the use of dextrin are drug targeting, improvement of circulation time, stabilization of the therapeutic agent, drug solubilization, reduction of side effects, sustained release action and depot properties [6].

The absorption of dextrin nanoparticles by cellular systems occurs through a process known as endocytosis and is influenced by the physicochemical characteristics of the nanoparticles, such as size, shape and the experimental conditions used [7].

The size of nanoparticles plays a key part in the use of dextrins as carrier systems as well as transmembrane transporters [8].

In this paper, the mass of α-dextrin, which is part of the FS-1 drug, was determined by the chromatographic method. Using the data of X-ray diffraction analysis for the structure of α-dextrins [9], the size of the α-dextrin nanocomplex is ~40–48 Å, which contains the active centers of the drug and determines its main pharmacological properties.

Based on the study of an aqueous solution of the system modeling the specific feature of the drug FS-1, the structure of the active nanocomplex FS-1 is proposed [10,11]. The nanocomplex of the FS-1drug contains a triiodide and two active centers located inside the dextrin helix: molecular iodine coordinated by a lithium halide and a polypeptide ($LiI(Cl)I_2$, Complex I), a binuclear complex of magnesium and lithium, including molecular iodine (MgI_3LiII_2, Complex II). In these complexes, molecular iodine exhibits acceptor properties with respect to the polypeptide in Complex II or ion I^- in Complex I and donor properties with respect to lithium halide in Complex II or Li^+ ion in Complex I. The polypeptide coordinates molecular iodine in Complex II and is located outside the dextrin helix.

For the purpose of this paper, the calculation was made using quantum-chemical approach DFT/B3PW91 with full optimization of the geometry of the spatial and electronic structure of the $LiI\ I_2$ and MgI_3LiII_2 complexes in the dextrin ring. In the calculations the polypeptide was replaced by an amide. The calculated UV spectra (TD-DFT/B3PW91 approach) of these complexes are in good agreement with the experimental UV spectra of the drug FS-1.

The ability of the FS-1 drug to penetrate the bactericidal cell membrane was proved by the electron spectroscopy method [12]. The active centers are protected from interaction with bioorganic ligands that are part of the cytoplasm of the cell by the α-dextrin helix and interaction with polypeptides. In earlier papers [13,14], we showed that only DNA nucleotides can compete with polypeptides for complexation with molecular iodine, which is part of the active centers of the drug FS-1.

In this paper, it is demonstrated that the active centers of the drug can be segregated from the dextrin helix and form complexes with nucleotide triplets of viral or bacterial DNA.

The interaction of active centers with nucleotide triplets is selective: the active centers of the FS-1 drug are only segregated on specific sections DNA. The mechanism of action of the drug is determined by the structure of the active center, which has formed a complex with a nucleotide triplet. The formation of a complex between the DNA nucleotide and the active center of the FS-1 drug (Complex I) is a key stage in the mechanisms of anti-HIV [14], anti-coronavirus (Complex I, II) [15] and antibacterial action (Complex II) [12].

2. Materials and Methods

The chromatographic method determined the α-dextrin mass, which is part of the FS-1 drug. Using the X-ray structural analysis data for the α-dextrins structure [9], the size of the nanocomplex α-dextrin was found ~40–48Å, containing active centers of the

drug and determining its basic pharmacological properties. Chromatographic studies were performed on an Agilent 1200 chromatograph with a refractometric detector on a gel-penetrating column Agilent PL Aquagel Mixed-H 8 μm (size exclusion column).

UV spectra were obtained using a Lambda-35 spectrophotometer (Perkin Elmer Inc., Waltham, MA, USA). Spectral range: 190–1100 nm, wavelength λ ± 0.5 nm. Optical density ± 0.02 units.

An adequate description of the structure and electronic properties of iodine complexes with the transfer of charge and polyiodide ions requires taking into account electron correlation. A detailed comparative analysis of various quantum chemical approaches including CCSD (T) and DFT (BLYP, BPW91, B3LYP, B3PW91) for calculations of dissociation energies, bond lengths, and harmonic frequencies for polyiodide anions and evaluation of the obtained data based on agreement with experimental IR and Raman Spectroscopy studies is presented in [16]. Comparison of the results obtained by DFT-methods with the results obtained by the CCSD (T) and experimental data show that the most reliable results are produced by an approximation of DFT-B3PW91. Based on these conclusions the DFT-B3PW91/6-31G ** for Atom I used basis midi approximation was selected in our investigations of molecular structures and characteristics of the complexes containing lithium and magnesium halides, molecular iodine and iodide anion.

The coincidence of the wavelength of electronic transitions for active centers and a triiodide, calculated using approach TD-DFT/B3PW91/midi, with experimentally obtained UV spectrum for drug FS-1 confirm the structures of active centers.

All calculations were performed on the Fujitsu PRIMERGY BX 920 S1 supercomputer (Fujitsu, Tokyo, Japan) with a performance of 10.9 TFLOPS with the help of the GAUSSIAN 09 program Gaussian 09 (Gaussian, Inc., Wallingford, CT, USA) [17].

3. Results

3.1. Determination of the Molecular Weight of α-Dextrin Nanoparticles in the FS-1 Drug by Chromatographic Method

To determine the molar masses of α-dextrins with a low and medium molar mass, oligomeric α-dextrins and α-dextrins with a molar mass of 75,000 g/mol were used as standards. The characteristics of the substances used are presented in Table 1.

Table 1. Properties of α-dextrins used as standards in calibrations to determine the molar masses of the catalytic reactions products.

Name	Formula	Retention Time, min	Molar Mass, g/mol	lg M	Number of Glucose Units
Maltotriose	$C_{18}H_{32}O_{16}$	9.4	504	2.70243	3
Maltotriose	$C_{24}H_{42}O_{21}$	9.356	666	2.82347	4
Maltopentaose	$C_{30}H_{52}O_{26}$	9.315	831	2.9196	5
Maltohexaose	$C_{36}H_{62}O_{31}$	9.289	990	2.99564	6
Maltoheptaose	$C_{42}H_{72}O_{36}$	9.259	1152	3.06145	7
High molecular weight α-dextrin		8.08	75,000	4.87506	417

To obtain a calibration, the results were subjected to mathematical treatment. The dependence of the logarithm of the molar mass of the calibration carbohydrates on the retention time was plotted.

Based on the obtained dependence after mathematical treatment, the following equation was obtained:

$$y = \lg M = -1.5968 \times x + 17.787 \quad (1)$$

The correlation coefficient was determined, which was −0.9983. This coefficient indicates the good linearity of the data obtained.

As can be seen in Figure 1 and Table 2 the high molecular weight peak at 5.665 min is 12 percent of the total α-dextrins. The main peak has a bimodal distribution. However, the average molar mass of the peak is quite high.

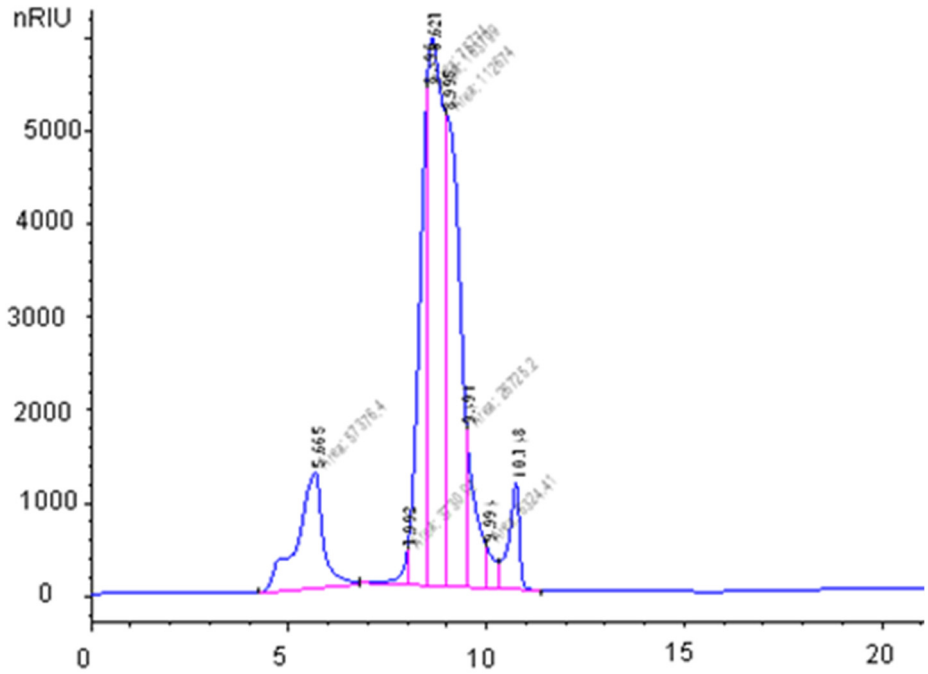

Figure 1. Chromatogram of the α-dextrin part of the FS-1 drug.

Table 2. Peaks and fractions properties in the chromatogram of α-dextrins of a part of the FS-1 drug.

Retention Time, min	Molecular Weight, g/mol	Polymerization Level	Content of the Total Amount of Carbohydrates in Solution, %
	Peaks		
5.665	4,800,000	26,667	12.25
8.627	10,260	57	83.09
	Peak Segments 8.627		
8.25	41.058	228.1	16.184
8.75	6531	36.28	34.986
9.25	1039	5.772	24.066
9.75	165	0.917	5.708

The main fraction in the FS-1drug is the fraction with a retention time of 8.75 min, its content in the total amount of α-dextrins was 34.986%. Since this fraction is in the middle of the peak and its share in the segments is maximum, it is reasonable to take its molecular weight as the average for the α-dextrin part of the FS-1drug. It means that the average molecular weight of the main component of α-dextrin in FS-1 with a retention time of 8.75 is 6531 (polymerization level—36.22). The higher molecular weight component of α-dextrins, apparently, should not be considered as capable of forming iodine-polymer complexes, since with such a large molecular weight—4,800,000 Da, the polymer structure is branched and cannot form iodine-polymer complexes.

The chromatographic method determined the average molecular weight of α-dextrin ~6531, which makes it possible to determine the size of α-dextrin nanoparticles. One dextrin ring of α-dextrin includes six glucose rings (the molecular weight of the glucose ring is 173), hence the dextrin nanomplex contains 6–7 rings. It is known from the data

of X-ray diffraction analysis that the distance between the dextrin rings is ~8 Å hence the nanoparticle size is ~40–48 Å.

3.2. FS-1 Active Nanocomplex Structure

The FS-1 drug is a chemically complex multicomponent drug containing molecular iodine, potassium and lithium halides, magnesium chloride, α-dextrins, and polypeptides. In terms of its physicochemical properties the drug FS-1 is an ionic nanostructured complex, which contains metal salts (LiCl (I), $MgCl_2$) of molecular iodine and its ionized forms.

It is not possible to identify active centers in the ionic nanostructured complex of the FS-1drug using physical techniques. We studied the structure of the active centers of the drug FS-1 on a model system, representing an aqueous solution containing potassium and lithium halides, molecular iodine, amino acid (glycine), and ethanol (system (a)) [10,11].

It was shown by UV spectroscopy in [18] that in an aqueous solution of KI—I_2-amylose, the number of units of the dextrin helix can affect the iodine-triiodide equilibrium. With an increase in the number of units ($N \geq 15$) by UV spectroscopy, iodine complexes and triiodide complexes can be detected in this system. Dextrin, which is a part of the drug, contains the number of units $N \geq 15$, therefore, molecular iodine and triiodide complexes can be present inside the dextrin helix and are identified in the UV spectra.

The glycine zwitterions cluster, such as the dextrin helix, creates conditions for the presence of I^-, I_3^- and I_2 ions in an aqueous solution of KI_3; therefore, a system containing glycine, potassium and lithium halides, and molecular iodine (system (a)) can be considered as a model for studying the interaction within the α-dextrin helix of lithium halides, triiodide and molecular iodine. System (a) was investigated by UV-IR spectroscopy and the quantum-chemical approach DFT/B3PW91 [10,11].

Quantum-chemical calculations of the stability of possible complexes in system (a) and spectroscopic studies indicate that lithium chloride interacts only with molecular iodine in system (a). When a complex of molecular iodine with the carboxy group of glycine is formed, a negative charge is transferred to molecular iodine, so I_2 can form a coordination bond with lithium chloride ($LiClI_2COO^-$). In such a complex, molecular iodine exhibits acceptor properties with respect to the carboxy group and donor properties with respect to lithium chloride.

The complex of lithium chloride with triiodide, which interacts with the protonated amino group of glycine, is significantly lower in the stability of the complex, in in which triiodide and lithium chloride are spatially separated: triiodide interacts with a protonated amino group, and lithium chloride with a positively charged carboxy group.

Consequently, three complexes are formed in system (a): $LiClI_2COO^-$, lithium chloride coordinated by the carboxy group, and triiodide, which forms a coordination bond with the protonated amino group.

These three complexes can also be formed within the α-dextrin helix.

The spatial and electronic structure of the LiI-I_2 complex in a dextrin ring containing six glucose rings and coordinated by an amide was calculated (Complex I). In the calculations, the polypeptide was replaced by an amide.

In Complex I, the lithium ion is not on the same straight line with triiodide; it coordinates two iodine atoms at once (Li-I^1 = 2.69 Å, Li-I^2 = 2.71 Å). This complex can be interpreted as a complex of molecular iodine (I^2-I^3 = 2.84 Å) with a lithium ion and an iodine ion I^1. When molecular iodine interacts with an iodine ion, I_2 acts as an acceptor; therefore, a negative charge is transferred to I_2. Negatively charged molecular iodine becomes a donor with respect to the lithium ion. In Complex I molecular iodine is in a special electronic form, not found in drugs containing iodine complexes with bioorganic ligands. The amide forms a hydrogen bond with one of the oxygen atoms of the dextrin ring (O-H = 1.87 Å) and does not interact with the LiI-I_2 complex. (Figure 2).

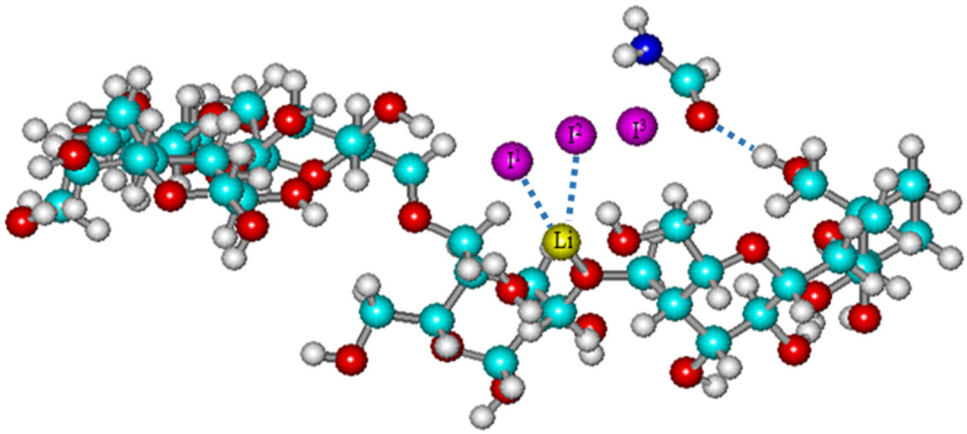

Figure 2. Complex I, LiI-I_2 in the dextrin ring. blue balls—carbon atoms, red—oxygen, dark blue—nitrogen, violet—iodine, yellow—lithium ion, white balls—hydrogen atoms.

The structure of the FS-1 drug also contains magnesium halides. Our calculations showed that magnesium ion can penetrate the dextrin ring and form a coordination bond with the OH group of α-dextrin. Inside the α-dextrin helix, the most energetically favorable structure is the one that combines the magnesium ion, triiodide, and LiCl (I)–I_2 (MgI_3LiII_2 Complex II, Figure 3).

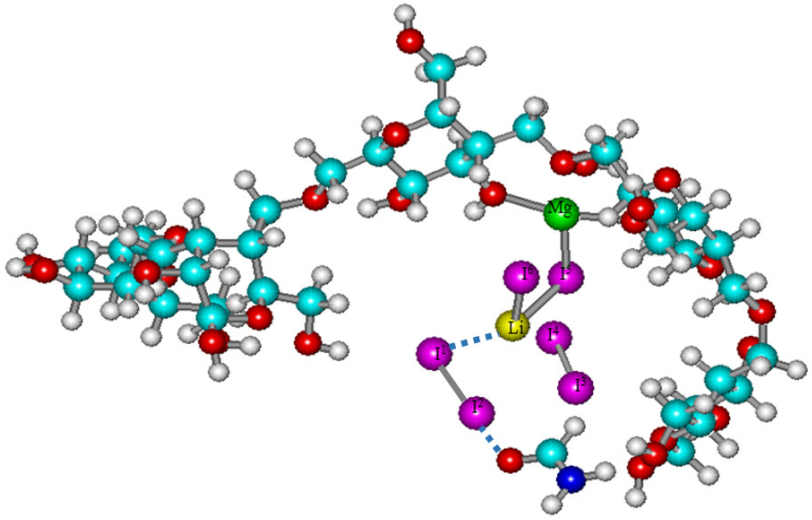

Figure 3. Complex II. A binuclear complex of magnesium and lithium, including molecular iodine and triiodide (MgI_3LiII_2) in the dextrin ring. Blue balls—carbon atoms, red balls—oxygen, dark balls—nitrogen, violet balls—iodine, green balls—magnesium ion, yellow balls—lithium ion, white balls—hydrogen atoms.

A calculation was performed with full optimization of the geometry of the spatial structure of the MgI_3LiII_2 complex in the dextrin ring (Complex II, Figure 3).

The MgI_3LiII_2 complex is a binuclear complex in which a magnesium ion and a lithium ion are bound by an iodine ion (Mg-I^5 = 2.81 Å, Li-I^5 = 2.67 Å). Molecular iodine (I^1-I^2 = 2.85 Å) is located inside the dextrin helix and is coordinated by a lithium ion (O-I^2 = 2.32 Å, Li-I^1 = 2.72 Å). A peptide located outside the α-dextrin helix. When a magnesium ion interacts with triiodide, triiodide decomposes into an iodine ion and molecular iodine (I^6-I^3 = 3.54 Å, I^3-I^4 = 2.72 Å). However, I^3-I^4 does not possess acceptor properties and cannot interact with either polypeptides or DNA nucleotides. The magnesium ion is coordinated by two iodine ions and three oxygen atoms of the dextrin ring.

Thus, molecular iodine inside active Complexes I and II of the drug is in a special electronic form, not found in other iodine-containing drugs. It is probably this electronic structure of iodine that ensures the low toxicity of the FS-1 drug.

A calculation was performed with full optimization of the geometry of the spatial structure of triiodide in the dextrin ring (complex III, Figure 4). Triiodide is located inside the dextrin helix (I^1-I^2 = 3.08 Å, I^2-I^3 = 2.91 Å).

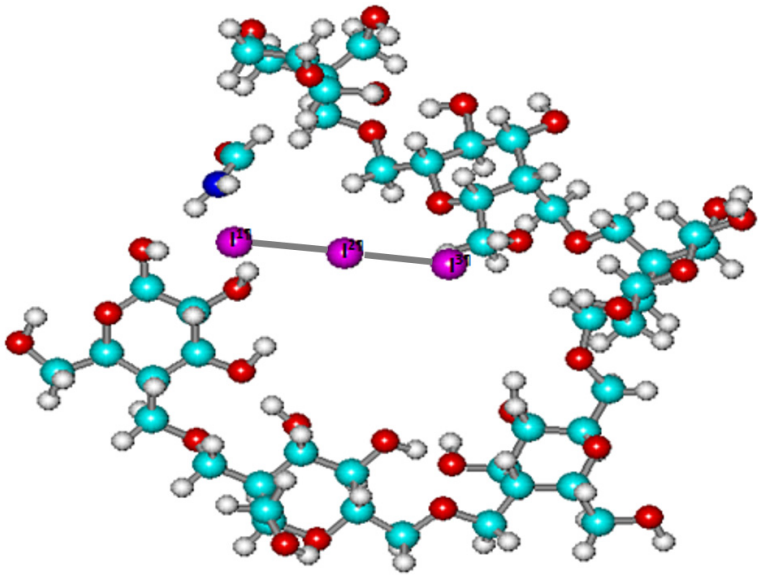

Figure 4. Complex III. Triiodide in the dextrin ring. Blue balls are carbon atoms, red—oxygen, dark blue—nitrogen, violet—iodine, and white balls—hydrogen atoms.

The experimental UV spectrum for the FS-1 drug was obtained for 1/1000 dilution of FS-1 in water.

The wavelengths of electronic transitions in Complexes I–III calculated using the quantum-chemical approach TD-DFT/B3PW91/midi (Table 3).

Table 3. The wavelengths of electronic transitions (nm) in Complexes I–III.

Complex I	
293	$^1A \rightarrow {}^1A$ ($I^3 \rightarrow I^1$-I^2-I^3)
263	$^1A \rightarrow {}^1A$ ($I^2 \rightarrow I^1$-I^2-I^3)
307	$^1A \rightarrow {}^1A$ ($I^3 \rightarrow I^1$-I^2-I^3)
Complex II	
339	$^1A \rightarrow {}^1A$ (I^6-I^5-$I^1 \rightarrow I^1$-I^2-I^5-Mg-Li)
	$^1A \rightarrow {}^1A$ (I^6,$I^5 \rightarrow I^1$-I^2-I^5-Mg-Li)
Complex III	
267	$^1A \rightarrow {}^1A$ (I^1-I^2-$I^3 \rightarrow I^1$-I^2-I^3)

The wavelengths of electronic transitions in Complexes I–II fall within the range in the experimental spectrum of 270–310 nm. The maximum of this interval is well described by the 293 nm band in Complex I, which corresponds to the transition between the occupied orbital with the main contribution of ion I^3 and the unoccupied orbital with the main contribution of triiodide. The 263 nm and 307 nm transitions in Complex I can also be attributed to transitions between the occupied and unoccupied triiodide orbitals. The 339 nm transition in Complex II is due to the orbital interaction between iodine ions (I^1, I^2, I^5, I^6) and magnesium and lithium ions. Transition 267 in Complex III is the transition between the occupied and unoccupied orbital of triiodide in the dextrin ring.

The wavelengths of electronic transitions in Complexes I–III, within the error of the method (~10 nm), are in good agreement of experimentally obtained UV spectrum of the FS-1 drug (Figure 5).

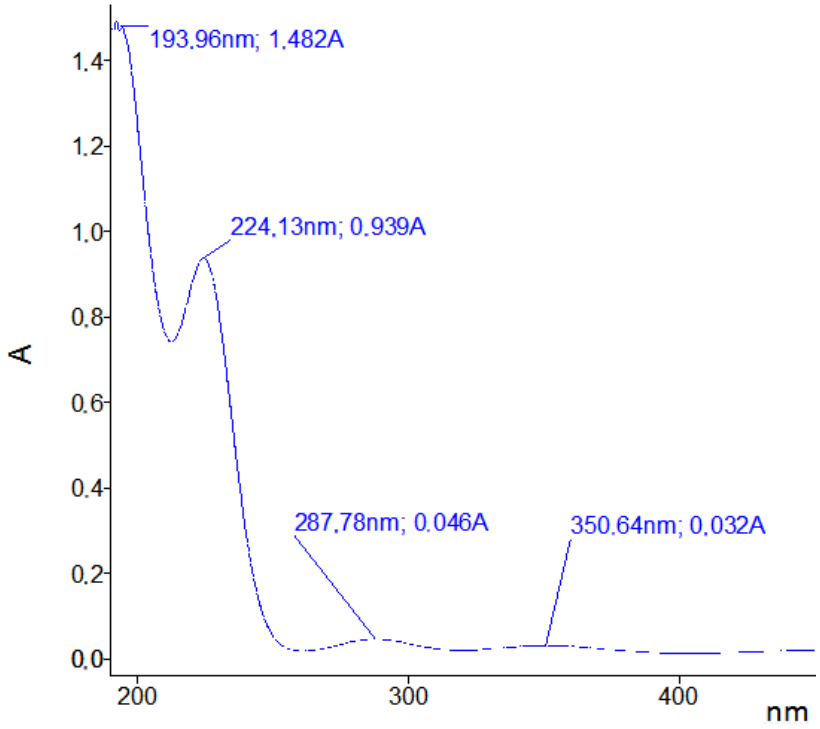

Figure 5. UV spectrum of the FS-1 drug.

Thus, nanocomplex of the FS-1 drug includes a triiodide and two active centers: a complex of iodine with lithium halide and a binuclear complex of magnesium and lithium with molecular iodine and triiodide.

3.3. Interaction of Active Centers of the FS-1 Drug with Nucleotide Triplets of Bacterial and Viral DNA

In earlier paper, using electron spectroscopy, we demonstrated that the FS-1 drug penetrates the bactericidal cell membrane [12].

The active centers of the FS-1 drug are protected from interaction with bioorganic ligands that are part of the cytoplasm of the cell by the α-dextrin helix and interaction with polypeptides. Only DNA nucleotides can compete with polypeptides for complexation with molecular iodine, which is part of the active centers of the FS-1 drug [13,14].

The structures of complexes in which of the active centers of the FS-1 drug interact with the AAG nucleotide triplet are shown in Figure 6.

We calculated the stability of complexes MgI_3LiII_2 and $LiII_2$ with nucleotide triplets and compared the results of calculations with the stability of these complexes with a dextrin ring.

The energy ΔE was calculated, which characterizes the difference in the stability of the complexes MgI_3LiII_2 and $LiII_2$ with a dextrin helix and with nucleotide triplets.

ΔE is calculated as follows:

$$\Delta E = (E^{tot}(\text{IV or V}) + E^{tot}(\text{dex}) + E^{tot}(\text{amid})) - (E^{tot}(\text{I or II}) + E^{tot}(\text{nucleotide trip})) \quad (2)$$

where:
E^{tot}(IV or V)—total energy of complex IV or V;
E^{tot}(dex)—total energy of the dextrin ring;
E^{tot}(amid)—total energy of amide;
E^{tot}(amid)—total energy of amide;
E^{tot}(nucleotide trip)—total energy of nucleotide triplet.

If ΔE is less than zero, when nanocomplex approaches bacterial or viral DNA, one or two active centers are segregated from the dextrin ring and form a complex with a nucleotide triplet (Table 4).

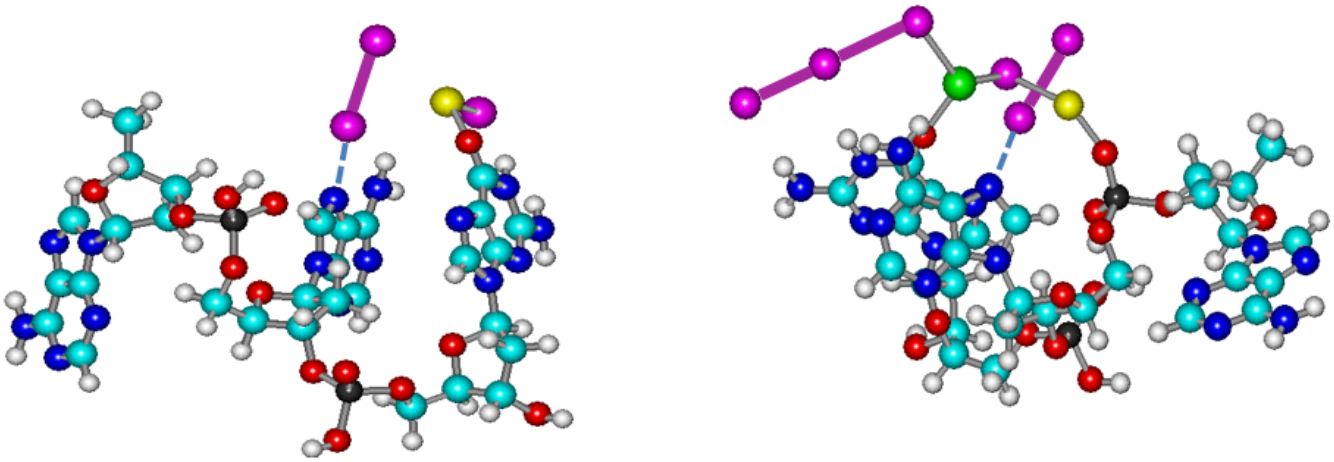

Figure 6. Complexes of active centers the FS-1 drug (LiI_3 complex IV, MgI_3LiI_3 complex V) with nucleotide triplet AAG. Blue balls are carbon atoms, red—oxygen, dark blue—nitrogen, violet—iodine, green ball—magnesium ion, yellow—lithium ion, black—phosphorus, and white balls—hydrogen atoms.

Table 4. Interaction energies (kcal/mol) of nucleotide triplets with active centers of the FS-1 drug.

	$LiII_2$	MgI_3LiII_2
GGT	−12.17	−10.72
GAA	−12.07	+19.02
GGG	+11.94	−13.61
CGG	−7.22	−17.60
CTG	+17.30	+26.40
ACC	+8.50	−6.30
GCG	1.26	32.47
CGC	2.89	52.91

Calculations have shown that ΔE depends on the nucleotide triplet structure. The active centers of the FS-1 drug are only segregated on specific sections of bacterial or viral DNA. The mechanism of action of the drug is determined by the structure of the active center, which has formed a complex with a nucleotide triplet.

The mechanism of anti-HIV action of the FS-1 drug was proposed by us earlier [14]. The complex of the active center $LiII_2$ with the nucleotide triplet (Complex IV) inhibits the active center of the HIV enzyme: integrase. The formation of complex IV destroys the pre-integration complex of the viral DNA with the active center of the integrase and forms a new nucleoprotein complex, where Complex IV binds both the viral DNA and the active center of the integrase.

In the recent work we proposed the mechanism of anti-coronavirus action of the FS-1 drug [15]. Active centers of the FS-1drug destroy the complex formed by the phosphate group of the viral RNA and the catalytic fragment of the ExoN domain of exoribonuclease and create a new nucleoprotein complex in which active centers bind both viral RNA and magnesium ions of the catalytic fragment.

The active complex MgI_3LiII_2 with a nucleotide triplet (Complex V) can inhibit the active site of the DNA-dependent RNA polymerase of bacteria [12].

For DNA S aureus analysis of epigenetic modifications in nucleotide triplets (Table 5) [19].

Table 5. Energy interactions (kcal/mol) of nucleotide triplets with active centers of the FS-1 drug and the frequency of epigenetic modifications in nucleotide triplets Staphylococcus aureus under the action of the FS-1 drug (N).

	$LiII_2$	MgI_3LiII_2	N
GGT	−12.17	−10.72	3645
GAA	−12.07	+19.02	2021
GGG	+11.94	−13.61	1866
ACC	+8.50	−6.30	298
CTG	+17.30	+26.40	234
CGC	2.89	52.91	276

Epigenetic modifications are any modifications to DNA that involve chemical modifications, such as methylation, halogenation, and DNA binding to proteins or other possible complexes.

As can be seen from Table 5. Between the stability of the complexes of active centers with nucleotide triplets and the frequency of epigenetic modifications in these nucleotide triplets (N) a qualitative correlation is observed.

The largest number of epigenetic modifications is observed in the GGT triplet. This triplet forms stable complexes immediately with two active centers. Triplet GAA and GGG form a complex only with one active center and the frequency of epigenetic modifications is significantly reduced. The energy of the ACC triplet interaction with the active center MgI_3LiII_2 is less than with the triplet GGG and N is also less. CTG and CGC triplets do not form complexes with active centers and in them N has further decreased.

It can be assumed that one of the reasons for epigenetic modifications in DNA under the influence of the FS-1drug is the formation of complexes of active centers of the FS-1 drug with nucleotide triplets Staphylococcus aureus.

This result allows to simulate the antibacterial efficacy of the FS-1drug. If the active center MgI_3LiII_2 interacts with nucleotide triplets, which are most common in the genome of bacteria, then the FS-1 drug has antibacterial properties.

4. Conclusions

An ionic nanostructured complex of the FS-1 drug contains nanocomplexes of α-dextrin ~40–48 Å in size. Active centers: molecular iodine complex with lithium halide, binuclear complex of magnesium and lithium, containing molecular iodine and triiodide, are located inside the dextrin helix. The polypeptide, which is located outside the dextrin helix, forms a hydrogen bond with dextrin in Complex I and coordinates molecular iodine, which is part of Complex II.

Molecular iodine inside the active Complexes I and II of the drug is found in a special electronic form, not found in other iodine-containing drugs. In these complexes molecular iodine exhibits acceptor properties in relation to polypeptide in Complex II or ion I^- in Complex I and donor properties—in relation to lithium halide in Complex II or ion Li^+ in Complex I. Probably, it is such a special electronic form of iodine that ensures low toxicity of the FS-1 drug.

It has been shown that the active centers of the drug can be segregated from dextrin helixes and form complexes with nucleotide triplets.

The interaction of active centers with nucleotide triplets carries a selective character: the active centers of the FS-1 drug are only segregated on specific sections of DNA. The formation of a complex between the nucleotide DNA and the active center of the FS-1 drug is a key stage in the anti-HIV mechanisms (Complex I), anti-coronavirus (Complex I, II) and antibacterial action (Complex II).

For S aureus DNA, the epigenetic modifications analysis in triplets was carried out. A qualitative correlation is observed between the stability of active sites complexes with nucleotide triplets and epigenetic modifications frequency in these nucleotide triplets (N). This result makes it possible to simulate the antibacterial efficacy of FS-1. If the active center of the MgI_3LiII_2 drug interacts with nucleotide triplets that are most often found in the bacterial genome, then it has antibacterial properties.

Author Contributions: G.A.-R.Y. created a model nanocomplex and model interaction active center with nucleotide triplets, A.K. determined the mass of the nanocomplex by chromatographic method, A.I. created the FS-1 drug. All authors have read and agreed to the published version of the manuscript.

Funding: The funding is provided from the National budget within the framework of Program-Targeted Financing (PTF) under the scientific and technical program "Development of New Anti-Infectious Drugs for 2018–2020"; 2020 Budget Program 057 "Applied Scientific Research of a Technological Nature in the Field of Industry". The code of the program is O.0777.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Cartesian coordinates are presented in Appendix A.

Acknowledgments: Calculations were made using a supercomputer in the Institute of Digital Equipment and Technology. All individuals included in this section have consented to the acknowledgement.

Conflicts of Interest: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Appendix A

Cartesian coordinates of the optimized structures.

Table A1. Complex I. LiI-I_2 in the dextrin ring.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	12.498804	−2.749244	−0.027672
2	6	0	12.733996	−1.705444	−1.139804
3	6	0	11.152795	−3.463461	−0.209549
4	1	0	12.481742	−2.260221	0.955937
5	6	0	13.648639	−3.788448	−0.032628
6	1	0	11.077233	−3.821553	−1.251832
7	8	0	10.089499	−2.571926	0.079984
8	6	0	11.037640	−4.677686	0.698190
9	8	0	13.393317	−4.885550	0.839623
10	1	0	11.053525	−4.326261	1.745793
11	8	0	9.815426	−5.312247	0.387874
12	6	0	12.230325	−5.603483	0.515079
13	1	0	12.266459	−5.987913	−0.516850
14	8	0	12.139923	−6.722433	1.343002
15	1	0	9.805368	−6.149466	0.869417
16	1	0	12.334330	−6.418248	2.240110
17	1	0	9.285390	−3.108879	0.120633

Table A1. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
18	1	0	12.823130	−2.232041	−2.098472
19	1	0	13.686674	−1.180441	−0.965734
20	8	0	11.705653	−0.763712	−1.322914
21	6	0	11.670494	0.259700	−0.344835
22	1	0	11.503949	−0.166791	0.656459
23	6	0	10.553112	1.246037	−0.683579
24	1	0	12.645776	0.779973	−0.327159
25	6	0	9.148847	0.669000	−0.420064
26	1	0	10.615811	1.448224	−1.760808
27	6	0	10.779042	2.579052	0.038909
28	1	0	9.083312	0.345219	0.634457
29	8	0	8.860979	−0.397940	−1.288192
30	6	0	8.057320	1.719181	−0.624994
31	1	0	11.677034	3.059285	−0.371101
32	6	0	10.970983	2.507419	1.557219
33	8	0	9.736058	3.506142	−0.261344
34	1	0	7.973089	1.884330	−1.713297
35	6	0	8.415583	3.057734	0.049096
36	8	0	6.874477	1.195836	−0.079951
37	1	0	8.284407	2.925036	1.134208
38	6	0	7.531629	4.211585	−0.413625
39	1	0	9.489149	−1.109211	−1.082109
40	1	0	11.888470	1.955482	1.791732
41	1	0	10.138025	1.965290	2.033476
42	8	0	11.108411	3.807131	2.085691
43	1	0	6.125499	1.733173	−0.387660
44	1	0	10.507046	4.353807	1.559888
45	8	0	6.198645	3.934423	−0.060578
46	1	0	7.637048	4.322486	−1.505734
47	1	0	7.883003	5.149230	0.048828
48	6	0	5.253884	4.815542	−0.620934
49	1	0	5.451185	4.956930	−1.697144
50	1	0	5.328277	5.809087	−0.142692
51	6	0	3.867327	4.215050	−0.394847
52	1	0	3.897146	3.748706	0.598385
53	6	0	3.503804	3.128905	−1.403815
54	6	0	2.739593	5.265097	−0.347319
55	8	0	4.489893	2.117207	−1.431279
56	1	0	3.418712	3.576879	−2.410910

Table A1. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
57	6	0	2.149292	2.526496	−1.051401
58	6	0	2.669093	6.177003	−1.572263
59	1	0	2.913681	5.924433	0.511572
60	8	0	1.492868	4.645764	−0.061574
61	1	0	2.230807	2.042936	−0.069972
62	8	0	1.852454	1.583393	−2.068777
63	6	0	1.087796	3.630129	−0.967572
64	6	0	−0.262997	3.122019	−0.499087
65	1	0	0.937972	4.036868	−1.982013
66	1	0	4.085633	1.379607	−1.911470
67	1	0	2.395158	5.606129	−2.472715
68	1	0	3.673427	6.594486	−1.751885
69	8	0	1.727045	7.191871	−1.295931
70	1	0	1.404601	0.817181	−1.680734
71	1	0	1.657619	7.752779	−2.074974
72	8	0	−0.097548	2.441497	0.728357
73	1	0	−0.671235	2.442286	−1.262482
74	1	0	−0.942952	3.980143	−0.397747
75	6	0	−1.252069	1.778750	1.202538
76	1	0	−1.765066	1.285628	0.362070
77	6	0	−2.269526	2.654663	1.947540
78	1	0	−0.878184	0.997805	1.874332
79	1	0	−2.469176	3.552981	1.346755
80	6	0	−1.785022	3.136715	3.330957
81	6	0	−3.613225	1.886970	2.078360
82	6	0	−0.559573	4.031274	3.291959
83	1	0	−1.536082	2.260611	3.957051
84	8	0	−2.810967	3.892258	3.973241
85	6	0	−3.482631	0.464136	2.664650
86	1	0	−4.035405	1.757710	1.073732
87	6	0	−4.601190	2.743482	2.877115
88	6	0	−3.976850	3.146302	4.205343
89	1	0	−4.770807	3.685161	2.329326
90	8	0	−5.807306	2.035720	3.057485
91	8	0	−4.903417	3.946331	4.870669
92	1	0	−3.729304	2.245915	4.803875
93	1	0	−0.849818	4.986323	2.825832
94	1	0	0.205053	3.570725	2.656724
95	8	0	−0.113605	4.212065	4.625054

Table A1. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
96	1	0	−6.317857	2.537825	3.705736
97	1	0	−4.500457	4.237879	5.697365
98	1	0	0.688731	4.742108	4.588884
99	1	0	−4.334539	0.241212	3.312825
100	1	0	−2.565901	0.341346	3.249738
101	8	0	−3.433362	−0.526143	1.620821
102	6	0	−4.672738	−1.216646	1.380851
103	1	0	−5.491416	−0.596143	1.753650
104	6	0	−4.676845	−2.592405	2.072990
105	1	0	−4.786362	−1.298199	0.295903
106	1	0	−3.797194	−2.621934	2.727665
107	6	0	−4.594467	−3.802674	1.119335
108	6	0	−5.919688	−2.789788	2.952042
109	6	0	−3.519226	−3.727055	0.039712
110	8	0	−5.789513	−3.987220	0.374139
111	1	0	−4.414427	−4.695803	1.744785
112	6	0	−7.143908	−2.958835	2.060392
113	8	0	−6.078128	−1.698387	3.827126
114	1	0	−5.791584	−3.722059	3.532973
115	6	0	−6.933725	−4.203894	1.192534
116	1	0	−7.216377	−2.102024	1.379077
117	8	0	−8.294696	−3.025615	2.874504
118	1	0	−6.759384	−5.080270	1.842422
119	6	0	−8.132658	−4.512449	0.314219
120	8	0	−2.276212	−3.289262	0.598986
121	1	0	−3.848199	−3.037453	−0.746151
122	1	0	−3.403527	−4.719130	−0.409383
123	1	0	−7.018518	−1.714946	4.062379
124	1	0	−9.001836	−2.568863	2.374649
125	1	0	−1.576465	−3.434269	−0.060448
126	1	0	−7.825265	−5.186117	−0.501126
127	8	0	−8.663687	−3.305766	−0.175500
128	1	0	−8.883177	−5.035462	0.927420
129	6	0	−9.921266	−3.420265	−0.793061
130	6	0	−10.606056	−2.044032	−0.835385
131	1	0	−10.560576	−4.128842	−0.238131
132	1	0	−9.811833	−3.816814	−1.818204
133	6	0	−9.605201	−1.045112	−1.437537
134	6	0	−11.106820	−1.655084	0.569918

Table A1. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
135	6	0	−11.865154	−2.228020	−1.718588
136	6	0	−12.084471	−0.489066	0.508082
137	8	0	−12.780825	−1.157020	−1.700409
138	1	0	−11.561363	−2.348774	−2.762847
139	8	0	−12.502584	−0.269230	1.856984
140	6	0	−13.247928	−0.865697	−0.404278
141	1	0	−13.787550	−1.723935	0.036135
142	1	0	−11.562504	0.382245	0.097747
143	8	0	−10.050057	−1.336432	1.469514
144	1	0	−11.669914	−2.518113	0.972292
145	1	0	−12.379797	−3.157724	−1.407211
146	1	0	−12.830299	0.633346	1.925337
147	1	0	−9.221422	−1.494365	−2.370676
148	1	0	−8.753895	−0.961995	−0.751236
149	8	0	−10.197630	0.207766	−1.685627
150	6	0	14.985755	−3.219592	0.417014
151	1	0	13.776011	−4.176041	−1.058607
152	1	0	−9.488087	0.787688	−2.015047
153	1	0	14.925842	−3.048467	1.503359
154	1	0	15.160532	−2.247185	−0.066340
155	8	0	15.991474	−4.148295	0.078180
156	1	0	−13.956266	−0.036629	−0.503403
157	1	0	16.810486	−3.871766	0.500899
158	1	0	−10.486718	−0.813571	2.161125
159	3	0	−1.867142	−1.332795	0.838527
160	53	0	0.376728	−1.727197	−1.097503
161	53	0	−2.455742	−0.534563	−1.980336
162	53	0	−5.085146	0.445349	−2.379244
163	8	0	−0.432339	−1.404846	2.239853
164	1	0	−0.468309	−2.223716	2.747678
165	1	0	0.312655	−1.510621	1.623230
166	8	0	−8.020414	1.634415	−2.806683
167	6	0	−8.062066	2.472679	−3.701558
168	7	0	−6.984931	2.927421	−4.363131
169	1	0	−9.010854	2.929517	−4.034479
170	1	0	−7.070178	3.602105	−5.104763
171	1	0	−6.075883	2.542716	−4.135150

Table A2. Complex II. MgI_3LiII_2 in the dextrin ring.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	7.293858	−1.325520	−1.157015
2	6	0	8.516226	−0.481913	−0.735216
3	6	0	7.284923	−1.520006	−2.672956
4	1	0	6.392985	−0.755040	−0.889236
5	6	0	7.145129	−2.697908	−0.470520
6	1	0	8.190804	−2.081033	−2.963633
7	8	0	7.296641	−0.253069	−3.302470
8	6	0	6.082957	−2.329546	−3.129613
9	8	0	5.990336	−3.367114	−0.977268
10	1	0	5.160021	−1.780494	−2.881168
11	8	0	6.224469	−2.507941	−4.519966
12	6	0	6.047412	−3.645239	−2.367815
13	1	0	6.954539	−4.235981	−2.587475
14	8	0	4.892909	−4.320050	−2.736217
15	1	0	5.451755	−2.991875	−4.836251
16	1	0	7.118362	−0.407514	−4.241034
17	1	0	9.364150	−0.687031	−1.396136
18	1	0	8.840255	−0.715103	0.287704
19	8	0	8.237252	0.904056	−0.856761
20	6	0	7.706799	1.486879	0.316737
21	1	0	7.061167	0.766453	0.843706
22	6	0	6.874056	2.710784	−0.065130
23	1	0	8.521545	1.764189	1.004610
24	6	0	5.700507	2.310025	−0.972195
25	1	0	7.505779	3.388787	−0.652328
26	6	0	6.407077	3.468846	1.206250
27	1	0	5.154696	1.467540	−0.506571
28	8	0	6.024535	2.023445	−2.311079
29	6	0	4.727715	3.465658	−1.105380
30	1	0	7.231598	4.099766	1.553750
31	6	0	5.972766	2.613970	2.400496
32	8	0	5.360802	4.429815	0.933734
33	1	0	5.241348	4.312177	−1.580013
34	6	0	4.231921	3.903023	0.255844
35	8	0	3.659270	3.041549	−1.964816
36	1	0	3.791798	3.049727	0.794893
37	6	0	3.191282	5.014162	0.216841
38	1	0	6.620816	1.254104	−2.403070

Table A2. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
39	1	0	6.807804	1.988667	2.732317
40	1	0	5.152891	1.927492	2.127335
41	8	0	5.625194	3.436665	3.484680
42	1	0	4.074371	2.406497	−2.584284
43	1	0	5.116952	4.171365	3.117908
44	8	0	1.910848	4.459846	−0.122025
45	1	0	3.469812	5.801473	−0.495676
46	1	0	3.131682	5.457331	1.217514
47	6	0	0.818796	5.368331	0.144642
48	1	0	0.653299	5.992123	−0.742184
49	1	0	1.124860	6.020901	0.970872
50	6	0	−0.417350	4.575936	0.557118
51	1	0	−0.061851	3.740149	1.173167
52	6	0	−1.225642	4.005912	−0.594456
53	6	0	−1.387874	5.384440	1.459005
54	8	0	−0.415643	3.215350	−1.487871
55	1	0	−1.670025	4.810816	−1.196338
56	6	0	−2.337940	3.123667	−0.062063
57	6	0	−1.870602	6.708803	0.863512
58	1	0	−0.861093	5.640560	2.385421
59	8	0	−2.452168	4.552841	1.885589
60	1	0	−1.877700	2.310585	0.525197
61	8	0	−3.000221	2.622916	−1.201706
62	6	0	−3.234294	3.950912	0.867406
63	6	0	−4.255169	3.086589	1.603553
64	1	0	−3.764685	4.699298	0.257969
65	1	0	−1.026556	2.602951	−1.936531
66	1	0	−2.533251	6.535447	0.001121
67	1	0	−0.995699	7.266203	0.484542
68	8	0	−2.523785	7.401095	1.896030
69	1	0	−3.825988	2.221617	−0.874311
70	1	0	−2.926998	8.196471	1.532936
71	8	0	−4.898172	2.260224	0.652082
72	1	0	−4.979680	3.730564	2.120804
73	1	0	−3.720939	2.498135	2.362545
74	6	0	−6.144902	1.682610	1.069913
75	1	0	−6.789983	2.485002	1.452149
76	6	0	−5.985885	0.591136	2.132962

Table A2. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
77	1	0	−6.608081	1.300654	0.161433
78	1	0	−5.169364	0.909062	2.797684
79	6	0	−5.598414	−0.808532	1.628160
80	6	0	−7.228025	0.434761	3.046399
81	6	0	−4.477051	−0.882896	0.610123
82	1	0	−6.480023	−1.265959	1.155413
83	8	0	−5.193228	−1.588432	2.754534
84	6	0	−8.503809	−0.083790	2.353298
85	1	0	−7.453071	1.416873	3.482128
86	6	0	−6.831719	−0.504992	4.192045
87	6	0	−6.257812	−1.819555	3.654272
88	1	0	−6.015560	−0.035359	4.767096
89	8	0	−7.955894	−0.748686	5.006163
90	8	0	−5.774814	−2.516219	4.758435
91	1	0	−7.045698	−2.396873	3.139542
92	1	0	−3.510554	−0.809373	1.127944
93	1	0	−4.552570	−0.044524	−0.093370
94	8	0	−4.599393	−2.125696	−0.072155
95	1	0	−7.688961	−1.425661	5.641616
96	1	0	−5.524149	−3.401745	4.470595
97	1	0	−3.844237	−2.220708	−0.666984
98	1	0	−9.378714	0.228919	2.939496
99	1	0	−8.519470	−1.180931	2.338263
100	8	0	−8.578474	0.424405	1.035790
101	6	0	−9.825128	0.206108	0.387837
102	1	0	−10.643776	0.518216	1.050249
103	6	0	−10.085727	−1.240698	−0.064278
104	1	0	−9.813263	0.865601	−0.485886
105	1	0	−9.724530	−1.933515	0.703386
106	6	0	−9.423226	−1.612773	−1.401883
107	6	0	−11.587605	−1.492059	−0.252534
108	6	0	−7.904448	−1.523117	−1.441864
109	8	0	−9.922094	−0.785519	−2.446929
110	1	0	−9.677761	−2.664684	−1.621440
111	6	0	−12.123483	−0.707972	−1.448426
112	8	0	−12.295324	−1.159616	0.921438
113	1	0	−11.726133	−2.562585	−0.488044
114	6	0	−11.300832	−1.015766	−2.708551

Table A2. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
115	1	0	−12.050013	0.368929	−1.228772
116	8	0	−13.485953	−1.094515	−1.582883
117	1	0	−11.456953	−2.082148	−2.949811
118	6	0	−11.690055	−0.164007	−3.901994
119	8	0	−7.402051	−2.508797	−0.567338
120	1	0	−7.583919	−0.509720	−1.158044
121	1	0	−7.592539	−1.695630	−2.483423
122	1	0	−13.229978	−1.203837	0.677648
123	1	0	−13.949471	−0.421893	−2.091996
124	1	0	−6.429684	−2.469247	−0.565001
125	1	0	−11.068100	−0.414396	−4.765215
126	1	0	−11.553281	0.899527	−3.678829
127	1	0	−12.734747	−0.338714	−4.176748
128	6	0	6.912277	−2.564061	1.024373
129	1	0	8.034587	−3.325004	−0.650103
130	1	0	6.061146	−1.886941	1.187976
131	1	0	7.796824	−2.120189	1.498698
132	8	0	6.649700	−3.845051	1.573249
133	1	0	6.397687	−3.696332	2.499303
134	12	0	1.625308	2.925498	−1.642061
135	53	0	1.467009	0.822978	0.406301
136	3	0	0.764942	−0.666040	−1.723335
137	53	0	−1.595027	−1.871870	−2.374441
138	53	0	1.408655	1.024935	−3.693801
139	1	0	4.974728	−5.248427	−2.488272
140	53	0	0.395432	−3.441732	−1.064203
141	8	0	1.539122	4.546486	−3.070242
142	1	0	0.795950	4.459358	−3.680927
143	1	0	2.335047	4.551097	−3.617449
144	53	0	3.424935	−0.836242	2.477603
145	53	0	4.949325	−2.227842	4.352481
146	6	0	3.191529	−4.308517	0.124364
147	7	0	4.116783	−4.978950	0.782914
148	1	0	3.536564	−3.388868	−0.355691
149	1	0	5.070217	−4.607538	0.880217
150	1	0	3.847544	−5.818197	1.278292
151	8	0	2.003961	−4.705603	0.039852

Table A3. Complex III. I_3^- in the dextrin ring.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	−6.154354	−3.477713	−1.331043
2	6	0	−5.923125	−4.507984	−2.463881
3	6	0	−5.015403	−2.457820	−1.266482
4	1	0	−6.216916	−3.973039	−0.350838
5	6	0	−7.468016	−2.709674	−1.590375
6	1	0	−4.844638	−2.024480	−2.270846
7	8	0	−3.810019	−3.039332	−0.754550
8	6	0	−5.365049	−1.318675	−0.303988
9	8	0	−7.677136	−1.658006	−0.620234
10	1	0	−5.515168	−1.750013	0.699432
11	8	0	−4.232631	−0.444383	−0.328700
12	6	0	−6.664360	−0.637776	−0.717314
13	1	0	−6.613744	−0.243078	−1.745680
14	8	0	−7.016275	0.442776	0.107404
15	1	0	−4.164473	−0.063297	0.589212
16	1	0	−6.725443	0.196728	1.031870
17	1	0	−3.308802	−2.220942	−0.467535
18	1	0	−6.110260	−4.009226	−3.428537
19	1	0	−6.641070	−5.345022	−2.363245
20	8	0	−4.589521	−4.998043	−2.567897
21	6	0	−4.293419	−6.000438	−1.583441
22	1	0	−4.415963	−5.599866	−0.562332
23	6	0	−2.840371	−6.449360	−1.797659
24	1	0	−4.987207	−6.857835	−1.708366
25	6	0	−1.849884	−5.340270	−1.377660
26	1	0	−2.699650	−6.592118	−2.879600
27	6	0	−2.559996	−7.778077	−1.084084
28	1	0	−2.054371	−5.032439	−0.335648
29	8	0	−1.926053	−4.239858	−2.269575
30	6	0	−0.403783	−5.827449	−1.410366
31	1	0	−3.103655	−8.598310	−1.575861
32	6	0	−2.913464	−7.832727	0.419643
33	8	0	−1.172864	−8.180130	−1.227413
34	1	0	−0.108975	−5.919801	−2.471504
35	6	0	−0.243236	−7.191801	−0.715838
36	8	0	0.357160	−4.851706	−0.715815
37	1	0	−0.364257	−7.037285	0.369024
38	6	0	1.132930	−7.816483	−0.976903
39	1	0	−2.729738	−3.745071	−1.942176
40	1	0	−4.006222	−7.852308	0.547891

Table A3. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
41	1	0	−2.530893	−6.939147	0.945432
42	8	0	−2.367295	−9.043176	0.942884
43	1	0	1.261199	−4.907660	−1.132147
44	1	0	−1.583509	−9.161444	0.337735
45	8	0	2.096673	−6.921035	−0.430442
46	1	0	1.264223	−7.939364	−2.068341
47	1	0	1.179647	−8.817111	−0.506468
48	6	0	3.451474	−7.178097	−0.806496
49	1	0	3.512560	−7.614786	−1.821056
50	1	0	3.929291	−7.884588	−0.099564
51	6	0	4.118573	−5.796881	−0.753431
52	1	0	3.609957	−5.271352	0.068911
53	6	0	3.880229	−4.992113	−2.033513
54	6	0	5.628698	−5.757265	−0.417443
55	8	0	2.491927	−4.934854	−2.383045
56	1	0	4.440720	−5.431182	−2.879666
57	6	0	4.381811	−3.581098	−1.784446
58	6	0	6.506323	−6.573317	−1.377798
59	1	0	5.790168	−6.167447	0.588424
60	8	0	6.089136	−4.395527	−0.295707
61	1	0	3.864633	−3.173656	−0.906796
62	8	0	4.073838	−2.817503	−2.963701
63	6	0	5.879644	−3.613010	−1.481660
64	6	0	6.400535	−2.197419	−1.232584
65	1	0	6.427948	−4.029871	−2.346045
66	1	0	2.447327	−4.073674	−2.886412
67	1	0	6.347217	−6.267847	−2.426462
68	1	0	6.203192	−7.635490	−1.295252
69	8	0	7.857764	−6.352278	−0.962637
70	1	0	3.961205	−1.895252	−2.624077
71	1	0	8.405967	−6.931811	−1.544453
72	8	0	5.395450	−1.460745	−0.527214
73	1	0	6.598403	−1.720873	−2.209672
74	1	0	7.344192	−2.267452	−0.669535
75	6	0	5.573620	−0.029630	−0.619876
76	1	0	5.687121	0.260505	−1.677401
77	6	0	6.760989	0.518931	0.194213
78	1	0	4.641846	0.402502	−0.233870
79	1	0	7.639309	−0.131408	0.045927
80	6	0	6.465544	0.538338	1.712358

Table A3. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
81	6	0	7.158907	1.933515	−0.312576
82	6	0	6.241514	−0.853628	2.318714
83	1	0	5.562435	1.149763	1.896551
84	8	0	7.593973	1.078885	2.439699
85	6	0	6.015723	2.960638	−0.368511
86	1	0	7.544613	1.846937	−1.340597
87	6	0	8.290333	2.458780	0.587128
88	6	0	7.858695	2.411794	2.050566
89	1	0	9.161442	1.782088	0.512072
90	8	0	8.630161	3.801946	0.237616
91	8	0	8.968442	2.907589	2.780713
92	1	0	6.965986	3.049359	2.213272
93	1	0	7.223013	−1.344930	2.380769
94	1	0	5.599461	−1.451473	1.658470
95	8	0	5.751493	−0.767077	3.663129
96	1	0	9.112104	4.108460	1.049025
97	1	0	8.658129	2.983573	3.716386
98	1	0	4.788957	−0.564011	3.567320
99	1	0	6.477109	3.950078	−0.514928
100	1	0	5.440459	2.965115	0.568384
101	8	0	5.147940	2.637476	−1.467776
102	6	0	4.406587	3.782609	−1.923810
103	1	0	5.096022	4.587532	−2.226003
104	6	0	3.424115	4.372796	−0.894200
105	1	0	3.850827	3.428624	−2.802941
106	1	0	3.923566	4.437317	0.080619
107	6	0	2.137010	3.537105	−0.714474
108	6	0	3.009428	5.798563	−1.312207
109	6	0	2.395282	2.053065	−0.449898
110	8	0	1.325464	3.569573	−1.905440
111	1	0	1.564334	3.953281	0.136784
112	6	0	2.072467	5.750926	−2.521027
113	8	0	4.157817	6.588768	−1.635198
114	1	0	2.433055	6.264303	−0.489178
115	6	0	0.853674	4.903467	−2.152887
116	1	0	2.593383	5.272484	−3.370119
117	8	0	1.766999	7.118724	−2.834652
118	1	0	0.348142	5.331875	−1.273036
119	6	0	−0.167377	4.803699	−3.280229
120	8	0	3.180896	1.887711	0.742641

Table A3. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
121	1	0	2.954439	1.629267	−1.290904
122	1	0	1.425780	1.537730	−0.374476
123	1	0	3.751262	7.324381	−2.164312
124	1	0	0.952742	7.056432	−3.407924
125	1	0	2.533650	1.622822	1.450572
126	1	0	0.292974	4.329752	−4.161647
127	8	0	−0.583127	6.137489	−3.657148
128	1	0	−1.021678	4.190849	−2.956860
129	6	0	−1.964752	6.465639	−3.429452
130	6	0	−2.308990	7.372924	−2.209157
131	1	0	−2.562268	5.541363	−3.364603
132	1	0	−2.273914	7.009622	−4.338577
133	6	0	−1.275366	8.524860	−2.112614
134	6	0	−2.349905	6.612904	−0.871696
135	6	0	−3.761272	7.847490	−2.540064
136	6	0	−3.232506	7.323623	0.162576
137	8	0	−4.482832	8.463612	−1.474728
138	1	0	−3.709907	8.602321	−3.337514
139	8	0	−3.154971	6.454665	1.321793
140	6	0	−4.634829	7.524210	−0.396083
141	1	0	−5.053047	6.558700	−0.732114
142	1	0	−2.788706	8.306706	0.357344
143	8	0	−1.031133	6.534408	−0.266014
144	1	0	−2.777402	5.606743	−1.022819
145	1	0	−4.335912	6.975121	−2.914737
146	1	0	−3.407977	7.005211	2.101290
147	1	0	−1.502681	9.293111	−2.866540
148	1	0	−0.288061	8.093324	−2.320454
149	8	0	−1.223416	9.183441	−0.838187
150	6	0	−8.749331	−3.541702	−1.457770
151	1	0	−7.446350	−2.263850	−2.604020
152	1	0	−0.830955	8.454320	−0.283093
153	1	0	−8.737855	−4.036482	−0.466864
154	1	0	−8.800293	−4.315709	−2.235050
155	8	0	−9.869648	−2.678127	−1.630210
156	1	0	−5.305301	7.992679	0.336729
157	1	0	−9.584003	−1.886281	−1.100621
158	1	0	−1.281040	6.243235	0.656377

Table A4. Complex LiI_2 with nucleotide triplet GGT.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	1	0	1.794747	4.507865	−1.731496
2	6	0	1.391624	4.759995	−2.716999
3	1	0	0.413439	5.228480	−2.577613
4	1	0	2.056962	5.484873	−3.193059
5	6	0	1.245168	3.524490	−3.576591
6	1	0	0.820348	3.792315	−4.554937
7	8	0	2.534373	2.920626	−3.785699
8	6	0	2.440032	1.521473	−3.817779
9	1	0	2.859190	1.131796	−4.752307
10	7	0	3.286179	0.993777	−2.731721
11	6	0	3.985241	1.720320	−1.801606
12	1	0	3.963733	2.798353	−1.783136
13	7	0	4.671753	0.957052	−0.987425
14	6	0	4.434128	−0.333318	−1.398377
15	6	0	4.815911	−1.591907	−0.853640
16	8	0	5.462891	−1.844915	0.172558
17	7	0	4.318055	−2.648297	−1.627216
18	1	0	4.509310	−3.584635	−1.242340
19	6	0	3.480858	−2.531941	−2.702107
20	7	0	3.092984	−3.692539	−3.284673
21	1	0	3.202424	−4.560937	−2.780847
22	1	0	2.354326	−3.626522	−3.965365
23	7	0	3.071774	−1.374384	−3.183347
24	6	0	3.572235	−0.327250	−2.497074
25	6	0	0.373714	2.403599	−2.996541
26	1	0	0.453259	2.369620	−1.905679
27	6	0	0.959933	1.158003	−3.655990
28	1	0	0.811807	0.233828	−3.096522
29	1	0	0.506821	1.045139	−4.645873
30	8	0	−0.982973	2.620762	−3.394676
31	15	0	−2.244873	2.742814	−2.409510
32	8	0	−3.389282	3.400085	−3.071307
33	8	0	−1.633478	3.355875	−1.086361
34	8	0	−2.572778	1.219988	−1.929994
35	6	0	−3.292784	0.387041	−2.849825
36	1	0	−4.106418	0.959503	−3.309619
37	1	0	−2.612031	0.042973	−3.636706
38	6	0	−3.848976	−0.822695	−2.119559
39	1	0	−4.430994	−1.401607	−2.848733
40	8	0	−2.788575	−1.637052	−1.629765

Table A4. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
41	6	0	−2.802834	−1.710817	−0.209628
42	1	0	−3.095635	−2.722795	0.090353
43	7	0	−1.466883	−1.526359	0.310214
44	6	0	−0.735489	−0.350070	0.425902
45	1	0	−1.164638	0.608312	0.170948
46	7	0	0.488715	−0.536832	0.831815
47	6	0	0.594574	−1.902606	0.982661
48	6	0	1.706295	−2.720222	1.325909
49	8	0	2.864431	−2.384431	1.623976
50	7	0	1.384091	−4.079587	1.263043
51	1	0	2.206020	−4.700649	1.295557
52	6	0	0.172471	−4.597067	0.899675
53	7	0	0.080654	−5.953051	0.881919
54	1	0	0.929644	−6.496491	0.820760
55	1	0	−0.739363	−6.326578	0.432014
56	7	0	−0.876678	−3.857607	0.601977
57	6	0	−0.602811	−2.539171	0.644850
58	6	0	−4.737809	−0.487990	−0.911403
59	1	0	−5.183691	0.506576	−0.970259
60	6	0	−3.798529	−0.650924	0.268049
61	1	0	−3.288549	0.299946	0.433134
62	1	0	−4.327848	−0.928690	1.179796
63	8	0	−5.800523	−1.470668	−0.811952
64	15	0	−7.339420	−1.026970	−0.967542
65	8	0	−7.836366	−1.579536	−2.388748
66	8	0	−7.606581	0.418906	−0.825594
67	8	0	−8.096094	−2.048417	0.009766
68	6	0	−7.688156	−2.397444	1.340990
69	1	0	−8.404964	−3.159055	1.654068
70	1	0	−6.686169	−2.836780	1.310480
71	6	0	−7.714033	−1.272831	2.356051
72	1	0	−7.696304	−1.753427	3.350303
73	8	0	−6.582005	−0.434373	2.195473
74	6	0	−6.811518	0.728433	2.995094
75	1	0	−6.414907	0.566026	4.000945
76	7	0	−6.017400	1.811718	2.447660
77	6	0	−6.304047	2.328992	1.203435
78	1	0	−7.199418	1.935961	0.733953
79	6	0	−5.516034	3.219650	0.549460
80	6	0	−5.882770	3.811596	−0.777202

Table A4. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
81	1	0	−6.047218	4.890813	−0.681547
82	1	0	−5.091873	3.677858	−1.521700
83	1	0	−6.798592	3.353908	−1.158072
84	6	0	−4.255872	3.576810	1.171045
85	8	0	−3.368891	4.271626	0.660709
86	7	0	−4.063338	3.065087	2.447101
87	1	0	−3.198405	3.318014	2.910516
88	6	0	−4.862078	2.175885	3.145378
89	8	0	−4.567985	1.755933	4.247772
90	6	0	−8.911920	−0.318285	2.325397
91	1	0	−9.158175	−0.095918	1.280484
92	6	0	−8.340235	0.938241	3.016316
93	1	0	−8.638996	1.866665	2.524055
94	1	0	−8.700319	0.971998	4.047971
95	8	0	−9.987431	−0.932936	2.996877
96	1	0	−7.885200	−2.543519	−2.417562
97	1	0	−10.804798	−0.501715	2.728163
98	1	0	−2.301835	3.774442	−0.474394
99	53	0	6.102182	2.016042	0.847208
100	53	0	7.624740	3.345605	2.770090
101	3	0	4.593561	−3.081267	1.335606
102	53	0	4.342910	−5.625503	0.339083

Table A5. Complex MgI_3LiII_2 with nucleotide triplet GGT.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	1	0	−4.773493	−3.973932	−4.929384
2	6	0	−5.111961	−4.840241	−4.352552
3	1	0	−6.199931	−4.916705	−4.437289
4	1	0	−4.669840	−5.737225	−4.793148
5	6	0	−4.704818	−4.719851	−2.898064
6	1	0	−5.111197	−5.551930	−2.309754
7	8	0	−3.262424	−4.753321	−2.821751
8	6	0	−2.879933	−3.827622	−1.840798
9	1	0	−2.980248	−4.254822	−0.833373
10	7	0	−1.467613	−3.494255	−1.970833
11	6	0	−0.912944	−2.445371	−2.644967
12	1	0	−1.469776	−1.746389	−3.258587
13	7	0	0.373007	−2.338193	−2.383366
14	6	0	0.688911	−3.353252	−1.507088

Table A5. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
15	6	0	1.853398	−3.611422	−0.739164
16	8	0	2.911622	−2.975010	−0.693111
17	7	0	1.686136	−4.738816	0.072870
18	1	0	2.480537	−4.934257	0.672193
19	6	0	0.515962	−5.449342	0.217122
20	7	0	0.518299	−6.484608	1.078374
21	1	0	1.366526	−6.865108	1.463176
22	1	0	−0.316767	−7.047619	1.115394
23	7	0	−0.594948	−5.138034	−0.421249
24	6	0	−0.458337	−4.092496	−1.247694
25	6	0	−5.140064	−3.398039	−2.216356
26	1	0	−5.866164	−2.841242	−2.811264
27	6	0	−3.826031	−2.652180	−2.029804
28	1	0	−3.587794	−2.101298	−2.943684
29	1	0	−3.840461	−1.954977	−1.192373
30	8	0	−5.739941	−3.731820	−0.948453
31	15	0	−6.328906	−2.618668	0.049306
32	8	0	−7.461843	−3.072495	0.875267
33	8	0	−6.514348	−1.377077	−0.925266
34	8	0	−5.033860	−2.186615	0.961483
35	6	0	−5.172530	−2.216155	2.385953
36	1	0	−6.230602	−2.170215	2.658744
37	1	0	−4.767885	−3.157693	2.772950
38	6	0	−4.429566	−1.064780	3.031082
39	1	0	−4.792185	−0.978411	4.067818
40	8	0	−3.022124	−1.325998	3.036325
41	6	0	−2.318224	−0.116937	3.208634
42	1	0	−1.903195	−0.055869	4.222682
43	7	0	−1.175792	−0.149711	2.287916
44	6	0	−0.758019	−1.214174	1.509784
45	1	0	−1.341811	−2.121262	1.470573
46	7	0	0.364383	−0.988946	0.874628
47	6	0	0.716008	0.284944	1.262463
48	6	0	1.800997	1.097258	0.905668
49	8	0	2.744768	0.791631	0.103188
50	7	0	1.804863	2.320215	1.524801
51	1	0	2.578138	2.956724	1.262579
52	6	0	0.835971	2.756456	2.393488
53	7	0	0.990490	3.996819	2.889099
54	1	0	1.805005	4.553715	2.684998

Table A5. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
55	1	0	0.336733	4.311323	3.586036
56	7	0	−0.204548	2.021841	2.749243
57	6	0	−0.222079	0.822372	2.154860
58	6	0	−4.528786	0.310013	2.365947
59	1	0	−4.484743	0.194215	1.279494
60	6	0	−3.306756	1.028824	2.935784
61	1	0	−2.905809	1.808482	2.287902
62	1	0	−3.592016	1.490957	3.885716
63	8	0	−5.749296	0.967617	2.747732
64	15	0	−6.718241	1.627499	1.645434
65	8	0	−7.965495	2.051219	2.539761
66	8	0	−7.001033	0.784599	0.461321
67	1	0	−8.634357	1.357842	2.621520
68	1	0	−6.767002	−0.548749	−0.438068
69	8	0	−6.079081	3.015902	1.212332
70	6	0	−5.589974	3.996665	2.146078
71	1	0	−5.217265	3.501248	3.046988
72	6	0	−4.482056	4.779715	1.475749
73	1	0	−4.111988	5.518538	2.204777
74	8	0	−3.448298	3.887716	1.084234
75	6	0	−2.780799	4.360112	−0.082491
76	1	0	−1.740028	4.583741	0.156828
77	7	0	−2.705655	3.272530	−1.056474
78	6	0	−3.844901	2.808085	−1.681071
79	1	0	−4.753848	3.337799	−1.422017
80	6	0	−3.873624	1.765006	−2.541997
81	6	0	−5.118805	1.278258	−3.214624
82	1	0	−4.963606	1.193206	−4.294204
83	1	0	−5.403237	0.287304	−2.847245
84	1	0	−5.955609	1.956701	−3.033778
85	6	0	−2.622801	1.064573	−2.796037
86	7	0	−1.517224	1.590680	−2.130238
87	1	0	−0.625430	1.130707	−2.295831
88	6	0	−1.476461	2.640131	−1.234919
89	8	0	−0.451250	2.972424	−0.660432
90	6	0	−4.883883	5.551269	0.215019
91	1	0	−5.645627	4.981372	−0.336364
92	6	0	−3.556294	5.598915	−0.556931
93	1	0	−3.666628	5.634351	−1.643431
94	1	0	−3.023783	6.502133	−0.243925

Table A5. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
95	8	0	−5.385432	6.800758	0.618004
96	1	0	−5.841315	7.214588	−0.122680
97	1	0	−6.405655	4.673803	2.416829
98	8	0	−2.501029	0.076006	−3.516176
99	53	0	1.675500	−0.524235	−2.958353
100	3	0	3.234648	−1.146775	−0.297193
101	53	0	3.229999	1.901601	−3.462516
102	12	0	4.210067	1.831324	−0.846221
103	53	0	5.915999	−0.282140	−0.812476
104	53	0	4.501481	4.190487	0.308288
105	53	0	4.794724	−1.463308	2.031894
106	53	0	3.414522	−2.638151	4.157254

Table A6. Complex LiI_3 with nucleotide triplet GAA.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	1	0	2.182434	3.198208	−3.638285
2	6	0	1.574574	2.974140	−4.520635
3	1	0	0.919417	3.827907	−4.719445
4	1	0	2.245387	2.852408	−5.375072
5	6	0	0.755449	1.711931	−4.321494
6	1	0	0.082190	1.548302	−5.170502
7	8	0	1.650498	0.579779	−4.233656
8	6	0	1.353298	−0.152369	−3.074818
9	1	0	0.634804	−0.957551	−3.280890
10	7	0	2.564138	−0.795594	−2.587552
11	6	0	3.879126	−0.429827	−2.785415
12	1	0	4.148570	0.324774	−3.508193
13	7	0	4.710234	−1.105813	−2.024411
14	6	0	3.895528	−1.933739	−1.292025
15	6	0	4.251316	−2.750284	−0.196448
16	8	0	5.396778	−2.891455	0.260652
17	7	0	3.129875	−3.370988	0.360859
18	1	0	3.313375	−3.968371	1.157834
19	6	0	1.823854	−3.165924	−0.054652
20	7	0	0.856326	−3.865554	0.582145
21	1	0	0.996932	−4.125651	1.548923
22	1	0	−0.088971	−3.537462	0.388236
23	7	0	1.499401	−2.361561	−1.049939

Table A6. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
24	6	0	2.563570	−1.762735	−1.616358
25	6	0	−0.074854	1.703448	−3.023383
26	1	0	−0.277224	2.707546	−2.643741
27	6	0	0.778116	0.860874	−2.089864
28	1	0	1.592152	1.464658	−1.675086
29	1	0	0.228159	0.405568	−1.267131
30	8	0	−1.334820	1.061042	−3.325268
31	15	0	−2.528627	0.942825	−2.253548
32	8	0	−3.843758	0.717749	−2.899556
33	8	0	−2.357608	2.188696	−1.305978
34	8	0	−2.114911	−0.280325	−1.260802
35	6	0	−2.308613	−1.631547	−1.712072
36	1	0	−3.022347	−1.656617	−2.542533
37	1	0	−1.342526	−2.031184	−2.035661
38	6	0	−2.845514	−2.490547	−0.582528
39	1	0	−3.089953	−3.468753	−1.008516
40	8	0	−1.869027	−2.680844	0.445289
41	6	0	−2.213906	−2.000882	1.653214
42	1	0	−2.344652	−2.753911	2.436407
43	6	0	−4.078460	−1.906703	0.121228
44	1	0	−4.621338	−1.205734	−0.518746
45	6	0	−3.505257	−1.229539	1.356688
46	1	0	−3.289018	−0.187601	1.118569
47	1	0	−4.205152	−1.254934	2.193226
48	8	0	−4.967994	−2.962518	0.551333
49	7	0	−1.114017	−1.174695	2.093008
50	6	0	−0.718016	0.076081	1.644235
51	1	0	−1.313445	0.639979	0.940555
52	7	0	0.425958	0.473314	2.133366
53	6	0	0.834272	−0.572224	2.935895
54	6	0	2.005860	−0.799244	3.694950
55	7	0	3.012483	0.085102	3.772141
56	1	0	3.075549	0.857911	3.117819
57	1	0	3.852870	−0.212289	4.242573
58	7	0	2.111364	−1.963120	4.371238
59	6	0	1.121682	−2.853930	4.274340
60	1	0	1.262810	−3.770473	4.846578
61	7	0	−0.009115	−2.783791	3.560801
62	6	0	−0.097701	−1.609304	2.923136

Table A6. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
63	15	0	−6.027369	−3.502734	−0.544375
64	8	0	−6.668375	−4.745986	0.245638
65	8	0	−5.473326	−3.762774	−1.885513
66	8	0	−7.213312	−2.426885	−0.544329
67	6	0	−8.018130	−2.213232	0.629001
68	1	0	−8.812877	−2.965557	0.650806
69	1	0	−7.408030	−2.313624	1.532382
70	6	0	−8.618726	−0.827537	0.586131
71	1	0	−9.385789	−0.770513	1.373002
72	8	0	−7.592226	0.127853	0.831748
73	6	0	−7.942472	1.307507	0.123299
74	1	0	−8.702914	1.877777	0.671770
75	6	0	−9.310747	−0.421995	−0.741201
76	1	0	−9.274062	−1.234620	−1.476998
77	6	0	−8.484350	0.787106	−1.204056
78	1	0	−7.663128	0.451142	−1.843994
79	1	0	−9.082160	1.523081	−1.747039
80	8	0	−10.645264	−0.086374	−0.408510
81	7	0	−6.777181	2.154794	0.063597
82	6	0	−5.644094	1.965311	−0.676555
83	1	0	−5.552299	1.247552	−1.482825
84	7	0	−4.666609	2.771296	−0.321269
85	6	0	−5.172681	3.531865	0.716491
86	6	0	−4.643580	4.554074	1.533987
87	7	0	−3.389759	5.032577	1.406679
88	1	0	−2.726192	4.604679	0.784155
89	1	0	−3.070027	5.705358	2.084449
90	7	0	−5.436159	5.081234	2.480614
91	6	0	−6.685223	4.619106	2.608500
92	1	0	−7.277034	5.087650	3.392310
93	7	0	−7.297275	3.661992	1.907278
94	6	0	−6.489184	3.156778	0.977290
95	1	0	−3.273374	2.501546	−0.915959
96	1	0	−6.293359	−5.580915	−0.062074
97	1	0	−11.132576	0.061760	−1.226581
98	53	0	4.009835	2.516720	1.056493
99	53	0	6.513631	1.122067	0.470927
100	3	0	6.406856	−1.420170	−0.704726
101	53	0	8.888825	−0.597105	−0.368681

Table A7. Complex MgI_3LiII_2 with nucleotide triplet GAA. Standard orientation.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	1	0	−0.174362	6.900008	1.096177
2	6	0	0.653504	6.855842	1.811352
3	1	0	1.394880	7.610288	1.532427
4	1	0	0.265288	7.111024	2.800370
5	6	0	1.287623	5.479244	1.846116
6	1	0	2.171975	5.475252	2.492448
7	8	0	0.330769	4.532629	2.383940
8	6	0	0.282654	3.414872	1.540244
9	1	0	1.027369	2.656194	1.811536
10	7	0	−1.008552	2.762136	1.691857
11	6	0	−2.242955	3.348819	1.767194
12	1	0	−2.356950	4.422903	1.790512
13	7	0	−3.227339	2.476391	1.814142
14	6	0	−2.598382	1.243620	1.779004
15	6	0	−3.090474	−0.074814	1.864188
16	8	0	−4.259468	−0.473151	2.057441
17	7	0	−2.086714	−1.028960	1.722012
18	1	0	−2.415171	−1.988075	1.747971
19	6	0	−0.748501	−0.760846	1.517510
20	7	0	0.080937	−1.795692	1.312974
21	1	0	−0.268519	−2.731426	1.184460
22	1	0	1.001660	−1.577042	0.934272
23	7	0	−0.271496	0.472331	1.525157
24	6	0	−1.214350	1.408100	1.669966
25	6	0	1.688265	4.928699	0.461251
26	1	0	1.822372	5.713921	−0.286076
27	6	0	0.549981	3.971567	0.146388
28	1	0	−0.325023	4.530198	−0.201929
29	1	0	0.797572	3.217655	−0.597863
30	8	0	2.939364	4.228496	0.632125
31	15	0	3.689508	3.379610	−0.507592
32	8	0	5.156006	3.410884	−0.401497
33	8	0	3.037887	3.882563	−1.891636
34	8	0	3.023468	1.901298	−0.439197
35	6	0	3.536406	0.977106	0.549566
36	1	0	4.514419	1.313325	0.908816
37	1	0	2.829321	0.943476	1.383335
38	6	0	3.690525	−0.408710	−0.041382
39	1	0	4.169968	−1.035747	0.716960
40	8	0	2.399303	−0.971480	−0.360633

Table A7. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
41	6	0	2.292907	−1.250754	−1.749677
42	1	0	2.358263	−2.328552	−1.930442
43	6	0	4.501908	−0.468939	−1.346356
44	1	0	5.192069	0.374992	−1.444632
45	6	0	3.427373	−0.479207	−2.422227
46	1	0	3.119669	0.546859	−2.637029
47	1	0	3.771575	−0.953764	−3.342188
48	8	0	5.212141	−1.711430	−1.451711
49	7	0	0.958013	−0.870968	−2.192799
50	6	0	0.397015	0.364379	−2.125183
51	1	0	0.944522	1.229700	−1.781744
52	7	0	−0.870792	0.351867	−2.488251
53	6	0	−1.173088	−0.962278	−2.806866
54	6	0	−2.335777	−1.648162	−3.236227
55	7	0	−3.503682	−1.052397	−3.511814
56	1	0	−3.651235	−0.072353	−3.326647
57	1	0	−4.299892	−1.643391	−3.699444
58	7	0	−2.249426	−2.984207	−3.377126
59	6	0	−1.084886	−3.599605	−3.148031
60	1	0	−1.089700	−4.678277	−3.286487
61	7	0	0.075040	−3.059677	−2.766714
62	6	0	−0.034172	−1.743289	−2.608822
63	15	0	6.592536	−1.867200	−0.620413
64	8	0	6.464373	−1.508758	0.813194
65	8	0	7.595045	−1.001620	−1.506743
66	8	0	6.929113	−3.411011	−0.877274
67	6	0	8.062163	−3.833221	−1.654714
68	1	0	7.862427	−4.870531	−1.933362
69	1	0	8.138980	−3.232779	−2.566307
70	6	0	9.351300	−3.767669	−0.860248
71	1	0	10.153434	−4.201116	−1.473533
72	8	0	9.659732	−2.399554	−0.561032
73	6	0	10.348491	−2.383358	0.711217
74	1	0	11.389685	−2.686277	0.551434
75	6	0	9.346718	−4.528050	0.490331
76	1	0	8.386753	−5.034290	0.657191
77	6	0	9.577838	−3.417539	1.521725
78	1	0	8.621429	−2.996841	1.847519
79	1	0	10.133414	−3.766343	2.395628
80	8	0	10.411681	−5.454955	0.414007

Table A7. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
81	7	0	10.393094	−1.052760	1.222940
82	6	0	9.372098	−0.260544	1.735485
83	1	0	8.349302	−0.616330	1.775102
84	7	0	9.776162	0.924391	2.110412
85	6	0	11.130912	0.928211	1.839386
86	6	0	12.146043	1.892022	2.017193
87	7	0	11.903429	3.112186	2.534551
88	1	0	10.983861	3.348407	2.865041
89	1	0	12.677268	3.737835	2.683580
90	7	0	13.400829	1.582236	1.649970
91	6	0	13.635838	0.371607	1.131013
92	1	0	14.669886	0.175949	0.853501
93	7	0	12.773357	−0.625019	0.910101
94	6	0	11.541013	−0.280856	1.283717
95	1	0	3.728091	4.211821	−2.483957
96	1	0	8.517931	−1.162935	−1.201286
97	1	0	10.401171	−6.001753	1.207700
98	53	0	−2.325856	2.194680	−2.130914
99	53	0	−4.074799	4.395836	−1.515241
100	3	0	−4.797656	2.757277	0.531614
101	53	0	−6.805183	1.195505	−0.085824
102	12	0	−6.182905	−0.665263	1.720483
103	53	0	−7.790997	−1.867455	3.448364
104	53	0	−6.298010	−3.364911	0.899019
105	53	0	−4.562510	−3.864761	−1.257896

Table A8. Complex LiI_3 with nucleotide triplet GGG. Standard orientation.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	1	0	−4.481189	5.359436	−1.705402
2	6	0	−3.829890	5.873447	−0.991065
3	1	0	−3.376555	6.735244	−1.490643
4	1	0	−4.450168	6.239409	−0.169118
5	6	0	−2.759340	4.940351	−0.452718
6	1	0	−2.052241	5.494306	0.177304
7	8	0	−3.382304	3.920793	0.343633
8	6	0	−2.922902	2.649397	−0.068665
9	1	0	−2.041203	2.330044	0.500904
10	7	0	−3.945896	1.670141	0.224284

Table A8. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
11	6	0	−5.298014	1.757737	−0.014213
12	1	0	−5.758201	2.649944	−0.411282
13	7	0	−5.931544	0.667158	0.334925
14	6	0	−4.966025	−0.185734	0.822099
15	6	0	−5.042782	−1.515826	1.315134
16	8	0	−6.027768	−2.257110	1.426567
17	7	0	−3.783171	−1.982518	1.710955
18	1	0	−3.789059	−2.936749	2.050286
19	6	0	−2.591558	−1.285326	1.636605
20	7	0	−1.481757	−1.877891	2.077711
21	1	0	−1.453586	−2.844188	2.357004
22	1	0	−0.586682	−1.364063	2.001126
23	7	0	−2.528841	−0.049285	1.155071
24	6	0	−3.716825	0.428778	0.772671
25	6	0	−1.966211	4.202762	−1.547723
26	1	0	−2.013601	4.717401	−2.511807
27	6	0	−2.588289	2.815247	−1.550760
28	1	0	−3.513219	2.822408	−2.137488
29	1	0	−1.920694	2.051643	−1.952508
30	8	0	−0.583306	4.133188	−1.112492
31	15	0	0.544216	3.731839	−2.183917
32	8	0	0.743601	5.125104	−2.981845
33	8	0	0.318495	2.557509	−3.042142
34	8	0	1.825020	3.579234	−1.234402
35	6	0	2.266619	4.612881	−0.346770
36	1	0	2.606983	5.478370	−0.927113
37	1	0	1.443633	4.919395	0.306262
38	6	0	3.402245	4.070911	0.500587
39	1	0	3.821484	4.906005	1.076577
40	8	0	2.888970	3.087134	1.404419
41	6	0	3.652601	1.906624	1.292175
42	1	0	4.468481	1.904990	2.027280
43	7	0	2.815767	0.767876	1.601166
44	6	0	1.443048	0.667408	1.623106
45	1	0	0.809939	1.520290	1.435568
46	7	0	1.040948	−0.546616	1.906396
47	6	0	2.191520	−1.282462	2.064581
48	6	0	2.377154	−2.673272	2.356735
49	8	0	1.557669	−3.552004	2.571087
50	7	0	3.772002	−2.973748	2.374932

Table A8. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
51	1	0	3.970464	−3.943353	2.586766
52	6	0	4.806458	−2.097002	2.155085
53	7	0	6.071056	−2.580308	2.235621
54	1	0	6.225564	−3.568755	2.119049
55	1	0	6.802498	−1.970367	1.875559
56	7	0	4.616980	−0.815193	1.909887
57	6	0	3.309150	−0.481381	1.876961
58	6	0	4.533213	3.387493	−0.291357
59	1	0	4.603656	3.717473	−1.330336
60	6	0	4.202651	1.914095	−0.130906
61	1	0	3.407188	1.639378	−0.828753
62	1	0	5.054483	1.247132	−0.269908
63	8	0	5.768237	3.712725	0.395755
64	15	0	7.175263	3.333666	−0.307468
65	8	0	8.191184	4.219408	0.572136
66	8	0	7.201480	3.486547	−1.771566
67	8	0	7.563349	1.858980	0.178185
68	6	0	7.580947	1.471540	1.568145
69	1	0	7.786514	2.340062	2.201810
70	1	0	6.606194	1.043629	1.821657
71	6	0	8.651160	0.421310	1.787376
72	1	0	8.735790	0.250033	2.868189
73	8	0	8.264903	−0.800471	1.147498
74	6	0	9.292962	−1.248832	0.257703
75	1	0	9.913995	−2.001620	0.754973
76	7	0	8.685842	−1.905055	−0.866289
77	6	0	7.843153	−1.362243	−1.827105
78	1	0	7.575677	−0.314467	−1.811707
79	7	0	7.421583	−2.241035	−2.693519
80	6	0	8.000845	−3.426334	−2.298224
81	6	0	7.904177	−4.745570	−2.865496
82	8	0	7.296058	−5.165360	−3.830077
83	7	0	8.689214	−5.657987	−2.081812
84	1	0	8.616412	−6.616325	−2.399394
85	6	0	9.424311	−5.357496	−0.970330
86	7	0	10.054698	−6.395900	−0.336649
87	1	0	10.359038	−7.179930	−0.893204
88	1	0	10.713358	−6.096057	0.366569
89	7	0	9.510263	−4.149184	−0.465259
90	6	0	8.780498	−3.244827	−1.160983

Table A8. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
91	6	0	10.043364	0.779380	1.242664
92	1	0	10.147853	1.862592	1.095254
93	6	0	10.091608	0.009371	−0.074662
94	1	0	9.591078	0.578057	−0.862403
95	1	0	11.109756	−0.220516	−0.399862
96	8	0	10.978297	0.290336	2.188982
97	1	0	11.864292	0.496031	1.869958
98	1	0	0.998960	4.943829	−3.896575
99	1	0	8.183155	5.148446	0.309096
100	53	0	−8.486750	0.245962	0.355703
101	53	0	−11.216245	−0.230969	0.433309
102	3	0	−7.512515	−2.490820	0.265934
103	53	0	−7.916077	−4.070562	−1.599814

Table A9. Complex MgI_3LiII_2 with nucleotide triplet GGG.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
1	1	0	−0.543387	3.857467	3.494376
2	6	0	−1.204796	4.675528	3.794309
3	1	0	−2.004107	4.270705	4.421602
4	1	0	−0.632976	5.384161	4.398604
5	6	0	−1.803324	5.372273	2.595733
6	1	0	−2.485031	6.173099	2.920231
7	8	0	−0.745180	5.947760	1.803948
8	6	0	−1.163489	6.099058	0.475309
9	1	0	−1.238353	7.155472	0.193721
10	7	0	−0.115386	5.531614	−0.391919
11	6	0	0.867654	4.650141	−0.047501
12	1	0	1.036961	4.319692	0.967882
13	7	0	1.575000	4.281632	−1.096565
14	6	0	1.041719	4.949023	−2.175524
15	6	0	1.294459	4.842030	−3.578324
16	8	0	2.018824	4.064061	−4.192506
17	7	0	0.501256	5.778033	−4.285952
18	1	0	0.640829	5.752369	−5.289113
19	6	0	−0.470008	6.587973	−3.747317
20	7	0	−1.162156	7.380907	−4.600747
21	1	0	−0.770795	7.642426	−5.491310
22	1	0	−1.780385	8.049102	−4.166566

Table A9. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
23	7	0	−0.782341	6.581763	−2.468668
24	6	0	−0.008248	5.752730	−1.743165
25	6	0	−2.551413	4.497389	1.584246
26	1	0	−2.043848	3.536218	1.456407
27	6	0	−2.502926	5.361391	0.327651
28	1	0	−2.581617	4.798476	−0.603774
29	1	0	−3.326475	6.080829	0.369234
30	8	0	−3.911464	4.272625	1.964815
31	15	0	−4.434331	2.848596	2.501152
32	8	0	−5.000162	3.161788	3.964135
33	8	0	−3.453910	1.738625	2.454258
34	8	0	−5.813743	2.672948	1.708539
35	6	0	−6.000769	2.989350	0.325706
36	1	0	−7.077545	3.134137	0.205181
37	1	0	−5.490398	3.926111	0.083769
38	6	0	−5.537980	1.883489	−0.603826
39	1	0	−5.916945	2.103782	−1.612710
40	8	0	−4.108809	1.848009	−0.614134
41	6	0	−3.716298	0.494920	−0.775632
42	1	0	−3.752668	0.221490	−1.838978
43	7	0	−2.335794	0.324277	−0.363413
44	6	0	−1.872077	−0.130453	0.859401
45	1	0	−2.521554	−0.360498	1.685866
46	7	0	−0.567950	−0.238492	0.890577
47	6	0	−0.160096	0.179545	−0.347885
48	6	0	1.153655	0.252176	−0.810474
49	8	0	2.147642	−0.118345	−0.128440
50	7	0	1.229334	0.753706	−2.092344
51	1	0	2.156291	0.875518	−2.488249
52	6	0	0.117314	1.128877	−2.833653
53	7	0	0.367310	1.603734	−4.073891
54	1	0	1.194391	2.176197	−4.234807
55	1	0	−0.460535	1.901562	−4.568241
56	7	0	−1.130076	1.012140	−2.404909
57	6	0	−1.223319	0.537406	−1.152795
58	6	0	−6.022843	0.467877	−0.209421
59	1	0	−6.667316	0.492656	0.672646
60	6	0	−4.728434	−0.298087	0.044731
61	1	0	−4.485409	−0.200105	1.104942

Table A9. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
62	1	0	−4.795927	−1.352304	−0.230122
63	8	0	−6.768871	−0.082557	−1.312219
64	15	0	−7.955048	−1.124768	−0.933475
65	8	0	−8.756725	−1.175272	−2.321871
66	8	0	−8.709176	−0.785728	0.285089
67	8	0	−7.249757	−2.562552	−0.860919
68	6	0	−6.760576	−3.233103	−2.035147
69	1	0	−7.608028	−3.524218	−2.663534
70	1	0	−6.109592	−2.562619	−2.606894
71	6	0	−5.983077	−4.459598	−1.617101
72	1	0	−5.777683	−5.050389	−2.521338
73	8	0	−4.756918	−4.052354	−1.010845
74	6	0	−4.451322	−5.005221	0.002845
75	1	0	−4.014259	−5.907714	−0.441753
76	7	0	−3.436288	−4.440717	0.855141
77	6	0	−3.567270	−3.425031	1.791363
78	1	0	−4.538235	−3.113511	2.150563
79	7	0	−2.430846	−2.923942	2.187158
80	6	0	−1.480651	−3.630795	1.474617
81	6	0	−0.079699	−3.492794	1.385148
82	8	0	0.671934	−2.671423	1.968178
83	7	0	0.498001	−4.403501	0.508969
84	1	0	1.516735	−4.328684	0.423934
85	6	0	−0.191085	−5.327706	−0.244955
86	7	0	0.520093	−6.144221	−1.033301
87	1	0	1.514404	−6.031463	−1.218612
88	1	0	−0.003833	−6.784483	−1.607773
89	7	0	−1.511265	−5.431541	−0.211860
90	6	0	−2.086477	−4.578898	0.639430
91	6	0	−6.693394	−5.405170	−0.613727
92	1	0	−7.717923	−5.074533	−0.403957
93	6	0	−5.804370	−5.306981	0.634262
94	1	0	−6.132716	−4.466593	1.252932
95	1	0	−5.812068	−6.220609	1.233134
96	8	0	−6.670946	−6.691221	−1.200963
97	1	0	−7.211251	−7.283491	−0.665727
98	1	0	−4.629778	2.545846	4.609838
99	1	0	−9.617926	−0.744963	−2.239244
100	53	0	3.715814	3.101446	−0.872044

Table A9. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
101	53	0	6.005037	1.534648	−0.335666
102	53	0	4.040243	−1.609332	2.370376
103	53	0	4.090468	−3.719451	0.075848
104	53	0	4.034849	−5.701600	−1.999259
105	12	0	1.337994	−0.813215	1.893811
106	53	0	1.856223	1.668211	2.910201
107	3	0	3.658260	0.746481	0.903832

Table A10. Complex LiI_3 with nucleotide triplet CGG. Framework group C1[X(C29H37I3LiN13O15P2)]. Deg. of freedom 294. Standard orientation.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
1	1	0	1.752941	−4.805442	2.318586
2	6	0	1.278768	−4.811718	3.304875
3	1	0	0.333235	−5.356956	3.234371
4	1	0	1.931318	−5.344493	4.001160
5	6	0	1.016688	−3.404332	3.790855
6	1	0	0.515995	−3.431424	4.770882
7	8	0	2.258775	−2.699664	3.913614
8	6	0	2.072271	−1.321259	3.702648
9	1	0	2.309794	−0.749605	4.607009
10	7	0	3.044328	−0.896653	2.690376
11	6	0	3.760576	−1.687624	1.827995
12	1	0	3.694192	−2.763886	1.845409
13	7	0	4.530709	−0.985449	1.034610
14	6	0	4.327438	0.328968	1.384852
15	6	0	4.792957	1.550846	0.820719
16	8	0	5.506337	1.741553	−0.174129
17	7	0	4.294764	2.653272	1.527293
18	1	0	4.547856	3.567434	1.123881
19	6	0	3.387112	2.611551	2.548914
20	7	0	3.012330	3.807718	3.062529
21	1	0	3.198091	4.652087	2.540298
22	1	0	2.231012	3.799054	3.697006
23	7	0	2.899356	1.489812	3.042194
24	6	0	3.400444	0.401124	2.426397
25	6	0	0.169062	−2.522064	2.869030
26	1	0	0.383642	−2.738355	1.817206

Table A10. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
27	6	0	0.609980	−1.116041	3.271394
28	1	0	0.505050	−0.367807	2.484904
29	1	0	0.018072	−0.800147	4.135959
30	8	0	−1.210863	−2.783609	3.146149
31	15	0	−2.392799	−2.697359	2.061843
32	8	0	−3.617077	−3.375085	2.543278
33	8	0	−1.754053	−3.208337	0.704819
34	8	0	−2.574986	−1.123441	1.729897
35	6	0	−3.291441	−0.285250	2.647198
36	1	0	−4.147631	−0.827988	3.063757
37	1	0	−2.622662	0.010086	3.462898
38	6	0	−3.763875	0.959128	1.913039
39	1	0	−4.317208	1.574410	2.635239
40	8	0	−2.645585	1.697028	1.433180
41	6	0	−2.668275	1.801188	0.011828
42	1	0	−2.936085	2.826222	−0.266777
43	7	0	−1.340879	1.589768	−0.514534
44	6	0	−0.638380	0.396271	−0.638009
45	1	0	−1.095573	−0.555459	−0.407340
46	7	0	0.593811	0.557509	−1.030612
47	6	0	0.734687	1.921602	−1.166590
48	6	0	1.869600	2.714305	−1.492153
49	8	0	3.022786	2.353353	−1.779541
50	7	0	1.579336	4.080713	−1.423462
51	1	0	2.415105	4.682955	−1.451679
52	6	0	0.377334	4.624813	−1.066696
53	7	0	0.317410	5.982103	−1.042816
54	1	0	1.177426	6.507595	−0.981312
55	1	0	−0.499155	6.375397	−0.603944
56	7	0	−0.690886	3.908735	−0.779553
57	6	0	−0.449322	2.584381	−0.832464
58	6	0	−4.658219	0.674522	0.694513
59	1	0	−5.159223	−0.292202	0.757032
60	6	0	−3.699608	0.780913	−0.474232
61	1	0	−3.231892	−0.193421	−0.626830
62	1	0	−4.203175	1.072703	−1.396185
63	8	0	−5.658774	1.713410	0.568389
64	15	0	−7.186164	1.423772	0.988989

Table A10. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
65	8	0	−7.466344	2.285211	2.313090
66	8	0	−7.528193	0.000580	1.187270
67	8	0	−8.009265	2.282266	−0.085535
68	6	0	−7.726799	2.333462	−1.494337
69	1	0	−8.422424	3.078630	−1.885315
70	1	0	−6.700820	2.683210	−1.644069
71	6	0	−7.939005	1.037723	−2.247640
72	1	0	−7.972763	1.302370	−3.319458
73	8	0	−6.874737	0.137073	−1.999744
74	6	0	−7.293998	−1.118335	−2.544444
75	1	0	−7.075688	−1.154776	−3.615679
76	7	0	−6.478643	−2.161850	−1.958801
77	6	0	−6.456463	−2.324150	−0.611461
78	1	0	−7.113407	−1.681672	−0.029677
79	6	0	−5.603515	−3.210529	−0.028561
80	6	0	−4.738546	−3.909466	−0.918955
81	7	0	−3.744272	−4.735986	−0.381423
82	7	0	−4.753190	−3.794036	−2.221102
83	6	0	−5.628166	−2.927202	−2.829164
84	8	0	−5.714214	−2.778837	−4.034986
85	6	0	−9.220034	0.249684	−1.938444
86	1	0	−9.447954	0.337560	−0.869620
87	6	0	−8.809874	−1.201518	−2.272839
88	1	0	−9.031623	−1.889172	−1.452848
89	1	0	−9.342166	−1.545572	−3.163233
90	8	0	−10.256526	0.786780	−2.731013
91	1	0	−7.481372	3.235389	2.141413
92	1	0	−11.098991	0.481368	−2.379518
93	1	0	−2.420364	−3.761384	0.193009
94	3	0	4.762612	2.985590	−1.422862
95	53	0	4.567897	5.566650	−0.490523
96	1	0	−5.541820	−3.327788	1.046181
97	1	0	−3.993248	−5.163923	0.504667
98	1	0	−3.401138	−5.399479	−1.068724
99	53	0	5.988039	−2.164896	−0.715091
100	53	0	7.513939	−3.616288	−2.541046

Table A11. Complex MgI_3LiII_2 with nucleotide triplet CGG. Standard orientation.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
1	1	0	−2.948276	−5.658886	−5.193347
2	6	0	−3.428778	−6.371236	−4.515290
3	1	0	−4.466441	−6.512150	−4.831447
4	1	0	−2.909868	−7.328500	−4.605320
5	6	0	−3.374185	−5.887769	−3.080176
6	1	0	−3.930675	−6.565312	−2.421302
7	8	0	−1.991619	−5.857348	−2.656856
8	6	0	−1.815792	−4.693597	−1.893251
9	1	0	−2.163079	−4.835325	−0.861216
10	7	0	−0.410947	−4.334919	−1.765544
11	6	0	0.319560	−3.526803	−2.594566
12	1	0	−0.004751	−3.236677	−3.581958
13	7	0	1.446616	−3.144648	−2.039051
14	6	0	1.478489	−3.730252	−0.793594
15	6	0	2.339712	−3.512130	0.315888
16	8	0	3.304542	−2.744334	0.390546
17	7	0	1.936519	−4.245244	1.432684
18	1	0	2.431862	−3.978407	2.291852
19	6	0	0.807355	−5.026800	1.493426
20	7	0	0.553897	−5.646732	2.662544
21	1	0	1.262932	−5.738635	3.371662
22	1	0	−0.218432	−6.293921	2.676569
23	7	0	−0.043000	−5.158271	0.489437
24	6	0	0.325332	−4.480681	−0.606520
25	6	0	−3.924079	−4.453063	−2.865050
26	1	0	−4.504415	−4.087772	−3.714660
27	6	0	−2.658114	−3.648705	−2.610950
28	1	0	−2.211539	−3.411036	−3.581764
29	1	0	−2.810014	−2.722887	−2.058303
30	8	0	−4.796122	−4.487828	−1.709597
31	15	0	−5.301786	−3.178159	−0.949594
32	8	0	−6.641027	−3.331836	−0.310977
33	8	0	−5.139248	−2.025077	−2.008523
34	8	0	−4.146908	−2.903998	0.161846
35	6	0	−4.464125	−2.927091	1.564133
36	1	0	−5.521072	−3.172559	1.695418
37	1	0	−3.860219	−3.708874	2.033437
38	6	0	−4.172527	−1.593775	2.228364
39	1	0	−4.738435	−1.563224	3.172046
40	8	0	−2.778763	−1.465264	2.506395

Table A11. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
41	6	0	−2.409234	−0.102327	2.535835
42	1	0	−2.136330	0.185646	3.558426
43	7	0	−1.178919	0.002284	1.727281
44	6	0	−0.306073	−1.050077	1.521428
45	1	0	−0.588104	−2.054081	1.796470
46	7	0	0.831214	−0.687904	0.980404
47	6	0	0.705987	0.674600	0.841102
48	6	0	1.633562	1.594541	0.355991
49	8	0	2.792578	1.266908	−0.068152
50	7	0	1.193409	2.888677	0.383660
51	1	0	1.845705	3.599940	0.011395
52	6	0	−0.060118	3.275657	0.844599
53	7	0	−0.344323	4.573994	0.802041
54	1	0	0.287848	5.208009	0.337598
55	1	0	−1.337589	4.861904	0.895741
56	7	0	−0.947152	2.403755	1.328365
57	6	0	−0.523968	1.140504	1.307593
58	6	0	−4.516624	−0.347004	1.412892
59	1	0	−4.289875	−0.506693	0.356619
60	6	0	−3.601525	0.715779	2.018137
61	1	0	−3.305741	1.499179	1.321663
62	1	0	−4.112883	1.195252	2.856481
63	8	0	−5.903328	−0.043690	1.570942
64	15	0	−6.927081	0.006266	0.320499
65	8	0	−7.934576	−1.185863	0.529500
66	8	0	−6.216261	0.041644	−0.997379
67	1	0	−7.566518	−2.061317	0.208395
68	1	0	−5.591028	−1.162495	−1.701371
69	8	0	−7.794561	1.308124	0.566205
70	6	0	−8.054571	1.854891	1.876770
71	1	0	−7.619781	1.215467	2.647119
72	6	0	−7.482444	3.253080	1.964817
73	1	0	−7.655968	3.613445	2.992215
74	8	0	−6.095569	3.219892	1.661305
75	6	0	−5.677134	4.467246	1.116834
76	1	0	−4.966559	4.951965	1.787635
77	7	0	−4.908594	4.215941	−0.105489
78	6	0	−5.469582	3.544635	−1.146973
79	1	0	−6.472673	3.166505	−0.990208
80	6	0	−4.791587	3.332610	−2.302271

Table A11. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
81	1	0	−5.240794	2.783286	−3.119762
82	6	0	−3.458822	3.850716	−2.356507
83	7	0	−2.878766	4.449224	−1.327232
84	6	0	−3.553898	4.631821	−0.167258
85	8	0	−3.045404	5.146490	0.837927
86	6	0	−8.097148	4.285168	1.017398
87	1	0	−8.311841	3.812265	0.047503
88	6	0	−6.952549	5.300644	0.899045
89	1	0	−6.931863	5.851918	−0.044021
90	1	0	−7.062728	6.024061	1.712880
91	8	0	−9.274975	4.770132	1.612407
92	1	0	−9.774010	5.274415	0.961182
93	1	0	−9.139012	1.896357	2.007320
94	7	0	−2.724443	3.712159	−3.481576
95	3	0	2.962302	−0.855091	0.428022
96	53	0	4.317914	1.033055	−3.439733
97	12	0	4.348693	2.244098	−0.881929
98	53	0	6.387422	1.249555	0.593605
99	53	0	3.744373	4.811137	−1.077575
100	53	0	2.795030	−1.307402	−2.722255
101	1	0	−3.149934	3.419327	−4.344481
102	1	0	−1.837170	4.189244	−3.520570
103	53	0	4.688120	−0.461436	2.583369
104	53	0	3.135438	−2.215858	4.250838

Table A12. Complex LiI_3 with nucleotide triplet CTG.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
1	1	0	6.629890	−1.646898	4.619939
2	6	0	6.245791	−0.710661	5.037708
3	1	0	5.416559	−0.944112	5.712496
4	1	0	7.043018	−0.246260	5.624113
5	6	0	5.791810	0.236640	3.941390
6	1	0	5.327157	1.129935	4.374701
7	8	0	6.934535	0.648540	3.168556
8	6	0	6.669869	0.452651	1.796479
9	1	0	6.220218	1.343712	1.343518
10	7	0	7.924126	0.224383	1.086526
11	6	0	9.072613	−0.102398	1.723970

Table A12. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
12	1	0	9.005253	−0.175422	2.802908
13	6	0	10.221836	−0.296932	1.023697
14	1	0	11.148063	−0.545311	1.526740
15	6	0	10.138823	−0.122941	−0.395455
16	7	0	11.249551	−0.265976	−1.156177
17	1	0	12.110616	−0.613927	−0.773951
18	1	0	11.141264	−0.202343	−2.155530
19	7	0	9.021738	0.193679	−1.026941
20	6	0	7.867966	0.369920	−0.334383
21	8	0	6.781261	0.639032	−0.839305
22	6	0	4.805683	−0.394126	2.941076
23	1	0	4.271505	−1.252603	3.353703
24	6	0	5.696102	−0.722808	1.755321
25	1	0	6.244180	−1.650717	1.953726
26	1	0	5.167007	−0.824246	0.809317
27	8	0	3.838951	0.633524	2.606051
28	15	0	2.507462	0.354988	1.771662
29	8	0	1.585357	1.512286	1.941015
30	8	0	2.050599	−1.060753	2.299798
31	8	0	2.903187	0.068342	0.244839
32	6	0	3.481148	1.140153	−0.544649
33	1	0	3.569544	2.053241	0.053296
34	1	0	4.481685	0.819208	−0.845763
35	6	0	2.635588	1.459418	−1.752512
36	1	0	3.120548	2.316159	−2.252430
37	8	0	2.548866	0.356122	−2.631101
38	6	0	1.553998	0.701325	−3.585809
39	1	0	1.979626	1.316395	−4.384885
40	7	0	1.096678	−0.509095	−4.233354
41	6	0	0.729431	−1.611238	−3.481302
42	1	0	0.843849	−1.480317	−2.410785
43	6	0	0.297858	−2.774916	−4.015853
44	6	0	−0.097495	−3.968829	−3.206013
45	1	0	−0.033961	−3.765342	−2.134538
46	1	0	−1.122762	−4.272367	−3.440233
47	1	0	0.542420	−4.825707	−3.441750
48	6	0	0.226148	−2.881198	−5.472395
49	8	0	−0.138639	−3.862440	−6.098578
50	7	0	0.627828	−1.720196	−6.150302

Table A12. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
51	1	0	0.591454	−1.759644	−7.160818
52	6	0	1.063125	−0.523185	−5.627562
53	8	0	1.373757	0.432285	−6.320388
54	6	0	1.175224	1.851883	−1.486525
55	1	0	0.774424	1.273863	−0.650629
56	6	0	0.474432	1.486913	−2.801380
57	1	0	−0.417359	0.878141	−2.635061
58	1	0	0.175535	2.386559	−3.343639
59	8	0	1.151629	3.246326	−1.162356
60	15	0	0.043396	3.918820	−0.204026
61	8	0	0.435962	5.292734	0.169688
62	8	0	−0.309673	2.850940	0.910197
63	8	0	−1.365105	3.835563	−1.003470
64	6	0	−1.837772	4.960500	−1.756094
65	1	0	−1.056063	5.721076	−1.853446
66	1	0	−2.102519	4.585238	−2.748777
67	6	0	−3.066944	5.576443	−1.108605
68	1	0	−3.421685	6.384191	−1.760759
69	8	0	−4.105265	4.594023	−1.002782
70	6	0	−4.435078	4.349437	0.342537
71	1	0	−5.438945	4.729429	0.559938
72	7	0	−4.522823	2.902192	0.555020
73	6	0	−3.479836	2.013525	0.534428
74	1	0	−2.448551	2.318236	0.417790
75	7	0	−3.889235	0.775455	0.673930
76	6	0	−5.258316	0.836556	0.780788
77	6	0	−6.228992	−0.181576	0.953095
78	8	0	−6.080975	−1.403741	1.056927
79	7	0	−7.521936	0.360247	1.010340
80	1	0	−8.249702	−0.326284	1.170673
81	6	0	−7.832973	1.696566	0.910027
82	7	0	−9.141332	2.036642	1.022789
83	1	0	−9.865590	1.364248	0.829492
84	1	0	−9.352532	3.001440	0.819890
85	7	0	−6.929373	2.637995	0.752787
86	6	0	−5.671595	2.164380	0.699723
87	6	0	−2.864382	6.152266	0.300350
88	1	0	−1.810455	6.392408	0.486998
89	6	0	−3.356867	5.017044	1.200284

Table A12. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
90	1	0	−2.540289	4.322666	1.413361
91	1	0	−3.753145	5.379686	2.151896
92	8	0	−3.695040	7.299093	0.390480
93	1	0	1.326224	−1.534959	1.825150
94	1	0	0.459818	2.363006	1.352380
95	1	0	−3.477667	7.758858	1.208807
96	53	0	−2.334287	−1.113165	0.831161
97	53	0	−0.381042	−3.125911	1.013299
98	3	0	−4.838667	−2.814960	0.973392
99	53	0	−4.398453	−5.224785	0.859966

Table A13. Complex MgI_3LiII_2 with nucleotide triplet CTG.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
1	1	0	−7.639123	−4.502558	−3.061891
2	6	0	−7.390859	−3.718542	−3.784334
3	1	0	−6.461669	−3.992024	−4.293409
4	1	0	−8.188301	−3.678344	−4.530539
5	6	0	−7.252330	−2.367169	−3.106644
6	1	0	−6.916904	−1.610481	−3.825539
7	8	0	−8.532329	−1.965717	−2.586267
8	6	0	−8.394114	−1.577645	−1.239025
9	1	0	−8.170823	−0.507181	−1.153339
10	7	0	−9.650969	−1.791893	−0.532467
11	6	0	−10.673159	−2.512054	−1.056870
12	1	0	−10.501335	−2.924094	−2.043871
13	6	0	−11.831269	−2.669496	−0.364344
14	1	0	−12.655111	−3.238424	−0.776770
15	6	0	−11.902833	−2.029322	0.915682
16	7	0	−13.024518	−2.137235	1.658853
17	1	0	−13.846484	−2.603741	1.318556
18	1	0	−13.061206	−1.640921	2.534624
19	7	0	−10.909056	−1.322436	1.432020
20	6	0	−9.748004	−1.177991	0.752430
21	8	0	−8.765343	−0.559377	1.163804
22	6	0	−6.287134	−2.368071	−1.905851
23	1	0	−5.562106	−3.183967	−1.940314
24	6	0	−7.227301	−2.413320	−0.715663
25	1	0	−7.565934	−3.443431	−0.559387

Table A13. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
26	1	0	−6.807314	−2.038603	0.216250
27	8	0	−5.552816	−1.110217	−1.959959
28	15	0	−4.336679	−0.734426	−1.007253
29	8	0	−3.473485	0.297516	−1.642849
30	8	0	−3.633281	−2.112156	−0.640200
31	8	0	−4.941635	−0.317548	0.417036
32	6	0	−5.884782	0.779194	0.532684
33	1	0	−6.116390	1.200436	−0.451874
34	1	0	−6.804224	0.369755	0.961175
35	6	0	−5.320341	1.889269	1.387202
36	1	0	−6.079169	2.684724	1.414099
37	8	0	−5.064391	1.444769	2.731703
38	6	0	−3.880116	2.010804	3.223714
39	1	0	−4.041592	2.389672	4.236011
40	7	0	−2.835333	0.933993	3.324667
41	6	0	−3.130066	−0.375715	3.065709
42	1	0	−4.170847	−0.558604	2.829570
43	6	0	−2.204013	−1.375611	3.068347
44	6	0	−2.546371	−2.810479	2.807255
45	1	0	−3.618110	−2.927221	2.634805
46	1	0	−2.014590	−3.189946	1.929760
47	1	0	−2.262808	−3.439697	3.657443
48	6	0	−0.835441	−1.000372	3.303794
49	8	0	0.152346	−1.752614	3.182654
50	7	0	−0.635388	0.305986	3.695753
51	1	0	0.307793	0.575335	3.949189
52	6	0	−1.578305	1.322079	3.767860
53	8	0	−1.306430	2.445059	4.150185
54	6	0	−3.997120	2.495683	0.927016
55	1	0	−3.331492	1.707677	0.560434
56	6	0	−3.468757	3.090483	2.224277
57	1	0	−2.403672	3.310396	2.232539
58	1	0	−4.018211	4.009987	2.452099
59	8	0	−4.255374	3.434567	−0.111004
60	15	0	−3.108238	3.895741	−1.155718
61	8	0	−3.666197	4.787265	−2.187843
62	8	0	−2.320164	2.581851	−1.570817
63	8	0	−1.920474	4.551092	−0.272612
64	6	0	−1.922489	5.959889	0.012067

Table A13. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
65	1	0	−2.856279	6.426414	−0.318091
66	1	0	−1.833944	6.059160	1.097435
67	6	0	−0.741663	6.644310	−0.653709
68	1	0	−0.717723	7.686629	−0.314287
69	8	0	0.475191	6.006758	−0.239687
70	6	0	1.140319	5.436238	−1.334829
71	1	0	2.067109	5.982550	−1.539285
72	7	0	1.582953	4.078993	−0.970016
73	6	0	0.806748	2.957661	−0.883504
74	1	0	−0.247074	2.929309	−1.133304
75	7	0	1.494876	1.922028	−0.454486
76	6	0	2.777021	2.373454	−0.229478
77	6	0	3.932437	1.733006	0.250195
78	8	0	4.030001	0.529335	0.587573
79	7	0	5.019053	2.584554	0.337968
80	1	0	5.871913	2.151182	0.715257
81	6	0	4.993842	3.920589	−0.001012
82	7	0	6.137065	4.608863	0.141310
83	1	0	6.981069	4.196721	0.502987
84	1	0	6.123419	5.592300	−0.076645
85	7	0	3.911454	4.530848	−0.452362
86	6	0	2.843846	3.732282	−0.541983
87	6	0	−0.733868	6.643971	−2.189839
88	1	0	−1.742637	6.505775	−2.597854
89	6	0	0.174575	5.456512	−2.521880
90	1	0	−0.416859	4.539305	−2.574040
91	1	0	0.693591	5.582546	−3.474718
92	8	0	−0.159800	7.875251	−2.585854
93	1	0	−2.662237	−2.133407	−0.724726
94	1	0	−2.833768	1.722824	−1.672452
95	1	0	−0.304722	7.989069	−3.531697
96	53	0	0.758858	−0.296796	−0.461773
97	53	0	−0.107069	−3.052740	−0.509631
98	12	0	5.216068	−0.920870	1.164852
99	3	0	1.267593	−2.346477	1.850400
100	53	0	7.508435	0.375790	1.798753
101	53	0	6.935746	−1.467487	−1.026343
102	53	0	5.834611	−3.006786	−3.036044
103	53	0	3.873527	−2.980459	2.126655

Table A14. Complex LiI_3 with nucleotide triplet ACC.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
1	1	0	−8.989693	0.566063	1.312841
2	6	0	−9.214552	0.180933	0.312778
3	1	0	−9.586982	−0.843359	0.411598
4	1	0	−10.009781	0.794651	−0.117795
5	6	0	−7.988452	0.221553	−0.583161
6	1	0	−8.202983	−0.259764	−1.544804
7	8	0	−7.630977	1.590638	−0.829909
8	6	0	−6.268711	1.804864	−0.530737
9	1	0	−5.635116	1.707952	−1.422277
10	6	0	−6.745506	−0.444767	0.032337
11	1	0	−6.988863	−1.151503	0.828797
12	6	0	−5.920419	0.740043	0.511408
13	1	0	−6.273771	1.063990	1.496064
14	1	0	−4.852694	0.524058	0.579391
15	8	0	−6.068066	−1.161255	−1.028292
16	7	0	−6.114690	3.170912	−0.078234
17	6	0	−6.987853	3.913692	0.691325
18	1	0	−7.927782	3.495184	1.021828
19	7	0	−6.578396	5.136172	0.921687
20	6	0	−5.367295	5.208428	0.268475
21	6	0	−4.423717	6.243813	0.113846
22	7	0	−4.575693	7.452719	0.696100
23	1	0	−5.461504	7.683582	1.115320
24	1	0	−3.957289	8.194780	0.411418
25	7	0	−3.321727	6.011362	−0.621233
26	6	0	−3.167838	4.801213	−1.174681
27	1	0	−2.265431	4.673659	−1.770005
28	7	0	−3.964538	3.732205	−1.088969
29	6	0	−5.057204	4.002632	−0.364586
30	15	0	−4.992144	−2.299542	−0.650183
31	8	0	−5.166182	−3.354497	−1.844542
32	8	0	−5.128957	−2.818286	0.727673
33	8	0	−3.555577	−1.680304	−0.961084
34	6	0	−3.112464	−1.394698	−2.306962
35	1	0	−3.327729	−2.254509	−2.947638
36	1	0	−3.647513	−0.516684	−2.682513
37	6	0	−1.623712	−1.133434	−2.316880
38	1	0	−1.294552	−1.148624	−3.363703
39	8	0	−1.343930	0.159467	−1.756581
40	6	0	−0.163221	0.010562	−0.999007

Table A14. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
41	1	0	0.722647	−0.016831	−1.645069
42	7	0	0.003891	1.188791	−0.140781
43	6	0	−0.986242	2.082723	0.102277
44	1	0	−1.956062	1.850748	−0.322690
45	6	0	−0.734819	3.223716	0.803097
46	1	0	−1.521525	3.942961	0.988881
47	6	0	0.611515	3.466901	1.199669
48	7	0	0.958497	4.594448	1.836942
49	1	0	0.290781	5.329763	1.994314
50	1	0	1.931173	4.758696	2.049270
51	7	0	1.579831	2.582198	0.939154
52	6	0	1.305835	1.423322	0.302686
53	8	0	2.169710	0.563931	0.068438
54	6	0	−0.758088	−2.145874	−1.522788
55	1	0	−1.298546	−3.067808	−1.295482
56	6	0	−0.340471	−1.332072	−0.303490
57	1	0	−1.162147	−1.272843	0.416719
58	1	0	0.552299	−1.720993	0.184573
59	8	0	0.406766	−2.415247	−2.309056
60	15	0	1.000499	−3.925237	−2.445954
61	8	0	2.214247	−3.659199	−3.426316
62	8	0	0.010676	−4.941609	−2.837814
63	8	0	1.626294	−4.274136	−0.994317
64	6	0	2.806526	−3.595145	−0.534402
65	1	0	3.665626	−3.889485	−1.147286
66	1	0	2.680334	−2.511859	−0.634407
67	6	0	3.059169	−3.944121	0.916256
68	1	0	3.978641	−3.425474	1.221796
69	8	0	1.963185	−3.491487	1.706214
70	6	0	1.512941	−4.534037	2.571731
71	1	0	1.955279	−4.436338	3.566243
72	7	0	0.084611	−4.384079	2.766017
73	6	0	−0.733495	−4.348467	1.682817
74	1	0	−0.249831	−4.486514	0.720639
75	6	0	−2.064504	−4.132086	1.815635
76	1	0	−2.731506	−4.112207	0.964655
77	6	0	−2.541306	−3.914983	3.153035
78	7	0	−3.859206	−3.674557	3.337649
79	1	0	−4.443599	−3.433879	2.547902
80	1	0	−4.146913	−3.429456	4.271405

Table A14. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
81	7	0	−1.762250	−3.945911	4.218198
82	6	0	−0.425217	−4.192247	4.098342
83	8	0	0.352157	−4.256002	5.039282
84	6	0	3.256292	−5.442237	1.220946
85	1	0	3.445719	−6.017081	0.303668
86	6	0	1.934743	−5.829499	1.876865
87	1	0	1.206451	−6.106704	1.108208
88	1	0	2.030696	−6.662859	2.578560
89	8	0	4.355880	−5.523400	2.112665
90	1	0	−5.798198	−4.052511	−1.630758
91	1	0	2.699487	−2.807242	−3.294178
92	1	0	4.470379	−6.447325	2.361706
93	53	0	4.193940	3.000864	0.926381
94	53	0	6.910488	3.501755	0.760462
95	3	0	3.823074	0.537696	−0.760612
96	53	0	4.188783	−0.754670	−2.912709

Table A15. Complex MgI_3LiII_2 with nucleotide triplet ACC.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
1	1	0	8.959696	3.373859	−1.368836
2	6	0	8.155195	3.760841	−2.001211
3	1	0	8.150811	4.852317	−1.920401
4	1	0	8.386999	3.494483	−3.034890
5	6	0	6.797128	3.187778	−1.622938
6	1	0	6.014347	3.663669	−2.222361
7	8	0	6.716894	1.780807	−1.879972
8	6	0	6.935362	1.031072	−0.695060
9	1	0	6.070191	0.377264	−0.551616
10	6	0	6.463256	3.316515	−0.137008
11	1	0	6.843308	4.237473	0.313005
12	6	0	7.060521	2.044542	0.455426
13	1	0	8.102257	2.230041	0.726196
14	1	0	6.538623	1.720487	1.357433
15	8	0	5.015166	3.307924	−0.037590
16	7	0	8.069745	0.139449	−0.848522
17	6	0	9.420710	0.391330	−0.656034
18	1	0	9.771728	1.297902	−0.183590
19	7	0	10.203778	−0.562644	−1.077620
20	6	0	9.339979	−1.497691	−1.602851

Table A15. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
21	6	0	9.564702	−2.743285	−2.229185
22	7	0	10.790460	−3.255523	−2.399373
23	1	0	11.602828	−2.749050	−2.088644
24	1	0	10.890794	−4.140450	−2.869802
25	7	0	8.500518	−3.437925	−2.675184
26	6	0	7.287364	−2.926891	−2.495587
27	1	0	6.464418	−3.529805	−2.876405
28	7	0	6.939304	−1.769757	−1.910061
29	6	0	8.014159	−1.087293	−1.482730
30	15	0	4.236767	3.767110	1.278105
31	8	0	4.778847	5.267030	1.491425
32	8	0	4.301062	2.911594	2.484474
33	8	0	2.746494	3.881469	0.714296
34	6	0	2.351943	4.825764	−0.300794
35	1	0	2.343089	5.829893	0.135850
36	1	0	3.061274	4.803833	−1.133610
37	6	0	0.959399	4.465740	−0.796661
38	1	0	0.566242	5.324549	−1.350502
39	8	0	0.985961	3.355188	−1.700027
40	6	0	0.435943	2.199189	−1.124427
41	1	0	−0.432127	1.864844	−1.703890
42	7	0	1.450768	1.101086	−1.213254
43	6	0	2.643919	1.295652	−1.837605
44	1	0	2.786958	2.281870	−2.255698
45	6	0	3.570393	0.309902	−1.923661
46	1	0	4.519875	0.478488	−2.416520
47	6	0	3.256276	−0.943391	−1.319949
48	7	0	4.149849	−1.922663	−1.289201
49	1	0	5.133650	−1.772380	−1.586765
50	1	0	3.902824	−2.793257	−0.838274
51	7	0	2.039428	−1.133859	−0.759714
52	6	0	1.117297	−0.143391	−0.698453
53	8	0	0.000349	−0.292023	−0.165174
54	6	0	0.005559	4.069706	0.330609
55	1	0	0.296667	4.499787	1.292184
56	6	0	0.080179	2.547030	0.323773
57	1	0	0.879915	2.224791	0.992343
58	1	0	−0.856707	2.090748	0.638976
59	8	0	−1.316327	4.533075	−0.003120
60	15	0	−2.326882	4.803861	1.234601

Table A15. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
61	8	0	−3.477446	5.658250	0.532656
62	8	0	−1.665306	5.324471	2.446992
63	8	0	−3.073740	3.421813	1.525606
64	6	0	−3.808360	2.668058	0.542120
65	1	0	−4.727504	3.200409	0.277621
66	1	0	−3.205139	2.526965	−0.359515
67	6	0	−4.151512	1.316822	1.130451
68	1	0	−4.709415	0.745549	0.382071
69	8	0	−2.924859	0.582946	1.445687
70	6	0	−2.783098	0.450923	2.881350
71	1	0	−3.009587	−0.586602	3.129366
72	7	0	−1.373525	0.655158	3.206358
73	6	0	−0.833919	1.805916	3.704956
74	1	0	−1.510752	2.624639	3.912163
75	6	0	0.505033	1.910642	3.907475
76	1	0	0.932783	2.821366	4.306866
77	6	0	1.309639	0.769521	3.591416
78	7	0	2.636791	0.787980	3.754156
79	1	0	3.156801	1.658752	3.756382
80	1	0	3.133716	−0.035507	3.446585
81	7	0	0.772116	−0.359590	3.109474
82	6	0	−0.526130	−0.402172	2.849048
83	8	0	−1.082658	−1.361273	2.233140
84	6	0	−4.924945	1.333372	2.450503
85	1	0	−5.583097	2.209366	2.511718
86	6	0	−3.804979	1.387290	3.500114
87	1	0	−3.447271	2.413255	3.587966
88	1	0	−4.133998	1.028286	4.477979
89	8	0	−5.637884	0.121400	2.510240
90	1	0	4.820315	5.505421	2.427404
91	1	0	−3.269007	6.597690	0.447658
92	1	0	−6.297879	0.169806	3.210533
93	53	0	1.523880	−3.178509	0.492575
94	53	0	0.806833	−5.360969	2.166837
95	3	0	−0.896134	−3.243538	1.964748
96	53	0	−2.909008	−3.419856	0.286995
97	12	0	−1.930565	−0.907199	0.190109
98	53	0	−2.728393	0.176795	−2.214050
99	53	0	−6.061406	−0.030694	−2.055002
100	53	0	−8.816317	−0.077005	−1.789848

Table A16. Complex LiI_3 with nucleotide triplet GCG.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
1	1	0	−3.598461	5.939027	−1.219990
2	6	0	−3.048759	6.556830	−0.502998
3	1	0	−2.591300	7.392568	−1.040597
4	1	0	−3.762856	6.962556	0.218162
5	6	0	−1.986485	5.746531	0.212872
6	1	0	−1.390597	6.387565	0.874455
7	8	0	−2.640190	4.739711	1.013935
8	6	0	−1.908276	3.550632	0.909952
9	1	0	−1.079836	3.510093	1.630865
10	7	0	−2.777989	2.426752	1.218014
11	6	0	−4.143343	2.326156	1.123958
12	1	0	−4.771209	3.188821	0.960738
13	7	0	−4.556351	1.089363	1.281097
14	6	0	−3.418476	0.335950	1.469797
15	6	0	−3.209176	−1.066868	1.588917
16	8	0	−4.038436	−1.986085	1.596703
17	7	0	−1.845655	−1.370784	1.685658
18	1	0	−1.644658	−2.363743	1.715841
19	6	0	−0.805767	−0.469877	1.624124
20	7	0	0.454953	−0.947355	1.707828
21	1	0	0.648576	−1.861460	1.308989
22	1	0	1.144304	−0.254840	1.416502
23	7	0	−1.003889	0.831449	1.516141
24	6	0	−2.299089	1.161101	1.434484
25	6	0	−1.013622	4.993486	−0.725595
26	1	0	−1.095172	5.320497	−1.765021
27	6	0	−1.388821	3.531962	−0.526735
28	1	0	−2.212859	3.261992	−1.195571
29	1	0	−0.560568	2.839342	−0.682606
30	8	0	0.335550	5.248311	−0.270936
31	15	0	1.537358	4.989401	−1.315043
32	8	0	2.618415	6.006465	−0.700284
33	8	0	1.207353	5.120243	−2.745284
34	8	0	2.101723	3.519188	−0.976655
35	6	0	2.602191	3.181123	0.327778
36	1	0	3.371818	3.900435	0.628251
37	1	0	1.779970	3.208456	1.050500
38	6	0	3.196952	1.787394	0.286295
39	1	0	3.649559	1.594627	1.267512
40	8	0	2.161400	0.833158	0.039033

Table A16. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
41	6	0	2.547492	−0.038856	−1.039031
42	1	0	3.027140	−0.928146	−0.629906
43	7	0	1.336906	−0.511901	−1.686205
44	6	0	0.605737	0.314400	−2.489179
45	1	0	1.040628	1.281417	−2.710898
46	6	0	−0.602873	−0.056393	−2.972531
47	1	0	−1.164509	0.597505	−3.628478
48	6	0	−1.115401	−1.326277	−2.538736
49	7	0	−2.329719	−1.722295	−2.924073
50	1	0	−2.930438	−1.109363	−3.450671
51	1	0	−2.790341	−2.531219	−2.507728
52	7	0	−0.415292	−2.130703	−1.735484
53	6	0	0.806198	−1.780512	−1.309526
54	8	0	1.495280	−2.503916	−0.558608
55	6	0	4.269959	1.560425	−0.798122
56	1	0	4.684752	2.504511	−1.160374
57	6	0	3.528354	0.775668	−1.872996
58	1	0	3.015356	1.485785	−2.526629
59	1	0	4.186781	0.139877	−2.468116
60	8	0	5.316392	0.754363	−0.229520
61	15	0	6.849785	1.297544	−0.361193
62	8	0	6.963458	2.751204	−0.126316
63	8	0	7.416270	0.787929	−1.740856
64	8	0	7.580980	0.315902	0.690077
65	6	0	7.455974	0.484680	2.104022
66	1	0	7.932270	1.423731	2.408246
67	1	0	6.398360	0.508220	2.387764
68	6	0	8.132719	−0.685870	2.801066
69	1	0	8.147652	−0.466186	3.876871
70	8	0	7.392228	−1.892116	2.607726
71	6	0	8.150227	−2.851433	1.904781
72	1	0	7.853027	−3.832776	2.279274
73	7	0	7.799780	−2.833862	0.480886
74	6	0	8.380131	−2.091875	−0.519985
75	1	0	9.380014	−1.693953	−0.435838
76	7	0	7.598043	−1.906397	−1.554016
77	6	0	6.426449	−2.560883	−1.226117
78	6	0	5.159703	−2.582006	−1.897570
79	8	0	4.813358	−2.046579	−2.942969
80	7	0	4.222669	−3.311086	−1.128126

Table A16. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
81	1	0	3.261961	−3.265025	−1.458759
82	6	0	4.436148	−3.854652	0.110451
83	7	0	3.375836	−4.489038	0.673945
84	1	0	2.451966	−4.204404	0.371404
85	1	0	3.493734	−4.723148	1.646973
86	7	0	5.594695	−3.807100	0.736894
87	6	0	6.527872	−3.137020	0.033742
88	6	0	9.583114	−0.960967	2.355623
89	1	0	9.779285	−0.452426	1.403179
90	6	0	9.605538	−2.491618	2.180729
91	1	0	10.303101	−2.854151	1.421229
92	1	0	9.890839	−2.926072	3.143282
93	8	0	10.453229	−0.483039	3.359935
94	1	0	3.191302	6.355685	−1.395661
95	1	0	7.471360	−0.210233	−1.850523
96	1	0	11.338944	−0.412709	2.988728
97	53	0	−6.948492	0.136076	1.146223
98	53	0	−9.472636	−1.001452	0.965631
99	3	0	−5.504860	−2.225454	0.424016
100	53	0	−5.344617	−3.323026	−1.835109

Table A17. Complex MgI_3LiII_2 with nucleotide triplet GCG.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
1	1	0	−0.345536	−6.673970	−3.646812
2	6	0	−0.850127	−7.467918	−3.087856
3	1	0	−1.691371	−7.831317	−3.684671
4	1	0	−0.148803	−8.294140	−2.947339
5	6	0	−1.344430	−6.960406	−1.750957
6	1	0	−1.891658	−7.745719	−1.213171
7	8	0	−0.200302	−6.573525	−0.953655
8	6	0	−0.617225	−5.530387	−0.128572
9	1	0	−1.150494	−5.884678	0.764192
10	7	0	0.553244	−4.796524	0.354766
11	6	0	1.754200	−4.607008	−0.262218
12	1	0	2.106225	−5.250347	−1.055244
13	7	0	2.407146	−3.579819	0.245127
14	6	0	1.590023	−3.047303	1.226325
15	6	0	1.593219	−1.815409	1.917465

Table A17. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
16	8	0	2.464545	−0.907914	1.880044
17	7	0	0.460874	−1.620485	2.676659
18	1	0	0.324401	−0.681126	3.051982
19	6	0	−0.593143	−2.511707	2.779168
20	7	0	−1.584701	−2.192991	3.621081
21	1	0	−1.791643	−1.190186	3.672074
22	1	0	−2.405110	−2.765967	3.478173
23	7	0	−0.631801	−3.639798	2.086398
24	6	0	0.433511	−3.822954	1.314113
25	6	0	−2.264621	−5.711501	−1.817742
26	1	0	−2.461525	−5.397450	−2.846136
27	6	0	−1.507485	−4.658173	−1.015793
28	1	0	−0.867015	−4.070306	−1.681940
29	1	0	−2.161669	−3.980404	−0.464887
30	8	0	−3.522631	−6.033400	−1.189115
31	15	0	−4.811517	−5.135435	−1.602847
32	8	0	−6.009062	−6.054649	−1.064892
33	8	0	−4.826638	−4.699695	−3.008856
34	8	0	−4.852118	−3.907966	−0.568924
35	6	0	−5.028113	−4.094704	0.842836
36	1	0	−5.982263	−4.596630	1.034259
37	1	0	−4.215817	−4.714741	1.238048
38	6	0	−5.015533	−2.742220	1.525746
39	1	0	−5.248199	−2.909285	2.587595
40	8	0	−3.721226	−2.156643	1.386859
41	6	0	−3.875672	−0.746634	1.182608
42	1	0	−3.956745	−0.239744	2.149013
43	7	0	−2.676902	−0.212145	0.563794
44	6	0	−2.491766	−0.264719	−0.790706
45	1	0	−3.260189	−0.751287	−1.374899
46	6	0	−1.412529	0.292242	−1.382203
47	1	0	−1.313937	0.321157	−2.459376
48	6	0	−0.473552	0.939700	−0.518065
49	7	0	0.575645	1.583400	−1.059214
50	1	0	0.485895	1.885304	−2.026211
51	1	0	1.130433	2.164577	−0.445065
52	7	0	−0.583166	0.905774	0.808075
53	6	0	−1.665826	0.352281	1.392323
54	8	0	−1.804139	0.311446	2.627782

Table A17. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
55	6	0	−6.039968	−1.712778	0.989736
56	1	0	−6.726269	−2.156526	0.264982
57	6	0	−5.167672	−0.624332	0.379255
58	1	0	−5.005585	−0.888117	−0.668113
59	1	0	−5.616152	0.369529	0.421924
60	8	0	−6.786551	−1.239323	2.125148
61	15	0	−8.244880	−0.569072	1.988122
62	8	0	−8.931599	−0.418141	3.279739
63	8	0	−8.942453	−1.496962	0.874634
64	8	0	−8.020254	0.791900	1.149508
65	6	0	−7.748021	1.993067	1.898164
66	1	0	−8.617846	2.243474	2.512953
67	1	0	−6.887455	1.839159	2.558681
68	6	0	−7.449273	3.123235	0.943914
69	1	0	−7.378928	4.045497	1.540958
70	8	0	−6.213136	2.876238	0.280681
71	6	0	−6.274111	3.604763	−0.943535
72	1	0	−6.133787	4.675404	−0.746830
73	7	0	−5.182685	3.201942	−1.787337
74	6	0	−5.040682	2.046233	−2.540354
75	1	0	−5.866689	1.365800	−2.692397
76	7	0	−3.845501	1.893901	−3.040852
77	6	0	−3.144536	2.996430	−2.598790
78	6	0	−1.766656	3.349801	−2.754867
79	8	0	−0.851009	2.755399	−3.323187
80	7	0	−1.494969	4.573218	−2.092077
81	1	0	−0.548996	4.912171	−2.217359
82	6	0	−2.381679	5.309083	−1.346663
83	7	0	−1.917700	6.463955	−0.798779
84	1	0	−0.942129	6.526519	−0.536527
85	1	0	−2.566112	6.903197	−0.162363
86	7	0	−3.637045	4.959270	−1.174810
87	6	0	−3.953480	3.818158	−1.815876
88	6	0	−8.507366	3.399246	−0.157204
89	1	0	−9.299571	2.640570	−0.147099
90	6	0	−7.684097	3.323736	−1.454144
91	1	0	−7.738549	2.313221	−1.869644
92	1	0	−8.022891	4.037996	−2.208145
93	8	0	−9.025049	4.688045	0.105399

Table A17. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
94	1	0	−6.339744	−6.657457	−1.743038
95	1	0	−9.888716	−1.582697	1.047556
96	1	0	−9.792409	4.832275	−0.459322
97	53	0	4.623433	−2.918878	−0.397892
98	53	0	7.243919	−2.106926	−1.195754
99	3	0	6.960777	0.313927	0.049885
100	12	0	4.174725	−0.409857	1.114388
101	53	0	6.349752	−0.148707	2.612541
102	53	0	4.592380	1.281558	−0.967265
103	53	0	3.204376	4.297085	−0.140545
104	53	0	1.938579	6.710870	0.237725

Table A18. Complex LiI_3 with nucleotide triplet CGC.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
1	8	0	−4.979731	−0.141693	−3.760330
2	6	0	−4.324374	0.862252	−4.499997
3	1	0	−3.689257	0.353053	−5.232010
4	1	0	−5.033465	1.493790	−5.057192
5	6	0	−3.455174	1.757607	−3.631597
6	1	0	−2.909803	2.471721	−4.261365
7	8	0	−4.317574	2.485524	−2.731146
8	6	0	−3.743940	2.460200	−1.440899
9	1	0	−3.020825	3.274730	−1.312824
10	7	0	−4.786064	2.662866	−0.435926
11	6	0	−6.105821	2.653482	−0.736870
12	1	0	−6.348823	2.529051	−1.784941
13	6	0	−7.042000	2.814466	0.236206
14	1	0	−8.098610	2.819293	−0.000251
15	6	0	−6.550721	2.987983	1.568690
16	7	0	−7.421382	3.160257	2.591306
17	1	0	−8.402418	2.976087	2.474341
18	1	0	−7.038128	3.174156	3.523138
19	7	0	−5.262747	3.018287	1.869547
20	6	0	−4.328986	2.869288	0.899490
21	8	0	−3.111811	2.892686	1.086914
22	6	0	−2.445202	0.997741	−2.747979
23	1	0	−2.293512	−0.037534	−3.065116
24	6	0	−3.052664	1.106298	−1.362398

Table A18. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
25	1	0	−3.808200	0.320930	−1.263639
26	1	0	−2.348396	1.025941	−0.538354
27	8	0	−1.178463	1.701857	−2.887806
28	15	0	0.068605	1.574529	−1.900029
29	8	0	1.283706	2.111199	−2.586254
30	8	0	0.125563	0.116917	−1.301132
31	8	0	−0.278187	2.363467	−0.545277
32	6	0	0.028916	3.756276	−0.390708
33	1	0	0.518224	4.146444	−1.288990
34	1	0	−0.915821	4.277278	−0.217494
35	6	0	0.949035	3.967633	0.793380
36	1	0	1.256859	5.023296	0.788751
37	8	0	0.262769	3.697169	2.029739
38	6	0	1.049203	2.874296	2.852869
39	1	0	0.906126	3.183594	3.891489
40	7	0	0.558833	1.471893	2.715263
41	6	0	−0.709302	1.143375	2.299703
42	1	0	−1.493776	1.878819	2.151973
43	7	0	−0.826866	−0.144347	2.071431
44	6	0	0.407160	−0.700508	2.338315
45	6	0	0.959588	−1.959830	1.983430
46	8	0	0.403737	−2.887219	1.351977
47	7	0	2.290563	−2.079386	2.355915
48	1	0	2.805319	−2.873016	1.942507
49	6	0	3.032524	−1.077200	2.945041
50	7	0	4.283438	−1.378023	3.325337
51	1	0	4.799016	−2.158738	2.898896
52	1	0	4.848298	−0.577729	3.563686
53	7	0	2.553926	0.141122	3.157731
54	6	0	1.278116	0.293771	2.780883
55	6	0	2.200610	3.088160	0.838289
56	1	0	1.959185	2.087142	0.466203
57	6	0	2.474497	3.024958	2.337342
58	1	0	3.140922	2.218700	2.635706
59	1	0	2.867844	3.986990	2.682048
60	8	0	3.242608	3.658661	0.051212
61	15	0	4.325071	2.661951	−0.641023
62	8	0	5.394284	3.433363	−1.321024
63	8	0	3.506370	1.591860	−1.451757

Table A18. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
64	8	0	4.855851	1.738853	0.571352
65	6	0	6.205511	1.896221	1.027071
66	1	0	6.584178	2.891851	0.775342
67	1	0	6.182155	1.789238	2.115195
68	6	0	7.129241	0.861850	0.426478
69	1	0	8.155792	1.141264	0.720069
70	8	0	6.813727	−0.438441	0.920404
71	6	0	7.118692	−1.419208	−0.063443
72	1	0	7.766183	−2.169492	0.394107
73	7	0	5.875273	−2.140937	−0.427620
74	6	0	5.253315	−2.042252	−1.633134
75	1	0	5.748122	−1.456520	−2.396678
76	6	0	4.066014	−2.651270	−1.879076
77	1	0	3.587773	−2.576580	−2.847004
78	6	0	3.450149	−3.330679	−0.782520
79	7	0	2.252332	−3.916614	−0.928937
80	1	0	1.636450	−3.667991	−1.697161
81	1	0	1.786247	−4.217445	−0.083552
82	7	0	4.035232	−3.409849	0.414044
83	6	0	5.271244	−2.884088	0.617692
84	8	0	5.871070	−2.985686	1.693123
85	6	0	7.103008	0.717323	−1.098088
86	1	0	6.053873	0.631188	−1.418198
87	6	0	7.769517	−0.653345	−1.217819
88	1	0	7.686411	−1.127716	−2.197122
89	1	0	8.838473	−0.543268	−1.006086
90	8	0	7.765738	1.731188	−1.789080
91	1	0	−5.587894	0.300368	−3.157225
92	1	0	−0.116443	−0.667553	−1.872345
93	1	0	2.679858	1.874204	−1.967938
94	1	0	7.139652	2.476177	−1.834432
95	53	0	−2.893033	−1.425801	1.611692
96	53	0	−5.146842	−2.980241	0.980863
97	3	0	−0.997847	−2.714348	0.102323
98	53	0	−0.881393	−2.809415	−2.499740

Table A19. Complex MgI_3LiII_2 with nucleotide triplet CGC.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
1	8	0	−3.463574	3.496236	−4.390126
2	6	0	−2.368250	4.259591	−4.847698
3	1	0	−1.944438	3.728899	−5.706403
4	1	0	−2.673928	5.257139	−5.193365
5	6	0	−1.295507	4.409430	−3.781595
6	1	0	−0.411455	4.911224	−4.194530
7	8	0	−1.838367	5.203428	−2.706644
8	6	0	−1.424742	4.628665	−1.489644
9	1	0	−0.406999	4.950359	−1.234820
10	7	0	−2.296388	5.072940	−0.405168
11	6	0	−3.367953	5.880460	−0.609249
12	1	0	−3.544335	6.181935	−1.634250
13	6	0	−4.141253	6.280131	0.434004
14	1	0	−4.994228	6.928696	0.278769
15	6	0	−3.762247	5.806760	1.730536
16	7	0	−4.493662	6.138228	2.812037
17	1	0	−5.271953	6.771529	2.754692
18	1	0	−4.167846	5.836918	3.716589
19	7	0	−2.703117	5.032991	1.936651
20	6	0	−1.922370	4.660787	0.902746
21	8	0	−0.897271	3.973317	1.011334
22	6	0	−0.862134	3.065786	−3.152424
23	1	0	−1.214688	2.212076	−3.737389
24	6	0	−1.468529	3.128420	−1.760121
25	1	0	−2.513657	2.811092	−1.823445
26	1	0	−0.956054	2.545557	−0.997221
27	8	0	0.586525	3.052629	−3.142172
28	15	0	1.491356	1.915851	−2.461070
29	8	0	2.834325	1.836483	−3.072149
30	8	0	0.709487	0.526001	−2.513637
31	8	0	1.489711	2.243472	−0.878053
32	6	0	2.012491	3.518134	−0.427056
33	1	0	2.412221	4.092031	−1.270167
34	1	0	1.176105	4.054563	0.028547
35	6	0	3.109447	3.339117	0.604989
36	1	0	3.514234	4.330720	0.830101
37	8	0	2.604069	2.811988	1.841819
38	6	0	2.870516	1.449726	1.946756
39	1	0	3.294055	1.242291	2.934665
40	7	0	1.569724	0.723463	1.895539

Table A19. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
41	6	0	0.339722	1.301392	1.947351
42	1	0	0.163496	2.371499	1.990914
43	7	0	−0.615347	0.388738	1.889347
44	6	0	0.011019	−0.837644	1.797783
45	6	0	−0.474074	−2.139788	1.631047
46	8	0	−1.682320	−2.501469	1.551475
47	7	0	0.525509	−3.079844	1.525953
48	1	0	0.206644	−4.023955	1.306451
49	6	0	1.888143	−2.799841	1.518623
50	7	0	2.727050	−3.810231	1.341498
51	1	0	2.372406	−4.724936	1.108817
52	1	0	3.727266	−3.596668	1.106870
53	7	0	2.345668	−1.558430	1.683907
54	6	0	1.394796	−0.640022	1.797680
55	6	0	4.239947	2.392743	0.198544
56	1	0	4.354371	2.351864	−0.888044
57	6	0	3.806300	1.050595	0.793013
58	1	0	3.262316	0.471249	0.046362
59	1	0	4.653187	0.455398	1.138650
60	8	0	5.439283	2.878950	0.810954
61	15	0	6.914276	2.831760	0.136951
62	8	0	7.677143	4.059336	0.386699
63	8	0	6.695696	2.447776	−1.401651
64	8	0	7.555483	1.449962	0.690795
65	6	0	7.708708	1.291924	2.111607
66	1	0	8.527644	1.924842	2.470859
67	1	0	6.783217	1.601537	2.608521
68	6	0	7.968345	−0.174184	2.423919
69	1	0	7.911291	−0.299225	3.512239
70	8	0	6.958264	−0.973222	1.813964
71	6	0	7.509919	−1.797524	0.794316
72	1	0	7.463870	−2.834990	1.128690
73	7	0	6.624955	−1.725387	−0.378783
74	6	0	6.829285	−0.883958	−1.423603
75	1	0	7.804783	−0.421525	−1.498188
76	6	0	5.862414	−0.639621	−2.348606
77	1	0	6.058443	−0.032848	−3.225436
78	6	0	4.602485	−1.302911	−2.150602
79	7	0	3.579710	−1.051810	−2.986384
80	1	0	3.532716	−0.158343	−3.463927

Table A19. *Cont.*

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Number	Number
81	1	0	2.691818	−1.464815	−2.741556
82	7	0	4.413880	−2.181479	−1.174811
83	6	0	5.395074	−2.435837	−0.279393
84	8	0	5.271923	−3.240146	0.653163
85	6	0	9.308420	−0.755236	1.954894
86	1	0	10.086765	0.017108	1.883264
87	6	0	8.950243	−1.330837	0.583393
88	1	0	9.031816	−0.522894	−0.145698
89	1	0	9.608886	−2.146650	0.275075
90	8	0	9.651852	−1.755479	2.891375
91	1	0	−3.941662	4.038219	−3.752670
92	1	0	−0.216784	0.479074	−2.211060
93	1	0	6.387424	1.536307	−1.538237
94	1	0	10.506649	−2.126735	2.645445
95	53	0	−2.835487	0.839894	1.951803
96	53	0	−5.702015	1.602434	2.036903
97	3	0	−6.477940	−0.805108	1.602046
98	12	0	−3.054269	−1.884113	0.297445
99	53	0	−5.454315	−2.985918	0.754656
100	53	0	−2.697292	−0.618259	−2.093301
101	53	0	−1.703846	−3.722005	−1.654609
102	53	0	−0.816063	−6.078672	−0.444238

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