Supporting Information for

Covalency in Resonance-Assisted Halogen Bonds demonstrated with Cooperativity in *N*-Halo-Guanine Quartets

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Appendix S1. Full computational details.

All calculations were carried out using the Amsterdam Density Functional (ADF) program developed by Baerends and co-workers[1,2,3] and QUILD.[4,5] The numerical integration was performed using the procedure developed by te Velde *et al.*[6,7] The MOs were expanded in a large uncontracted set of Slater type orbitals (STOs): TZ2P. The TZ2P basis set[8] is of triple-ζ quality for all atoms and has been augmented with two sets of polarization functions, that is, 2p and 3d on H; 3d and 4f on carbon, nitrogen, oxygen, fluorine, chlorine and potassium; 4d and 4f on bromine; 5d and 4f on iodine. Core shells of the atoms (1s for C, N, O and F; 1s2s2p for Cl and K; up to 3p for Br and up to 4p for I) were treated by the frozen-core approximation. An auxiliary set of s, p, d, f and g STOs was used to fit the molecular density and to represent the Coulomb and exchange potentials accurately in each self-consistent field (SCF) cycle. Equilibrium structures were obtained by optimizations using analytical gradient techniques.[9] Geometries and energies were calculated at the BLYP level of the generalized gradient approximation (GGA): exchange is described by Slater's Xα potential,[10] with nonlocal corrections due to Becke[11,12] added self-consistently, and correlation is treated using the gradient-corrected functional of Lee, Yang and Parr.[13,14,15] Dispersion corrections are applied using the DFT-D3(BJ) method, developed by Grimme,[16] which contains the damping function proposed by Becke and Johnson.[17] In this approach, the density functional is augmented with an empirical term correcting for long-range dispersion effects, described by a sum of damped interatomic potentials of the form $C_6/(R^6+c)$ added to the usual DFT energy. Scalar relativistic effects were accounted for using the zeroth-order regular approximation (ZORA).[18,19]

A very similar approach has been shown to accurately reproduce CCSD(T) structural and energy data of stacked as well as hydrogen-bonded AT and GC complexes.[20,21] Energy minima of the bases, base pairs and quartets have been verified to be equilibrium structures through vibrational analysis.[22,23,24] All global minima were found to have zero imaginary frequencies.

The Voronoi Deformation Density (VDD) charge Q_A is computed as the (numerical) integral of the deformation density $\Delta\rho(\mathbf{r}) = \rho(\mathbf{r}) - \sum_B \rho_B(\mathbf{r})$ associated with the formation of the molecule from its atoms in the volume of the Voronoi cell of atom A (eq 7).[25]

$$Q_A = -\int_{\text{Voronoi cell A}} \left(\rho(\mathbf{r}) - \sum_B \rho_B(\mathbf{r})\right) d\mathbf{r} \qquad (9)$$

The Voronoi cell of an atom A is defined as the compartment of space bounded by the bond midplanes on and perpendicular to all bond axes between nucleus A and its

neighboring nuclei (cf. the Wigner-Seitz cells in crystals). Here, $\rho(\mathbf{r})$ is the electron density of the molecule and $\sum_B \rho_B(\mathbf{r})$ is the superposition of atomic densities ρ_B of a fictitious promolecule without chemical interactions that is associated with the situation in which all atoms are neutral. Q_A monitors how much charge flows, due to chemical interactions, out of ($Q_A > 0$) or into ($Q_A < 0$) the Voronoi cell of atom A, that is, the region of space that is closer to nucleus A than to any other nucleus.

1. G. te Velde, F. M. Bickelhaupt, E. J. Baerends, C. Fonseca Guerra, S. J. A. van Gisbergen, J. G. Snijders and T. Ziegler, *J. Comput. Chem.*, 2001, **22**, 931-967.

2. C. Fonseca Guerra, J. G. Snijders, G. te Velde and E. J. Baerends, *Theor. Chem. Acc.*, 1998, **99**, 391-403.

3. ADF2012, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com/. E. J. Baerends, T. Ziegler, J. Autschbach, D. Bashford, A. Bérces, F. M. Bickelhaupt, C. Bo, P. M. Boerrigter, L. Cavallo, D. P. Chong, L. Deng, R. M. Dickson, D. E. Ellis, M. van Faassen, L. Fan, T. H. Fischer, C. Fonseca Guerra, A. Ghysels, A. Giammona, S. J. A. van Gisbergen, A. W. Götz, J. A. Groeneveld, O. V. Gritsenko, M. Grüning, S. Gusarov, F. E. Harris, P. van den Hoek, C. R. Jacob, H. Jacobsen, L. Jensen, J. W. Kaminski, G. van Kessel, F. Kootstra, A. Kovalenko, M. V. Krykunov, E. van Lenthe, D. A. McCormack, A. Michalak, M. Mitoraj, J. Neugebauer, V. P. Nicu, L. Noodleman, V. P. Osinga, S. Patchkovskii, P. H. T. Philipsen, D. Post, C. C. Pye, W. Ravenek, J. I. Rodríguez, P. Ros, P. R. T. Schipper, G. Schreckenbach, J. S. Seldenthuis, M. Seth, J. G. Snijders, M. Solà, M. Swart, D. Swerhone, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T. A. Wesolowski, E. M. van Wezenbeek, G. Wiesenekker, S. K. Wolff, T. K. Woo and A. L. Yakovlev.

4. M. Swart and F. M. Bickelhaupt, *Int. J. Quantum Chem.*, 2006, **106**, 2536-2544.

5. M. Swart and F. M. Bickelhaupt, *J. Comput. Chem.*, 2008, **29**, 724-734.

6. P. M. Boerrigter, G. te Velde and E. J. Baerends, *Int. J. Quantum Chem.*, 1988, **33**, 87-113.

7. G. te Velde and E. J. Baerends, *J. Comput. Phys.*, 1992, **99**, 84-98.

8. E. van Lenthe and E. J. Baerends, *J. Comput. Chem.*, 2003, **24**, 1142-1156.

9. L. Versluis and T. Ziegler, *J. Chem. Phys.*, 1988, **88**, 322-328.

10. J. C. Slater, *Quantum Theory of Molecules and Solids, Vol. 4*, McGraw-Hill, New York, 1974.

11. A. D. Becke, *J. Chem. Phys.*, 1986, **84**, 4524-4529.

12. A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098-3100.

13. C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785-789.

14. B. G. Johnson, P. M. W. Gill and J. A. Pople, *J. Chem. Phys.*, 1993, **98**, 5612-5626.

15. T. V. Russo, R. L. Martin and P. J. Hay, *J. Chem. Phys.*, 1994, **101**, 7729-7737.

16. S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456-1465.

17. E. R. Johnson and A. D. Becke, *J. Chem. Phys.*, 2005, **123**, 024101-024107.

18. E. van Lenthe, E. J. Baerends and J. G. Snijders, *J. Chem. Phys.*, 1994, **101**, 9783-9792.

19. E. van Lenthe, R. van Leeuwen, E. J. Baerends and J. G. Snijders, *Int. J. Quantum Chem.*, 1996, **57**, 281-293.

20. T. van der Wijst, C. Fonseca Guerra, M. Swart, F. M. Bickelhaupt and B. Lippert, *Angew. Chem. Int. Ed.*, 2009, **48**, 3285-3287.

21. C. Fonseca Guerra, T. van der Wijst, J. Poater, M. Swart and F. M. Bickelhaupt, *Theor. Chem. Acc.*, 2010, **125**, 245-252.

22. A. Bérces, R. M. Dickson, L. Fan, H. Jacobsen, D. Swerhone and T. Ziegler, *Comput. Phys. Commun.*, 1997, **100**, 247-262.

23. H. Jacobsen, A. Bérces, D. Swerhone and T. Ziegler, *Comput. Phys. Commun.*, 1997, **100**, 263-276.

24. S. K. Wolff, *Int. J. Quantum Chem.*, 2005, **104**, 645-659.

25. C. Fonseca Guerra, J.-W. Handgraaf, E. J. Baerends and F. M. Bickelhaupt, *J. Comput. Chem.*, 2004, **25**, 189-210.

Appendix S2. Description of back-donation occuring in I-G_4.

As alluded to in the main text, there is, in the case of the iodine-bonded I-G_4 quartet, bidirectional charge transfer which perturbs the trend in VDD charges as shown in Figure 5b of the paper. To explain this, we start with the Br-G_4 quartet for which this bidirectional charge transfer does not occur. Thus, when constructing Br-G_4 by stepwise adding Br-G bases, we find that the charge separation increases from ±270 to ±299 upon going from Br-G_2 to Br-G_3 due to enhanced donation from the increasingly destabilized σ_{HOMO} on the Br-G_{n-1} fragment to the σ_{LUMO} on the n^{th} Br-G fragment. Along Br-G_2, Br-G_3 and Br-G_4, the population of the σ_{LUMO} on the accepting Br-G fragment increases from 0.20 to 0.22 to 0.26 electrons, respectively.

For I-G_4, we found an even stronger increase in σ_{LUMO} populations of the n^{th} I-G fragment along I-G_2, I-G_3 and I-G_4: it increases from 0.23 to 0.31 to 0.38 electrons, respectively. However, the VDD charges of the fragment in Figure 5b do not show an increased charge separation upon going from I-G_2 (±254) to I-G_3 (±255). This is because the charges as revealed by the VDD analyses are partially quenched due to bidirectional donor–acceptor interactions: there is, besides the charge transfer from I-G_{n-1} to I-G, also charge transfer from I-G to I-G_{n-1}. This is because the σ_{HOMO} on I-G and the σ_{LUMO} on I-G_{n-1} are more delocalized over the molecular fragments and therefore overlap, which is not the case for the natural G_4 or the other X-G_4 quartets.

Table S1. Bond energy decomposition (in kcal mol^{-1}) for the hydrogen- and halogen-bonded base pairs, without symmetry constraints.[a]

	ΔE	ΔE_{prep}	ΔE_{int}	ΔV_{elstat}	ΔE_{Pauli}	ΔE_{oi}	ΔE_{disp}
AT	–16.6	+1.9	–18.5	–32.1	+40.2	–21.2	–5.4
F-AT	[b]						
Cl-AT	–5.9	+0.4	–6.2	–11.7	+18.0	–8.0	–4.6
Br-AT	–9.1	+1.1	–10.2	–20.3	+30.4	–14.4	–5.8
I-AT	–11.1	+1.9	–13.0	–26.1	+38.3	–18.0	–7.2
GC	–30.0	+4.0	–34.0	–47.6	+51.7	–31.8	–6.3
F-GC	[b]						
Cl-GC	–6.7	+0.4	–7.1	–10.8	+16.7	–7.4	–5.6
Br-GC	–11.4	+2.0	–13.4	–20.5	+29.6	–16.6	–5.9
I-GC	–17.3	+3.7	–20.9	–31.8	+43.4	–24.4	–8.1

[a] Computed at ZORA-BLYP-D3(BJ)/TZ2P. [b] Stacked conformation, no stable halogen-bonded base pair found.

Table S2. Bond energies (in kcal mol^{-1}) and hydrogen or halogen bond lengths (Å) of G_4 and Xan_4 in the gas phase. Bond energies for C_{4h}-symmetric quartets are relative to C_s-symmetric G or Xan.[a]

Quartet	Symmetry	ΔE_{bond}	Inner bond length	Outer bond length
G_4	S_4	–81.0	2.742	2.961
	C_{4h}	–82.3	2.771	2.920
F-G_4	C_4 / S_4	[b]		
	C_{4h}	–3.0	4.164[c]	[c]
Cl-G_4	C_2 ("C_4")	–22.6	[d]	4.388 / 4.389
	C_{4h}	–33.9	4.270	4.540
Br-G_4	C_4	–40.0	4.776	4.480
	C_{4h}	–58.4	4.356	4.587
I-G_4	S_4	–65.4	[e]	4.844
	C_{4h}	–74.9	4.602	4.895
Xan_4	C_4	–67.5	2.763	2.790
	C_{4h}	–66.6	2.715	2.858
F-Xan_4	C_4 / S_4	[b]		
	C_{4h}	–2.8	4.255	4.455
Cl-Xan_4	C_4 / S_4	[f]		
	C_{4h}	–25.1	4.417	4.743
Br-[illegible]	C_4	–39.5	4.711	4.501
	C_{4h}	–39.3	4.485	4.822
I-Xan_4	C_4	–48.6	4.801	5.091
	C_{4h}	–48.3	4.801	5.187

[a] Computed at ZORA-BLYP-D3(BJ)/TZ2P in C_{4h}, C_4 or S_4 symmetry and E_{base} is the energy of the guanine or xanthine, optimized in C_1 symmetry
[b] Does not form a halogen-bonded complex.
[c] Weakly bound via one fluorine bond from the outer fluorine of one guanine to the oxygen of the other guanine.
[d] Essentially no halogen-bonding interaction.
[e] Interaction between inner iodine atoms.
[f] Global minimum is C_{4h}-symmetric.

Table S3. Energy decomposition (in kcal mol^{-1}) for the formation of hydrogen- and halogen-bonded G_4 from G_{n-1} + G in C_{4h} symmetry.[a]

		G_2	G_3	G_3*	G_4	G_2^{diag}	ΔE_{sum}	Synergy
G_4	ΔE_{oi}^{σ}	–14.7	–16.4	–16.1	–36.1	–0.1	–59.1	–8.2
	ΔE_{oi}^{π}	–1.8	–2.4	–2.3	–6.2	–0.1	–7.3	–3.1
	ΔE_{oi}	–16.5	–18.8	–18.5	–42.3	–0.2	–66.4	–11.3
	ΔE_{Pauli}	30.9	31.4	30.2	61.3	0.1	123.8	–0.2
	ΔV_{elstat}	–26.4	–30.9	–30.1	–60.9	–1.6	–108.8	–9.4
	ΔE_{disp}	–4.5	–4.7	–4.7	–9.1	–0.2	–18.3	0.0
	$\Delta E_{int}(G_n)$	–16.5	–23.0	–23.0	–51.1	–1.9	–69.7	–20.9
F-G_4	ΔE_{oi}^{σ}	–0.7	–0.7	–0.7	–1.5	0.0	–2.7	–0.2
	ΔE_{oi}^{π}	–0.1	–0.2	–0.1	–0.4	0.0	–0.5	–0.1
	ΔE_{oi}	–0.8	–0.9	–0.8	–1.8	0.0	–3.2	–0.3
	ΔE_{Pauli}	1.3	1.3	1.3	2.5	0.0	5.0	0.0
	ΔV_{elstat}	–0.4	–0.3	–0.4	–1.0	0.2	–1.3	–0.4
	ΔE_{disp}	–0.7	–0.8	–0.8	–1.5	0.0	–3.0	0.0
	$\Delta E_{int}(G_n)$	–0.7	–0.7	–0.7	–1.8	0.1	–2.4	–0.7
Cl-G_4	ΔE_{oi}^{σ}	–9.2	–10.3	–9.8	–22.3	0.0	–36.9	–5.0
	ΔE_{oi}^{π}	–0.8	–1.0	–0.9	–2.3	0.0	–3.3	–0.9
	ΔE_{oi}	–10.0	–11.3	–10.8	–24.6	0.0	–40.2	–5.8
	ΔE_{Pauli}	22.6	22.9	22.4	45.2	0.0	90.4	0.4
	ΔV_{elstat}	–15.5	–16.5	–16.5	–33.7	0.0	–61.9	–3.8
	ΔE_{disp}	–4.6	–4.7	–4.7	–9.3	–0.1	–18.5	0.0
	$\Delta E_{int}(G_n)$	–7.5	–9.6	–9.6	–22.4	–0.1	–30.3	–9.2
Br-G_4	ΔE_{oi}^{σ}	–20.2	–23.0	–22.0	–51.5	–0.1	–81.1	–13.7
	ΔE_{oi}^{π}	–1.8	–2.0	–2.1	–5.2	0.0	–7.1	–2.0
	ΔE_{oi}	–22.0	–25.0	–24.2	–56.8	–0.1	–88.1	–15.6
	ΔE_{Pauli}	47.6	48.4	46.8	95.0	0.0	190.6	0.4
	ΔV_{elstat}	–32.6	–35.5	–34.7	–71.2	–0.3	–131.0	–8.3
	ΔE_{disp}	–6.3	–6.4	–6.4	–12.7	–0.2	–25.5	0.0
	$\Delta E_{int}(G_n)$	–13.2	–18.6	–18.6	–45.7	–0.6	–54.0	–23.5
I-G_4	ΔE_{oi}^{σ}	–23.2	–27.0	–27.5	–61.1	–0.1	–93.0	–18.3
	ΔE_{oi}^{π}	–2.4	–2.6	–2.7	–6.2	0.0	–9.5	–1.7
	ΔE_{oi}	–25.6	–29.5	–30.2	–67.3	–0. 1	–102.4	–20.0
	ΔE_{Pauli}	55.2	55.8	55.5	111.4	0.0	221.0	1.4
	ΔV_{elstat}	–39.0	–42.1	–41.2	–83.0	–0.9	–157.7	–6.3
	ΔE_{disp}	–8.3	–8.6	–8.6	–16.8	–0.3	–33.7	0.0
	$\Delta E_{int}(G_n)$	–17.6	–24.4	–24.4	–55.8	–1.3	–72.9	–24.9

[a] Computed at ZORA-BLYP-D3(BJ)/TZ2P.

Table S4. Energy decomposition (in kcal mol^{-1}) for the formation of hydrogen- and halogen-bonded Xan_4 from Xan_{n-1} + Xan in C_{4h} symmetry.[a]

		Xan_2	Xan_3	Xan_3*	Xan_4	Xan_2^{diag}	ΔE_{sum}	Synergy
Xan_4	ΔE_{oi}^{σ}	–16.6	–16.8	–16.9	–34.0	–0.1	–66.6	–0.8
	ΔE_{oi}^{π}	–2.2	–2.2	–2.3	–4.2	0.0	–8.8	0.2
	ΔE_{oi}	–18.8	–19.0	–19.2	–38.2	–0.1	–75.4	–0.6
	ΔE_{Pauli}	31.7	31.7	31.9	63.3	0.1	127.2	–0.4
	ΔV_{elstat}	–26.6	–26.7	–26.7	–53.5	0.0	–106.4	–0.5
	ΔE_{disp}	–4.2	–4.4	–4.4	–8.6	–0.2	–17.3	0.0
	$\Delta E_{int}(Xan_n)$	–17.9	–18.5	–18.5	–37.0	–0.2	–71.9	–1.5
F-Xan_4	ΔE_{oi}^{σ}	–0.8	–0.8	–0.8	–1.6	0.0	–3.1	–0.1
	ΔE_{oi}^{π}	–0.1	–0.1	–0.1	–0.2	0.0	–0.4	–0.1
	ΔE_{oi}	–0.9	–0.9	–0.9	–1.8	0.0	–3.5	–0.1
	ΔE_{Pauli}	1.9	1.9	1.9	3.9	0.0	7.8	–0.0
	ΔV_{elstat}	–0.6	–0.2	–0.2	–0.9	0.5	–1.3	–0.3
	ΔE_{disp}	–1.3	–1.4	–1.4	–2.7	0.0	–5.4	0.0
	$\Delta E_{int}(Xan_n)$	–0.8	–0.5	–0.5	–1.6	0.4	–2.4	–0.5
Cl-Xan_4	ΔE_{oi}^{σ}	–4.5	–4.5	–4.6	–9.2	0.0	–18.1	–0.1
	ΔE_{oi}^{π}	–0.5	–0.5	–0.5	–1.0	0.0	–2.1	0.0
	ΔE_{oi}	–5.0	–5.0	–5.1	–10.2	0.0	–20.2	–0.1
	ΔE_{Pauli}	12.3	12.3	12.3	24.6	0.0	49.4	–0.1
	ΔV_{elstat}	–9.7	–9.6	–9.5	–19.4	0.1	–38.4	–0.2
	ΔE_{disp}	–4.1	–4.2	–4.2	–8.3	–0.1	–16.5	0.0
	$\Delta E_{int}(Xan_n)$	–6.5	–6.5	–6.5	–13.2	0.1	–25.7	–0.4
Br-Xan_4	ΔE_{oi}^{σ}	–9.7	–9.7	–9.8	–19.7	0.0	–38.7	–0.4
	ΔE_{oi}^{π}	–1.1	–1.1	–1.2	–2.2	0.0	–4.6	0.0
	ΔE_{oi}	–10.8	–10.9	–11.0	–22.0	0.0	–43.3	–0.3
	ΔE_{Pauli}	24.9	24.8	24.9	49.7	0.0	99.6	–0.2
	ΔV_{elstat}	–18.7	–18.8	–18.7	–37.5	0.0	–74.7	–0.3
	ΔE_{disp}	–5.8	–5.9	–5.9	–11.7	–0.1	–23.3	0.0
	$\Delta E_{int}(Xan_n)$	–10.4	–10.7	–10.7	–21.5	–0.1	–41.7	–0.8
I-Xan_4	ΔE_{oi}^{σ}	–9.8	–9.9	–10.0	–20.0	0.0	–39.3	–0.4
	ΔE_{oi}^{π}	–1.3	–1.3	–1.4	–2.6	0.0	–5.3	0.1
	ΔE_{oi}	–11.1	–11.2	–11.3	–22.6	0.0	–44.6	–0.3
	ΔE_{Pauli}	26.5	26.4	26.5	52.8	0.0	106.0	–0.3
	ΔV_{elstat}	–20.5	–20.7	–20.6	–41.2	–0.1	–82.2	–0.2
	ΔE_{disp}	–7.3	–7.5	–7.5	–14.7	–0.2	–29.5	0.0

$\Delta E_{int}(Xan_n)$	–12.4	–12.9	–12.9	–25.7	–0.3	–50.3	–0.8

[a] Computed at ZORA-BLYP-D3(BJ)/TZ2P.

Table S5. Orbital energies (eV) of the relevant HOMOs in the σ-electron system of the fragments of C_{4h}-symmetric G_4 and X-G_4.[a]

	G		G_2		G_3	
G_4	σ_{HOMO}	–5.7	σ_{HOMO}	–4.6	σ_{HOMO}	–4.3
	σ_{HOMO-1}	–6.1	σ_{HOMO-1}	–5.2	σ_{HOMO-1}	–5.0
	–		σ_{HOMO-2}	–6.4	σ_{HOMO-3}	–6.2
	σ_{HOMO-3}	–9.7	σ_{HOMO-6}	–8.6	σ_{HOMO-9}	–8.4
Cl-G_4	σ_{HOMO}	–6.3	σ_{HOMO}	–5.5	σ_{HOMO}	–5.3
	σ_{HOMO-1}	–6.5	σ_{HOMO-1}	–5.9	σ_{HOMO-1}	–5.7
	–		–		σ_{HOMO-7}	–7.0
	σ_{HOMO-5}	–10.3	σ_{HOMO-}	–9.5	σ_{HOMO-}	–9.3
Br-G_4	σ_{HOMO}	–6.0	σ_{HOMO}	–5.0	σ_{HOMO}	–4.6
	–		–		σ_{HOMO-1}	–5.2
	σ_{HOMO-1}	–6.4	σ_{HOMO-1}	–5.5	σ_{HOMO-2}	–5.3
	–		–		σ_{HOMO-5}	–6.4
	σ_{HOMO-5}	–10.1	σ_{HOMO-}	–9.1	σ_{HOMO-}	–8.8
I-G_4	σ_{HOMO}	–5.7	σ_{HOMO}	–4.8	σ_{HOMO}	–4.6
	σ_{HOMO-1}	–6.3	σ_{HOMO-1}	–5.5	σ_{HOMO-2}	–5.3
	–		σ_{HOMO-2}	–5.7	σ_{HOMO-3}	–5.5
	–		σ_{HOMO-5}	–6.8	σ_{HOMO-6}	–6.5
	σ_{HOMO-5}	–10.0	σ_{HOMO-}	–9.1	σ_{HOMO-}	–8.9
	–		σ_{HOMO-}	–9.5	σ_{HOMO-}	–9.3

[a] Computed at ZORA-BLYP-D3(BJ)/TZ2P.

Table S6. Orbital energies (eV) of the relevant LUMOs in the σ-electron system of the fragments of C_{4h}-symmetric G_4 and X-G_4.[a]

	G		G_2		G_3	
G_4	σ_{LUMO+3}	0.8	σ_{LUMO+5}	0.4	σ_{LUMO+6}	0.6
	σ_{LUMO+2}	0.1	σ_{LUMO+2}	–0.3	σ_{LUMO+3}	–0.1
	σ_{LUMO}	–1.1	σ_{LUMO}	–1.4	σ_{LUMO}	–1.2
Cl-G_4	σ_{LUMO+1}	–2.8	σ_{LUMO+1}	–3.1	σ_{LUMO+1}	–2.9
	σ_{LUMO}	–3.2	σ_{LUMO}	–3.5	σ_{LUMO}	–3.4
Br-G_4	σ_{LUMO+1}	–3.5	σ_{LUMO+1}	–4.0	σ_{LUMO+1}	–4.0
	σ_{LUMO}	–4.2	σ_{LUMO}	–4.6	σ_{LUMO}	–4.6
I-G_4	σ_{LUMO+1}	–3.7	σ_{LUMO+1}	–4.1	σ_{LUMO+1}	–4.0
	σ_{LUMO}	–4.6	σ_{LUMO}	–4.8	σ_{LUMO}	–4.6

[a] Computed at ZORA-BLYP-D3(BJ)/TZ2P in C_{4h} symmetry.

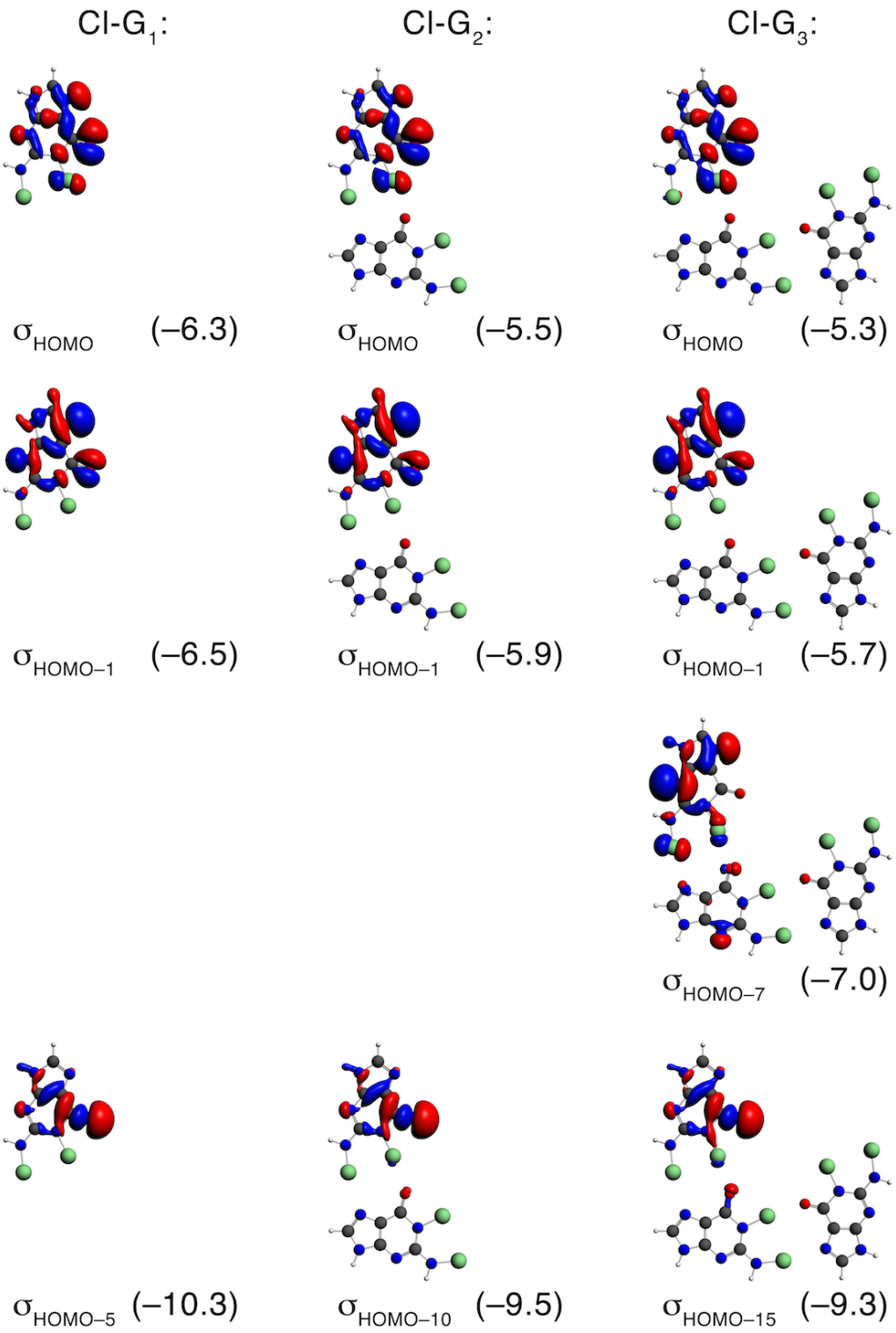

Figure S1. Electron-donating highest occupied molecular orbitals (HOMOs) and their energies (eV) in the σ-electron system of the fragments of the C_{4h}-symmetric Cl-G_4 quartet. Computed at ZORA-BLYP-D3(BJ)/TZ2P.

Table S7. Cartesian coordinates (in Å) and ADF total bonding energies (in kcal mol^{-1}) of all hydrogen-bonding species in this work, computed at ZORA-BLYP-D3(BJ)/TZ2P.

Adenine (C_s)			[-2306.56]	Adenine (C_1)			[-2306.56]
N	-1.97967626	-0.55625902	0.00000000	N	0.89117276	-0.10057037	-0.38595116
C	-1.21597972	0.55856065	0.00000000	C	1.65075754	-0.07168223	0.73068721
C	0.19019953	0.41986809	0.00000000	C	3.05540973	-0.00841230	0.59657814
C	0.68215044	-0.89727777	0.00000000	C	3.55116802	0.01522812	-0.71933819
N	-0.04666962	-2.02531957	0.00000000	N	2.82645035	-0.01752243	-1.84920202
C	-1.36462114	-1.75647706	0.00000000	C	1.50886794	-0.07467668	-1.58464060
N	1.23123600	1.34762752	0.00000000	N	4.09221201	0.04776309	1.52746079
C	2.32469877	0.60970956	0.00000000	C	5.18641861	0.10233900	0.79274417
N	2.06056616	-0.75381468	0.00000000	N	4.92724262	0.08523977	-0.57167488
N	-1.82549843	1.77330148	0.00000000	N	1.03784106	-0.12698382	1.94636147
H	-2.02605721	-2.61984136	0.00000000	H	0.85064788	-0.10146951	-2.44997100
H	3.33759380	0.98916781	0.00000000	H	6.19671984	0.15584986	1.17528636
H	2.73282738	-1.51082399	0.00000000	H	5.60085645	0.12270131	-1.32656096
H	-2.83469292	1.81830213	0.00000000	H	0.03296756	-0.01697359	1.97822885
H	-1.27279193	2.61805730	0.00000000	H	1.58312832	0.04931446	2.77897435
Thymine (C_s)			[-2306.56]	Thymine ( )			[-]
N	1.58285637	-0.87635294	0.00000000				
C	0.22911992	-1.16386584	0.00000000	Global minimum is C_s-symmetric.			
C	-0.72416763	-0.19966402	0.00000000				
C	-0.29548064	1.20620912	0.00000000				
N	1.11020523	1.39080309	0.00000000				
C	2.10512159	0.41933940	0.00000000				
C	-2.20171862	-0.48573175	0.00000000				
O	-1.04669449	2.17826984	0.00000000				
O	3.30612117	0.65726490	0.00000000				
H	2.27303293	-1.61768433	0.00000000				
H	1.43470641	2.35491717	0.00000000				
H	-0.01534058	-2.22186579	0.00000000				
H	-2.68124219	-0.03925582	0.87906452				
H	-2.68124219	-0.03925582	-0.87906452				
H	-2.39489599	-1.56339161	0.00000000				
Guanine (C_s)			[-2461.45]	Guanine (C_1)			[-2461.92]
O	-0.02824683	2.96305717	0.00000000	O	1.02287883	2.02736998	0.05276676
C	0.00968596	1.73954214	0.00000000	C	1.65172753	0.97772343	0.05168244
N	1.30495676	1.07514050	0.00000000	N	0.92596489	-0.28254342	0.08455004
C	1.52926930	-0.28203521	0.00000000	C	1.47397637	-1.54277453	0.08940044
N	0.55790571	-1.17605607	0.00000000	N	2.77186253	-1.76872622	0.06682332
C	-0.67792636	-0.61064042	0.00000000	C	3.50612968	-0.62339719	0.05093902
C	-1.03339348	0.74798531	0.00000000	C	3.06729474	0.70968319	0.03026358
N	-2.41657525	0.89578989	0.00000000	N	4.14813578	1.58351941	0.00112198
C	-2.88760398	-0.33122393	0.00000000	C	5.21001193	0.80792559	0.00341412
N	-1.87588161	-1.29093283	0.00000000	N	4.88129799	-0.54593934	0.03306132
N	2.82912563	-0.71153862	0.00000000	N	0.59812706	-2.61229822	0.17475466
H	2.08534351	1.72659248	0.00000000	H	-0.08061182	-0.16478436	0.16649051
H	-3.93218703	-0.61000891	0.00000000	H	6.23845707	1.14071159	-0.01671721
H	-1.97717517	-2.29835641	0.00000000	H	5.51299536	-1.33728043	0.04126259
H	2.99546492	-1.70725917	0.00000000	H	1.04847738	-3.50478548	-0.00013109
H	3.61166927	-0.07713588	0.00000000	H	-0.30267364	-2.51020906	-0.27973831
Cytosine (C_s)			[-1904.29]	Cytosine (C_1)			[-1904.30]
C	1.58574578	-0.74276426	0.00000000	C	-2.69326421	-1.09671399	0.05465054
N	1.60928557	0.69970399	0.00000000	N	-4.12266101	-0.90642199	0.03166392
C	0.48789839	1.46569411	0.00000000	C	-4.71435320	0.31580040	0.01368144
C	-0.73896634	0.87212065	0.00000000	C	-3.94536166	1.44125394	0.01743914
C	-0.75192838	-0.56972658	0.00000000	C	-2.51838557	1.24078425	0.04621433
N	0.33930377	-1.32342794	0.00000000	N	-1.93464817	0.05113649	0.06782225
O	2.65775801	-1.33821063	0.00000000	O	-2.26220802	-2.24441639	0.06666474
N	-1.95105029	-1.22254776	0.00000000	N	-1.69285663	2.33426372	0.02268979
H	2.53468010	1.11571533	0.00000000	H	-4.67110934	-1.76007006	0.02899360
H	0.62496907	2.54228564	0.00000000	H	-5.79924730	0.33920652	-0.00488091
H	-1.65000662	1.45994701	0.00000000	H	-4.39095534	2.42932554	-0.00671614
H	-2.82858125	-0.72629051	0.00000000	H	-2.05801685	3.25272903	0.23015173
H	-1.94437260	-2.23396985	0.00000000	H	-0.70747284	2.16339180	0.18373988
Xanthine (C_s)			[-2356.97]	Xanthine ( )			[-]
N	-4.74341031	2.64817058	0.00000000				
C	-2.17474559	2.41727251	0.00000000	Global minimum is C_s-symmetric.			
C	-3.43407624	3.11036196	0.00000000				

C	-3.55100099	4.49276392	0.00000000
N	-2.43455725	5.29950780	0.00000000
C	-1.14395844	4.76377043	0.00000000
N	-1.10607105	3.35715772	0.00000000
O	-0.13401256	5.45389879	0.00000000
O	-1.97772151	1.20357227	0.00000000
C	-5.55184207	3.75074379	0.00000000
H	-6.63015929	3.67963795	0.00000000
N	-4.85860491	4.89338606	0.00000000
H	-0.16874916	2.96305280	0.00000000
H	-2.51599291	6.31030348	0.00000000
H	-5.01952858	1.67363464	0.00000000

AT base pair (C_s) [-4490.53] AT base pair ( ) [-]

N	-1.24983318	0.59951765	0.00000000
C	-1.99719242	-0.53630819	0.00000000
C	-3.40449286	-0.38395960	0.00000000
C	-3.89463892	0.93271100	0.00000000
N	-3.17019675	2.06759966	0.00000000
C	-1.85580793	1.80749708	0.00000000
N	-4.44491954	-1.31019503	0.00000000
C	-5.53861205	-0.57249866	0.00000000
N	-5.27211259	0.79082482	0.00000000
N	-1.37909549	-1.73362665	0.00000000
H	-1.17806900	2.65837263	0.00000000
H	-6.55167682	-0.95117360	0.00000000
H	-5.94220528	1.54984662	0.00000000
H	-0.35264573	-1.79191508	0.00000000
H	-1.94491141	-2.57054898	0.00000000
N	3.54876531	1.74263756	0.00000000
C	4.25718553	0.55801734	0.00000000
C	3.64418174	-0.65303340	0.00000000
C	2.17819889	-0.67787972	0.00000000
N	1.54384225	0.56523327	0.00000000
C	2.14953278	1.80859303	0.00000000
C	4.38412833	-1.96385535	0.00000000
O	1.51109944	-1.72834440	0.00000000
O	1.54227292	2.87593856	0.00000000
H	4.02392697	2.63737075	0.00000000
H	0.48217391	0.57148000	0.00000000
H	5.33803651	0.66338487	0.00000000
H	4.11401343	-2.56093818	0.87923639
H	4.11401343	-2.56093818	-0.87923639
H	5.46759319	-1.80508815	0.00000000

GC base pair (C_s) [-4396.19] GC base pair ( ) [-]

C	2.71658083	-1.07021999	0.00000000
N	4.12480196	-0.89142290	0.00000000
C	4.70798790	0.34260220	0.00000000
C	3.93637517	1.46165787	0.00000000
C	2.50327201	1.27930722	0.00000000
N	1.94879912	0.05291093	0.00000000
O	2.27148288	-2.23026128	0.00000000
N	1.67742571	2.33560952	0.00000000
H	4.67853231	-1.74110309	0.00000000
H	5.79227140	0.36871606	0.00000000
H	4.38099967	2.45040319	0.00000000
H	2.06149998	3.26987453	0.00000000
H	0.63738171	2.20608272	0.00000000
O	-1.04898883	2.02078908	0.00000000
C	-1.65444589	0.92792705	0.00000000
N	-0.92199760	-0.28376847	0.00000000
C	-1.46200393	-1.55247180	0.00000000
N	-2.77340561	-1.78700638	0.00000000
C	-3.50413153	-0.65116226	0.00000000
C	-3.06393491	0.68593473	0.00000000
N	-4.14578916	1.56458596	0.00000000
C	-5.20706007	0.79024476	0.00000000
N	-4.88107752	-0.56739937	0.00000000
N	-0.58893460	-2.58827167	0.00000000
H	0.11421520	-0.18289031	0.00000000
H	-6.23558269	1.12409983	0.00000000
H	-5.51398739	-1.35738431	0.00000000
H	-0.98373766	-3.51724480	0.00000000
H	0.43009284	-2.45874008	0.00000000

Global minimum is C_s-symmetric.

Global minimum is C_s-symmetric.

G_4 quartet (C_{4h})			[-9928.10]
N	5.48799540	-0.19464775	0.00000000
O	1.24331387	-2.08408495	0.00000000
N	3.37744739	-1.20703300	0.00000000
C	4.75118501	-1.32715496	0.00000000
N	5.39211920	-2.50352007	0.00000000
C	4.55239519	-3.55441653	0.00000000
C	3.15226742	-3.54925201	0.00000000
C	2.46575678	-2.29298610	0.00000000
N	4.89948861	-4.89533722	0.00000000
C	3.71917076	-5.62805164	0.00000000
N	2.65467087	-4.84930954	0.00000000
H	5.12140198	0.76870480	0.00000000
H	6.48944380	-0.32738237	0.00000000
H	2.94474886	-0.25836054	0.00000000
H	5.84538221	-5.25567631	0.00000000
H	3.71551787	-6.70859636	0.00000000
N	0.19464775	5.48799540	0.00000000
O	2.08408495	1.24331387	0.00000000
N	1.20703300	3.37744739	0.00000000
C	1.32715496	4.75118501	0.00000000
N	2.50352007	5.39211920	0.00000000
C	3.55441653	4.55239519	0.00000000
C	3.54925201	3.15226742	0.00000000
C	2.29298610	2.46575678	0.00000000
N	4.89533722	4.89948861	0.00000000
C	5.62805164	3.71917076	0.00000000
N	4.84930954	2.65467087	0.00000000
H	-0.76870480	5.12140198	0.00000000
H	0.32738237	6.48944380	0.00000000
H	0.25836054	2.94474886	0.00000000
H	5.25567631	5.84538221	0.00000000
H	6.70859636	3.71551787	0.00000000
N	-5.48799540	0.19464775	0.00000000
O	-1.24331387	2.08408495	0.00000000
N	-3.37744739	1.20703300	0.00000000
C	-4.75118501	1.32715496	0.00000000
N	-5.39211920	2.50352007	0.00000000
C	-4.55239519	3.55441653	0.00000000
C	-3.15226742	3.54925201	0.00000000
C	-2.46575678	2.29298610	0.00000000
N	-4.89948861	4.89533722	0.00000000
C	-3.71917076	5.62805164	0.00000000
N	-2.65467087	4.84930954	0.00000000
H	-5.12140198	-0.76870480	0.00000000
H	-6.48944380	0.32738237	0.00000000
H	-2.94474886	0.25836054	0.00000000
H	-5.84538221	5.25567631	0.00000000
H	-3.71551787	6.70859636	0.00000000
N	-0.19464775	-5.48799540	0.00000000
O	-2.08408495	-1.24331387	0.00000000
N	-1.20703300	-3.37744739	0.00000000
C	-1.32715496	-4.75118501	0.00000000
N	-2.50352007	-5.39211920	0.00000000
C	-3.55441653	-4.55239519	0.00000000
C	-3.54925201	-3.15226742	0.00000000
C	-2.29298610	-2.46575678	0.00000000
N	-4.89533722	-4.89948861	0.00000000
C	-5.62805164	-3.71917076	0.00000000
N	-4.84930954	-2.65467087	0.00000000
H	0.76870480	-5.12140198	0.00000000
H	-0.32738237	-6.48944380	0.00000000
H	-0.25836054	-2.94474886	0.00000000
H	-5.25567631	-5.84538221	0.00000000
H	-6.70859636	-3.71551787	0.00000000

G_4 quartet (S_4)			[-9928.70]
N	2.22615799	-4.76757047	1.07301841
N	0.45025437	-3.44456317	0.32978282
C	0.90405523	-4.66163884	0.78827245
N	0.11029142	-5.72043990	0.98836749
C	-1.18020551	-5.46544333	0.69849078
C	-1.74463011	-4.27938119	0.21309526
C	-0.89243966	-3.14986905	-0.00290398
N	-2.24634722	-6.34290172	0.80628736
C	-3.38496624	-5.66389204	0.39036756
N	-3.11697314	-4.42453510	0.02650291
O	-1.20092282	-2.02316730	-0.42229106
H	2.93467121	-4.12428716	0.68818808
H	2.53072993	-5.69959960	1.32115701
H	1.10678560	-2.63156879	0.30417349
H	-2.18752637	-7.29942335	1.13231206
H	-4.35898409	-6.13168420	0.38021429
N	4.76757047	2.22615799	-1.07301841
N	3.44456317	0.45025437	-0.32978282
C	4.66163884	0.90405523	-0.78827245
N	5.72043990	0.11029142	-0.98836749
C	5.46544333	-1.18020551	-0.69849078
C	4.27938119	-1.74463011	-0.21309526
C	3.14986905	-0.89243966	0.00290398
N	6.34290172	-2.24634722	-0.80628736
C	5.66389204	-3.38496624	-0.39036756
N	4.42453510	-3.11697314	-0.02650291
O	2.02316730	-1.20092282	0.42229106
H	4.12428716	2.93467121	-0.68818808
H	5.69959960	2.53072993	-1.32115701
H	2.63156879	1.10678560	-0.30417349
H	7.29942335	-2.18752637	-1.13231206
H	6.13168420	-4.35898409	-0.38021429
N	-2.22615799	4.76757047	1.07301841
N	-0.45025437	3.44456317	0.32978282
C	-0.90405523	4.66163884	0.78827245
N	-0.11029142	5.72043990	0.98836749
C	1.18020551	5.46544333	0.69849078
C	1.74463011	4.27938119	0.21309526
C	0.89243966	3.14986905	-0.00290398
N	2.24634722	6.34290172	0.80628736
C	3.38496624	5.66389204	0.39036756
N	3.11697314	4.42453510	0.02650291
O	1.20092282	2.02316730	-0.42229106
H	-2.93467121	4.12428716	0.68818808
H	-2.53072993	5.69959960	1.32115701
H	-1.10678560	2.63156879	0.30417349
H	2.18752637	7.29942335	1.13231206
H	4.35898409	6.13168420	0.38021429
N	-4.76757047	-2.22615799	-1.07301841
N	-3.44456317	-0.45025437	-0.32978282
C	-4.66163884	-0.90405523	-0.78827245
N	-5.72043990	-0.11029142	-0.98836749
C	-5.46544333	1.18020551	-0.69849078
C	-4.27938119	1.74463011	-0.21309526
C	-3.14986905	0.89243966	0.00290398
N	-6.34290172	2.24634722	-0.80628736
C	-5.66389204	3.38496624	-0.39036756
N	-4.42453510	3.11697314	-0.02650291
O	-2.02316730	1.20092282	0.42229106
H	-4.12428716	-2.93467121	-0.68818808
H	-5.69959960	-2.53072993	-1.32115701
H	-2.63156879	-1.10678560	-0.30417349
H	-7.29942335	2.18752637	-1.13231206
H	-6.13168420	4.35898409	-0.38021429

Xan_4 quartet (C_{4h})			[-9494.91]
N	2.64050498	4.74974742	0.00000000
N	-2.64050498	-4.74974742	0.00000000
N	4.74974742	-2.64050498	0.00000000
C	2.44388117	2.18227440	0.00000000
C	-2.44388117	-2.18227440	0.00000000
C	2.18227440	-2.44388117	0.00000000
C	3.11103321	3.44438244	0.00000000
C	-3.11103321	-3.44438244	0.00000000
C	3.44438244	-3.11103321	0.00000000
C	4.49638763	3.55621472	0.00000000
C	-4.49638763	-3.55621472	0.00000000
C	3.55621472	-4.49638763	0.00000000
N	5.29314284	2.42618221	0.00000000
N	-5.29314284	-2.42618221	0.00000000
N	2.42618221	-5.29314284	0.00000000
C	4.73798669	1.15206206	0.00000000
C	-4.73798669	-1.15206206	0.00000000
C	1.15206206	-4.73798669	0.00000000
N	3.35590747	1.10532026	0.00000000
N	-3.35590747	-1.10532026	0.00000000
N	1.10532026	-3.35590747	0.00000000
O	5.44841049	0.13100989	0.00000000
O	-5.44841049	-0.13100989	0.00000000
O	0.13100989	-5.44841049	0.00000000
O	1.22529569	1.96376461	0.00000000
O	-1.22529569	-1.96376461	0.00000000
O	1.96376461	-1.22529569	0.00000000
C	5.54846886	-3.74407861	0.00000000
C	3.74407861	5.54846886	0.00000000
C	-3.74407861	-5.54846886	0.00000000
H	6.62694537	-3.67633631	0.00000000
H	3.67633631	6.62694537	0.00000000
H	-3.67633631	-6.62694537	0.00000000
N	4.89765929	4.85856569	0.00000000
N	-4.89765929	-4.85856569	0.00000000
N	4.85856569	-4.89765929	0.00000000
H	-2.91639552	-0.15805295	0.00000000
H	2.91639552	0.15805295	0.00000000
H	0.15805295	-2.91639552	0.00000000
H	-6.30491987	-2.49777336	0.00000000
H	6.30491987	2.49777336	0.00000000
H	2.49777336	-6.30491987	0.00000000
H	-1.64265697	-5.02934960	0.00000000
H	1.64265697	5.02934960	0.00000000
H	5.02934960	-1.64265697	0.00000000
N	-4.74974742	2.64050498	0.00000000
C	-2.18227440	2.44388117	0.00000000
C	-3.44438244	3.11103321	0.00000000
C	-3.55621472	4.49638763	0.00000000
N	-2.42618221	5.29314284	0.00000000
C	-1.15206206	4.73798669	0.00000000
N	-1.10532026	3.35590747	0.00000000
O	-0.13100989	5.44841049	0.00000000
O	-1.96376461	1.22529569	0.00000000
C	-5.54846886	3.74407861	0.00000000
H	-6.62694537	3.67633631	0.00000000
N	-4.85856569	4.89765929	0.00000000
H	-0.15805295	2.91639552	0.00000000
H	-2.49777336	6.30491987	0.00000000
H	-5.02934960	1.64265697	0.00000000

Xan_4 quartet (C_4)			[-9495.39]
N	-2.59845597	-4.71191638	-0.15697233
N	2.59845597	4.71191638	-0.15697233
N	-4.71191638	2.59845597	-0.15697233
N	4.71191638	-2.59845597	-0.15697233
C	-2.45208850	-2.20382083	0.40900704
C	2.45208850	2.20382083	0.40900704
C	-2.20382083	2.45208850	0.40900704
C	2.20382083	-2.45208850	0.40900704
C	-3.07841005	-3.41934640	-0.00658119
C	3.07841005	3.41934640	-0.00658119
C	-3.41934640	3.07841005	-0.00658119
C	3.41934640	-3.07841005	-0.00658119
C	-4.42298384	-3.49179489	-0.35239603
C	4.42298384	3.49179489	-0.35239603
C	-3.49179489	4.42298384	-0.35239603
C	3.49179489	-4.42298384	-0.35239603
N	-5.21676895	-2.36228759	-0.32183193
N	5.21676895	2.36228759	-0.32183193
N	-2.36228759	5.21676895	-0.32183193
N	2.36228759	-5.21676895	-0.32183193
C	-4.69297813	-1.12351308	0.01747832
C	4.69297813	1.12351308	0.01747832
C	-1.12351308	4.69297813	0.01747832
C	1.12351308	-4.69297813	0.01747832
N	-3.35476721	-1.11296680	0.37268664
N	3.35476721	1.11296680	0.37268664
N	-1.11296680	3.35476721	0.37268664
N	1.11296680	-3.35476721	0.37268664
O	-5.40043411	-0.10032154	0.00038914
O	5.40043411	0.10032154	0.00038914
O	-0.10032154	5.40043411	0.00038914
O	0.10032154	-5.40043411	0.00038914
O	-1.28058843	-2.03443028	0.77151430
O	1.28058843	2.03443028	0.77151430
O	-2.03443028	1.28058843	0.77151430
O	2.03443028	-1.28058843	0.77151430
C	5.46217716	-3.65325967	-0.57766885
C	-5.46217716	3.65325967	-0.57766885
C	-3.65325967	-5.46217716	-0.57766885
C	3.65325967	5.46217716	-0.57766885
H	6.51876868	-3.56392396	-0.78586909
H	-6.51876868	3.56392396	-0.78586909
H	-3.56392396	-6.51876868	-0.78586909
H	3.56392396	6.51876868	-0.78586909
N	-4.78988866	-4.75520960	-0.70363953
N	4.78988866	4.75520960	-0.70363953
N	-4.75520960	4.78988866	-0.70363953
N	4.75520960	-4.78988866	-0.70363953
H	2.93862099	0.18212417	0.58609652
H	-2.93862099	-0.18212417	0.58609652
H	0.18212417	-2.93862099	0.58609652
H	-0.18212417	2.93862099	0.58609652
H	6.19517838	2.40018236	-0.58654819
H	-6.19517838	-2.40018236	-0.58654819
H	2.40018236	-6.19517838	-0.58654819
H	-2.40018236	6.19517838	-0.58654819
H	1.60771261	4.99993102	-0.04310287
H	-1.60771261	-4.99993102	-0.04310287
H	4.99993102	-1.60771261	-0.04310287
H	-4.99993102	1.60771261	-0.04310287

G_4-[G_4^{con}]-G_4 (C_4)			[-29852.35]
N	-4.09034629	3.64371873	-3.36032859
O	0.38257005	2.40402865	-3.48865017
N	-1.81996473	3.08100217	-3.37475696
C	-2.80073207	4.04545761	-3.30056711
N	-2.54629464	5.35919416	-3.20470203
C	-1.22934822	5.63190136	-3.19863431
C	-0.15494101	4.73921784	-3.28775659
C	-0.42605598	3.33604005	-3.38775813
N	-0.63982065	6.88402951	-3.12143409
C	0.73869187	6.69711081	-3.18213704
N	1.05629342	5.42245103	-3.28132609
H	-4.40977870	2.66507153	-3.30837475
H	-4.76917658	4.35770442	-3.13591332
H	-2.09176619	2.07484159	-3.41509183
H	-1.13919455	7.76309484	-3.08921139
H	1.43223399	7.52496413	-3.14681551
N	-3.64371873	-4.09034629	-3.36032859
O	-2.40402865	0.38257005	-3.48865017
N	-3.08100217	-1.81996473	-3.37475696
C	-4.04545761	-2.80073207	-3.30056711
N	-5.35919416	-2.54629464	-3.20470203
C	-5.63190136	-1.22934822	-3.19863431
C	-4.73921784	-0.15494101	-3.28775659
C	-3.33604005	-0.42605598	-3.38775813
N	-6.88402951	-0.63982065	-3.12143409
C	-6.69711081	0.73869187	-3.18213704
N	-5.42245103	1.05629342	-3.28132609
H	-2.66507153	-4.40977870	-3.30837475
H	-4.35770442	-4.76917658	-3.13591332
H	-2.07484159	-2.09176619	-3.41509183
H	-7.76309484	-1.13919455	-3.08921139
H	-7.52496413	1.43223399	-3.14681551
N	4.09034629	-3.64371873	-3.36032859
O	-0.38257005	-2.40402865	-3.48865017
N	1.81996473	-3.08100217	-3.37475696
C	2.80073207	-4.04545761	-3.30056711
N	2.54629464	-5.35919416	-3.20470203
C	1.22934822	-5.63190136	-3.19863431
C	0.15494101	-4.73921784	-3.28775659
C	0.42605598	-3.33604005	-3.38775813
N	0.63982065	-6.88402951	-3.12143409
C	-0.73869187	-6.69711081	-3.18213704
N	-1.05629342	-5.42245103	-3.28132609
H	4.40977870	-2.66507153	-3.30837475
H	4.76917658	-4.35770442	-3.13591332
H	2.09176619	-2.07484159	-3.41509183
H	1.13919455	-7.76309484	-3.08921139
H	-1.43223399	-7.52496413	-3.14681551
N	3.64371873	4.09034629	-3.36032859
O	2.40402865	-0.38257005	-3.48865017
N	3.08100217	1.81996473	-3.37475696
C	4.04545761	2.80073207	-3.30056711
N	5.35919416	2.54629464	-3.20470203
C	5.63190136	1.22934822	-3.19863431
C	4.73921784	0.15494101	-3.28775659
C	3.33604005	0.42605598	-3.38775813
N	6.88402951	0.63982065	-3.12143409
C	6.69711081	-0.73869187	-3.18213704
N	5.42245103	-1.05629342	-3.28132609
H	2.66507153	4.40977870	-3.30837475
H	4.35770442	4.76917658	-3.13591332
H	2.07484159	2.09176619	-3.41509183
H	7.76309484	1.13919455	-3.08921139
H	7.52496413	-1.43223399	-3.14681551
N	-5.22206531	-1.64723282	3.41235070
O	-1.86808758	1.55660496	3.25789385

G_4-K^+-[G_4^{con}]-K^+-G_4 (C_4)			[-29856.65]
N	4.08855429	-3.74565467	-3.35073865
O	-0.33007379	-2.33702292	-3.07472222
N	1.84330119	-3.10178486	-3.23063004
C	2.78994656	-4.10534361	-3.34534359
N	2.47450859	-5.40240866	-3.43698720
C	1.15086106	-5.62516034	-3.42404755
C	0.11311760	-4.68607553	-3.31830047
C	0.44918785	-3.30995121	-3.20170672
N	0.51001439	-6.84918510	-3.50243533
C	-0.85720807	-6.60468053	-3.45397738
N	-1.12691123	-5.31979193	-3.33908568
H	4.43615829	-2.77103789	-3.34215482
H	4.74547408	-4.49195477	-3.53277406
H	2.15014673	-2.10983448	-3.18999034
H	0.96535755	-7.74225709	-3.64866099
H	-1.58319007	-7.40297863	-3.50899533
N	3.74565467	4.08855429	-3.35073865
O	2.33702292	-0.33007379	-3.07472222
N	3.10178486	1.84330119	-3.23063004
C	4.10534361	2.78994656	-3.34534359
N	5.40240866	2.47450859	-3.43698720
C	5.62516034	1.15086106	-3.42404755
C	4.68607553	0.11311760	-3.31830047
C	3.30995121	0.44918785	-3.20170672
N	6.84918510	0.51001439	-3.50243533
C	6.60468053	-0.85720807	-3.45397738
N	5.31979193	-1.12691123	-3.33908568
H	2.77103789	4.43615829	-3.34215482
H	4.49195477	4.74547408	-3.53277406
H	2.10983448	2.15014673	-3.18999034
H	7.74225709	0.96535755	-3.64866099
H	7.40297863	-1.58319007	-3.50899533
N	-4.08855429	3.74565467	-3.35073865
O	0.33007379	2.33702292	-3.07472222
N	-1.84330119	3.10178486	-3.23063004
C	-2.78994656	4.10534361	-3.34534359
N	-2.47450859	5.40240866	-3.43698720
C	-1.15086106	5.62516034	-3.42404755
C	-0.11311760	4.68607553	-3.31830047
C	-0.44918785	3.30995121	-3.20170672
N	-0.51001439	6.84918510	-3.50243533
C	0.85720807	6.60468053	-3.45397738
N	1.12691123	5.31979193	-3.33908568
H	-4.43615829	2.77103789	-3.34215482
H	-4.74547408	4.49195477	-3.53277406
H	-2.15014673	2.10983448	-3.18999034
H	-0.96535755	7.74225709	-3.64866099
H	1.58319007	7.40297863	-3.50899533
N	-3.74565467	-4.08855429	-3.35073865
O	-2.33702292	0.33007379	-3.07472222
N	-3.10178486	-1.84330119	-3.23063004
C	-4.10534361	-2.78994656	-3.34534359
N	-5.40240866	-2.47450859	-3.43698720
C	-5.62516034	-1.15086106	-3.42404755
C	-4.68607553	-0.11311760	-3.31830047
C	-3.30995121	-0.44918785	-3.20170672
N	-6.84918510	-0.51001439	-3.50243533
C	-6.60468053	0.85720807	-3.45397738
N	-5.31979193	1.12691123	-3.33908568
H	-2.77103789	-4.43615829	-3.34215482
H	-4.49195477	-4.74547408	-3.53277406
H	-2.10983448	-2.15014673	-3.18999034
H	-7.74225709	-0.96535755	-3.64866099
H	-7.40297863	1.58319007	-3.50899533
N	3.76654957	4.06967075	3.34886716
O	2.33555245	-0.34188074	3.07392908

N	-3.58226596	0.01306330	3.25809045	N	3.11130836	1.82764121	3.22940575
C	-4.91328077	-0.33585137	3.30736475	C	4.11960255	2.76920103	3.34423116
N	-5.91575445	0.55600621	3.29323028	N	5.41499266	2.44719211	3.43655568
C	-5.47713907	1.82864759	3.28101544	C	5.63098441	1.12239857	3.42468302
C	-4.15693549	2.29444186	3.28202373	C	4.68666644	0.08940000	3.31905677
C	-3.08730390	1.34197204	3.26514674	C	3.31237049	0.43243858	3.20132315
N	-6.25427863	2.97568623	3.27949542	N	6.85168106	0.47539073	3.50404591
C	-5.38765013	4.06272994	3.28488740	C	6.60026961	-0.89058677	3.45605574
N	-4.12495458	3.68621805	3.29008371	N	5.31408968	-1.15383045	3.34062022
H	-4.55488764	-2.42670487	3.31290910	H	2.79362068	4.42201158	3.34185405
H	-6.20436425	-1.86160712	3.31607363	H	4.51598513	4.72259754	3.53241813
H	-2.85580159	-0.73502257	3.24169830	H	2.12097159	2.13955304	3.18837695
H	-7.26556989	2.99833098	3.28503261	H	7.74701753	0.92628856	3.65018600
H	-5.74790164	5.08119447	3.28312707	H	7.39488336	-1.62055511	3.51177413
N	1.64723282	-5.22206531	3.41235070	N	-4.06967075	3.76654957	3.34886716
O	-1.55660496	-1.86808758	3.25789385	O	0.34188074	2.33555245	3.07392908
N	-0.01306330	-3.58226596	3.25809045	N	-1.82764121	3.11130836	3.22940575
C	0.33585137	-4.91328077	3.30736475	C	-2.76920103	4.11960255	3.34423116
N	-0.55600621	-5.91575445	3.29323028	N	-2.44719211	5.41499266	3.43655568
C	-1.82864759	-5.47713907	3.28101544	C	-1.12239857	5.63098441	3.42468302
C	-2.29444186	-4.15693549	3.28202373	C	-0.08940000	4.68666644	3.31905677
C	-1.34197204	-3.08730390	3.26514674	C	-0.43243858	3.31237049	3.20132315
N	-2.97568623	-6.25427863	3.27949542	N	-0.47539073	6.85168106	3.50404591
C	-4.06272994	-5.38765013	3.28488740	C	0.89058677	6.60026961	3.45605574
N	-3.68621805	-4.12495458	3.29008371	N	1.15383045	5.31408968	3.34062022
H	2.42670487	-4.55488764	3.31290910	H	-4.42201158	2.79362068	3.34185405
H	1.86160712	-6.20436425	3.31607363	H	-4.72259754	4.51598513	3.53241813
H	0.73502257	-2.85580159	3.24169830	H	-2.13955304	2.12097159	3.18837695
H	-2.99833098	-7.26556989	3.28503261	H	-0.92628856	7.74701753	3.65018600
H	-5.08119447	-5.74790164	3.28312707	H	1.62055511	7.39488336	3.51177413
N	5.22206531	1.64723282	3.41235070	N	-3.76654957	-4.06967075	3.34886716
O	1.86808758	-1.55660496	3.25789385	O	-2.33555245	0.34188074	3.07392908
N	3.58226596	-0.01306330	3.25809045	N	-3.11130836	-1.82764121	3.22940575
C	4.91328077	0.33585137	3.30736475	C	-4.11960255	-2.76920103	3.34423116
N	5.91575445	-0.55600621	3.29323028	N	-5.41499266	-2.44719211	3.43655568
C	5.47713907	-1.82864759	3.28101544	C	-5.63098441	-1.12239857	3.42468302
C	4.15693549	-2.29444186	3.28202373	C	-4.68666644	-0.08940000	3.31905677
C	3.08730390	-1.34197204	3.26514674	C	-3.31237049	-0.43243858	3.20132315
N	6.25427863	-2.97568623	3.27949542	N	-6.85168106	-0.47539073	3.50404591
C	5.38765013	-4.06272994	3.28488740	C	-6.60026961	0.89058677	3.45605574
N	4.12495458	-3.68621805	3.29008371	N	-5.31408968	1.15383045	3.34062022
H	4.55488764	2.42670487	3.31290910	H	-2.79362068	-4.42201158	3.34185405
H	6.20436425	1.86160712	3.31607363	H	-4.51598513	-4.72259754	3.53241813
H	2.85580159	0.73502257	3.24169830	H	-2.12097159	-2.13955304	3.18837695
H	7.26556989	-2.99833098	3.28503261	H	-7.74701753	-0.92628856	3.65018600
H	5.74790164	-5.08119447	3.28312707	H	-7.39488336	1.62055511	3.51177413
N	-1.64723282	5.22206531	3.41235070	N	4.06967075	-3.76654957	3.34886716
O	1.55660496	1.86808758	3.25789385	O	-0.34188074	-2.33555245	3.07392908
N	0.01306330	3.58226596	3.25809045	N	1.82764121	-3.11130836	3.22940575
C	-0.33585137	4.91328077	3.30736475	C	2.76920103	-4.11960255	3.34423116
N	0.55600621	5.91575445	3.29323028	N	2.44719211	-5.41499266	3.43655568
C	1.82864759	5.47713907	3.28101544	C	1.12239857	-5.63098441	3.42468302
C	2.29444186	4.15693549	3.28202373	C	0.08940000	-4.68666644	3.31905677
C	1.34197204	3.08730390	3.26514674	C	0.43243858	-3.31237049	3.20132315
N	2.97568623	6.25427863	3.27949542	N	0.47539073	-6.85168106	3.50404591
C	4.06272994	5.38765013	3.28488740	C	-0.89058677	-6.60026961	3.45605574
N	3.68621805	4.12495458	3.29008371	N	-1.15383045	-5.31408968	3.34062022
H	-2.42670487	4.55488764	3.31290910	H	4.42201158	-2.79362068	3.34185405
H	-1.86160712	6.20436425	3.31607363	H	4.72259754	-4.51598513	3.53241813
H	-0.73502257	2.85580159	3.24169830	H	2.13955304	-2.12097159	3.18837695
H	2.99833098	7.26556989	3.28503261	H	0.92628856	-7.74701753	3.65018600
H	5.08119447	5.74790164	3.28312707	H	-1.62055511	-7.39488336	3.51177413
N	-5.32984595	1.20410022	-0.00859977	N	5.57580216	0.13818128	-0.00018065
O	-0.82156464	2.28998579	-0.08861042	O	1.36352231	-1.80204448	-0.00030799
N	-3.07793440	1.81547792	-0.07251171	N	3.49054561	-0.90846867	-0.00060494
C	-4.40447336	2.18219925	-0.02471561	C	4.87208408	-1.00650145	-0.00058668
N	-4.82339798	3.45950370	0.00404721	N	5.52014405	-2.17792721	-0.00080680
C	-3.80351347	4.33616388	0.03695497	C	4.69647780	-3.23522270	-0.00024061
C	-2.42822862	4.07326245	0.02996767	C	3.29085131	-3.24322906	0.00026259
C	-1.98249187	2.71352557	-0.04295558	C	2.60715748	-2.00086953	-0.00014349
N	-3.89600808	5.71812750	0.09113483	N	5.05495564	-4.57140350	-0.00019401
C	-2.59736081	6.22073279	0.10016034	C	3.88318574	-5.31649354	0.00028606
N	-1.69938381	5.25718124	0.07055427	N	2.81084804	-4.55182529	0.00052868
H	-5.14431907	0.19084932	0.01803352	H	5.15184213	1.08453979	0.00028537
H	-6.28533344	1.51027337	0.09681511	H	6.58075434	0.03905356	0.00001240
H	-2.82624652	0.80314253	-0.09274775	H	3.03134429	0.02273321	-0.00075033

H	-4.75649332	6.24826797	0.05479873	H	6.00327662	-4.92625099	-0.00073533
H	-2.39338486	7.28131089	0.12960804	H	3.89163660	-6.39650456	0.00037088
N	-1.20410022	-5.32984595	-0.00859977	N	-0.13818128	5.57580216	-0.00018065
O	-2.28998579	-0.82156464	-0.08861042	O	1.80204448	1.36352231	-0.00030799
N	-1.81547792	-3.07793440	-0.07251171	N	0.90846867	3.49054561	-0.00060494
C	-2.18219925	-4.40447336	-0.02471561	C	1.00650145	4.87208408	-0.00058668
N	-3.45950370	-4.82339798	0.00404721	N	2.17792721	5.52014405	-0.00080680
C	-4.33616388	-3.80351347	0.03695497	C	3.23522270	4.69647780	-0.00024061
C	-4.07326245	-2.42822862	0.02996767	C	3.24322906	3.29085131	0.00026259
C	-2.71352557	-1.98249187	-0.04295558	C	2.00086953	2.60715748	-0.00014349
N	-5.71812750	-3.89600808	0.09113483	N	4.57140350	5.05495564	-0.00019401
C	-6.22073279	-2.59736081	0.10016034	C	5.31649354	3.88318574	0.00028606
N	-5.25718124	-1.69938381	0.07055427	N	4.55182529	2.81084804	0.00052868
H	-0.19084932	-5.14431907	0.01803352	H	-1.08453979	5.15184213	0.00028537
H	-1.51027337	-6.28533344	0.09681511	H	-0.03905356	6.58075434	0.00001240
H	-0.80314253	-2.82624652	-0.09274775	H	-0.02273321	3.03134429	-0.00075033
H	-6.24826797	-4.75649332	0.05479873	H	4.92625099	6.00327662	-0.00073533
H	-7.28131089	-2.39338486	0.12960804	H	6.39650456	3.89163660	0.00037088
N	5.32984595	-1.20410022	-0.00859977	N	-5.57580216	-0.13818128	-0.00018065
O	0.82156464	-2.28998579	-0.08861042	O	-1.36352231	1.80204448	-0.00030799
N	3.07793440	-1.81547792	-0.07251171	N	-3.49054561	0.90846867	-0.00060494
C	4.40447336	-2.18219925	-0.02471561	C	-4.87208408	1.00650145	-0.00058668
N	4.82339798	-3.45950370	0.00404721	N	-5.52014405	2.17792721	-0.00080680
C	3.80351347	-4.33616388	0.03695497	C	-4.69647780	3.23522270	-0.00024061
C	2.42822862	-4.07326245	0.02996767	C	-3.29085131	3.24322906	0.00026259
C	1.98249187	-2.71352557	-0.04295558	C	-2.60715748	2.00086953	-0.00014349
N	3.89600808	-5.71812750	0.09113483	N	-5.05495564	4.57140350	-0.00019401
C	2.59736081	-6.22073279	0.10016034	C	-3.88318574	5.31649354	0.00028606
N	1.69938381	-5.25718124	0.07055427	N	-2.81084804	4.55182529	0.00052868
H	5.14431907	-0.19084932	0.01803352	H	-5.15184213	-1.08453979	0.00028537
H	6.28533344	-1.51027337	0.09681511	H	-6.58075434	-0.03905356	0.00001240
H	2.82624652	-0.80314253	-0.09274775	H	-3.03134429	-0.02273321	-0.00075033
H	4.75649332	-6.24826797	0.05479873	H	-6.00327662	4.92625099	-0.00073533
H	2.39338486	-7.28131089	0.12960804	H	-3.89163660	6.39650456	0.00037088
N	1.20410022	5.32984595	-0.00859977	N	0.13818128	-5.57580216	-0.00018065
O	2.28998579	0.82156464	-0.08861042	O	-1.80204448	-1.36352231	-0.00030799
N	1.81547792	3.07793440	-0.07251171	N	-0.90846867	-3.49054561	-0.00060494
C	2.18219925	4.40447336	-0.02471561	C	-1.00650145	-4.87208408	-0.00058668
N	3.45950370	4.82339798	0.00404721	N	-2.17792721	-5.52014405	-0.00080680
C	4.33616388	3.80351347	0.03695497	C	-3.23522270	-4.69647780	-0.00024061
C	4.07326245	2.42822862	0.02996767	C	-3.24322906	-3.29085131	0.00026259
C	2.71352557	1.98249187	-0.04295558	C	-2.00086953	-2.60715748	-0.00014349
N	5.71812750	3.89600808	0.09113483	N	-4.57140350	-5.05495564	-0.00019401
C	6.22073279	2.59736081	0.10016034	C	-5.31649354	-3.88318574	0.00028606
N	5.25718124	1.69938381	0.07055427	N	-4.55182529	-2.81084804	0.00052868
H	0.19084932	5.14431907	0.01803352	H	1.08453979	-5.15184213	0.00028537
H	1.51027337	6.28533344	0.09681511	H	0.03905356	-6.58075434	0.00001240
H	0.80314253	2.82624652	-0.09274775	H	0.02273321	-3.03134429	-0.00075033
H	6.24826797	4.75649332	0.05479873	H	-4.92625099	-6.00327662	-0.00073533
H	7.28131089	2.39338486	0.12960804	H	-6.39650456	-3.89163660	0.00037088
				K	0.00000000	0.00000000	-1.77687348
				K	0.00000000	0.00000000	1.77676278

Table S8. Cartesian coordinates (in Å) and ADF total bonding energies (in kcal mol^{-1}) of all fluorine-bonding species in this work, computed at ZORA-BLYP-D3(BJ)/TZ2P.

F-Adenine (C_s)			[-2254.39]
N	-1.63715900	-1.25778321	0.00000000
C	-1.32670492	0.04762554	0.00000000
C	0.03179753	0.45206131	0.00000000
C	0.96935364	-0.59338800	0.00000000
N	0.70372883	-1.91069840	0.00000000
C	-0.61771482	-2.14687363	0.00000000
N	0.65449512	1.69639124	0.00000000
C	1.94413462	1.41172910	0.00000000
N	2.19805558	0.04800513	0.00000000
N	-2.28403643	1.00955011	0.00000000
H	-0.91713735	-3.19209791	0.00000000
H	2.74530772	2.13792781	0.00000000
H	3.10152149	-0.40923175	0.00000000
F	-3.63859595	0.65699374	0.00000000
H	-2.14349525	2.01065802	0.00000000

F-Adenine (C_1)			[-2258.29]
N	0.90451660	-0.16513133	-0.41122843
C	1.66173967	-0.15201512	0.69083079
C	3.06246680	-0.04190190	0.58465735
C	3.56618421	0.02305005	-0.73177588
N	2.84456799	0.00795379	-1.85871852
C	1.52581961	-0.07929237	-1.60769825
N	4.08963914	0.03750933	1.52182993
C	5.18439828	0.14351788	0.79344554
N	4.93693542	0.13835819	-0.57213166
N	1.09992559	-0.36398283	1.95590814
H	0.87278051	-0.08342342	-2.47650696
H	6.18887321	0.22881958	1.18520397
H	5.61499238	0.21850354	-1.32018785
F	-0.22378678	0.19841103	2.06569745
H	1.63438011	0.10121565	2.69480266

F-Thymine (C_s)			[-2116.07]
N	1.30990481	-1.25372715	0.00000000
C	-0.07147795	-1.19931623	0.00000000
C	-0.76241339	-0.03320304	0.00000000
C	-0.03007868	1.24320456	0.00000000
N	1.38860655	1.03993464	0.00000000
C	2.15331292	-0.13841300	0.00000000
C	-2.26642293	0.04681857	0.00000000
O	-0.51589903	2.36107343	0.00000000
O	3.36787905	-0.19315250	0.00000000
H	1.79581649	-2.14318257	0.00000000
F	2.15587487	2.19901719	0.00000000
H	-0.56721859	-2.16475189	0.00000000
H	-2.62355665	0.59461514	0.87965741
H	-2.62355665	0.59461514	-0.87965741
H	-2.71058036	-0.95356481	0.00000000

F-Thymine ( )	[-]
Global minimum is C_s-symmetric.	

F-Guanine (C_s)			[-2357.49]
O	0.16504420	-2.97028482	0.00000000
C	0.09339582	-1.76435558	0.00000000
N	1.36073408	-0.94657313	0.00000000
C	1.49298437	0.41367544	0.00000000
N	0.43542457	1.20641506	0.00000000
C	-0.74953237	0.55043720	0.00000000
C	-0.99917807	-0.83187716	0.00000000
N	-2.36616848	-1.08669782	0.00000000
C	-2.92965530	0.09985009	0.00000000
N	-1.99617125	1.13575813	0.00000000
N	2.69762095	1.06148245	0.00000000
F	2.52702827	-1.72682342	0.00000000
H	-3.99277227	0.29655306	0.00000000
H	-2.17691490	2.13216501	0.00000000
H	2.77966510	2.07007323	0.00000000
F	3.93127004	0.40912751	0.00000000

F-Guanine (C_1)			[-2367.01]
O	1.62449006	-1.86605615	0.08739214
C	2.25815888	-0.83752476	0.05763358
N	1.57838382	0.47446289	-0.06096008
C	2.13138931	1.72723558	-0.12017453
N	3.43300480	1.91373391	-0.04500170
C	4.14793170	0.76234899	0.02626524
C	3.67952132	-0.55963784	0.10094409
N	4.73341329	-1.44973943	0.19458191
C	5.81510656	-0.69440146	0.17951343
N	5.52182892	0.65701439	0.07858024
N	1.30072467	2.81765253	-0.41028928
F	0.19508871	0.39551791	-0.21541797
H	6.83349041	-1.05229662	0.23973564
H	6.17372684	1.43236686	0.05387432
H	1.88294030	3.65826809	-0.33587322
F	0.34918158	3.01599341	0.71123117

F-Cytosine (C_s)			[-1852.10]
C	-1.13381678	-1.35168845	0.00000000
N	-1.76384038	-0.05533014	0.00000000
C	-1.07317899	1.11483129	0.00000000
C	0.28853330	1.10148413	0.00000000
C	0.89717777	-0.21084415	0.00000000
N	0.24669377	-1.35511616	0.00000000
O	-1.84908392	-2.34434680	0.00000000
N	2.26240895	-0.21158066	0.00000000
H	-2.77842375	-0.06903643	0.00000000
H	-1.65224589	2.03249586	0.00000000
H	0.86527753	2.01914322	0.00000000
H	2.89127135	0.57857259	0.00000000
F	2.96374442	-1.41982085	0.00000000

F-Cytosine (C_1)			[-1855.66]
C	-3.48490047	0.78521323	0.06199877
N	-4.92013017	0.69197985	0.09535480
C	-5.59996965	-0.48378354	0.08188157
C	-4.91312368	-1.66093068	0.03597116
C	-3.47828926	-1.54174932	0.00669992
N	-2.80226789	-0.42222481	0.01840235
O	-2.96757021	1.89158883	0.07848373
N	-2.80109966	-2.77064791	-0.13709443
H	-5.40865711	1.58134848	0.12893252
H	-6.68325144	-0.42996385	0.11032764
H	-5.42329674	-2.61673709	0.00628971
H	-3.14765419	-3.49269032	0.49914437
F	-1.40992410	-2.67811998	0.17807922

F-Xanthine (C_s)			[-2252.38]
C	-4.26739583	5.26039925	0.00000000
H	-3.36979999	7.14504710	0.00000000
O	-0.92078329	6.46330638	0.00000000

F-Xanthine ( )	[-]
Global minimum is C_s-symmetric.	

N	-5.35964442	3.39800472	0.00000000
C	-1.87900631	5.71953193	0.00000000
F	-5.69343966	2.05172164	0.00000000
N	-3.21100849	6.14238292	0.00000000
C	-2.76711657	3.23993945	0.00000000
N	-5.59299778	5.59026748	0.00000000
H	-7.31836696	4.27203206	0.00000000
O	-2.47727502	2.06066567	0.00000000
C	-4.06028461	3.88529565	0.00000000
C	-6.24924020	4.42384416	0.00000000
N	-1.78209350	4.29816256	0.00000000
F	-0.47027842	3.84817932	0.00000000

F-AT base pair (C_s)			[-4371.83]
N	-1.95857159	-0.40518171	0.00000000
C	-3.17936458	-0.95917366	0.00000000
C	-4.33233163	-0.13437186	0.00000000
C	-4.07874943	1.24637702	0.00000000
N	-2.87646327	1.84403442	0.00000000
C	-1.87447840	0.94740662	0.00000000
N	-5.69866024	-0.40353497	0.00000000
C	-6.26255240	0.79081646	0.00000000
N	-5.33904556	1.82585300	0.00000000
N	-3.35637431	-2.30609034	0.00000000
H	-0.86606106	1.35101636	0.00000000
H	-7.32721810	0.98066215	0.00000000
H	-5.52879724	2.82034885	0.00000000
F	-2.25101637	-3.16581753	0.00000000
H	-4.23530593	-2.80504062	0.00000000
N	3.60091869	2.23148210	0.00000000
C	4.80094249	1.54419570	0.00000000
C	4.87213356	0.19087292	0.00000000
C	3.63136925	-0.60128125	0.00000000
N	2.46680210	0.23585962	0.00000000
C	2.34027748	1.63102849	0.00000000
C	6.16724528	-0.57766130	0.00000000
O	3.54483199	-1.81635463	0.00000000
O	1.28862606	2.24658621	0.00000000
H	3.58019552	3.24476993	0.00000000
F	1.24913373	-0.43164483	0.00000000
H	5.68704968	2.17077035	0.00000000
H	6.22877158	-1.22883127	0.87960931
H	6.22877158	-1.22883127	-0.87960931
H	7.02506043	0.10220615	0.00000000

F-AT base pair (C_1)			[-4386.45]
N	-2.43396041	0.99040260	1.92491077
C	-3.24088139	0.43805886	1.01087556
C	-2.69758231	-0.23291362	-0.10046809
C	-1.28571365	-0.28714894	-0.15389783
N	-0.44524469	0.25462416	0.74291995
C	-1.10206612	0.87337772	1.74110927
N	-3.26316953	-0.85436671	-1.20873253
C	-2.21929447	-1.27336165	-1.90552889
N	-1.00342053	-0.96664537	-1.32280327
N	-4.63003651	0.41186739	1.19706905
H	-0.48361037	1.33835565	2.50526794
H	-2.27417618	-1.80652907	-2.84489536
H	-0.06228620	-1.14911343	-1.68541045
F	-5.11630092	1.62361593	1.82064183
H	-5.12694365	0.37627539	0.30234271
N	2.96025643	0.82969040	1.56736715
C	2.97364443	1.59291487	0.41935083
C	2.65664027	1.08857576	-0.79921915
C	2.24589159	-0.31071658	-0.89591800
N	2.43035656	-1.02214176	0.31355152
C	2.60067925	-0.51855669	1.62250822
C	2.61344662	1.91155056	-2.05983898
O	1.79408688	-0.86303136	-1.90065415
O	2.50379263	-1.16863273	2.64109399
H	3.13402696	1.25107259	2.47293821
F	1.95852871	-2.33128896	0.29732292
H	3.24053366	2.63485048	0.56242599
H	3.24849156	1.46874976	-2.83552161
H	1.59405643	1.94689708	-2.46138103
H	2.95101145	2.93458310	-1.86739581

F-GC base pair (C_s)			[-4211.03]
C	-3.50138510	0.94280657	0.00000000
N	-4.93253638	0.78441019	0.00000000
C	-5.55269205	-0.42570114	0.00000000
C	-4.81346997	-1.56843732	0.00000000
C	-3.37795365	-1.38412151	0.00000000
N	-2.76031446	-0.21863047	0.00000000
O	-3.04684275	2.08148801	0.00000000
N	-2.64827682	-2.53380243	0.00000000
H	-5.46251574	1.64939896	0.00000000
H	-6.63770268	-0.42621384	0.00000000
H	-5.28061263	-2.54659089	0.00000000
H	-2.98560691	-3.48586525	0.00000000
F	-1.25681493	-2.48354701	0.00000000
O	1.80110497	-2.03077230	0.00000000
C	2.37012489	-0.96144905	0.00000000
N	1.57096521	0.30412119	0.00000000
C	2.02676999	1.59365111	0.00000000
N	3.32355908	1.86830896	0.00000000
C	4.11690417	0.77282827	0.00000000
C	3.75682684	-0.58483640	0.00000000
N	4.88742105	-1.39610956	0.00000000
C	5.90122915	-0.56060409	0.00000000
N	5.49541883	0.77365997	0.00000000
N	1.20527343	2.68260744	0.00000000
F	0.18797679	0.09315671	0.00000000
H	6.94734691	-0.83345633	0.00000000
H	6.08064385	1.59976777	0.00000000
H	1.55990020	3.63003559	0.00000000
F	-0.18446346	2.60924226	0.00000000

F-GC base pair (C_1)			[-4236.96]
C	-1.66970783	0.55964622	-2.47287677
N	-1.95835859	-0.53754689	-3.34221291
C	-2.06006360	-1.82705220	-2.91232977
C	-1.94643686	-2.10464862	-1.58552525
C	-1.75510897	-0.96933875	-0.72424171
N	-1.64779566	0.27894932	-1.12104331
O	-1.43635998	1.66045182	-2.97134305
N	-1.76484151	-1.28555606	0.64340729
H	-2.02345987	-0.30674047	-4.32837297
H	-2.22592110	-2.58698283	-3.66808438
H	-2.01602047	-3.11636229	-1.20479111
H	-1.06529842	-1.99652981	0.89781873
F	-1.41816718	-0.16541678	1.46337001
O	1.15069199	-2.20996551	1.30975400
C	1.41020858	-1.06493142	0.97231591
N	1.62006340	-0.01225062	1.95888893
C	1.62363193	1.34788730	1.75325129
N	1.57332840	1.86182918	0.54384407
C	1.55572617	0.94125794	-0.44899891
C	1.52454339	-0.45972345	-0.33091454
N	1.43737679	-1.05484904	-1.57787371
C	1.41749975	-0.04171699	-2.42702176
N	1.49859501	1.18980859	-1.80068767
N	1.86339107	2.19106440	2.84558232
F	1.59699781	-0.44656534	3.28431997
H	1.35237274	-0.12383738	-3.50265457
H	1.28417392	2.08869625	-2.22022991
H	1.77017964	3.15089491	2.49731276
F	0.72420273	2.10849459	3.79088621

F-G_4 quartet (C_{4h})			[-9432.99]
N	6.20651397	-1.23606886	0.00000000
O	2.34583237	-4.00581402	0.00000000
N	4.28883235	-2.69133994	0.00000000
C	5.64058562	-2.47565936	0.00000000
N	6.49748180	-3.48730940	0.00000000
C	5.91275326	-4.70649382	0.00000000
C	4.54806667	-5.03770546	0.00000000
C	3.55600432	-3.99879017	0.00000000
N	6.57081504	-5.91804774	0.00000000
C	5.59219195	-6.91102471	0.00000000
N	4.37381883	-6.41866051	0.00000000
F	5.48167141	-0.05029455	0.00000000
H	7.20845408	-1.09443070	0.00000000
F	3.44029814	-1.57860813	0.00000000
H	7.57605014	-6.03871381	0.00000000
H	5.85172953	-7.96052216	0.00000000
N	1.23606886	6.20651397	0.00000000
O	4.00581402	2.34583237	0.00000000
N	2.69133994	4.28883235	0.00000000
C	2.47565936	5.64058562	0.00000000
N	3.48730940	6.49748180	0.00000000
C	4.70649382	5.91275326	0.00000000
C	5.03770546	4.54806667	0.00000000
C	3.99879017	3.55600432	0.00000000
N	5.91804774	6.57081504	0.00000000
C	6.91102471	5.59219195	0.00000000
N	6.41866051	4.37381883	0.00000000
F	0.05029455	5.48167141	0.00000000
H	1.09443070	7.20845408	0.00000000
F	1.57860813	3.44029814	0.00000000
H	6.03871381	7.57605014	0.00000000
H	7.96052216	5.85172953	0.00000000
N	-6.20651397	1.23606886	0.00000000
O	-2.34583237	4.00581402	0.00000000
N	-4.28883235	2.69133994	0.00000000
C	-5.64058562	2.47565936	0.00000000
N	-6.49748180	3.48730940	0.00000000
C	-5.91275326	4.70649382	0.00000000
C	-4.54806667	5.03770546	0.00000000
C	-3.55600432	3.99879017	0.00000000
N	-6.57081504	5.91804774	0.00000000
C	-5.59219195	6.91102471	0.00000000
N	-4.37381883	6.41866051	0.00000000
F	-5.48167141	0.05029455	0.00000000
H	-7.20845408	1.09443070	0.00000000
F	-3.44029814	1.57860813	0.00000000
H	-7.57605014	6.03871381	0.00000000
H	-5.85172953	7.96052216	0.00000000
N	-1.23606886	-6.20651397	0.00000000
O	-4.00581402	-2.34583237	0.00000000
N	-2.69133994	-4.28883235	0.00000000
C	-2.47565936	-5.64058562	0.00000000
N	-3.48730940	-6.49748180	0.00000000
C	-4.70649382	-5.91275326	0.00000000
C	-5.03770546	-4.54806667	0.00000000
C	-3.99879017	-3.55600432	0.00000000
N	-5.91804774	-6.57081504	0.00000000
C	-6.91102471	-5.59219195	0.00000000
N	-6.41866051	-4.37381883	0.00000000
F	-0.05029455	-5.48167141	0.00000000
H	-1.09443070	-7.20845408	0.00000000
F	-1.57860813	-3.44029814	0.00000000
H	-6.03871381	-7.57605014	0.00000000
H	-7.96052216	-5.85172953	0.00000000

F-G_4 quartet (C_4/S_4) [-]

Does not form a halogen-bonded complex.

F-Xan$_4$ quartet (C_{4h}) [-9012.27]

N	3.39574457	5.36055853	0.00000000
N	-3.39574457	-5.36055853	0.00000000
N	5.36055853	-3.39574457	0.00000000
N	-5.36055853	3.39574457	0.00000000
C	3.23963657	2.76866341	0.00000000
C	-3.23963657	-2.76866341	0.00000000
C	2.76866341	-3.23963657	0.00000000
C	-2.76866341	3.23963657	0.00000000
C	3.88461092	4.06236809	0.00000000
C	-3.88461092	-4.06236809	0.00000000
C	4.06236809	-3.88461092	0.00000000
C	-4.06236809	3.88461092	0.00000000
C	5.25979306	4.26851415	0.00000000
C	-5.25979306	-4.26851415	0.00000000
C	4.26851415	-5.25979306	0.00000000
C	-4.26851415	5.25979306	0.00000000
N	6.14099554	3.20926184	0.00000000
N	-6.14099554	-3.20926184	0.00000000
N	3.20926184	-6.14099554	0.00000000
N	-3.20926184	6.14099554	0.00000000
C	5.71549708	1.87831637	0.00000000
C	-5.71549708	-1.87831637	0.00000000
C	1.87831637	-5.71549708	0.00000000
C	-1.87831637	5.71549708	0.00000000
N	4.30092577	1.77971933	0.00000000
N	-4.30092577	-1.77971933	0.00000000
N	1.77971933	-4.30092577	0.00000000
N	-1.77971933	4.30092577	0.00000000
O	6.46527253	0.91961615	0.00000000
O	-6.46527253	-0.91961615	0.00000000
O	0.91961615	-6.46527253	0.00000000
O	-0.91961615	6.46527253	0.00000000
O	2.06366632	2.47571973	0.00000000
O	-2.06366632	-2.47571973	0.00000000
O	2.47571973	-2.06366632	0.00000000
O	-2.47571973	2.06366632	0.00000000
C	-6.24867969	4.42211635	0.00000000
C	6.24867969	-4.42211635	0.00000000
C	4.42211635	6.24867969	0.00000000
C	-4.42211635	-6.24867969	0.00000000
H	-7.31752673	4.26918665	0.00000000
H	7.31752673	-4.26918665	0.00000000
H	4.26918665	7.31752673	0.00000000
H	-4.26918665	-7.31752673	0.00000000
N	5.59098245	5.59356904	0.00000000
N	-5.59098245	-5.59356904	0.00000000
N	5.59356904	-5.59098245	0.00000000
N	-5.59356904	5.59098245	0.00000000
F	-3.84783494	-0.47045495	0.00000000
F	3.84783494	0.47045495	0.00000000
F	-0.47045495	3.84783494	0.00000000
F	0.47045495	-3.84783494	0.00000000
H	-7.14335999	-3.36707021	0.00000000
H	7.14335999	3.36707021	0.00000000
H	-3.36707021	7.14335999	0.00000000
H	3.36707021	-7.14335999	0.00000000
F	-2.05289625	-5.69547747	0.00000000
F	2.05289625	5.69547747	0.00000000
F	-5.69547747	2.05289625	0.00000000
F	5.69547747	-2.05289625	0.00000000

F-Xan$_4$ quartet (C_4/S_4) [-]

Does not form a halogen-bonded complex.

Table S9. Cartesian coordinates (in Å) and ADF total bonding energies (in kcal mol^{-1}) of all chlorine-bonding species in this work, computed at ZORA-BLYP-D3(BJ)/TZ2P.

Cl-Adenine (C_s)			[-2236.46]
N	-1.50007649	-1.37567434	0.00000000
C	-1.29919697	-0.04970995	0.00000000
C	0.02561477	0.45164386	0.00000000
C	1.04281234	-0.51757892	0.00000000
N	0.87966407	-1.85138580	0.00000000
C	-0.42018994	-2.18823623	0.00000000
N	0.55138589	1.74008835	0.00000000
C	1.85897820	1.55683098	0.00000000
N	2.21823100	0.21659870	0.00000000
N	-2.34087181	0.82952935	0.00000000
H	-0.63981457	-3.25311237	0.00000000
H	2.60161242	2.34288086	0.00000000
H	3.15441693	-0.16915216	0.00000000
Cl	-3.99483068	0.34718936	0.00000000
H	-2.17537357	1.82830273	0.00000000

Cl-Adenine (C_1)			[-2237.34]
N	0.93588756	-0.17008156	-0.46109841
C	1.67315428	-0.15953018	0.65611573
C	3.07746395	-0.04229272	0.55948308
C	3.59541773	0.02994805	-0.74838388
N	2.88889177	0.00930665	-1.88765389
C	1.56935220	-0.08912991	-1.65104825
N	4.09247778	0.03393939	1.50925115
C	5.19689106	0.14721617	0.79585674
N	4.96417933	0.14956939	-0.57227944
N	1.09914894	-0.34281171	1.90282297
H	0.92477890	-0.10172879	-2.52632502
H	6.19652899	0.23231340	1.19978527
H	5.65008169	0.23159781	-1.31277018
Cl	-0.57621383	0.13463282	2.13759697
H	1.66676686	0.00338223	2.67455082

Cl-Thymine (C_s)			[-2096.91]
N	0.71316722	-1.66521586	0.00000000
C	-0.54503380	-1.09920153	0.00000000
C	-0.73746384	0.24074876	0.00000000
C	0.42686602	1.13656827	0.00000000
N	1.69369015	0.44376739	0.00000000
C	1.91353536	-0.95178805	0.00000000
C	-2.09734063	0.88804288	0.00000000
O	0.37258908	2.35555538	0.00000000
O	3.00406121	-1.49366677	0.00000000
H	0.83156632	-2.67148327	0.00000000
Cl	3.12042334	1.42897677	0.00000000
H	-1.36883926	-1.80585143	0.00000000
H	-2.21901678	1.53077555	0.87943945
H	-2.21901678	1.53077555	-0.87943945
H	-2.88906421	0.13201376	0.00000000

Cl-Thymine ( )	[-]
Global minimum is C_s-symmetric.	

Cl-Guanine (C_s)			[-2315.83]
O	0.11030740	-2.99104979	0.00000000
C	0.06247577	-1.78250321	0.00000000
N	1.36957479	-0.99112874	0.00000000
C	1.46453050	0.38165079	0.00000000
N	0.38831899	1.15746949	0.00000000
C	-0.79409708	0.51153261	0.00000000
C	-1.03501664	-0.86728647	0.00000000
N	-2.40234995	-1.13179365	0.00000000
C	-2.97165065	0.05151638	0.00000000
N	-2.04300540	1.09367820	0.00000000
N	2.63034192	1.12096119	0.00000000
Cl	2.76518176	-2.04645678	0.00000000
H	-4.03574763	0.24299535	0.00000000
H	-2.22865955	2.08901059	0.00000000
H	2.46566821	2.12106768	0.00000000
Cl	4.29984048	0.70751147	0.00000000

Cl-Guanine (C_1)			[-2324.46]
O	1.72315762	-1.88722247	0.35639099
C	2.30970875	-0.84159774	0.18955569
N	1.55474897	0.41447527	-0.10537337
C	2.11410895	1.66326965	-0.29751653
N	3.41554649	1.87754957	-0.25519207
C	4.16159153	0.76605926	-0.05497167
C	3.72057159	-0.53992734	0.19060875
N	4.79355125	-1.39347155	0.38912543
C	5.85920028	-0.62665135	0.26796946
N	5.53790283	0.69690022	-0.00273822
N	1.28579261	2.73327215	-0.65737854
Cl	-0.15773856	0.18262219	-0.31990930
H	6.88519136	-0.95403582	0.36363682
H	6.17361744	1.47569302	-0.12765932
H	1.90860065	3.52629897	-0.82842221
Cl	0.23599802	3.34218975	0.71133794

Cl-Cytosine (C_s)			[-1834.14]
C	-0.90346448	-1.51120527	0.00000000
N	-1.75498405	-0.34881659	0.00000000
C	-1.28256451	0.92541103	0.00000000
C	0.06010373	1.15375492	0.00000000
C	0.89880065	-0.02356785	0.00000000
N	0.45258978	-1.26188497	0.00000000
O	-1.42776519	-2.61726650	0.00000000
N	2.25162566	0.20117513	0.00000000
H	-2.75092967	-0.54265135	0.00000000
H	-2.01571371	1.72540402	0.00000000
H	0.46195416	2.16041687	0.00000000
H	2.64491729	1.13205283	0.00000000
Cl	3.41761941	-1.06702930	0.00000000

Cl-Cytosine (C_1)			[-1834.83]
C	-3.50563186	0.79452734	0.05512671
N	-4.94246169	0.73000037	0.11111863
C	-5.64198182	-0.43464579	0.10229511
C	-4.97932244	-1.62387630	0.03792164
C	-3.53986000	-1.54039543	-0.01237360
N	-2.85262061	-0.42293952	0.00418003
O	-2.96734242	1.89254570	0.06367375
N	-2.87501446	-2.75525070	-0.15578148
H	-5.41366013	1.62756704	0.16093463
H	-6.72362980	-0.36276859	0.14930651
H	-5.51227709	-2.56723876	0.01322152
H	-3.32847023	-3.55933764	0.26933803
Cl	-1.15579836	-2.82462943	0.16166633

Cl-Xanthine (C_s)			[-2215.42]
C	-4.48728804	5.40577625	0.00000000
Cl	-6.16095933	1.91101908	0.00000000
O	-1.11137300	6.48464067	0.00000000

Cl-Xanthine ( )	[-]
Global minimum is C_s-symmetric.	

N	-5.66237544	3.56223562	0.00000000
H	-7.56663612	4.55257113	0.00000000
Cl	-0.40135920	3.67474066	0.00000000
C	-2.08232479	5.75335782	0.00000000
C	-3.07904763	3.33943222	0.00000000
N	-3.39255243	6.23467240	0.00000000
N	-5.79885273	5.79223518	0.00000000
O	-2.86804217	2.13996835	0.00000000
C	-4.34248706	4.02795867	0.00000000
N	-2.00572754	4.32331135	0.00000000
C	-6.49139769	4.65242514	0.00000000
H	-3.50115094	7.24354212	0.00000000

Cl-AT base pair (C_s)			[-4339.69]	Cl-AT base pair ( )			[-4340.15]
N	-1.96926926	0.32458987	0.00000000	N	-1.96256126	0.24585809	0.13917350
C	-2.89606994	-0.64947444	0.00000000	C	-2.93317550	-0.67960991	0.11324591
C	-4.26504300	-0.28046909	0.00000000	C	-4.27713362	-0.25066883	0.01794643
C	-4.53147827	1.09759226	0.00000000	C	-4.47893716	1.14126898	-0.00985569
N	-3.62521705	2.09114259	0.00000000	N	-3.52840967	2.08774234	0.03202138
C	-2.37273330	1.61798130	0.00000000	C	-2.29956740	1.55684687	0.10045992
N	-5.43927861	-1.02559439	0.00000000	N	-5.48342902	-0.93864195	-0.06712657
C	-6.39898085	-0.11841661	0.00000000	C	-6.39497744	0.01300039	-0.14270969
N	-5.91410718	1.18157574	0.00000000	N	-5.85189906	1.28969975	-0.11112399
N	-2.57055469	-1.96927137	0.00000000	N	-2.67200587	-2.02462819	0.25574844
H	-1.57000911	2.35040852	0.00000000	H	-1.46380236	2.25074367	0.12402809
H	-7.45971417	-0.32833638	0.00000000	H	-7.46156939	-0.14683189	-0.22286401
H	-6.45246722	2.03927514	0.00000000	H	-6.34804686	2.17120088	-0.16094544
Cl	-0.95828257	-2.57096908	0.00000000	Cl	-1.10141406	-2.66229809	-0.17365728
H	-3.30360540	-2.66802622	0.00000000	H	-3.41600802	-2.63724465	-0.07084168
N	4.29102002	2.01670490	0.00000000	N	4.21902240	2.09254491	-0.04407535
C	5.12820442	0.92046699	0.00000000	C	5.11984301	1.04755377	-0.05143535
C	4.65433861	-0.34789642	0.00000000	C	4.72247780	-0.24631978	-0.02374630
C	3.20112836	-0.57075347	0.00000000	C	3.28541099	-0.55574635	0.01163438
N	2.42017879	0.63101959	0.00000000	N	2.43469375	0.59912315	0.02967593
C	2.89335260	1.95291892	0.00000000	C	2.82874708	1.94678308	-0.00156892
C	5.53721899	-1.56753433	0.00000000	C	5.67556443	-1.41189474	-0.02763153
O	2.67171650	-1.67546700	0.00000000	O	2.82180665	-1.68835625	0.02641930
O	2.19541591	2.95519938	0.00000000	O	2.07256093	2.90617918	0.00628794
H	4.66341237	2.95873321	0.00000000	H	4.53476217	3.05471620	-0.06788472
Cl	0.67042218	0.43333998	0.00000000	Cl	0.70176913	0.30852393	0.08579433
H	6.18973948	1.14775450	0.00000000	H	6.16558110	1.33740637	-0.08109188
H	5.33537670	-2.19047357	0.87916092	H	5.53176412	-2.03043839	0.86599900
H	5.33537670	-2.19047357	-0.87916092	H	5.48935833	-2.06053682	-0.89142257
H	6.59506863	-1.28491288	0.00000000	H	6.71461805	-1.06790636	-0.05814954

Cl-GC base pair (C_s)			[-4159.06]	Cl-GC base pair ( )			[-4165.98]
C	-3.52911402	0.80807823	0.00000000	C	-3.56943757	0.71121470	-0.41861523
N	-4.96017378	0.73058195	0.00000000	N	-4.99673982	0.64630830	-0.29760117
C	-5.64556672	-0.44473033	0.00000000	C	-5.67333719	-0.50317659	-0.03236442
C	-4.96920439	-1.62440434	0.00000000	C	-4.99200653	-1.67067469	0.12622211
C	-3.52543062	-1.53918093	0.00000000	C	-3.55488974	-1.59804226	-0.00005619
N	-2.85551687	-0.39510431	0.00000000	N	-2.89274058	-0.48090738	-0.24252214
O	-3.00570863	1.91758247	0.00000000	O	-3.04578363	1.79117529	-0.65777155
N	-2.85819472	-2.72818449	0.00000000	N	-2.88437476	-2.79680770	0.08958908
H	-5.44083974	1.62379096	0.00000000	H	-5.48059518	1.52976152	-0.41909305
H	-6.72880030	-0.38482873	0.00000000	H	-6.75347559	-0.43411963	0.04264477
H	-5.49211124	-2.57382553	0.00000000	H	-5.50860674	-2.60256611	0.32443382
H	-3.36034134	-3.60557738	0.00000000	H	-3.34039257	-3.55277311	0.58840044
Cl	-1.14290824	-2.87094230	0.00000000	Cl	-1.15709181	-2.84720238	0.26608697
O	1.72331707	-1.87879931	0.00000000	O	1.68598723	-1.82865518	0.31454148
C	2.34856568	-0.83252022	0.00000000	C	2.28428209	-0.78446738	0.12714465
N	1.61392170	0.47457149	0.00000000	N	1.55814924	0.48689783	-0.07192482
C	2.21551072	1.71140649	0.00000000	C	2.15144890	1.71691111	-0.25245271
N	3.53866962	1.86415632	0.00000000	N	3.46178115	1.89571666	-0.30238329
C	4.24098073	0.71642967	0.00000000	C	4.17702587	0.75208770	-0.20512725
C	3.75955726	-0.59811782	0.00000000	C	3.70291531	-0.54448211	0.02674408
N	4.81238904	-1.51160107	0.00000000	N	4.75443244	-1.44611624	0.10842093
C	5.89761282	-0.77162867	0.00000000	C	5.83724518	-0.71620058	-0.06984161
N	5.61519718	0.59556899	0.00000000	N	5.55013113	0.62910177	-0.26545066
N	1.55676283	2.92189659	0.00000000	N	1.34125212	2.83078477	-0.50691194
Cl	-0.13685244	0.25261168	0.00000000	Cl	-0.18493786	0.31636781	-0.18688786
H	6.91489124	-1.13798022	0.00000000	H	6.85355041	-1.08518024	-0.06978002
H	6.27309978	1.36483079	0.00000000	H	6.20435115	1.38782218	-0.41361858
H	2.18495311	3.71655590	0.00000000	H	1.97946143	3.61224411	-0.67084862
Cl	-0.11027994	3.34560348	0.00000000	Cl	0.37498850	3.39342718	0.93142437

Cl-G_4 quartet (C_{4h})			[-9297.18]
N	-6.52391161	1.03571809	0.00000000
O	-2.07805425	2.72251516	0.00000000
N	-4.25018595	1.90948968	0.00000000
C	-5.61879301	2.06687119	0.00000000
N	-6.18721151	3.27732933	0.00000000
C	-5.32450115	4.30865388	0.00000000
C	-3.92314927	4.27835947	0.00000000
C	-3.26363481	3.01096025	0.00000000
N	-5.65200757	5.65219476	0.00000000
C	-4.45684787	6.36474733	0.00000000
N	-3.40409702	5.57562071	0.00000000
Cl	-6.34750173	-0.70559973	0.00000000
H	-7.48651409	1.35151413	0.00000000
Cl	-3.49559215	0.32997740	0.00000000
H	-6.59227250	6.02706924	0.00000000
H	-4.43630486	7.44516681	0.00000000
N	-1.03571809	-6.52391161	0.00000000
O	-2.72251516	-2.07805425	0.00000000
N	-1.90948968	-4.25018595	0.00000000
C	-2.06687119	-5.61879301	0.00000000
N	-3.27732933	-6.18721151	0.00000000
C	-4.30865388	-5.32450115	0.00000000
C	-4.27835947	-3.92314927	0.00000000
C	-3.01096025	-3.26363481	0.00000000
N	-5.65219476	-5.65200757	0.00000000
C	-6.36474733	-4.45684787	0.00000000
N	-5.57562071	-3.40409702	0.00000000
Cl	0.70559973	-6.34750173	0.00000000
H	-1.35151413	-7.48651409	0.00000000
Cl	-0.32997740	-3.49559215	0.00000000
H	-6.02706924	-6.59227250	0.00000000
H	-7.44516681	-4.43630486	0.00000000
N	6.52391161	-1.03571809	0.00000000
O	2.07805425	-2.72251516	0.00000000
N	4.25018595	-1.90948968	0.00000000
C	5.61879301	-2.06687119	0.00000000
N	6.18721151	-3.27732933	0.00000000
C	5.32450115	-4.30865388	0.00000000
C	3.92314927	-4.27835947	0.00000000
C	3.26363481	-3.01096025	0.00000000
N	5.65200757	-5.65219476	0.00000000
C	4.45684787	-6.36474733	0.00000000
N	3.40409702	-5.57562071	0.00000000
Cl	6.34750173	0.70559973	0.00000000
H	7.48651409	-1.35151413	0.00000000
Cl	3.49559215	-0.32997740	0.00000000
H	6.59227250	-6.02706924	0.00000000
H	4.43630486	-7.44516681	0.00000000
N	1.03571809	6.52391161	0.00000000
O	2.72251516	2.07805425	0.00000000
N	1.90948968	4.25018595	0.00000000
C	2.06687119	5.61879301	0.00000000
N	3.27732933	6.18721151	0.00000000
C	4.30865388	5.32450115	0.00000000
C	4.27835947	3.92314927	0.00000000
C	3.01096025	3.26363481	0.00000000
N	5.65219476	5.65200757	0.00000000
C	6.36474733	4.45684787	0.00000000
N	5.57562071	3.40409702	0.00000000
Cl	-0.70559973	6.34750173	0.00000000
H	1.35151413	7.48651409	0.00000000
Cl	0.32997740	3.49559215	0.00000000
H	6.02706924	6.59227250	0.00000000
H	7.44516681	4.43630486	0.00000000

Cl-G_4 quartet (C_2, pseudo-C_4)			[-9320.44]
N	3.94271713	4.68496641	1.15512325
O	-0.55216505	3.17679672	0.87053982
N	1.66998773	3.94400265	0.96606050
C	2.64515154	4.89465826	0.71609838
N	2.36957772	6.06503749	0.15147062
C	1.06206991	6.26604641	-0.11367508
C	-0.00127725	5.37570036	0.05747677
C	0.22636877	4.07458789	0.63148299
N	0.49888302	7.40489560	-0.66110416
C	-0.85936443	7.16344033	-0.79414032
N	-1.18495562	5.95839283	-0.37298868
Cl	4.83624786	3.26744987	0.40690776
H	4.48374657	5.50891792	0.89211153
Cl	2.07076961	2.47814364	1.81536457
H	1.00205709	8.24677337	-0.91279734
H	-1.54319205	7.89591483	-1.19750029
N	5.20795270	-4.25899219	0.05416302
O	4.24074820	0.03877005	1.81256508
N	4.70857914	-2.06765664	0.88001581
C	5.28156362	-2.88072063	-0.08358429
N	5.98524055	-2.39036403	-1.09567216
C	6.12204864	-1.04798589	-1.08734696
C	5.56502531	-0.12575435	-0.19637971
C	4.77531284	-0.58326131	0.91895268
N	6.82610098	-0.28967287	-2.00464172
C	6.66898814	1.03771597	-1.63988745
N	5.92446132	1.16505636	-0.56056331
Cl	3.51438785	-4.97086622	-0.14102252
H	5.73278036	-4.65651184	-0.72584005
Cl	3.92431706	-2.77273833	2.26280810
H	7.34159764	-0.65462406	-2.79613792
H	7.11200661	1.84937564	-2.19841511
N	-3.94271713	-4.68496641	1.15512325
O	0.55216505	-3.17679672	0.87053982
N	-1.66998773	-3.94400265	0.96606050
C	-2.64515154	-4.89465826	0.71609838
N	-2.36957772	-6.06503749	0.15147062
C	-1.06206991	-6.26604641	-0.11367508
C	0.00127725	-5.37570036	0.05747677
C	-0.22636877	-4.07458789	0.63148299
N	-0.49888302	-7.40489560	-0.66110416
C	0.85936443	-7.16344033	-0.79414032
N	1.18495562	-5.95839283	-0.37298868
Cl	-4.83624786	-3.26744987	0.40690776
H	-4.48374657	-5.50891792	0.89211153
Cl	-2.07076961	-2.47814364	1.81536457
H	-1.00205709	-8.24677337	-0.91279734
H	1.54319205	-7.89591483	-1.19750029
N	-5.20795270	4.25899219	0.05416302
O	-4.24074820	-0.03877005	1.81256508
N	-4.70857914	2.06765664	0.88001581
C	-5.28156362	2.88072063	-0.08358429
N	-5.98524055	2.39036403	-1.09567216
C	-6.12204864	1.04798589	-1.08734696
C	-5.56502531	0.12575435	-0.19637971
C	-4.77531284	0.58326131	0.91895268
N	-6.82610098	0.28967287	-2.00464172
C	-6.66898814	-1.03771597	-1.63988745
N	-5.92446132	-1.16505636	-0.56056331
Cl	-3.51438785	4.97086622	-0.14102252
H	-5.73278036	4.65651184	-0.72584005
Cl	-3.92431706	2.77273833	2.26280810
H	-7.34159764	0.65462406	-2.79613792
H	-7.11200661	-1.84937564	-2.19841511

Cl-Xan$_4$ quartet (C_{4h})			[-8886.76]
N	3.56292103	5.66931565	0.00000000
N	-3.56292103	-5.66931565	0.00000000
N	5.66931565	-3.56292103	0.00000000
N	-5.66931565	3.56292103	0.00000000
C	3.35330899	3.08240303	0.00000000
C	-3.35330899	-3.08240303	0.00000000
C	3.08240303	-3.35330899	0.00000000
C	-3.08240303	3.35330899	0.00000000
C	4.02901353	4.34968826	0.00000000
C	-4.02901353	-4.34968826	0.00000000
C	4.34968826	-4.02901353	0.00000000
C	-4.34968826	4.02901353	0.00000000
C	5.40902692	4.49022222	0.00000000
C	-5.40902692	-4.49022222	0.00000000
C	4.49022222	-5.40902692	0.00000000
C	-4.49022222	5.40902692	0.00000000
N	6.23400051	3.38963551	0.00000000
N	-6.23400051	-3.38963551	0.00000000
N	3.38963551	-6.23400051	0.00000000
N	-3.38963551	6.23400051	0.00000000
C	5.74438475	2.08450266	0.00000000
C	-5.74438475	-2.08450266	0.00000000
C	2.08450266	-5.74438475	0.00000000
C	-2.08450266	5.74438475	0.00000000
N	4.32674168	2.00804804	0.00000000
N	-4.32674168	-2.00804804	0.00000000
N	2.00804804	-4.32674168	0.00000000
N	-2.00804804	4.32674168	0.00000000
O	6.48482581	1.10978663	0.00000000
O	-6.48482581	-1.10978663	0.00000000
O	1.10978663	-6.48482581	0.00000000
O	-1.10978663	6.48482581	0.00000000
O	2.15475756	2.84891805	0.00000000
O	-2.15475756	-2.84891805	0.00000000
O	2.84891805	-2.15475756	0.00000000
O	-2.84891805	2.15475756	0.00000000
C	-6.49181969	4.65554466	0.00000000
C	6.49181969	-4.65554466	0.00000000
C	4.65554466	6.49181969	0.00000000
C	-4.65554466	-6.49181969	0.00000000
H	-7.56746074	4.55913753	0.00000000
H	7.56746074	-4.55913753	0.00000000
H	4.55913753	7.56746074	0.00000000
H	-4.55913753	-7.56746074	0.00000000
N	5.79880915	5.79887433	0.00000000
N	-5.79880915	-5.79887433	0.00000000
N	5.79887433	-5.79880915	0.00000000
N	-5.79887433	5.79880915	0.00000000
Cl	-3.66642664	-0.40468664	0.00000000
Cl	3.66642664	0.40468664	0.00000000
Cl	-0.40468664	3.66642664	0.00000000
Cl	0.40468664	-3.66642664	0.00000000
H	-7.24302407	-3.49528598	0.00000000
H	7.24302407	3.49528598	0.00000000
H	-3.49528598	7.24302407	0.00000000
H	3.49528598	-7.24302407	0.00000000
Cl	-1.90406710	-6.15917954	0.00000000
Cl	1.90406710	6.15917954	0.00000000
Cl	-6.15917954	1.90406710	0.00000000
Cl	6.15917954	-1.90406710	0.00000000

Cl-Xan$_4$ quartet ( )	[-]
Global minimum is C_{4h}-symmetric.	

Table S10. Cartesian coordinates (in Å) and ADF total bonding energies (in kcal mol^{-1}) of all bromine-bonding species in this work, computed at ZORA-BLYP-D3(BJ)/TZ2P.

Br-Adenine (C_s)			[-2229.60]
N	-1.44304917	-1.42483047	0.00000000
C	-1.28856452	-0.09129075	0.00000000
C	0.02298606	0.44885879	0.00000000
C	1.06973521	-0.48908686	0.00000000
N	0.94867972	-1.82746829	0.00000000
C	-0.33997429	-2.20447262	0.00000000
N	0.51029639	1.75246224	0.00000000
C	1.82273574	1.60912237	0.00000000
N	2.22233610	0.28023027	0.00000000
N	-2.35762002	0.74936930	0.00000000
H	-0.52680950	-3.27554130	0.00000000
H	2.54148875	2.41710183	0.00000000
H	3.16968744	-0.07725496	0.00000000
Br	-4.14806371	0.16521306	0.00000000
H	-2.22087186	1.75292584	0.00000000

Br-Adenine (C_1)			[-2228.56]
N	1.02309203	-0.22540362	-0.51160825
C	1.75697359	-0.22163306	0.61019035
C	3.15878937	-0.06500223	0.51382118
C	3.67542124	0.04658410	-0.79294540
N	2.97040180	0.03115053	-1.93254219
C	1.65304749	-0.10556622	-1.69872842
N	4.17219144	0.01951655	1.46464854
C	5.27279449	0.17788101	0.75424166
N	5.04017878	0.20103562	-0.61385880
N	1.18521752	-0.45521281	1.84742962
H	1.00948971	-0.11582085	-2.57476179
H	6.26974785	0.28317825	1.16001875
H	5.72336579	0.31802047	-1.35220894
Br	-0.63501879	0.10331157	2.13571897
H	1.75809109	-0.12064995	2.62204267

Br-Thymine (C_s)			[-]
N	0.17832381	-1.80477110	0.00000000
C	-0.85741707	-0.89408404	0.00000000
C	-0.64439003	0.44255041	0.00000000
C	0.73623986	0.95159397	0.00000000
N	1.74012932	-0.07757564	0.00000000
C	1.53618088	-1.47251445	0.00000000
C	-1.75141169	1.46378318	0.00000000
O	1.03661969	2.13615932	0.00000000
O	2.41534377	-2.31728298	0.00000000
H	-0.00329509	-2.80157372	0.00000000
Br	3.55438930	0.49661225	0.00000000
H	-1.85329201	-1.32603938	0.00000000
H	-1.67786196	2.11373230	0.87945968
H	-1.67786196	2.11373230	-0.87945968
H	-2.73141613	0.97560815	0.00000000

Br-Thymine ( )	[-]
Global minimum is C_s-symmetric.	

Br-Guanine (C_s)			[-2299.18]
O	-0.01425944	-2.97824645	0.00000000
C	-0.03504059	-1.76514815	0.00000000
N	1.27175893	-1.00149103	0.00000000
C	1.38180408	0.37016510	0.00000000
N	0.31012682	1.15698294	0.00000000
C	-0.88066017	0.52921989	0.00000000
C	-1.13153661	-0.84662000	0.00000000
N	-2.50077829	-1.10131878	0.00000000
C	-3.06136067	0.08628122	0.00000000
N	-2.12459561	1.12218583	0.00000000
N	2.54802015	1.10765474	0.00000000
Br	2.76652811	-2.21879599	0.00000000
H	-4.12397200	0.28607145	0.00000000
H	-2.30346569	2.11872176	0.00000000
H	2.36445282	2.10480090	0.00000000
Br	4.39141403	0.73722124	0.00000000

Br-Guanine (C_1)			[-2309.83]
O	0.98815398	1.90101729	0.69398558
C	1.59457462	0.90307547	0.36415420
N	0.87797405	-0.31280123	-0.08527669
C	1.47253668	-1.50175373	-0.46553287
N	2.78647234	-1.67049713	-0.48438627
C	3.49981189	-0.57443830	-0.14652700
C	3.01863690	0.66518370	0.29376853
N	4.06371549	1.52247560	0.59124156
C	5.15380771	0.82325692	0.33839991
N	4.87451085	-0.45890402	-0.11409393
N	0.66997921	-2.54001101	-0.93875155
Br	-1.01709837	-0.07452706	-0.23638252
H	6.16926597	1.17425592	0.45984825
H	5.53521609	-1.18598941	-0.36128801
H	1.31895629	-3.26804161	-1.25057867
Br	-0.31094252	-3.51864659	0.51737689

Br-Cytosine (C_s)			[-1826.32]
C	-0.76572725	1.57712763	0.00000000
N	-1.73094117	0.50771656	0.00000000
C	-1.38966458	-0.80779536	0.00000000
C	-0.07740313	-1.17207515	0.00000000
C	0.88080073	-0.08726555	0.00000000
N	0.55667472	1.19019793	0.00000000
O	-1.17469772	2.73120909	0.00000000
N	2.20131363	-0.44314125	0.00000000
H	-2.70202485	0.80162720	0.00000000
H	-2.20016363	-1.52945891	0.00000000
H	0.21841613	-2.21472986	0.00000000
H	2.49621117	-1.41017871	0.00000000
Br	3.60763339	0.80992616	0.00000000

Br-Cytosine (C_1)			[-1827.05]
C	-4.20705120	-0.62501165	0.04872459
N	-5.64268070	-0.57520891	0.13733287
C	-6.35389745	0.58225992	0.13396652
C	-5.70592249	1.77799462	0.04383036
C	-4.26515473	1.71298874	-0.03739561
N	-3.56937962	0.59863544	-0.02192306
O	-3.65699575	-1.71755603	0.05029384
N	-3.61496656	2.92749771	-0.21331723
H	-6.10296747	-1.47703695	0.20763605
H	-7.43343983	0.49996525	0.20774390
H	-6.25085540	2.71450499	0.02326676
H	-4.07478449	3.73278091	0.20421977
Br	-1.73712257	3.03347750	0.13865052

Br-Xanthine (C_s)			[-2200.32]
Br	-6.30428401	1.79797929	0.00000000
O	-2.96598156	2.15539524	0.00000000
N	-5.73851819	3.60203886	0.00000000

Br-Xanthine ( )	[-]
Global minimum is C_s-symmetric.	

C	-2.13578814	5.75201097	0.00000000
C	-6.55511289	4.70013638	0.00000000
C	-3.15530652	3.36158292	0.00000000
Br	-0.32142495	3.59078653	0.00000000
N	-2.07258466	4.32455236	0.00000000
C	-4.41502819	4.05819521	0.00000000
H	-3.53381990	7.26298109	0.00000000
H	-7.63166523	4.61544997	0.00000000
C	-4.54480522	5.43711478	0.00000000
N	-3.43966122	6.25264999	0.00000000
O	-1.15801886	6.47741061	0.00000000
N	-5.85295171	5.83575486	0.00000000

Br-AT base pair (C_s)			[-4327.48]	Br-AT base pair (C_1)			[-4327.98]
N	-2.00880796	0.51634407	0.00000000	N	-1.95763813	0.44331344	0.21876229
C	-2.88422264	-0.51163039	0.00000000	C	-2.84357150	-0.50364217	-0.14357743
C	-4.27051685	-0.19675141	0.00000000	C	-4.20028837	-0.12546254	-0.27653908
C	-4.60570236	1.16439457	0.00000000	C	-4.50043586	1.22817622	-0.03366184
N	-3.74816722	2.20155321	0.00000000	N	-3.63145662	2.18501398	0.32557549
C	-2.47738766	1.79203967	0.00000000	C	-2.38330146	1.71271337	0.43014613
N	-5.40537696	-0.99914108	0.00000000	N	-5.34533572	-0.84621685	-0.59726949
C	-6.40987350	-0.14158874	0.00000000	C	-6.31524590	0.04760283	-0.55260110
N	-5.99002953	1.18078017	0.00000000	N	-5.86863325	1.31860355	-0.21767144
N	-2.52727841	-1.81923719	0.00000000	N	-2.47246193	-1.78668230	-0.47465898
H	-1.71114667	2.56190054	0.00000000	H	-1.60882934	2.41959808	0.71291744
H	-7.45866674	-0.40427342	0.00000000	H	-7.35984688	-0.15172909	-0.74880286
H	-6.56982986	2.01114481	0.00000000	H	-6.42403001	2.15954580	-0.11570108
Br	-0.77806806	-2.51050424	0.00000000	Br	-1.03173068	-2.65458461	0.45066184
H	-3.26693176	-2.51245312	0.00000000	H	-3.26746729	-2.42341527	-0.51347439
N	4.51169536	2.00417057	0.00000000	N	4.42276491	2.18785412	-0.11626591
C	5.26048501	0.84667790	0.00000000	C	5.26567693	1.10724775	-0.27077557
C	4.68542349	-0.37943967	0.00000000	C	4.79978772	-0.16263465	-0.32537063
C	3.21688661	-0.47722474	0.00000000	C	3.34998171	-0.39701542	-0.21354654
N	2.53295319	0.77064064	0.00000000	N	2.56258734	0.78210802	-0.07177385
C	3.10996128	2.04352758	0.00000000	C	3.02807597	2.09857336	-0.00781675
C	5.46578566	-1.66701401	0.00000000	C	5.68317333	-1.36984873	-0.49502447
O	2.60833003	-1.54647995	0.00000000	O	2.83736240	-1.51224177	-0.23945412
O	2.49765057	3.10306818	0.00000000	O	2.33102714	3.09596483	0.12780128
H	4.95476178	2.91498897	0.00000000	H	4.78454664	3.13280560	-0.07263760
Br	0.58582041	0.67499572	0.00000000	Br	0.63365211	0.53672536	0.05923028
H	6.33698855	0.98855301	0.00000000	H	6.32197309	1.34779595	-0.34430777
H	5.21407220	-2.27188611	0.87903190	H	5.56049413	-2.06054004	0.34740104
H	5.21407220	-2.27188611	-0.87903190	H	5.40707375	-1.92630939	-1.39844212
H	6.54342420	-1.47205638	0.00000000	H	6.73642237	-1.07812514	-0.56549754

Br-GC base pair (C_s)			[-4138.43]	Br-GC base pair (C_1)			[-4148.31]
C	-4.23379208	-0.69298233	0.00000000	C	-4.28460282	0.01474107	-0.31548782
N	-5.66057797	-0.63447981	0.00000000	N	-5.69993590	0.06022706	-0.42316760
C	-6.35989786	0.53357726	0.00000000	C	-6.39073649	1.23657197	-0.45999488
C	-5.69856030	1.72060417	0.00000000	C	-5.72743452	2.42476145	-0.39836890
C	-4.25085310	1.66581087	0.00000000	C	-4.28966258	2.34765291	-0.29218891
N	-3.57325349	0.51942621	0.00000000	N	-3.63046647	1.20148073	-0.25365899
O	-3.69083197	-1.79359440	0.00000000	O	-3.73611754	-1.10198776	-0.27604303
N	-3.61071010	2.86391214	0.00000000	N	-3.56748951	3.50985194	-0.27712946
H	-6.12921092	-1.53393529	0.00000000	H	-6.17754983	-0.83462747	-0.45653319
H	-7.44217512	0.46004387	0.00000000	H	-7.46990632	1.16529080	-0.53703637
H	-6.23487390	2.66246671	0.00000000	H	-6.26082221	3.36770285	-0.43527103
H	-4.14985723	3.71949942	0.00000000	H	-4.02588748	4.36602023	0.01607303
Br	-1.74112470	3.09683814	0.00000000	Br	-1.72597547	3.42813019	0.19736453
O	1.02023263	1.97205984	0.00000000	O	0.44819443	1.46719213	0.85307130
C	1.68357008	0.94131127	0.00000000	C	1.21328833	0.63238385	0.39263094
N	1.01699639	-0.38217127	0.00000000	N	0.74309474	-0.68376789	-0.02861291
C	1.68443183	-1.58208766	0.00000000	C	1.55924424	-1.68459570	-0.49707642
N	3.01703632	-1.67022788	0.00000000	N	2.87424161	-1.55999807	-0.66200330
C	3.66130855	-0.49002439	0.00000000	C	3.34291026	-0.32691485	-0.37706529
C	3.10675299	0.79445542	0.00000000	C	2.63215315	0.75726822	0.15111258
N	4.10623418	1.76654159	0.00000000	N	3.46950260	1.84427989	0.35335676
C	5.23162777	1.08897735	0.00000000	C	4.65784847	1.43121529	-0.04338752
N	5.02712208	-0.29272423	0.00000000	N	4.64504568	0.11879990	-0.49785903
N	1.09814463	-2.83087766	0.00000000	N	0.98061072	-2.88408863	-0.92536577
Br	-0.92964502	-0.18537737	0.00000000	Br	-1.21118168	-0.86653438	-0.08429260
H	6.22656988	1.51236573	0.00000000	H	5.56545278	2.01865831	-0.03079613
H	5.72788639	-1.02300079	0.00000000	H	5.42681247	-0.42604124	-0.84030873
H	1.78462342	-3.57598990	0.00000000	H	1.75737349	-3.44633276	-1.28398910
Br	-0.66890610	-3.47646163	0.00000000	Br	0.34106513	-4.05159004	0.57694116

Br-G_4 quartet (C_{4h})			[-9255.08]
N	6.53817271	-1.05144880	0.00000000
O	2.12580658	-2.72279280	0.00000000
N	4.27955698	-1.94241008	0.00000000
C	5.65183850	-2.08998489	0.00000000
N	6.21924454	-3.31159847	0.00000000
C	5.35747497	-4.33861946	0.00000000
C	3.95330886	-4.30582600	0.00000000
C	3.32024101	-3.02566667	0.00000000
N	5.68310447	-5.68606661	0.00000000
C	4.49417715	-6.40159490	0.00000000
N	3.44084961	-5.61044945	0.00000000
Br	6.37285031	0.89902772	0.00000000
H	7.50010878	-1.37151150	0.00000000
Br	3.41381618	-0.20658695	0.00000000
H	6.62269710	-6.06257504	0.00000000
H	4.46966328	-7.48140037	0.00000000
N	1.05144880	6.53817271	0.00000000
O	2.72279280	2.12580658	0.00000000
N	1.94241008	4.27955698	0.00000000
C	2.08998489	5.65183850	0.00000000
N	3.31159847	6.21924454	0.00000000
C	4.33861946	5.35747497	0.00000000
C	4.30582600	3.95330886	0.00000000
C	3.02566667	3.32024101	0.00000000
N	5.68606661	5.68310447	0.00000000
C	6.40159490	4.49417715	0.00000000
N	5.61044945	3.44084961	0.00000000
Br	-0.89902772	6.37285031	0.00000000
H	1.37151150	7.50010878	0.00000000
Br	0.20658695	3.41381618	0.00000000
H	6.06257504	6.62269710	0.00000000
H	7.48140037	4.46966328	0.00000000
N	-6.53817271	1.05144880	0.00000000
O	-2.12580658	2.72279280	0.00000000
N	-4.27955698	1.94241008	0.00000000
C	-5.65183850	2.08998489	0.00000000
N	-6.21924454	3.31159847	0.00000000
C	-5.35747497	4.33861946	0.00000000
C	-3.95330886	4.30582600	0.00000000
C	-3.32024101	3.02566667	0.00000000
N	-5.68310447	5.68606661	0.00000000
C	-4.49417715	6.40159490	0.00000000
N	-3.44084961	5.61044945	0.00000000
Br	-6.37285031	-0.89902772	0.00000000
H	-7.50010878	1.37151150	0.00000000
Br	-3.41381618	0.20658695	0.00000000
H	-6.62269710	6.06257504	0.00000000
H	-4.46966328	7.48140037	0.00000000
N	-1.05144880	-6.53817271	0.00000000
O	-2.72279280	-2.12580658	0.00000000
N	-1.94241008	-4.27955698	0.00000000
C	-2.08998489	-5.65183850	0.00000000
N	-3.31159847	-6.21924454	0.00000000
C	-4.33861946	-5.35747497	0.00000000
C	-4.30582600	-3.95330886	0.00000000
C	-3.02566667	-3.32024101	0.00000000
N	-5.68606661	-5.68310447	0.00000000
C	-6.40159490	-4.49417715	0.00000000
N	-5.61044945	-3.44084961	0.00000000
Br	0.89902772	-6.37285031	0.00000000
H	-1.37151150	-7.50010878	0.00000000
Br	-0.20658695	-3.41381618	0.00000000
H	-6.06257504	-6.62269710	0.00000000
H	-7.48140037	-4.46966328	0.00000000

Br-G_4 quartet (C_4)			[-9279.28]
N	-0.68062148	6.57080287	-0.53983490
O	-2.99970744	2.60711183	-1.69484977
N	-1.86169208	4.56399905	-1.06996793
C	-1.72257342	5.70907569	-0.29458624
N	-2.61841237	6.03728969	0.64125959
C	-3.65215916	5.18546611	0.75827806
C	-3.86556666	3.99115488	0.06629107
C	-2.94738646	3.57959817	-0.96516587
N	-4.71697948	5.29414806	1.63941857
C	-5.51807351	4.18251793	1.45881477
N	-5.03251818	3.39114149	0.52111851
Br	1.18160247	5.87082984	-0.06364951
H	-0.80254915	7.36088238	0.09551559
Br	-0.63473600	4.18688746	-2.49142907
H	-4.85929558	6.04947553	2.29860221
H	-6.41645562	4.00265332	2.02991575
N	6.57080287	0.68062148	-0.53983490
O	2.60711183	2.99970744	-1.69484977
N	4.56399905	1.86169208	-1.06996793
C	5.70907569	1.72257342	-0.29458624
N	6.03728969	2.61841237	0.64125959
C	5.18546611	3.65215916	0.75827806
C	3.99115488	3.86556666	0.06629107
C	3.57959817	2.94738646	-0.96516587
N	5.29414806	4.71697948	1.63941857
C	4.18251793	5.51807351	1.45881477
N	3.39114149	5.03251818	0.52111851
Br	5.87082984	-1.18160247	-0.06364951
H	7.36088238	0.80254915	0.09551559
Br	4.18688746	0.63473600	-2.49142907
H	6.04947553	4.85929558	2.29860221
H	4.00265332	6.41645562	2.02991575
N	0.68062148	-6.57080287	-0.53983490
O	2.99970744	-2.60711183	-1.69484977
N	1.86169208	-4.56399905	-1.06996793
C	1.72257342	-5.70907569	-0.29458624
N	2.61841237	-6.03728969	0.64125959
C	3.65215916	-5.18546611	0.75827806
C	3.86556666	-3.99115488	0.06629107
C	2.94738646	-3.57959817	-0.96516587
N	4.71697948	-5.29414806	1.63941857
C	5.51807351	-4.18251793	1.45881477
N	5.03251818	-3.39114149	0.52111851
Br	-1.18160247	-5.87082984	-0.06364951
H	0.80254915	-7.36088238	0.09551559
Br	0.63473600	-4.18688746	-2.49142907
H	4.85929558	-6.04947553	2.29860221
H	6.41645562	-4.00265332	2.02991575
N	-6.57080287	-0.68062148	-0.53983490
O	-2.60711183	-2.99970744	-1.69484977
N	-4.56399905	-1.86169208	-1.06996793
C	-5.70907569	-1.72257342	-0.29458624
N	-6.03728969	-2.61841237	0.64125959
C	-5.18546611	-3.65215916	0.75827806
C	-3.99115488	-3.86556666	0.06629107
C	-3.57959817	-2.94738646	-0.96516587
N	-5.29414806	-4.71697948	1.63941857
C	-4.18251793	-5.51807351	1.45881477
N	-3.39114149	-5.03251818	0.52111851
Br	-5.87082984	1.18160247	-0.06364951
H	-7.36088238	-0.80254915	0.09551559
Br	-4.18688746	-0.63473600	-2.49142907
H	-6.04947553	-4.85929558	2.29860221
H	-4.00265332	-6.41645562	2.02991575

Br-Xan$_4$ quartet (C_{4h})			[-8840.62]
N	3.60622081	5.75246581	0.00000000
C	3.38690980	3.15655632	0.00000000
C	4.05851155	4.42558123	0.00000000
C	5.44233205	4.54751132	0.00000000
N	6.25302959	3.43629627	0.00000000
C	5.74356139	2.13917852	0.00000000
N	4.33322959	2.07549774	0.00000000
O	6.48740090	1.15976332	0.00000000
O	2.18131446	2.91948107	0.00000000
C	4.71082803	6.55499313	0.00000000
H	4.63497009	7.63231324	0.00000000
N	5.84906470	5.84991405	0.00000000
Br	3.58377463	0.31704224	0.00000000
H	7.26349374	3.52840141	0.00000000
Br	1.78771318	6.31323951	0.00000000
N	-3.60622081	-5.75246581	0.00000000
N	5.75246581	-3.60622081	0.00000000
N	-5.75246581	3.60622081	0.00000000
C	-3.38690980	-3.15655632	0.00000000
C	3.15655632	-3.38690980	0.00000000
C	-3.15655632	3.38690980	0.00000000
C	-4.05851155	-4.42558123	0.00000000
C	4.42558123	-4.05851155	0.00000000
C	-4.42558123	4.05851155	0.00000000
C	-5.44233205	-4.54751132	0.00000000
C	4.54751132	-5.44233205	0.00000000
C	-4.54751132	5.44233205	0.00000000
N	-6.25302959	-3.43629627	0.00000000
N	3.43629627	-6.25302959	0.00000000
N	-3.43629627	6.25302959	0.00000000
C	-5.74356139	-2.13917852	0.00000000
C	2.13917852	-5.74356139	0.00000000
C	-2.13917852	5.74356139	0.00000000
N	-4.33322959	-2.07549774	0.00000000
N	2.07549774	-4.33322959	0.00000000
N	-2.07549774	4.33322959	0.00000000
O	-6.48740090	-1.15976332	0.00000000
O	1.15976332	-6.48740090	0.00000000
O	-1.15976332	6.48740090	0.00000000
O	-2.18131446	-2.91948107	0.00000000
O	2.91948107	-2.18131446	0.00000000
O	-2.91948107	2.18131446	0.00000000
C	-6.55499313	4.71082803	0.00000000
C	6.55499313	-4.71082803	0.00000000
C	-4.71082803	-6.55499313	0.00000000
H	-7.63231324	4.63497009	0.00000000
H	7.63231324	-4.63497009	0.00000000
H	-4.63497009	-7.63231324	0.00000000
N	-5.84906470	-5.84991405	0.00000000
N	5.84991405	-5.84906470	0.00000000
N	-5.84991405	5.84906470	0.00000000
Br	-3.58377463	-0.31704224	0.00000000
Br	-0.31704224	3.58377463	0.00000000
Br	0.31704224	-3.58377463	0.00000000
H	-7.26349374	-3.52840141	0.00000000
H	-3.52840141	7.26349374	0.00000000
H	3.52840141	-7.26349374	0.00000000
Br	-1.78771318	-6.31323951	0.00000000
Br	-6.31323951	1.78771318	0.00000000
Br	6.31323951	-1.78771318	0.00000000

Br-Xan$_4$ quartet (C_4)			[-8840.82]
N	2.36383123	-6.28897778	0.08762772
C	2.69235427	-3.75485773	-0.41233387
C	3.07381961	-5.08681309	-0.03594715
C	4.38443883	-5.44333773	0.25557901
N	5.39532514	-4.51114722	0.23090804
C	5.16122120	-3.16344603	-0.03024920
N	3.81690217	-2.85948511	-0.33112530
O	6.07794180	-2.34202389	0.00357258
O	1.59435687	-3.33665295	-0.77042644
C	3.26327979	-7.25051371	0.44915977
H	2.96520118	-8.27260152	0.63064589
N	4.50976103	-6.77043956	0.54585035
Br	3.43055174	-1.01131950	-0.63002769
H	6.35191086	-4.77339478	0.44485137
Br	0.46625713	-6.46203589	0.02982804
N	-2.36383123	6.28897778	0.08762772
N	6.28897778	2.36383123	0.08762772
N	-6.28897778	-2.36383123	0.08762772
C	-2.69235427	3.75485773	-0.41233387
C	3.75485773	2.69235427	-0.41233387
C	-3.75485773	-2.69235427	-0.41233387
C	-3.07381961	5.08681309	-0.03594715
C	5.08681309	3.07381961	-0.03594715
C	-5.08681309	-3.07381961	-0.03594715
C	-4.38443883	5.44333773	0.25557901
C	5.44333773	4.38443883	0.25557901
C	-5.44333773	-4.38443883	0.25557901
N	-5.39532514	4.51114722	0.23090804
N	4.51114722	5.39532514	0.23090804
N	-4.51114722	-5.39532514	0.23090804
C	-5.16122120	3.16344603	-0.03024920
C	3.16344603	5.16122120	-0.03024920
C	-3.16344603	-5.16122120	-0.03024920
N	-3.81690217	2.85948511	-0.33112530
N	2.85948511	3.81690217	-0.33112530
N	-2.85948511	-3.81690217	-0.33112530
O	-6.07794180	2.34202389	0.00357258
O	2.34202389	6.07794180	0.00357258
O	-2.34202389	-6.07794180	0.00357258
O	-1.59435687	3.33665295	-0.77042644
O	3.33665295	1.59435687	-0.77042644
O	-3.33665295	-1.59435687	-0.77042644
C	-7.25051371	-3.26327979	0.44915977
C	7.25051371	3.26327979	0.44915977
C	-3.26327979	7.25051371	0.44915977
H	-8.27260152	-2.96520118	0.63064589
H	8.27260152	2.96520118	0.63064589
H	-2.96520118	8.27260152	0.63064589
N	-4.50976103	6.77043956	0.54585035
N	6.77043956	4.50976103	0.54585035
N	-6.77043956	-4.50976103	0.54585035
Br	-3.43055174	1.01131950	-0.63002769
Br	-1.01131950	-3.43055174	-0.63002769
Br	1.01131950	3.43055174	-0.63002769
H	-6.35191086	4.77339478	0.44485137
H	-4.77339478	-6.35191086	0.44485137
H	4.77339478	6.35191086	0.44485137
Br	-0.46625713	6.46203589	0.02982804
Br	-6.46203589	-0.46625713	0.02982804
Br	6.46203589	0.46625713	0.02982804

G_4-[Br-G_4^{con}]-G_4 (C_4)			[-29209.26]
N	5.31209580	1.25906031	3.55168161
O	0.84549072	2.33445716	4.32435883
N	3.07254723	1.85177166	3.91995074
C	4.34697610	2.20602815	3.53051493
N	4.69147141	3.44630460	3.15430476
C	3.66872029	4.31667023	3.22813862
C	2.35444616	4.07537608	3.64016277
C	1.96830736	2.74277043	3.99316863
N	3.69638899	5.66100851	2.89632953
C	2.41804954	6.16238592	3.10083700
N	1.59618415	5.23893399	3.55653793
H	5.13948664	0.24118943	3.61496126
H	6.17967364	1.54004604	3.11392324
H	2.85498100	0.85118106	4.10458270
H	4.47437078	6.13570109	2.45808733
H	2.16268675	7.18959253	2.88896217
N	1.25906031	-5.31209580	3.55168161
O	2.33445716	-0.84549072	4.32435883
N	1.85177166	-3.07254723	3.91995074
C	2.20602815	-4.34697610	3.53051493
N	3.44630460	-4.69147141	3.15430476
C	4.31667023	-3.66872029	3.22813862
C	4.07537608	-2.35444616	3.64016277
C	2.74277043	-1.96830736	3.99316863
N	5.66100851	-3.69638899	2.89632953
C	6.16238592	-2.41804954	3.10083700
N	5.23893399	-1.59618415	3.55653793
H	0.24118943	-5.13948664	3.61496126
H	1.54004604	-6.17967364	3.11392324
H	0.85118106	-2.85498100	4.10458270
H	6.13570109	-4.47437078	2.45808733
H	7.18959253	-2.16268675	2.88896217
N	-5.31209580	-1.25906031	3.55168161
O	-0.84549072	-2.33445716	4.32435883
N	-3.07254723	-1.85177166	3.91995074
C	-4.34697610	-2.20602815	3.53051493
N	-4.69147141	-3.44630460	3.15430476
C	-3.66872029	-4.31667023	3.22813862
C	-2.35444616	-4.07537608	3.64016277
C	-1.96830736	-2.74277043	3.99316863
N	-3.69638899	-5.66100851	2.89632953
C	-2.41804954	-6.16238592	3.10083700
N	-1.59618415	-5.23893399	3.55653793
H	-5.13948664	-0.24118943	3.61496126
H	-6.17967364	-1.54004604	3.11392324
H	-2.85498100	-0.85118106	4.10458270
H	-4.47437078	-6.13570109	2.45808733
H	-2.16268675	-7.18959253	2.88896217
N	-1.25906031	5.31209580	3.55168161
O	-2.33445716	0.84549072	4.32435883
N	-1.85177166	3.07254723	3.91995074
C	-2.20602815	4.34697610	3.53051493
N	-3.44630460	4.69147141	3.15430476
C	-4.31667023	3.66872029	3.22813862
C	-4.07537608	2.35444616	3.64016277
C	-2.74277043	1.96830736	3.99316863
N	-5.66100851	3.69638899	2.89632953
C	-6.16238592	2.41804954	3.10083700
N	-5.23893399	1.59618415	3.55653793
H	-0.24118943	5.13948664	3.61496126
H	-1.54004604	6.17967364	3.11392324
H	-0.85118106	2.85498100	4.10458270
H	-6.13570109	4.47437078	2.45808733
H	-7.18959253	2.16268675	2.88896217
N	3.45592290	-4.17017290	-3.61478812
O	2.44344840	0.29645261	-2.80764253

G_4-K^+-[Br-G_4^{con}]-K^+-G_4 (C_4)			[-29184.93]
N	5.54882472	-0.06673717	3.47265344
O	1.35886154	1.92043499	3.61428412
N	3.47458659	1.00458025	3.56199374
C	4.85024051	1.08280793	3.42059217
N	5.49966921	2.24004120	3.24460920
C	4.68610117	3.30971331	3.24918244
C	3.28868830	3.33786858	3.38868237
C	2.59790728	2.10608581	3.53573744
N	5.04848890	4.63517422	3.09215650
C	3.88568523	5.39305008	3.14303358
N	2.81454351	4.64598182	3.31550929
H	5.12609109	-1.01015459	3.42626356
H	6.53129598	0.01456528	3.24726083
H	3.02512947	0.07307051	3.64761926
H	5.99717460	4.97661865	3.00042975
H	3.89749547	6.46824190	3.04172498
N	-0.06673717	-5.54882472	3.47265344
O	1.92043499	-1.35886154	3.61428412
N	1.00458025	-3.47458659	3.56199374
C	1.08280793	-4.85024051	3.42059217
N	2.24004120	-5.49966921	3.24460920
C	3.30971331	-4.68610117	3.24918244
C	3.33786858	-3.28868830	3.38868237
C	2.10608581	-2.59790728	3.53573744
N	4.63517422	-5.04848890	3.09215650
C	5.39305008	-3.88568523	3.14303358
N	4.64598182	-2.81454351	3.31550929
H	-1.01015459	-5.12609109	3.42626356
H	0.01456528	-6.53129598	3.24726083
H	0.07307051	-3.02512947	3.64761926
H	4.97661865	-5.99717460	3.00042975
H	6.46824190	-3.89749547	3.04172498
N	-5.54882472	0.06673717	3.47265344
O	-1.35886154	-1.92043499	3.61428412
N	-3.47458659	-1.00458025	3.56199374
C	-4.85024051	-1.08280793	3.42059217
N	-5.49966921	-2.24004120	3.24460920
C	-4.68610117	-3.30971331	3.24918244
C	-3.28868830	-3.33786858	3.38868237
C	-2.59790728	-2.10608581	3.53573744
N	-5.04848890	-4.63517422	3.09215650
C	-3.88568523	-5.39305008	3.14303358
N	-2.81454351	-4.64598182	3.31550929
H	-5.12609109	1.01015459	3.42626356
H	-6.53129598	-0.01456528	3.24726083
H	-3.02512947	-0.07307051	3.64761926
H	-5.99717460	-4.97661865	3.00042975
H	-3.89749547	-6.46824190	3.04172498
N	0.06673717	5.54882472	3.47265344
O	-1.92043499	1.35886154	3.61428412
N	-1.00458025	3.47458659	3.56199374
C	-1.08280793	4.85024051	3.42059217
N	-2.24004120	5.49966921	3.24460920
C	-3.30971331	4.68610117	3.24918244
C	-3.33786858	3.28868830	3.38868237
C	-2.10608581	2.59790728	3.53573744
N	-4.63517422	5.04848890	3.09215650
C	-5.39305008	3.88568523	3.14303358
N	-4.64598182	2.81454351	3.31550929
H	1.01015459	5.12609109	3.42626356
H	-0.01456528	6.53129598	3.24726083
H	-0.07307051	3.02512947	3.64761926
H	-4.97661865	5.99717460	3.00042975
H	-6.46824190	3.89749547	3.04172498
N	3.02328609	-4.59611647	-3.58648820
O	2.35822674	-0.05446718	-2.86327698

N	3.01115680	-1.91408103	-3.17788797	N	2.75952813	-2.30260952	-3.21283624
C	3.90734564	-2.90174282	-3.52839437	C	3.58609534	-3.37590196	-3.50448904
N	5.20127572	-2.67411994	-3.79602301	N	4.90151112	-3.25307641	-3.70747425
C	5.52987145	-1.37494041	-3.69806141	C	5.33491625	-1.98767761	-3.60545565
C	4.70166220	-0.29276279	-3.38072940	C	4.58616613	-0.83449039	-3.32032376
C	3.31909557	-0.53114203	-3.09570281	C	3.18631576	-0.96402731	-3.11377594
N	6.78554183	-0.81883478	-3.87655305	N	6.63481213	-1.53894239	-3.74344172
C	6.66900159	0.54833387	-3.65324972	C	6.62668365	-0.16864136	-3.53124115
N	5.42978962	0.89162262	-3.36090305	N	5.41395931	0.28595021	-3.27716443
H	2.49193073	-4.49260043	-3.43525752	H	2.02044449	-4.80231471	-3.43766433
H	4.14734407	-4.85617091	-3.88029396	H	3.64187322	-5.34459205	-3.86585152
H	2.01484843	-2.16349007	-3.00205379	H	1.73953745	-2.45733795	-3.09501157
H	7.62985306	-1.33718117	-4.08137344	H	7.43886279	-2.12174662	-3.94259000
H	7.51468127	1.21721334	-3.71769352	H	7.52787827	0.42519030	-3.57916299
N	-4.17017290	-3.45592290	-3.61478812	N	-4.59611647	-3.02328609	-3.58648820
O	0.29645261	-2.44344840	-2.80764253	O	-0.05446718	-2.35822674	-2.86327698
N	-1.91408103	-3.01115680	-3.17788797	N	-2.30260952	-2.75952813	-3.21283624
C	-2.90174282	-3.90734564	-3.52839437	C	-3.37590196	-3.58609534	-3.50448904
N	-2.67411994	-5.20127572	-3.79602301	N	-3.25307641	-4.90151112	-3.70747425
C	-1.37494041	-5.52987145	-3.69806141	C	-1.98767761	-5.33491625	-3.60545565
C	-0.29276279	-4.70166220	-3.38072940	C	-0.83449039	-4.58616613	-3.32032376
C	-0.53114203	-3.31909557	-3.09570281	C	-0.96402731	-3.18631576	-3.11377594
N	-0.81883478	-6.78554183	-3.87655305	N	-1.53894239	-6.63481213	-3.74344172
C	0.54833387	-6.66900159	-3.65324972	C	-0.16864136	-6.62668365	-3.53124115
N	0.89162262	-5.42978962	-3.36090305	N	0.28595021	-5.41395931	-3.27716443
H	-4.49260043	-2.49193073	-3.43525752	H	-4.80231471	-2.02044449	-3.43766433
H	-4.85617091	-4.14734407	-3.88029396	H	-5.34459205	-3.64187322	-3.86585152
H	-2.16349007	-2.01484843	-3.00205379	H	-2.45733795	-1.73953745	-3.09501157
H	-1.33718117	-7.62985306	-4.08137344	H	-2.12174662	-7.43886279	-3.94259000
H	1.21721334	-7.51468127	-3.71769352	H	0.42519030	-7.52787827	-3.57916299
N	-3.45592290	4.17017290	-3.61478812	N	-3.02328609	4.59611647	-3.58648820
O	-2.44344840	-0.29645261	-2.80764253	O	-2.35822674	0.05446718	-2.86327698
N	-3.01115680	1.91408103	-3.17788797	N	-2.75952813	2.30260952	-3.21283624
C	-3.90734564	2.90174282	-3.52839437	C	-3.58609534	3.37590196	-3.50448904
N	-5.20127572	2.67411994	-3.79602301	N	-4.90151112	3.25307641	-3.70747425
C	-5.52987145	1.37494041	-3.69806141	C	-5.33491625	1.98767761	-3.60545565
C	-4.70166220	0.29276279	-3.38072940	C	-4.58616613	0.83449039	-3.32032376
C	-3.31909557	0.53114203	-3.09570281	C	-3.18631576	0.96402731	-3.11377594
N	-6.78554183	0.81883478	-3.87655305	N	-6.63481213	1.53894239	-3.74344172
C	-6.66900159	-0.54833387	-3.65324972	C	-6.62668365	0.16864136	-3.53124115
N	-5.42978962	-0.89162262	-3.36090305	N	-5.41395931	-0.28595021	-3.27716443
H	-2.49193073	4.49260043	-3.43525752	H	-2.02044449	4.80231471	-3.43766433
H	-4.14734407	4.85617091	-3.88029396	H	-3.64187322	5.34459205	-3.86585152
H	-2.01484843	2.16349007	-3.00205379	H	-1.73953745	2.45733795	-3.09501157
H	-7.62985306	1.33718117	-4.08137344	H	-7.43886279	2.12174662	-3.94259000
H	-7.51468127	-1.21721334	-3.71769352	H	-7.52787827	-0.42519030	-3.57916299
N	4.17017290	3.45592290	-3.61478812	N	4.59611647	3.02328609	-3.58648820
O	-0.29645261	2.44344840	-2.80764253	O	0.05446718	2.35822674	-2.86327698
N	1.91408103	3.01115680	-3.17788797	N	2.30260952	2.75952813	-3.21283624
C	2.90174282	3.90734564	-3.52839437	C	3.37590196	3.58609534	-3.50448904
N	2.67411994	5.20127572	-3.79602301	N	3.25307641	4.90151112	-3.70747425
C	1.37494041	5.52987145	-3.69806141	C	1.98767761	5.33491625	-3.60545565
C	0.29276279	4.70166220	-3.38072940	C	0.83449039	4.58616613	-3.32032376
C	0.53114203	3.31909557	-3.09570281	C	0.96402731	3.18631576	-3.11377594
N	0.81883478	6.78554183	-3.87655305	N	1.53894239	6.63481213	-3.74344172
C	-0.54833387	6.66900159	-3.65324972	C	0.16864136	6.62668365	-3.53124115
N	-0.89162262	5.42978962	-3.36090305	N	-0.28595021	5.41395931	-3.27716443
H	4.49260043	2.49193073	-3.43525752	H	4.80231471	2.02044449	-3.43766433
H	4.85617091	4.14734407	-3.88029396	H	5.34459205	3.64187322	-3.86585152
H	2.16349007	2.01484843	-3.00205379	H	2.45733795	1.73953745	-3.09501157
H	1.33718117	7.62985306	-4.08137344	H	2.12174662	7.43886279	-3.94259000
H	-1.21721334	7.51468127	-3.71769352	H	-0.42519030	7.52787827	-3.57916299
N	0.20883434	-6.57421383	0.16035368	N	-0.58930747	-6.70737568	0.40807575
O	2.62404572	-2.55961009	0.67197051	O	1.87857605	-2.69539977	0.28861479
N	1.42296619	-4.47992851	0.21391112	N	0.67487420	-4.64375879	0.19354724
C	1.33260896	-5.81340646	-0.11713289	C	0.55336022	-6.01087671	0.04284348
N	2.38660015	-6.49899465	-0.58503746	N	1.58086960	-6.78518836	-0.30629138
C	3.53130327	-5.79657580	-0.64320831	C	2.75707384	-6.14917949	-0.40075969
C	3.75013311	-4.45986089	-0.29061528	C	3.01791024	-4.78049690	-0.21960282
C	2.65065888	-3.70041446	0.23296714	C	1.91212819	-3.92780303	0.09601932
N	4.75776019	-6.25590667	-1.10160985	N	3.97062029	-6.71600666	-0.73566448
C	5.65299108	-5.19829706	-1.01295492	C	4.90572827	-5.69082362	-0.74686074
N	5.08048000	-4.11402237	-0.52672833	N	4.37274487	-4.52567271	-0.44276254
Br	-1.68148570	-6.08598545	-0.30504784	Br	-2.38424973	-6.18003798	-0.19823938
H	0.36822436	-7.49428802	-0.24811926	H	-0.44838035	-7.68035866	0.13594961
Br	-0.12138302	-3.45099087	0.69470996	Br	-0.87175078	-3.43438465	0.38808574

H	4.95542562	-7.20211851	-1.40151067	H	4.13314869	-7.70117840	-0.90879164
H	6.68018602	-5.27797104	-1.33626060	H	5.94320926	-5.86422712	-0.99444198
N	-6.57421383	-0.20883434	0.16035368	N	-6.70737568	0.58930747	0.40807575
O	-2.55961009	-2.62404572	0.67197051	O	-2.69539977	-1.87857605	0.28861479
N	-4.47992851	-1.42296619	0.21391112	N	-4.64375879	-0.67487420	0.19354724
C	-5.81340646	-1.33260896	-0.11713289	C	-6.01087671	-0.55336022	0.04284348
N	-6.49899465	-2.38660015	-0.58503746	N	-6.78518836	-1.58086960	-0.30629138
C	-5.79657580	-3.53130327	-0.64320831	C	-6.14917949	-2.75707384	-0.40075969
C	-4.45986089	-3.75013311	-0.29061528	C	-4.78049690	-3.01791024	-0.21960282
C	-3.70041446	-2.65065888	0.23296714	C	-3.92780303	-1.91212819	0.09601932
N	-6.25590667	-4.75776019	-1.10160985	N	-6.71600666	-3.97062029	-0.73566448
C	-5.19829706	-5.65299108	-1.01295492	C	-5.69082362	-4.90572827	-0.74686074
N	-4.11402237	-5.08048000	-0.52672833	N	-4.52567271	-4.37274487	-0.44276254
Br	-6.08598545	1.68148570	-0.30504784	Br	-6.18003798	2.38424973	-0.19823938
H	-7.49428802	-0.36822436	-0.24811926	H	-7.68035866	0.44838035	0.13594961
Br	-3.45099087	0.12138302	0.69470996	Br	-3.43438465	0.87175078	0.38808574
H	-7.20211851	-4.95542562	-1.40151067	H	-7.70117840	-4.13314869	-0.90879164
H	-5.27797104	-6.68018602	-1.33626060	H	-5.86422712	-5.94320926	-0.99444198
N	-0.20883434	6.57421383	0.16035368	N	0.58930747	6.70737568	0.40807575
O	-2.62404572	2.55961009	0.67197051	O	-1.87857605	2.69539977	0.28861479
N	-1.42296619	4.47992851	0.21391112	N	-0.67487420	4.64375879	0.19354724
C	-1.33260896	5.81340646	-0.11713289	C	-0.55336022	6.01087671	0.04284348
N	-2.38660015	6.49899465	-0.58503746	N	-1.58086960	6.78518836	-0.30629138
C	-3.53130327	5.79657580	-0.64320831	C	-2.75707384	6.14917949	-0.40075969
C	-3.75013311	4.45986089	-0.29061528	C	-3.01791024	4.78049690	-0.21960282
C	-2.65065888	3.70041446	0.23296714	C	-1.91212819	3.92780303	0.09601932
N	-4.75776019	6.25590667	-1.10160985	N	-3.97062029	6.71600666	-0.73566448
C	-5.65299108	5.19829706	-1.01295492	C	-4.90572827	5.69082362	-0.74686074
N	-5.08048000	4.11402237	-0.52672833	N	-4.37274487	4.52567271	-0.44276254
Br	1.68148570	6.08598545	-0.30504784	Br	2.38424973	6.18003798	-0.19823938
H	-0.36822436	7.49428802	-0.24811926	H	0.44838035	7.68035866	0.13594961
Br	0.12138302	3.45099087	0.69470996	Br	0.87175078	3.43438465	0.38808574
H	-4.95542562	7.20211851	-1.40151067	H	-4.13314869	7.70117840	-0.90879164
H	-6.68018602	5.27797104	-1.33626060	H	-5.94320926	5.86422712	-0.99444198
N	6.57421383	0.20883434	0.16035368	N	6.70737568	-0.58930747	0.40807575
O	2.55961009	2.62404572	0.67197051	O	2.69539977	1.87857605	0.28861479
N	4.47992851	1.42296619	0.21391112	N	4.64375879	0.67487420	0.19354724
C	5.81340646	1.33260896	-0.11713289	C	6.01087671	0.55336022	0.04284348
N	6.49899465	2.38660015	-0.58503746	N	6.78518836	1.58086960	-0.30629138
C	5.79657580	3.53130327	-0.64320831	C	6.14917949	2.75707384	-0.40075969
C	4.45986089	3.75013311	-0.29061528	C	4.78049690	3.01791024	-0.21960282
C	3.70041446	2.65065888	0.23296714	C	3.92780303	1.91212819	0.09601932
N	6.25590667	4.75776019	-1.10160985	N	6.71600666	3.97062029	-0.73566448
C	5.19829706	5.65299108	-1.01295492	C	5.69082362	4.90572827	-0.74686074
N	4.11402237	5.08048000	-0.52672833	N	4.52567271	4.37274487	-0.44276254
Br	6.08598545	-1.68148570	-0.30504784	Br	6.18003798	-2.38424973	-0.19823938
H	7.49428802	0.36822436	-0.24811926	H	7.68035866	-0.44838035	0.13594961
Br	3.45099087	-0.12138302	0.69470996	Br	3.43438465	-0.87175078	0.38808574
H	7.20211851	4.95542562	-1.40151067	H	7.70117840	4.13314869	-0.90879164
H	5.27797104	6.68018602	-1.33626060	H	5.86422712	5.94320926	-0.99444198
				K	0.00000000	0.00000000	2.38329433
				K	0.00000000	0.00000000	-1.59762950

Table S11. Cartesian coordinates (in Å) and ADF total bonding energies (in kcal mol^{-1}) of all iodine-bonding species in this work, computed at ZORA-BLYP-D3(BJ)/TZ2P.

I-Adenine (C_s)			[-2225.35]
N	-1.41826277	-1.40929990	0.00000000
C	-1.26518753	-0.07374275	0.00000000
C	0.04933244	0.45936784	0.00000000
C	1.09361550	-0.48232846	0.00000000
N	0.96929964	-1.82071456	0.00000000
C	-0.32029693	-2.19453937	0.00000000
N	0.54199590	1.76104607	0.00000000
C	1.85370530	1.61320609	0.00000000
N	2.24874373	0.28263103	0.00000000
N	-2.34374853	0.75217950	0.00000000
H	-0.51145121	-3.26485924	0.00000000
H	2.57551374	2.41850040	0.00000000
H	3.19470520	-0.07837793	0.00000000
I	-4.29952946	0.08784621	0.00000000
H	-2.19408165	1.75435949	0.00000000

I-Adenine (C_1)			[-2225.79]
N	1.10211818	-0.19176926	-0.50372178
C	1.85398465	-0.18964409	0.60895286
C	3.25748750	-0.05543714	0.48041541
C	3.74884092	0.03778519	-0.83669913
N	3.02246667	0.02153077	-1.96460134
C	1.70890998	-0.09526875	-1.70462594
N	4.29153234	0.01598109	1.40967508
C	5.38046095	0.14974152	0.67643886
N	5.11949144	0.16893927	-0.68675284
N	1.28773227	-0.38279190	1.84528742
H	1.04718615	-0.10639768	-2.56713129
H	6.38747996	0.23877045	1.06093460
H	5.78898414	0.26586087	-1.44027588
I	-0.72681370	0.09548365	2.16938255
H	1.87575579	-0.09167073	2.62362964

I-Thymine (C_s)			[-2086.57]
N	-0.00583049	-1.81696143	0.00000000
C	-0.95316411	-0.81482866	0.00000000
C	-0.61457603	0.49582189	0.00000000
C	0.80992753	0.86520627	0.00000000
N	1.71800574	-0.24171449	0.00000000
C	1.37613468	-1.60587224	0.00000000
C	-1.61865823	1.61821632	0.00000000
O	1.21832541	2.02044107	0.00000000
O	2.17284288	-2.53212425	0.00000000
H	-0.27726513	-2.79307672	0.00000000
I	3.76544038	0.21405379	0.00000000
H	-1.98505690	-1.15204392	0.00000000
H	-1.48304028	2.25831499	0.87939687
H	-1.48304028	2.25831499	-0.87939687
H	-2.64107968	1.22646967	0.00000000

I-Thymine ( )	[-]
Global minimum is C_s-symmetric.	

I-Guanine (C_s)			[-2291.53]
O	0.84597690	-2.73416364	0.00000000
C	0.47930795	-1.56946311	0.00000000
N	-0.98164790	-1.26873583	0.00000000
C	-1.50746072	0.00558423	0.00000000
N	-0.73157021	1.08977035	0.00000000
C	0.59391655	0.86452427	0.00000000
C	1.25352112	-0.36825590	0.00000000
N	2.63518455	-0.19330538	0.00000000
C	2.80590820	1.10881029	0.00000000
N	1.59694799	1.80972144	0.00000000
N	-2.84628880	0.34011343	0.00000000
I	-2.05845503	-3.11319986	0.00000000
H	3.75673112	1.62352999	0.00000000
H	1.46321564	2.81318858	0.00000000
H	-2.94189544	1.35027287	0.00000000
I	-4.70654628	-0.55391634	0.00000000

I-Guanine (C_1)			[-2302.40]
O	1.07542243	1.89083674	0.74116322
C	1.67779749	0.89376870	0.38331344
N	0.95301048	-0.28841764	-0.10114535
C	1.54896749	-1.46804812	-0.51030007
N	2.86537429	-1.64303448	-0.53762958
C	3.58188637	-0.56182733	-0.16598932
C	3.10204231	0.66376222	0.31458276
N	4.14813013	1.50980981	0.64123446
C	5.23734207	0.81815235	0.36595128
N	4.95683358	-0.44875383	-0.12934590
N	0.73834669	-2.49468260	-0.98723874
I	-1.12954481	0.04895022	-0.28072428
H	6.25318039	1.16367996	0.49927075
H	5.61672219	-1.16818920	-0.39949308
H	1.38134996	-3.20114496	-1.35560640
I	-0.29307105	-3.65480852	0.56554519

I-Cytosine (C_s)			[-1823.32]
C	0.67181120	-1.60964068	0.00000000
N	1.70412946	-0.60516770	0.00000000
C	1.44834210	0.72997026	0.00000000
C	0.16251844	1.17945438	0.00000000
C	-0.86724054	0.16282606	0.00000000
N	-0.62004179	-1.13431845	0.00000000
O	1.00350820	-2.78860043	0.00000000
N	-2.16654969	0.58170706	0.00000000
H	2.65404466	-0.96144261	0.00000000
H	2.30432256	1.39706859	0.00000000
H	-0.06442174	2.23919270	0.00000000
H	-2.39077556	1.56803477	0.00000000
I	-3.76919169	-0.72436332	0.00000000

I-Cytosine (C_1)			[-1823.55]
C	-4.25017232	-0.64639852	0.05202940
N	-5.68789654	-0.63542184	0.12285513
C	-6.42913273	0.50366302	0.11271454
C	-5.81376144	1.71694079	0.03206602
C	-4.36990657	1.69572990	-0.03149090
N	-3.64858082	0.59300374	-0.00738918
O	-3.67068185	-1.72446782	0.05880682
N	-3.73151201	2.90763781	-0.17916948
H	-6.12451037	-1.54914901	0.18766631
H	-7.50701295	0.39240575	0.17221751
H	-6.38426237	2.63794318	0.00671610
H	-4.23245046	3.73026232	0.14138389
I	-1.67431458	3.06277781	0.13730854

I-Xanthine (C_s)			[-2194.75]
N	-5.98328923	3.79102938	0.00000000
C	-3.40635323	3.52261993	0.00000000
C	-4.65514203	4.23432756	0.00000000

I-Xanthine ( )	[-]
Global minimum is C_s-symmetric.	

C	-4.75750570	5.61531387	0.00000000
N	-3.63372459	6.40575802	0.00000000
C	-2.34411919	5.87060953	0.00000000
N	-2.30081671	4.44610447	0.00000000
O	-3.24673976	2.30683581	0.00000000
C	-6.77476526	4.90943206	0.00000000
O	-1.34939747	6.57785494	0.00000000
H	-3.70209163	7.41796659	0.00000000
I	-6.64230492	1.81689084	0.00000000
H	-7.85313377	4.84768203	0.00000000
N	-6.05799641	6.03693529	0.00000000
I	-0.39112130	3.58848316	0.00000000

I-AT base pair (C_s)			[-4322.60]
N	-2.12120610	0.50706189	0.00000000
C	-3.04212430	-0.48447558	0.00000000
C	-4.41337348	-0.10484297	0.00000000
C	-4.69357902	1.26739352	0.00000000
N	-3.79143843	2.26625396	0.00000000
C	-2.54055785	1.80436348	0.00000000
N	-5.57977701	-0.86055085	0.00000000
C	-6.54902978	0.03661072	0.00000000
N	-6.07577640	1.34105252	0.00000000
N	-2.75561627	-1.80944505	0.00000000
H	-1.74404706	2.54278719	0.00000000
H	-7.60774532	-0.18342204	0.00000000
H	-6.62158885	2.19420014	0.00000000
I	-0.92800941	-2.76625719	0.00000000
H	-3.55949004	-2.42844843	0.00000000
N	4.69263287	2.21149310	0.00000000
C	5.49389418	1.08969840	0.00000000
C	4.97314698	-0.16057760	0.00000000
C	3.50943551	-0.31730952	0.00000000
N	2.76316160	0.89049304	0.00000000
C	3.29070192	2.18194953	0.00000000
C	5.80882920	-1.41300226	0.00000000
O	2.94848579	-1.41461194	0.00000000
O	2.63208635	3.21599771	0.00000000
H	5.09231047	3.14212929	0.00000000
I	0.62754470	0.68330436	0.00000000
H	6.56300236	1.28002923	0.00000000
H	5.58372693	-2.02852896	0.87901115
H	5.58372693	-2.02852896	-0.87901115
H	6.87716390	-1.17168852	0.00000000

I-AT base pair (C_1)			[-4323.49]
N	-2.03107216	0.46357427	0.33836413
C	-2.86232988	-0.42638435	-0.24783897
C	-4.20310923	-0.02779147	-0.45871868
C	-4.55375332	1.26774250	-0.03363339
N	-3.74400464	2.15535687	0.56432323
C	-2.50208121	1.68128759	0.70943185
N	-5.29629753	-0.69156489	-1.00366225
C	-6.28367836	0.17937969	-0.91527461
N	-5.89819842	1.38136342	-0.33622495
N	-2.43163667	-1.64740833	-0.70451379
H	-1.77114861	2.33921670	1.17005924
H	-7.29929061	0.01088689	-1.24654015
H	-6.47815210	2.19230859	-0.15663061
I	-1.11741840	-2.85386668	0.41962421
H	-3.21615667	-2.22471070	-1.00576481
N	4.60907606	2.35770460	-0.16764397
C	5.45609010	1.29775815	-0.41372363
C	4.99803754	0.02809037	-0.52112974
C	3.55400634	-0.21936561	-0.36690698
N	2.75659335	0.93028618	-0.12717898
C	3.22050219	2.23983972	-0.01113410
C	5.88350703	-1.15933058	-0.79032662
O	3.05023700	-1.34045386	-0.43798438
O	2.52071863	3.22373959	0.20654773
H	4.96135328	3.30365173	-0.08559477
I	0.63735421	0.61380393	0.09147596
H	6.50676328	1.55358541	-0.51355380
H	5.79793077	-1.89694104	0.01634393
H	5.57821423	-1.66807377	-1.71244566
H	6.93138733	-0.85433255	-0.88340483

I-GC base pair (C_s)			[-4132.10]
C	-4.41811835	0.09501841	0.00000000
N	-5.83440592	0.08124782	0.00000000
C	-6.56889016	1.23477317	0.00000000
C	-5.95027007	2.44780205	0.00000000
C	-4.50496056	2.43488398	0.00000000
N	-3.80986509	1.29879880	0.00000000
O	-3.81578094	-1.00162354	0.00000000
N	-3.80374661	3.59177673	0.00000000
H	-6.28087887	-0.82977958	0.00000000
H	-7.64731014	1.12243431	0.00000000
H	-6.52350215	3.36802773	0.00000000
H	-4.28093862	4.48425143	0.00000000
I	-1.72099248	3.54572591	0.00000000
O	0.65521564	1.71848550	0.00000000
C	1.47551158	0.80022803	0.00000000
N	1.01155495	-0.59115572	0.00000000
C	1.87083982	-1.66094029	0.00000000
N	3.20491429	-1.54078961	0.00000000
C	3.65724284	-0.27639103	0.00000000
C	2.90117280	0.89893374	0.00000000
N	3.72832507	2.02234889	0.00000000
C	4.94943958	1.53720681	0.00000000
N	4.97345820	0.14005817	0.00000000
N	1.50254612	-2.99542229	0.00000000
I	-1.17632599	-0.66688793	0.00000000
H	5.86202188	2.11716498	0.00000000
H	5.78407887	-0.46577805	0.00000000
H	2.33413076	-3.57557884	0.00000000
I	-0.18754075	-4.18237079	0.00000000

I-GC base pair (C_1)			[-4143.22]
C	-4.52882242	0.32089107	-0.52545407
N	-5.92609275	0.43499861	-0.71814116
C	-6.57176996	1.63671941	-0.61526680
C	-5.88010200	2.77242570	-0.32015784
C	-4.45495422	2.62828981	-0.12855941
N	-3.84935236	1.44647455	-0.23579943
O	-4.00538790	-0.81262236	-0.63406015
N	-3.67542640	3.69419323	0.16284687
H	-6.42904780	-0.41876291	-0.93648527
H	-7.64345627	1.62519551	-0.77957363
H	-6.38477063	3.72838541	-0.23719608
H	-4.08290935	4.61062298	0.30006636
I	-1.63160193	3.40232425	0.49441735
O	0.59873062	1.50746231	0.72975574
C	1.31840437	0.64734203	0.22171007
N	0.78330475	-0.62283294	-0.21591454
C	1.56543465	-1.64444154	-0.70050350
N	2.88464462	-1.56800447	-0.88832177
C	3.40051394	-0.35754263	-0.59750492
C	2.73376137	0.74107044	-0.04043476
N	3.61074969	1.79637755	0.16778214
C	4.77799276	1.35104066	-0.25508045
N	4.71472838	0.04702608	-0.73179574
N	0.93834602	-2.82536371	-1.10270968
I	-1.40056486	-0.69780964	-0.32641695
H	5.70499004	1.90770024	-0.24787853
H	5.47304636	-0.51847587	-1.09281536
H	1.68064188	-3.40280655	-1.50687249
I	0.24975248	-4.11463013	0.52874455

I-G_4 quartet (C_{4h})			[-9241.06]
N	6.55024760	-1.19678798	0.00000000
O	2.23572675	-3.10797535	0.00000000
N	4.34096083	-2.19824056	0.00000000
C	5.72773049	-2.28074066	0.00000000
N	6.34431197	-3.48741527	0.00000000
C	5.52961061	-4.55069681	0.00000000
C	4.12757704	-4.57002519	0.00000000
C	3.45313150	-3.31884971	0.00000000
N	5.89665993	-5.89116793	0.00000000
C	4.73337286	-6.64779846	0.00000000
N	3.65357664	-5.88732663	0.00000000
I	6.43439872	0.98955330	0.00000000
H	7.51804526	-1.50393532	0.00000000
I	3.24846281	-0.37069033	0.00000000
H	6.84690854	-6.24039914	0.00000000
H	4.74352374	-7.72748287	0.00000000
N	1.19678798	6.55024760	0.00000000
O	3.10797535	2.23572675	0.00000000
N	2.19824056	4.34096083	0.00000000
C	2.28074066	5.72773049	0.00000000
N	3.48741527	6.34431197	0.00000000
C	4.55069681	5.52961061	0.00000000
C	4.57002519	4.12757704	0.00000000
C	3.31884971	3.45313150	0.00000000
N	5.89116793	5.89665993	0.00000000
C	6.64779846	4.73337286	0.00000000
N	5.88732663	3.65357664	0.00000000
I	-0.98955330	6.43439872	0.00000000
H	1.50393532	7.51804526	0.00000000
I	0.37069033	3.24846281	0.00000000
H	6.24039914	6.84690854	0.00000000
H	7.72748287	4.74352374	0.00000000
N	-6.55024760	1.19678798	0.00000000
O	-2.23572675	3.10797535	0.00000000
N	-4.34096083	2.19824056	0.00000000
C	-5.72773049	2.28074066	0.00000000
N	-6.34431197	3.48741527	0.00000000
C	-5.52961061	4.55069681	0.00000000
C	-4.12757704	4.57002519	0.00000000
C	-3.45313150	3.31884971	0.00000000
N	-5.89665993	5.89116793	0.00000000
C	-4.73337286	6.64779846	0.00000000
N	-3.65357664	5.88732663	0.00000000
I	-6.43439872	-0.98955330	0.00000000
H	-7.51804526	1.50393532	0.00000000
I	-3.24846281	0.37069033	0.00000000
H	-6.84690854	6.24039914	0.00000000
H	-4.74352374	7.72748287	0.00000000
N	-1.19678798	-6.55024760	0.00000000
O	-3.10797535	-2.23572675	0.00000000
N	-2.19824056	-4.34096083	0.00000000
C	-2.28074066	-5.72773049	0.00000000
N	-3.48741527	-6.34431197	0.00000000
C	-4.55069681	-5.52961061	0.00000000
C	-4.57002519	-4.12757704	0.00000000
C	-3.31884971	-3.45313150	0.00000000
N	-5.89116793	-5.89665993	0.00000000
C	-6.64779846	-4.73337286	0.00000000
N	-5.88732663	-3.65357664	0.00000000
I	0.98955330	-6.43439872	0.00000000
H	-1.50393532	-7.51804526	0.00000000
I	-0.37069033	-3.24846281	0.00000000
H	-6.24039914	-6.84690854	0.00000000
H	-7.72748287	-4.74352374	0.00000000

I-G_4 quartet (S_4)			[-9274.96]
N	3.06304475	3.84841920	-2.29701983
N	1.74527135	3.74954987	-0.31794810
C	2.23276454	4.46006874	-1.39720952
N	1.87759463	5.72961816	-1.65786088
C	0.90926506	6.20150936	-0.85118843
C	0.39424068	5.60221068	0.29951842
C	0.89697271	4.31472995	0.70061126
N	0.20082479	7.38616703	-0.98838176
C	-0.72913846	7.43302082	0.03696541
N	-0.63487973	6.37944917	0.83084461
O	0.61726454	3.68484532	1.71807840
I	4.75114897	2.61057226	-1.73926381
H	3.34745472	4.52634573	-3.00170475
I	1.67205627	1.50134954	-0.18496403
H	0.32690808	8.06487621	-1.72927001
H	-1.44316778	8.23685901	0.13812261
N	3.84841920	-3.06304475	2.29701983
N	3.74954987	-1.74527135	0.31794810
C	4.46006874	-2.23276454	1.39720952
N	5.72961816	-1.87759463	1.65786088
C	6.20150936	-0.90926506	0.85118843
C	5.60221068	-0.39424068	-0.29951842
C	4.31472995	-0.89697271	-0.70061126
N	7.38616703	-0.20082479	0.98838176
C	7.43302082	0.72913846	-0.03696541
N	6.37944917	0.63487973	-0.83084461
O	3.68484532	-0.61726454	-1.71807840
I	2.61057226	-4.75114897	1.73926381
H	4.52634573	-3.34745472	3.00170475
I	1.50134954	-1.67205627	0.18496403
H	8.06487621	-0.32690808	1.72927001
H	8.23685901	1.44316778	-0.13812261
N	-3.06304475	-3.84841920	-2.29701983
N	-1.74527135	-3.74954987	-0.31794810
C	-2.23276454	-4.46006874	-1.39720952
N	-1.87759463	-5.72961816	-1.65786088
C	-0.90926506	-6.20150936	-0.85118843
C	-0.39424068	-5.60221068	0.29951842
C	-0.89697271	-4.31472995	0.70061126
N	-0.20082479	-7.38616703	-0.98838176
C	0.72913846	-7.43302082	0.03696541
N	0.63487973	-6.37944917	0.83084461
O	-0.61726454	-3.68484532	1.71807840
I	-4.75114897	-2.61057226	-1.73926381
H	-3.34745472	-4.52634573	-3.00170475
I	-1.67205627	-1.50134954	-0.18496403
H	-0.32690808	-8.06487621	-1.72927001
H	1.44316778	-8.23685901	0.13812261
N	-3.84841920	3.06304475	2.29701983
N	-3.74954987	1.74527135	0.31794810
C	-4.46006874	2.23276454	1.39720952
N	-5.72961816	1.87759463	1.65786088
C	-6.20150936	0.90926506	0.85118843
C	-5.60221068	0.39424068	-0.29951842
C	-4.31472995	0.89697271	-0.70061126
N	-7.38616703	0.20082479	0.98838176
C	-7.43302082	-0.72913846	-0.03696541
N	-6.37944917	-0.63487973	-0.83084461
O	-3.68484532	0.61726454	-1.71807840
I	-2.61057226	4.75114897	1.73926381
H	-4.52634573	3.34745472	3.00170475
I	-1.50134954	1.67205627	0.18496403
H	-8.06487621	0.32690808	1.72927001
H	-8.23685901	-1.44316778	-0.13812261

I-Xan$_4$ quartet (C_{4h})			[-8827.25]
N	3.80291265	6.00305585	0.00000000
N	-3.80291265	-6.00305585	0.00000000
N	6.00305585	-3.80291265	0.00000000
N	-6.00305585	3.80291265	0.00000000
C	3.54942020	3.41295408	0.00000000
C	-3.54942020	-3.41295408	0.00000000
C	3.41295408	-3.54942020	0.00000000
C	-3.41295408	3.54942020	0.00000000
C	4.23924063	4.66984984	0.00000000
C	-4.23924063	-4.66984984	0.00000000
C	4.66984984	-4.23924063	0.00000000
C	-4.66984984	4.23924063	0.00000000
C	5.62528516	4.76235064	0.00000000
C	-5.62528516	-4.76235064	0.00000000
C	4.76235064	-5.62528516	0.00000000
C	-4.76235064	5.62528516	0.00000000
N	6.40876355	3.63160141	0.00000000
N	-6.40876355	-3.63160141	0.00000000
N	3.63160141	-6.40876355	0.00000000
N	-3.63160141	6.40876355	0.00000000
C	5.86490362	2.34868307	0.00000000
C	-5.86490362	-2.34868307	0.00000000
C	2.34868307	-5.86490362	0.00000000
C	-2.34868307	5.86490362	0.00000000
N	4.45372370	2.30805969	0.00000000
N	-4.45372370	-2.30805969	0.00000000
N	2.30805969	-4.45372370	0.00000000
N	-2.30805969	4.45372370	0.00000000
O	6.58863731	1.35134359	0.00000000
O	-6.58863731	-1.35134359	0.00000000
O	1.35134359	-6.58863731	0.00000000
O	-1.35134359	6.58863731	0.00000000
O	2.33037166	3.21561185	0.00000000
O	-2.33037166	-3.21561185	0.00000000
O	3.21561185	-2.33037166	0.00000000
O	-3.21561185	2.33037166	0.00000000
C	-6.77855647	4.92840986	0.00000000
C	6.77855647	-4.92840986	0.00000000
C	4.92840986	6.77855647	0.00000000
C	-4.92840986	-6.77855647	0.00000000
H	-7.85759790	4.87718845	0.00000000
H	7.85759790	-4.87718845	0.00000000
H	4.87718845	7.85759790	0.00000000
H	-4.87718845	-7.85759790	0.00000000
N	6.05688271	6.05633399	0.00000000
N	-6.05688271	-6.05633399	0.00000000
N	6.05633399	-6.05688271	0.00000000
N	-6.05633399	6.05688271	0.00000000
I	-3.58273461	-0.38610025	0.00000000
I	3.58273461	0.38610025	0.00000000
I	-0.38610025	3.58273461	0.00000000
I	0.38610025	-3.58273461	0.00000000
H	-7.42121213	-3.69750573	0.00000000
H	7.42121213	3.69750573	0.00000000
H	-3.69750573	7.42121213	0.00000000
H	3.69750573	-7.42121213	0.00000000
I	-1.80817252	-6.64517925	0.00000000
I	1.80817252	6.64517925	0.00000000
I	-6.64517925	1.80817252	0.00000000
I	6.64517925	-1.80817252	0.00000000

I-Xan$_4$ quartet (C_4)			[-8827.61]
N	3.75807161	5.96382117	-0.05685717
N	-3.75807161	-5.96382117	-0.05685717
N	5.96382117	-3.75807161	-0.05685717
N	-5.96382117	3.75807161	-0.05685717
C	3.53394638	3.40306249	0.34493151
C	-3.53394638	-3.40306249	0.34493151
C	3.40306249	-3.53394638	0.34493151
C	-3.40306249	3.53394638	0.34493151
C	4.19836024	4.63510647	0.03573700
C	-4.19836024	-4.63510647	0.03573700
C	4.63510647	-4.19836024	0.03573700
C	-4.63510647	4.19836024	0.03573700
C	5.56345340	4.70635431	-0.21168874
C	-5.56345340	-4.70635431	-0.21168874
C	4.70635431	-5.56345340	-0.21168874
C	-4.70635431	5.56345340	-0.21168874
N	6.34315165	3.57314178	-0.19990843
N	-6.34315165	-3.57314178	-0.19990843
N	3.57314178	-6.34315165	-0.19990843
N	-3.57314178	6.34315165	-0.19990843
C	5.80864768	2.30452291	0.01268771
C	-5.80864768	-2.30452291	0.01268771
C	2.30452291	-5.80864768	0.01268771
C	-2.30452291	5.80864768	0.01268771
N	4.42107432	2.28498085	0.26560375
N	-4.42107432	-2.28498085	0.26560375
N	2.28498085	-4.42107432	0.26560375
N	-2.28498085	4.42107432	0.26560375
O	6.52670908	1.30206772	-0.02155732
O	-6.52670908	-1.30206772	-0.02155732
O	1.30206772	-6.52670908	-0.02155732
O	-1.30206772	6.52670908	-0.02155732
O	2.35070778	3.23487886	0.65559400
O	-2.35070778	-3.23487886	0.65559400
O	3.23487886	-2.35070778	0.65559400
O	-3.23487886	2.35070778	0.65559400
C	-6.71435310	4.86026230	-0.35724800
C	6.71435310	-4.86026230	-0.35724800
C	4.86026230	6.71435310	-0.35724800
C	-4.86026230	-6.71435310	-0.35724800
H	-7.78305495	4.79937017	-0.50287396
H	7.78305495	-4.79937017	-0.50287396
H	4.79937017	7.78305495	-0.50287396
H	-4.79937017	-7.78305495	-0.50287396
N	5.98003292	5.98374682	-0.44664183
N	-5.98003292	-5.98374682	-0.44664183
N	5.98374682	-5.98003292	-0.44664183
N	-5.98374682	5.98003292	-0.44664183
I	-3.55049807	-0.38149871	0.53859942
I	3.55049807	0.38149871	0.53859942
I	-0.38149871	3.55049807	0.53859942
I	0.38149871	-3.55049807	0.53859942
H	-7.34104143	-3.62337288	-0.37642812
H	7.34104143	3.62337288	-0.37642812
H	-3.62337288	7.34104143	-0.37642812
H	3.62337288	-7.34104143	-0.37642812
I	-1.75375819	-6.58605891	-0.03015221
I	1.75375819	6.58605891	-0.03015221
I	-6.58605891	1.75375819	-0.03015221
I	6.58605891	-1.75375819	-0.03015221