

Exploiting the optical sensing of Fluorophore tagged DNA Nucleobases on hexagonal BN and Al-doped BN sheet: A Computational study

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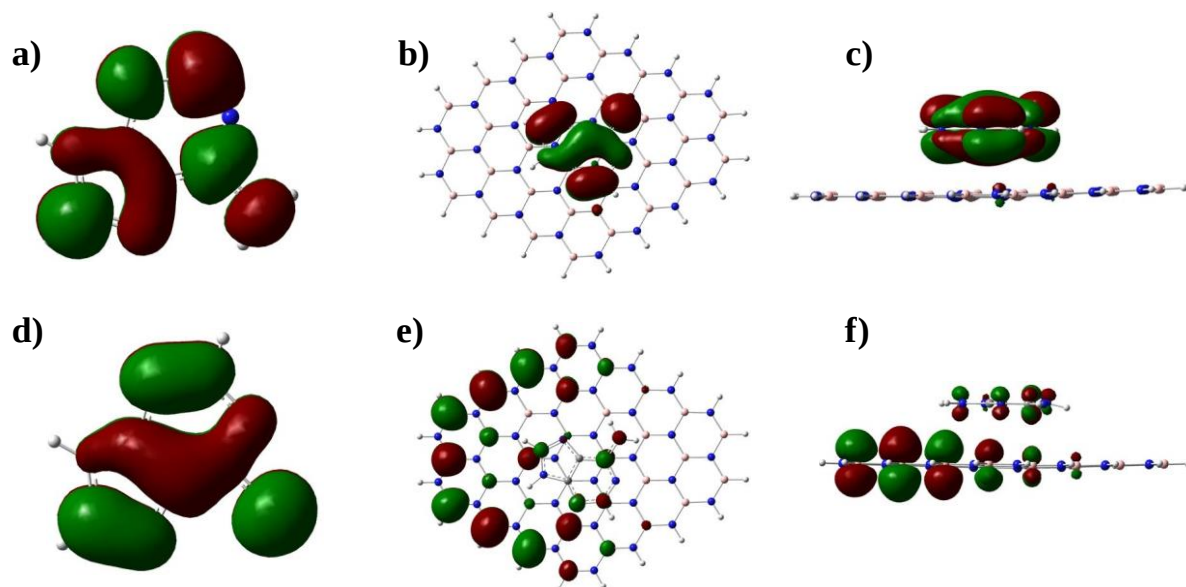


Figure S1. HOMO and LUMO of the isolated and complex systems. HOMOs of a) isolated adenine nucleobase and adsorbed adenine on *h*-BN sheet b) top view c) side view, LUMOs of d) isolated adenine and adsorbed adenine on *h*-BN sheet e) top view and f) side view.

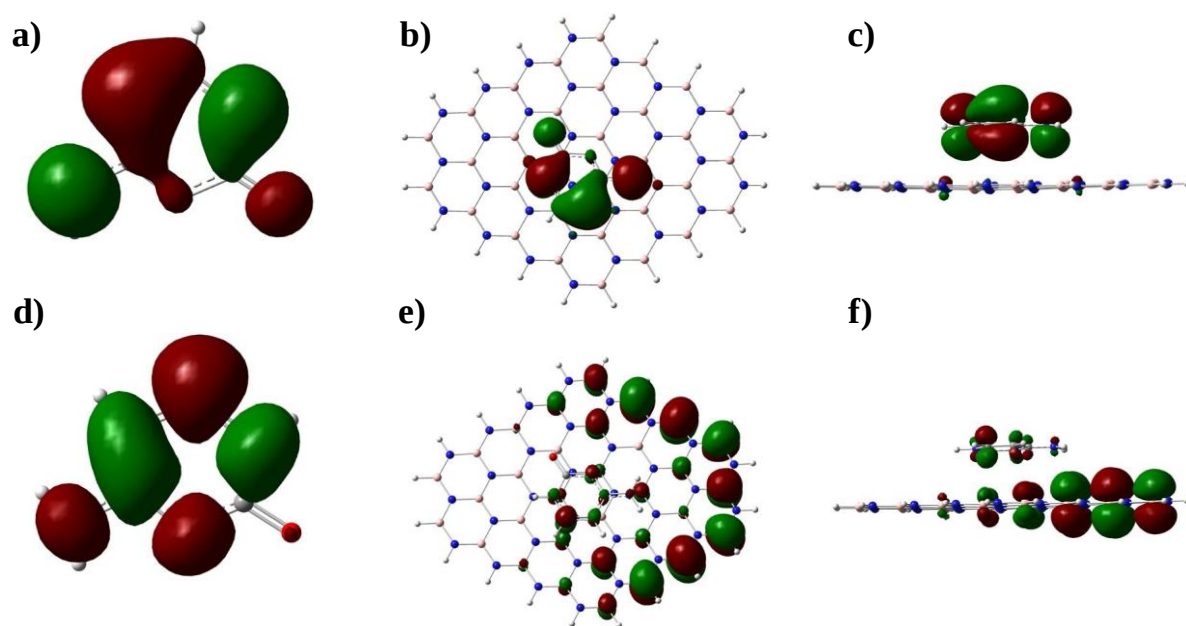


Figure S2. HOMO and LUMO of the isolated and complex systems. HOMOs of a) isolated cytosine nucleobase and adsorbed cytosine on *h*-BN sheet b) top view c) side view, LUMOs of d) isolated cytosine and adsorbed cytosine on *h*-BN sheet e) top view and f) side view.

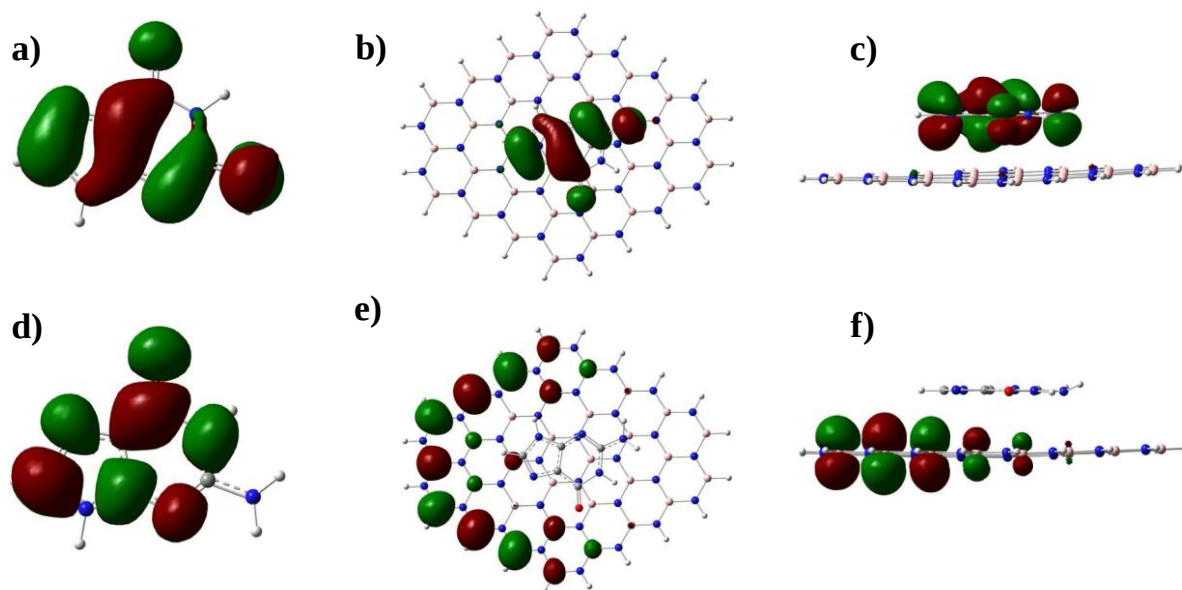


Figure S3. HOMO and LUMO of the isolated and complex systems. HOMOs of a) isolated guanine nucleobase and adsorbed guanine on *h*-BN sheet b) top view c) side view, LUMOs of d) isolated guanine and adsorbed guanine on *h*-BN sheet e) top view and f) side view.

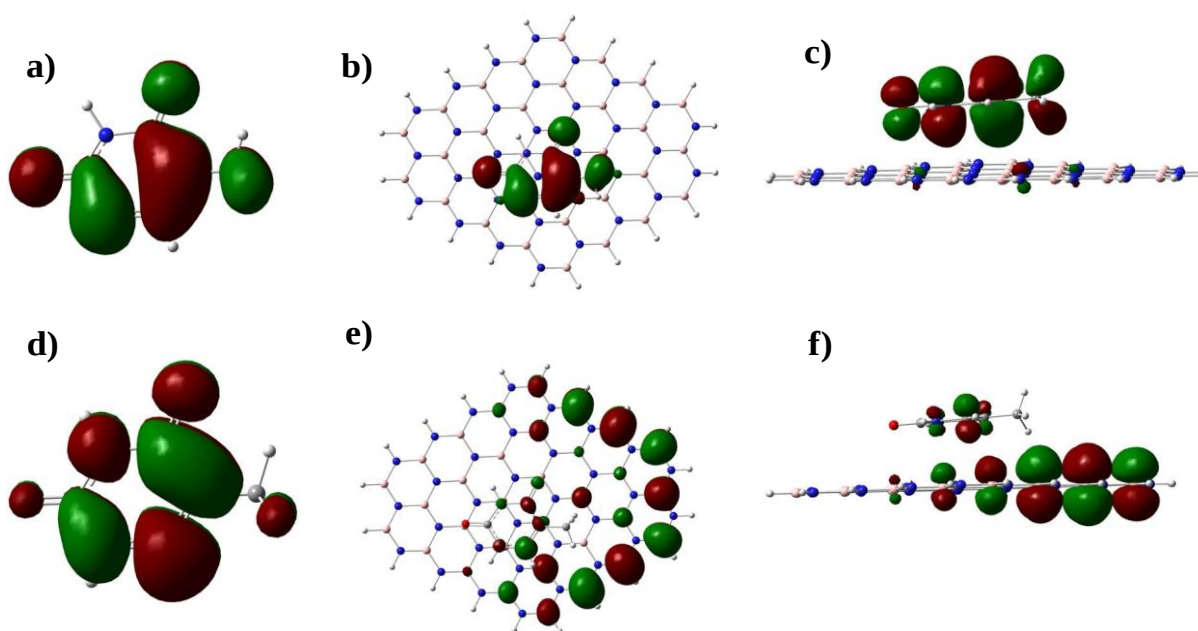


Figure S4. HOMO and LUMO of the isolated and complex systems. HOMOs of a) isolated thymine nucleobase and adsorbed thymine on *h*-BN sheet b) top view c) side view, LUMOs of d) isolated thymine and adsorbed thymine on *h*-BN sheet e) top view and f) side view.

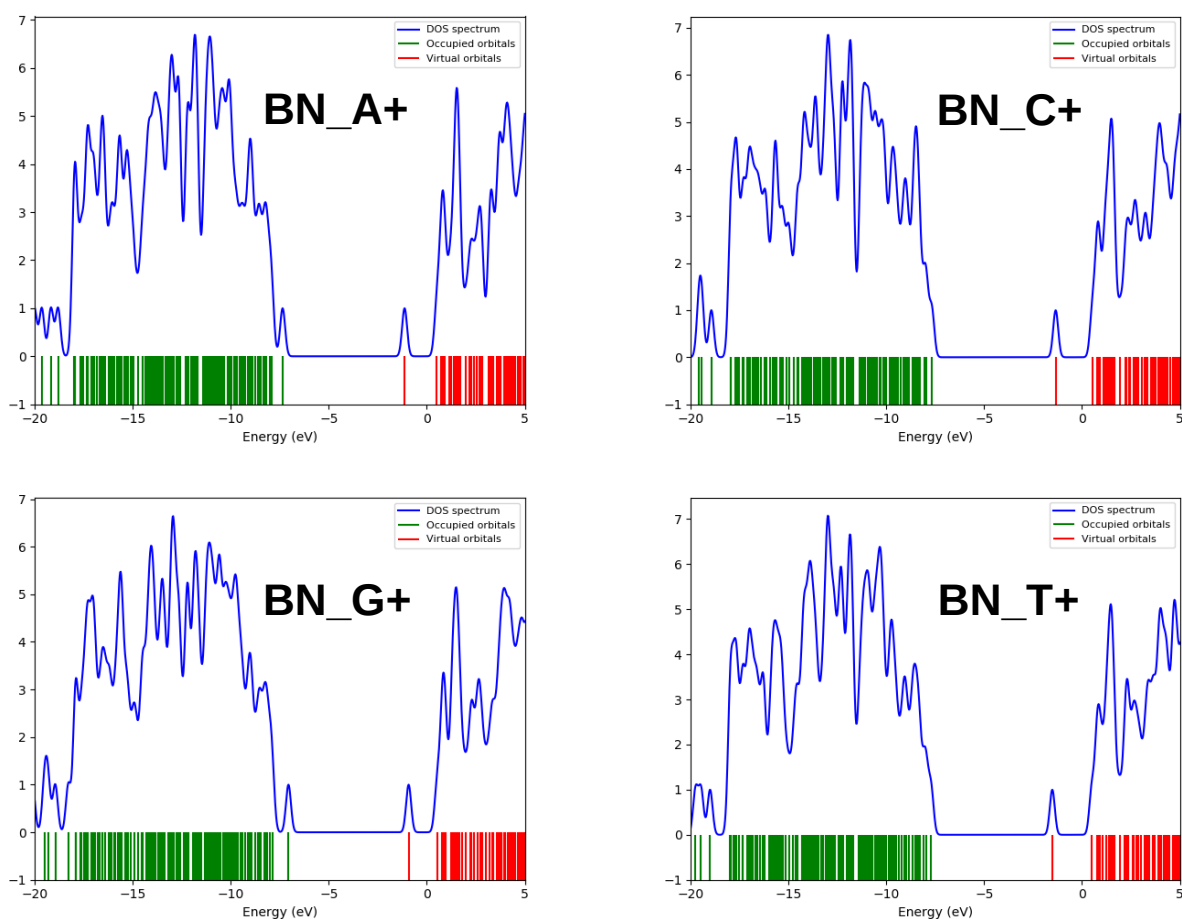


Figure S5. Total density of states of adsorbed nucleobases with attached fluorophore on the *h*-BN sheet calculated using the M062X/6-31G* level of theory using Gausssum software.

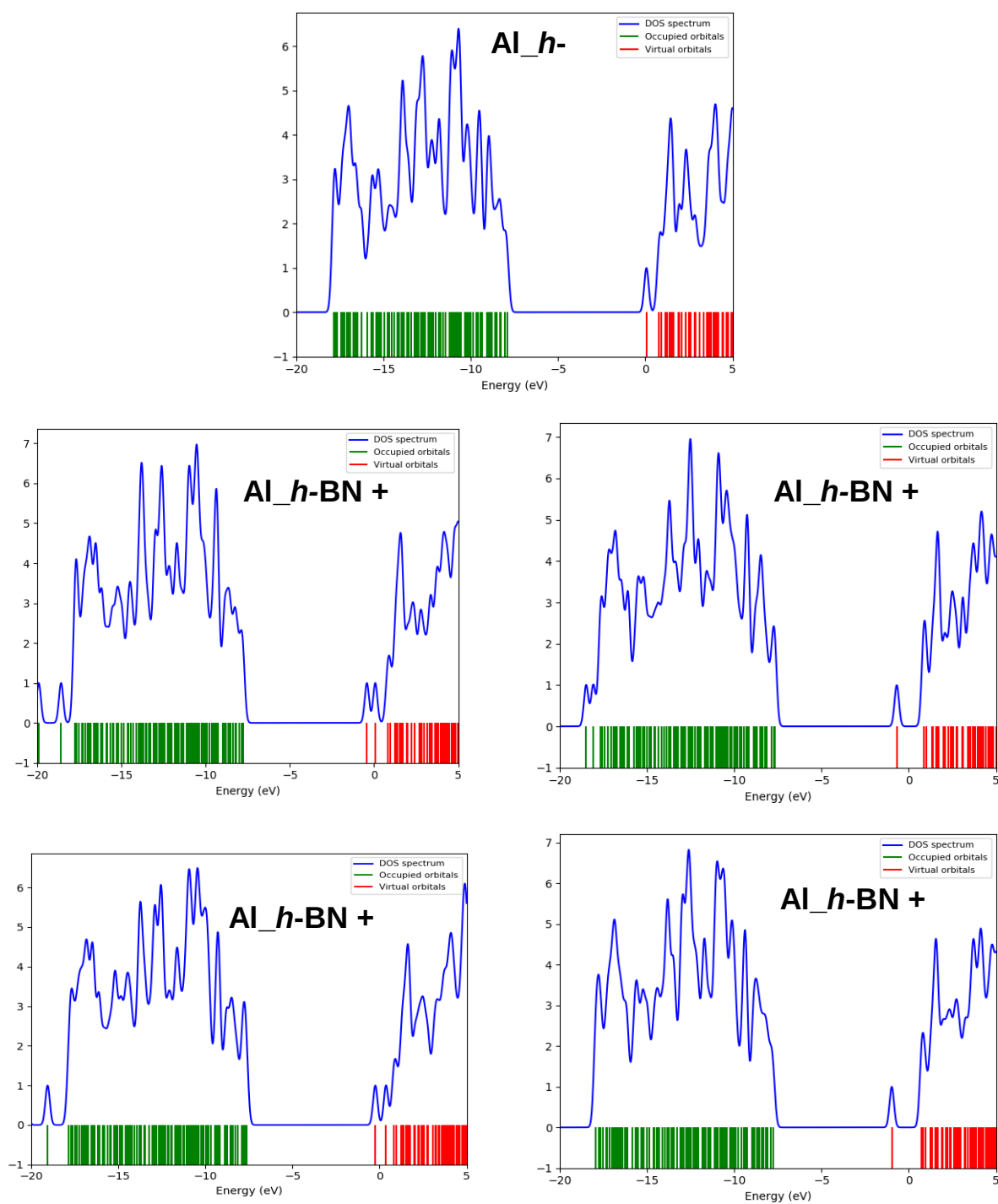


Figure S6. Total density of states of adsorbed nucleobases on the aluminium doped hexagonal boron nitride (Al_hBN) sheet calculated using the M062X/6-31G* level of theory using Gausssum software.

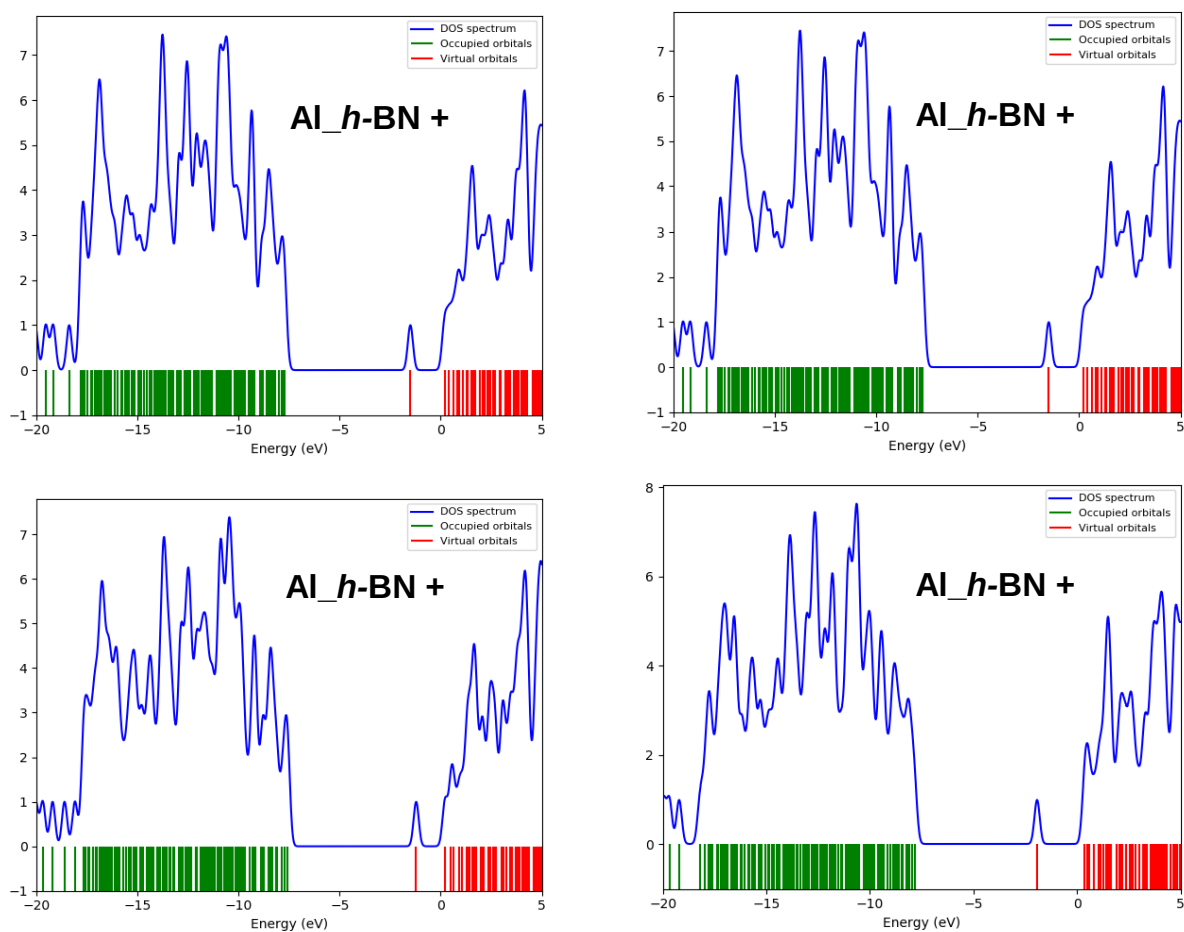


Figure S7. Total density of states of adsorbed nucleobases with attached fluorophore on the aluminium doped hexagonal boron nitride (Al_hBN) sheet calculated using the M062X/6-31G* level of theory using Gausssum software.

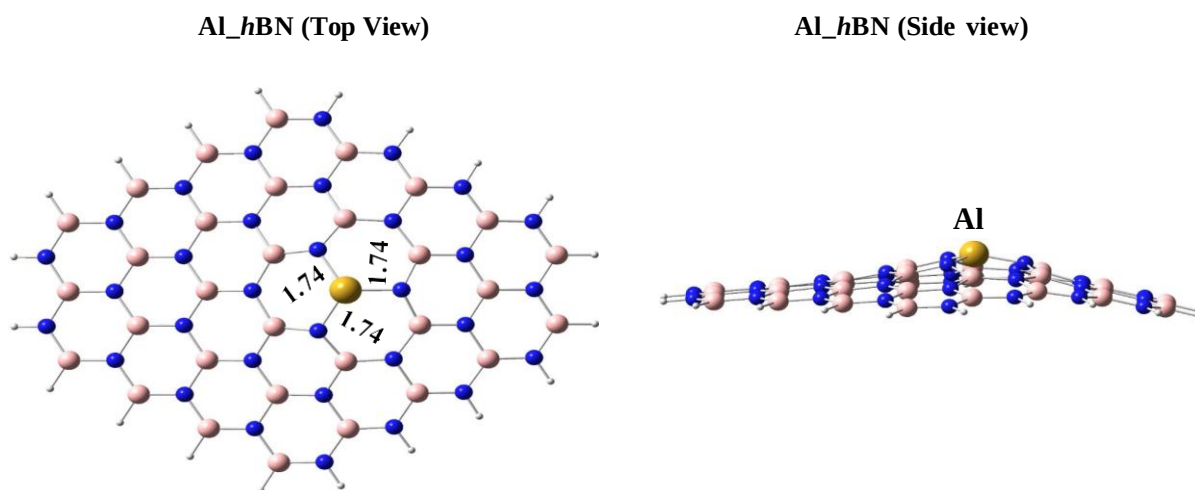


Figure S8. The optimized structures of Al_hBN sheet (top view and side view) calculated at M062X/6-31G* level of theory in the aqueous phase. Blue, white, golden, and light orange spheres represent N, H, Al, and B atoms, respectively. Distances are given in Angstrom (Å).

Table S1: The calculated binding energies (eV) of nucleobases with pristine *h*-BN sheet in aqueous phase.

Systems	B3LYP-D3/6-31G* level of theory ΔE (eV)
<i>h</i> -BN+A	-0.92
<i>h</i> -BN+C	-0.81
<i>h</i> -BN+G	-0.97
<i>h</i> -BN+T	-0.94
Al- <i>h</i> -BN+A	-2.09
Al- <i>h</i> -BN+C	-2.28
Al- <i>h</i> -BN+G	-2.12
Al- <i>h</i> -BN+T	-1.09

Table S2: Atoms in molecules (AIM) analyses of aluminium doped *h*-BN sheet complexed with the studied nucleobases calculated using the M06-2X/6-31G* level of theory in aqueous phase.

Table S3: The absorption (λ_{nm}) of different *h*-BN size sheets calculated at M06-2X/6-31G* level of theory in aqueous phase.

Different <i>h</i> -BN size	Absorption (λ_{nm})
B ₃₂ N ₃₂ H ₂₀ (Our studied model)	174.3 nm (main peak), 185.8 nm (Shoulder Peak)
B ₃₅ N ₃₅ H ₂₂ (Big)	177.3 nm (main peak), 186.0 nm (Shoulder Peak)
B ₂₇ N ₂₇ H ₁₈ (Middle)	171.2 nm (Main peak), 185.7 nm (Shoulder Peak)
B ₁₂ N ₁₂ H ₁₂ (Small)	165.3 nm (main peak), 179.5 nm (Shoulder Peak)

Cartesian coordinates of Individual *h*-BN, Al_*h*BN, nucleobase, nucleobase tagged fluorophore, and complexed systems using M062X/6-31G* level of theory in aqueous phase.

Systems	Critical-points (CP)	Density of all electrons	Laplacian of electron density, ($\nabla^2 r$)	Total Energy density H(r)	Potential energy density V(r)	Lagrangian kinetic energy, G(r)	$ V(r) / G(r)$
Al_ <i>h</i> -BN+A	CP- 141	0.02592	0.07230	-0.00107	-0.02023	0.01915	1.05
	CP-174	0.05950	0.34810	0.00079	-0.08543	0.08622	1.00
	CP-205	0.00420	0.01450	-0.00080	-0.00200	0.00281	0.71
Al_ <i>h</i> -BN+C	CP-125	0.01836	0.05394	0.00003	-0.01341	0.01345	0.99
	CP-164	0.05839	0.32898	-0.00001	-0.08228	0.08226	1.00
	CP-189	0.01219	0.03393	-0.00005	-0.00858	0.00853	1.00
Al_ <i>h</i> BN+G	CP-161	0.00434	0.01425	0.00051	-0.00254	0.00305	0.83
	CP-177	0.05398	0.29803	-0.00016	-0.07482	0.07466	1.00
	CP-189	0.01019	0.03459	0.00089	-0.00685	0.00775	0.88
Al_ <i>h</i> -BN+T	CP-179	0.04151	0.19327	-0.00133	-0.05099	0.04965	1.02
	CP-181	0.00584	0.01922	0.00089	-0.00300	0.00390	0.76
	CP-143	0.00639	0.01725	0.00055	-0.00319	0.00375	0.85
<i>h</i>-BN sheet				B	-1.42248100	2.50860700	-0.00000200
H	1.3547160	-	0.00000500	B	-	-	0.00000000
O	0	7.30504300			3.59349100	3.76846800	0.00000300
H	-	-	0.00000400	B	-	-	-0.00000100
	1.14949900	7.12837600			1.41729500	5.01956400	-0.00000200
H	-	-	0.00000300	B	-	3.7684680	0.00000100
	3.35040900	5.87142000			3.59348700	0	0.00001200
H	-	-	0.00000000	B	-	5.0195640	-0.00001300
	5.53402600	4.61224700			1.41729300	0	-0.00000200
H	-	-	0.00000500	B	-	2.5111160	-0.00000200
	7.72241600	3.34034500			5.76566600	0	-0.00000300
H	-	1.2645740	0.00000000	B	-	1.2539400	0.00000100
	9.13282500	0			7.93713200	0	0.00000400
H	-	3.3403500	0.00000000	B	-	-	0.00000400
	7.72241000	0			7.93713200	1.25393700	0.00000100
H	-	-	0.00000500	B	0.7500990	3.7586040	0.00000300
	9.13282500	1.26457000			0	0	0.00000100
H	-	4.6122480	0.00000100	B	0.7605980	6.2684450	0.00000100
	5.53402100	0			0	0	0.00000200
H	-	5.8714190	-0.00000100	B	-	-	
	3.35041000	0					
H	-	7.1283730	-0.00000200				

	1.14950300	0		B	5.76566800	2.51111500
H	1.3547220	7.3050410	-0.00000200		0.7500950	-
	0	0		B	0	3.75860500
H	3.5241820	6.0378370	-0.00000200		0.7605970	-
	0	0		B	0	6.26844300
H	5.6836430	4.7889850	-0.00000100		2.9221200	-
	0	0		B	0	5.00585100
H	7.8658700	3.5365250	0.00000000		2.9171470	-
	0	0		B	0	2.50171000
H	3.5241800	-	0.00000500		5.0877340	-
	0	6.03783700		B	0	3.75359900
H	5.6836410	-	0.00000400		5.0881520	-
	0	4.78898900		B	0	1.25160600
				B	7.2609960	0.0000020
					0	0
					7.2608670	-
					0	2.50686700

H	7.86587300	-3.53652200	0.00000500	B	7.26086500	2.50686900	0.00000000
H	8.95805400	1.27469600	0.00000200	B	5.08815100	1.25160000	-0.00000100
H	8.95805300	-1.27470300	0.00000500	B	2.91679300	-0.00000100	-0.00000100
B	0.74656000	-1.25243600	-0.00000100	B	2.91714700	2.50171100	-0.00000200
B	0.74656100	1.25243300	-0.00000200	B	5.08773400	3.75359500	-0.00000200
B	-1.42341700	0.00000000	-0.00000200	N	-0.65641000	-6.24412200	0.00000400
N	1.47176100	-0.00000100	-0.00000100	N	1.48671600	-5.01435400	0.00000300
N	-0.69786800	-1.25321100	-0.00000100	N	-0.69174900	-3.75981000	0.00000100
N	-0.69786800	1.25321000	-0.00000200	N	1.47380200	-2.50490900	0.00000100
N	-2.86689400	-2.50708800	-0.00000100	N	3.64199500	1.25217900	-0.00000100
N	-2.86874400	-0.00000100	-0.00000200	N	1.47380100	2.50490600	-0.00000200
B	-1.42248500	-2.50860500	-0.00000100	N	3.64199600	-1.25217900	0.00000000
B	-3.59323000	-1.25536900	-0.00000200	N	3.64694800	-3.75958900	0.00000300
B	-5.76477500	0.00000200	-0.00000100	N	3.64694700	3.75958800	-0.00000200
B	-3.59322600	1.25537000	-0.00000100	B	2.92212100	5.00585100	-0.00000200
				N	1.48671700	5.01435300	-0.00000200
				N	-0.65640700	6.24412300	-0.00000200
				N	-0.69174800	3.75981000	-0.00000200
				N	5.81233600	-2.51255700	0.00000200
				N	5.80980400	-0.00000200	0.00000000
				N	5.81233500	2.51255200	-0.00000100
				N	7.94571900	1.26371600	0.00000100
				N	7.94571900	-1.26371300	0.00000300
				N	-2.84594700	4.99285600	-0.00000100
				N	-2.86689200	2.50708800	-0.00000100
				N	-2.84595000	-4.99285500	0.00000200
				N	-5.02599800	-3.73575800	-0.00000100
				N	-5.04056000	-1.25193200	-0.00000200
				N	-5.04055800	1.25193200	0.00000000
				N	-5.02599500	3.73575900	0.00000000
				N	-7.20541500	2.47007000	0.00000400
				N	-7.22080300	0.00000100	-0.00000100
				N	-7.20541700	-2.47006800	-0.00000300

<i>h</i>-BN sheet +Adenine				B	-7.92362800	1.15665200	-0.38630700
N	2.03557600	0.80962200	2.56930900	B	-7.91613700	-1.35026100	-0.33288400
C	2.10738500	-0.55964400	2.60101900	B	0.75208700	3.68057100	-0.56016500
H	3.06164000	-1.06998600	2.61253500	B	0.75635600	6.19183100	-0.54172500
N	0.93497800	-1.14303400	2.61325300	B	-5.74195500	-2.60203400	-0.36210800
C	0.04271100	-0.09046100	2.58795300	B	0.77655700	-3.83198400	-0.40121600
C	-1.36663500	-0.03654500	2.57709500	B	0.79294200	-6.34084900	-0.29915200
N	-2.12847600	-1.15265600	2.63842600	B	2.95061000	-5.07343700	-0.33388300
H	-3.10892900	-1.06110500	2.40686100	B	2.93701300	-2.57098200	-0.42071500
H	-1.69307400	-2.04545600	2.44985900	B	5.11182900	-3.81449700	-0.33512600
N	-1.96422900	1.16232300	2.53607100	B	5.10447000	-1.31314400	-0.39535200
C	-1.19142500	2.26017300	2.50240300	B	7.27301500	-0.05435700	-0.36693100
H	-1.73203400	3.20408400	2.45151300	B	7.28062800	-2.56054400	-0.31710300
N	0.13453400	2.34912400	2.51542500	B	7.26547100	2.45207800	-0.40489800
C	0.70450800	1.13645100	2.55840300	B	5.09706600	1.18964200	-0.43891000
H	2.81668900	1.45296000	2.55963000	B	2.92840700	-0.06933100	-0.48710100
H	1.39011900	-7.37489900	-0.25673800	B	2.92153500	2.43250500	-0.51754600
H	-1.11563100	-7.20462600	-0.26672100	B	5.08867100	3.69133700	-0.46423300
H	-3.31804600	-5.95527400	-0.29997400	N	-0.62407400	-6.32023800	-0.30234400
H	-5.50506400	-4.70212500	-0.30831400	N	1.51542800	-5.08575900	-0.34674400
H	-7.69497200	-3.43604000	-0.28802800	N	-0.66617400	-3.83717200	-0.39795300
H	-9.11902900	1.16361700	-0.35595500	N	1.49613600	-2.57921200	-0.45802700
H	-7.71408900	3.24338000	-0.43010500	N	3.65124800	1.18505000	-0.47805700
H	-9.11141100	-1.36308400	-0.30104900	N	1.48110200	2.42991800	-0.56467100
H	-5.53137000	4.51967100	-0.49684600	N	3.65845100	-1.31847300	-0.43286800
H	-3.35224500	5.78410700	-0.53637300	N	3.67170600	-3.82542900	-0.36578900
H	-1.15632400	7.04696700	-0.55508500	N	3.64866200	3.69215700	-0.49919500
H	1.34858000	7.22969500	-0.52791300	B	2.91953700	4.93620500	-0.51164600
H	3.51868200	5.96997600	-0.49845400	N	1.48509000	4.93934100	-0.53705800
H	5.68127500	4.72862700	-0.45677500	N	-0.66011900	6.16452600	-0.56048400
H	7.86663900	3.48401900	-0.40513200	N	-0.68899300	3.68006900	-0.59321200
H	3.55557400	-6.10294000	-0.29218700	N	5.83239400	-2.57099400	-0.35061200
H	5.71104800	-4.84718100	-0.29458700	N	5.82233800	-0.05936800	-0.40108000
H	7.88803300	-3.58815000	-0.28038900	N	5.81720500	2.45262000	-0.43721400
H	8.96608900	1.22543900	-0.35041100	N	7.95404800	1.21144000	-0.37322800

H	8.97377300	-1.32250000	-0.30237900	N	7.96170300	-1.31544100	-0.32780900
B	0.76496600	-1.32900800	-0.49716300	N	-2.84554800	4.90711700	-0.55638700
B	0.75628700	1.17561900	-0.57004300	N	-2.85962600	2.42187900	-0.56918700
B	-1.40851700	-0.08162800	-0.55318400	N	-2.81647400	-5.07606300	-0.34216300
N	1.48542400	-0.07441800	-0.53781400	N	-4.99972800	-3.82508200	-0.35048000
N	-0.68016300	-1.33372200	-0.51515800	N	-5.02011400	-1.34200300	-0.41390200
N	-0.68765500	1.17241400	-0.60237600	N	-5.02728200	1.16123400	-0.46821000
N	-2.84475000	-2.59237500	-0.43851000	N	-5.02129500	3.64449800	-0.50744100
N	-2.85444600	-0.08674700	-0.53320600	N	-7.19572400	2.37392600	-0.42795800
B	-1.39946900	-2.58857300	-0.45478000	N	-7.20332400	-0.09527600	-0.38041900
B	-3.57323700	-1.34144000	-0.46736500	N	-7.18133700	-2.56449200	-0.32405200
B	-5.74774900	-0.09117700	-0.42151500				
B	-3.57947600	1.16827200	-0.51886400				
B	-1.41508400	2.42586800	-0.58883100				
B	-3.56737000	-3.85434600	-0.37680200				
B	-1.38760900	-5.09806900	-0.34685600				
B	-3.58873100	3.67980500	-0.54538600				
B	-1.41655500	4.93653200	-0.57180300				
B	-5.75605600	2.41791300	-0.46848100				
h-BN sheet + cytosine				B	5.14921300	-3.64449900	-0.42887500
N	-1.81091000	-0.81203200	2.55178400	N	-0.65405300	6.31489200	-0.18359800
C	-1.18990900	-2.01411200	2.63204600	N	1.49475100	5.09699900	-0.19884700
H	-1.82878200	-2.88987900	2.66086800	N	-0.67513300	3.83257900	-0.30951900
C	0.16319900	-2.07535900	2.65891900	N	1.49723500	2.59082200	-0.33778300
H	0.69184700	-3.01764400	2.71760100	N	3.69016300	-1.15117500	-0.43882200
C	0.85560500	-0.81724800	2.58415300	N	1.52925700	-2.41324500	-0.50139700
N	2.20187100	-0.81135800	2.59584300	N	3.67210100	1.34985100	-0.33148400
H	2.68684200	0.06734100	2.47584100	N	3.66130700	3.85469300	-0.20925200
H	2.73729900	-1.66554800	2.55145800	N	3.70853500	-3.65747400	-0.45461800
N	0.24282200	0.35601500	2.50845600	B	2.99051400	-4.90748600	-0.45853700
C	-1.12037000	0.41090400	2.50606100	N	1.55535800	-4.92258400	-0.46740300
O	-1.77099100	1.45136700	2.45682300	N	-0.58024800	-6.16385600	-0.44716500
H	-2.82175700	-0.75073900	2.52857300	N	-0.62915300	-3.67945200	-0.48987000
H	1.35056700	7.38398700	-0.08302600	N	5.83368700	2.62065400	-0.21086100
H	-1.15372000	7.19465800	-0.14794900	N	5.84830300	0.11121000	-0.32258200
H	-3.34371700	5.93089500	-0.24550600	N	5.86675000	-2.40001900	-0.39674100
H	-5.52054400	4.66167100	-0.29671100	N	7.99168700	-1.14016900	-0.30815700
H	-7.70122500	3.37700500	-0.30307300	N	7.97496700	1.38530400	-0.20882400
H	-9.08315900	-1.23607000	-0.32672300	N	-2.77512600	-4.92408200	-0.42787100
H	-7.65865300	-3.30365500	-0.35439500	N	-2.80943800	-2.43833100	-0.45503500
H	-9.09941100	1.29160900	-0.30689800	N	-2.83505300	5.05595100	-0.28917300
H	-5.46308300	-4.56040200	-0.38454600	N	-5.00830800	3.78858600	-0.33582100
H	-3.27452700	-5.80522300	-0.40496400	N	-5.00682600	1.30563900	-0.38155000
H	-1.06968900	-7.04996200	-0.43040500	N	-4.99115300	-1.19749700	-0.40604700
H	1.43688000	-7.21380700	-0.44242700	N	-4.96121000	-3.68051600	-0.40002700
H	3.59779500	-5.93637100	-0.44968500	N	-7.14826500	-2.42952100	-0.36245500
H	5.75027800	-4.67691600	-0.43027500	N	-7.17920900	0.04012800	-0.35319800
H	7.92563600	-3.41273500	-0.37261100	N	-7.17977800	2.50966800	-0.32470900
H	3.52526800	6.12941800	-0.09747700				
H	5.69039900	4.89366900	-0.10474900				
H	7.87909800	3.65541800	-0.10809900				
H	9.00371700	-1.14510400	-0.28064700				
H	8.98673400	1.40164200	-0.17737600				
B	0.77604200	1.33599500	-0.43347400				
B	0.79481100	-1.16276100	-0.52074300				
B	-1.38225100	0.07834800	-0.50922100				
N	1.51333400	0.09091400	-0.49956800				
N	-0.66521300	1.33227300	-0.49207100				
N	-0.64976600	-1.17155600	-0.54358500				
N	-2.84294100	2.57433800	-0.41261400				
N	-2.82897000	0.06764700	-0.47612900				
B	-1.39840600	2.57702300	-0.39004700				
B	-3.55773800	1.31949900	-0.41859700				
B	-5.72302700	0.05050300	-0.38168700				
B	-3.54363400	-1.18979300	-0.45079800				
B	-1.36436300	-2.43021500	-0.49929600				
B	-3.57454000	3.82727100	-0.34586700				
B	-1.40671800	5.08639600	-0.25977700				
B	-3.52889100	-3.70363300	-0.42711100				

B	-1.34650700	-4.94236400	-0.45515600		
B	-5.70836500	-2.46031500	-0.38956700		
B	-7.88762300	-1.21801700	-0.34665700		
B	-7.90367300	1.28943300	-0.32710900		
B	0.81242000	-3.67004100	-0.48848800		
B	0.83655000	-6.18080600	-0.45260800		
B	-5.73946900	2.55954800	-0.34750600		
B	0.76544500	3.83801200	-0.28173600		
B	0.76188000	6.34610100	-0.15029600		
B	2.92902600	5.09596800	-0.16473200		
B	2.93800400	2.59498700	-0.29346500		
B	5.10094400	3.85658500	-0.17101900		
B	5.11769400	1.35751500	-0.28854500		
B	7.29853700	0.11903000	-0.27971500		
B	7.28159200	2.62323100	-0.17165900		
B	7.31487800	-2.38650400	-0.36005200		
B	5.13479000	-1.14333400	-0.38731600		
B	2.95378000	0.09621300	-0.42716700		
B	2.97169600	-2.40316800	-0.46989800		
h-BN sheet +Guanine					
N	-1.38976500	1.29396900	2.56542400	B	-2.99613400 0.01913100 -0.51182400
C	-2.30352300	0.26641400	2.56531800	B	-2.99581000 -2.47991300 -0.47734500
H	-3.36760000	0.46001300	2.58571500	B	-5.16427900 -3.73146900 -0.34473600
N	-1.74035300	-0.91272800	2.53721600	N	0.57605100 6.26165900 -0.45532200
C	-0.38847800	-0.64220600	2.51724500	N	-1.56742300 5.03435800 -0.48001900
C	0.73412600	-1.53281500	2.43955600	N	0.60934600 3.77730400 -0.52245400
O	0.75730600	-2.75356300	2.37307500	N	-1.55633800 2.52563700 -0.54377500
N	1.94116600	-0.80060900	2.42287300	N	-3.72242400 -1.23100100 -0.46284100
C	2.06309100	0.56741300	2.47649000	N	-1.55670000 -2.48572400 -0.56473100
N	1.03706000	1.38307000	2.53605300	N	-3.72225700 1.27299400 -0.47051000
C	-0.14909000	0.72673800	2.53525900	N	-3.72741100 3.78068600 -0.45310400
H	-1.59264500	2.28531700	2.58266300	N	-3.72616000 -3.73758600 -0.41725700
H	2.77671900	-1.37050200	2.32498900	B	-3.00256600 -4.98440900 -0.43643800
N	3.32374200	1.06749200	2.40150700	N	-1.56977300 -4.99455300 -0.50877800
H	3.40598800	2.05544300	2.60283900	N	0.57104900 -6.22669400 -0.54905900
H	4.10209600	0.49797500	2.70531600	N	0.60631000 -3.74426200 -0.62833400
H	-1.43426800	7.32440900	-0.42815200	N	-5.89088400 2.53398900 -0.37274400
H	1.07113600	7.14446000	-0.43158300	N	-5.88751900 0.02174100 -0.35922600
H	3.26860800	5.88603400	-0.43245800	N	-5.88926300 -2.49038700 -0.32911400
H	5.44874200	4.62643500	-0.41669800	N	-8.02081400 -1.24148800 -0.24368300
H	7.63748200	3.35554700	-0.41494300	N	-8.02193300 1.28552500 -0.27141800
H	9.04611400	-1.25023700	-0.42455800	N	2.75965000 -4.97447000 -0.55485700
H	7.63290300	-3.32538900	-0.44766500	N	2.78043400 -2.48840700 -0.57025200
H	9.04806000	1.27807800	-0.41614000	N	2.76345500 5.00855300 -0.46570300
H	5.44584100	-4.59467900	-0.49026000	N	4.94155900 3.75025600 -0.45322200
H	3.26382200	-5.85262000	-0.52472800	N	4.95727600 1.26849000 -0.52136800
H	1.06498700	-7.11022100	-0.53181800	N	4.95359800 -1.23433900 -0.52027800
H	-1.44022800	-7.28496900	-0.47160300	N	4.93855200 -3.71795200 -0.50740900
H	-3.60490900	-6.01564300	-0.38980700	N	7.11780800 -2.45410800 -0.46246500
H	-5.75960600	-4.76641900	-0.29771500	N	7.13536500 0.01548300 -0.46801500
H	-7.93938800	-3.51420300	-0.21304200	N	7.12141700 2.48513100 -0.44145200
H	-3.60384800	6.05881000	-0.42759500		
H	-5.76245000	4.81050700	-0.37382400		
H	-7.94225300	3.55851800	-0.28673800		
H	-9.03188100	-1.25182800	-0.19290900		
H	-9.03319900	1.29591400	-0.22450200		
B	-0.82949300	1.27052700	-0.59891600		
B	-0.83163700	-1.23360400	-0.60371100		
B	1.33783300	0.01735300	-0.63880300		
N	-1.55562200	0.02047500	-0.60684200		
N	0.61339600	1.27126500	-0.63719700		
N	0.61343600	-1.23587200	-0.64710900		
N	2.78250500	2.52396100	-0.53792000		
N	2.78378100	0.01764300	-0.61160000		
B	1.33873600	2.52387800	-0.55945100		
B	3.50849300	1.27172800	-0.54516800		
B	5.67900000	0.01775200	-0.50485100		
B	3.50584300	-1.23623400	-0.57349300		
B	1.33406700	-2.49311200	-0.60840200		
B	3.50865000	3.78223700	-0.48414600		

B	1.33509200	5.03529200	-0.48062300				
B	3.50568700	-3.75003200	-0.54266800				
B	1.32992500	-4.99993500	-0.57848700				
B	5.67790000	-2.49355000	-0.49591800				
B	7.85054900	-1.23875400	-0.45047000				
B	7.85240700	1.26889200	-0.44124300				
B	-0.83248300	-3.73845200	-0.56606700				
B	-0.84516900	-6.24906800	-0.50939900				
B	5.68090000	2.52525200	-0.47168000				
B	-0.83156400	3.77787200	-0.51872500				
B	-0.84051100	6.28772400	-0.45374500				
B	-3.00228600	5.02675500	-0.45441800				
B	-2.99818700	2.52237500	-0.49339900				
B	-5.16707500	3.77503500	-0.39958600				
B	-5.16678000	1.27294200	-0.40155700				
B	-7.33668600	0.02177900	-0.29017600				
B	-7.33810000	2.52846700	-0.30862400				
B	-7.33565400	-2.48458900	-0.25818100				
B	-5.16499600	-1.23027400	-0.38329300				
h-BN sheet +Thymine							
N	1.59668200	2.31513700	2.46730700	B	-3.01176800	-0.12256100	-0.43599900
C	0.23276500	2.45133400	2.57348600	B	-3.04606000	-2.61849800	-0.27548900
H	0.12651100	3.47512000	2.58424600	B	-5.23425600	-3.83707200	-0.17835400
C	-0.59847800	1.39154400	2.65295600	N	0.65097300	6.06693000	-0.56496700
C	-2.08620000	1.50691100	2.77526700	N	-1.51005100	4.86852800	-0.54504200
H	-2.58013200	0.88937800	2.01918400	N	0.64933700	3.58206500	-0.57863100
H	-2.42920600	1.15413800	3.75346100	N	-1.53545700	2.35997200	-0.54836300
H	-2.40855900	2.54358900	2.64524500	N	-3.75441600	-1.36124400	-0.35121000
C	-0.01268000	0.05238500	2.60746900	N	-1.60427300	-2.64217200	-0.29005700
O	-0.64791700	-0.99137300	2.63132500	N	-3.72072500	1.13880400	-0.48575100
N	1.38146700	0.02462500	2.52198000	N	-3.68909800	3.64628200	-0.52309800
H	1.81711700	-0.89239700	2.49155500	N	-3.79392700	-3.86311900	-0.18624900
C	2.24414300	1.10078800	2.44812900	B	-3.08637700	-5.11655500	-0.10354900
O	3.45455400	0.98584800	2.36491400	N	-1.65135100	-5.14499000	-0.11240400
H	2.19024100	3.13311200	2.40112800	N	0.47455500	-6.40192000	-0.04348400
H	-1.34464300	7.15711400	-0.54142800	N	0.54350100	-3.92448500	-0.22274200
H	1.15717400	6.94375600	-0.56724200	N	-5.87215300	2.43087500	-0.48226600
H	3.33902700	5.65359600	-0.58769600	N	-5.90499800	-0.07996600	-0.39064500
H	5.50403200	4.36399200	-0.65362000	N	-5.94186300	-2.58826000	-0.25228900
H	7.67381400	3.06024800	-0.69067000	N	-8.05798600	-1.31117100	-0.29821700
H	9.01815200	-1.56143200	-0.50851200	N	-8.02279300	1.21353000	-0.41563500
H	7.57683100	-3.61287200	-0.36455600	N	2.68022100	-5.18557000	-0.16199500
H	9.05472500	0.96433300	-0.63610300	N	2.73539000	-2.70608400	-0.33748100
H	5.37232200	-4.84668000	-0.23714300	N	2.82165000	4.78253300	-0.58646100
H	3.17268000	-6.06917200	-0.10664800	N	4.98370800	3.49489700	-0.64088300
H	0.95659500	-7.29015000	0.01713500	N	4.96379900	1.01193500	-0.60155000
H	-1.55109800	-7.43100000	0.05379300	N	4.92657400	-1.48711100	-0.45757200
H	-3.70266800	-6.13726400	-0.02667300	N	4.87674500	-3.96469400	-0.28966300
H	-5.84454300	-4.86163000	-0.10788900	N	7.07357000	-2.73581100	-0.41175800
H	-8.00882300	-3.58148300	-0.17221700	N	7.12473300	-0.27032000	-0.55521000
H	-3.53217900	5.92262500	-0.52998000	N	7.14501000	2.19782600	-0.65543000
H	-5.71092600	4.70507100	-0.52373900				
H	-7.91083400	3.48398100	-0.49205700				
H	-9.07028600	-1.30727000	-0.28281200				
H	-9.03476600	1.23899300	-0.40237600				
B	-0.82497100	1.09744500	-0.52407500				
B	-0.85970300	-1.40268200	-0.37434400				
B	1.32815200	-0.18731400	-0.51191100				
N	-1.56776200	-0.14183500	-0.45614900				
N	0.62009800	1.07622200	-0.56272600				
N	0.58470100	-1.42557500	-0.41560900				
N	2.80709100	2.29804300	-0.60803900				
N	2.77223200	-0.20764300	-0.53087300				
B	1.36336700	2.31989400	-0.59035600				
B	3.51744700	1.03602400	-0.57067000				
B	5.66831500	-0.24750300	-0.53924900				
B	3.47954600	-1.46800800	-0.44194400				
B	1.29039100	-2.68709400	-0.32558400				
B	3.55250700	3.54693000	-0.61413300				

B	1.39335000	4.83132000	-0.57850800
B	3.44422900	-3.97531300	-0.26056100
B	1.25130500	-5.19102600	-0.14087400
B	5.63325100	-2.75368900	-0.38486100
B	7.82269200	-1.53294200	-0.49320000
B	7.85893600	0.97180900	-0.61883300
B	-0.89837900	-3.90207200	-0.20761800
B	-0.94250800	-6.40600900	-0.02797700
B	5.70543300	2.25857100	-0.63495300
B	-0.79326800	3.60166900	-0.56008800
B	-0.76549300	6.11215300	-0.55029600
B	-2.94589000	4.88163000	-0.53296000
B	-2.97795300	2.37773800	-0.52138900
B	-5.13011400	3.66121400	-0.51130200
B	-5.16624200	1.15998500	-0.45447200
B	-7.35565200	-0.05890500	-0.36851200
B	-7.32071800	2.44599000	-0.46517900
B	-7.39011200	-2.56203500	-0.23705200
B	-5.20029500	-1.34007600	-0.33290600
Adenine+ F (Benzoxazole)			
N	1.16768500	-1.34955900	0.00032700
C	0.47205100	-0.16695300	0.00091600
N	1.23898100	0.89730900	0.00219100
C	2.51074100	0.37794400	0.00253800
C	3.78675100	0.98702100	0.00139200
N	3.94025700	2.32036500	0.02464900
H	4.86523200	2.71138100	-0.08161600
H	3.14093400	2.92658700	-0.08617400
N	4.87148300	0.19738200	-0.00254700
C	4.69392300	-1.13221700	-0.00239800
H	5.60998800	-1.71870300	-0.00516300
N	3.56144100	-1.82858200	-0.00071300
C	2.49433800	-1.01895100	0.00105000
H	0.75913100	-2.27660600	-0.00079100
C	-2.94422200	0.68477400	0.00003000
C	-3.02553200	-0.70979300	-0.00048500
C	-4.27225400	-1.33779300	-0.00094600
C	-5.39256900	-0.51623400	-0.00086800
C	-5.28189100	0.88616200	-0.00036900
C	-4.04571200	1.52530900	0.00009300
C	-0.98065700	-0.17568200	0.00024600
H	-4.35369400	-2.41914500	-0.00132300
H	-6.38071800	-0.96430600	-0.00119800
H	-6.18496400	1.48728000	-0.00032200
H	-3.94694500	2.60435400	0.00051100
O	-1.61784700	1.02046000	0.00048900
N	-1.73070400	-1.22777700	-0.00034000
Cytosine+ F			
N	1.67335500	1.10866900	-0.00047800
C	1.11331700	-0.12981100	-0.00005500
C	1.89986600	-1.23331700	0.00021900
H	1.47374300	-2.22723300	0.00053300
C	3.32009600	-0.99657900	0.00009800
N	4.14682600	-2.05366200	0.00013800
H	5.14460600	-1.89793200	0.00014700
H	3.80242300	-3.00147500	0.00027200
N	3.86233700	0.21103500	-0.00005900
C	3.06347800	1.31762300	-0.00009000
O	3.48000800	2.46924700	0.00010500
H	1.09011500	1.93766300	-0.00016600
C	-2.38076200	-0.79169500	-0.00010500
C	-2.33909100	0.60435400	0.00007500
C	-3.46266800	1.41556300	0.00019300
C	-4.67946800	0.74175700	0.00017400
C	-4.75156300	-0.66408000	-0.00001300
C	-3.61007700	-1.45452200	-0.00018800
C	-0.34907900	-0.20982200	-0.00004700
H	-3.39372600	2.49680200	0.00032100
C	3.29130200	-0.68464400	-0.00532100
C	4.37337200	-1.54906800	-0.01010500
C	5.62411100	-0.93730500	-0.00239700
C	5.76468300	0.46169600	0.00955100
C	4.66167200	1.30715800	0.01388500
C	1.34252300	0.23043500	-0.00179100
H	4.25101500	-2.62570400	-0.01935300
H	6.51380100	-1.55805000	-0.00552000
H	6.76211200	0.88874500	0.01572300
H	4.76676800	2.38650100	0.02326300
O	1.95662900	-0.98672200	-0.01025600
N	2.12044600	1.26043600	0.00788100
N	-5.46763400	-1.65679500	-0.04302700
H	-5.35572000	-2.64383100	0.14536000
H	-6.34142900	-1.24935300	0.26107100
Thymine+ F			
N	1.50902300	1.26937500	-0.00036300
C	1.03865000	-0.03169200	-0.00005900
C	1.87156300	-1.10292800	0.00024700
C	1.43833000	-2.53832600	0.00069400
H	0.83167900	-2.77128000	-0.87828800
H	2.32758500	-3.16908100	0.00200200
H	0.82976600	-2.77014300	0.87864000
C	3.31894900	-0.83398600	0.00017500
O	4.18291600	-1.69445300	0.00040600
N	3.67694100	0.51098900	-0.00016200
H	4.67123200	0.71389900	-0.00016500
C	2.84001300	1.60800500	-0.00037200
O	3.23966700	2.75650800	-0.00057700
H	0.85160800	2.04044300	-0.00046700
C	-2.46385100	-0.70140500	-0.00048400
C	-2.41241100	0.69334600	0.00040900
C	-3.52987800	1.51296100	0.00092800
C	-4.75153500	0.84796100	0.00048700
C	-4.83374700	-0.55728500	-0.00042600
C	-3.69776300	-1.35572600	-0.00092900
C	-0.42230500	-0.13802100	-0.00008900
H	-3.45291900	2.59366400	0.00163100
H	-5.66690900	1.43014900	0.00084600
H	-5.81276600	-1.02479000	-0.00075700
H	-3.75637500	-2.43847900	-0.00164300
O	-1.09418700	1.05004200	0.00066000
N	-1.16112900	-1.19730500	-0.00078900

H	-5.59905100	1.31724500	0.00029000		
H	-5.72717400	-1.13870300	-0.00003300		
H	-3.66106600	-2.53767000	-0.00033000		
O	-1.02187700	0.97158600	0.00007600		
N	-1.07383500	-1.27635300	-0.00017800		
Guanine+ F					
N	-0.80552200	-0.98663100	-0.00246900		
C	-0.10909200	0.20252300	-0.00356700		
N	-0.89248100	1.25346700	-0.00418700		
C	-2.15650200	0.72809900	-0.00300500		
C	-3.43204000	1.39327300	-0.00399500		
O	-3.68246800	2.58655900	-0.00807800		
N	-4.47494100	0.44175300	-0.00243600		
H	-5.40878500	0.83936300	-0.02368100		
C	-4.33005300	-0.92399500	0.00454300		
N	-3.16411300	-1.53184000	0.00695600		
C	-2.12815200	-0.66591800	-0.00176100		
H	-0.40983600	-1.91913000	-0.00126200		
C	3.40125500	0.70775200	0.00597200		
Adenine+ F + <i>h</i>-BN					
H	-1.76705100	7.29767300	-0.39960200		
H	0.74397100	7.22988600	-0.44236200		
H	2.99327300	6.07348300	-0.54526400		
H	5.22677000	4.91298100	-0.60391900		
H	7.46356900	3.74026100	-0.61211900		
H	9.07312700	-0.79752200	-0.67993200		
H	7.75254300	-2.93196500	-0.75623400		
H	8.96452400	1.72545900	-0.63523000		
H	5.62869900	-4.29270900	-0.82717000		
H	3.50410700	-5.64441600	-0.80312500		
H	1.36353700	-6.99517600	-0.75232400		
H	-1.13158400	-7.28105200	-0.69679500		
H	-3.35183200	-6.10968100	-0.66378800		
H	-5.55936200	-4.95785800	-0.60221400		
H	-7.79005400	-3.80614500	-0.51799900		
H	-3.87804100	5.94170400	-0.45634000		
H	-5.98079000	4.60199300	-0.47641300		
H	-8.10206000	3.25721000	-0.43355200		
H	-8.98352100	-1.59495800	-0.48166600		
H	-9.09596000	0.94974700	-0.44997600		
B	-0.90043100	1.29278600	-0.84957600		
B	-0.79105700	-1.20905100	-0.88391100		
B	1.32291500	0.13598400	-0.91921700		
N	-1.56945100	0.01166400	-0.89137400		
N	0.54334800	1.35630200	-0.86803300		
N	0.65169100	-1.14711600	-0.92064500		
N	2.65602800	2.69972400	-0.78890000		
N	2.76547100	0.19786900	-0.93593500		
B	1.21416200	2.63726100	-0.77935500		
B	3.43543100	1.48177100	-0.86054400		
B	5.65722000	0.32203000	-0.84732900		
B	3.54573700	-1.02469700	-0.93242800		
B	1.43088600	-2.36972200	-0.89728900		
B	3.32589700	3.98768600	-0.69325400		
B	1.09891200	5.14017400	-0.59460000		
B	3.65417100	-3.53349800	-0.87931800		
B	1.53553700	-4.87729900	-0.81650400		
B	5.76585500	-2.18281900	-0.85767300		
B	7.87931800	-0.83768000	-0.74427200		
B	7.77144800	1.66533000	-0.69426600		
B	-0.68443100	-3.71161900	-0.81746800		
B	-0.58294900	-6.22030700	-0.73967000		
B	5.54890400	2.82708400	-0.73900900		
B	-1.01229300	3.79002400	-0.67128700		
B	-1.12904600	6.29101300	-0.48387400		
B	-3.23386200	4.93889500	-0.54120400		
B	-3.12218400	2.44325100	-0.71060800		
B	-5.34092600	3.59619000	-0.55676800		
B	-5.23454800	1.09822900	-0.68884400		
B	-7.34665900	-0.24649000	-0.58830600		
N	-6.01099000	2.32503200	-0.58918000		
N	-5.90306000	-0.18172100	-0.69871000		
N	-5.78953000	-2.68959300	-0.64750900		
N	-7.97488700	-1.53925800	-0.54834700		
N	-8.08636100	0.98475600	-0.51776900		
N	2.96149700	-4.78941000	-0.83181600		
N	2.87290400	-2.30729300	-0.92779000		
N	2.52672200	5.17645900	-0.60879100		
N	4.75790400	4.01836200	-0.68185800		
N	4.88088800	1.54337000	-0.84886100		
N	4.98937400	-0.95759700	-0.91946900		
N	5.08318500	-3.44030100	-0.87164200		
N	7.20179200	-2.08329600	-0.78894300		
N	7.11110300	0.38447700	-0.77594000		
N	6.98828900	2.84910400	-0.68090800		
N	-0.72245700	1.24371300	2.23602100		
C	-0.14739300	-0.00249200	2.20151900		
N	-1.01816000	-0.98461900	2.22889900		
C	-2.23102200	-0.34159800	2.28705400		
C	-3.56185700	-0.81909200	2.33709600		
N	-3.85112200	-2.12921400	2.34736400		
H	-4.81617900	-2.42804000	2.33294300		
H	-3.11999600	-2.82166900	2.27278400		
N	-4.55958400	0.07757300	2.38248200		
C	-4.24919200	1.38325400	2.38262600		
H	-5.10181800	2.05897400	2.41575200		
N	-3.05241700	1.96140600	2.34164800		
C	-2.07464200	1.04756500	2.29220300		
H	-0.22452700	2.12678500	2.23469800		
C	3.16625700	-1.20005200	2.22900800		
C	3.38952100	0.17786900	2.29166500		
C	4.69439100	0.67026500	2.37011300		
C	5.72210400	-0.26522900	2.39272200		
C	5.46635400	-1.64810800	2.33347000		
C	4.17260600	-2.15237500	2.24342500		
C	1.30052600	-0.14035100	2.19297500		
H	4.88772700	1.73743100	2.40774800		
H	6.75057800	0.07646300	2.45023300		
H	6.30240600	-2.34013300	2.34075000		
H	3.96174500	-3.21423200	2.18111500		
O	1.81337600	-1.39499200	2.15573600		
N	2.15476300	0.82761600	2.26537500		
Cytosine+ F + <i>h</i>-BN					
H	1.25971600	7.29219500	-0.52242800		
H	-1.24678200	7.13339000	-0.49232800		
H	-3.45626000	5.89343600	-0.50659100		
H	-5.64830900	4.65093000	-0.50253000		
H	-7.84533900	3.39703500	-0.48965600		
H	-9.29085200	-1.19686800	-0.51594300		
H	-7.89499600	-3.28318600	-0.55340200		
H	-9.27208400	1.33065600	-0.48858900		
H	-5.71557700	-4.56843900	-0.56608100		

B	-7.45558600	2.25575800	-0.50913700	H	-3.54030700	-5.84108000	-0.54734500
B	-7.23494800	-2.74967100	-0.56831000	H	-1.34785800	-7.11127300	-0.51114600
B	-5.12414300	-1.39709600	-0.72226200	H	1.15571100	-7.30456100	-0.52284300
B	-3.01334700	-0.05180700	-0.83323000	H	3.33251100	-6.05407800	-0.60612300
B	-2.90339100	-2.54991000	-0.79940200	H	5.50122600	-4.81653600	-0.66001600
B	-5.01144200	-3.89749900	-0.65674800	H	7.69004600	-3.58360600	-0.79500000
N	0.28737500	6.32827500	-0.50223200	H	3.41824300	6.01110400	-0.62523500
N	-1.80024000	5.01000000	-0.56794600	H	5.56508600	4.75173400	-0.78126300
N	0.42894900	3.85244100	-0.67697800	H	7.73753500	3.48765200	-0.92837100
N	-1.68030100	2.51046500	-0.76079200	H	8.79659200	-1.33045000	-0.88893100
N	-3.68282600	-1.33440500	-0.81875500	H	8.81385700	1.21665500	-0.94694600
N	-1.46307000	-2.49200700	-0.84653200	B	0.60182100	1.25101600	-0.76718700
N	-3.79227400	1.16517600	-0.77283100	B	0.58566500	-1.25374300	-0.74616000
N	-3.90442000	3.66621400	-0.61423200	N	-1.57802400	0.01423500	-0.75732900
N	-3.57411000	-3.83949100	-0.72534400	B	1.31857800	-0.00661400	-0.78900300
B	-2.79592800	-5.05314200	-0.71465200	N	-0.84206500	1.26100500	-0.76689100
N	-1.36291500	-4.99897300	-0.75995300	N	-0.85893600	-1.24392200	-0.74315900
N	0.83086000	-6.13440200	-0.76973900	N	4.37810800	-0.13239600	2.24821900
N	0.75562200	-3.65105500	-0.84643600	C	3.60092300	-1.25353800	2.23409300
N	-3.00021000	2.52957600	-0.67664000	O	4.03571800	-2.39644100	2.14962000
N	-3.02209200	0.02290000	-0.74670500	H	1.64329300	-1.91527900	2.28122100
B	-1.55612000	2.51966500	-0.69597600	C	-1.88257700	0.72161700	2.46889800
B	-3.73614100	1.28223700	-0.69464100	C	-1.80311100	-0.67360600	2.44699900
B	-5.91527700	0.04353300	-0.64921300	C	-2.90292800	-1.51640300	2.46111000
B	-3.75422300	-1.22622800	-0.71273700	C	-4.13808400	-0.87599500	2.49266800
B	-1.59234000	-2.49372100	-0.69837100	C	-4.24871400	0.52775500	2.51209600
B	-3.71556100	3.79372600	-0.59882500	C	-3.12960500	1.35062000	2.50226400
B	-1.53017500	5.02830200	-0.58118500	C	0.16359300	0.19501500	2.41418800
B	-3.77014100	-3.73813600	-0.64024100	H	-2.80329400	-2.59577900	2.44073200
B	-1.60170300	-5.00245600	-0.59361100	H	-5.04214700	-1.47660800	2.49722800
B	-5.93398200	-2.46623000	-0.63129600	H	-5.23778800	0.97472200	2.53066200
B	-8.09578800	-1.19498700	-0.56047300	H	-3.21154500	2.43242300	2.51192400
B	-8.07724000	1.31228100	-0.53508000	O	-0.47693100	-1.00527300	2.41381200
B	0.57408400	-3.75730600	-0.64846400	N	-0.58940500	1.24155700	2.44793700
B	0.56830400	-6.26450200	-0.55771200				
B	-5.89701300	2.55265700	-0.58819800				
B	0.62602400	3.75357300	-0.66902500				
B	0.65688900	6.26121900	-0.55914000				
B	2.80784900	4.98448700	-0.65696700				
B	2.78324800	2.48171100	-0.76850500				
B	4.96339000	3.71951800	-0.79565300				
B	4.94514000	1.21866700	-0.86511900				

N	-5.18393900	1.29068300	-0.66533300	B	-1.84649900	-4.92841200	-0.72047600
N	-5.20220400	-1.21370500	-0.68755800	B	-3.25878300	4.00531500	-0.81387300
N	-5.20259400	-3.69626100	-0.61579000	B	-0.98494200	5.06442700	-0.82616600
N	-7.37323600	-2.41628700	-0.58366300	B	-5.52752800	2.93968400	-0.74113200
N	-7.37084200	0.05372000	-0.58628600	B	-7.79170400	1.87626200	-0.56622400
N	-7.33676400	2.52302300	-0.53622500	B	-8.00400300	-0.61967000	-0.52031700
N	2.20948600	-1.07409200	2.30311500	B	1.06609300	3.62441700	-0.91196600
C	1.62578900	0.15171800	2.37512600	B	1.28982900	6.12296700	-0.79651900
C	2.38975600	1.27120300	2.39064900	B	-5.95538800	-2.05655300	-0.68074700
H	1.94399200	2.25588200	2.44362000	B	0.41871000	-3.85965100	-0.80353500
C	3.81233200	1.06313000	2.31612200	B	0.21301700	-6.35846400	-0.63831900
N	4.61843200	2.13694400	2.30987400	B	2.47161600	-5.28501000	-0.65485800
H	5.61523100	2.00275000	2.21107700	B	2.68277100	-2.79227700	-0.80450900
H	4.25247100	3.07747000	2.30154800	B	4.73066800	-4.22386100	-0.60036300
				B	4.94519700	-1.73625600	-0.70256100
				B	7.21411400	-0.67488600	-0.56134500
				B	6.99603100	-3.16983300	-0.49171600
				H	-6.09769300	4.45232200	-0.08761800
				H	-4.01274700	5.86148400	-0.18916100
				H	-1.90425200	7.26564400	-0.22986300
B	7.43142800	1.82148500	-0.61135000	H	0.58192100	7.61120500	-0.30988900
B	5.16594600	0.75700300	-0.77795800	H	2.82692800	6.49431900	-0.44450200
B	2.89822100	-0.30462300	-0.92531200	H	5.06172500	5.39223900	-0.52537200
B	3.11491300	2.19087100	-0.91334500	H	7.31954900	4.28046300	-0.51236400
B	5.37939300	3.24821600	-0.74122000	H	3.61151700	-5.53037900	-1.22687400
N	-1.19607200	-6.21345200	-0.65002600	H	5.67799600	-4.15540100	-0.99636000
N	1.04236700	-5.17284200	-0.70778800	H	7.76911400	-2.77361700	-0.80307500
N	-1.01724600	-3.73916900	-0.81541200	H	8.55145700	2.09091800	-0.54084100
N	1.24718900	-2.67618300	-0.87935900	H	8.71074200	-0.45203500	-0.61330200
N	3.72875300	0.88239500	-0.89285500	B	0.52747200	-0.94277900	-0.99390600
N	1.67789400	2.31580500	-0.98291100	B	0.36460400	1.55084500	-0.79443600
N	3.51235700	-1.61153700	-0.84874800	B	-1.71826000	0.15854000	-0.81743600
N	3.29881600	-4.10625300	-0.69074500	N	1.17061400	0.35266400	-0.91500600
N	3.94937200	3.38017800	-0.85198300	N	-0.91131300	-1.03838800	-0.94462100
B	3.33410500	4.68070100	-0.81974500	N	-1.07509500	1.45661400	-0.76614600
N	1.90480000	4.81288900	-0.85220100	N	-2.98541400	-2.44192600	-0.85145600
N	-0.12380600	6.21982400	-0.79217100	N	-3.15457700	0.05703700	-0.72926100
N	-0.37121300	3.74764600	-0.88909500	B	-1.54954800	-2.34121500	-0.95390500
N	5.55920900	-3.05146100	-0.60936000	B	-3.78914500	-1.24522600	-0.71293400
N	5.77379700	-0.55079400	-0.68180000	B	-6.02494900	-0.15360100	-0.40246900
N	5.99609200	1.94797200	-0.73630300	B	-3.95429000	1.25270000	-0.55541300
N	8.00545000	0.52541900	-0.53190100	B	-1.87839000	2.65308400	-0.61258500
N	7.78625200	-1.99041300	-0.47245600	B	-3.62226100	-3.74986000	-0.83973800
N	-2.40940800	5.16114000	-0.79877600	B	-1.37890500	-4.84438200	-1.08709000
N	-2.64540600	2.68731900	-0.88692800	B	-4.11781700	3.75287700	-0.34952200
N	-3.26693200	-4.78010400	-0.69588400	B	-2.03354400	5.14972300	-0.38415800
N	-5.32764400	-3.34172200	-0.68592100	B	-6.19112900	2.34503000	-0.23209700
N	-5.13164200	-0.86833400	-0.81488100	B	-8.26064500	0.93650700	-0.07322500
N	-4.91716500	1.62618500	-0.83438400	B	-8.09452000	-1.56100300	-0.22325900
N	-4.68639500	4.09735200	-0.75230600	B	0.20807300	4.04239400	-0.57275500
N	-6.96078600	3.02541100	-0.62663500	B	0.05606000	6.54004300	-0.37023900
N	-7.18818400	0.56671600	-0.62941000	B	-5.85928200	-2.65349800	-0.54372800
N	-7.38132100	-1.89359600	-0.55203500	B	0.69523300	-3.43965000	-1.13701600
N	0.62775100	1.25965200	2.09293100	B	0.87092500	-5.94093700	-1.27085500
C	0.16243900	-0.03828000	2.09925600	B	2.94289600	-4.54109500	-1.18741700
N	1.12833900	-0.92533000	2.14373400	B	2.77428400	-2.04581000	-1.06627200
C	2.27458800	-0.17445000	2.16868700	B	5.01888000	-3.15991800	-0.99702600
C	3.65445200	-0.58147200	2.22339900	B	4.86144500	-0.66238500	-0.92818900
O	4.13297400	-1.70418100	2.23250400	B	6.94142400	0.71825200	-0.71116100
N	4.49840400	0.55168200	2.26613100	B	7.10160900	-1.78366600	-0.81118200
H	5.48965400	0.33188900	2.29953700	B	6.78175300	3.21692400	-0.59364500
C	4.09733100	1.86550900	2.24459700	B	4.69825300	1.83251400	-0.76674800
N	2.83641800	2.23725300	2.17492400	B	2.61307000	0.44892700	-0.92090100
C	1.98586000	1.19092100	2.14355900	B	2.45208800	2.93610100	-0.71582800
H	0.06628100	2.10353400	2.07806400	B	4.53608500	4.32203100	-0.60228200
C	-3.19988000	-1.16311200	2.27323700	N	-0.54284100	-6.01250900	-1.21048100
C	-3.34145500	0.22646400	2.27280900	N	1.51159800	-4.64231400	-1.22362600
C	-4.55872500	0.88114900	2.37144100	N	-0.74019400	-3.53852700	-1.06867800
C	-5.67401100	0.05350700	2.48125100	N	1.33394600	-2.14149500	-1.09361200
C	-5.55966200	-1.34863000	2.48155200	N	3.25485800	1.74122900	-0.82702500
C	-4.32698000	-1.98096500	2.37191200	N	1.01108200	2.84310600	-0.69493300
C	-1.26337900	-0.32509900	2.12814600				

H	-4.63428900	1.96287300	2.36185600	N	3.41754100	-0.75278900	-0.99182300
H	-6.65809100	0.50429900	2.56122200	N	3.58277400	-3.25323000	-1.09343400
H	-6.46138600	-1.94846700	2.55268700	N	3.09734500	4.23514300	-0.61669600
H	-4.23354100	-3.06194600	2.36062500	B	2.29374300	5.42738100	-0.51455500
O	-2.08510300	0.76375700	2.17459200	N	0.86092300	5.34074100	-0.49110600
N	-1.84496100	-1.47701400	2.17112100	N	-1.35497600	6.42006700	-0.32161400
N	5.06633800	2.80810000	2.24682200	N	-1.22962600	3.94653500	-0.52718700
H	4.75594200	3.75605900	2.41391200	N	5.66215700	-1.87502600	-0.93256300
H	6.00080900	2.58263900	2.55885000	N	5.49876500	0.62922900	-0.82673900
Thymine + F + h-BN				N	5.33900700	3.13396200	-0.67267500
H	1.53182200	-6.93270900	-1.35364300	N	7.54391300	2.01902100	-0.60914000
H	-0.97845600	-6.92608400	-1.23584200	N	7.70295800	-0.50225900	-0.69777000
H	-3.24444400	-5.82882000	-0.97618400	N	-3.45437100	5.02423500	-0.30584900
H	-5.48972100	-4.73116600	-0.67502800	N	-3.31602300	2.55233000	-0.52990000
H	-7.74056800	-3.62479400	-0.36325900	N	-2.80088600	-4.91803100	-0.97609100
H	-9.44662300	0.85997800	0.05970600	B	3.55446100	3.74941500	0.06944100
H	-8.18364100	3.03045900	0.04001100	B	1.39008200	5.03771100	-0.06142200
H	-9.27894800	-1.65702200	-0.08893400	B	5.73075300	2.51887600	-0.26401500
N	-5.04509600	-3.82103900	-0.68778900	B	7.83317200	1.25413100	-0.77454500
N	-5.22581800	-1.34725800	-0.56547000	B	7.83317200	-1.25413100	-0.77454500
N	-5.39062000	1.14581300	-0.40691200	B	-0.78564700	3.78034500	0.09856600
N	-5.53790100	3.61771800	-0.21562200	B	-0.78184600	6.25608400	-0.34591200
N	-7.61583400	2.20058000	-0.07677300	B	5.73075300	-2.51887600	-0.26401500
N	-7.46744200	-0.25993500	-0.23173200	B	-0.78564700	-3.78034500	0.09856600
N	-7.28866200	-2.71904300	-0.37527900	B	-0.78184600	-6.25608400	-0.34591200
N	2.59864500	0.25642700	2.12972400	B	-2.94486300	-4.99967600	-0.26021000
C	1.94990900	-0.96651500	2.14153400	B	-2.95893000	-2.51362100	0.05248000
C	2.63075900	-2.14116700	2.10511000	B	-5.11030100	-3.74923400	-0.26681900
C	2.00934900	-3.50413500	2.11441200	B	-5.10347000	-1.24863400	-0.08278500
H	1.16589400	-3.56411900	1.42444200	B	-7.27212600	0.00000000	-0.26968600
H	2.76937000	-4.23696700	1.83753000	B	-7.26984900	-2.50121800	-0.33749500
H	1.62631900	-3.75425300	3.10982200	B	-7.26984900	2.50121800	-0.33749500
C	4.10142500	-2.07350100	2.07138200	B	-5.10347000	1.24863400	-0.08278500
O	4.83720800	-3.04536500	2.01696700	B	-2.93423900	0.00000000	0.23747700
N	4.64487600	-0.79137300	2.09568400	B	-2.95893000	2.51362100	0.05248000
H	5.65861000	-0.72678900	2.08818000	B	-5.11030100	3.74923400	-0.26681900
C	3.96412200	0.40831200	2.12818600	N	0.63548100	-6.24271200	-0.30033400
O	4.51639500	1.49311000	2.13896000	N	-1.51226700	-5.01646700	-0.16180800
H	2.05738900	1.11251900	2.18159400	N	0.66038900	-3.81057700	0.18147200
C	-1.61171200	-1.12190500	2.35481500	N	-1.53310300	-2.53764800	0.22719700
C	-1.35559200	0.25055400	2.34605400	N	-3.66529500	1.25148300	0.08948200
C	-2.33347300	1.22761900	2.44177000	N	-1.53310300	2.53764800	0.22719700
C	-3.63612000	0.75220200	2.55088100	N	-3.66529500	-1.25148300	0.08948200
C	-3.92721800	-0.62583000	2.55265000	N	-3.67621700	-3.76093100	-0.15817700
C	-2.92689100	-1.58494000	2.45404800	N	-3.67621700	3.76093100	-0.15817700
C	0.48766600	-0.86487500	2.20274300	B	-2.94486300	4.99967600	-0.26021000
H	-2.09617500	2.28576200	2.42773400	N	-1.51226700	5.01646700	-0.16180800
H	-4.45186000	1.46534700	2.62145500	N	0.63548100	6.24271200	-0.30033400
H	-4.96270100	-0.94309800	2.62593200	N	0.66038900	3.81057700	0.18147200
H	-3.14778200	-2.64718400	2.45048900	N	-5.82658700	-2.50576000	-0.21759400
O	-0.00327600	0.40956300	2.23468100	N	-5.82743000	0.00000000	-0.12694800
N	-0.39813800	-1.80385900	2.26713200	N	-5.82658700	2.50576000	-0.21759400
Al_h-BN				N	-7.95692700	1.26081400	-0.34127800
H	-1.37603300	-7.27386100	-0.54397500	N	-7.95692700	-1.26081400	-0.34127800
H	1.12812100	-7.11426300	-0.45048800	N	2.81719400	4.97972300	-0.05463300
H	3.33598500	-5.82339900	-0.26857000	N	2.85269900	2.51054900	0.41300200
H	5.43177100	-4.60431400	-0.38041100	N	2.81719400	-4.97972300	-0.05463300
H	7.61833800	-3.34249100	-0.79921400	N	4.97412600	-3.72784900	-0.15905800
H	8.98701400	1.25904100	-1.08835300	N	5.05329700	-1.26812100	0.00365100
H	7.61833800	3.34249100	-0.79921400	N	5.05329700	1.26812100	0.00365100
H	8.98701400	-1.25904100	-1.08835300	N	4.97412600	3.72784900	-0.15905800
H	5.43177100	4.60431400	-0.38041100	N	7.12468300	2.47611000	-0.62503500
H	3.33598500	5.82339900	-0.26857000	N	7.14737800	0.00000000	-0.55708200
H	1.12812100	7.11426300	-0.45048800	N	7.12468300	-2.47611000	-0.62503500
H	-1.37603300	7.27386100	-0.54397500	Al	1.43478200	0.00000000	1.20468500
H	-3.54151300	6.01947700	-0.43906400	Al_h-BN +Adenine			
H	-5.70591500	4.77566300	-0.40323000	N	-2.35947900	-0.87384700	4.52266200
H	-7.86779200	3.53054200	-0.43385000	C	-2.26756500	-0.99787100	3.18963000
H	-3.54151300	-6.01947700	-0.43906400	H	-2.71337900	-1.81474700	2.63554400

H	-5.70591500	-4.77566300	-0.40323000	N	-1.57177600	-0.00840500	2.64956800
H	-7.86779200	-3.53054200	-0.43385000	C	-1.19137600	0.80903500	3.70988400
H	-8.96501100	1.26904700	-0.43358500	C	-0.45253100	2.01471900	3.83201300
H	-8.96501100	-1.26904700	-0.43358500	N	0.08791900	2.66698600	2.79768800
B	-0.82648400	-1.31992400	0.57159900	H	0.58584300	3.52612000	2.98555500
B	-0.82648400	1.31992400	0.57159900	H	-0.01996800	2.34570800	1.83800000
N	-1.50416600	0.00000000	0.52150300	N	-0.29137300	2.51977400	5.06679800
N	0.55915000	-1.47820700	0.91236600	C	-0.82559100	1.88125800	6.11247500
N	0.55915000	1.47820700	0.91236600	H	-0.65536500	2.34831700	7.07945600
N	2.85269900	-2.51054900	0.41300200	N	-1.53547600	0.75705300	6.12541800
N	3.14141000	0.00000000	0.85607800	C	-1.68403300	0.26933300	4.89220800
B	1.37825500	-2.59672400	0.51972700	H	-2.84261800	-1.51064500	5.14601700
B	3.67253300	-1.27382300	0.44329000	H	1.66935100	7.04583800	-1.74805500
B	5.74360400	0.00000000	-0.16435100	H	-0.83938200	6.89996500	-1.77470400
B	3.67253300	1.27382300	0.44329000	H	-3.05798800	5.64696900	-1.60499100
B	1.37825500	2.59672400	0.51972700	N	-2.69125200	-2.61513000	-0.26252900
B	3.55446100	-3.74941500	0.06944100	N	-2.55942200	4.81760900	-1.30485600
B	1.39008200	-5.03771100	-0.06142200	N	-4.71243000	3.56665500	-1.44705500
H	-5.15413900	4.42672100	-1.74976800	N	-4.79893200	1.11902000	-1.14944400
H	-7.30710700	3.14394700	-2.21901100	N	-4.82623200	-1.39738800	-0.94527700
H	-8.70387500	-1.46162100	-2.23255000	N	-4.79346200	-3.86274700	-0.82318700
H	-7.37732400	-3.51856200	-1.66900500	N	-6.88279200	-2.64260800	-1.55694700
H	-8.67854000	1.05198000	-2.43760500	N	-6.87865200	-0.17349700	-1.72150300
H	-5.25307600	-4.75188400	-0.98032600	N	-6.83126700	2.28812900	-1.96270300
H	-3.17371300	-5.97254600	-0.64392000	Al	-1.31826700	-0.03224400	0.69796600
H	-0.97431300	-7.27410200	-0.63014100	Al_h-BN +Cytosine			
H	1.53134300	-7.45431400	-0.61586900	N	1.07734300	-0.92584700	4.94171400
H	3.69997700	-6.20340900	-0.52133300	C	1.06430700	0.25690000	5.60570700
H	5.86470700	-4.97387900	-0.46545800	H	0.85450300	0.20847400	6.66709100
H	8.03990200	-3.74876700	-0.47374100	C	1.32981900	1.41300100	4.95579500
H	3.81524000	5.79494100	-1.42064300	H	1.36363200	2.36105300	5.47341700
H	5.95959200	4.55022100	-1.15906400	C	1.60293800	1.33303700	3.55363900
H	8.11182000	3.29492300	-0.97511400	N	1.97734300	2.42271400	2.89619200
H	9.15934900	-1.50039400	-0.57828700	H	2.31464400	2.40393800	1.93575300
H	9.18489600	1.03266500	-0.75601500	H	2.06014100	3.30112300	3.39044100
B	0.99146100	1.19021400	-0.22062700	N	1.48794000	0.15989900	2.88909400
B	0.95735800	-1.41979000	-0.04734000	C	1.34205000	-1.03370000	3.58577600
N	1.67209700	-0.11988600	-0.13703100	O	1.43402500	-2.11944900	3.04267400
N	-0.40087000	1.37979600	0.07795100	H	0.94293100	-1.80022300	5.43666900
N	-0.43775000	-1.51927100	0.21991300	H	-1.68342700	-7.29796600	-0.88432800
N	-2.63564200	2.38822200	-0.67489800	H	0.82582000	-7.16211900	-0.89892200
N	-2.92238600	-0.08120500	-0.09790800	H	3.04652300	-5.90185200	-0.85996400
B	-1.17472100	2.45699700	-0.48824700	H	5.14500800	-4.70311300	-1.13476000
B	-3.44064000	1.14172300	-0.62194900	H	7.29531200	-3.46998000	-1.73778900
B	-5.49392700	-0.14923800	-1.25734200	H	8.70970800	1.11590700	-2.12928400
B	-3.46730400	-1.36137100	-0.42133500	H	7.39380500	3.21560500	-1.72294300
B	-1.22062100	-2.67075500	-0.10844900	H	8.67257000	-1.40716900	-2.13603600
B	-3.30835700	3.59923400	-1.13878400	H	5.27640400	4.50717600	-1.13728600
B	-1.13432800	4.85877900	-1.24753200	H	3.19864300	5.75603100	-0.93945900
B	-3.38753600	-3.87200900	-0.51886300	H	1.00967700	7.05317300	-1.09616100
B	-1.23207400	-5.16690700	-0.45223900	H	-1.49557700	7.24553800	-1.13921000
B	-5.51145500	-2.65941700	-1.11032100	H	-3.67341100	6.01998800	-0.94181000
B	-7.56701300	-1.43600500	-1.86034000	H	-5.84544800	4.80991400	-0.78056400
B	-7.54163900	1.06297000	-2.06499900	H	-8.02849800	3.59534600	-0.69040300
B	0.93971200	-3.91098400	-0.32873000	H	-3.82850400	-6.01169300	-0.72011200
B	0.93787500	-6.41938200	-0.53693600	H	-5.97089700	-4.73972100	-0.60549300
B	-5.45822600	2.34899000	-1.52539100	H	-8.12058800	-3.46569300	-0.56137800
B	1.01440400	3.61084600	-0.88403900	H	-9.15412400	1.34988900	-0.60331900
B	1.05734400	6.04775400	-1.50751900	H	-9.18757500	-1.19000500	-0.55428700
B	3.19997100	4.79375200	-1.20235200	B	-0.98923300	-1.31777700	0.02931600
B	3.16924900	2.33752600	-0.70473300	B	-0.95531300	1.28536100	-0.00216200
B	5.34870500	3.53836700	-0.98400700	N	-1.68021000	-0.00565400	0.01046500
B	5.30963900	1.05968700	-0.61981800	N	0.39861900	-1.45463500	0.29266100
B	7.47283600	-0.21172200	-0.59575900	N	0.43962600	1.40125200	0.27791500
B	7.49893900	2.27859900	-0.84013900	N	2.63138300	-2.56800900	-0.25962200
B	7.44816600	-2.71114100	-0.48500300	N	2.93215800	-0.06359000	0.13511000
B	5.28352000	-1.43020000	-0.44258600	B	1.16233100	-2.60302600	-0.08292100
B	3.11160900	-0.14960500	-0.33789800	B	3.43998000	-1.32876200	-0.29759100
B	3.11676200	-2.66527900	-0.34714900				
B	5.27356100	-3.93564200	-0.44159300				
N	-0.35936600	6.04124700	-1.53609200				

N	1.76546800	4.82274600	-1.19179000	B	5.49819700	-0.10258000	-1.04151800
N	-0.43075000	3.64673200	-0.88201500	B	3.47768900	1.17706600	-0.30137900
N	1.73553800	2.37741100	-0.61918900	B	1.21713100	2.51193300	-0.16299400
N	3.83931900	-1.41151800	-0.35554400	B	3.30009400	-3.81640100	-0.60023000
N	1.68413800	-2.66466300	-0.26767900	B	1.12281000	-5.07466000	-0.59012100
N	3.86536500	1.08254700	-0.53206200	B	3.40545500	3.67701500	-0.61950000
N	3.91120100	3.56326300	-0.96292100	B	1.25166300	4.97060400	-0.72517600
N	3.83658700	-3.92961500	-0.41639200	B	5.52597800	2.41050800	-1.09537700
B	3.10258000	-5.16970000	-0.45955500	B	7.57425100	1.12321800	-1.75184000
N	1.66866300	-5.17153900	-0.43810600	B	7.53762700	-1.38433700	-1.75740700
N	-0.47915500	-6.39505200	-0.54651200	B	-0.92775000	3.74066500	-0.52008500
N	-0.50467100	-3.92403700	-0.31384400	B	-0.90948500	6.21931700	-0.95783200
N	6.05182000	2.29989300	-0.80247100	B	5.45273300	-2.61358500	-1.10100800
N	6.02323900	-0.19271900	-0.53360200	B	-1.02209400	-3.78970200	-0.38382500
N	6.00126600	-2.69775300	-0.44490000	B	-1.07040500	-6.28066500	-0.74427300
N	8.14798600	-1.47880400	-0.54064600	H	-3.04858200	6.49910200	-0.57659000
N	8.17326900	1.03698200	-0.71840900	H	-5.27622700	5.35329700	-0.69666700
N	-2.65880200	-5.11360200	-0.49047300	H	-7.49980800	4.20918200	-0.83305700
B	-3.21051900	-4.99529300	-0.59731600	H	-3.59913900	-5.52213500	-1.49720200
B	-3.17309700	-2.50160500	-0.34726500	H	-5.72059900	-4.18674300	-1.32515400
B	-5.35691100	-3.71763700	-0.52256600	H	-7.82869400	-2.83755500	-1.26462500
B	-5.31234600	-1.21576500	-0.39064500	H	-8.69685200	2.00588200	-0.98446200
B	-7.47210500	0.05926000	-0.49434400	H	-8.81566700	-0.53182200	-1.13374500
B	-7.50468900	-2.44312300	-0.51420100	B	-0.65457500	-0.97188600	-0.43132900
B	-7.43954800	2.55941100	-0.60554000	B	-0.56685500	1.59891800	0.00120800
B	-5.28038000	1.28064200	-0.43472000	N	-1.30505900	0.34431300	-0.28431200
B	-3.11336800	0.00825200	-0.20159000	N	0.73566600	-1.14034000	-0.22761500
B	-3.10789900	2.51023000	-0.43499900	N	0.78446200	1.62988400	0.45994000
B	-5.25901100	3.77565400	-0.65942600	N	2.94014100	-2.35288900	-0.40292900
N	0.34662400	-6.28172600	-0.75735300	N	3.26874900	0.05253300	0.43598200
N	-1.77711200	-5.02777800	-0.56954900	B	1.46652600	-2.32285700	-0.50389000
N	0.42129900	-3.83147800	-0.36142700	B	3.78136900	-1.15822400	-0.14227400
N	-1.74254600	-2.53586500	-0.26030600	B	5.94682300	0.05812200	-0.44634000
N	-3.83819100	1.26597300	-0.33564100	B	3.87986600	1.32969800	0.20190200
N	-1.67541400	2.51062500	-0.34375800	B	1.65679000	2.74126400	0.25947300
N	-3.87033900	-1.23466100	-0.29302600	B	3.60438800	-3.59080200	-0.79062700
N	-3.92053200	-3.74510300	-0.48866700	B	1.38591400	-4.75725200	-1.12829600
N	-3.82195400	3.76644800	-0.62597400	B	3.90392000	3.84381500	0.12292600
B	-3.08198000	4.99343200	-0.78086000	B	1.81094600	5.23865100	-0.03765100
N	-1.64794200	4.98995200	-0.75187300	B	6.04049100	2.55788000	-0.21342100
N	0.50760300	6.18712600	-0.94568200	B	8.12723700	1.27097700	-0.74294200
N	0.51715700	3.74535400	-0.49858800	B	8.02398200	-1.21581100	-1.05831000
N	-6.05850500	-2.46552000	-0.46462200	B	-0.41530600	4.08662900	-0.17502600
N	-6.02360200	0.04171600	-0.42111800	B	-0.28300100	6.59256900	-0.32730100
N	-5.99314900	2.54586400	-0.55485400	B	5.83707100	-2.42652700	-0.84515300
N	-8.14313800	1.32867100	-0.55666400	B	-0.73768400	-3.41382500	-0.96456800
N	-8.17624000	-1.19356200	-0.50956300	B	-0.83881300	-5.87191400	-1.47191600
N	2.67912100	4.91480100	-0.71813300	B	-2.95666100	-4.53429200	-1.29371300
N	2.69971700	2.44851300	-0.25189400	B	-2.86207500	-2.06757700	-0.86410100
N	2.54946800	-5.04550900	-0.64582800	B	-5.07442600	-3.19489800	-1.16000800
N	4.70613800	-3.81784600	-0.91123100	B	-4.95617600	-0.70795600	-0.84003400
N	4.79986800	-1.35346000	-0.82785200	B	-7.06496800	0.64957600	-0.91449700
N	4.83486800	1.16989700	-0.83077600	B	-7.17914800	-1.84476600	-1.12422700
N	4.81358900	3.63670900	-0.90372700	B	-6.94677800	3.15025800	-0.81222700
N	6.89617600	2.35325700	-1.54070800	B	-4.84212100	1.78645200	-0.66336900
N	6.88138500	-0.12089200	-1.51168200	B	-2.73072700	0.42475700	-0.50000400
N	6.82399000	-2.59393800	-1.55101800	B	-2.63610800	2.93683100	-0.42363700
Al	1.31577100	-0.04673400	0.92354900	B	-4.72810300	4.29245700	-0.64163900
Al_h-BN +Guanine				N	0.57921700	-5.91947800	-1.42263500
N	0.78721000	-2.92053200	2.95682000	N	-1.52254300	-4.61282100	-1.24627300
C	1.67588800	-1.92701800	2.75792300	N	0.70449800	-3.50612600	-0.88710100
H	2.74088600	-2.09523200	2.67513000	N	-1.43340500	-2.15195000	-0.77944300
N	1.07609200	-0.75208300	2.61822500	N	-3.40852200	1.71350100	-0.50812800
C	-0.28284100	-1.02137300	2.75320600	N	-1.21666000	2.87946100	-0.23424800
C	-1.42700500	-0.14963900	2.73347000	N	-3.51921900	-0.78467300	-0.71536700
O	-1.47451500	1.06739700	2.71139500	N	-3.63915800	-3.27556300	-1.10523600
N	-2.60815400	-0.91840100	2.74391500	N	-3.29641200	4.23194200	-0.51998900
C	-2.68849200	-2.28414100	2.86679300	B	-2.50439100	5.43864200	-0.47958000
N	-1.63171400	-3.06263200	3.00318200	N	-1.07769000	5.37982900	-0.32742700
				N	1.12584400	6.50113900	-0.19294100
				N	1.01978100	4.03000700	-0.00227000

C	-0.47762900	-2.37950100	2.92339100	N	-5.73680100	-1.92486900	-1.02823600
H	1.01250600	-3.90036900	3.09083600	N	-5.62237400	0.57460900	-0.78921900
H	-3.46406700	-0.37416300	2.68014800	N	-5.50550700	3.08349000	-0.69727900
N	-3.91476300	-2.83449400	2.80529400	N	-7.68992900	1.94415000	-0.89981900
H	-3.98099300	-3.81695600	3.03384000	N	-7.80722600	-0.57398500	-1.05419700
H	-4.74645600	-2.27739000	2.94035800	N	3.22945500	5.11734100	0.08230900
H	-1.47155900	-6.86047400	-1.70057100	N	3.13359100	2.61279000	0.26639700
H	1.03267600	-6.80937300	-1.58801700	N	2.81617200	-4.76868200	-1.06587400
H	3.30533800	-5.62591600	-1.29516100	N	5.03840200	-3.61389100	-0.91418500
H	5.48450200	-4.48302600	-1.18280200	N	5.19410200	-1.17991800	-0.49283900
H	7.72660900	-3.27470700	-1.34131500	N	5.29367300	1.32143400	-0.16094200
H	9.30122700	1.26091300	-0.97498200	N	5.33696800	3.78387100	0.00059100
H	7.99352100	3.35296900	-0.50885300	N	7.45687800	2.49508500	-0.48296200
H	9.19733300	-1.24219300	-1.29229000	N	7.37810100	0.03575900	-0.73676900
H	5.84650900	4.65548900	-0.08317200	N	7.25665500	-2.41036400	-1.10345100
H	3.79611300	5.95395200	0.00841800	B	-5.53829700	1.20394000	-0.12340600
H	1.66510500	7.35783800	-0.20539100	B	-3.30819000	0.02534400	-0.03631400
H	-0.81595600	7.65649600	-0.44525000	B	-3.43001000	2.53825000	-0.10198600
Al	1.52909000	0.05977800	0.84744500	B	-5.64264200	3.70701100	-0.19207500
Al_h-BN + Thymine				N	0.41860000	-6.03276600	-1.20248600
N	1.78399500	-2.44009600	3.04841600	N	-1.75424300	-4.90076300	-0.84003800
C	3.14421900	-2.27366300	2.85331000	N	0.39298400	-3.62329800	-0.61799700
H	3.69452500	-3.19983900	2.73197100	N	-1.82703400	-2.44494000	-0.32094800
C	3.75153700	-1.07056700	2.82662100	N	-4.09336300	1.25311200	-0.06484600
C	5.22153200	-0.86318400	2.62658900	N	-1.99722300	2.60591100	-0.04115300
H	5.72008700	-1.81261100	2.42057100	N	-4.00783100	-1.24416400	-0.19252700
H	5.38902500	-0.18668300	1.78146600	N	-3.95109000	-3.73576500	-0.57547100
H	5.67645600	-0.41017700	3.51241400	N	-4.20620900	3.76661300	-0.19695500
C	2.92594400	0.11481100	2.99308800	B	-3.52816600	5.03506300	-0.29740200
O	3.29609600	1.25358900	3.13385400	N	-2.09473000	5.10086200	-0.30514200
N	1.48614000	-0.13368200	2.86986400	N	-0.00588800	6.41116700	-0.52089700
H	0.94908500	0.62095600	3.31041000	N	0.13595300	3.95792600	-0.17793000
C	0.90225400	-1.41167800	3.19855300	N	-6.14138400	-2.56542000	-0.38238100
O	-0.25965400	-1.50838300	3.50042600	N	-6.22167600	-0.06775200	-0.16895100
H	1.40464500	-3.37160400	3.17524800	N	-6.31284600	2.43796000	-0.14304700
H	-1.56747100	-7.12954800	-1.34842500	N	-8.40280200	1.12061900	-0.15720800
H	0.92937100	-6.87742000	-1.42735700	N	-8.31620700	-1.39783000	-0.27466500
H	3.10136100	-5.52907000	-1.30342200	N	2.23093900	5.22946400	-0.46450500
H	5.16633100	-4.22515200	-1.44416500	N	2.37857600	2.74361500	-0.15595300
H	7.28499000	-2.85793500	-1.89177100	N	2.57096700	-4.71073200	-1.02848100
H	8.47441100	1.80493900	-2.00598800	N	4.68304600	-3.37696400	-1.17281700
H	7.04799100	3.81700400	-1.53683100	N	4.66662800	-0.91944600	-0.93984800
H	8.56446300	-0.71543900	-2.13581100	N	4.58367600	1.60645300	-0.78473000
H	4.84090000	4.97280300	-0.94335200	N	4.42335800	4.06805800	-0.75979700
H	2.70352300	6.10521500	-0.65483300	N	6.58907400	2.92437900	-1.40528600
H	0.44672500	7.30667700	-0.65520800	N	6.69790600	0.45098300	-1.49469600
H	-2.06275600	7.37740700	-0.58293900	N	6.76318400	-2.01950500	-1.66949500
H	-4.17133800	6.03881600	-0.38415900	Al	1.12887600	0.13011700	0.78095900
H	-6.28064300	4.71627100	-0.23465400	Al_h-BN + Adenine +F			
H	-8.39795100	3.39389500	-0.15135900	N	-1.69708200	2.37211100	3.56198900
H	-3.76282900	-5.96941900	-0.99388800	C	-0.98316200	1.54366100	2.77864900
H	-5.95727700	-4.81679700	-0.69603200	N	-1.71512400	0.53368000	2.31878000
H	-8.15698400	-3.65605800	-0.48191700	C	-2.97474900	0.71016200	2.87966100
H	-9.41475400	1.09530300	-0.17086100	C	-4.16235400	-0.06750900	2.91929400
H	-9.32747100	-1.44083400	-0.28840300	N	-4.29167300	-1.28174000	2.37416100
B	-1.12950900	-1.21915900	0.03695900	H	-5.17125400	-1.76673100	2.49036600
B	-1.21811100	1.40204800	0.20616700	H	-3.54327500	-1.76327900	1.89279900
N	-1.86507400	0.06672100	0.13651600	N	-5.20969800	0.44099300	3.58868400
N	0.27912500	-1.32514700	0.23882000	C	-5.07867600	1.60686000	4.22817300
N	0.17557900	1.58937100	0.47664900	H	-5.97007800	1.95871200	4.74146300
N	2.54811700	-2.26713300	-0.46733800	N	-3.99957200	2.37793700	4.33679700
N	2.73119000	0.22673300	0.03829000	C	-2.97845500	1.87160100	3.64729000
B	1.08763500	-2.39330600	-0.27114100	H	-1.33389800	3.19066000	4.04030900
B	3.30210300	-0.99248000	-0.44319300	C	2.45264700	0.94307800	2.42098000
B	5.30653400	0.37814200	-1.06027200	C	2.44673800	2.33713500	2.33293700
B	3.22056600	1.53008200	-0.28221400	C	3.65008600	3.03233300	2.18311100
B	0.91432900	2.75140800	0.06131400	C	4.81487200	2.27625300	2.16597200
B	3.27438700	-3.46172500	-0.88708100	C	4.79209100	0.87358200	2.29841400
				C	3.60160700	0.16668500	2.42470900

B	1.14686000	-4.81136700	-0.95697900	C	0.45086500	1.69679200	2.55162300
B	3.01691800	4.02234700	-0.45565400	H	3.66512200	4.11317100	2.09377200
B	0.80436900	5.22366100	-0.39245400	H	5.77180400	2.77493300	2.05085000
B	5.20968600	2.89413000	-0.98502600	H	5.73030700	0.32755500	2.28535800
B	7.33208900	1.73999600	-1.65633900	H	3.56680900	-0.91352400	2.51096800
B	7.42065500	-0.76572200	-1.78868700	O	1.15258400	0.53529900	2.54487100
B	-1.30803900	3.88024500	-0.16077500	N	1.12701300	2.78601200	2.43624700
B	-1.42220400	6.37390600	-0.47505800	H	1.85001900	6.71729000	-2.26012700
B	5.38324500	-2.13203000	-1.26597900	H	-0.65843600	6.64036400	-2.33575900
B	-1.05266000	-3.64809600	-0.57974900	H	-2.92434200	5.45122100	-2.15844700
B	-0.99659000	-6.09926900	-1.14383600	H	-5.06172100	4.27264500	-2.26555200
B	-3.18862900	-4.93689900	-0.81154400	H	-7.24686000	3.01671100	-2.67434900
B	-3.26088300	-2.47181600	-0.36204200	H	-8.78637000	-1.53387000	-2.34882900
B	-5.38793900	-3.77546300	-0.55771900	H	-7.53570500	-3.57861300	-1.60392200
B	-5.45305400	-1.28866400	-0.24484000	H	-8.67809300	0.95641100	-2.75149100
B	-7.67153500	-0.11597100	-0.19764500	N	-4.96387700	-3.93795700	-0.71516300
B	-7.58831100	-2.61014000	-0.38478100	N	-7.00730600	-2.71588500	-1.57184800
B	-7.75947000	2.38452800	-0.14967600	N	-6.91765500	-0.27000600	-1.94484500
H	-5.45466700	-4.82100600	-0.79319700	N	-6.79487500	2.16729700	-2.35985600
H	-3.42130900	-6.08132600	-0.34921900	Al	-1.36019000	-0.12023700	0.46116800
H	-1.26801300	-7.45216200	-0.26037300	Al_h-BN + Cytosine +F			
H	1.22927800	-7.71920000	-0.25937100	N	-0.82107900	-0.79396800	2.97908500
H	3.44298900	-6.53836500	-0.28311000	C	-1.44143200	0.40840800	2.84046900
H	5.65051100	-5.37601100	-0.32660900	C	-0.73422600	1.56880100	2.88550200
H	7.86630200	-4.21713400	-0.36884700	H	-1.22488500	2.52992400	2.81126400
H	3.96005100	5.41324600	-1.84832100	C	0.68679600	1.44131700	2.85192800
H	6.06438000	4.10695600	-1.48924900	N	1.46447300	2.51068900	2.85460400
H	8.16805100	2.79383600	-1.18380800	H	2.47270900	2.41785900	2.80580400
H	9.05456100	-2.01012200	-0.55390200	H	1.07473000	3.44424600	2.82790600
H	9.16315800	0.51378300	-0.82800600	N	1.28396400	0.22840200	2.69560700
B	0.97831300	0.93423600	-0.58361700	C	0.56468300	-0.92930600	3.00250200
B	0.86741700	-1.64147900	-0.13881300	O	1.08884800	-2.00478200	3.19248400
N	1.61713800	-0.38919800	-0.39792600	H	-1.36380200	-1.65110800	3.02645300
N	-0.40539500	1.15986200	-0.34159300	C	-4.87319700	0.80799500	2.04270700
N	-0.52200200	-1.67909100	0.20604200	C	-4.72578000	-0.58253900	2.06386900
N	-2.60386400	2.23284600	-1.06655500	C	-5.74587100	-1.47901200	1.78595200
N	-2.95918900	-0.18602000	-0.33668400	C	-6.96923600	-0.89841700	1.47148900
B	-1.13533600	2.25583600	-0.90178800	C	-7.14616100	0.49937600	1.43779400
B	-3.44094200	1.01695800	-0.93914700	C	-6.10851100	1.37606400	1.71906900
B	-5.53170000	-0.25470600	-1.48476500	C	-2.87452100	0.38065600	2.56379900
B	-3.54833800	-1.46348300	-0.55534500	H	-5.59472800	-2.55183200	1.81001500
B	-1.34954900	-2.81839300	-0.06153600	H	-7.81151400	-1.54028000	1.23600400
B	-3.23856800	3.43484500	-1.59632200	H	-8.12067400	0.89667200	1.17436300
B	-1.02444800	4.62466500	-1.74966900	H	-6.23969700	2.45225600	1.69021800
B	-3.56081400	-3.97282400	-0.40023600	O	-3.42998700	-0.84831900	2.40495000
B	-1.45209200	-5.33074100	-0.23080000	N	-3.65288900	1.39075500	2.37231600
B	-5.63697600	-2.74283500	-1.12430400	H	-0.60785300	-7.34499300	-1.19642800
B	-7.64871300	-1.51555800	-1.97880200	H	1.87491400	-7.17382300	-0.86675600
B	-7.54146000	0.95933100	-2.37770000	H	4.05554800	-5.87947700	-0.49398600
B	0.76294200	-4.14643700	-0.22124000	H	6.16190000	-4.66048100	-0.41111600
B	0.67341900	-6.66063200	-0.24874700	H	8.37174400	-3.40897500	-0.64395200
B	-5.42150300	2.21996200	-1.92043900	H	9.77477100	1.18792300	-0.92917700
B	1.08369100	3.32456100	-1.32381700	H	8.38166300	3.27320000	-0.83907800
B	1.20725900	5.74165100	-2.00615200	H	9.77287100	-1.33627900	-0.85089500
B	3.31045200	4.43424500	-1.62555700	H	6.17961100	4.54812500	-0.65109700
B	3.19436500	1.99025600	-1.08281300	H	4.06089200	5.77934000	-0.74495600
B	5.41499600	3.11846800	-1.31475200	H	1.86213000	7.07075900	-1.07882300
B	5.28636500	0.65334700	-0.87764400	H	-0.62735300	7.23196300	-1.34308300
B	7.40949800	-0.67536600	-0.69342300	H	-2.80420500	5.97304500	-1.38303500
B	7.51881700	1.80104100	-1.04073900	H	-4.96581800	4.72290200	-1.51450700
B	7.30594500	-3.16541400	-0.45304900	H	-7.09692600	3.46641100	-1.84854600
B	5.18292000	-1.82138800	-0.54808300	H	-2.78004300	-6.08940700	-1.32121600
B	3.05259800	-0.47392300	-0.59101000	H	-4.93745900	-4.84635200	-1.52662200
B	2.97750800	-2.97916300	-0.37611600	H	-7.07380700	-3.59982200	-1.87768700
B	5.09234700	-4.32026600	-0.37466100	H	-8.15630300	1.19979200	-2.09081700
N	-0.20945500	5.77450700	-2.06469900	H	-8.14830500	-1.33822100	-2.09727500
N	1.87683600	4.50792700	-1.64524800	B	-0.13116300	-1.35423500	-0.26949400
N	-0.35884800	3.40759600	-1.34158000	B	-0.11913900	1.24851800	-0.37983300
N	1.76310900	2.07586800	-1.03365400	N	-0.83028700	-0.05156000	-0.39068400
N	3.74013800	-1.75579000	-0.49528200				
N	1.54708900	-2.92562400	-0.26936600				

N	3.84325500	0.71636100	-0.87481400	N	1.21746500	-1.46847500	0.16528200
N	3.98031100	3.18806500	-1.35048600	N	1.25620200	1.35948200	-0.04999800
N	3.65577100	-4.26837600	-0.35231200	N	3.51759900	-2.54827900	0.02874200
B	2.88111100	-5.48296900	-0.29173800	N	3.74495200	-0.02591400	0.46098700
N	1.44778300	-5.43532500	-0.24905800	B	2.04011000	-2.61030400	-0.05463200
N	-0.74231200	-6.58716200	-0.24456800	B	4.31358900	-1.29742200	0.11627200
N	-0.68134800	-4.10708900	-0.18581000	B	6.44695800	-0.05396900	-0.33039200
N	6.07388700	1.86425600	-1.07484400	B	4.31968300	1.21707000	0.03211700
N	5.96069400	-0.61270200	-0.69406100	B	2.05776600	2.51317500	-0.25478000
N	5.85978100	-3.10848300	-0.45257300	B	4.24408600	-3.79279300	-0.19615100
N	8.04363000	-1.95786200	-0.55299900	B	2.10140500	-5.08222400	-0.52715800
N	8.15138900	0.54688800	-0.83907300	B	4.25707700	3.70083400	-0.39345100
N	-2.87700900	-5.23124600	-0.26191600	B	2.10569200	4.98163100	-0.73193800
N	-2.82050400	-2.72155400	-0.24348400	B	6.44546000	2.45843000	-0.48904100
N	-2.45173800	4.62104500	-1.82094900	B	8.59241400	1.18662100	-0.74354400
N	-4.64279400	3.42037700	-1.91253300	H	3.94477900	0.60234700	2.69317400
N	-4.79992800	0.99674700	-1.46465200	O	1.11804200	-2.73399900	2.22751300
N	-4.90289400	-1.49903300	-1.08402800	N	1.29860100	-0.52092400	2.60869300
B	8.59028300	-1.32119600	-0.66729500	N	-6.22510200	-2.37917500	4.45715300
B	-0.07265300	3.71900200	-0.77338500	H	-6.12276400	-3.17403500	5.07243100
B	-0.04733800	6.20701000	-1.13554100	H	-7.06675400	-1.82838600	4.54454300
B	6.43853600	-2.56827500	-0.34190200	H	1.59318300	7.74900100	-0.04622900
B	-0.07368000	-3.82753600	-0.62970100	H	-0.90955900	7.57275400	-0.16914000
B	-0.03562300	-6.31786700	-0.97822600	H	-3.10718200	6.28431900	-0.35128700
B	-2.19983600	-5.06342800	-1.11941100	H	-5.18475100	5.10614000	-0.82948500
B	-2.24022700	-2.56959200	-0.86994000	H	-7.32390400	3.94697000	-1.61971300
B	-4.35675900	-3.81542500	-1.35728800	H	-8.61541100	-0.51691300	-2.88569200
B	-4.37175500	-1.31044900	-1.22054800	H	-7.23988700	-2.61371700	-2.91186000
B	-6.49604000	-0.06512700	-1.69774300	H	-8.64889600	1.96112700	-2.39555800
B	-6.48824500	-2.56843300	-1.73105800	H	-5.07518000	-3.93890200	-2.59742100
B	-6.50383700	2.43739500	-1.71563800	H	-2.96265800	-5.17734900	-2.54763800
B	-4.37612100	1.18912000	-1.22649400	H	-0.73296600	-6.41537400	-2.76659700
B	-2.23813600	-0.05581700	-0.73528900	H	1.77084400	-6.57170300	-2.66930600
B	-2.24545000	2.45690100	-0.92357100	H	3.91139800	-5.35868700	-2.16234700
B	-4.37625200	3.69453100	-1.36072600	H	6.04712100	-4.15427300	-1.66528100
N	1.37093900	-6.29855200	-0.79825200	H	8.18187900	-2.95239900	-1.16697700
N	-0.78041000	-5.07609500	-0.90447000	H	3.76266400	6.48711100	0.02319700
N	1.35700700	-3.84818700	-0.41744300	H	5.92773900	5.23979500	0.07817100
N	-0.82888500	-2.58634700	-0.60964600	H	8.09876700	3.99305400	0.11356800
N	-2.95878900	1.19565700	-0.93386200	H	9.24017900	-0.74932000	-0.58762900
N	-0.82612200	2.47741900	-0.71257500	H	9.21141800	1.75482200	-0.13928300
N	-2.95900200	-1.31163200	-0.90404600	B	1.00769000	1.68719900	-0.11265400
N	-2.94038400	-3.82488800	-1.10629100	B	1.04355300	-0.86934800	-0.66620800
N	-2.95386900	3.70992700	-1.14635600	N	1.72208200	0.42003800	-0.40249400
B	-2.21582900	4.94906900	-1.19521200	N	-0.38808400	1.76497300	0.18688600
N	-0.78883800	4.96502100	-1.03272400	N	-0.35221800	-1.05767600	-0.47325300
N	1.36450500	6.19327800	-0.99380500	N	-2.62694700	2.90539300	-0.32478700
N	1.36459000	3.74714000	-0.60405100	N	-2.83734400	0.37724800	-0.51449600
N	-5.07431900	-2.57267200	-1.41916100	B	-1.16888800	2.93916000	-0.08177100
N	-5.08391500	-0.06218100	-1.36780800	B	-3.40213400	1.67829800	-0.63427400
N	-5.08815700	2.44819200	-1.41122600	B	-5.42408300	0.56069700	-1.60252800
N	-7.16888400	1.19454700	-1.86749500	B	-3.36362500	-0.78639000	-1.13729500
N	-7.16181500	-1.32833700	-1.86990500	B	-1.10219400	-2.09804800	-1.10689500
N	3.52891000	4.92981400	-0.59655200	B	-3.32126600	4.17922600	-0.44991900
N	3.53015900	2.46512000	-0.12679300	B	-1.17092100	5.45830800	-0.19197800
N	3.52050800	-5.02857700	-0.36634800	B	-3.23010500	-3.18181700	-1.88809400
N	5.68179900	-3.77975800	-0.26897200	B	-1.04724200	-4.42416200	-2.07482500
N	5.73824600	-1.31224900	-0.19606200	B	-5.38382200	-1.89684900	-2.14789400
N	5.74299100	1.21269200	-0.27692100	B	-7.47491300	-0.56345000	-2.52499400
N	5.69401500	3.67700000	-0.47262200	B	-7.50781900	1.89801500	-2.03895000
N	7.87159700	2.40963200	-0.70289000	B	1.09158700	-3.21767600	-1.54118600
N	7.88822700	-0.06247500	-0.56811600	B	1.15364400	-5.59368700	-2.36508500
N	7.86551400	-2.53692100	-0.55545900	B	-5.44729500	3.03782500	-1.17620800
Al	2.00128700	-0.00912300	0.83533900	B	0.99711400	4.19545700	-0.11939000
Al_h-BN + Guanine +F				B	1.00010300	6.71123100	-0.08686400
N	-1.64677100	-2.37950700	3.38205900	B	3.16400800	5.45420800	-0.04673800
C	-0.92692600	-1.50304200	2.64364200	B	3.17332300	2.95295300	-0.20849100
N	-1.69118900	-0.53646900	2.15862300	B	5.33356900	4.21001900	-0.04553300
C	-2.96305600	-0.79271500	2.63432800	B	5.34004400	1.72010800	-0.33211300
				B	7.52740000	0.49839300	-0.44942400
				B	7.50394500	2.97138900	-0.05956600

C	-4.17517100	-0.01914800	2.55482400	B	7.56225500	-1.94867400	-0.97571500
O	-4.36047200	1.07312900	2.05116200	B	5.36769400	-0.73036700	-0.81529000
N	-5.21624800	-0.70136900	3.21405000	B	3.16490000	0.45958300	-0.53263200
H	-6.11190700	-0.22266500	3.18857600	B	3.23856200	-1.97307400	-1.17226800
C	-5.10461200	-1.88001000	3.91194500	B	5.42620200	-3.15882900	-1.43459000
N	-3.96836600	-2.53950900	4.04373200	N	-0.41556200	6.68936300	-0.15044200
C	-2.95141900	-1.94908600	3.39720200	N	1.72990600	5.45916400	-0.08021800
H	-1.28024300	-3.18333000	3.88167900	N	-0.44674500	4.20757700	-0.14577200
C	2.57500900	-1.05442500	2.42865600	N	1.73976200	2.94978200	-0.17140600
C	2.45292200	-2.42346500	2.18226800	N	3.92431400	-0.74128900	-0.85846400
C	3.53033800	-3.26546000	1.95094200	N	1.80473600	-2.01425100	-1.15564400
C	4.78070500	-2.65778800	2.00848900	N	3.89563600	1.70709600	-0.34179500
C	4.93268000	-1.28562400	2.28693300	N	3.89730200	4.21399100	-0.10393000
C	3.83701500	-0.45872600	2.49421900	N	3.99200300	-3.17429700	-1.51329700
C	0.52333100	-1.54287100	2.48013700	B	3.28861200	-4.37684700	-1.88219000
H	3.40358400	-4.32180700	1.74389700	N	-0.88957000	0.11207800	-0.42963000
H	5.66648800	-3.26014900	1.83287000	N	1.14024900	-1.37061100	0.02984500
H	5.93318400	-0.86561500	2.32328900	N	1.15981300	1.51744500	0.17877200
N	1.85418900	-4.40438100	-1.92325700	N	3.43359000	-2.45361000	-0.21986200
N	-0.26215800	-5.58041800	-2.44114900	N	3.69381500	0.03177500	0.36828200
N	-0.35175100	-3.25237700	-1.59144500	B	1.95746500	-2.50366100	-0.27929200
N	6.05884800	2.97316400	-0.13585900	B	4.24640700	-1.22089800	-0.06987600
N	6.07935500	0.49350200	-0.51988500	B	6.37756900	0.03856600	-0.46094900
N	6.11968200	-1.95169300	-1.07879200	B	4.27121000	1.30483200	0.03546600
N	8.22959000	-0.74025600	-0.64605600	B	2.00469800	2.64849300	-0.06195600
N	8.20051400	1.74249000	-0.19224300	B	4.14645400	-3.69092700	-0.52748700
N	-2.47289100	-4.37714200	-2.16521700	B	1.98526800	-4.94645400	-0.86960700
N	-2.56560600	-2.02556500	-1.30206200	B	4.22049500	3.80210000	-0.23632000
N	-2.59575600	5.41298700	-0.27622600	B	2.08941200	5.12115800	-0.50997400
N	-4.72575400	4.20499800	-0.76887100	B	6.39852500	2.55511800	-0.44516900
N	-4.76022000	1.76953500	-1.15944400	B	8.52612800	1.28725400	-0.83304800
N	-4.72927100	-0.71182100	-1.64575500	B	8.50021300	-1.21856200	-0.93700300
N	-4.63367300	-3.11531600	-2.20580700	B	-0.10041300	3.88971000	-0.60716100
N	-6.76145400	-1.79114200	-2.56692700	B	-0.03861400	6.38448400	-0.91771700
N	-6.81537900	0.63028900	-2.04981900	B	6.34769100	-2.47187400	-0.64966100
N	-6.82488500	3.06648400	-1.60916900	B	-0.17679400	-3.66066900	-0.88629900
Al	-1.28985600	0.22843000	0.36096000	B	-0.17643400	-6.13649000	-1.32146400
Al_h-BN + Thymine +F				B	-2.32714800	-4.85122400	-1.37697800
N	-0.57299700	0.80636700	2.90012500	B	-2.32845700	-2.36488800	-1.05845800
C	-1.11291800	-0.46763300	2.73731100	B	-4.47019600	-3.56872900	-1.53392600
C	-0.37160400	-1.60049000	2.83097100	B	-4.44410400	-1.06909700	-1.32952900
C	-0.89554100	-3.00107800	2.70877200	B	-6.57179000	0.21381700	-1.66074200
H	-1.36284200	-3.15544800	1.73185100	B	-6.59655700	-2.28509200	-1.78836400
H	-0.06596700	-3.69945400	2.82571000	B	-6.54672500	2.71605000	-1.59824500
H	-1.65323400	-3.20810900	3.46842300	B	-4.41960900	1.42659100	-1.23603800
C	1.07006800	-1.44320100	3.02069800	B	-2.29191600	0.14085300	-0.81407700
O	1.87570200	-2.31780500	3.21802900	B	-2.27671600	2.65727300	-0.87391000
N	1.57337600	-0.08444900	2.82791000	B	-4.38930100	3.93411500	-1.28514700
H	2.49076300	0.02414400	3.27311600	N	1.23399900	-6.14121400	-1.17176000
C	0.74770400	1.06237200	3.10634500	N	-0.90338900	-4.88811200	-1.19090600
O	1.22552000	2.12505000	3.40674100	N	1.25585000	-3.70967800	-0.69268000
H	-1.20033100	1.60129700	2.97433400	N	-0.91420000	-2.40849300	-0.80996100
C	-4.56811000	-0.86591100	1.97490400	N	-2.99923800	1.40590500	-0.95440000
C	-4.41949600	0.52181400	2.03376700	N	-0.86632500	2.65364300	-0.60474200
C	-5.45457800	1.42460900	1.84469400	N	-3.02188500	-1.09550100	-1.05675900
C	-6.69549800	0.85319300	1.58322700	N	-3.04827200	-3.60345400	-1.31539100
C	-6.87403600	-0.54251100	1.51171300	N	-2.96722800	3.92371800	-1.06727200
C	-5.81971700	-1.42498700	1.70208200	B	-2.21652000	5.15554500	-1.05738000
C	-2.54229400	-0.45977400	2.43052100	N	-0.79476000	5.14850200	-0.85659500
H	-5.30361700	2.49649400	1.90020600	N	1.36949500	6.34789900	-0.75402300
H	-7.54972400	1.50258500	1.42268700	N	1.33218500	3.89294300	-0.40463800
H	-7.86261500	-0.93421900	1.29680100	N	-5.16952600	-2.31528200	-1.54428100
H	-5.95227100	-2.50015400	1.64805900	N	-5.14376200	0.19003200	-1.40916500
O	-3.10936900	0.77632800	2.32392900	N	-5.11832900	2.69950800	-1.36273200
N	-3.33584500	-1.46036600	2.23596000	N	-7.23782800	1.48570400	-1.73713500
H	-0.76693900	-7.14774600	-1.56145200	N	-7.26114800	-1.03419300	-1.84626100
H	1.72440300	-7.01982400	-1.28274300	N	3.50923900	5.04791200	-0.37085400
H	3.93214700	-5.75944400	-0.91566000	N	3.48150000	2.56112800	-0.01379700
H	6.05115300	-4.55356200	-0.84133400	N	3.40784400	-4.91054100	-0.73920500
				N	5.58094000	-3.67967000	-0.63706400
				N	5.66136400	-1.22248000	-0.40403500

H	8.26617000	-3.30161600	-1.05268900	N	5.68670600	1.30470000	-0.29882200
H	9.70347900	1.29083500	-1.04610000	N	5.65497100	3.77215000	-0.34138600
H	8.33310100	3.37718200	-0.78086300	N	7.81881300	2.51010600	-0.68981000
H	9.67724800	-1.22824600	-1.15150500	N	7.81198100	0.03516700	-0.73072500
H	6.14145500	4.64959900	-0.48239000	N	7.76839200	-2.43479500	-0.89339700
H	4.05218400	5.89417800	-0.49606500	Al	1.96246400	0.03629500	0.71917700
H	1.88208200	7.21870900	-0.81572700				
H	-0.60307100	7.42004300	-1.11288000				
H	-2.78834100	6.19134600	-1.22806500				
H	-4.96423200	4.97443100	-1.40861000				
H	-7.12962300	3.75594900	-1.67936200				
H	-2.92492900	-5.86310500	-1.59520500				
H	-5.06886700	-4.58680900	-1.71638600				
H	-7.20041200	-3.30433000	-1.94457700				
H	-8.23544400	1.50978700	-1.90725800				
H	-8.25819700	-1.02554000	-2.02137300				
B	-0.21121500	-1.20609400	-0.39669700				
B	-0.18963200	1.41121500	-0.27401100				
Adenine				Thymine			
N	2.06731000	0.58480800	0.00118700	N	-1.11211400	-1.24231500	-0.00046600
C	2.28232000	-0.76899900	-0.00039900	C	0.24306500	-1.47248200	-0.00005400
H	3.28421400	-1.17597400	-0.00022700	H	0.52559800	-2.51964700	0.00001300
N	1.17819200	-1.47163700	-0.00058400	C	1.15650400	-0.47943200	0.00000600
C	0.18044300	-0.51746900	-0.00011000	C	2.64123300	-0.71868800	0.00016300
C	-1.22754100	-0.60998100	0.00027900	H	2.95600300	-1.28140000	-0.88304000
N	-1.86478900	-1.79261900	0.00029600	H	3.15996900	0.24119200	-0.00254300
H	-2.87334200	-1.81902000	0.00032700	H	2.95670300	-1.27665100	0.88615600
H	-1.34646800	-2.65774400	0.00036500	C	0.66452700	0.89902500	-0.00003600
N	-1.94732300	0.52399600	-0.00003800	O	1.36182100	1.90165700	0.00003900
C	-1.29105700	1.69397800	-0.00040900	N	-0.72719500	1.02224700	-0.00027000
H	-1.92542900	2.57783900	0.00019500	H	-1.09516600	1.96783400	-0.00026200
N	0.01814700	1.92050500	-0.00011100	C	-1.67064000	0.01470300	0.00008000
C	0.71005200	0.77113000	-0.00030900	O	-2.87091700	0.21924100	0.00032500
H	2.77496400	1.30756600	-0.00023800	H	-1.76331900	-2.01678700	0.00094900
Cytosine							
N	-1.27593000	0.88956300	0.00000100				
C	-0.19398600	1.70640200	-0.00000100				
H	-0.39338300	2.77162800	-0.00000400				
C	1.05270100	1.17881700	0.00000000				
H	1.93673000	1.80143800	-0.00000200				
C	1.13192900	-0.25703600	0.00000100				
N	2.34215900	-0.84183900	-0.00000100				
H	2.40166700	-1.84967100	-0.00000300				
H	3.19546000	-0.30500700	-0.00000400				
N	0.07056600	-1.05174300	0.00000200				
C	-1.18161500	-0.51159600	0.00000800				
O	-2.21741400	-1.17028600	-0.00000500				
H	-2.21290300	1.27250800	-0.00000300				
Guanine							
N	-1.73357600	-1.49430900	-0.00067000				
C	-2.70489400	-0.52184400	0.00064300				
H	-3.75517300	-0.77758300	-0.00026500				
N	-2.21190000	0.68798100	0.00301800				
C	-0.84531000	0.49713300	0.00332600				
C	0.22419100	1.45367300	0.00152200				
O	0.17929400	2.67455300	-0.00099000				
N	1.47221300	0.78959500	-0.00093000				
H	2.27790100	1.40614500	-0.03155500				
C	1.66981900	-0.56854500	-0.00047300				
N	0.69213900	-1.44273600	0.00497800				
C	-0.52889500	-0.85543300	0.00062500				
H	-1.87841800	-2.49542500	-0.00283900				
N	2.96046000	-0.99597300	-0.06680800				
H	3.68984200	-0.39345400	0.29059600				
H	3.08667800	-1.97791500	0.14100700				

