Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
This journal is © The Owner Societies 2011

Supplementary Information

Theoretical studies on interactions between low energy electrons and protein-DNA fragments: Valence anions of AT-Amino Acids Side Chain Complexes.

Anna Szyperska,[a] Agnieszka Gajewicz,[a] Kamil Mazurkiewicz,[a] Jerzy Leszczynski,[*b] Janusz Rak[*a]

[a] *Department of Chemistry, University of Gdańsk, Sobieskiego 18, 80-952 Gdańsk, Poland. E-mail: janusz@raptor.chem.univ.gda.pl; Fax: (+4858) 523 5571; Tel.:(+4858) 523 5322*

[b] *Interdisciplinary Center for Nanotoxicity, Department of Chemistry, Jackson State University, Jackson, MS 39217, USA. E-mail: jerzy@icnanotox.org; Fax: (+01601) 979 6865; Tel.: (+01601) 979 3723*

[†] *Electronic supplementary information (ESI) available.*

This journal is © The Owner Societies 2011

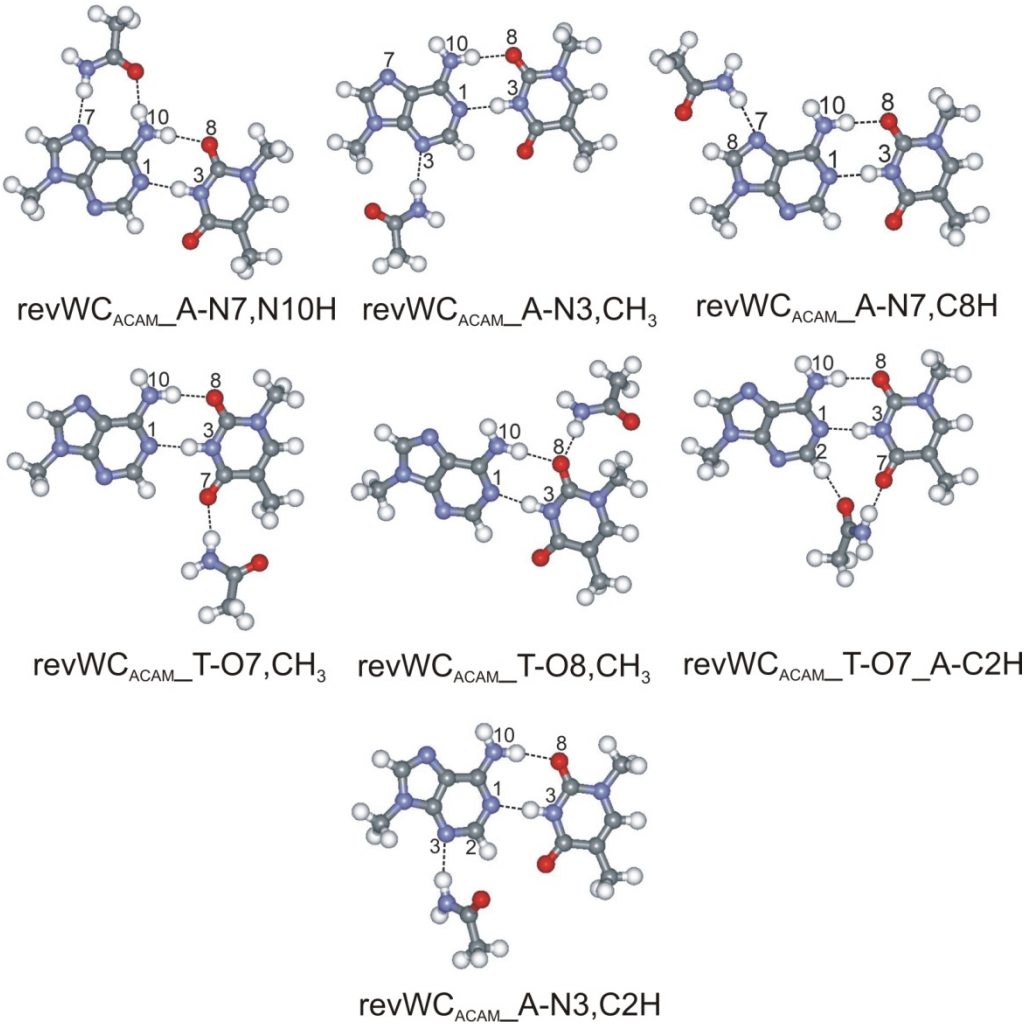
Table S1. Thermodynamic characteristics of neutral 9-methyladenine…1-methylthymine - acetamide in reversed WC, Hoogsteen and reversed Hoogsteen configurations. ΔE, E_{stab}, ΔG and G_{stab} stand for the relative energy, stabilization energy, relative Gibbs free energy and stabilization free energy, respectively. ΔE and ΔG were calculated with respect to the most stable neutral complex, WC_{ACAM}_A-N7,N10H. The values were calculated at the B3LYP/6-31++G(d,p) level. All energies in kcal/mol.

Structure	ΔE	E_{stab}	ΔG	G_{stab}
reversed Watson-Crick				
$revWC_{ACAM}$_A-N7,N10H	0.28	-10,19	-0.03	2.32
$revWC_{ACAM}$_A-N3,CH_3	2.30	-8.17	1.92	4.27
$revWC_{ACAM}$_A-N7,C8H	2.53	-7.93	1.24	3.59
$revWC_{ACAM}$_T-O7,CH_3	3.41	-7.06	1.59	3.94
$revWC_{ACAM}$_T-O8,CH_3[(a)]	3.56	-6.90	3.26	5.61
$revWC_{ACAM}$_T-O7_A-C2H	6.06	-4.41	3.89	6.24
$revWC_{ACAM}$_A-N3,C2H	6.94	-3.53	2.95	5.30
Hoogsteen				
$Hoog_{ACAM}$_A-N1,N10H	-1.36	-10.44	-0.91	2.49
$Hoog_{ACAM}$_T-O7_A-C8H	0.35	-8.73	0.65	4.06
$Hoog_{ACAM}$_A-N3,CH_3	1.35	-7.73	1.32	4.72
$Hoog_{ACAM}$_T-O7,CH_3	1.87	-7.21	1.23	4.63
$Hoog_{ACAM}$_T-O8_A-N10H	2.40	-6.69	1.86	5.26
$Hoog_{ACAM}$_T-O8,CH_3	3.02	-6.07	2.25	5.65
$Hoog_{ACAM}$_A-N1,C2H	3.37	-5.71	1.94	5.34
$Hoog_{ACAM}$_A-N3,C2H	4.03	-5.05	2.43	5.83
reversed Hoogsteen				
$revHoog_{ACAM}$_A-N1,N10H	-1.42	-10.79	-1.03	2.03
$revHoog_{ACAM}$_T-O7_A-C8H	-0.29	-9.66	0.12	3.18
$revHoog_{ACAM}$_A-N3,CH_3	1.74	-7.62	1.55	4.61
$revHoog_{ACAM}$_T-O8,CH_3	2.13	-7.23	1.52	4.58
$revHoog_{ACAM}$_T-O7,CH_3	3.02	-6.34	1.66	4.72
$revHoog_{ACAM}$_T-O8_A-N10H	3.61	-5.75	2.78	5.84
$revHoog_{ACAM}$_A-N1,C2H	3.75	-5.62	2.57	5.63
$revHoog_{ACAM}$_A-N3,C2H	4.26	-5.10	2.94	6.00

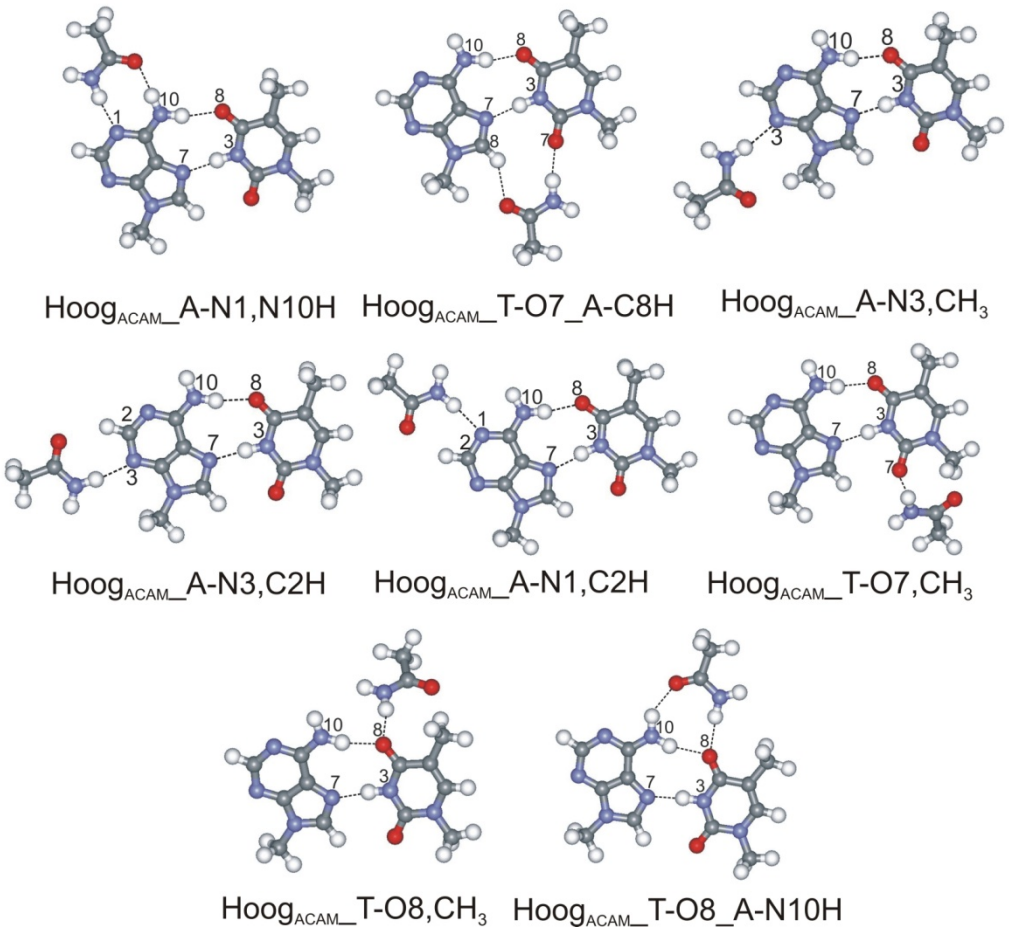
[a] revWC$_{ACAM}$_T-O8_A-N10H converged to revWC$_{ACAM}$_T-O8,CH$_3$ structure

Fig. S1 Optimized structures of the neutral complexes of MAMT-ACAM complex in (A) reversed Watson-Crick, (B) Hoogsteen, (C) reversed Hoogsteen configurations.

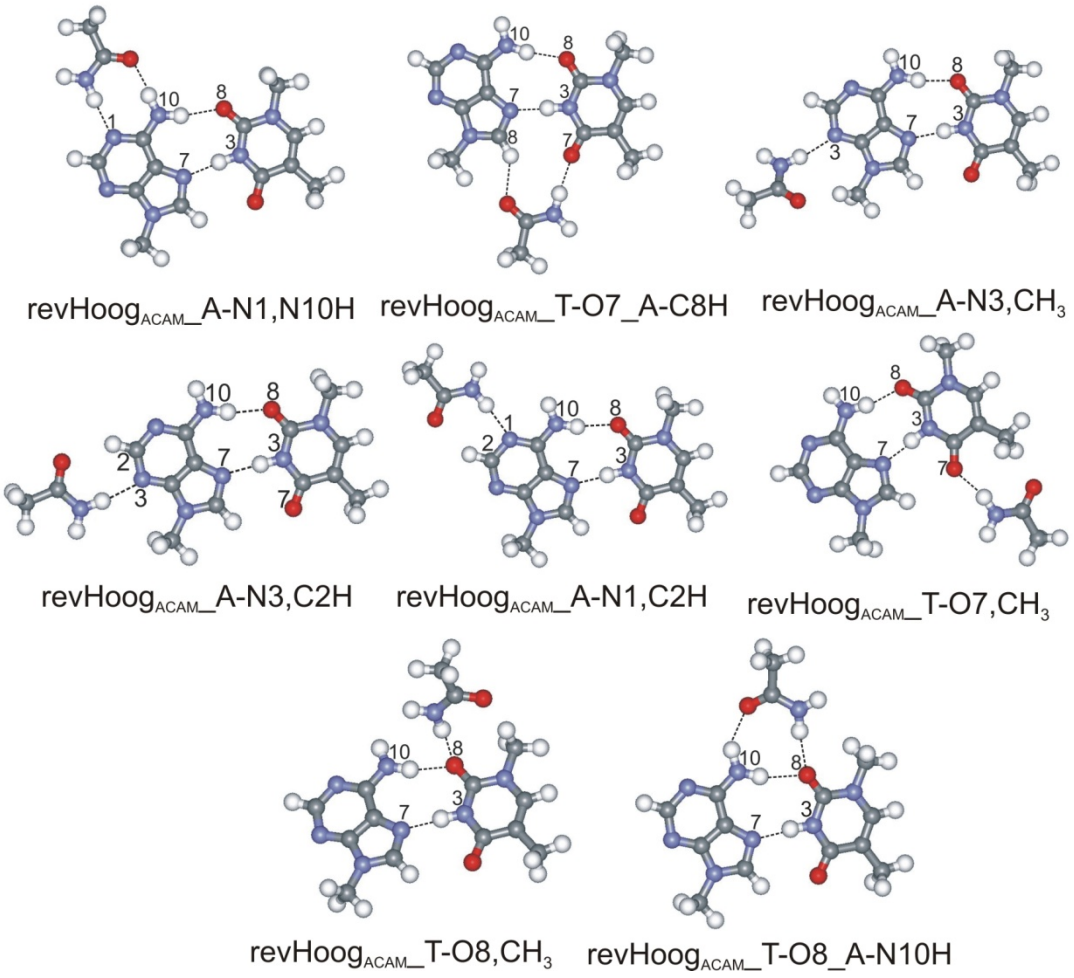
(A)



(B)


Hoog$_{ACAM}$_A-N1,N10H
Hoog$_{ACAM}$_T-O7_A-C8H
Hoog$_{ACAM}$_A-N3,CH$_3$
Hoog$_{ACAM}$_A-N3,C2H
Hoog$_{ACAM}$_A-N1,C2H
Hoog$_{ACAM}$_T-O7,CH$_3$
Hoog$_{ACAM}$_T-O8,CH$_3$
Hoog$_{ACAM}$_T-O8_A-N10H

(C)


revHoog$_{ACAM}$_A-N1,N10H
revHoog$_{ACAM}$_T-O7_A-C8H
revHoog$_{ACAM}$_A-N3,CH$_3$
revHoog$_{ACAM}$_A-N3,C2H
revHoog$_{ACAM}$_A-N1,C2H
revHoog$_{ACAM}$_T-O7,CH$_3$
revHoog$_{ACAM}$_T-O8,CH$_3$
revHoog$_{ACAM}$_T-O8_A-N10H