

Complete family of h-bonded 1-methylcytosine homoassociates: Quantum-mechanical investigation

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Summary. On the MP2/6-311++G(2df,pd)//B3LYP/6-311++G(d,p) theory level in vacuum for the first time was shown that stabilized by specific intermolecular contacts complete family of m¹Cyt-m¹Cyt homoassociates counts 37 structures in diapason of 0+34.42 kcal/mol relative Gibbs energies. Centrally symmetric homoassociate corresponds to global minima which is stabilized by pair of antiparallel H-bonds N4H...N1 and has enthalpy of formation practically the same as in mass-spectrometry experiment (L.F. Sukhodub et al., 1976). Detail analysis of intermolecular H-bonds, especially weak CH...O/N, physico-chemical properties has been performed. Briefly discussed application of results in spontaneous point mutations of DNA theory.

Keywords: nucleic base, nucleic base pairs, non-canonical base pairs, homoassociate, self-associate, cytosine, 1-methylcytosine.

Introduction. Nucleic bases (NB) play major role in coding genetic information, RNA spatial structure, engineering synthetic DNA. It's generally known that DNA strands hold complementary NB pairs of Gua-Cyt and Ade-Thy [2]. The complimentary principle is key factor supplying the transmission of genetic information in heredity line. Point changes of NB — mutations are possible through creation of incorrect pairs by rare NB tautomeric forms [3] which in turn leads to transformation of canonical NB pairs into non-canonical and errors during biosynthesis of DNA. RNA spatial structure in many respects is defined by intermolecular H-bonds between NB. Special emphasis in literature gives attention to non-canonical NB pairs in RNA [4-7]. At the same time synthetic DNA can be designed to have non-canonical NB pairs. Every mentioned aspect demands knowledge about geometrical and physico-chemical prop-

erties of isolated NB as well as of their H-bonded associates.

Object and methods. The goal of this paper is to obtain geometrical and physico-chemical properties of all possible 1-methylcytosine (m¹Cyt) homoassociates which involve all of it's seven possible tautomeric forms. Input structures automatically generated by original algorithm. Geometrical and electronic structure of molecules and complexes as well as their wavefunctions were obtained using density functional theory on B3LYP/6-311++G(d,p) theory level in vacuum. All optimized structures has been checked on stability by absence of imaginary frequencies in their spectra. Electronic energies of NB interaction and NB Gibbs free energies were obtained on MP2/6-311++G(2df,pd)//B3LYP/6-311++G(d,p) theory level. Quantum-mechanical calculations were done in Gaussian 03 for Win32 application [8].

Intermolecular H-bond identification were done by QTAIM method [9]. For identification of CH...O/N H-bonds NBO-analysis [10] and Grunenberg constant [11, 12] methods were addi-

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tionally used. Grunenberg constants calculations were done in Compliance 3.0.2 application [13]. Classical H-bond energies were calculated by Iogansen method [14, 15]. Non-canonical CH...O/N H-bond energies and van-der-Waals contacts were calculated by Espinosa-Mollins-Lecomte method (EML) [16].

Results and discussion. *Fundamental physico-chemical properties of m¹Cyt-m¹Cyt homoassociates.* Results are presented in table 1. Atomic numbering based on standard scheme [17]. Belonging to the same plane as molecule methyl group hydrogen atom has index 1. Complete family of H-bonded homoassociates m¹Cyt-m¹Cyt contains 37 structures. These structures consists of NB pairs in common tautomeric form as well as rare tautomeric forms. Most energetically favorable conformer **1** has centrosymmetrical structure, stabilized by two antiparallel H-bonds on m¹Cyt Watson-Crick binding site (naming convention by [18]) and has zero dipole moment. Ten homoassociates m¹Cyt-m¹Cyt has planesymmetrical structure (3 of them are centrosymmetrical); other 27 are significantly non-planar.

Conformer **1**'s population in standard conditions is 99,97 % and conformers **2**, **3** has total population of ~0,03 %.

It was established that homoassociates m¹Cyt-m¹Cyt are stabilized by bond types: NH...N; NH...O; OH...N; OH...O; CH...N; CH...O. Classic H-bond energies lie in diapason 0,39÷2,80 kcal/mol (table 1).

Identification of weak CH...O/N H-bonds. Weak CH...O and CH...N bonds attract special interest in literature. One of the problems discussed are their physicochemical properties and classification. It was established [19] that in such conditions that type of specific contacts is true H-bond. Our interest has been attracted to this H-bonds because 20 out 37 conformers in complete conformational family of m¹Cyt-m¹Cyt homoassociates are stabilized through CH...O/N H-bonds. In 16 conformers m-group in position 1 takes part in CH...O/N H-bonds as proton donor. As we can see from table 1 QTAIM method identifies all specific CH...O/N contacts as H-bond. Although for their robust identification as a true H-bonds we additionally used NBO-analysis [10] and Grunenberg constants methods [11, 12].

Quantum-mechanical calculations' results of

stabilization energies $E^{(2)}$ and Grunenberg constants for these H-bonds are presented in table 2. As we can see all values $E^{(2)} > 0$ which means charge transfer from atom-acceptor lone pair to C-H antibond. Also all Grunenberg constants are positive which means stabilization (pull not push) nature of specific CH...O/N contacts. No charge transfer in complex **3** means borderline case of transformation H-bond into van-der-Waals contact and can be useful for future investigations of lower bounds for electron density and it's laplacian in corresponding H-bond critical point. Obviously, that by using QTAIM theory only, it's hard if not possible at all to tell the difference between AH...B H-bond and A...B van-der-Waals contact. It's seen from table 1 that for van-der-Waals contacts electron density values belong to 0.002-0.012 a.u. diapason and laplacian of electron density values belong to 0.006-0.038 a.u. diapason. At the same time for weak H-bonds electron density values belong to 0.006-0.019 a.u. and laplacian of electron density values belong to 0.009-0.052 a.u. Comparability of values in both cases shows us the necessity of QTAIM usage in pair with NBO-analysis for identification and investigation of weak H-bonds nature. Although this fact doesn't diminish the value of QTAIM analysis as most generic and relatively cheap method for modeling electronic clouds.

We'll add that for CH...O/N contacts we found linear relation of H-bond energy E_{HB} from electron density in bond critical point ρ . Relations for data in table 1 are $E_{HB}^{CH...O} = 175.121\rho + 0.107$ and $E_{HB}^{CH...N} = 163.684\rho + 0.044$ with RMSD values of 0.0003 kcal/mol and 0.0043 kcal/mol respectively. Data extrapolation on base of these relations to minimal electron density value of $\rho = 0,002$ a.u. gives adequate minimal H-bond energy values of $E_{HB}^{CH...O}(min) = 0,46$ kcal/mol and $E_{HB}^{CH...N}(min) = 0,28$ kcal/mol.

Interpretation of classic mass-spectrometry experiment. In [20, 21] is described mass-spectrometry experiment with registration of associating biomolecules in vacuum. In this experiment reaction $m^1Cyt + m^1Cyt \leftrightarrow m^1Cyt \cdot m^1Cyt$ has been registered and it's reported standard enthalpy of formation has value of $\Delta H = 73,3$ kJ/mol for $T = 383$ K. Basing our hypothesis on population value of most energetically favorable homo-

Table 1

Fundamental physicochemical properties of *m*'Cyt-*m*'Cyt homoassociates

Complex	ΔG° , kcal/mol	μ , D	H-bond/vdW contact AH...B/A...B	P, a.u.	$\Delta\rho$, a.u.	100 ϵ	d_{AB} , Å	d_{HB} , Å	Δd_{AH} , Å	$\angle AHB$, deg	E_{HB} , kcal/mol
1	2	3	4	5	6	7	8	9	10	11	12
1	0.00	0.00	N4H1...N3	0.032	0.088	0.08	2.946	1.917	0.023	175.7	6.39
			N4H1...N3	0.032	0.088	0.08	2.946	1.917	0.023	175.7	6.39
2	5.31	6.54	N3H...N3	0.028	0.080	0.07	3.005	1.977	0.020	174.6	5.90
			N4H...O2	0.016	0.054	0.02	3.187	2.164	0.004	177.8	3.11
			N4H1...O2	0.031	0.031	0.05	2.864	1.840	0.017	176.6	5.42
3	5.49	4.79	N3...C2	0.007	0.024	139.4	3.202	–	–	–	1.22
			N4H1...N3	0.020	0.063	0.05	3.096	2.110	0.012	161.8	4.20
			C1H...O2	0.002	0.009	0.41	3.794	3.289	0.000	109.5	0.39
4	6.47	2.99	C1H...N3	0.014	0.041	0.05	3.427	2.349	0.000	168.9	2.19
			N4H1...O2	0.027	0.105	0.06	2.888	1.867	0.014	176.3	4.67
5	6.64	13.38	N4H2...O2	0.025	0.088	0.06	2.970	1.953	0.011	179.8	4.16
6	7.48	14.93	C5H...N3	0.006	0.017	0.05	3.762	2.746	0.000	156.5	0.96
			N4H2...O2	0.024	0.089	0.04	2.967	1.952	0.011	176.0	4.06
7	7.54	10.60	N4H2...N3	0.022	0.068	0.02	3.032	2.109	0.015	149.5	4.71
			N4H1...N4	0.014	0.044	0.12	3.190	2.298	0.006	146.1	2.63
8	7.81	13.28	N4H2...N3	0.019	0.060	0.08	3.152	2.149	0.009	169.4	3.67
			C5H...O2	0.009	0.030	0.04	3.456	2.440	0.000	156.0	1.69
9	7.85	10.64	C6H...O2	0.012	0.037	0.03	3.372	2.345	0.000	157.3	2.14
			C1H1...O2	0.006	0.019	0.23	3.675	2.689	-0.002	150.4	1.15
10	8.01	1.00	N1...O2	0.004	0.017	170.5	3.360	–	–	–	0.92
			C1H...O2	0.008	0.025	0.13	3.403	2.599	0.000	129.9	1.44
			O2...N1	0.005	0.018	232.2	3.317	–	–	–	1.02
			C1H...O2	0.006	0.022	0.38	3.476	2.685	0.000	129.0	1.24
			C1H...N3	0.006	0.018	0.70	3.794	2.751	0.000	160.0	0.99
11	8.16	5.54	N3...C5	0.005	0.014	109.4	3.568	–	–	–	0.72
			N4H1...N4	0.011	0.033	0.04	3.416	2.408	0.005	172.7	2.22
			C1H...O2	0.007	0.022	0.20	3.368	2.659	0.000	122.2	1.28
12	8.82	12.25	C6H...O2	0.013	0.042	0.04	3.352	2.294	0.001	164.5	2.35
			C1H1...O2	0.007	0.021	0.22	3.637	2.621	-0.001	155.0	1.28
13	8.83	3.99	N3H...N3	0.029	0.080	5.81	2.977	1.946	0.025	173.0	6.76
			N4H1...N4	0.033	0.088	5.46	2.927	1.898	0.025	174.0	6.75
			O2...O2	0.002	0.002	4.74	3.701	–	–	–	0.34
14	8.97	13.90	C6H...O2	0.014	0.045	0.03	3.316	2.264	0.001	162.8	2.50
			C1H1...O2	0.008	0.025	0.20	3.552	2.527	-0.001	156.4	1.43
15	9.52	12.69	C6H...O2	0.015	0.052	0.04	3.277	2.201	0.001	171.0	2.80
			C1H1...N3	0.006	0.016	0.02	3.875	2.791	0.000	172.8	0.89
16	9.75	0.41	N3H...O2	0.027	0.100	3.38	2.902	1.879	0.017	172.5	5.22
			N3H...N4	0.037	0.092	5.44	2.883	1.846	0.030	172.5	7.48
17	10.16	6.31	N4H...N3	0.019	0.060	0.05	3.185	2.170	0.002	171.7	2.45
			N3H...O2	0.023	0.082	0.05	3.001	1.978	0.014	176.4	3.77

1	2	3	4	5	6	7	8	9	10	11	12
20	10.63	3.89	N4H1...O2	0.028	0.101	0.04	2.903	1.887	0.014	172.7	4.85
			N3H...N3	0.027	0.077	0.06	3.010	1.988	0.022	169.3	6.13
			O2...N4	0.002	0.007	20.11	3.862	–	–	–	0.28
21	10.95	10.81	C5H...N3	0.010	0.030	0.09	3.529	2.477	0.001	163.9	1.58
			N4H2...N4	0.011	0.031	0.06	3.437	2.429	0.002	178.3	1.15
	11.21	0.97	C1H...O2	0.013	0.043	0.07	3.352	2.267	0.000	172.3	2.34
			C1H...O2	0.013	0.043	0.07	3.357	2.271	0.000	172.3	2.32
23	11.48	4.05	C1H...O2	0.012	0.040	0.07	3.340	2.311	-0.002	156.9	2.16
			C1H...O2	0.012	0.045	0.04	3.350	2.262	0.000	175.1	2.34
24	11.96	6.81	N4H2...N4	0.014	0.041	0.05	3.288	2.325	0.004	159.0	2.23
25	12.68	0.00	N3H...O2	0.026	0.097	0.03	2.913	1.903	0.014	167.2	4.70
			N3H...O2	0.026	0.097	0.03	2.913	1.904	0.014	167.2	4.70
26	16.62	1.30	N4H1...N3	0.038	0.098	0.07	2.868	1.843	0.027	170.1	6.98
			O2H...N3	0.058	0.093	0.06	2.689	1.667	0.057	175.3	10.72
27	17.70	4.89	O2H...N3	0.057	0.096	0.05	2.686	1.671	0.052	173.3	10.34
			N4H1...N3	0.035	0.090	0.07	2.923	1.894	0.026	173.0	6.90
28	21.55	3.42	C1H...N3	0.011	0.034	0.11	3.313	2.469	-0.002	133.4	1.87
			O2H...O2	0.050	0.143	0.05	2.630	1.627	0.036	177.5	8.54
29	22.05	2.81	C1H...N3	0.010	0.026	0.05	3.517	2.558	-0.001	146.3	1.49
			O2H...O2	0.047	0.146	0.05	2.637	1.640	0.029	176.2	7.77
30	22.54	6.82	N3H...N3	0.033	0.084	0.06	2.950	1.918	0.028	171.0	7.15
			N4H...N4	0.015	0.045	0.05	3.312	2.289	0.002	178.3	2.41
			O2H...O2	0.048	0.142	0.03	2.647	1.658	0.028	171.3	7.69
31	23.22	0.96	N3...N3	0.012	0.038	9.80	2.972	–	–	–	2.18
			O2H...O2	0.045	0.127	0.04	2.674	1.687	0.038	166.0	8.62
			N4H1...N4	0.027	0.076	0.08	3.019	1.988	0.027	173.2	6.78
32	23.53	4.34	N3H...N3	0.034	0.087	0.06	2.920	1.903	0.029	164.8	7.12
			O2H...N4	0.078	0.084	0.05	2.594	1.547	0.081	175.8	12.59
			N4...O2	0.002	0.008	8.96	3.733	–	–	–	0.39
33	28.30	4.17	N3H...N3	0.025	0.077	5.88	2.998	2.001	0.021	161.4	5.90
			N4...N4	0.002	0.006	9.11	3.948	–	–	–	0.29
			O2H...O2	0.050	0.128	1.53	2.631	1.631	0.034	175.2	8.33
34	29.70	12.35	C1H...O2	0.008	0.027	0.39	3.359	2.565	-0.002	129.0	1.55
			C1H...O2	0.010	0.035	0.19	3.308	2.421	-0.005	137.4	1.89
			O2H...O2	0.041	0.140	0.04	2.680	1.705	0.023	168.9	6.79
35	30.72	15.03	O2H...O2	0.039	0.126	0.05	2.720	1.746	0.024	168.5	6.87
			C1H...O2	0.011	0.038	0.23	3.278	2.379	-0.006	138.7	2.10
36	31.68	0.06	O2H...N3	0.081	0.073	0.05	2.591	1.534	0.089	179.2	13.10
			O2H...N3	0.081	0.074	0.05	2.594	1.537	0.089	179.5	13.06
37	34.42	13.38	O2H...O2	0.039	0.125	0.05	2.723	1.750	0.024	168.1	6.80
			C1H...O2	0.010	0.037	0.24	3.294	2.396	-0.006	138.7	2.00

*Note ΔG^0 – relative Gibbs free energy ($T=298,15$ K; $P=1$ atm); μ – dipole moment; AH...B/A...B – atoms forming H-bond and/or van-der-Waals contact; ρ – electron density at BCP; $\Delta\rho$ – laplacian of electron density at the BCP; ε – ellipticity at the BCP; E_{HB} – H-bond energy; distances d_{AB} , d_{HB} and angle $\angle AHB$ between H-bond atoms; elongation Δd_{AH} of H-bonded AH group.

Table 2

Stabilization energies $E^{(2)}$ and linear Grunenberg constant *Cstr* values for intermolecular CH...O/N H-bonds in *m*¹Cyt-*m*¹Cyt homoassociates (calculations on B3LYP/6-311++G(d,p) theory level)

Complex	AH...B	$E^{(2)}$, kcal/mol	<i>Cstr</i> , Å/mdyn
3	C1H...O2	0.00	210.862
4	C1H...N3	3.32	11.904
6	C5H...N3	0.96	56.735
8	C5H...O2	1.79	35.720
9	C6H...O2	2.36	29.497
	C1H1...O2	0.37	66.103
10	C1H...O2	0.16	55.063
	C1H...O2	0.08	81.740
	C1H...N3	0.21	58.270
11	C1H...O2	0.06	233.045
12	C6H...O2	3.03	20.523
	C1H1...O2	0.42	71.288
14	C6H...O2	3.30	16.476
	C1H1...O2	0.60	42.019
15	C6H...O2	4.41	9.990
	C1H1...N3	0.89	49.176
18	C5H...N3	5.53	8.214
19	C1H...O2	1.66	14.329
	C1H...O2	1.62	15.430
21	C5H...N3	1.46	18.925
22	C1H...O2	1.41	14.395
	C1H...O2	1.35	14.539
23	C1H...O2	1.12	25.317
	C1H...O2	2.49	13.805
28	C1H...N3	0.90	17.845
29	C1H...N3	1.08	56.163
34	C1H...O2	0.51	30.099
	C1H...O2	0.75	24.909
35	C1H...O2	0.72	21.020
37	C1H...O2	0.71	21.897

associate **1**, we calculated for it standard enthalpy of formation with account of so-called BSSE correction. We report theoretical value of $\Delta H=72,09$ kJ/mol which coincides with experimental value with precision of 1.65 %. This tells us that experimental value of standard enthalpy of formation corresponds to most energetically favorable complex **1** (table 1, fig. 1). By the way,

exceptional coincidence of theoretical and experimental data which were obtained through extrapolation on zero field technique points on legitimacy of the last.

Spontaneous point mutations theory. Obtained data is also useful in spontaneous point mutations theory which is today far from it's complete and non-contradiction state. Such in paper

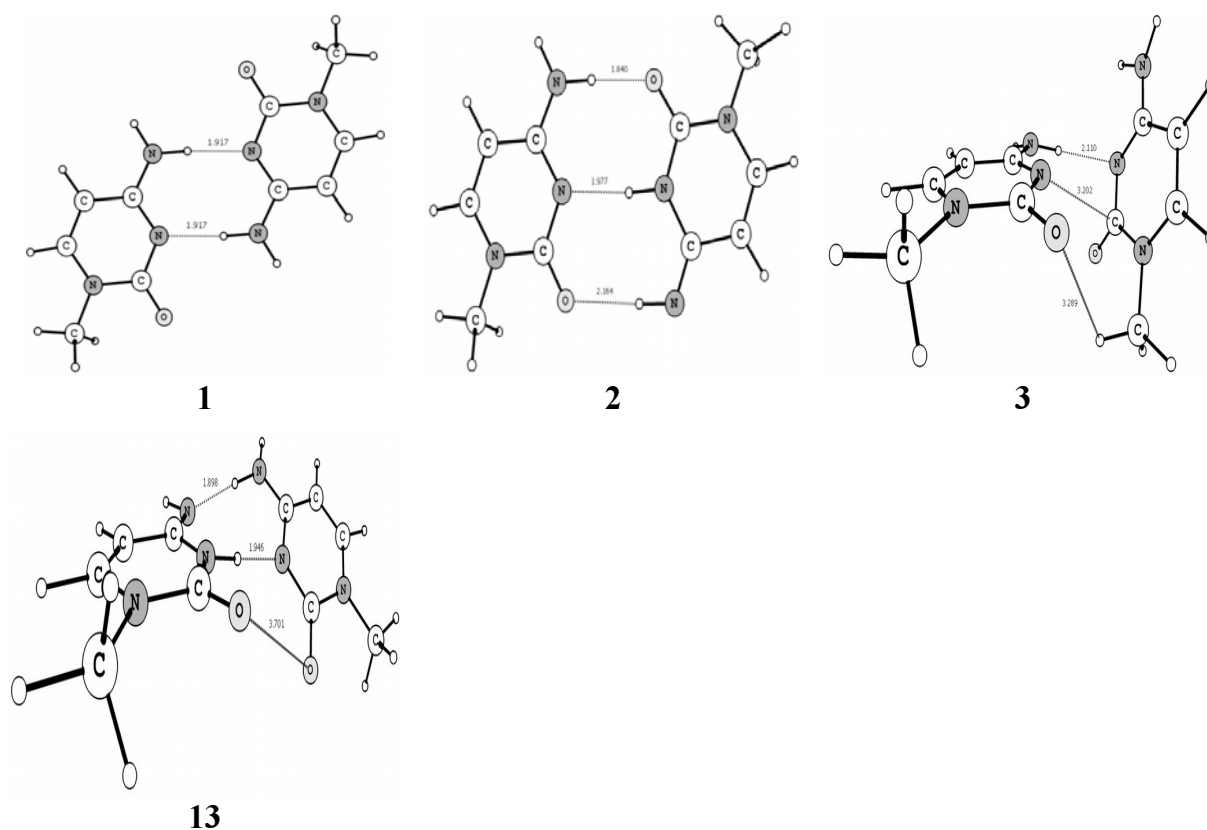


Fig. 1. Chosen $m^1\text{Cyt}\cdot m^1\text{Cyt}^*$ homoassociates (see also tables 1 and 2). Intermolecular H-bonds and van-der-Waals contacts are depicted by dotted lines. Their distances $\text{H}\dots\text{B}$ and $\text{A}\dots\text{B}$ are shown in Å.

[24] propeller-like homoassociate is postulated. It's so-called short Watson-Crick pair of $\text{Cyt}\cdot\text{Cyt}^*$ which is stabilized by two H-bonds $\text{N3}\dots\text{N3}$, $\text{N4}\dots\text{H4-1}\dots\text{N4}$ and van-der-Waals contact $\text{O2}\dots\text{O2}$ and is transversion. Our data shows that this same complex is homoassociate 13 ($\Delta G^0=8,83$ kcal/mol) and is most energetically favorable among all other homoassociates with syn-oriented glycosidic bonds N1-C1m . This fact strongly evidences against all other possible alternatives and pair of $\text{Cyt}\cdot\text{Cyt}^*$ is responsible for spontaneous point mutations of this type during DNA biosynthesis.

Conclusions. First to obtain complete family of $m^1\text{Cyt}\cdot m^1\text{Cyt}^*$ homoassociates for standard conditions. Complete family contains 37 structures with relative Gibbs free energies in

$0\div 34,42$ kcal/mol. Homoassociates are stabilized through classic ($\text{NH}\dots\text{N}$; $\text{NH}\dots\text{O}$; $\text{OH}\dots\text{N}$; $\text{OH}\dots\text{O}$) and weak ($\text{CH}\dots\text{N}$; $\text{CH}\dots\text{O}$) H-bonds as well as van-der-Waals contacts. It's shown that sugar-replacing methyl group is proton donor in H-bonds and influences Gibbs distribution for homoassociates. We show that QTAIM theory should be used in concert with NBO-analysis while investigating specific intermolecular contacts. Linear relation between $\text{CH}\dots\text{O/N}$ H-bond energy E_{HNB} and electron density in bond critical point ρ . First to interpret theoretically result of classical mass-spectrometry experiment (L.F. Sukhodub et al., 1976). Showed theoretically that homoassociate $m^1\text{Cyt}\cdot m^1\text{Cyt}^*$ is responsible for spontaneous point mutations during DNA biosynthesis.

Повне сімейство Н-зв'язаних гомоасоціатів 1-метилцитозину: квантово-механічне дослідження

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Резюме. На рівні квантово-механічної теорії MP2/6-311++G(2df,pd)//B3LYP/6-311++G(d,p) у вакуумному наближенні вперше показано, що повне сімейство гомоасоціатів m¹Cyt:m¹Cyt, стабілізованих специфічними міжмолекулярними контактами за нормальних умов, нараховує 37 структур у діапазоні відносних енергій Гіббса 0÷34,42 ккал/моль. Глобальному мінімуму енергії відповідає центросиметричний гомоасоціат, стабілізований парою антипаралельних Н-зв'язків N4H...N1: ентальпія його утворення практично збігається з результатами мас-спектрометричного експерименту (Л.Ф. Суходуб та ін., 1976). Детально проаналізовано основні фізико-хімічні властивості міжмолекулярних, особливо слабких СН...O/N, Н-зв'язків. Коротко обговорюється застосування отриманих результатів у теорії спонтаних точкових мутацій ДНК.

Ключові слова: нуклеотидна основа, пари нуклеотидних основ, неканонічні пари нуклеотидних основ, гомоасоціат, самоасоціат, цитозин, 1-метилцитозин.

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