Journal of Physical & Theoretical Chemistry
Islamic Azad University of Iran 1(1)
Science and Research Campus

Ab initio study & Density functional investigational of Adenine & Thymine; Comparison of primitive Gaussian and NBO calculation

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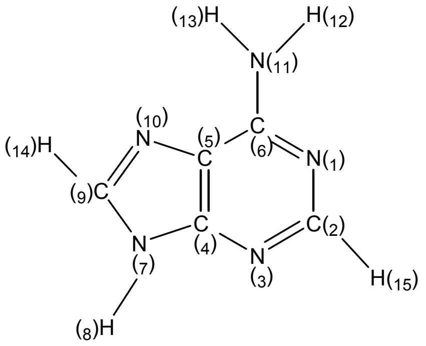
Abstract

We have performed quantum-chemical ab initio in various basis sets at the Hartree-Fock and B3LYP levels for Adenine and Thymine with the program GAUSSIAN98. The Dipole, Quadrupole, Octapole and Hexadecapole moments and primitive in nine basis sets for these molecules are presented. The most stabilized forms of these molecules are observed in 6-311++G** basis set. We have evaluated coefficient hybridation of bonds and occupancy orbital, donor and acceptors. NBO calculations show that hybridation of coefficient and occupancy in several basis sets is different.

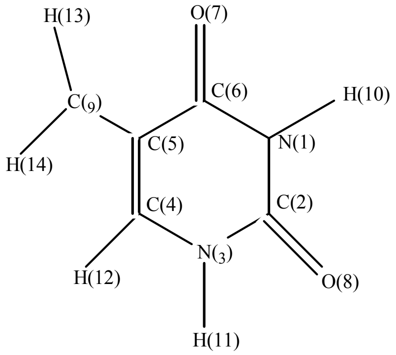
INTRODUCTION

The uracil moiety is one of the important nucleobase residues in nucleotides and nucleic acids[1]. Nucleotides, are playing a key role in biology [2-4] e.g., in the information storage via RNA and DNA or in energy-transfer processes. The use structurally altered nucleotides as probes provide one way to study the involved enzymic reactions. Ab initio quantum-chemical calculations with inclusion of electron correlation have recently provided a relatively consistent picture on base pair interaction energies and geometries. We have therefore performed calculations of this type for A and T. This can lead to a more detailed information on structure, charge distribution and energetic of these bases. In addition, the results obtained have been related to geometrical data for the A and T derived from an analysis of a set of experimental high resolution molecule structure. Adenine and Thymine (Fig. 1) is the important nucleobase residue in nucleotides and nucleic acids. Nucleotides are playing a key role in biology e.g. in the information storage via RNA and DNA or energy transfer processes[5].

Thymine and uracil are weak acids in which two position namely C2=0 and C4=0 have approximately equal tendencies for enolization and ionization[6]. However one of these positions enolization, inhibits that of the other. Thymine has then only one dissociation constant. Electrostatic properties (Dipole, Quadrupole,….) were studied with ab-initio density functional method and so for Adenine and Thymine are discussed and compared to various basis set calculated at the HF & B3LYP levels[7,8]. NBO analysis is based on a method for optically transforming a given wave function into localized form corresponding to the one center (lone pair) and two-center (bond) elements of the chemist's Lewis structure picture[9].



Adenine



Thymine

Fig. 1 Molecular structure of Adenine and Thymine.

The second-order perturbative estimates of donor-acceptor (bond-antibond) interactions in the NBO basis[10]. This is carried out by examining all possible interactions between filled (donor) Lewis-type NBOs and empty(acceptor) non-Lewis NBOs and estimating their energetic importance by 2nd-order perturbation theory[11]. Since these interactions

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lead to loss of occupancy from the localized NBOs of the idealized Lewis structure into the empty non-Lewis orbital (and thus to departures from the idealized Lewis structure description) they are referred to as delocalization corrections to the zeroth-order natural Lewis structure[12]. For each donor NBO(i) and acceptor NBO(j) the stabilization energy E_2 associated with delocalization (2e-stabilization) $i \rightarrow j$ is :

$$E_2 = \Delta E_{(ij)} = \frac{q_i}{F_{(ij)}^{\;2}}(\varepsilon_j - \varepsilon_i)$$

Where q_i is the donor orbital occupancy, ε_i and ε_j are diagonal elements (orbital energies) and $F_{(ij)}$ is the aff-diagonal NBO fock matrix element[13,14].

In HF theory the energy has the form:

$$E_{HF} = V + \langle hp\rangle + ½ \langle p_j(p)\rangle - 1/2 \langle p_k(p)\rangle$$

Where V is the nuclear repulsion energy, P is the density matrix, <hp> is the one-electron(kinetic plus potential) energy 1/2 $\langle p_j(p)\rangle$ is the classical coulomb repulsion of the electrons and -1/2 $\langle p_k(p)\rangle$ is the exchange energy resulting from the quantum (fermions) nature of electrons[15,16]. In density functional theory the exact exchange (HF) for a single determinant is replaced by a more general expression the exchange-correlation functional which can include terms accounting for both exchange energy and the electron correlation which is omitted from Hartree-Fock theory[17,18].

$$E_{ks} = V + \langle hp\rangle + 1/2\langle p_j(p)\rangle + E\chi[p] + E_c[p]$$

Where $E\chi[p]$ is the exchange functional and $E_c[p]$is the correlation functional. The correlation functional of Lee,Yang and parr which includes both local and nonlocal term. BLYP request the Beck exchange functional and LYP correlation functional[19,20].

Basis set effects:

A basis set is the mathematical description of the orbital within a system (which is turn combine to approximate the total electronic wave function used to perform the theoretical calculation[21,22]. Larger basis set more accurately approximate the orbital by imposing fewer restrictions on the location of the electron in space. In the true quantum mechanical picture electrons have a finite probability of existing anywhere in space[23,24]. This limit corresponds to the infinite basis set expansion in the chart in the previous section. The standard basis sets use linear combination of Gaussian function to form the orbital. Basis sets assign a group of basis functions to each atom within a molecule to approximate its orbital[25]. These basis function themselves are composed of Gaussian functions. The former are then referred to as contracted Gaussian (or contracted functions) and the latter referred to as primitives[26].

COMPUTATIONAL DETAILS

Ab initio calculations at the HF/6-31G, HF/6-31G*,HF/6-311G, HF/6-311*G,HF/6-311G**, HF/6-311+G, HF/6-311++G, HF/6-311++G*, HF/6-311++G** [27,28] and B3LYP/6-31G , B3LYP/6-31G* , B3LYP/6-311G , B3LYP/6-311G* , B3LYP/6-311G** , B3LYP/6-311+G , B3LYP/6-311++G , B3LYP/6-311++G* , and B3LYP/6-311++G** [29,30] for Adenine and Thymine were carried out to determine the molecule structure with the program GAUSSIAN98[31]. Energy minima of the optimized molecule have been verified at the Hartree-Fock and B3LYP levels[32].

The Natural Bond Orbital (NBO) analysis was performed by using the NBO as implement in Gaussian 98. NBO calculations have been done at HF and B3LYP levels. We have computed hybridation coefficient of four bonds for Adenine and Thymine at HF and B3LYP levels in nine basis sets. We evaluated lowest occupancy orbital, highest energy, donor, acceptor and lowest charge atoms in nine basis sets[33].

RESULT AND DISCUSSION

The calculated amounts of dipole, quadrupole, octapole and hexadecapole moments at the HF and B3LYP levels in various basis sets are given in table 1-4.

Figure 2 shows the change in Dipole moments corresponds to primitive for Adenine and also figure 3-5 show variation of quadrupole, octapole and hexadecapole of those molecules versus primitive.

These data shows that for Adenine at the HF and B3LYP levels and also for Thymine at the HF level, we have the least energy in 6-311++G** basis set but the least amount of hexadecapole moment at XXXX tensor element obtained in 6-311+G basis set. Whereas the calculated energy for Thymine at the B3LYP level is minimum in 6-311++G** basis set but the amount of hexadecapole moment at XXXX tensor element is the least amount in 6-311++G basis set.

We have computed hybridation coefficient of four bonds in Adenine and Thymine in HF and B3LYP levels (table 5-8). Hybridation coefficient is different in various methods and basis sets. In Adenine at HF and B3LYP levels the lowest occupancy orbital with the highest energy is N7. In Thymine at HF and B3LYP levels the lowest occupancy orbital with the highest energy is N1 (see tables 9-12). N7 in Adenine and N1 in Thymine is site for complexation with cations.

Table 1. Calculated Dipole, Quadropole, Octapole and Hexadecapole Moments in various basis sets at HF level for Adenine.

		Adenine								
		Hartree-Fock								
		6-31g	6-31g*	6-311g	6-311g*	6-31g**	6-311+g	6-311++g	6-311++g*	6-311++g**
	Primitive	240	300	285	345	315	325	330	390	405
Dipole Moment	X	2.3533	2.1837	2.3930	2.1985	-2.1843	2.4484	2.4437	2.2741	2.2767
	Y	-1.0683	-1.1272	-1.0582	-1.1275	-1.1191	-0.9908	-0.9858	-1.1021	-1.0657
	Z	0.0004	-0.0003	0.0003	0.0019	0.0040	0.0003	0.0004	-0.0004	0.0006
Quadrupole Moment	XX	-44.590	-43.133	-44.942	-43.282	-43.123	-45.430	-45.402	-43.974	-44.166
	YY	-58.426	-56.362	-58.698	-56.504	-56.346	-59.604	-59.608	-57.673	-57.822
	ZZ	-60.152	-59.098	-60.360	-59.503	-59.011	-61.070	-61.068	-60.350	-60.167
	XY	6.3801	6.7033	6.4716	6.7806	-6.6511	6.2933	6.2775	6.7235	6.4875
	XZ	0.0018	-0.0087	0.0017	-0.0153	-0.0003	0.0021	0.0022	-0.0072	-0.0087
	YZ	0.0004	-0.0050	0.0005	-0.0109	-0.0042	0.0002	0.0004	-0.0033	-0.0057
Octapole Moment	XXX	46.178	41.291	46.624	41.630	-41.316	48.313	48.273	43.823	43.823
	YYY	-18.679	-17.884	18.912	-17.785	-17.750	-18.381	-18.250	-17.846	-17.205
	ZZZ	0.0002	0.0004	0.0003	0.0023	0.0026	0.0006	0.0007	0.0008	0.0015
	XYY	-21.459	-19.207	-21.607	-19.460	19.170	-21.774	-21.768	-20.013	-19.756
	XXY	-5.8083	-5.7806	-5.6216	-5.7111	-5.7319	-5.4162	-5.3872	-5.6314	-5.4647
	XXZ	0.0081	0.0044	0.0091	0.0147	0.0161	0.0098	0.0101	0.0025	0.0084
	XZZ	0.2621	0.3886	0.3692	0.4057	-0.3363	0.6850	0.6773	0.7368	0.6951
	YZZ	0.5686	0.6851	0.6814	0.7697	0.5952	0.9771	0.9763	1.0279	0.9192
	YYZ	-0.0024	0.0031	-0.0025	0.0176	0.0187	-0.0009	-0.0005	0.0027	0.0088
	XYZ	-0.0005	0.0060	-0.0002	0.0177	-0.0125	-0.0010	-0.0012	0.0039	0.0091
Hexadecapole Moment	XXXX	-708.69	-687.86	-715.81	-691.44	-687.51	-727.87	-727.63	-706.01	-707.41
	YYYY	-587.99	-571.93	-593.14	-574.24	-571.84	-607.87	-608.11	-592.34	-593.42
	ZZZZ	-57.735	-55.994	-59.692	-58.424	-55.838	-63.977	-63.973	-63.207	-62.888
	XXXY	60.966	63.003	61.995	62.655	-62.690	61.244	60.995	63.534	61.700
	XXXZ	0.0115	-0.0729	0.0121	-0.1171	-0.0193	0.0165	0.0160	-0.0647	-0.0718
	YYYX	34.835	34.913	35.060	34.514	-34.623	33.448	33.331	34.070	32.454
	YYYZ	0.0038	-0.0171	0.0062	-0.0517	-0.0373	0.0047	0.0061	-0.0085	-0.0247
	ZZZX	0.0012	-0.0068	0.0008	-0.0119	0.0004	0.0010	0.0008	-0.0059	-0.0070
	ZZZY	0.0013	-0.0033	0.0014	-0.0072	-0.0042	0.0013	0.0017	-0.0011	-0.0032
	XXYY	-177.89	-176.86	-179.45	-177.28	-176.69	-183.39	-183.46	-181.26	-182.06
	XXZZ	-166.98	-162.25	-167.87	-163.70	-162.07	-172.34	-172.40	-168.64	-168.02
	YYZZ	-116.87	-114.17	-118.05	-115.25	-114.05	-122.36	-122.39	-120.10	-119.78
	XXYZ	0.0066	-0.0220	0.0039	-0.0485	-0.0206	0.0023	0.0031	-0.0133	-0.0233
	YYXZ	0.0016	-0.0302	0.0009	-0.0607	0.0112	0.0008	0.0003	-0.0250	-0.0344
	ZZXY	1.1260	1.1994	1.1279	1.4064	-1.4005	0.6015	0.6093	0.8606	1.0623

Table 2. Calculated Dipole, Quadropole, Octapole and Hexadecapole Moments in various basis sets at B3LYP level for Adenine.

		Adenine								
		B3LYP								
		6-31g	6-31g*	6-311g	6-311g*	6-31g**	6-311+g	6-311++g	6-311++g*	6-311++g**
	Primitive	240	300	285	345	315	325	330	390	405
Dipole moment	X	-2.0855	-1.9614	-2.1472	-2.0032	-1.9585	-2.2519	-2.2476	-2.1266	-2.1255
	Y	-1.3439	-1.3289	-1.3287	-1.3195	-1.3232	-1.2352	-1.2300	-1.2655	-1.2319
	Z	0.0014	0.0187	0.0010	0.0063	0.0141	0.0017	0.0017	0.0052	0.0048
Quadrupole moment	XX	-43.843	-42.846	-44.555	-43.347	-42.931	-45.414	-45.384	-44.344	-44.592
	YY	-56.822	-55.322	-57.677	-55.954	-55.347	-59.159	-59.170	-57.647	-57.828
	ZZ	-58.904	-58.075	-59.800	-59.029	-57.986	-60.799	-60.795	-60.144	-59.954
	XY	-7.7099	-7.6225	-7.6206	-7.5563	-7.5865	-7.3496	-7.3427	-7.4036	-7.1941
	XZ	0.0046	0.0403	0.0038	0.0139	0.0319	0.0031	0.0031	0.0142	0.0127
	YZ	-0.0041	-0.0451	-0.0032	-0.0127	-0.0331	-0.0024	-0.0021	-0.0119	-0.0105
Octapole moment	XXX	-40.815	-36.554	-42.638	-38.036	-36.519	-45.698	-45.649	-41.471	-41.420
	YYY	-20.785	-19.380	-20.791	-19.116	-19.299	-20.231	-20.089	-19.084	-18.487
	ZZZ	0.0014	0.0145	0.0015	0.0056	0.0115	0.0020	0.0022	0.0047	0.0044
	XYY	20.133	17.956	20.850	18.498	17.925	21.320	21.322	19.313	19.084
	XXY	-6.4021	-6.2997	-6.3478	-6.2896	-6.2520	-6.1567	-6.1284	-6.2447	-6.0880
	XXZ	0.0094	0.0983	0.0087	0.0424	0.0857	0.0175	0.0189	0.0379	0.0354
	XZZ	-0.1680	-0.2856	-0.2593	-0.3076	-0.2388	-0.7241	-0.7147	-0.7775	0.7355
	YZZ	0.3582	0.4854	0.4442	0.5663	0.4067	0.8649	0.8661	0.9751	0.8695
	YYZ	0.0156	0.1135	0.0111	0.0393	0.0863	0.0129	0.0125	0.0361	0.0330
	XYZ	0.0006	-0.0937	0.0031	-0.0253	-0.0659	0.0002	0.0010	-0.0211	-0.0189
Hexadecapole moment	XXXX	-721.17	-703.05	-732.94	-710.74	-704.04	-753.19	-752.76	-731.96	-734.36
	YYYY	-591.51	-577.89	-603.02	-585.34	-578.14	-627.19	-627.58	-612.26	-613.60
	ZZZZ	-55.214	-53.883	-59.116	-57.988	-53.717	-65.077	-65.072	-64.408	-64.077
	XXXY	-69.056	-68.739	-68.321	-67.117	-68.409	-67.568	-67.493	-68.089	-66.365
	XXXZ	0.0330	0.2512	0.0251	0.0901	0.2067	0.0218	0.0204	0.0958	0.0855
	YYYX	-41.487	-39.741	-40.480	-38.166	-39.652	-38.066	-38.047	-36.970	-35.576
	YYYZ	-0.0234	-0.2790	-0.0141	-0.0645	-0.1895	-0.0094	-0.0054	-0.0603	-0.0534
	ZZZX	0.0038	0.0323	0.0027	0.0108	0.0246	0.0022	0.0024	0.0113	0.0101
	ZZZY	-0.0031	-0.0369	-0.0023	-0.0084	-0.0249	-0.0011	-0.0008	-0.0082	-0.0072
	XXYY	-182.22	-181.95	-184.31	-182.99	-182.00	-190.37	-190.36	-188.71	-189.72
	XXZZ	-166.97	-162.85	-170.20	-166.18	-162.59	-176.33	-176.37	-172.65	-171.99
	YYZZ	-116.59	-114.32	-119.53	-116.86	-114.16	-125.51	-125.54	-123.27	-122.91
	XXYZ	-0.0242	-0.2081	-0.0226	-0.0653	-0.1598	-0.0200	-0.0215	-0.0671	-0.0592
	YYXZ	0.0315	0.2110	0.0253	0.0824	0.1738	0.0257	0.0256	0.0831	0.0758
	ZZXY	-1.9426	-1.9296	-2.0128	-2.1352	-2.1081	-1.1751	-1.1954	-1.2827	-1.4854

Table 3. Calculated Dipole, Quadropole, Octapole and Hexadecapole Moments in various basis set at HF level for Thymine.

		Thymine								
		Hartree-Fock								
		6-31g	6-31g*	6-311g	6-311g*	6-31g**	6-311+g	6-311++g	6-311++g*	6-311++g**
	Primitive	222	276	264	318	294	300	306	360	378
Dipole moment	X	-1.4558	-1.0803	-1.4512	-1.0469	-1.1043	-1.5676	-1.5651	-1.2177	-1.2711
	Y	-5.0053	-4.4640	-4.9933	-4.4489	-4.4548	-5.1138	-5.1136	-4.6240	-40598
	Z	-0.0015	0.0001	-0.0025	0.0011	-0.0002	-0.0023	-0.0020	0.0026	0.0023
Quadrupole moment	XX	-66.377	-63.327	-66.663	-63.582	-63.220	-67.477	-67.474	-64.591	-64.502
	YY	-48.243	-46.798	-48.471	-46.951	-46.786	-49.056	-49.037	-47.647	-47.754
	ZZ	-52.967	-52.048	-53.188	-52.423	-51.992	-53.588	-53.591	-52.926	-52.792
	XY	3.9392	3.2219	3.8321	3.1744	3.2382	4.0319	4.0445	3.4564	3.4938
	XZ	-0.0036	0.0026	-0.0066	-0.0005	0.0012	-0.0090	-0.0092	-0.0034	-0.0013
	YZ	0.0043	-0.0064	0.0081	-0.0025	-0.0066	0.0088	0.0085	-0.0053	-0.0041
Octapole moment	XXX	-46.486	-35.267	-46.548	-35.321	-35.686	-49.403	-49.273	-39.421	-40.018
	YYY	-23.403	-19.438	-23.332	-19.876	-19.398	-25.071	-25.074	-22.015	-21.893
	ZZZ	-0.0009	0.0084	0.0014	0.0046	0.0109	0.0071	0.0081	0.0073	0.0044
	XYY	26.191	24.558	26.245	24.736	24.531	26.493	26.503	25.029	24.710
	XXY	-18.556	-14.808	-18.300	-14.744	-14.859	-18.855	-18.892	-15.603	-15.565
	XXZ	-0.0052	-0.0061	-0.0111	-0.0004	-0.0102	-0.0201	-0.0207	-0.0089	-0.0038
	XZZ	1.9627	2.4457	2.1379	2.6675	2.4482	1.7009	1.6878	2.0594	2.0575
	YZZ	4.0461	4.2603	4.0761	4.4772	4.2586	3.7807	3.7731	4.0720	4.0012
	YYZ	-0.0050	-0.0063	-0.0095	-0.0012	-0.0078	-0.0076	-0.0065	0.0135	0.0111
	XYZ	0.0080	-0.0002	0.0169	-0.0066	0.0009	0.0214	0.0213	-0.0151	-0.0155
Hexadecapole moment	XXXX	-1097.8	-1054.1	-1102.3	-1061.1	-1051.7	-1120.9	-1121.3	-1081.4	-1078.3
	YYYY	-388.48	-378.37	-391.40	-380.74	-378.23	-400.60	-400.49	-390.46	-390.41
	ZZZZ	-54.908	-53.484	-56.636	-55.706	-53.525	-59.295	-59.374	-58.635	-58.402
	XXXY	-17.491	-18.781	-18.017	-19.086	-18.739	-17.116	-17.040	-17.421	-17.051
	XXXZ	-0.0052	0.0057	-0.0182	0.0012	-0.0112	-0.0475	-0.0504	-0.0431	-0.0251
	YYYX	20.298	14.099	19.589	14.453	14.340	21.477	21.632	16.854	17.290
	YYYZ	0.0183	-0.0230	0.0339	0.0010	-0.0253	0.0430	0.0425	-0.0018	-0.0001
	ZZZX	-0.0045	-0.0140	-0.0087	-0.0102	-0.0149	-0.0137	-0.0152	-0.0021	-0.0010
	ZZZY	0.0019	-0.0036	0.0036	-0.0078	-0.0028	0.0270	0.0020	-0.0114	-0.0089
	XXYY	-223.96	-216.20	-224.75	-217.32	-215.94	-228.83	-228.64	-221.56	-221.40
	XXZZ	-163.28	-159.79	-164.47	-160.83	-159.65	-167.54	-167.61	-164.16	-163.88
	YYZZ	-84.572	-82.779	-85.282	-83.752	-82.867	-87.458	-87.481	-86.058	-85.890
	XXYZ	0.0144	-0.0177	0.0239	-0.0104	-0.0206	0.0205	0.0184	-0.0230	-0.0222
	YYXZ	-0.0134	0.0198	-0.0197	0.0112	0.0217	-0.0114	-0.0089	0.0206	0.0229
	ZZXY	-4.3481	-4.6801	-4.4320	-5.0608	-4.7246	-4.0621	-4.0343	-4.3959	-4.3808

Table 4. Calculated Dipole, Quadropole, Octapole and Hexadecapole Moments in various basis sets at B3LYP level for Thymine.

		Thymine								
		B3LYP								
		6-31g	6-31g*	6-311g	6-311g*	6-31g**	6-311+g	6-311++g	6-311++g*	6-311++g**
	Primitive	222	276	264	318	294	300	603	360	378
Dipole moment	X	1.0219	-0.7785	1.0555	-0.7571	-0.7988	-1.2731	-1.2703	-1.0326	-1.0802
	Y	-4.4540	-4.0675	-4.5484	-4.1275	-4.0525	-4.7939	-4.7928	-4.4306	-4.4021
	Z	0.0013	-0.0003	0.0012	-0.0001	-0.0004	-0.0011	-0.0015	-0.0001	-0.0002
Quadrupole moment	XX	-63.088	-60.946	-64.213	-61.933	-60.865	-65.689	-65.689	-63.593	-63.534
	YY	-47.019	-46.092	-47.750	-46.685	-46.145	-48.780	-48.757	-47.783	-47.931
	ZZ	-52.118	-51.407	-52.967	-52.313	-51.365	-53.586	-53.590	-53.029	-52.903
	XY	-3.2316	2.7236	-3.2839	2.7633	2.7334	3.6491	3.6629	3.2125	3.2410
	XZ	0.0019	0.0015	0.0018	0.0010	-0.0002	-0.0004	0.0016	0.0024	0.0010
	YZ	0.0005	0.0010	-0.0005	0.0007	0.0021	0.0028	-0.0007	-0.0012	-0.0014
Octapole moment	XXX	39.108	-30.915	39.970	-31.050	-31.287	-45.275	-45.164	-37.622	-38.137
	YYY	-18.999	-15.988	-20.013	-17.116	-15.826	-23.250	-23.220	-20.744	-20.539
	ZZZ	-0.0006	0.0031	-0.0010	0.0031	0.0025	0.0036	0.0075	0.0039	0.0079
	XYY	-25.214	23.813	-25.555	24.283	23.743	25.929	25.793	24.773	24.454
	XXY	-17.361	-14.453	-17.590	-14.684	-14.493	-18.802	-18.837	-16.210	-16.136
	XXZ	-0.0031	0.0048	-0.0029	0.0035	0.0021	0.0016	0.0009	0.0051	0.0012
	XZZ	-1.8706	2.2537	-2.1645	2.6475	2.2901	1.4868	1.4737	1.8194	1.8515
	YZZ	4.0370	4.1756	4.1619	4.4858	4.1619	3.6654	3.6570	3.8918	3.8137
	YYZ	0.0068	-0.0087	0.0063	-0.0068	-0.0085	-0.0074	-0.0106	-0.0064	-0.0114
	XYZ	0.0036	0.0020	0.0055	-0.0004	0.0031	0.0079	0.0111	0.0006	-0.0013
Hexadecapole moment	XXXX	-1081.0	-1046.7	-1102.4	-1066.9	-1044.1	-1134.6	-1134.9	-1100.7	-1097.9
	YYYY	-393.87	-385.83	-400.63	-391.47	-386.12	-415.93	-415.67	-406.70	-407.00
	ZZZZ	-53.582	-52.480	-57.192	-56.421	-52.503	-61.018	-61.102	-60.556	-60.327
	XXXY	18.875	-19.956	19.013	-20.233	-19.769	-16.987	-16.927	-17.539	-17.146
	XXXZ	0.0241	0.0176	0.0226	0.0146	0.0075	0.0148	0.0210	0.0210	0.0117
	YYYX	-15.077	10.618	-15.469	11.404	10.697	18.957	19.157	15.444	15.722
	YYYZ	0.0083	0.0131	0.0042	0.0138	0.0179	0.0152	-0.0058	0.0037	0.0103
	ZZZX	-0.0079	-0.0171	-0.0070	-0.0146	-0.0145	-0.0121	-0.0177	-0.0147	-0.0234
	ZZZY	-0.0016	-0.0029	-0.0018	-0.0037	-0.0026	-0.0007	-0.0007	-0.0037	-0.0069
	XXYY	-223.88	-217.75	-228.06	-221.49	-217.60	-235.15	-234.91	-228.59	-228.62
	XXZZ	-162.85	-159.91	-166.64	-163.23	-159.86	-171.20	-171.29	-168.09	-167.93
	YYZZ	-84.640	-83.080	-86.867	-85.366	-83.107	-90.093	-90.093	-88.681	-88478
	XXYZ	0.0009	-0.0046	-0.0023	-0.0033	-0.0007	0.0048	-0.0056	-0.0076	-0.0160
	YYXZ	0.0041	0.0110	0.0028	0.0110	0.0052	0.0036	0.0152	0.0136	0.0240
	ZZXY	4.4283	-4.6439	4.7284	-5.2297	-4.6631	-4.0925	-4.0591	-4.3353	-4.3056

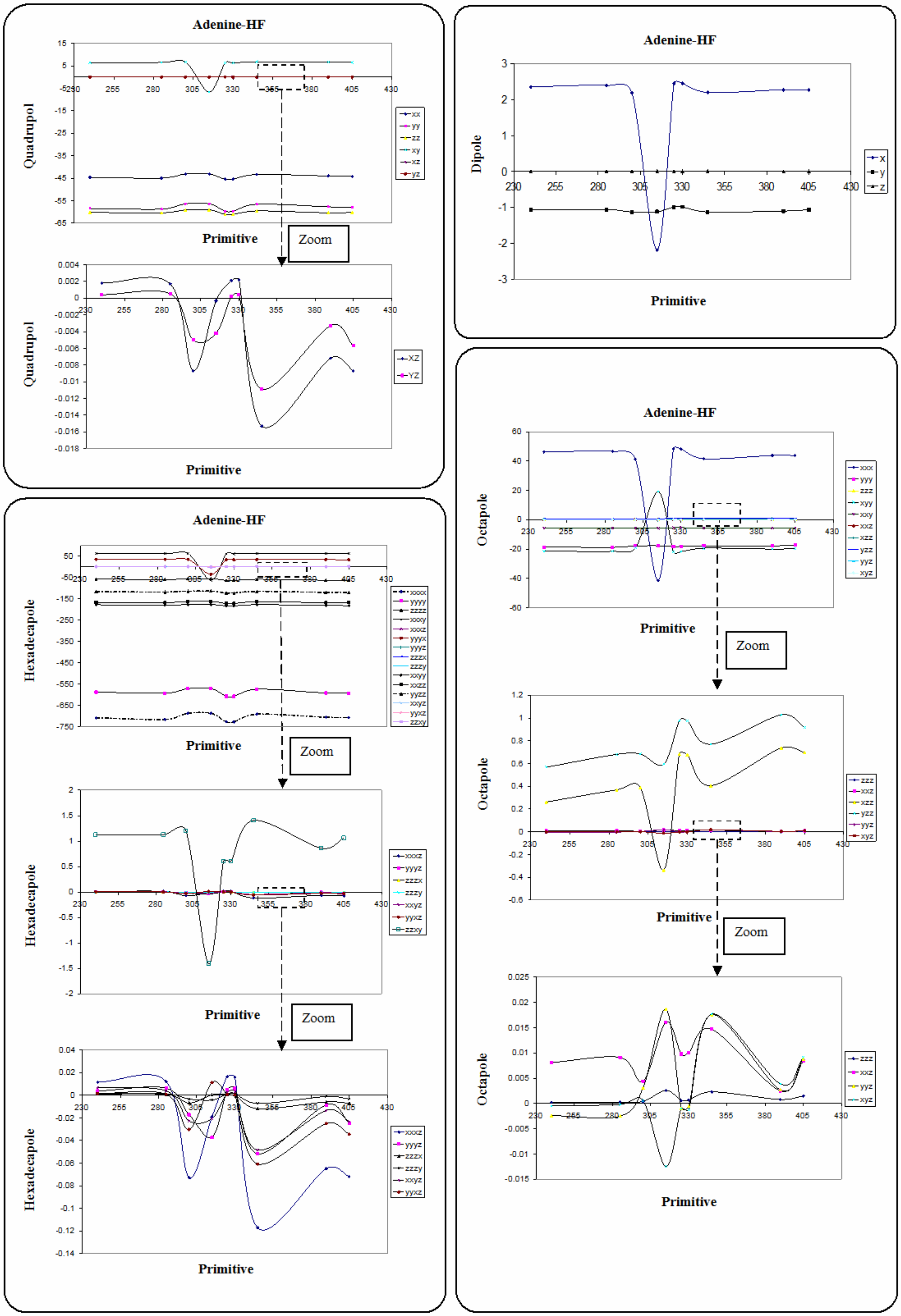

Fig. 2 Dipole, Quadrupole, Octapole, Hexadecapole moments VS. Primitive Gaussian Function for Adenine at the different basis sets.

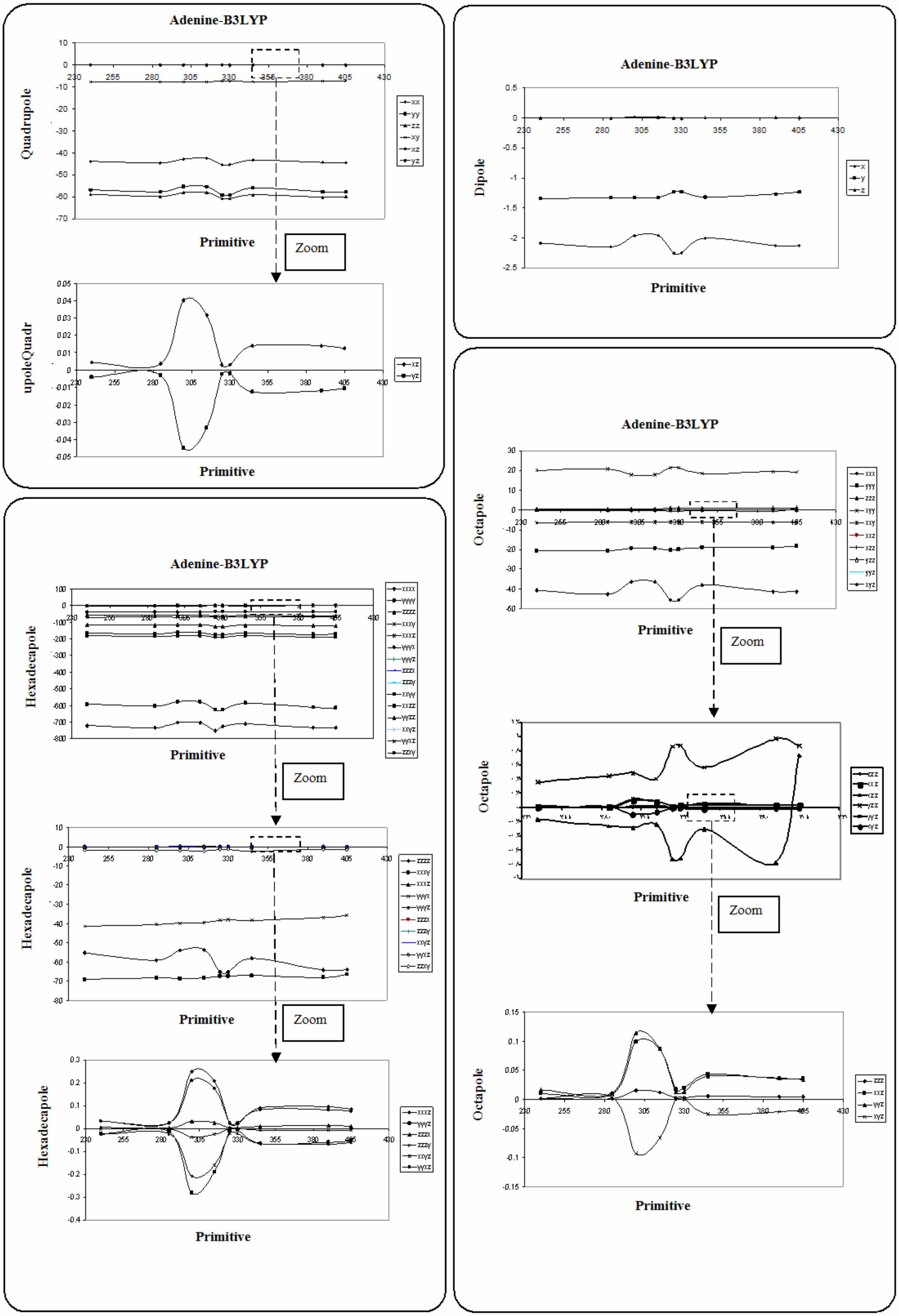

Fig. 3 Dipole, Quadrupole, Octapole, Hexadecapole moments VS. Primitive Gaussian Function for Adenine at the different basis sets.

For Thymine at HF and B3LYP levels, hybridation coefficient:
in C4 – C5 : $\sigma_{C4} > \pi_{C4}$, $\sigma_{C5} < \pi_{C5}$
in C6 – O7 : $\sigma_{C6} > \pi_{C6}$, $\sigma_{O7} < \pi_{O7}$ and $\sigma, \pi_O > \sigma, \pi_C$
These below results are due to polarized basis sets and at HF and B3LYP levels:

N1 – C2	sp^n	$n\sigma_{C,N}$ 6-31G > $n\ \sigma_{C,N}$ 6-31G*
N3 – C4	sp^n	$n\ \sigma_N$ 6-311G> $n\ \sigma_N$ 6-311G*
		$n\sigma_N$6-311++G>$n\sigma_N$6-311++G*
C4 – C5	sp^n	$n\sigma_C$ 6-31G> $n\ \sigma_C$ 6-31G*
		$n\ \sigma_C$ 6-311G > $n\ \sigma_C$ 6-311G*
		$n\sigma_C$6-311++G>$n\sigma_C$6-311++G*

These below results are due to diffused basis sets:

N1 – C2	sp^n	$n\ \sigma_N$ 6-311G < $n\ \sigma_N$ 6-311+G	HF , B3LYP
N3 – C4	sp^n	$n\ \sigma_C$ 6-311G < $n\ \sigma_C$ 6-311+G	HF
C4 – C5	sp^n	$n\ \sigma_C$ 6-311G < $n\ \sigma_C$ 6-311+G	HF , B3LYP
C6 – O7	sp^n	$n\ \sigma_O$ 6-311G < $n\ \sigma_O$ 6-311+G	HF , B3LYP

We find that: For Adenine at HF and B3LYP levels, hybridation coefficient :
in N1 – C6 $\sigma_N < \pi_N$, $\sigma_C > \pi_C$,
in C2 – N3 $\sigma_N < \pi_N$, $\sigma_C > \pi_C$,
in C4 – C5 $\sigma_{C4} > \pi_{C4}$, $\sigma_{C5} < \pi_C5$
These below results are due to polarized basis sets at HF level:

N1 – C6	sp^n	$n\ \sigma_{N,C}$ 6-31G > $n\ \sigma_{N,C}$ 6-31G*
C2 – N3	sp^n	$n\ \sigma_{N,C}$ 6-311G > $n\ \sigma_{N,C}$ 6-311G*
		$n\ \sigma_{N,C}$ 6-311+G > $n\ \sigma_{N,C}$ 6-311+G*

This below result is due to diffused basis sets at HF and B3LYP levels:

C2 – N3	sp^n	$n\ \sigma_O$ 6-311G* < $n\ \sigma_O$ 6-311+G*
C6 – N10		

Table 5. Hybridation coefficient of six bonds calculated by NBO method in HF level at different basis sets for Adenine.

		N1-C6	**C2-N3**	**C4-C5**	**C6-N10**
6-31g	σ	$0.7607(SP^{1.78})_N+0.6491(SP^{2.18})_C$	$0.6308(SP^{1.97})_C+0.7759(SP^{1.73})_N$	$0.7068(SP^{1.75})_C+0.7074(SP^{2.03})_C$	$0.6366(SP^{2.21})_C+0.7712(SP^{1.59})_N$
	π	$0.8405(SP^{1.00})_N+0.5418(SP^{1.00})_C$	$0.5758(SP^{1.00})_C+0.8176(SP^{1.00})_N$	$0.6322(SP^{1.00})_C+0.7748(SP^{1.00})_C$	
6-31g*	σ	$0.7633(SP^{1.76})_N+0.6460(SP^{2.12})_C$	$0.6277(SP^{1.88})_C+0.7785(SP^{1.71})_N$	$0.7063(SP^{1.71})_C+0.7079(SP^{2.00})_C$	$0.6310(SP^{2.28})_C+0.7758(SP^{1.53})_N$
	π	$0.8505(SP^{1.00})_N+0.5259(SP^{1.00})_C$	$0.5602(SP^{1.00})_C+0.8284(SP^{1.00})_N$	$0.6240(SP^{1.00})_C+0.7814(SP^{1.00})_C$	
6-311g	σ	$0.7599(SP^{1.79})_N+0.6501(SP^{2.15})_C$	$0.6329(SP^{1.89})_C+0.7742(SP^{1.77})_N$	$0.7064(SP^{1.76})_C+0.7078(SP^{2.03})_C$	$0.6347(SP^{2.22})_C+0.7728(SP^{1.52})_N$
	π	$0.8432(SP^{1.00})_N+0.5376(SP^{1.00})_C$	$0.5715(SP^{1.00})_C+0.8206(SP^{1.00})_N$	$0.6318(SP^{1.00})_C+0.7751(SP^{1.00})_C$	
6-311g*	σ	$0.7630(SP^{1.75})_N+0.6464(SP^{2.08})_C$	$0.6290(SP^{1.81})_C+0.7774(SP^{1.73})_N$	$0.7057(SP^{1.72})_C+0.7085(SP^{2.01})_C$	$0.6287(SP^{2.29})_C+0.7777(SP^{1.46})_N$
	π	$0.8528(SP^{1.00})_N+0.5223(SP^{1.00})_C$	$0.5558(SP^{1.00})_C+0.8313(SP^{1.00})_N$	$0.6229(SP^{1.00})_C+0.7823(SP^{1.00})_C$	
6-31g**	σ	$0.7635(SP^{1.76})_N+0.6458(SP^{2.12})_C$	$0.6277(SP^{1.88})_C+0.7784(SP^{1.71})_N$	$0.7063(SP^{1.71})_C+0.7079(SP^{2.00})_C$	$0.6311(SP^{2.28})_C+0.7757(SP^{1.55})_N$
	π	$0.8503(SP^{1.00})_N+0.5263(SP^{1.00})_C$	$0.5607(SP^{1.00})_C+0.8280(SP^{1.00})_N$	$0.6241(SP^{1.00})_C+0.7814(SP^{1.00})_C$	
6-311+g	σ	$0.7582(SP^{1.83})_N+0.6520(SP^{2.15})_C$	$0.6343(SP^{1.90})_C+0.7731(SP^{1.78})_N$	$0.7065(SP^{1.76})_C+0.7077(SP^{2.05})_C$	$0.6372(SP^{2.21})_C+0.7707(SP^{1.56})_N$
	π	$0.8426(SP^{1.00})_N+0.5385(SP^{1.00})_C$	$0.5712(SP^{1.00})_C+0.8208(SP^{1.00})_N$	$0.6325(SP^{1.00})_C+0.7746(SP^{1.00})_C$	
6-31++g	σ	$0.7582(SP^{1.83})_N+0.6520(SP^{2.16})_C$	$0.6343(SP^{1.90})_C+0.7731(SP^{1.78})_N$	$0.7066(SP^{1.76})_C+0.7076(SP^{2.05})_C$	$0.6372(SP^{2.21})_C+0.7707(SP^{1.56})_N$
	π	$0.8427(SP^{1.00})_N+0.5384(SP^{1.00})_C$	$0.5711(SP^{1.00})_C+0.8209(SP^{1.00})_N$	$0.6324(SP^{1.00})_C+0.7747(SP^{1.00})_C$	
6-311++g*	σ	$0.7615(SP^{1.79})_N+0.6481(SP^{2.18})_C$	$0.6303(SP^{1.83})_C+0.7763(SP^{1.74})_N$	$0.7058(SP^{1.73})_C+0.7084(SP^{2.02})_C$	$0.6315(SP^{2.27})_C+0.7754(SP^{1.50})_N$
	π	$0.8526(SP^{1.00})_N+0.5226(SP^{1.00})_C$	$0.5549(SP^{1.00})_C+0.8319(SP^{1.00})_N$	$0.6238(SP^{1.00})_C+0.7816(SP^{1.00})_C$	
6-311++g**	σ	$0.7616(SP^{1.78})_N+0.6480(SP^{2.09})_C$	$0.6304(SP^{1.83})_C+0.7763(SP^{1.74})_N$	$0.7058(SP^{1.73})_C+0.7084(SP^{2.02})_C$	$0.6318(SP^{2.27})_C+0.7752(SP^{1.52})_N$
	π	$0.8517(SP^{1.00})_N+0.5241(SP^{1.00})_C$	$0.5560(SP^{1.00})_C+0.8311(SP^{1.00})_N$	$0.6241(SP^{1.00})_C+0.7813(SP^{1.00})_C$	

Table 6. Hybridation coefficient of six bonds calculated by NBO method in B3LYP level at different basis sets for Adenine.

		N1-C6	C2-N3	C4-C5	C6-N10
6-31g	σ	$0.7591(SP^{1.93})_N+0.6510(SP^{2.20})_C$	$0.6330(SP^{1.98})_C+0.7742(SP^{1.89})_N$	$0.7066(SP^{1.73})_C+0.7076(SP^{2.05})_C$	$0.6364(SP^{2.24})_C+0.7713(SP^{1.57})_N$
	π	$0.8052(SP^{1.00})_N+0.5929(SP^{1.00})_C$	$0.6143(SP^{1.00})_N+0.7891(SP^{1.00})_C$	$0.6693(SP^{1.00})_C+0.7430(SP^{1.00})_C$	
6-31g*	σ	$0.7610(SP^{1.88})_N+0.6487(SP^{2.13})_C$	$0.6306(SP^{1.90})_C+0.7761(SP^{1.85})_N$	$0.7064(SP^{1.70})_C+0.7079(SP^{2.03})_C$	$0.6329(SP^{2.30})_C+0.7742(SP^{1.53})_N$
	π	$0.8124(SP^{1.00})_N+0.5831(SP^{1.00})_C$	$0.6037(SP^{1.00})_N+0.7972(SP^{1.00})_C$	$0.6647(SP^{1.00})_C+0.7471(SP^{1.00})_C$	
6-311g	σ	$0.7599(SP^{1.79})_N+0.6501(SP^{2.15})_C$	$0.6329(SP^{1.89})_C+0.7742(SP^{1.77})_N$	$0.7064(SP^{1.76})_C+0.7078(SP^{2.04})_C$	$0.6374(SP^{2.22})_C+0.7728(SP^{1.52})_N$
	π	$0.8432(SP^{1.00})_N+0.5376(SP^{1.00})_C$	$0.5714(SP^{1.00})_N+0.8207(SP^{1.00})_C$	$0.6317(SP^{1.00})_C+0.7752(SP^{1.00})_C$	
6-311g*	σ	$0.7609(SP^{1.85})_N+0.6488(SP^{2.11})_C$	$0.6311(SP^{1.84})_C+0.7757(SP^{1.85})_N$	$0.7064(SP^{1.72})_C+0.7078(SP^{2.04})_C$	$0.6310(SP^{2.32})_C+0.7758(SP^{1.46})_N$
	π	$0.8159(SP^{1.00})_N+0.5782(SP^{1.00})_C$	$0.5985(SP^{1.00})_N+0.8012(SP^{1.00})_C$	$0.6635(SP^{1.00})_C+0.7481(SP^{1.00})_C$	
6-31g**	σ	$0.7611(SP^{1.88})_N+0.6487(SP^{2.13})_C$	$0.6307(SP^{1.90})_C+0.7761(SP^{1.85})_N$	$0.7063(SP^{1.70})_C+0.7079(SP^{2.03})_C$	$0.6329(SP^{2.30})_C+0.7743(SP^{1.54})_N$
	π	$0.8122(SP^{1.00})_N+0.5834(SP^{1.00})_C$	$0.6043(SP^{1.00})_N+0.7968(SP^{1.00})_C$	$0.6648(SP^{1.00})_C+0.7470(SP^{1.00})_C$	
6-311+g	σ	$0.7564(SP^{1.97})_N+0.6541(SP^{2.18})_C$	$0.6360(SP^{1.92})_C+0.7717(SP^{1.93})_N$	$0.7070(SP^{1.75})_C+0.7072(SP^{2.07})_C$	$0.6381(SP^{2.23})_C+0.7700(SP^{1.55})_N$
	π	$0.8087(SP^{1.00})_N+0.5882(SP^{1.00})_C$	$0.6076(SP^{1.00})_N+0.7942(SP^{1.00})_C$	$0.6690(SP^{1.00})_C+0.7433(SP^{1.00})_C$	
6-31++g	σ	$0.7566(SP^{1.98})_N+0.6539(SP^{2.19})_C$	$0.6351(SP^{1.98})_C+0.7724(SP^{1.92})_N$	$0.7070(SP^{1.75})_C+0.7072(SP^{2.07})_C$	$0.6391(SP^{2.20})_C+0.7691(SP^{1.65})_N$
	π	$0.8071(SP^{1.00})_N+0.5904(SP^{1.00})_C$	$0.6102(SP^{1.00})_N+0.7923(SP^{1.00})_C$	$0.6695(SP^{1.00})_C+0.7428(SP^{1.00})_C$	
6-311++g*	σ	$0.7588(SP^{1.89})_N+0.6514(SP^{2.11})_C$	$0.6332(SP^{1.85})_C+0.7740(SP^{1.86})_N$	$0.7067(SP^{1.73})_C+0.7075(SP^{2.06})_C$	$0.6348(SP^{2.28})_C+0.7727(SP^{1.50})_N$
	π	$0.8159(SP^{1.00})_N+0.5782(SP^{1.00})_C$	$0.5966(SP^{1.00})_N+0.8025(SP^{1.00})_C$	$0.6642(SP^{1.00})_C+0.7476(SP^{1.00})_C$	
6-311++g**	σ	$0.7587(SP^{1.89})_N+0.6514(SP^{2.11})_C$	$0.6333(SP^{1.85})_C+0.7739(SP^{1.86})_N$	$0.7065(SP^{1.73})_C+0.7077(SP^{2.06})_C$	$0.6348(SP^{2.28})_C+0.7727(SP^{1.52})_N$
	π	$0.8148(SP^{1.00})_N+0.5797(SP^{1.00})_C$	$0.5979(SP^{1.00})_N+0.8015(SP^{1.00})_C$	$0.6641(SP^{1.00})_C+0.7476(SP^{1.00})_C$	

Table 7. Hybridation coefficient of six bonds calculated by NBO method in HF level at different basis sets for Thymine.

7		N1-C2	N3-C4	C4-C5	C6-O7
6-31g	σ	$0.7913(SP^{1.82})_N+0.6114(SP^{2.10})_C$	$0.7887(SP^{1.76})_N+0.6148(SP^{2.60})_C$	$0.7053(SP^{1.47})_C+0.7089(SP^{1.74})_C$	$0.5960(SP^{2.05})_C+0.8030(SP^{1.48})_0$
	π			$0.6642(SP^{1.00})_C+0.7475(SP^{1.00})_C$	$0.5301(SP^{1.00})_C+0.8480(SP^{1.00})_0$
6-31g*	σ	$0.7953(SP^{1.79})_N+0.6062(SP^{2.10})_C$	$0.7890(SP^{1.74})_N+0.6144(SP^{2.56})_C$	$0.7054(SP^{1.44})_C+0.7088(SP^{1.73})_C$	$0.5854(SP^{2.01})_C+0.8107(SP^{1.20})_0$
	π			$0.6608(SP^{1.00})_C+0.7505(SP^{1.00})_C$	$0.5215(SP^{1.00})_C+0.8532(SP^{1.00})_0$
6-311g	σ	$0.7890(SP^{1.81})_N+0.6144(SP^{2.11})_C$	$0.7892(SP^{1.71})_N+0.6142(SP^{2.53})_C$	$0.7073(SP^{1.39})_C+0.7069(SP^{1.72})_C$	$0.6003(SP^{2.01})_C+0.7998(SP^{1.56})_0$
	π			$0.6642(SP^{1.00})_C+0.7476(SP^{1.00})_C$	$0.5262(SP^{1.00})_C+0.8503(SP^{1.00})_0$
6-311g*	σ	$0.7933(SP^{1.78})_N+0.6089(SP^{2.12})_C$	$0.7899(SP^{1.69})_N+0.6133(SP^{2.50})_C$	$0.7070(SP^{1.37})_C+0.7072(SP^{1.71})_C$	$0.5897(SP^{1.97})_C+0.8076(SP^{1.23})_0$
	π			$0.6596(SP^{1.00})_C+0.7516(SP^{1.00})_C$	$0.5205(SP^{1.00})_C+0.8539(SP^{1.00})_0$
6-31g**	σ	$0.7954(SP^{1.79})_N+0.6061(SP^{2.10})_C$	$0.7889(SP^{1.75})_N+0.6146(SP^{2.56})_C$	$0.7054(SP^{1.44})_C+0.7088(SP^{1.73})_C$	$0.5854(SP^{2.01})_C+0.8108(SP^{1.20})_0$
	π			$0.6617(SP^{1.00})_C+0.7498(SP^{1.00})_C$	$0.5215(SP^{1.00})_C+0.8532(SP^{1.00})_0$
6-311+g	σ	$0.7887(SP^{1.83})_N+0.6147(SP^{2.11})_C$	$0.7906(SP^{1.71})_N+0.6123(SP^{2.60})_C$	$0.7058(SP^{1.41})_C+0.7085(SP^{1.73})_C$	$0.6044(SP^{2.01})_C+0.7967(SP^{1.60})_0$
	π			$0.6656(SP^{1.00})_C+0.7463(SP^{1.00})_C$	$0.5241(SP^{1.00})_C+0.8516(SP^{1.00})_0$
6-31++g	σ	$0.7887(SP^{1.83})_N+0.6147(SP^{2.11})_C$	$0.7907(SP^{1.70})_N+0.6123(SP^{2.60})_C$	$0.7058(SP^{1.41})_C+0.7084(SP^{1.73})_C$	$0.6044(SP^{2.01})_C+0.7967(SP^{1.60})_0$
	π			$0.6656(SP^{1.00})_C+0.7463(SP^{1.00})_C$	$0.5241(SP^{1.00})_C+0.8516(SP^{1.00})_0$
6-311++g*	σ	$0.7926(SP^{1.80})_N+0.6098(SP^{2.12})_C$	$0.7913(SP^{1.69})_N+0.6115(SP^{2.56})_C$	$0.7056(SP^{1.39})_C+0.7086(SP^{1.72})_C$	$0.5937(SP^{1.97})_C+0.8047(SP^{1.27})_0$
	π			$0.6610(SP^{1.00})_C+0.7404(SP^{1.00})_C$	$0.5184(SP^{1.00})_C+0.8552(SP^{1.00})_0$
6-311++g**	σ	$0.7927(SP^{1.81})_N+0.6096(SP^{2.12})_C$	$0.7911(SP^{1.69})_N+0.6117(SP^{2.56})_C$	$0.7057(SP^{1.39})_C+0.7085(SP^{1.72})_C$	$0.5937(SP^{1.97})_C+0.8047(SP^{1.27})_0$
	π			$0.6624(SP^{1.00})_C+0.7491(SP^{1.00})_C$	$0.5188(SP^{1.00})_C+0.8549(SP^{1.00})_0$

Table 8. Hybridation coefficient of six bonds calculated by NBO method in B3LYP level at different basis sets for Thymine.

		N1-C2	N3-C4	C4-C5	C6-O7
6-31g	σ	$0.7889(SP^{1.80})_N+0.6145(SP^{2.06})_C$	$0.7872(SP^{1.71})_N+0.6167(SP^{2.59})_C$	$0.7050(SP^{1.48})_C+0.7092(SP^{1.78})_C$	$0.5990(SP^{2.09})_C+0.8007(SP^{1.69})_O$
	π			$0.6846(SP^{1.00})_C+0.7289(SP^{1.00})_C$	$0.5664(SP^{1.00})_C+0.8241(SP^{1.78})_O$
6-31g*	σ	$0.7919(SP^{1.78})_N+0.6107(SP^{2.07})_C$	$0.7876(SP^{1.69})_N+0.6162(SP^{2.55})_C$	$0.7050(SP^{1.46})_C+0.7092(SP^{1.77})_C$	$0.5917(SP^{2.05})_C+0.8062(SP^{1.39})_O$
	π			$0.6801(SP^{1.00})_C+0.7331(SP^{1.00})_C$	$0.5580(SP^{1.00})_C+0.8298(SP^{1.78})_O$
6-311g	σ	$0.7873(SP^{1.79})_N+0.6166(SP^{2.07})_C$	$0.7880(SP^{1.66})_N+0.6157(SP^{2.53})_C$	$0.7072(SP^{1.40})_C+0.7070(SP^{1.76})_C$	$0.6010(SP^{2.07})_C+0.7990(SP^{1.75})_O$
	π			$0.6831(SP^{1.00})_C+0.7303(SP^{1.00})_C$	$0.5611(SP^{1.00})_C+0.8277(SP^{1.78})_O$
6-311g*	σ	$0.7902(SP^{1.76})_N+0.6129(SP^{2.08})_C$	$0.7883(SP^{1.63})_N+0.6153(SP^{2.49})_C$	$0.7072(SP^{1.38})_C+0.7071(SP^{1.75})_C$	$0.5939(SP^{2.03})_C+0.8046(SP^{1.40})_O$
	π			$0.6781(SP^{1.00})_C+0.7350(SP^{1.00})_C$	$0.5538(SP^{1.00})_C+0.8326(SP^{1.78})_O$
6-31g**	σ	$0.7920(SP^{1.78})_N+0.6105(SP^{2.07})_C$	$0.7876(SP^{1.70})_N+0.6162(SP^{2.55})_C$	$0.7051(SP^{1.46})_C+0.7091(SP^{1.77})_C$	$0.5917(SP^{2.05})_C+0.8062(SP^{1.39})_O$
	π			$0.6807(SP^{1.00})_C+0.7325(SP^{1.00})_C$	$0.5581(SP^{1.00})_C+0.8297(SP^{1.78})_O$
6-311+g	σ	$0.7860(SP^{1.82})_N+0.6182(SP^{2.09})_C$	$0.7889(SP^{1.66})_N+0.6145(SP^{2.59})_C$	$0.7059(SP^{1.42})_C+0.7084(SP^{1.78})_C$	$0.6066(SP^{2.05})_C+0.7950(SP^{1.81})_O$
	π			$0.6843(SP^{1.00})_C+0.7292(SP^{1.00})_C$	$0.5581(SP^{1.00})_C+0.8298(SP^{1.78})_O$
6-31++g	σ	$0.7871(SP^{1.86})_N+0.6168(SP^{2.08})_C$	$0.7885(SP^{1.72})_N+0.6150(SP^{2.64})_C$	$0.7047(SP^{1.50})_C+0.7096(SP^{1.79})_C$	$0.6051(SP^{2.04})_C+0.7961(SP^{1.78})_O$
	π			$0.6850(SP^{1.00})_C+0.7285(SP^{1.00})_C$	$0.5591(SP^{1.00})_C+0.8291(SP^{1.78})_O$
6-311++g*	σ	$0.7887(SP^{1.79})_N+0.6148(SP^{2.10})_C$	$0.7893(SP^{1.64})_N+0.6141(SP^{2.54})_C$	$0.7058(SP^{1.41})_C+0.7084(SP^{1.76})_C$	$0.5992(SP^{2.00})_C+0.8006(SP^{1.46})_O$
	π			$0.6793(SP^{1.00})_C+0.7339(SP^{1.00})_C$	$0.5506(SP^{1.00})_C+0.8348(SP^{1.78})_O$
6-311++g**	σ	$0.7888(SP^{1.80})_N+0.6147(SP^{2.10})_C$	$0.7892(SP^{1.65})_N+0.6142(SP^{2.55})_C$	$0.7060(SP^{1.41})_C+0.7082(SP^{1.76})_C$	$0.5992(SP^{2.00})_C+0.8006(SP^{1.46})_O$
	π			$0.6805(SP^{1.00})_C+0.7328(SP^{1.00})_C$	$0.5510(SP^{1.00})_C+0.8345(SP^{1.78})_O$

AKNOWLEDGMENT

We are grateful to Dr. M. Monajjemi , Department of Chemistry, Science & Research Campus, I.A. University, P.O.Box 14515-755, Tehran, Iran.

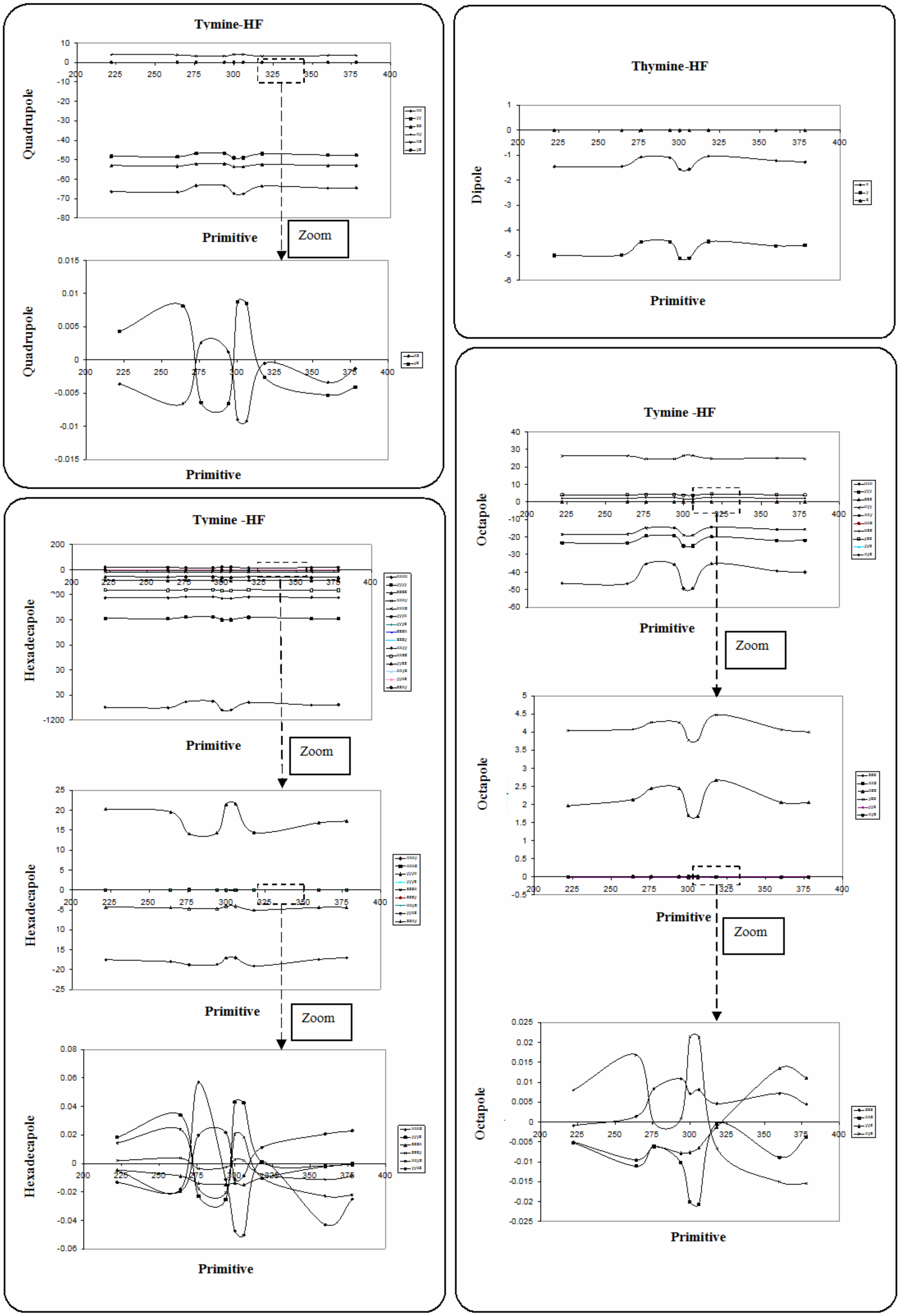

Fig. 4 Dipole, Quadrupole, Octapole, Hexadecapole moments VS. Primitive Gaussian Function for Tymine at the different basis sets.

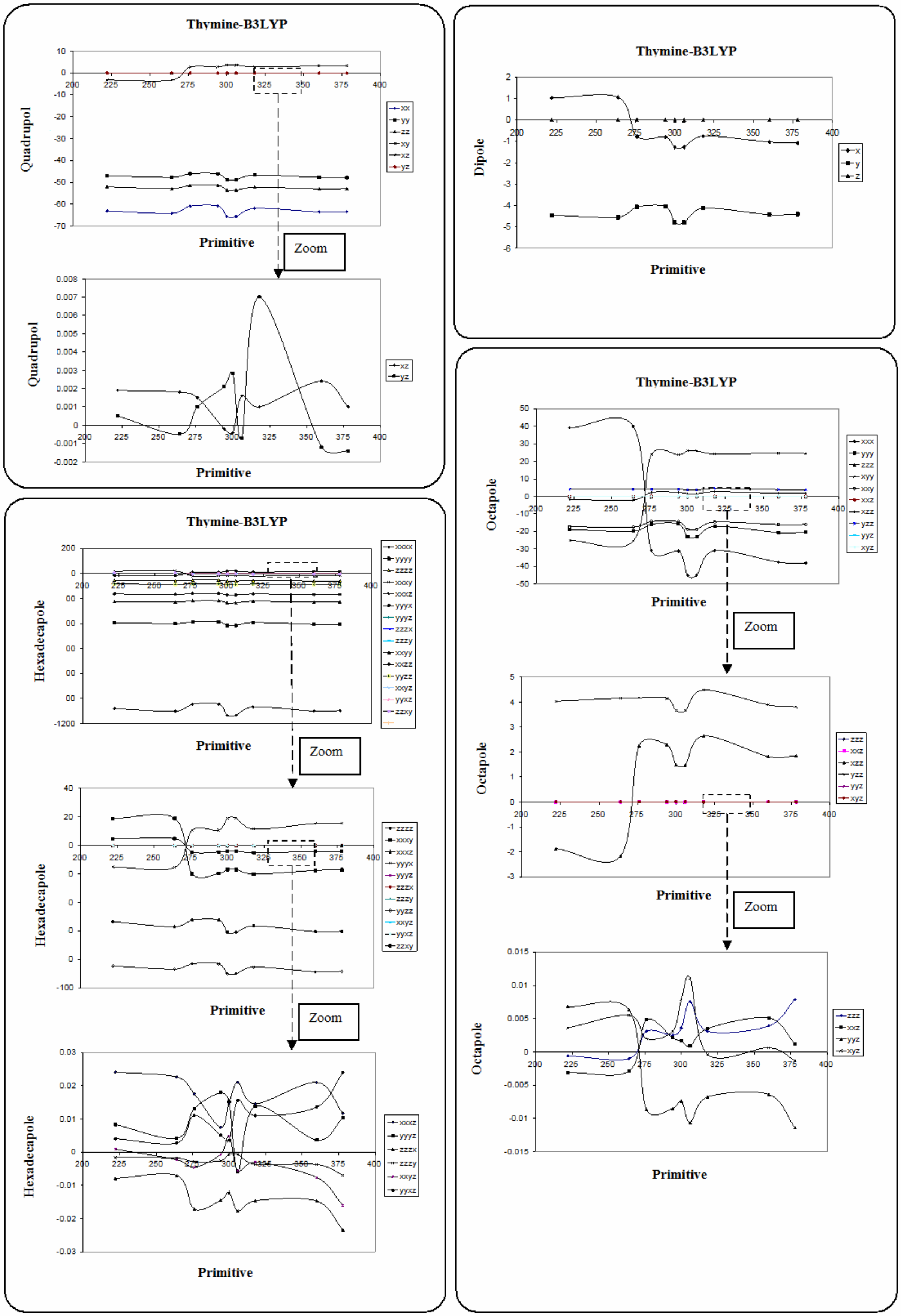

Fig. 5 Dipole, Quadrupole, Octapole, Hexadecapole moments VS. Primitive Gaussian Function for Thymine at the different basis sets.

Table 9. Occupancy orbital, Energy, Donor, Acceptor, Natural charge and Total Lewis for Adenine at HF level.

	Lowest Occupancy	Highest Energy (kcal/mol)	Donor	Acceptor	Natural charge	Total Lewis (%)
6-31g	1.67243	-0.39338	N 7	BD*(2) C 4-C 5 BD*(2) C 8- N 9	N 10 -0.87236	97.3465
6-31g*	1.67093	-0.37767	N 7	BD*(2) C 4- C 5 BD*(2) C 8- N 9	N 10 -0.86178	97.3402
6-311g	1.67449	-0.39654	N 7	BD*(2) C 4- C 5 BD*(2) C 8- N 9	N 10 -0.80200	97.3558
6-311g*	1.67409	-0.38265	N 7	BD*(2) C 4- C 5 BD*(2) C 8- N 9	N 10 -0.79465	97.3447
6-31g**	1.67183	-0.37748	N 7	BD*(2) C 4- C 5 BD*(2) C 8- N 9	N 10 -0.87702	97.3407
6-311+g	1.67311	-0.39974	N 7	BD*(2) C 4- C 5 BD*(2) C 8- N 9	N 10 -0.81126	97.3688
6-31++g	1.67311	-0.39965	N 7	BD*(2) C 4- C 5 BD*(2) C 8- N 9	N 10 -0.80851	97.3689
6-311++g*	1.67316	-0.38782	N 7	BD*(2) C 4- C 5 BD*(2) C 8- N 9	N 10 -0.80016	97.3591
6-311++g**	1.67426	-0.38826	N 7	BD*(2) C 4- C 5 BD*(2) C 8- N 9	N 10 -0.81236	97.3614

Table 10. Occupancy orbital, Energy, Donor, Acceptor, Natural charge and Total Lewis for Adenine at B3LYP level.

	Lowest Occupancy	**Highest Energy (kcal/mol)**	**Donor**	**Acceptor**	**Natural charge**	**Total Lewis (%)**
6-31g	1.60319	-0.28320	N 7	BD*(2) C 4- C 5 BD*(2) C 8- N 9	N 10 -0.80443	96.9440
6-31g*	1.60386	-0.27281	N 7	BD*(2) C 4- C 5 BD*(2) C 8- N 9	N 10 -0.80477	96.9341
6-311g	1.67460	-0.39654	N 7	BD*(2) C 4- C 5 BD*(2) C 8- N 9	N 10 -0.80195	97.3552
6-311g*	1.60674	-0.28090	N 7	BD*(2) C 4- C 5 BD*(2) C 8- N 9	N 10 -0.74130	96.9166
6-31g**	1.60435	-0.27267	N 7	BD*(2) C 4- C 5 BD*(2) C 8- N 9	N 10 -0.81769	96.9338
6-311+g	1.60543	-0.29706	N 7	BD*(2) C 4- C 5 BD*(2) C 8- N 9	N 10 -0.74979	96.9559
6-31++g	1.60120	-0.29546	N 7	BD*(2) C 4- C 5 BD*(2) C 8- N 9	N 10 -0.80498	96.9499
6-311++g*	1.60672	-0.28918	N 7	BD*(2) C 4- C 5 BD*(2) C 8- N 9	N 10 -0.74935	96.9383
6-311++g**	1.60783	-0.28996	N 7	BD*(2) C 4- C 5 BD*(2) C 8- N 9	N 10 -0.76335	96.9411

Table 11. Occupancy orbital, Energy, Donor, Acceptor, Natural charge and Total Lewis for Thymine at HF level.

	Lowest Occupancy	**Highest Energy (kcal/mol)**	**Donor**	**Acceptor**	**Natural charge**	**Total Lewis (%)**
6-31g	1.71842	-0.41440	N 1	BD*(2) C 2- O 8 BD*(2) C 6- O 7	N 1 -0.74756	98.2515
6-31g*	1.72465	-0.39619	N 1	BD*(2) C 2- O 8 BD*(2) C 6- O 7	N 1 -0.76252	98.2455
6-311g	1.72011	-0.41790	N 1	BD*(1) C 2- O 8 BD*(2) C 6- O 7	O 8 -0.70923	98.2656
6-311g*	1.72802	-0.40085	N 1	BD*(1) C 2- O 8 BD*(2) C 6- O 7	N 1 -0.72344	98.2524
6-31g**	1.72505	-0.39601	N 1	BD*(2) C 2- O 8 BD*(2) C 6- O 7	N 1 -0.77005	98.2474
6-311+g	1.71756	-0.42059	N 1	BD*(1) C 2- O 8 BD*(2) C 6- O 7	N 1 -0.70667	98.2689
6-31++g	1.71743	-0.42049	N 1	BD*(1) C 2- O 8 BD*(2) C 6- O 7	O 8 -0.70568	98.2677
6-311++g*	1.72532	-0.40508	N 1	BD*(2) C 2- O 8 BD*(2) C 6- O 7	N 1 -0.72201	98.2549
6-311++g**	1.72645	-0.40554	N 1	BD*(2) C 2- O 8 BD*(2) C 6- O 7	N 1 -0.72777	98.2589

Table 12. Occupancy orbital, Energy, Donor, Acceptor, Natural charge and Total Lewis for Thymine at B3LYP level.

	Lowest Occupancy	**Highest Energy (kcal/mol)**	**Donor**	**Acceptor**	**Natural charge**	**Total Lewis (%)**
6-31g	1.63869	-0.28569	N 1	BD*(2) C 2- O 8 BD*(2) C 6- O 7	C 9 -0.70986	97.7948
6-31g*	1.64755	-0.27410	N 1	BD*(2) C 2- O 8 BD*(2) C 6- O 7	C 9 -0.68207	97.7948
6-311g	1.64116	-0.29421	N 1	BD*(2) C 2- O 8 BD*(2) C 6- O 7	N 1 -0.62153	97.7977
6-311g*	1.65113	-0.28263	N 1	BD*(2) C 2- O 8 BD*(2) C 6- O 7	N 1 -0.64127	97.7881
6-31g**	1.64803	-0.27409	N 1	BD*(2) C 2- O 8 BD*(2) C 6- O 7	C 9 -0.69455	97.9762
6-311+g	1.63900	-0.30082	N 1	BD*(2) C 2- O 8 BD*(2) C 6- O 7	N 1 -0.61978	97.8079
6-31++g	1.63509	-0.29900	N 1	BD*(2) C 2- O 8 BD*(2) C 6- O 7	C 9 -0.68064	97.7969
6-311++g*	1.64906	-0.29088	N 1	BD*(2) C 2- O 8 BD*(2) C 6- O 7	N 1 -0.63657	97.8006
6-311++g**	1.65022	-0.29131	N 1	BD*(2) C 2- O 8 BD*(2) C 6- O 7	N 1 -0.64244	97.8036

REFERENCES

1. *Hohenberg P. and Kohn W. , inhomogeneous electron gas Physical Review 1964, 136, 138.*
2. *A Sigel, H. Sigel(Eds.) Introductions of Metal Ions with Nucleotides, Nucleic Acids, and their constituents, Metal Ions in Biological systems, Vol. 32, Marcel Dekker, New York, 1996, pp. 1-814.*
3. *(a)Cooperman, B. S. Met. Ions Biol. Syst. 1976, 5, 79-125. (b)Mildvan, A. S. Adv. Enzymol. Relat. Areas Mol. Biol. 1979,49,103-26. (c)Eichhorn, G. L. Met. Ions Biol. 1980, 10, 1-21.*
4. *(a)Sigel, H., Ed. "Metal Ions in Biological Systems" ; Dekker: New York and Basel, 1979; Vol. 8. (b)Spiro, T.G., Ed.; "Metal Ions in Biology"; Wiley: New York, 1980; Vol. 1. (c)Eichhorn, G. L.; Marzilli, L. G., Eds. "Advances in Inorganic Biochemistry"; Elsevier/North-Holland: New York, Amesterdam, and Oxford, 1981; Vol.3.*
5. *Monajjemi M. and Ghiasi R., Journal of Chemical Research 2004, 11, 11-18.*
6. *Migross L.M and Strauss U. P., Chemical Physics of Ionic solution. Conwax B. F. and Baradus, Eds. Wiely New York, 1966, 361-389 Dove W. F. and Davidson N. J. Mol. Bio. 1962, 5, 467.*
7. *Martin, R. B.; Mariam, Y. H. Met. Ions Biol. Syst. 1979, 8, 57-124.*
8. *Kresse, G.; Furthmuller, J. Comp Mater Sci 1996,6,15.*
9. *Salahub D. R. and Zorner M. C. Eds. The challenge of d and f electrons(Acs, Washington, D. C. 1989).*
10. *10. Alkorta, I.; Rozas I. and Eleguero, J. J. Mol. Struct(THEOCHEM). 2001, 537,139.*
11. *Reed J. F. and Wienhold F. J. Chem. Phy. 1985, 65, 1736-1740.*
12. *Foster J. P. and Wienhold F. J. Am. Chem. Soc. 1980, 102, 7211-7218.*
13. *Beeke A. D. Phys. Rev. 1988, 38, 3098.*
14. *Kohn, W. Rev. Mod. Phys. 1999, 71, 1253.*
15. *Šponer, J.; Leszczynski, J.; Hobza, P. Biopolymers 2002, 61,3.*
16. *Suhnel, J. Biopolymers 2002,61,32.*
17. *Tetas M. and Louenstien J. Biochemistry 1963, 2, 350.*
18. *Parr R. G. and Yang W. Density functional theory of atoms molecules (Oxford, 1989).*
19. *Markov, G.; Payn, M. C. Phys. Rev. B 1995, 51, 4014.*
20. *Neugebauer, J.; Scheffler, M. Phys. Rev. B. 1992, 46, 16067.*
21. *Mark H. F. and Gaylord N. G., Encyclopedia of polymer science and technology, interscience publisher, New York, 1969, 10, 781-861.*
22. *Šponer, J.; Leszczynski, J.; Hobza, P. Biomol. Struc. Dyn. 1997,14,117.*
23. *Halvin R. and Michaes M., J. Phy. Chem. A. 1977, 101, 8908.*
24. *Starikov, E. B. Int J Quantum Chem 2000,77,859.*
25. *Hozba, P.; Šponer, J. Chem. Rev. 1999, 99, 3247.*
26. *Miehlich, B., Sarin A., Stolland H. and Preuss H. Chem. Phys. Lett, 1989, 157, 200.*
27. *Hehre, W. J.; Ditchfield, R. and Pople, J. A. J. Chem. Phys. 1972, 56, 2257.*
28. *Hariharan, P.C. and Pople, J. A. Theoret. Chim. Acta. 1973, 38, 213.*
29. *Becke, A. D. J. Chem. Phys. 1993, 98, 5648.*
30. *Lee, C.; Yang, G. and Parr, R. G. Physical Review 1988, B37, 785.*
31. *Frisch, M.J.; Trucks, G.W.; Schlegel, H. B.; Gill, P. M. W.; Johnson, B. G.; Robb, M. A.; Cheeseman, R.; Keith, T. A.; Petersson, G. A.; Montgomery, J. A.; Raghavachari, K.; Al-Laham, M. A.; Zakrzewski, V. G.; Ortiz, J. V.; Foresman, J. B.; Cioslowski, J.; Stefanov, B. B., Nanayakkara, A.; Challacombe, M.; Peng, C. Y.; Ayala, P. Y.; Chen, W.; Wong, M. W.; Andres, J. L.; Replogle,E. S.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Binkly, J. S.; Defrees, D. J.; Baker, J.; Stewart, J. P.; Head-Gordon, M.; Gonzalez, C.; Pople, J. A. GAUSSIAN 94, Revision E. 1, Gaussian, Inc., Pittsburgh PA (1995).*
32. *Boys, S. F. and Bernardi, F. Mol. Phys. 1970, 19, 553.*
33. *Carpenter J. F. and Wienhold F. J. Chem . Phy. 1989, 65, 1716-1740.*