

Quantum Chemical Analysis of ATP, GTP and Related Compounds in Gas Phase

A.H. Pakiari^{a,*}, M. Farrokhnia^a and A. Moradshahi^b

^aDepartment of Chemistry, College of Sciences, Shiraz University, Shiraz 71454, Iran

^bDepartment of Biology, College of Sciences, Shiraz University, Shiraz 71454, Iran

(Received 25 July 2008, Accepted 28 October 2008)

Adenosine 5'-triphosphate (ATP) and Guanine 5'-triphosphate (GTP), which are highly significant species for biological system as sources of energy, along with two other compounds, ribose 5'-triphosphate (RTP) and triphosphate (TP), have been investigated theoretically. The capability of releasing terminal phosphoric acid and existent intramolecular bonds in their structure have been studied in gas phase. Due to the presence of hydrogen bonds in the above molecules, several inner and stable rings have been formed by atoms in molecules. The Quantum Theory of Atoms in Molecules (QTAIM) has been used in order to discover the intramolecular interactions properties in terms of charge densities. We have also demonstrated that the release of terminal phosphoric acid in ATP and GTP are both facilitated in the presence of ribose and base in comparison with TP and RTP. Our calculations have been done using density functional procedure.

Keywords: ATP, GTP, QTAIM, Intramolecular hydrogen bond

INTRODUCTION

Adenosine 5'-triphosphate (ATP), an adenine nucleotide, is extremely important to metabolism because it is the currency of energy exchange in metabolic process. ATP is produced by catabolism of food molecules (and the light reactions of photosynthesis in plants) and consumed by cellular processes that require energy, such as biosynthesis, active transport of substances across cell membranes, cell motility and muscle contraction. ATP stores free energy in its two phosphoanhydride bonds and transfers this energy when it is hydrolyzed to adenosine 5'-diphosphate and orthophosphate (P) or adenosine 5'-monophosphate and pyrophosphate [1]. The P-O-P linkage is not found in nature except as produced by living organisms because of its high susceptibility to hydrolysis [2]. ATP, ADP and AMP are made up of three

units: an adenine, a ribose and one phosphate group. These molecules are involved in a vast variety of chemical environments and applications from inorganic to biological systems [3,4]. Guanosine 5'-triphosphate (GTP) is a similar molecule to ATP and the chemical energy derived from the hydrolysis of P-O-P linkage of guanine di- and triphosphate (*i.e.* GDP and GTP) is used by the cells to carry out different biological functions such as ATP [5].

In physiological pH range pyrophosphate and adenosine triphosphate have two or three negative charges. The coulomb repulsion between the excess charges, at least partly, renders pyrophosphate and ATP as "energy-rich" molecules [6].

Chemical evolution of biological systems shows that there is no difficulty to account for the appearance of the bases and sugars of nucleic acids on the primitive earth. An unexpected stumbling block arises, however, when one tries to account for the particular reason and way in which the bases and sugars are joined to make nucleoside, such as the coupling of adenine

*Corresponding author. E-mail: pakari@shirazu.ac.ir

and ribose to form the adenosine molecules. As regards evolutionary changes of living cells, one of the probable explanations for selecting adenosine and not guanosine, cytidine or uridine for coupling to the triphosphate tail in ATP, is the relative simplicity of the synthesis of adenine which resulted in its being present in greater concentrations than the other bases in the primitive environment of living cells. Adenine is the most readily synthesized hydrogen cyanide: four HCN first yields tetramer of HCN, diaminomaleonitrile, and the rearrangement takes place in the presence of light and one more HCN leads to form adenine. This synthesis proceeds under conditions that would have been reasonable on the primitive earth. According to this point of view, "The use of ATP may represent nothing more than another cosmic throw of dice" [7].

In the present article, we have addressed the question of biological superiority of ATP in living systems. Although the idea of "high energy" phosphate has been current for over 70 years [8,9] and has been proved essential for understanding of energy storage and energy transfer in biological systems to date, there has not yet appeared any clear explanation as to why certain phosphate compounds contain more energy than ordinary ester phosphate or other similar compounds. Our primary aim is to find a suitable answer to this question so that roles of adenine and ribose would be deliberated in ATP molecule. To this end, properties of terminal P-O bond have been studied in three molecules that all are similar in their pyrophosphate tails but differ in parts involving adenine and ribose. The influence of adenine and ribose on terminal P-O bond has been investigated computationally. Finally, effects of ribose and other organic nucleobase, guanine have been considered in other similar molecule, GTP, and the results were in good agreement with those obtained from ATP.

METHODOLOGY

Molecular geometries and their electronic wave functions have been optimized with the help of *Gaussian 98* program [10]. All species have been optimized in gas phase using density functional theory (DFT) [11,12] and the hybrid B3LYP exchange-correlation functional [13,14] by using 6-31+G* basis set. Frequency analysis was also performed for the structures to make sure that they were indeed minimum

structures.

Bader's Quantum Theory of Atoms in Molecules (QTAIM) [15,16] was applied to characterize the influence of organic nucleobase and sugar on terminal P-O bond in the investigated systems. The quantum theory of atoms in molecules is based on the analysis of electronic density topology and identifies chemical bond as a bond critical point (BCP) and corresponding bond paths (BP). Because of flexibility and reliability of this method, many researches have been devoted to obtain chemical bond strength and nature in both organic and inorganic chemistry, *via* QTAIM analysis [17-19]. What distinguishes this research from others is the characterization of terminal P-O bond in terms of QTAIM parameters and analysis of the effect of different segments on the strength of such a P-O bond. Furthermore, we have investigated different intramolecular interactions which have significant roles in stabilizing ATP molecules in biological systems. AIM2000 package [20] has been used to obtain bond properties, plot molecular graphs as well as virial paths.

RESULTS AND DISCUSSION

There is valuable experimental information concerning the protonation state, conformation, and metal-chelation of ATP [21-23]. H NMR experiments [24,25] show that the molecule exists in water in an anti-configuration, and the triphosphate tail is fully deprotonated under neutral conditions especially when complexed with Mg^{2+} . Mg^{2+} has a strong catalytic activity related to its ability to elongate one of the anhydride P-O bonds, with an estimated reaction barrier of 13.5 kcal mol⁻¹ for a pyrophosphate dianion [26-28].

There have been several theoretical studies on the hydrolysis of pyrophosphate in the gas phase [26,29-31] in addition to several other attempts made to model the break of anhydride P-O-P linkage and to understand the underlying mechanism. These approaches range from simple molecular orbital calculations to sophisticated quantum mechanical calculations of isolated active site of protein such as myosin [26,27,30,32-37]. In the field of quantum chemistry, many investigations have been carried out at the Hartree Fock level. Similar to many other compounds in chemistry, electron correlation plays a major role in imparting the unusual properties to these molecules [38]. Various studies [39-42]

have indicated that the electrostatic effects play an important role both in the molecular structure and thermochemistry of the hydrolysis of pyrophosphates.

The traditional way to think of energetic character of ATP is to assign its terminal P-O bond in pyrophosphate tail of the molecules as an energy rich bond, that releases energy upon hydrolysis due to the coulomb repulsion of product, resonance effects and changes in protonation [2]. The schematic representation of ATP is shown in Fig. 1.

In the present study, main focus is on the effect of different segments in ATP on the terminal anhydride P-O bond. We have examined molecules that have similar triphosphate tail. Since charge density and bond length can be criteria of bond strength, these properties of terminal P-O bond have been compared in the systems of interest in gas phase. The fully optimized geometries of ATP, GTP, ribose 5'-triphosphate (RTP) and triphosphate (TP) system, are presented in Fig. 2. These geometries have been analyzed in terms of bond length of terminal anhydride P-O bond in all systems. Because of the crucial role of Mg^{2+} in ATP molecule and its important effect on lengthening of terminal P-O bond in ATP^{2-} , fully optimized structures of $ATPMg^{2-}$ and $RTPMg^{2-}$, which have been presented in Fig. 3, were studied to support our results.

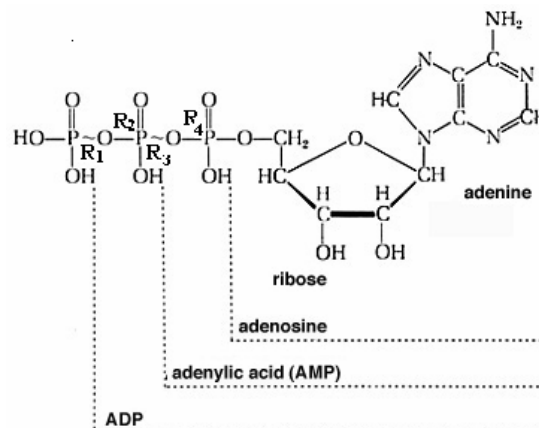


Fig. 1. Schematic representation of ATP.

According to these pieces of evidence obtained computationally, it seems that organic nucleobase and ribose result in elongating terminal P-O bond and decreasing its charge density so that its strength decreases in ATP molecules. Other research results in negatively charged molecules and Mg-chelation of ATP and RTP support our analysis strongly which are presented below.

The results of QTAIM parameters (in atomic units), bond distances (in angstrom) and fully optimized structures of

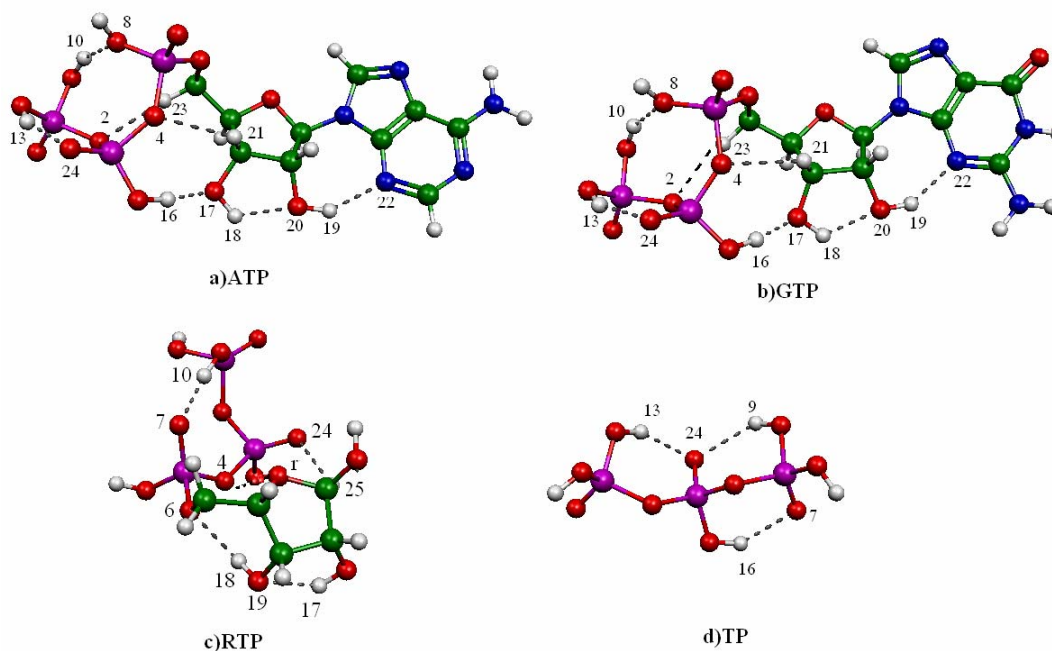


Fig. 2. ATP, GTP, RTP and TP and their atom numbers.

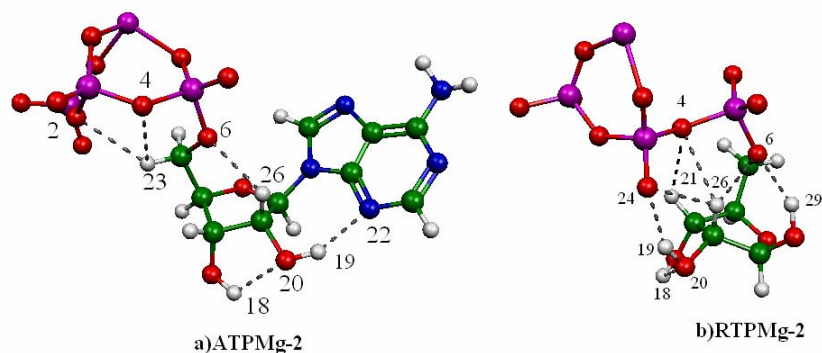


Fig. 3. ATPMg⁻² and RTPMg⁻² and their atom numbers.

Table 1. The Results of P-O Bond Distance (R, Angstrom) and Charge Density (ρ , Atomic Units) in Investigated Systems. R₁ is the Terminal P-O Bond

Molecule	R ₁	ρ_{BCP1}	R ₂	ρ_{BCP2}	R ₃	ρ_{BCP3}	R ₄	ρ_{BCP4}
ATP	1.682	0.143	1.613	0.168	1.636	0.156	1.626	0.161
GTP	1.682	0.143	1.613	0.168	1.636	0.156	1.626	0.161
RTP	1.673	0.146	1.596	0.173	1.643	0.154	1.609	0.167
TP	1.651	0.158	1.635	0.164	1.585	0.178	1.681	0.148
ATPMg ⁻²	1.638	0.157	1.667	0.148	1.565	0.152	1.651	0.155
RTPMg ⁻²	1.629	0.161	1.669	0.149	1.598	0.168	1.713	0.132
ATP ⁻⁴	1.629	0.160	1.691	0.140	1.683	0.142	1.645	0.155
RTP ⁻⁴	1.624	0.162	1.702	1.137	1.675	0.145	1.658	0.151
TP ⁻⁵	1.621	0.163	1.630	0.164	1.623	0.162	1.621	0.163

investigated molecules are shown in Table 1 and Figs. 2 to 4. From the above analysis (Table 1), in both ATP and GTP molecules charge densities ($\rho_{BCP1} = 0.143$) and bond distances (1.682) of terminal anhydride P-O bond (R₁) are absolutely the least and the most values in comparison with corresponding values in other molecules in series of interest to us, respectively. According to these results, a descending order is also seen in charge densities in addition to increase in bond distance of terminal anhydride P-O bond (R₁). The above trends in R₁ for lengthening bond distance and declining electron density are true for RTPMg⁻² and ATPMg⁻² alike as shown in Table 1. ATPMg⁻² has less charge density ($\rho_{BCP1} = 0.157$) than RTPMg⁻² ($\rho_{BCP1} = 0.161$), which indicates the P-O bond is more apt to break in former compound relative to latter one. All the computations have been performed for

negatively charged molecules ATP⁻⁴, RTP⁻⁴ and TP⁻⁵. The results in both charge density and bond distances at such a P-O bond follow an identical order with those have observed in neutral molecules of ATP series.

However in other P-O bonds (R₂, R₃ and R₄) there is not any clear trend toward decreasing charge density or increasing bond distances. This observation, however, is in accord with our main aim because the terminal anhydride P-O is the most reactive and important bond in ATP. Moreover, our theoretical results in this part are in agreement with experimental evidence. Thus, it sounds reasonable to consider this bond and investigate its individual character separately from other P-O bonds in series.

In the second part of our study, we would like to consider other aspects of the problem and focus upon ATP, GTP and

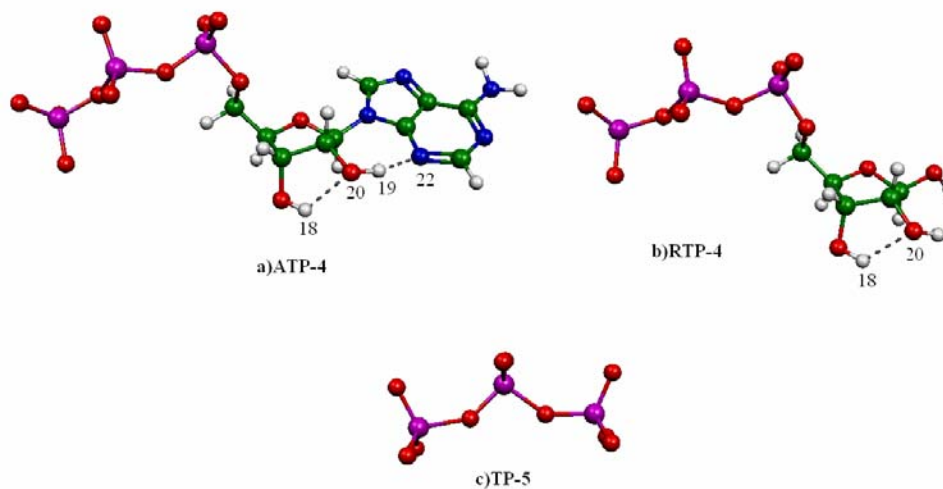


Fig. 4. ATP⁴, RTP⁴, TP⁵ and their atom numbers.

other above-mentioned molecules structurally. Their intramolecular hydrogen bonds have been detected according to the QTAIM criteria. The existence of BCP between different atoms, which are not chemically connected, is an indication of intramolecular interactions that stabilize molecules.

In ATP and GTP, TP is connected to ribose through single bond C₃₃ (ribose)-O₆ (TP), and organic nucleobase is also connected to ribose through single bond C₃₂ (ribose)-N₃₁ (base), as shown in Fig. 2. Therefore, they are able to have free rotation along those single bonds and make different conformations. In present research, we have considered only one of the possible conformers of ATP and GTP in gas phase and studied the existent intramolecular interactions. The stabilization energy related to intramolecular H-bonds has been estimated by using the local potential energy density proposed by Espinosa. In this method, the energy of the hydrogen bond is equal to one-half of the local potential energy density at the hydrogen bond critical point multiplied by the atomic volume element a_0^3 [43].

$$E_{HB}^{(3)} = -\frac{a_0^3}{2} V_{CP} \approx -\frac{V_{CP}}{2}$$

Although there are other procedures in literature [44,45] to estimate hydrogen bond strength in accordance with QTAIM analysis, Espinosa's procedure is more suitable for our purpose. The second approach is to estimate the stabilization

energy by comparing the BCP charge density of intramolecular hydrogen bonds with hydrogen bond in H₂O dimer. Charge density of BCP for hydrogen bond in water dimer is 0.0286 (a.u.) that stabilizes the dimer about 6.0 kcal mol⁻¹. Therefore, the relative stabilization energies can be estimated by the ratio of the corresponding charge density at the BCP. The former and latter estimation of hydrogen bond strength are denoted by E_{SE}^1 and E_{SE}^2 in Table 2, respectively.

ATP has seven hydrogen bonds with estimated total stabilization energy (E_{SE}^1) 46.91 kcal mol⁻¹ as indicated in Table 2. Three of these hydrogen bonds are between TP and ribose with total charge density at BCPs 6.52 and estimated stabilization energy of 16.53 kcal mol⁻¹. There is one hydrogen bond between ribose and adenine with charge density at BCP 2.96 and estimated stabilization energy of 6.90 kcal mol⁻¹.

GTP has seven hydrogen bonds, too, with E_{SE}^1 equals to 45.76 kcal mol⁻¹, as shown in Table 2. For stopping free rotation, there exist three hydrogen bonds between TP and ribose with total charge density at BCPs 6.43 and estimated stabilization energy of 16.02 kcal mol⁻¹, and there is one hydrogen bond between ribose and guanine with electron density at BCP 2.81 and E_{SE}^1 equals to 6.59 kcal mol⁻¹, as shown in Table 2.

On the basis of these estimated stabilization energies, it sounds that two energetic molecules, ATP and GTP are more stable than other above-mentioned molecules due to intramolecular interactions. To study the overall stability of

Table 2. Charge Density (a.u.) of BCP, Bond Length (Å) and Estimated Energy of Hydrogen Bonds in ATP, GTP, RTP, TP, ATPMg⁻², RTPMg⁻² and ATP⁴⁻

Molecule	Intramolecular interaction	Interaction	$\rho_{BCP}[10^{-2}]$	$r_{\text{Å}}$	$V_{\text{kcal/mol}}[10^{-2}]$	E_{SE}^1	E_{SE}^2
ATP	H ₁₀ -O ₈	TP	2.25	1.99	1.94	6.09	4.7
	H ₁₃ -O ₂₄	TP	3.52	1.83	2.99	9.38	7.3
	H ₂₁ -O ₄	Ribose-TP	1.05	2.47	0.76	2.39	2.2
	H ₂₃ -O ₂	Ribose-TP	0.95	2.49	0.68	2.13	2.0
	H ₁₆ -O ₁₇	Ribose-TP	4.52	1.69	3.83	12.02	9.4
	H ₁₉ -N ₂₂	Ribose adenine	2.96	1.97	2.21	6.93	6.2
	O ₂₀ -H ₁₈	Ribose	2.77	1.92	2.54	7.97	5.8
Total stabilization energy						46.91	37.6
GTP	H ₁₀ -O ₈	TP	2.23	1.99	1.92	6.02	4.7
	H ₁₃ -O ₂₄	TP	3.48	1.82	2.96	9.38	7.3
	H ₁₉ -N ₂₂	Ribose guanine	2.81	1.99	2.10	6.59	5.9
	H ₂₁ -O ₄	Ribose-TP	1.01	2.49	0.72	2.26	2.2
	H ₂₃ -O ₂	Ribose-TP	0.90	2.51	0.64	2.01	1.9
	H ₁₆ -O ₁₇	Ribose-TP	4.43	1.70	3.75	11.77	9.3
	O ₂₀ -H ₁₈	Ribose	2.69	1.93	2.47	7.75	5.6
Total stabilization energy						45.76	36.7
RTP	H ₁₀ -O ₇	TP	4.00	1.72	3.43	10.76	8.3
	H ₁₉ -O ₁₇	Ribose	2.74	1.98	2.44	7.66	5.7
	H ₂₅ -O ₂₄	Ribose-TP	0.96	2.47	0.68	2.13	2.0
	H ₁₈ -O ₆	Ribose-TP	2.07	2.06	1.83	5.74	4.3
	O _{ribos} -O ₄	Ribose-TP	0.86	3.06	0.66	2.07	-
Total stabilization energy						28.36	20.3
TP	H ₁₃ -O ₂₄	TP	2.88	1.91	2.46	7.72	6.0
	H ₉ -O ₂₄	TP	1.46	2.24	1.18	3.70	3.0
	H ₁₆ -O ₇	TP	2.16	2.05	1.80	5.65	4.5
Total stabilization energy						17.07	13.5
ATPMg ⁻²	H ₁₈ -O ₂₀	Ribose	2.12	2.07	1.93	6.05	4.4
	H ₂₆ -O ₆	Ribose-TP	1.28	2.40	0.93	2.92	2.7
	H ₂₈ -O ₂	Ribose-TP	0.77	2.61	0.52	1.63	1.6
	H ₁₉ -N ₂₂	Ribose adenine	2.45	2.05	1.82	5.71	5.1
	H ₂₈ -O ₁₄	Ribose-TP	0.50	2.85	0.28	0.88	1.1
Total stabilization energy						17.19	14.9
RTPMg ⁻²	H ₁₈ -O ₂₀	Ribose	2.30	2.07	2.05	6.43	4.8
	H ₁₉ -O ₂₄	Ribose-TP	2.73	1.90	2.32	7.28	5.7
	H ₂₆ -O ₂₄	Ribose-TP	1.31	2.42	0.97	3.04	2.8
	H ₂₆ -O ₄	Ribose-TP	0.88	2.57	0.64	2.01	1.8
	H ₂₆ -O ₆	Ribose-TP	1.58	2.34	1.21	3.79	3.3
	H ₂₉ -O ₆	Ribose-TP	1.77	2.14	1.50	4.71	3.7
	H ₂₁ -O ₄	Ribose-TP	0.82	2.61	0.54	1.69	1.7
Total stabilization energy						28.95	23.8
ATP ⁴⁻	H ₁₈ -O ₂₀	Ribose	2.59	1.99	2.35	7.37	5.4
	H ₁₉ -N ₂₂	Ribose adenine	3.47	1.89	2.66	8.35	7.2
Total stabilization energy						15.18	12.6

E_{SE}^1 and E_{SE}^2 are in kcal mol⁻¹, and they are evaluated by [43] and estimated by H₂O dimer, respectively.

these molecules in biological system, it is also necessary to consider solvent effects and influences of biological environment on intermolecular interactions. However, our focus is primarily on the structural and topological properties of ATP, GTP and their related compounds in gas phase without considering any effect of biological environment.

Finally, the hydrogen bonds in each component and also between three components of ATP and GTP keep fixed conformation with internal rotation. However, ATP⁴⁻ can have many conformations since there are two hydrogen bonds in it which stabilize ATP⁴⁻ just about 15.18 kcal mol⁻¹. There is one hydrogen bond in RTP⁴⁻ with 7 kcal mol⁻¹ stabilization energy.

SUMMARY AND CONCLUDING REMARKS

ATP (Adenosine 5'-Triphosphate) includes three different parts, the most important of which is its triphosphate tail. ATP owes its energy-rich character to this particular part. According to our present research the role of remaining segments, including adenine and ribose, is to elongate that remarkable P-O bond, which is involved in ATP hydrolysis and energy-releasing mechanisms directly. This elongation of bond goes along with reducing charge density of this interesting bond. Our investigations cover negatively charged ATP and similar anions which were similar in their triphosphate tails, in addition to two Mg-chelation anion ATPMg²⁻ and RTPMg²⁻. The intramolecular hydrogen bonds and the stabilization energy due to their existence in molecules investigated here are two other pieces of evidence which show that ATP and GTP are the most stable molecules in biological environments.

REFERENCES

- [1] J.D. Rawn, Biochemistry, Neil Patterson Publishers, Carolina Biological Supply Company 1 (1989) 238.
- [2] J. Akola, R.O. Jones, J. Phys. Chem. B. 107 (2003) 11774.
- [3] M. Baltscheffsky, P. Nyren, in: L. Ernster (Ed.), Bioenergetics, Elsevier, Amsterdam, 1984.
- [4] M. Baltscheffsky, H. Baltscheffsky, in: L. Ernster (Ed.), Molecular Mechanism in Bioenergetics, Elsevier, Amsterdam, 1992.
- [5] Y. Sugawara, N. Kamiya, H. Isawaki, T. Ito, Y. Satow, J. Am. Chem. Soc. 113 (1991) 5440.
- [6] X. Wang, E.R. Vorpagel, X. Yang, Lai-Sheng Wang, J. Phys. Chem. A. 105 (2001) 10468.
- [7] R.E. Dickerson, Scientific American 239 (1978) 62.
- [8] F. Lipmann, Adv. Enzymol. 1 (1941) 99.
- [9] J.S. Sowden, H.O.L. Fischer, Ann. Rev. Biochem. 11 (1942) 203.
- [10] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, V.G. Zakrzewski, J.A. Montgomery, R.E. Stratmann, J.C. Burant, S. Dapprich, J.M. Millam, A.D. Daniels, K.N. Kudin, M.C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G.A. Petersson, P.Y. Ayala, Q. Cui, K. Morokuma, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J. Cioslowski, J.V. Ortiz, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, J.L. Andres, C. Gonzalez, M. Head-Gordon, E.S. Replogle, J.A. Pople, Gaussian 98 Revision A.7, Gaussian Inc., Pittsburgh, PA, 1998.
- [11] J.W. Andzelm, in: J.K. Labanowski, J.W. Andzelm (Eds.), Density Functional Methods in Chemistry, Springer, New York, 1991.
- [12] T. Ziegler, Chem. Rev. 91 (1991) 651.
- [13] A.P. Becke, J. Chem. Phys. 98 (1993) 5648.
- [14] C. Lec, W. Yang, R.G. Parr, Phys. Rev. B 37 (1988) 785.
- [15] R.F.W. Bader, Atoms in Molecules: A Quantum Theory, Oxford University Press, Oxford, UK, 1990.
- [16] P.L.A. Popelier, Atoms in Molecules, an Introduction, Prentice Hall, Pearson Education Limited, 2000.
- [17] G.F. Matta, R.F.W. Bader, PROTEINS: Structure, Function, and Genetics. 40 (2000) 310.
- [18] G.F. Matta, R.F.W. Bader, PROTEINS: Structure, Function, and Genetics 48 (2002) 519.
- [19] G.F. Matta, R.F.W. Bader, PROTEINS: Structure, Function, and Genetics. 52 (2003) 360.
- [20] R.F.W. Bader, F. Biegler-König, J. Schönbohm, AIM2000 Program Package, Ver. 2.0, University of

- Applied Sciences, Bielefeld, Germany, 2002.
- [21] J. Granot, D. Fiat, *J. Am. Chem. Soc.* 99 (1977) 70.
- [22] H. Sigel, R. Tribolet, R. Malini-Balakrishnan, R.B. Martin, *Inorg. Chem.* 26 (1987) 2149.
- [23] H. Sigel, *Chimia* 41 (1987) 11.
- [24] P. Wang, J.L. Oscarson, R.M. Izatt, G.D. Watt, C.D. Larsen, *J. Sol. Chem.* 24 (1995) 989.
- [25] P. Wang, R.M. Izatt, J.L. Oscarson, S.E. Gillespie, *J. Phys. Chem.* 100 (1996) 9556.
- [26] H. Saint-Marin, L.E. Ruiz-Vicent, A. Romirez-Solis, I. Ortega, *J. Am. Chem. Soc.* 118 (1996) 12167.
- [27] K. Yoshikawa, Y. Shinohara, H. Terada, S. Kato, *Biophys. Chem.* 27 (1987) 251.
- [28] L. Jiang, X. Mao, *Polyhedron.* 21 (2002) 435.
- [29] B. Ma, C. Meredith, H.F. Schaefer III, *J. Phys. Chem.* 98 (1994) 8216.
- [30] B. Ma, C. Meredith, H.F. Schaefer III, *J. Phys. Chem.* 99 (1995) 3815.
- [31] M.E. Colvin, E. Evleth, Y. Akacem, *J. Am. Chem. Soc.* 117 (1995) 4357.
- [32] K. Fukui, A. Imamura, C. Nagata, *Bull. Chem. Soc. Jpn.* 36 (1963) 1450.
- [33] M. Tajima, M. Honda, *J. Mol. Struct. (Theochem).* 228 (1991) 201.
- [34] J.R.T. Johnson, I. Panas, *Chem. Phys.* 276 (2002) 45.
- [35] H. Kagawa, K. Mori, *J. Phys. Chem. B* 103 (1999) 7346.
- [36] N. Okimoto, K. Yamanaka, J. Ueno, M. Hata, T. Hoshino, M. Tsuda, *Biophys. J.* 81 (2001) 2786.
- [37] T.J. Minehardt, N. Marzari, R. Cooke, E. Pate, P.A. Kollman, R. Car, *Biophys. J.* 82 (2002) 660.
- [38] P. Hansia, N. Guruprasad, S. Vishveshwara, *Biophys. Chem.* 119 (2006) 127.
- [39] T.L. Hill, M.F. Morales, *J. Am. Chem. Soc.* 37 (1951) 1656.
- [40] D.M. Hayes, G.L. Kenyon, P.A. Kollman, *J. Am. Chem. Soc.* 100 (1978) 4331.
- [41] C.S. Ewing, J.R. Van Wazer, *J. Am. Chem. Soc.* 110 (1988) 79.
- [42] H. Saint-Martin, I. Ortega-Blake, A. Les, L. Adamowicz, *Biochem. Biophys. Acta* 1080 (1991) 205.
- [43] E. Espinosa, E. Molins, C. Lecomte, *Chem. Phys. Lett.* 285 (1998) 170.
- [44] S.J. Grabowski, *Monatsh. Chem.* 133 (2002) 1373.
- [45] S.J. Grabowski, *J. Phys. Org. Chem.* 17 (2004) 18.