Contents lists available at *Dergipark*

Journal of Scientific Reports-A

journal homepage: *https://dergipark.org.tr/tr/pub/jsr-a*

E-ISSN: 2687-6167 ***Number 61, June 2025***

RESEARCH ARTICLE

Receive Date: 18.12.2024 *Accepted Date: 08.04.2025*

A useful utility program for all Gaussian version users: ZEKA

Zeki Kartal[a*], Kamil Kartal[b]

[a]*Retired Professor of Atomic and Molecular Physics, Kütahya Dumlupınar University, Kütahya, 43020, Türkiye, ORCID: 0000-0001-9739-0858*
[b]*Retired from TFKB (TÜRKİYE FINANCE PARTICIPATION BANK) Information Technologies, Assistant Manager, and IT Manager at TGS between 2011-2015, İstanbul, 34584, Türkiye, ORCID: 0009-0003-2157-1689*

Abstract

This study focuses on ZEKA, a time-saving utility calculation program for researchers using the Gaussian 03, Gaussian 09 and Gaussian 16 molecular modeling and calculation programs. The magnetic, vibrational, electro-optic, some NLO and NBO properties of the compound whose structure is resolved with the Gaussian program are calculated by taking the necessary data from its .log output file and placing them in the relevant formulas. The ZEKA utility program completes such calculations in a very short time interval of approximately **300-400 milliseconds (ms)** for an average-sized molecular structure, depending on the size of its log file. These processes require the researcher to spend a lot of time on this work. In addition, the fact that the calculations are performed by the human factor may cause some unwanted errors. The ZEKA utility program will enable researchers to both make the best use of their limited time and prevent errors caused by human factors.

Keywords: Gaussian molecular modeling program, Gaussian calculation program, structural properties of compounds, Gaussian output file (.log), ZEKA utility program

1. Introduction

Human beings began to watch the various events taking place around them in this world, first with fear, then with curiosity, and then with interest. As a result, humankind has gained insights into the events of interest. Later, human beings began to investigate the events around them, wondering why and how they happened. Thus, the foundation of the first scientific thought and scientific study in human history was laid.

As time passed, studies and developments in science reached a dizzying pace in every field. Especially in the last fifty years, developments in the fields of computers and software have enabled many physical and chemical events to be simulated in the computer environment and the results of the events to be obtained in the form of new data. For example, obtaining new compounds and investigating their physical, chemical, electronic and magnetic properties is one of the most important areas in this regard.

Quantum chemistry and solid-state physics computer programs apply quantum chemistry methods in these fields. These programs may also use Hartree-Fock (HF), Density Functional Theory (DFT), Molecular Mechanics (MM), Semi-Empirical Quantum Chemistry (SEQCM), and a number of other methods. Some of these programs are suitable for both free use and

* Corresponding author. Tel.: 05326831144
E-mail address: zekikartal52@gmail.com

commercial use. Many experts have made great contributions in bringing these programs to their current state. Programs such as AMPAC [1], CASTEP [2], CRYSTAL [3], GAMESS [4], GAUSSIAN [5], MOPAC [6], SIESTA [7] and SPARTAN [8] … etc. can be given as examples of such programs. Many researchers are increasingly using some of these programs in their own studies. Many researchers make decisions about which program to use in their scientific studies based on their own observations, sensations, and the results of using and testing various programs to the extent of their possibilities.

It is a well-known fact that there are many auxiliary programs such as GAUSSSUM, MULTIWFN and others that make it easier to understand the outputs of the computational molecular modeling programs mentioned above. None of the other programs provided as an auxiliary to the Gaussian program provide those who use it with the concrete calculated results that the ZEKA utility does. However, the ZEKA utility offers a new type of service that those programs do not provide, namely automatic calculation of μ, α_0, Δα, β_0 and γ values. Thus, it saves for researchers a significant amount of time.

Gaussian software easily indicates the most complex interactions in electronic structures, revealing even the smallest differences in them. Gaussian enables in-depth examination of electronic interactions in molecular structures, and presents the results accurately in the shortest possible time. Due to such features, it is widely used in academic studies. The purpose of this study is definitely not to compare similar programs with each other in terms of quality or functionality, but only to save time for researchers using various variants of the Gaussian program and to make their work easier on some issues.

Whichever program is used to determine the structural properties of a compound, the result gives the information in an output file as various file extensions (for example, chk, gjf and log etc. in the Gaussian program). These new outputs contain raw information used to calculate many properties of the compound of interest. Extracting this raw information from the file, applying it to the necessary formulas, and obtaining the desired result relies almost entirely on human effort. Especially in complex compounds formed by the combination of many atoms, the number of raw data in question can reach quite large values. Therefore, the number of human errors that can be made when using large amounts of raw data also increases.

2. Material and method

When conducting an experimental scientific study, various chemical substances such as ligands, different atoms and solvents are used. As a result of experimental studies, new synthesized products emerge in various forms. Some physical and chemical properties of these new products are investigated either with some technical instruments (for example: IR, Raman, NMR, powder and single crystal data analyzers ...) or with some quantum mechanical calculation programs mentioned earlier.

Like many researchers, we use the Gaussian program in computational chemistry studies. We calculated various properties of some of the compounds we examined with the help of the Gaussian program [9-12]. We wanted to create a utility that would save time and eliminate human errors for researchers who will use the Gaussian program in their future studies. Thus, as a result of long efforts, the "ZEKA" program emerged. The purpose of this study is to introduce the ZEKA utility to Gaussian users. Later, efforts will be made to improve it in line with the requests and suggestions that may come from the users.

2.1. Why the ZEKA utility was needed?

By using the data (mol or cif files) of a compound that has been theoretically designed or whose crystal structure has been analyzed experimentally, theoretical analyzes can be made about that compound with the Gaussian program. The Gaussian program saves theoretical calculation results as files with gjf, chk, and log extensions. The first two documents give the visual data of the relevant compound, and the last document gives the raw data as a txt file. The raw data to be taken from the txt file of the relevant compound is used in the formulae below (Eqs. 1-8) to calculate its magnetic, electrical or structural properties [13,14].

The values that can be calculated for the relevant compound; dipole moment (μ), mean polarizability (α_0), anisotropies of polarizability (Δα), first order static hyperpolarizability (β_0) and its components (β_x, β_y, β_z) and second order static hyperpolarizability (γ) values are given in Equations (1-8), respectively.

$$\mu = \sqrt{\mu_x^2 + \mu_y^2 + \mu_z^2} \tag{1}$$

$$\alpha_0 = \frac{\alpha_{xx}+\alpha_{yy}+\alpha_{zz}}{3} \tag{2}$$

$$\Delta\alpha = \sqrt{\frac{(\alpha_{xx}-\alpha_{yy})^2+(\alpha_{yy}-\alpha_{zz})^2+(\alpha_{zz}-\alpha_{xx})^2+6(\alpha_{xy}^2+\alpha_{xz}^2+\alpha_{zy}^2)}{2}} \tag{3}$$

$$\beta_x = \beta_{xxx} + \beta_{xyy} + \beta_{xzz} \quad (4)$$

$$\beta_y = \beta_{yyy} + \beta_{xxy} + \beta_{yzz} \quad (5)$$

$$\beta_z = \beta_{zzz} + \beta_{xxz} + \beta_{yyz} \quad (6)$$

$$\beta_0 = \sqrt{\beta_x^2 + \beta_y^2 + \beta_z^2} \quad (7)$$

$$\gamma = \frac{1}{5}\{\gamma_{xxxx} + \gamma_{yyyy} + \gamma_{zzzz} + 2[\gamma_{xxyy} + \gamma_{xxzz} + \gamma_{yyzz}]\} \quad (8)$$

Even the log file calculated by the Gaussian program for a small compound consisting of about five or six atoms has a very large volume. It would take a researcher a very long time to calculate some properties of the compound by taking the relevant values from this file and using them in equations (Eqs. 1-8). Small research on this subject will reveal the sizes of the log files of the relevant compounds (approximately between 100 – 10.000 KB or over 100.000 in terms of number of lines). Especially when some researchers want to calculate the various properties of different derivatives of a ligand or a large number of compounds formed by a ligand or ligands with different transition metals, the time required for this becomes much longer [15,16]. In addition to wasting time, this will also add possible errors caused by the human factor to the results. It can only be understood whether there is an error in the results obtained by repeating the process. This results in a significant waste of time. For this reason, the ZEKA utility program was created by us so that researchers can allocate their valuable time to new research topics.

All values calculated from the equations for the compounds are expressed in atomic units (au). These calculated values are converted into electrostatic units (esu) by multiplying them with appropriate coefficients [17,18]. The ZEKA utility simultaneously performs the unit conversions and presents the results in both systems.

2.2. Promotion and use of the ZEKA utility

ZEKA program is a utility that calculates and presents various properties of a compound by using the data calculated and presented by various versions of the Gaussian program in the relevant formulas. ZEKA program can run on any laptop or desktop computer with Windows operating system. When the needle at the bottom left of the ZEKA utility program is moved to the left, the program screen becomes increasingly transparent. This allows you to see and access any information in the background without leaving the program.

To easily obtain some features of a molecular structure analyzed in the Gaussian program, you can use the ZEKA utility in two ways, depending on the language selection, “TURKISH” or “ENGLISH”. To do this, all you have to do is select the language you want to use in the "ZEKA" utility, which you have made available for operation by performing the necessary operations on your computer (see Fig. 1).

An important tip: It is important that there are no programs running in the background when using the ZEKA utility, so that it can perform its operations smoothly and quickly.

Fig. 1. First boot view of the ZEKA utility program.

3. Results and discussion

If your ZEKA utility program language selection is English, it will turn into a new window as seen in the picture below (Fig. 2).

Fig. 2. View of the ZEKA utility program after selecting the user language as English.

When you select the log extension file of the compound you want to analyze among your Gaussian data, the appearance of the ZEKA utility is as shown in Fig. 3. If the selected log file is a file created by a higher version program such as Gaussian 09 or Gaussian 16, a green mark will appear inside the "SELECT LOG FILE" button. If the selected log file is a file created by a lower version program such as Gaussian 03, this green mark will not appear (see Fig. 3).

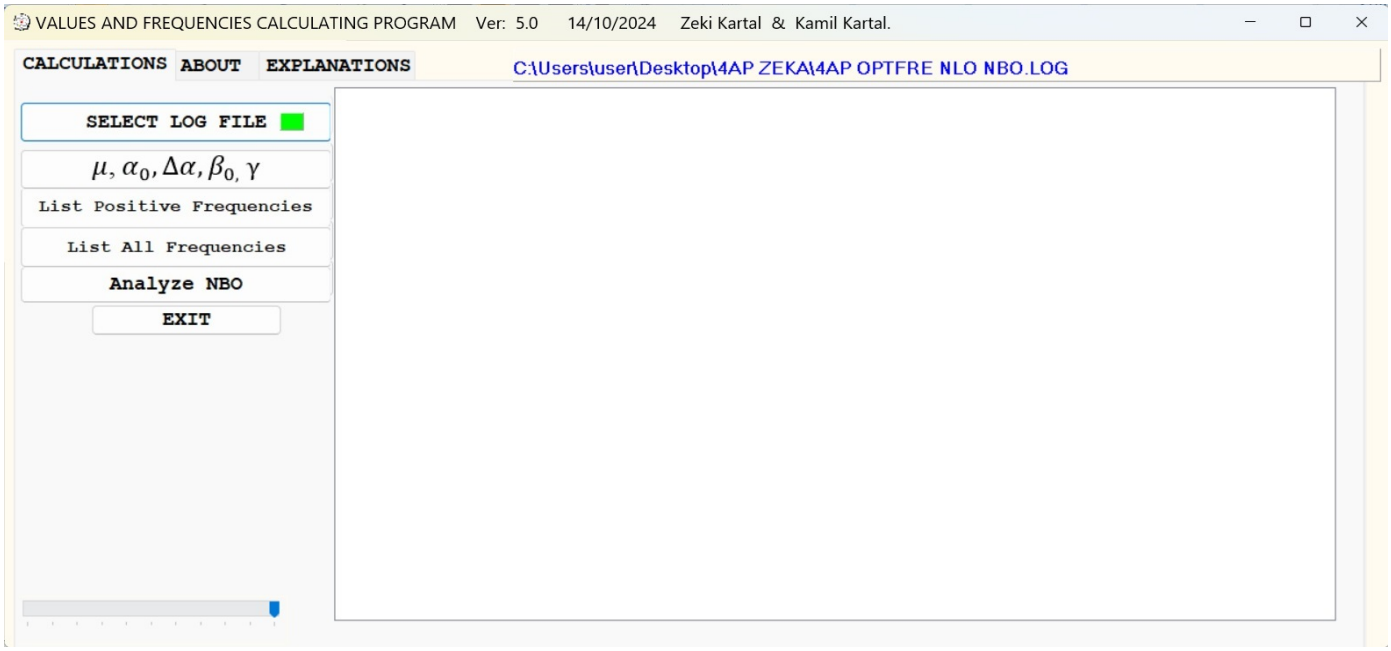

Fig. 3. View of the ZEKA utility after selecting the relevant log file.

3.1. Calculating the NLO values of a compound.

The ZEKA utility automatically displays in a window on the screen, at the moment a button is pressed for any task, the total number of lines in the relevant log file, the start and end times of the operation, the time taken to perform the operation and the number of operations performed.

When you ask the ZEKA utility to calculate the NLO values of the compound you are interested in (that is, when you touch the

button on which the μ, α_0, Δα, β_0 and γ values are written), the ZEKA utility lists the values calculated for all steps using the data in the log file of the relevant compound. Which of the values listed by the ZEKA utility will be taken will be found with the help of the values in the chk file of the relevant compound. When the relevant compound's chk file is opened in GaussView, the dipole moment value in the "Gaussian Calculation Summary" section of the "Results" tab seen in GaussView and the matching dipole moment value calculated by the ZEKA utility are found. The calculated values in the step where the matching dipole moment value is found are the correct values sought. Another benefit of these ranked values is that they help us understand how some of the properties of the compound change as its energy changes.

To better understand the use of the ZEKA utility, the calculation procedures for the 4-aminopyridine (4AP) ligand molecule [9,10 and 19,20], which we use in many of our studies, are given as examples in Figures (4-7). The GaussView image of the chk file created by the Gaussian program for the 4AP molecule is given in Fig. 4. Here, the dipole moment value of the 4AP molecule is seen as 4.017742 Debye. This value is found as 4.0177 Debye in the document calculated by the ZEKA utility. When the relative error value resulting from the representation of the relevant dipole moment value with only two different decimal places is calculated, it is seen that the result is 00105%. This result is also at a level that can be neglected within scientific limits. The all values in that step where this dipole moment value is located are the real values sought for the 4AP molecule. As can be seen from Fig. 5, the NLO values of the relevant compound calculated by the ZEKA utility are given in both atomic units (au) and electrostatic units (esu).

Then, the ZEKA utility will ask you to specify a file name to save the results as a docx file into the relevant file (Fig. 5). When you specify the file name, the results will be saved as a docx file into the relevant file. If desired and if the operating system on your computer is suitable, this docx file can be saved too in PDF format with the same name by clicking the PDF button seen under the analysis labels.

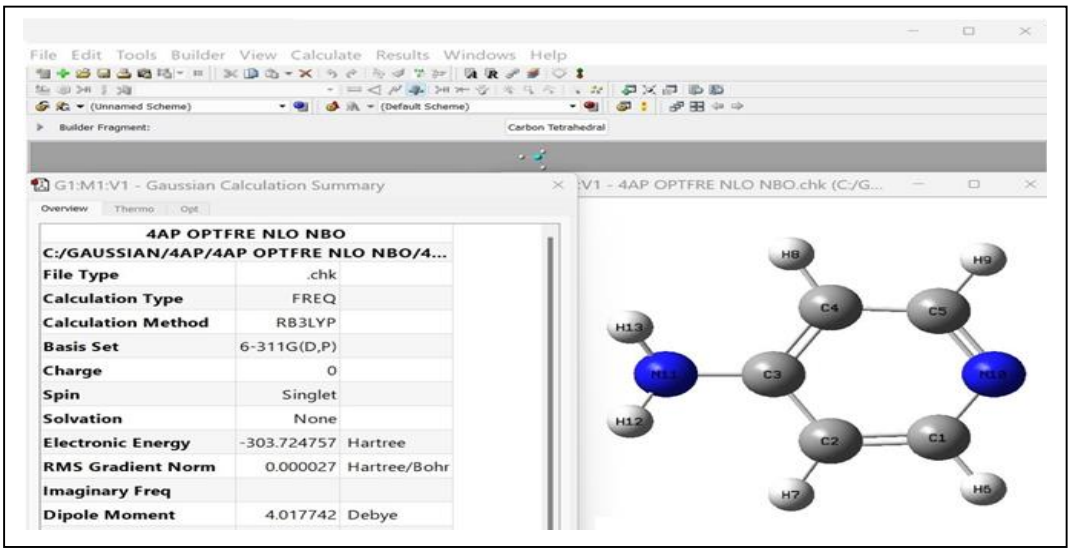

Fig. 4. The image of the chk file created by the Gaussian program for the 4AP molecule in GaussView.

The point that program users should pay attention to here is that the scientific notation of (esu) units is ($\times 10^{-30}$) or similar.

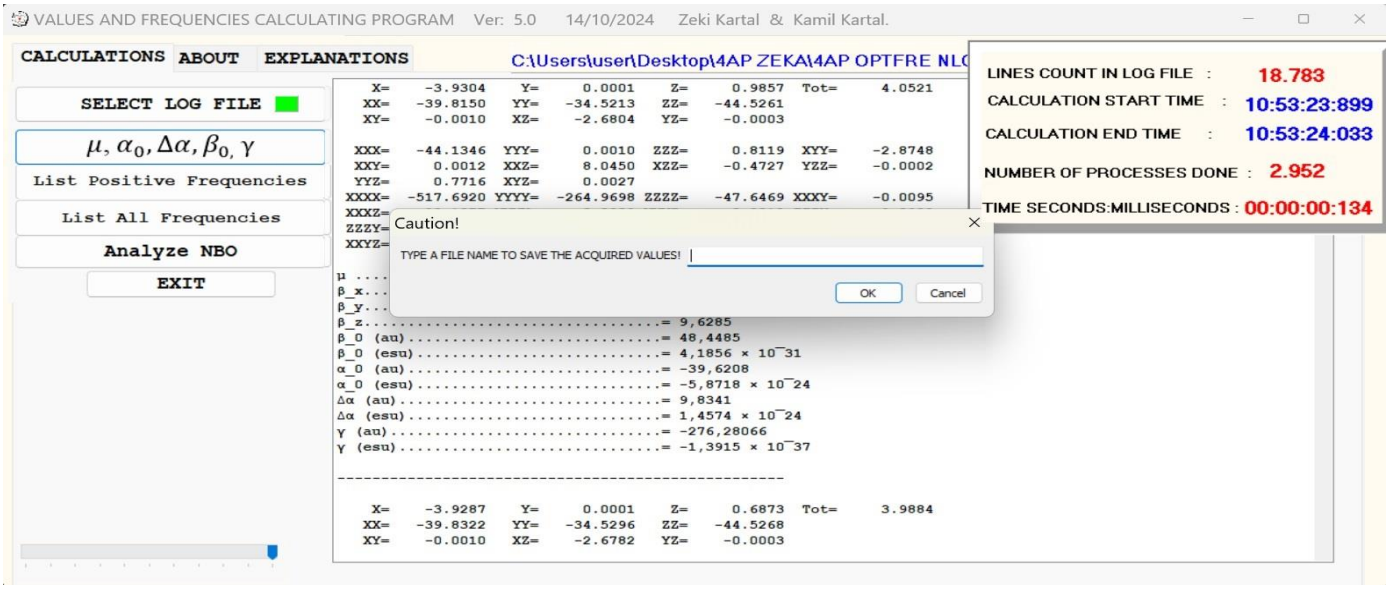

Fig. 5. View of the ZEKA utility after calculating the NLO values of the compound of interest.

The magnetic moment and NLO values obtained by the ZEKA utility for the 4AP molecule using the values in the .log file generated by the Gaussian program are given in Table 1 in terms of both (au) and (esu) values.

Table 1. Magnetic moment and NLO values obtained by the ZEKA utility for the 4AP molecule.

Symbols	In (au) unit	Symbols	In (au) unit	In (esu) unit
μ	4.0177 D	β_0	48.2372	4.1673×10^{-31}
$\boldsymbol{\beta_x}$	-47.432	α_0	-39.6249	-5.8724×10^{-24}
$\boldsymbol{\beta_y}$	0.002	$\Delta\alpha$	9.8302	1.4568×10^{-24}
$\boldsymbol{\beta_z}$	8.7772	γ	-276.33848	-1.3918×10^{-37}

Similar processes will be repeated to perform vibration (IR and Raman) frequencies (Fig. 6) and natural bond analysis (NBO) (Fig. 7) of the same compound.

3.2. Calculating the vibration (IR and Raman) values of a compound.

When some properties of a molecular structure are to be calculated with the Gaussian program, if the molecular structure is not optimized enough or if the appropriate basis set is not selected for the calculation, some vibration frequencies of that molecular structure may take negative values. If desired, only positive frequencies or all frequencies, both positive and negative, of the molecule of interest will be calculated. The calculated vibration frequencies along with the IR intensities and Raman activity values of the relevant molecule are listed by the ZEKA utility from the largest vibration to the smallest (Fig. 6).

When the "List all frequencies" button is used for a molecular structure, the ZEKA utility will warn "No negative frequency values found" if the molecular structure is fully optimized and the appropriate calculation basis set is selected.

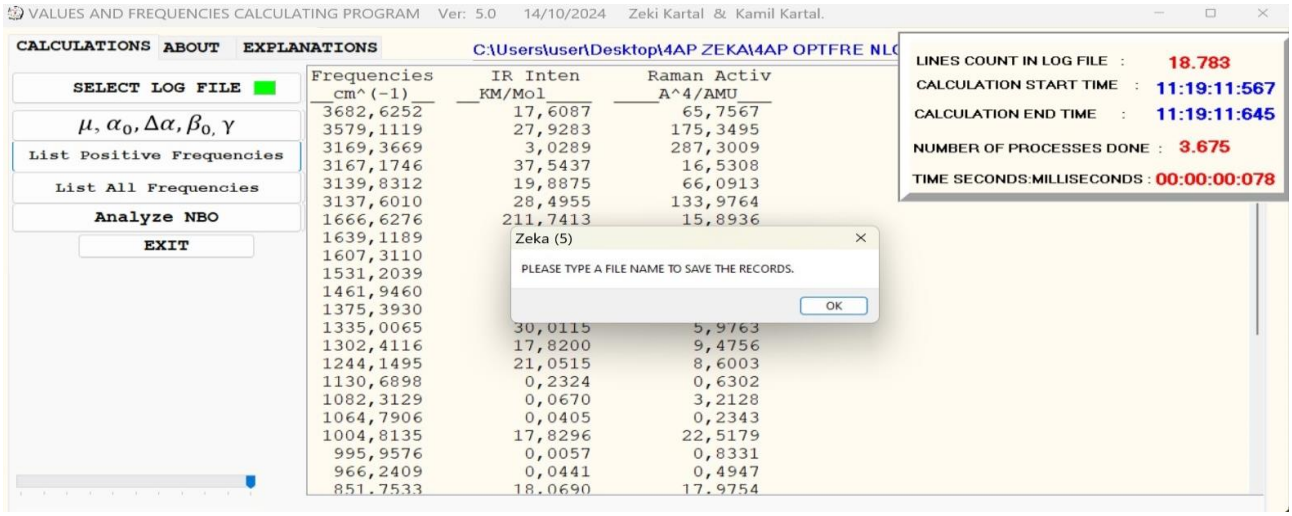

Fig. 6. View of the ZEKA utility after calculating the vibration frequencies of the compound of interest.

The values of vibrational frequencies in the .log file calculated by the Gaussian program were tabulated for the 4AP molecule by the ZEKA utility (see Table 2). In this table, the IR and Raman frequencies (cm^{-1}), IR intensities (KM/Mol) and Raman activities (A^4/AMU) are in units.

Table 2. Table of vibration frequency values arranged by the ZEKA utility for the 4AP molecule. The units of frequencies, IR intensities and Raman activities are (cm^{-1}), (KM/Mol) and (A^4/AMU), respectively.

Frequencies	IR intensities	Raman activities	Frequencies	IR intensities	Raman activities
3682.6252	17.6087	65.7567	1082.3129	0.067	3.2128
3579.1119	27.9283	175.3495	1064.7906	0.0405	0.2343
3169.3669	3.0289	287.3009	1004.8135	17.8296	22.5179
3167.1746	37.5437	16.5308	995.9576	0.0057	0.8331
3139.8312	19.8875	66.0913	966.2409	0.0441	0.4947
3137.601	28.4955	133.9764	851.7533	18.069	17.9754
1666.6276	211.7413	15.8936	840.5563	0.0702	1.3705
1639.1189	95.402	7.7507	822.6253	53.0769	1.8792
3682.6252	17.6087	65.7567	749.6183	0.278	0.1587
3579.1119	27.9283	175.3495	684.7527	0.0531	5.2105
1607.311	31.7898	0.6878	544.8463	18.3842	1.3007
1531.2039	34.6126	4.0246	532.0932	6.9096	5.932
1461.946	11.8774	1.6015	473.2431	324.8051	2.0192
1375.393	0.1127	1.232	394.8566	0.0092	0.0173
1335.0065	30.0115	5.9763	384.3669	0.5189	1.0215
1302.4116	17.82	9.4756	356.4313	14.245	0.6391
1244.1495	21.0515	8.6003	218.2846	1.5046	0.2216
1130.6898	0.2324	0.6302			

3.3. Calculating the NBO values of a compound.

The magnitude of the interaction energy between electron donor and electron acceptor parts in a molecular structure indicates the intensity of the interaction in that structure and is shown with the symbol $E^{(2)}$. The Gaussian program calculates the transitions of a compound separately for each different part of that compound. In the NBO analysis of a compound, the ZEKA utility lists all transition values of that compound from largest to smallest according to the $E^{(2)}$ energy value (Fig. 7). By taking the desired parts from this table, the parts that need to be drawn attention to in the study can be further emphasized.

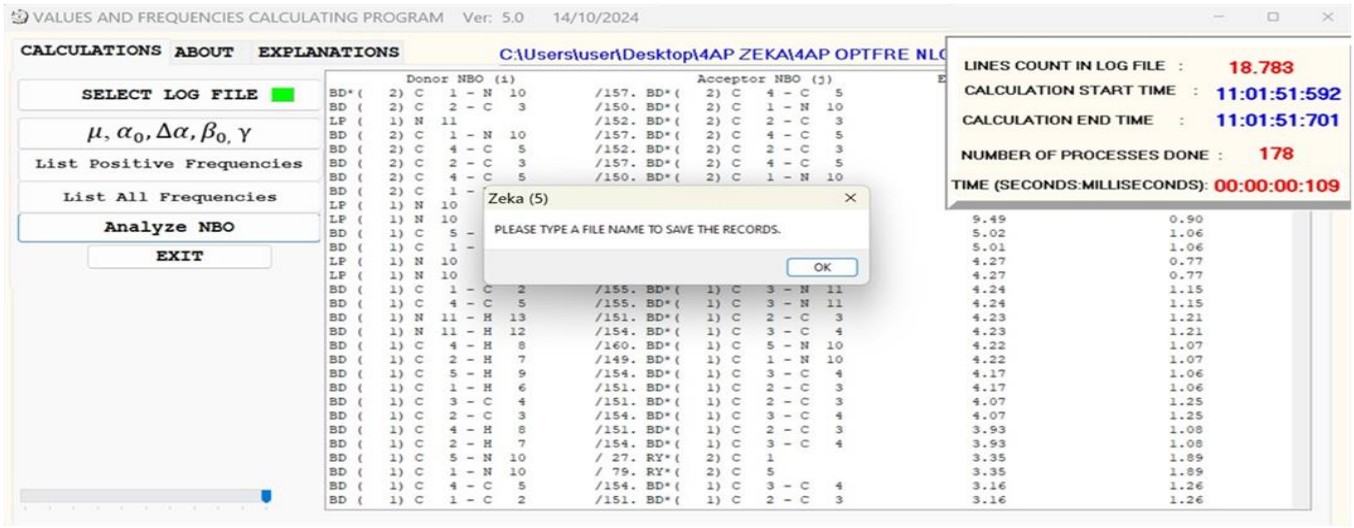

Fig. 7. View of the ZEKA utility after performing the NBO analysis of the compound of interest.

Both the results of the vibration frequencies and the NBO analysis were recorded in Excel table format by the ZEKA utility for easier conversion into tables by users. There are a total of 174 NBO transitions with different stabilization energies [$E^{(2)}$] calculated by the Gaussian program for the 4AP ligand molecule. The first ten NBO analysis results of the 4AP ligand molecule are listed in Table 3, sorted from largest to smallest, for the purpose of example.

Table 3. Ranking of the first ten values of the stabilization energy of the 4AP molecule by the ZEKA utility from largest to smallest.

Donor NBO(i)	Acceptor NBO(j)	$E^{(2)}$ [a] kcal/mol	E(j)-E(i) [b] (a.u.)	F(i,j) [c] (a.u.)
BD* (2) [d] C1 - N10	BD*(2) C4 - C5	221.43	0.01	0.08
BD (2) C2 - C3	BD*(2) C1 - N10	32.87	0.27	0.085
LP (1) N11	BD*(2) C2 - C3	32.45	0.32	0.096
BD (2) C1 - N10	BD*(2) C4 - C5	29.53	0.32	0.087
BD (2) C4 - C5	BD*(2) C2 - C3	24.93	0.28	0.077
BD (2) C2 - C3	BD*(2) C4 - C5	13.98	0.29	0.058
BD (2) C4 - C5	BD*(2) C1 - N10	13.12	0.27	0.055
BD (2) C1 - N10	BD*(2) C2 - C3	11.47	0.31	0.055
LP (1) N10	BD*(1) C4 - C5	9.49	0.9	0.084
LP (1) N10	BD*(1) C1 - C2	9.49	0.9	0.084

[a] $E^{(2)}$: stabilization energy, [b] Energy difference between i and j NBO orbitals, [c] F(i,j) is the Fock matrix elements, [d] (*) indicates anti-bonding, LP (A) is a valence lone pair orbital.

The accuracy and consistency of the all results obtained by the ZEKA utility have been confirmed by repeated calculations of the same results at different times by us and other people.

If it assumes that 30 minutes are required for each calculation step, it is seen that the time that should be spent on this part of an average article is approximately three or four hours. This situation shows how important the ZEKA utility is for a researcher in terms of using time effectively.

4. Conclusions

The biggest deficiency of people or groups doing scientific research is that they cannot spend enough time on the subjects they are working on. Because there are many research subjects today and the number of these subjects is increasing at a dizzying pace every day. In this case, researchers spend their valuable and limited time on subjects that can be solved in other ways. These expenditures are a great loss for the future of science. The ZEKA utility was prepared to save time for researchers working on molecular mechanics calculations theoretically or experimentally so that they can use it on new research topics. A problem can be solved by a human. The time required for this is a few hours. The same problem can be solved by ZEKA utility. The time required for this is a few hundred milliseconds (ms). When the times spent by humans and the ZEKA utility to solve the same problem are compared with each other, the importance of using the ZEKA utility becomes apparently. In future versions of the ZEKA utility, it is planned to add some properties obtained from the HOMO and LUMO states of the relevant compounds, some values of their thermochemical properties, and examinations of UV-visible region and NMR spectroscopic values. In addition, studies will be

carried out to make the program more functional in line with the suggestions or new requests of the researchers who use this ZEKA utility program.

Researchers who want to use the ZEKA utility can contact via e-mail and use it after completing the necessary procedures. Valuable researchers who use the ZEKA utility are requested to cite this article as a reference.

Acknowledgement

As the authors, we would like to express our greatest gratitude to our parents and all our teachers who provided us with this opportunity to deliver the ZEKA utility to the users.

Author contribution statement

The authors contributed equally to the preparation of this article.
Zeki Kartal: Research, Writing–review and editing, original draft.
Kamil Kartal: Research, program design, program creation, and program development.

References

[1] D. C. Young, *Computational Chemistry*. Wiley-Interscience, 2001, Appendix A. A.3.1 pp. 341, AMPAC, doi: 10.1002/0471220655.app1.

[2] S. J. Clark *et al.*, "First principles methods using CASTEP," *Z. Kristallog.*, vol. 220, no. 5-6, pp. 567-570, 2005, doi: 10.1524/zkri.220.5.567.65075.

[3] R. Dovesi *et al*., "Quantum-mechanical condensed matter simulations with crystal," *WIREs Comput. Mol. Sci.*, vol. 8, no. 4, 2018, doi: 10.1002/wcms.1360.

[4] G. M. J. Barca *et al*., "Recent developments in the general atomic and molecular electronic structure system," *J. Chem. Phys.*, vol. 152, no. 15, pp. 154102, 2020, doi: 10.1063/5.0005188.

[5] M. J. Frisch *et al.*, Gaussian 03 Revision D.01. Gaussian. Inc., Wallingford CT (2004).

[6] J. J. Stewart, "MOPAC: A semiempirical molecular orbital program." *J. Comput. Aided Mol. Des.*, vol. 4. no. 1, pp. 1-105, 1990, doi:10.1007/BF00128336.

[7] A. García *et al*., "Siesta: Recent developments and applications." *J. Chem. Phys.* vol. 152, no. 20, 2020. 204108, doi:10.1063/5.0005077.

[8] D. C. Young, *Computational Chemistry*, Wiley-Interscience, 2001, Appendix A. A. 1.6 pp 330, Spartan, doi: 10.1002/0471220655.app1.

[9] Z. Kartal and O. Şahin, "Synthesis. X-ray crystallography characterization and DFT theoretical studies of a new metal compound $[CdCl_2(4\text{-aminopyridine})_2]_n$," *J. Mol. Struct.*, vol. 1243, 2020, 130720, doi:10.1016/j.molstruc.2021.130720.

[10] Z. Kartal and O. Şahin, "Synthesis of two Hofmann type and Hofmann-type-like compounds in crystal form from 4-aminopyridine and their characterizations by various methods," *J. Mol. Struct.*, vol. 1252, 2022, 132088, doi: 10.1016/j.molstruc.2021.132088.

[11] Z. Kartal and Z. S. Şahin, "Synthesis and characterization of two new Hofmann-Type-Like compounds from some alkali metal atoms and glycine anhydride," *JOTCSA*, vol. 11, no. 1, pp. 125-36, 2024, doi: 10.18596/jotcsa.1368425.

[12] Z. Kartal and Z. S. Şahin, "Crystal structure and Hirshfeld surface analysis of a heterometallic Hofmann-type-like compound," *Sinop Univ. J. Nat. Sci.*, vol. 9, no. 1, pp. 72-95, 2024, doi: 10.33484/sinopfbd.1370598.

[13] D. A. Kleinman, "Nonlinear Dielectric Polarization in Optical Media," *Phys. Rev.*, vol. 126, no. 6, pp. 1977-1979, 1962, doi: 10.1103/PhysRev.126.1977.

[14] H. A. Kurtz D. S. Dudis, "Quantum Mechanical Methods for Predicting Nonlinear Optical Properties," *Reviews in Computational Chemistry*, vol. 12, K. B. Lipkowitz. D. B. Boyd. Ed., New York. USA: VCH Publishers, 1998, pp 241-279.

[15] M. G. Vivas D. L. da Silva, C. R. Mendonca, L. De Boni, "Chapter 8 - First-order hyperpolarizability of organic molecules: hyper-Rayleigh scattering and applications." *Molecular and Laser Spectroscopy*. V.P. Gupta. Yukihiro Ozaki. Ed., Elsevier, 2020, pp. 275-314, doi: 10.1016/B978-0-12-818870-5.00008-3.

[16] Ö. Tamer *et al*., "First and second order hyperpolarizabilities of flavonol derivatives: A density functional theory study," *Spectrochim. Acta. Part A*, 283, 2022, 121728, doi: 10.1016/j.saa.2022.121728.

[17] A. B. Ahmed, H. Feki, Y. Abid, H. Boughzala, A. Mlayah, "Structural. vibrational and theoretical studies of l-histidine bromide," *J. Mol. Struct.*, vol. 888, no. (1-3), pp. 180–186, 2008, doi:10.1016/j.molstruc.2007.11.056.

[18] M. Nakano *et al*., "Second hyperpolarizability (gamma) of singlet diradical system: dependence of gamma on the diradical character," *J Phys Chem A*., vol. 109, no. 5, pp. 885-891, 2005, doi:10.1021/jp046322x.

[19] Z. Kartal and O. Şahin, "Synthesis, spectroscopic, thermal, crystal structure properties and characterization of new Hofmann-type-like clathrates with 4-aminopyridine and water," *Turk. J. Chem.*, vol. 45, no. 3, pp. 616–633, 2021, doi:10.3906/ kim-2011-29.

[20] Z. Kartal and O. Şahin, "The synthesis of heteroleptic cyanometallate aminopyridine complexes and an investigation into their structural properties with various spectroscopic methods." *J. Mol. Struct.*, 2021, 1227, 129514, doi:10.1016/j.molstruc.2020.129514.