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Some aminonitroethylenes and their interactions with each other – A DFT treatment

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Abstract

The main backbone of some explosive materials contains some of aminonitroethylenes in the embedded form such as 1,l -diamino-2,2-dinitroethylene (FOX-7). In the present study, *cis*, *trans* and *geminal* aminonitroethylenes and their mutual composites are considered within the constraints of density functional theory (DFT) mainly at the level of B3LYP/6-311++G(d,p). For the thermo chemical data also some thermo chemical recipes have been employed. At the level of B3LYP/6-311++G(d,p), all of the structures possess exothermic heat of formation values and also have favorable Gibbs free energy of formation values. The calculations reveal that they are electronically stable. Various quantum chemical data have been collected and discussed including UV-VIS spectra.

1. Introduction

1-Amino-2-nitroethylene which possesses push-pull type character is the main backbone of some explosive materials (in embedded form) such as in FOX-7 (1,l -diamino-2,2-dinitroethylene) structure [1,2] or in some dyes as it is or its heteroanalogs [3]. Monoaminomononitroethylenes in the form of *cis*, *trans* and *geminal* (constitutional isomers) isomers have different extents of push-pull resonance effects which dictate various structural properties. Restricted rotation about carbon-carbon double bonds has long been a subject of interest and study [4-8]. However, positioning one or more electron-donating groups (typically amino groups) at one end of the sp^2-sp^2 bond and one or more electron-accepting groups ($-NO_2$, -CN, etc.) at the other end affords a significant decrease in the C=C rotational barrier [l]. The diminution of the C=C rotational barrier in push-pull type ethylenes is a consequence of electronic/resonance effects, steric interactions between the donor and acceptor groups, or a combination of both of these [6-8]. Push-pull type double bonds have long been a subject of interest and study for various purposes [8-12].

Amino and nitro groups have donor and acceptor properties, respectively in terms of classical resonance theory. When they are attached to a double or a triple bond, a polar system may arise depending on the positions of the donor and acceptor groups.

Molecular interactions refer to the attractive or repulsive forces *between* molecules and non-bonded atoms. These interactions can be cohesive (attraction between like substances), adhesive (attraction between different substances), or repulsive. These interactions play crucial roles in fields such as chemistry, biochemistry, biophysics, and materials science, influencing processes like protein folding, drug design, pathogen detection, sensor technology, nanotechnology, separations, gecko feet, and studies related to the origins of life. Known interchangeably as noncovalent interactions, intermolecular interactions, non-bonding interactions, noncovalent forces, and intermolecular forces, these terms all describe the same fundamental phenomena [6].

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Non-covalent interactions can be classified into different categories, such as electrostatic, π-effects, van der Waals forces, and hydrophobic effects [6, 13-18]. Ion-dipole and dipole-dipole interactions depend on the orientations of the dipole. Dipole-induced dipole interactions are important even between molecules with permanent dipoles.

In the present study, mutual interaction of *cis, trans and geminal* aminonitroethylenes are considered within the constraints of density functional theory (DFT).

2. Method of Calculations

In the present study, all the initial optimizations of the structures leading to energy minima have been achieved first by employing MM2 method which is then followed by semi empirical PM3 self consistent fields molecular orbital method [19-21]. Afterwards, the structure optimizations have been achieved within the framework of Hartree-Fock and finally by using density functional theory (DFT) at the level of B3LYP/6-311++G(d,p) [22,23]. Note that the exchange term of B3LYP consists of hybrid Hartree-Fock and local spin density (LSD) exchange functions with Becke's gradient correlation to LSD exchange [24]. The correlation term of B3LYP consists of the Vosko, Wilk, Nusair (VWN3) local correlation functional [25] and Lee, Yang, Parr (LYP) correlation correction functional [26]. In the present study, the normal mode analysis for each structure yielded no imaginary frequencies for the $3N–6$ vibrational degrees of freedom, where N is the number of atoms in the system. This search has indicated that the structure of each molecule considered corresponds to at least a local minimum on the potential energy surface. Furthermore, all the bond lengths have been thoroughly searched in order to find out whether any bond cleavage occurred or not during the geometry optimization process. All these computations were performed by using SPARTAN 06 program [27].

3. Results and Discussion

Any molecule with a dipole moment (or any ion) is surrounded by an electrostatic field. This electrostatic field shifts the electron density (alters the dipole moments) nearby molecules. A permanent dipole is perturbed by an adjacent dipole, thus the polarization changes. Note that the ease with which electron density is shifted by an electronic field is called polarizability. Dipole-induced dipole interactions are important even between molecules with permanent dipoles.

Figure 1 shows the optimized structures and the direction of the dipole moment vectors of the aminonitroethylenes considered where the capital letters C, T and G mean *cis*, *trans* and *geminal* isomers.

In their planar forms, parent isomers are alternant systems isoconjugate with certain even alternant hydrocarbon (even AH) anions [28,29]. Structures C and G (see figure 2) are non-Kekulé and Kekulé [28,29] structures, respectively that have certain numbers of starred (n^*) and unstarred (n^o) positions. A non-Kekulé structure is characterized with $\Delta n \geq 2$ where $\Delta n= n^*-n^o$ [28,30]. According to Dewar, a nitro group should be considered as a nitroso (N=O group) [28]. Although, structures C and T are classified initially as non-Kekule and G as a Kekule' structures, their isoconjugates C' (also T') and G' are odd-alternant hydrocarbon (odd-AH) anions. In those systems, centric perturbations [28,29] by a heteroatom(s) or a substitution of an electron attracting group at the starred position(s) lower both the HOMO and LUMO energy levels at unequal extents. Whereas, electron donors raise up both of the interfrontier molecular orbital energy levels at unequal extents (HOMO and LUMO) [31]. Thus, the interfrontier molecular orbital energy gap (Δε, the LUMO-HOMO energy difference) is dictated by the characteristics of π-electron topology of the system (aminonitroethylenes) presently considered (see the below pages for spectral (UV-VIS) discussion). Note also that NO_2 and NH_2 groups in structure of G are cross conjugated.

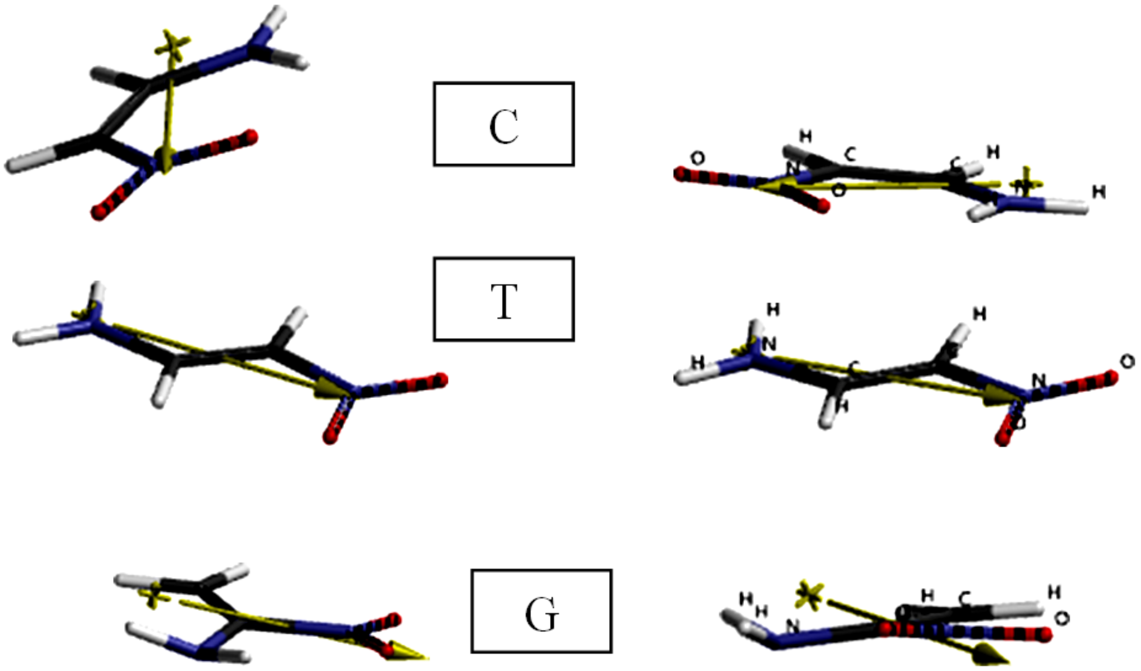


Figure 1. Optimized structures of the aminonitroethylenes considered.

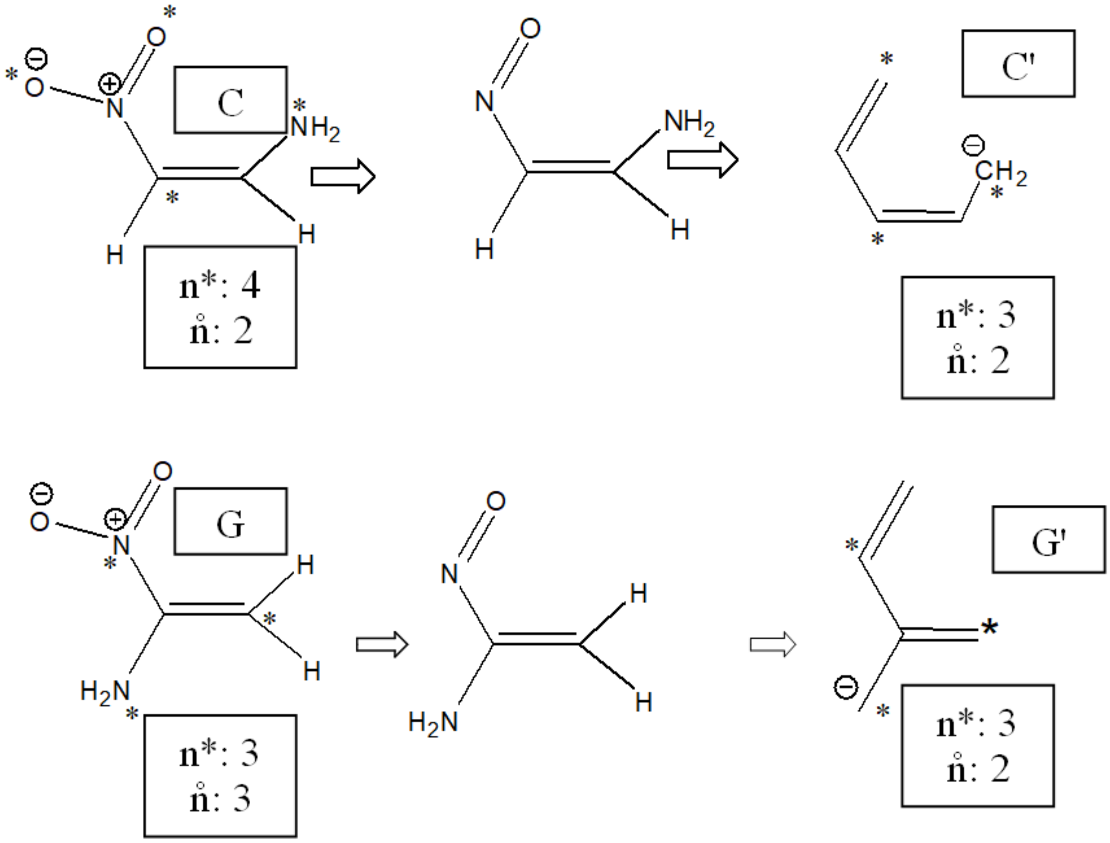


Figure 2. Structures C, G and their isoconjugate alternant hydrocarbon anions.

Figure 3 stands for the composites of aminonitroethylenes which arise from mutual interaction of the parent structures (which are mostly head to tail type).

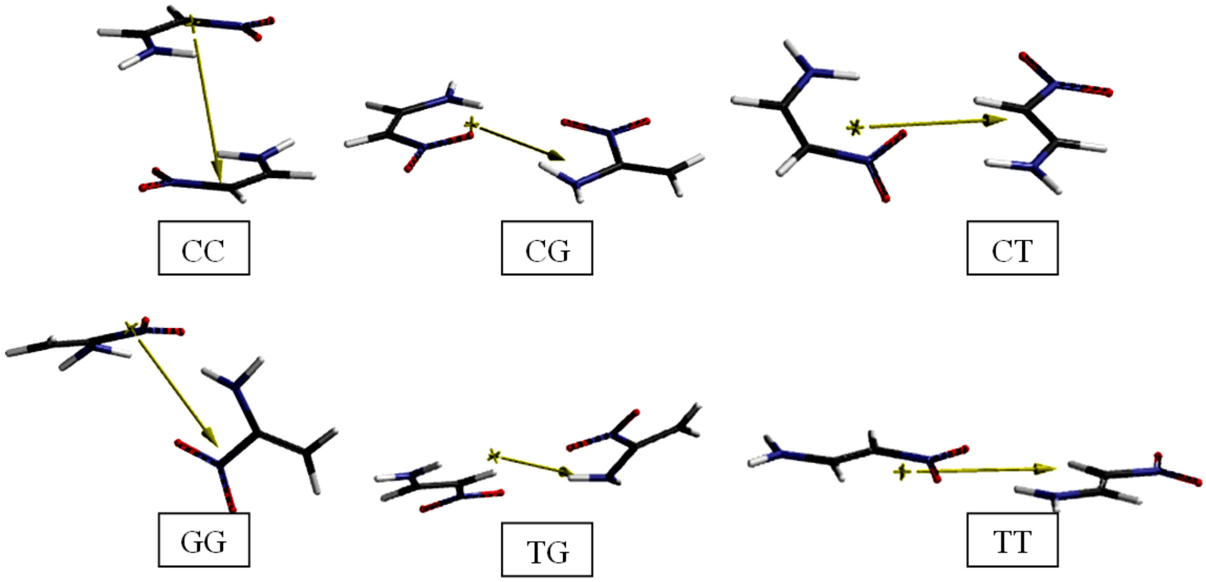


Figure 3. Optimized structures of the aminonitroethylene composites considered.

Note that the parent aminonitroethylenes are constitutional isomers of each other and so do their considered composites.

Table 1 lists some thermo chemical properties of the parent isomers considered. The data reveal that the standard heat of formation (H^o) values of all the parent isomers are exothermic and they are favored according to their G^o (Gibbs free energy of formation) values. The algebraic order of H^o and G^o values are C<T<G. Hence, structure-C has the most exothermic one and possesses the most favorable G^o value.

Table 1. Some thermo chemical properties of the parent isomers considered.

Specie	H^o	S^o (J/mol^o)	G^o
C	-888729.5839	311.22	-888822.3752
T	-888712.7044	321.02	-888808.4153
G	-888690.8653	312.07	-888783.9087

Energies in kJ/mol. B3LYP/6-311++G(d,p) calculations.

Table 2 shows some thermo chemical data for the parent structures considered. The algebraic order of heat of formation energies (gas phase) for the parent compounds is C<T<G so that C is the most and G is the least exothermic structures.

Table 3 shows some energies of the parent isomers considered where E, ZPE and E_C stand for the total electronic energy, zero point vibrational energy and the corrected total electronic energy, respectively. According to the data, they are all electronically stable structures. The stability order based on E_C values is C>T>G.

Table 2. Some thermo chemical data (advanced level) for the parent structures considered.

	Compounds		
Calculation	C	G	T
G3(MP2) H_{298}	-887463.9585	-887440.3621	-887447.4865
G3(MP2) E_e	-887668.2977	-887642.7823	-887651.0272
G3(MP2) E_o	-887482.0646	-887458.6497	-887466.4294
dH(298)	-887463.9585	-887440.3621	-887447.4865
MP2 total energy	-887668.2977	-887642.7823	-887651.0271

Energies in kJ/mol.

Table 3. Some energies of the parent isomers considered.

Specie	E	ZPE	E_C
C	-888929.00	190.67	-888738.33
T	-888911.30	189.03	-888722.27
G	-888887.13	187.21	-888699.92

Energies in kJ/mol. B3LYP/6-311++G(d,p) level.

Some thermo chemical properties of the composites (they are isomers too) considered are listed in Table 4. All composites are exothermic (H^o) and they are favored according to their G^o (standard Gibbs free energy of formation) values. The algebraic order of H^o and G^o values are CC<CT<TT<CG<TG<GG and CT<CC<TT<CG<TG<GG, respectively.

Table 4. Some thermo chemical properties of the composites considered.

Specie	H^o	S^o (J/mol^o)	G^o
CC	-1777480.177	420.29	-1777605.488
CG	-1777449.052	425.31	-1777575.857
CT	-1777476.861	431.95	-1777605.649
GG	-1777398.395	429.44	-1777526.431
TG	-1777431.148	436.69	-1777561.351
TT	-1777457.241	439.89	-1777588.396

Energies in kJ/mol. B3LYP/6-311++G(d,p) level.

A simplified recipe (T1) based on G3(MP2) and intended to reproduce G3(MP2) heats of formation values (rather than experimental heats) has been developed. It eliminates the QCISD(T)/6-31G(d) energy calculation, the zero point energy calculation and the temperature correction to the enthalpy (ΔH(T)) and replaces the large basis set MP2 energy calculation with dual basis set RI-MP2 calculation where 6-311++G(2df,p) is the large and 6-311G(d) is the small basis set. The T1 calculations use HF/6-31G(d) equilibrium geometries instead of

MP2/6-31(d) geometries in G3(MP2) calculation [27]. On the other hand, semi emprical PM3 calculations also yield the enthalpy of formation data. The PM3 type semi emprical calculations (based on some advanced optimized geometry calculations) could be good alternatives to yield heat of formation values.

Table 5 shows heat of formation data for parent aminonitroethylenes and their mutual composites considered. The PM3//B3LYP/6-311++G(d,p) and T1 calculations yield parallel results to the others (see Tables 1 and 2) for the parent structure but not for the rest. According to the data, (B3LYP/6-311++G(d,p) level) present in Table 6 the composites are all electronically stable structures. The stability order is CC>CT>TT>CG>TG>GG.

Table 5. Heat of formation data for parent aminonitroethylenes and their composites considered.

Specie	PM3//B3LYP/ 6-311++G(d,p)	T1
C	19.197	(20.72)
T	20.248	(37.44)
G	55.707	(43.04)
CC	34.032	(0.61)
CG	60.600	(27.91)
CT	19.217	(19.08)
GG	98.926	(57.71)
TG	60.848	(48.48)
TT	27.727	(37.85)

Energies in kJ/mol.

Table 6. Some energies of the composites considered.

Specie	E	ZPE	E_C
CC	-1777880.00	385.82	-1777494.18
CG	-1777845.86	382.31	-1777463.55
CT	-1777876.06	384.43	-1777491.63
GG	-1777790.71	376.88	-1777413.83
TG	-1777826.52	379.65	-1777446.87
TT	-1777855.77	382.75	-1777473.02

Energies in kJ/mol. B3LYP/6-311++G(d,p) level.

Aqueous and solvation energy (E_{aq} and E_{solv}, respectively) values for the composites considered are tabulated in Table 7. The algebraic order of aqueous and solvation energy values are CT<CC<CG<TT<TG<TG

and CG<TT<CT<CC<TG<GG, respectively. Orientation of the structures and/or groups with respect to each other, thus their hydrogen bond formation possibilities and their stabilities, etc., dictate the orders obtained presently. The solvation energies were calculated by adopting SM5.4/A model [27].

Table 7. Aqueous and solvation energy values for the composites considered.

Specie	E_{aq}	E_{solv}
CC	-1777940.21	-60.215
CG	-1777936.98	-91.124
CT	-1777946.86	-70.798
GG	-1777824.90	-34.186
TG	-1777875.08	-48.562
TT	-1777934.38	-78.609

Energies in kJ/mol. Solvation energy by SM5.4/A model.

Table 8 shows the calculated dipole moment and polarizability values for the species considered. The orders of dipole moments and polarizability values are TT>CT>T>C>G>TG>CG>GG>CC and TT>GG>TG>CT>CG>CC>G>T>C, respectively.

Table 8. Dipole moment and polarizability values for the species considered.

Specie	Dipole moment	Polarizability
C	6.34	46.65
T	7.45	46.68
G	4.19	46.89
CC	0.03	53.12
CG	2.64	53.27
CT	9.18	53.37
GG	2.09	53.44
TG	3.61	53.34
TT	15.68	53.47

Dipole moments in debye units. Polarizabilities in 10^{-30} m^3 units. B3LYP/6-311++G(d,p) level.

Figure 4 displays the electrostatic potential (ESP) charges and ESP maps of the parent aminonitroethylenes considered where negative potential regions reside on red/reddish and positive ones on blue/bluish parts of the maps. Note that the ESP charges are obtained by the program based on a numerical method that generates charges that reproduce the electrostatic potential field from the entire wavefunction [27].

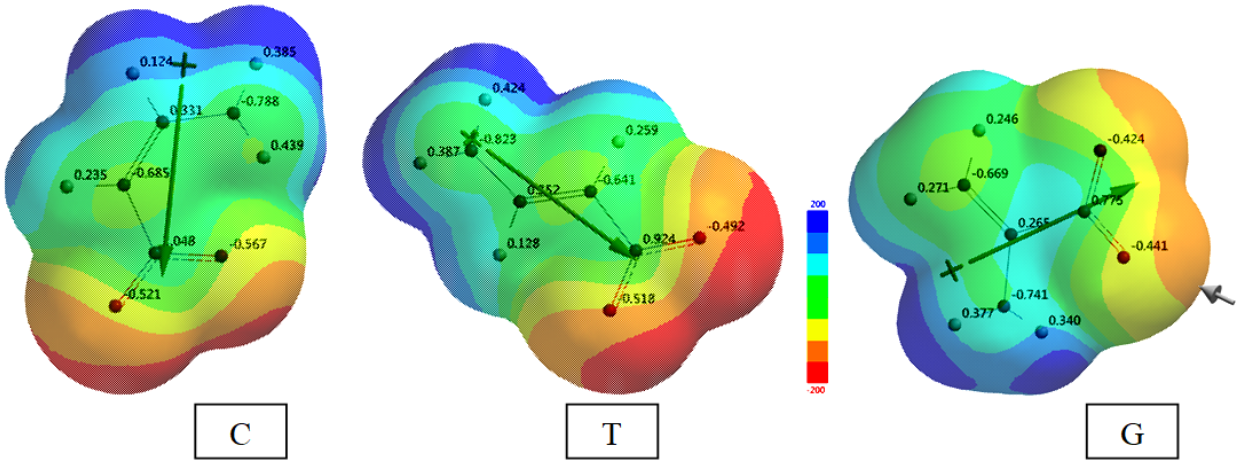
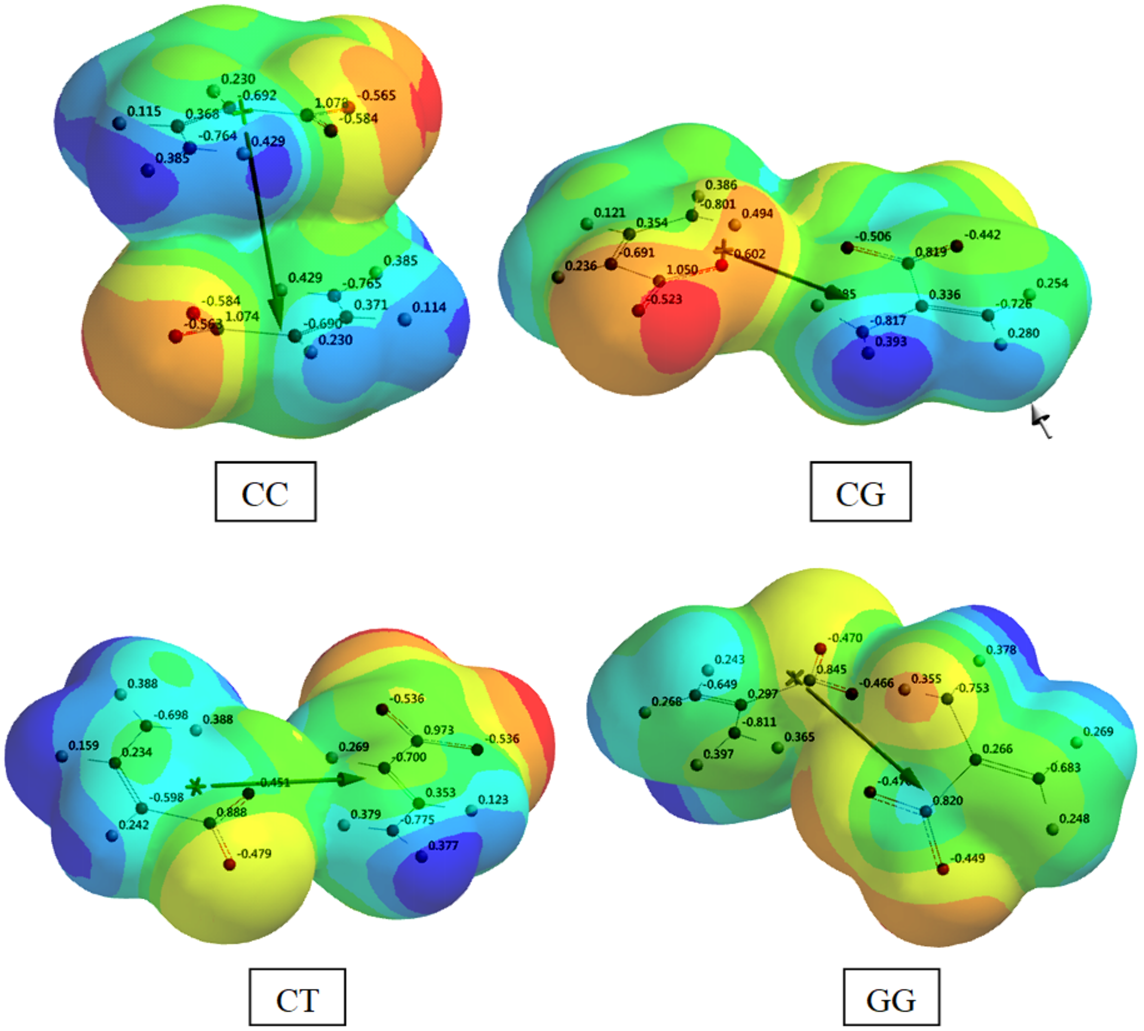


Figure 4. The ESP charges and ESP maps of the parent aminonitroethylenes considered.

Figure 5 shows the ESP charges and ESP maps of the aminonitroethylene composites considered. Note that the structural variations greatly affect the values and locations of the positive and negative charges and the potential regions of the composites.



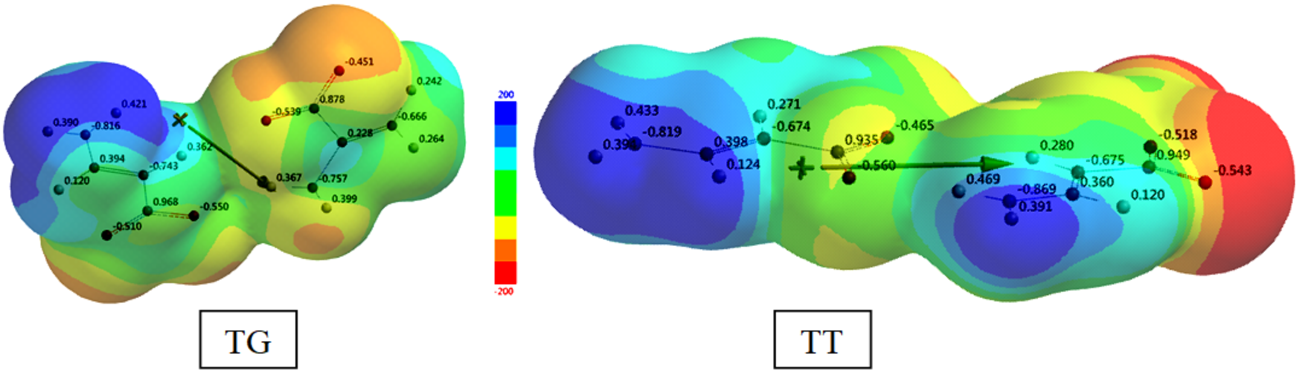
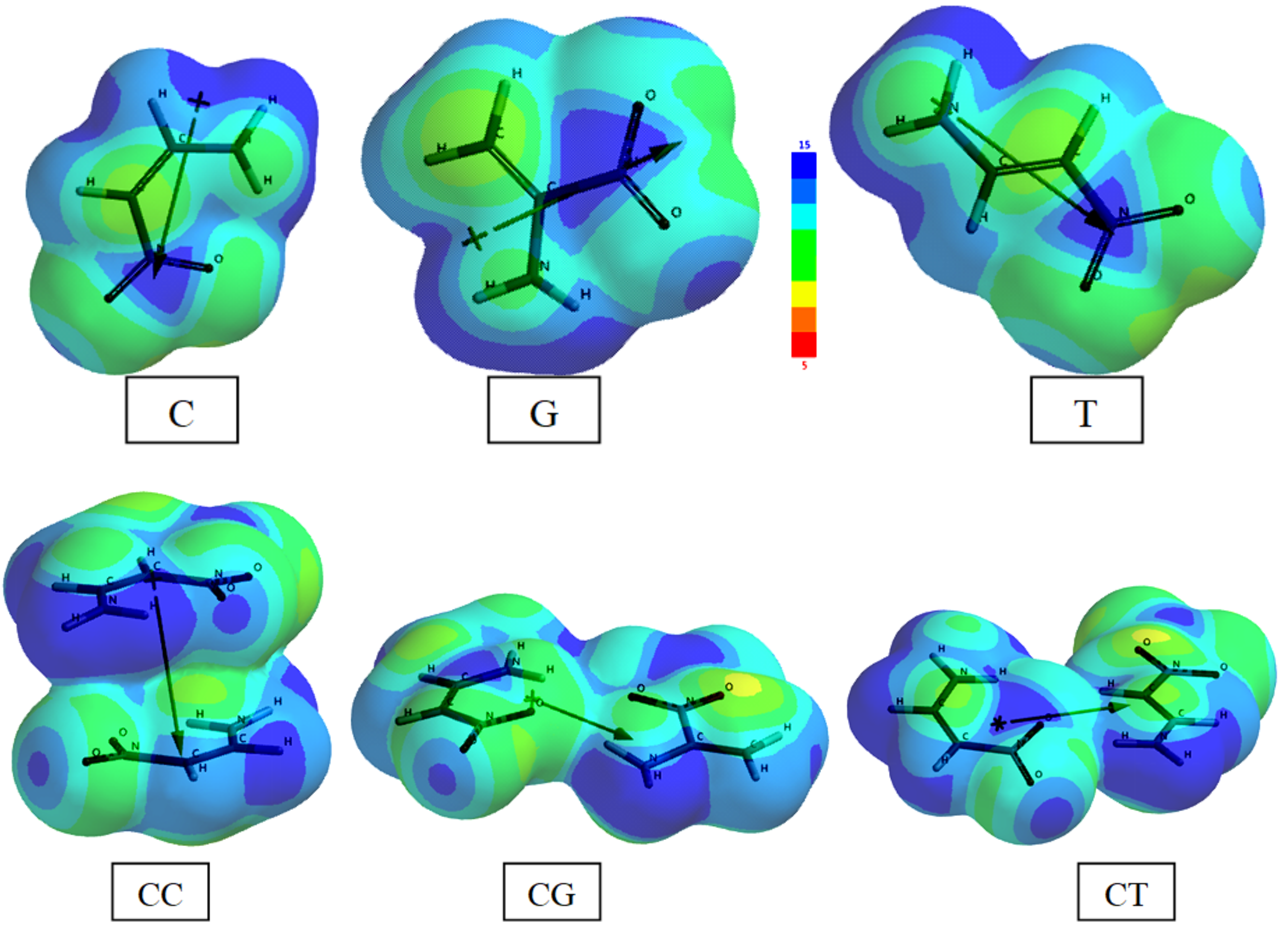
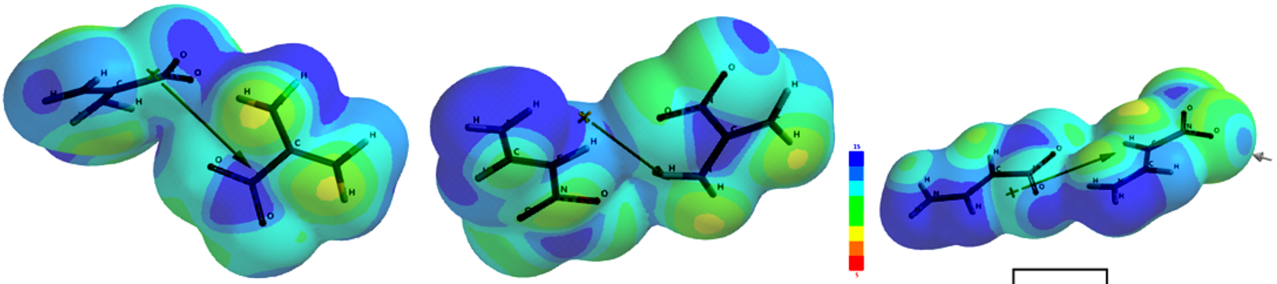


Figure 5. The ESP charges and ESP maps of the aminonitroethylene composites considered.

Figure 6 shows the local ionization potential maps of the species considered where conventionally red/reddish regions (if any exists) on the density surface indicate areas from which electron removal is relatively easy, meaning that they are subject to electrophilic attack. It is worth remembering that the local ionization potential map is a graph of the value of the local ionization potential on an isodensity surface corresponding to a van der Waals surface.

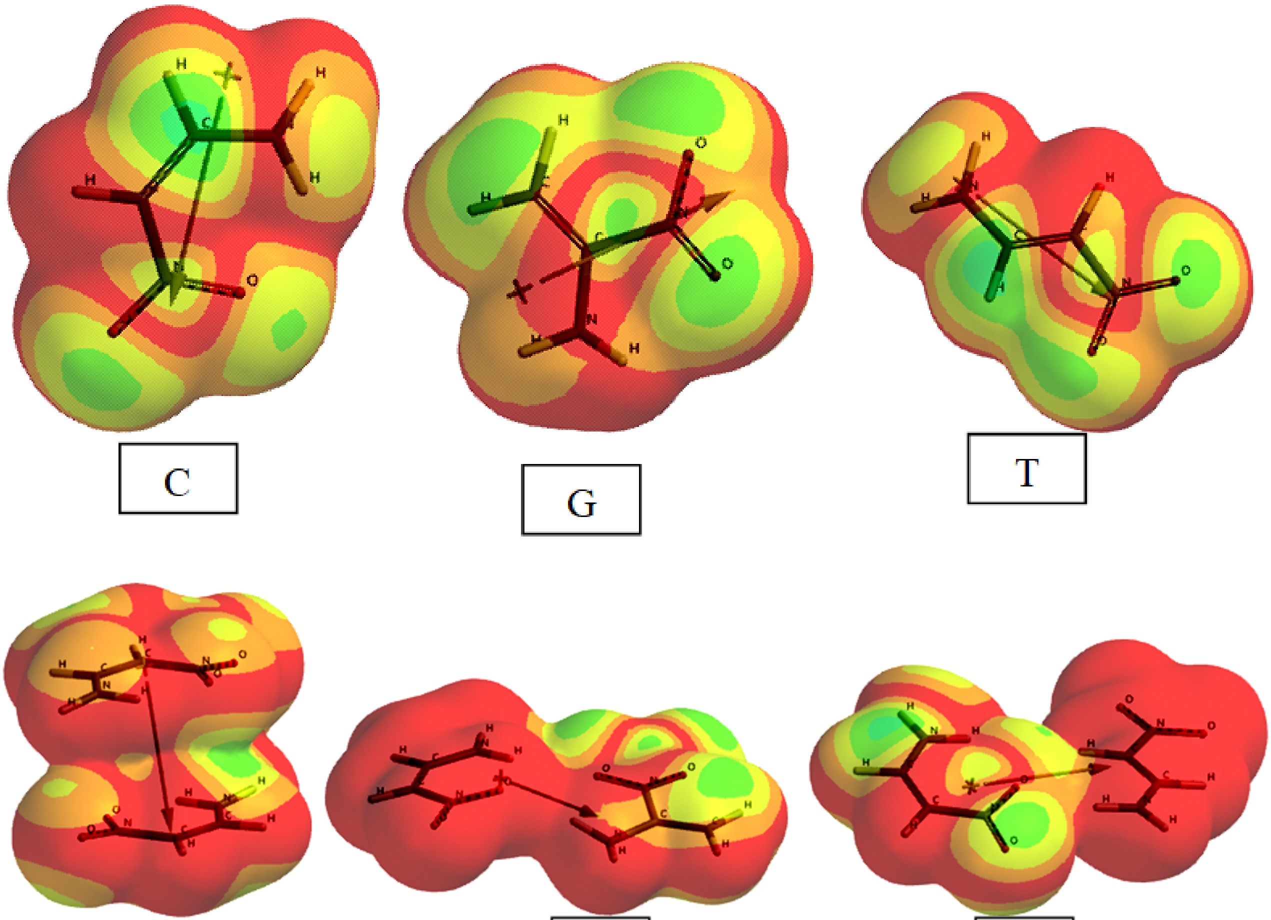




GG TG TT

Figure 6. The local ionization potential maps of the species considered.

The LUMO maps of the isomers considered are displayed in Figure 7. Note that a LUMO map displays the absolute value of the LUMO on the electron density surface. The blue color (if any exists) stands for the maximum value of the LUMO and the red colored region, associates with the minimum value. Note that the LUMO and NEXTLUMO are the major orbitals directing the molecule towards of the attack of nucleophiles [27]. Positions where the greatest LUMO coefficient exists is the most vulnerable site in nucleophilic reactions.



C G T

CC CG CT

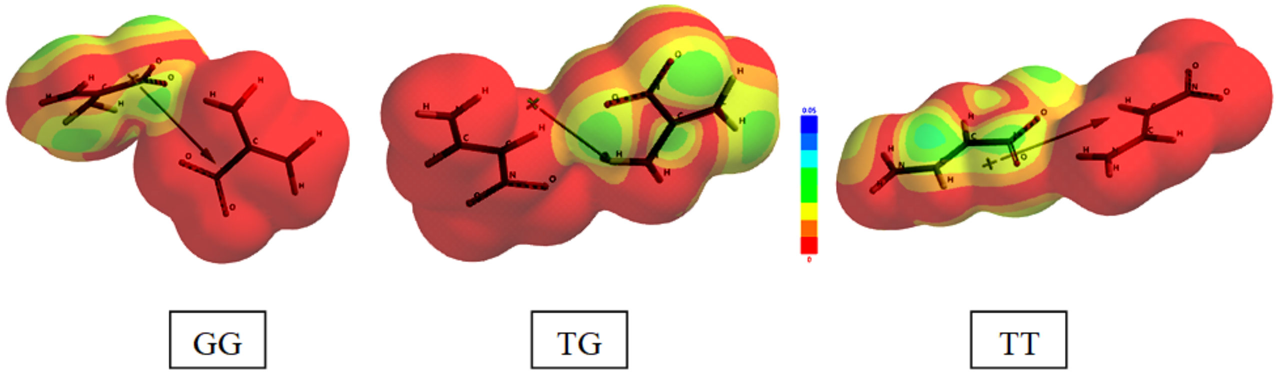


Figure 7. The LUMO maps of the species considered.

Figure 8 displays the bond densities of the aminonitroethylene composites considered. As seen in the figure, there is no bond density between components of the composites, in spite of the fact that some, charge-charge, charge dipole or dipole-dipole interactions between them presumably exist.

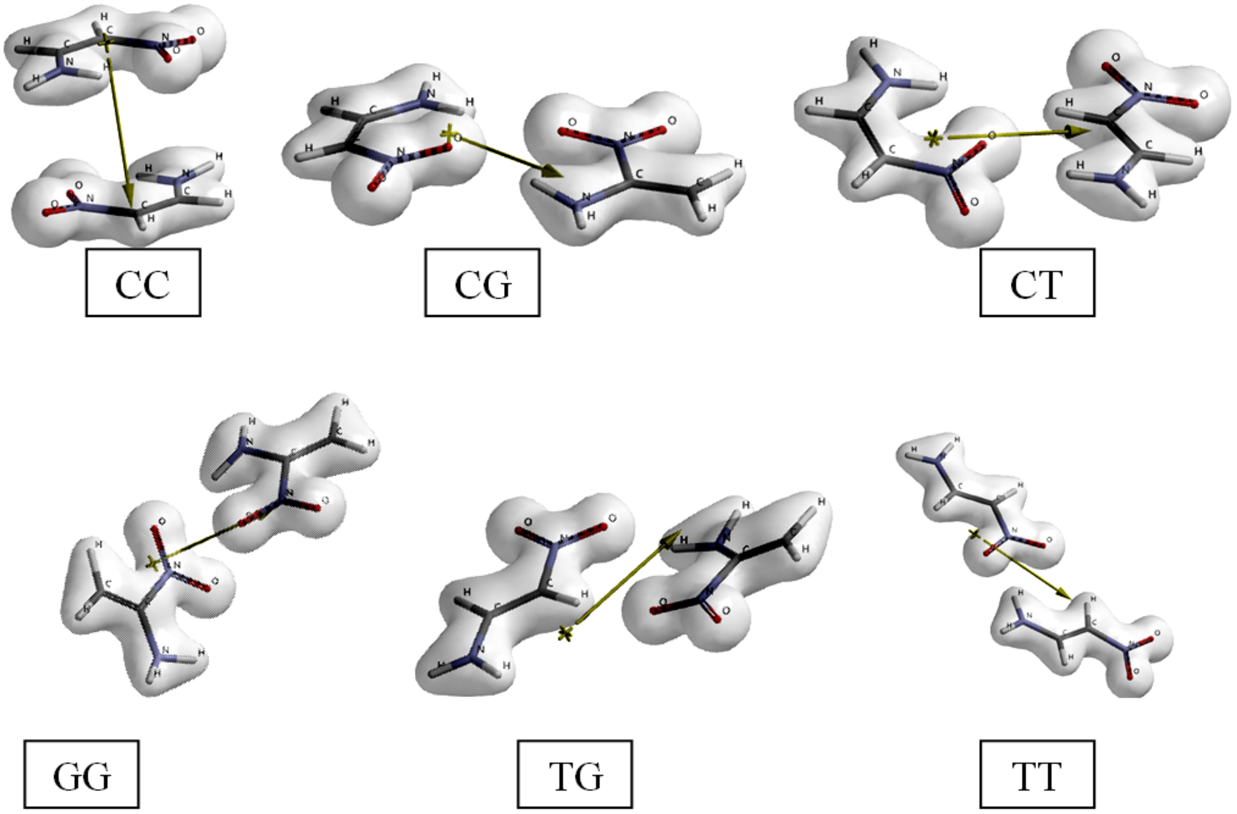


Figure 8. The bond densities of the aminonitroethylene composites considered.

Figure 9 shows some of the orbital energy levels of aminonitroethylenes considered.

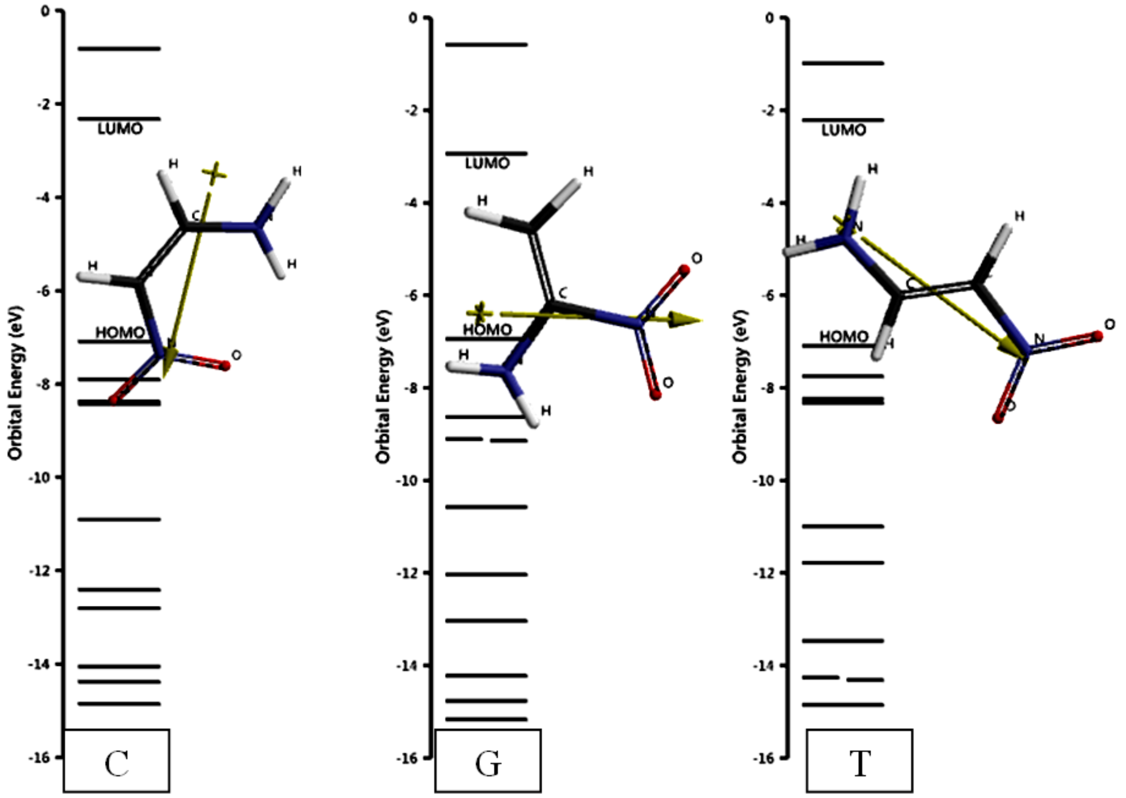
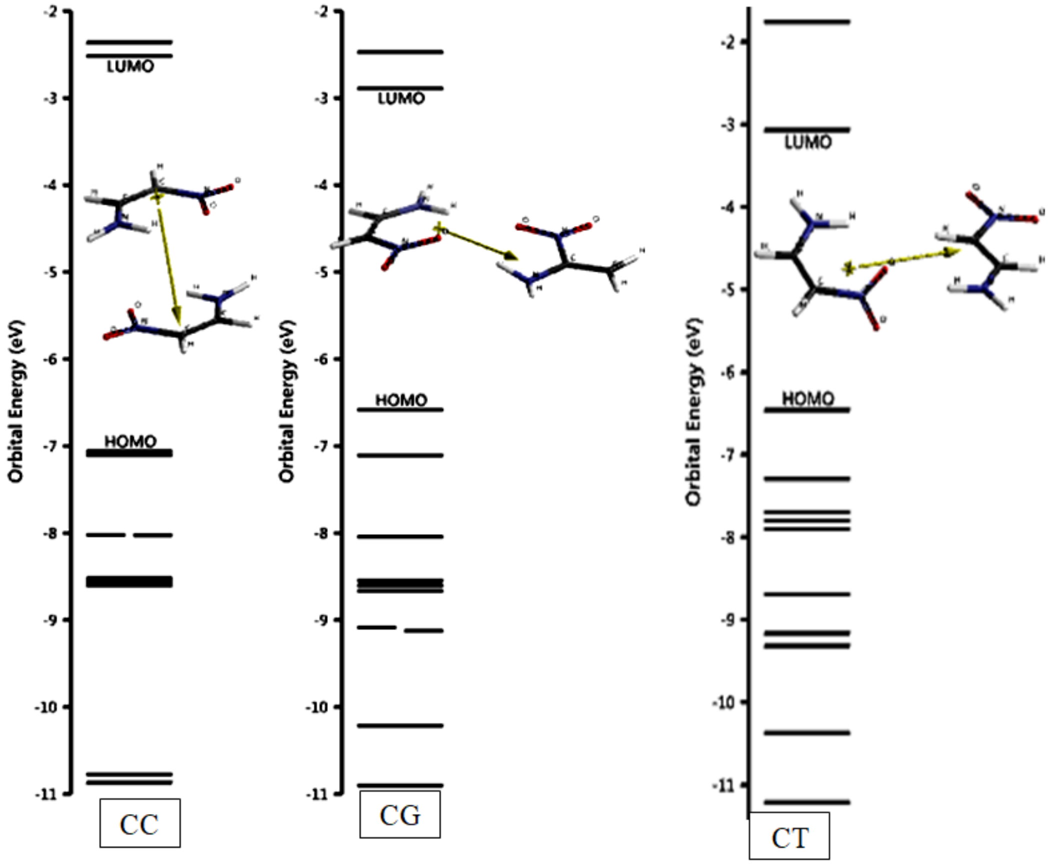


Figure 9. Some of the orbital energy levels of aminonitroethylenes considered.

Figure 10 displays some of the orbital energy levels of aminonitroethylene composites considered.



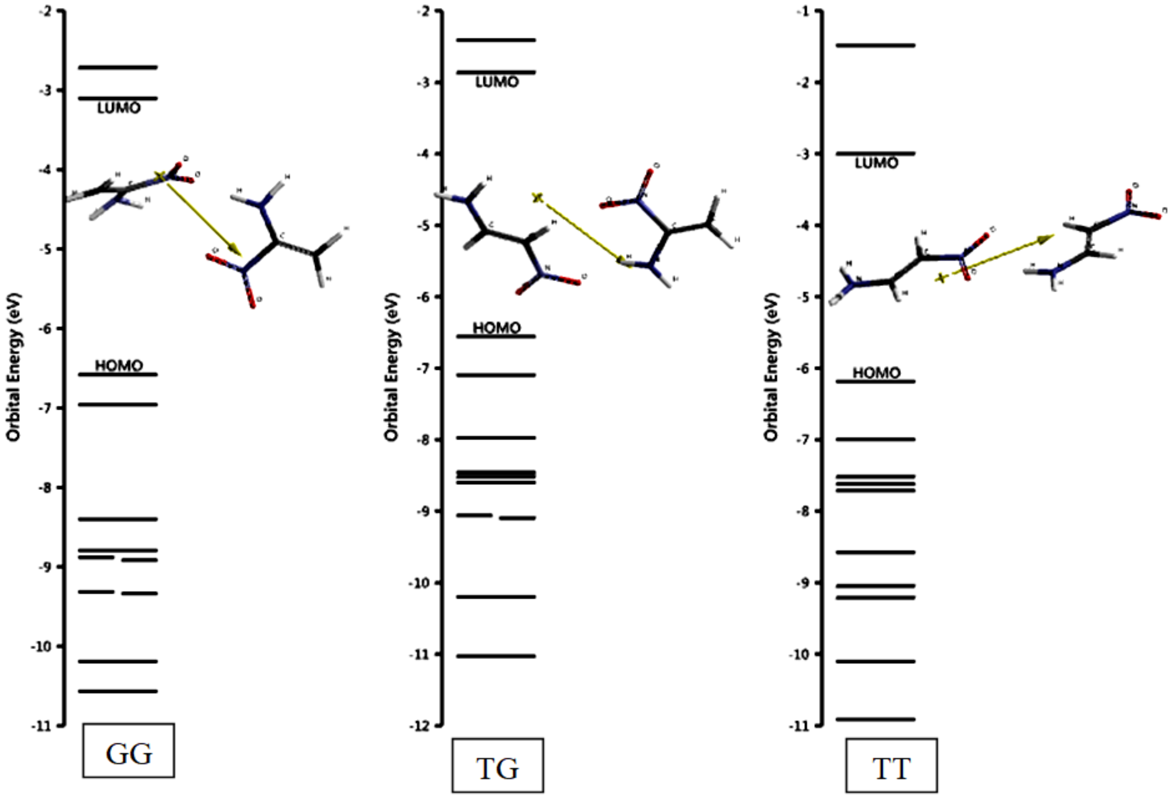


Figure 10. Some of the orbital energy levels of aminonitroethylene composites considered.

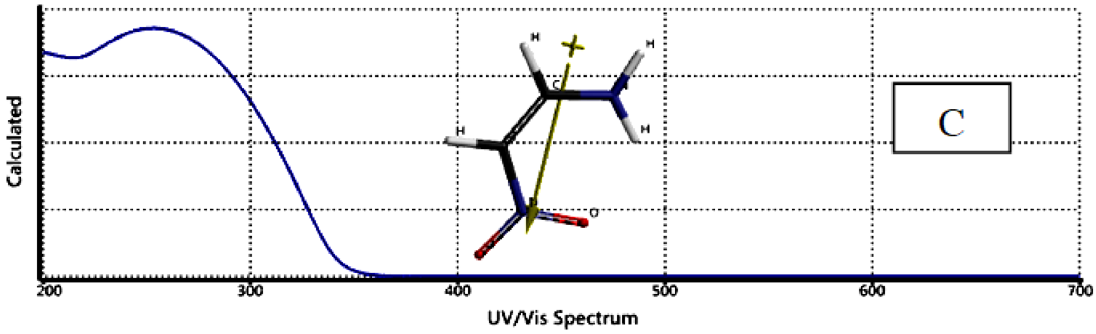
Table 9 shows the HOMO, LUMO energies and the interfrontier molecular orbital energy gap values, Δε, (Δε= ε_{LUMO}-ε_{HOMO}) for the species considered. The algebraic orders of the HOMO and LUMO energies are C<T<CC<G<CG<GG<TG<CT<TT and GG<CT<TT<G<CG<TG<CC<C<T, respectively. Thus, the interfrontier molecular orbital energy gap values, constitute the order of TT<CT<GG<TG<CG<G<C<T.

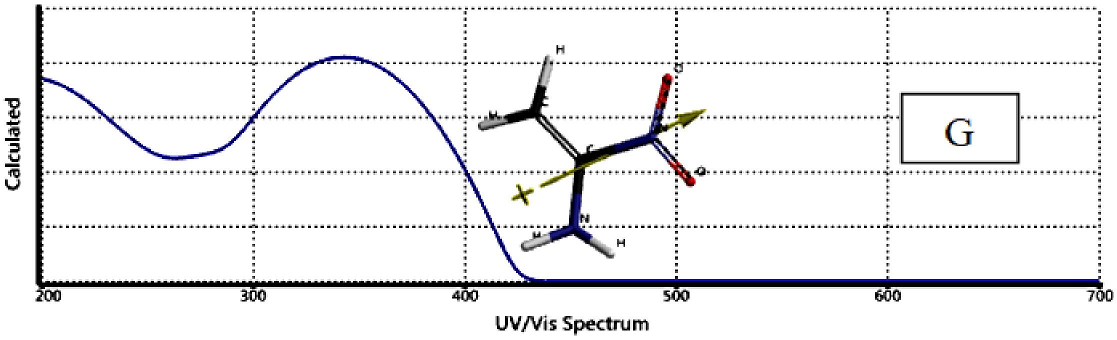
Table 9. The HOMO, LUMO energies and Δε values for the species considered.

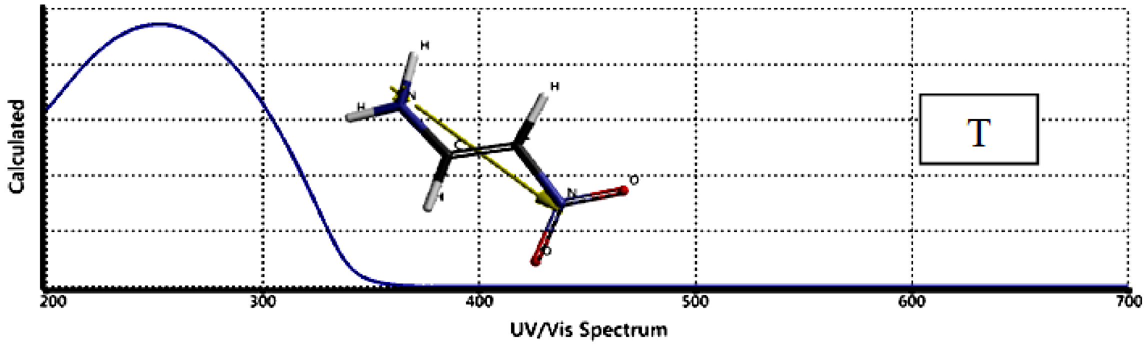
Specie	HOMO	LUMO	Δε
C	-684.39	-223.99	460.40
T	-683.87	-213.81	470.06
G	-669.52	-283.23	386.29
CC	-680.99	-242.56	438.43
CG	-635.19	-278.30	356.89
CT	-623.27	-296.49	326.78
GG	-634.50	-299.49	335.01
TG	-632.52	-276.21	356.31
TT	-596.93	-289.13	307.80

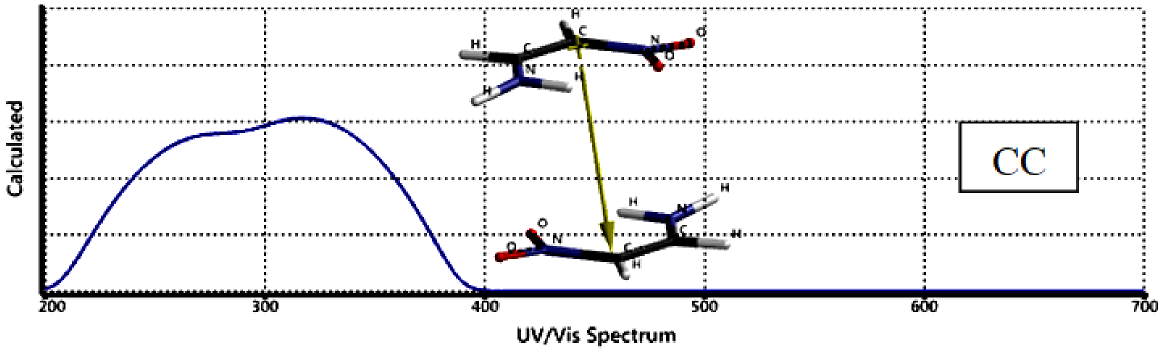
Energies in kJ/mol. B3LYP/6-311++G(d,p) level.

Figure 11 displays the calculated (time dependent, TDDFT) UV-VIS spectra of the species considered. The spectrums of the parent structures C and T are all confined to UV region whereas the geminal one shows a bathochromic shift as compared to the other isomers. The order of Δε values is G<C<T for the parent structures. The order of λ_{max} values G>C>T (342.67, 253.18 and 252.09 nm, respectively) are in good accord with the adverse order of Δε values. All the composites considered except, CC, absorb both in UV and VIS regions of the spectrum and exhibit some bathochromic effect at varying extends arising from nonbonding intermolecular interactions (see Figure 8 for the bond densities). The spectra vary much in shape for the species, so do the intensities and positions. Intensities of the spectra (and value of the transition moment which is responsible for the excitations) [31, 32] seem to be rather sensitive to molecular regio/stereochemistry of the composites.









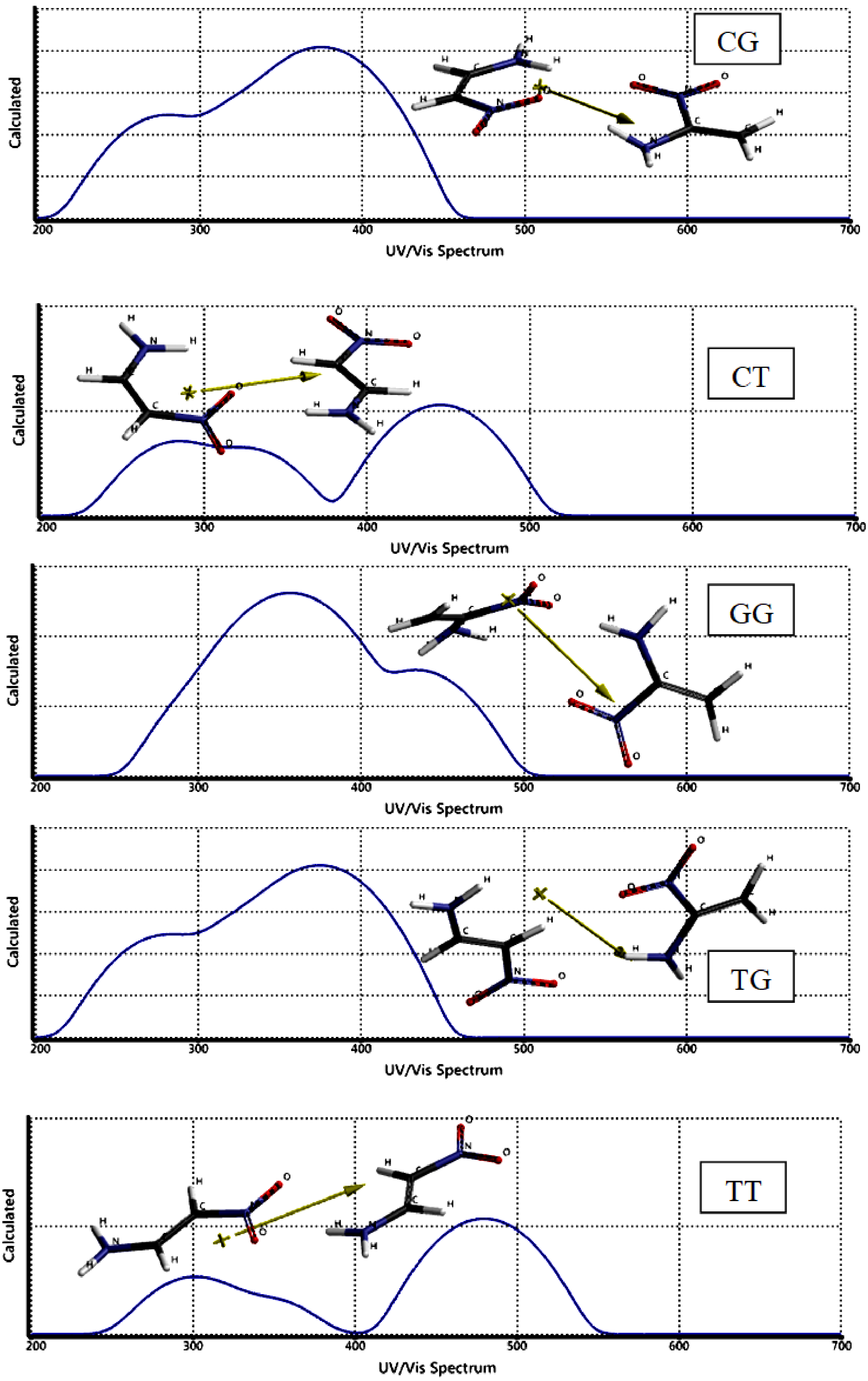


Figure 11. The calculated UV-VIS spectra of the species considered.

The outcome of calculated order of $\lambda_{\max}$ values for the parent compounds could be contemplated in the framework of resonance theory in order to visualize some spectral facts better. Two sets of resonance structures for G are shown in Figure 12. Set I stands for electron attracting character of NO_2 group whereas set II indicates the electron donating behavior of the amino substituent.

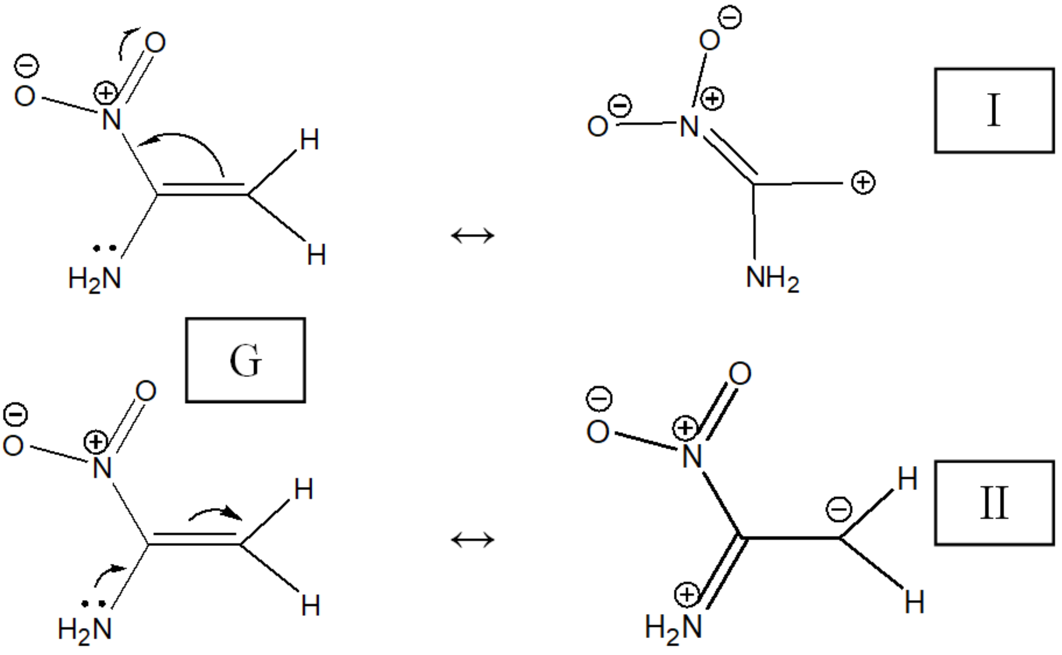


Figure 12. Two sets of resonance structures for G.

On the other hand, figure 13 stands for the optimized structure of isomer G which shows that nitrogen atom of the amino group seems to be in sp^3-hybridized form whereas NO_2 group is almost coplanar with π-skeleton of the ethylene system, thus constituting a 4π-skeleton. Although, the resonance structure I appears to possess better extended conjugation compared to II, its statistical weigh should however be less because electron donating effect of the NH_2 group somehow resists/blocs to flow of electrons leading to resonance form I. Hence, the competing possibilities of resonance structures I and II, biasing for II, should dictate the calculated order of $\lambda_{\max}$ values. Note that in addition to those resonance effects, inductive effects operating through the σ-skeleton might interfere fine aspects of the spectra.

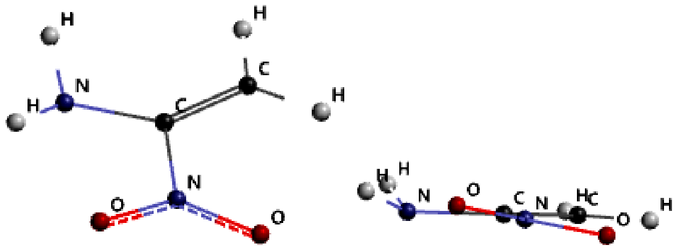


Figure 13. The optimized structure of isomer G.

4. Conclusion

The present study, performed on, the *cis*, *trans* and *geminal* aminonitroethylenes and their interactions with each other, within the restrictions of density functional theory has revealed that the parent structures and their composites are thermally and electronically stable at the vacuum conditions. Results indicate that the composites have some nonbonded interactions which are charge-charge, charge-dipole and /or dipole-dipole type. The parent structures have push-pull type character at different extents. The interfrontier molecular orbital energy gap values vary depending on the π-topology of the structures and regio and stereochemistry of the components in the case of composites. All the composites considered exhibit some bathochromic effect at varying extends arising from nonbonding intermolecular interactions.

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