Adsorption of Industrial Gases (CH$_4$, CO$_2$, and CO) on Olympicene: A DFT and CCSD(T) Investigation

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ABSTRACT: Olympicene C$_{19}$H$_{12}$, an organic semiconductor, is investigated as an adsorption material for toxic industrial gas molecules such as CH$_4$, CO$_2$, and CO. A deep insight of complexation of CH$_4$, CO$_2$, and CO with olympicene (analyte@OLY) was obtained by interaction energy, symmetry-adopted perturbation theory (SAPT2+), quantum theory of atoms in molecules (QTAIM), density of states (DOS), noncovalent interaction (NCI), and frontier molecular orbital and natural bond orbital analysis. Domain-based local pair natural orbital coupled cluster theory single-point energy calculations were performed using the cc-pVTZ basis set in combination with corresponding auxiliary cc-pVTZ/JK and cc-pVTZ/C basis sets. For all property calculations of doped olympicene complexes, the ωB97M-V functional was employed. The stability trend for interaction energies is CO$_2$@OLY > CH$_4$@OLY > CO@OLY. QTAIM and NCI analysis confirmed the presence of NCIs, where the dispersion factor (in CH$_4$@OLY) has the highest contribution, as revealed from SAPT2+. The chemical sensitivity of the system was evidenced by the origination of new energy states in DOS spectra. The recovery time for the analyte@OLY complex was calculated at 300 K, and an excellent recovery response was observed. All results evidently indicated weak interactions of the olympicene surface with CH$_4$, CO$_2$, and CO.

INTRODUCTION

Adsorption studies of industrial gases have attracted much attention due to increasing environmental concerns.$^{1-3}$ The demand for the development of highly selective and sensitive gas sensors for the detection of environmental toxic gas molecules is increasing constantly.$^4$ Among these gases, methane, carbon dioxide, and carbon monoxide are hazardous environmental pollutants which are majorly produced due to endless growth of automobiles and industries.$^5$ Cement production, burning of fossil fuel, agriculture, increased manufacture of chemicals, industrial products, and mining activities are the main sources of these gases.$^6,7$ CH$_4$ is a flammable, colorless, odorless, and explosive gas that is widely used as in the manufacture of organic chemicals and fuel in industries and houses.$^8$ The repeated release of CH$_4$ gas in the atmosphere results in climatic change and global warming. CH$_4$ reduces the amount of oxygen in air, which gives rise to difficulty in breathing, blurred vision, and cardiac disturbances.$^{10}$ CO is a colorless, tasteless, odorless, and toxic gas.$^{11}$ CO reacts with hemoglobin and blocks oxygen transport due to the formation of carboxyhemoglobin.$^{12}$ Even small traces of CO must be sensed because a concentration of CO > 150 ppm is lethal to health and can even cause death.$^{12,13}$ Greenhouse effect is the utmost threat from increased CO$_2$ in the atmosphere.$^{14}$ An increased concentration of CO$_2$ is an alarming point for the earth’s climate.$^{15}$ Weather patterns are greatly influenced by excessive CO$_2$ in the atmosphere.$^{16}$ Ocean acidification is one of the major problems caused by CO$_2$.$^{17}$ The formation of carbonic acid from CO$_2$ and H$_2$O decreases the pH of oceans, which is a serious threat to the survival of marine organisms.$^{18}$ Humans exposed to high levels of CO$_2$ can have elevated blood pressure, coma, increased heart rate, and sweating.$^{19}$

In an effort to protect the environment, research for highly effective gas sensors for detection of CH$_4$, CO$_2$, and CO is the subject of experimental and theoretical studies. Therefore, different types of solid materials are employed as gas sensors to adsorb these toxic gases such as activated carbon, zeolites, metal–organic frameworks, graphene, and covalent organic frameworks. Recently, carbon nanostructures have been extensively explored for their adsorption and sensing properties.$^{20-23}$ Already reported gas sensors for CO and CO$_2$ are Pt-
doped armchair graphene nanoribbons and carbon nanotubes. Different graphene-based materials have been studied for the detection of CO and CO gases. For methane gas, resistive gas sensors are used, but such sensors have poor conductivity at low temperature. In this study, we introduce a polyaromatic five-ringed structure named olympicene (C_{19}H_{12}) as an effective adsorption material for the detection of methane, carbon dioxide, and carbon monoxide.

Olympicene, a modification of the pentacene molecule, has been recently synthesized and reported to exist in a stable form. Pentacene commonly serves as a semiconductor in organic field-effect transistors, organic light emitting diodes, and other electronic devices, for instance, thin-film sensors. Olympicene, which is structurally similar to pentacene, has been proposed as a potential alternative for organic-based electronics due to its promising electrical and optical characteristics. It is believed that the olympicene can be used in the semiconductor industry similarly to pentacene. Olympicene offers a wide range of potential uses in the field of high-tech LEDs, energy storage devices, sensors, and solar cells. To the best of our knowledge, theoretical study of adsorption behavior of olympicene has been rarely carried out. It is predicted that this flat molecule can be a better adsorption material for toxic gases.

## COMPUTATIONAL METHODOLOGY

All-quantum chemical calculations were carried out using version 5.0.1 of the ORCA computational code. All DFT calculations were accelerated using the RIJCCOSX algorithm, while domain-based local pair natural orbital coupled cluster theory [DLPNO-CCSD(T)] calculations were accelerated using the RIJK algorithm. Geometry optimizations were performed using the RI-B3LYP hybrid functional including D3BJ dispersion correction with Becke–Johnson damping and the def2-TZVP basis set in combination with the corresponding auxiliary def2/J basis set.

At the RI-B3LYP-D3/def2-TZVP final optimized geometries, DLPNO-CCSD(T) with single, double, and perturbative triple excitation single-point energy calculations were performed using the cc-pVTZ basis set in combination with corresponding auxiliary cc-pVTZ/JK and cc-pVTZ/C basis sets. From the accurate energies of DLPNO-CCSD(T) calculations, the interaction energy of methane, carbon dioxide, and carbon monoxide over olympicene was calculated from the following formula

\[ E_{\text{int}} = E_{\text{complex}} - (E_{\text{analyte}} + E_{\text{olympicene}}) \]

In addition, the ωB97M-V functional was employed along with the def2-TZVP basis set in combination with the corresponding auxiliary def2/J basis set for noncovalent interactions (NCIs), quantum theory of atoms in molecules (QTAIM), and natural bond orbital (NBO) calculations of doped olympicene complexes. The wave function files of all complexes generated by ORCA at the ωB97M-V/def2-TZVP level of theory were analyzed by Multiwfn software for NCI and QTAIM analysis. The isosurfaces of NCI and QTAIM analysis were visualized using VMD and reduced density gradient (RDG) scatter maps of NCIs were plotted using gnuplot. NCI analysis was carried out using 3D isosurfaces and reduced density gradient (RGG) plots to get an idea of NCIs. Furthermore, the NCIs between olympicene and toxic gases were quantified by bond critical point using QTAIM analysis. NBO 7.0 software was employed to perform NBO charge analysis of analyte@OLY complexes.

Energies of the HOMO, LUMO, HOMO–LUMO energy gaps, and density of states (DOS) were calculated at the RI-B3LYP-D3/def2-TZVP level of theory. The change in energy states of the olympicene surface after the adsorption of analytes was evaluated by DOS analysis, and DOS spectra were generated using Multitwnf software. The components of energies (exchange, induction, dispersion, and electrostatic) in CH_{4}@OLY, CO_{2}@OLY, and CO@OLY were analyzed by the symmetry-adapted perturbation theory (SAPT) in the PSI4 software (version 1.4.1) at the SAPT2+/aug-cc-pVDZ level of theory. The recovery time at 300 K was computed by using transition state theory for the determination of reusability of the olympicene surface.

## RESULTS AND DISCUSSION

### Interaction Energies

DFT calculations were performed to evaluate olympicene as an adsorption material for CH_{4}, CO_{2}, and CO. The final optimized structure of olympicene from both sides and front view are shown in Figure 1.

![Figure 1](https://doi.org/10.1021/acsomega.2c01796)

**Figure 1.** Front (A) and side views (B) of optimized geometry of the olympicene molecule.

Olympicene has three noticeable six-membered rings. The adsorption of analytes CH_{4}, CO_{2}, and CO is investigated over these rings. After optimization of different configurations of analyte@OLY complexes, we selected the most stable ones for further examination. The geometries of the most stable analyte@OLY complexes are shown in Figure 2.

The interaction distances and interaction energies of CH_{4}, CO_{2}, and CO gases adsorbed on the surface of olympicene are calculated and listed in Table 1. The results show that the interaction energies of CH_{4}, CO_{2}, and CO are −13.0, −19.3, and −11.7 kJ mol⁻¹, respectively. Among all considered analytes, the highest adsorption energy is observed for CO@OLY due to efficient overlapping of orbitals and strong van der Waals interaction (vide infra). The highest stability of the CO@OLY complex is advocated by the least adsorption distance (H-20···O-33), which is 2.84 Å. The values of interaction energies for all three gases show a decreasing trend with increasing interaction distance. The outcome of interaction energies of all complexes supported the mechanism of physisorption. The stability trend for interaction energies is CO_{2}@OLY > CH_{4}@OLY > CO@OLY. To account for the basis-set superposition error (BSSE) in interaction energies, we used the counterpoise correction. The BSSE-corrected interaction energies for CH_{4}@OLY, CO_{2}@OLY, and CO@OLY complexes were found to be −11.4, −14.9, and −9.1 kJ mol⁻¹, respectively. For all complexes, the same order of stability for interaction energies was found even after inclusion of BSSE corrections; that is, no changes were observed in the trend of interaction energies before and after inclusion of BSSE corrections, as shown in Table 1.
SAPT2+. SAPT gives quantitative information regarding NCIs between two entities, that is, the analytes and complex. Division of interaction energy into different parts such as dispersion, exchange, electrostatic, and induction has been performed using SAPT ($E_{\text{int}} = E_{\text{ele}} + E_{\text{ind}} + E_{\text{disp}} + E_{\text{exch}}$). SAPT2+ is regarded as the silver standard of SAPT. SAPT2+ is superior to SAPT0 because of inclusion of second-order corrections with intramonomer electronic correlation to dispersion and induction, which are ignored in SAPT0.51

The results of the SAPT2+ analysis are given in Table 2. In all analyte@OLY complexes, a negative sign of $E_{\text{SAPT2+}}$ indicates the existence of attractive interactions. The attractive parts of SAPT2+ analysis are distributed into $\Delta E_{\text{ind}}, \Delta E_{\text{disp}}$, and $\Delta E_{\text{elst}}$. The positive sign of the exchange part of SAPT2+ energies corresponds to repulsive interactions due to filled orbitals of the olympicene surface and analytes. The SAPT2+ values obtained for analyte@OLY were $-12.7 \text{ kJ mol}^{-1}$ (CH$_4$@OLY), $-20.4 \text{ kJ mol}^{-1}$ (CO$_2$@OLY), and $-8.5 \text{ kJ mol}^{-1}$ (CO@OLY). The results obtained from the SAPT2+ energy components agree with the interaction energy $E_{\text{int}}$ results. The components of the SAPT2+ energy for CH$_4$@OLY were $-6.4 \text{ kJ mol}^{-1}$ ($E_{\text{elst}}$), $-1.3 \text{ kJ mol}^{-1}$ ($E_{\text{ind}}$), and $-21.5 \text{ kJ mol}^{-1}$ ($E_{\text{disp}}$). These results showed that $E_{\text{disp}}$ was the major stabilizing element (73.7%), whereas $E_{\text{elst}}$ (21.9%) and $E_{\text{ind}}$ (4.3%) were less notable in the total energy. In case of the CO$_2$@OLY complex, the contributions of each part of energy toward the total SAPT2+ were $-11.3 \text{ kJ mol}^{-1}$ ($E_{\text{elst}}$), $-2.9 \text{ kJ mol}^{-1}$ ($E_{\text{ind}}$), and $-28.9 \text{ kJ mol}^{-1}$ ($E_{\text{disp}}$). The $E_{\text{disp}}$ component in CO$_2$@OLY (67%) was less as compared to $E_{\text{disp}}$ (73.7%) of the CH$_4$@OLY complex. For the CO@OLY complex, $\Delta E_{\text{disp}}$ is
the main contributing factor toward $E_{\text{SAPT2}+}$ (61.4%), while $\Delta E_{\text{elst}}$ is the next highest attractive stabilization factor (29.06%). The results in Table 2 prove that the contribution from $E_{\text{elst}}$ and $E_{\text{ind}}$ remained appreciable, but the largest contribution toward the total SAPT2+ was observed from $E_{\text{disp}}$ in all of the complexes.

**Electronic Properties.** The nature of interactions between CH₄, CO₂, CO, and olympicene can be estimated by electronic properties. The electronic properties of systems are studied by NBO and frontier molecular orbital (FMO) analysis.

**FMO and NBO Analysis.** Quantum mechanics affirms that the interaction occurs when the FMOs of two species interact with one another. The HOMO of the molecule having the highest energy has the power to give electrons to the LUMO of the molecule having the lowest energy. The difference in energy between the e-donating HOMO and e-receiving LUMO can be employed to figure out the nature of interaction and the stability of complexes. Moreover, the electrical conductivity of the interacting species is estimated by the band gap or $E_{\text{H-L}}$ gap.

Table 3: FMO and NBO Analysis of Analyte@OLY Complexes

| complexes     | $E_{\text{HOMO}}$ (eV) | $E_{\text{LUMO}}$ (eV) | $E_{\text{H-L}}$ gap (eV) | $Q_{\text{NBO}}$ |
|---------------|------------------------|------------------------|--------------------------|-----------------|
| olympicene    | −5.511                 | −1.496                 | 4.015                    | 0.0008          |
| CH₄@OLY      | −5.539                 | −1.508                 | 4.031                    | 0.0008          |
| CO₂@OLY      | −5.551                 | −1.539                 | 4.012                    | 0.0028          |
| CO@OLY       | −5.548                 | −1.528                 | 4.020                    | 0.0031          |

olympicene are −5.511 and −1.496 eV, respectively. The $E_{\text{H-L}}$ gap of olympicene surface is 4.015 eV. The $E_{\text{H-L}}$ gap of CH₄, CO₂, and CO, respectively. Slight variations in the $E_{\text{H-L}}$ gap of olympicene are observed on adsorbing CH₄, CO₂, and CO, which indicates weak interactions between olympicene and the absorbed gases. The $E_{\text{H-L}}$ gap of the CO₂@OLY complex decreased as compared to pristine olympicene, while the adsorption of CH₄ and CO onto the olympicene surface altered the energy of the HOMO and LUMO in such a way that the $E_{\text{H-L}}$ gap of these complexes increased as compared to that of the pristine olympicene.

NBO charge analysis was executed to study the amount of charge transferred during interactions between the analytes and olympicene surface. The calculated results of NBO analysis are presented in Table 3. The values of $Q_{\text{NBO}}$ are positive on CH₄, CO₂, and CO in analyte@OLY complexes, which indicate that charges are transferred to the olympicene surface. For the CH₄@OLY complex, the amount of charge transferred is 0.0008 lel. The amount of charge transferred from the analyte to surface in the CO₂@OLY and CO@OLY complex is 0.0031 and 0.0028 lel, respectively. The NBO results for CO declare that olympicene extracted a relatively higher amount of charge (0.0031 lel) from the carbon monoxide as compared to carbon dioxide (0.0028 lel) and methane (0.0008 lel). The electron-rich oxygen transfers the electronic cloud toward olympicene. The results of $Q_{\text{NBO}}$ are quite opposite to those of $E_{\text{ind}}$ that is, a higher amount of charge transfer is observed for CO₂@OLY, whereas the highest $E_{\text{ind}}$ is observed for CO@OLY. Similarly, the lowest $E_{\text{ind}}$ for CO@OLY reflects the highest $Q_{\text{NBO}}$ for CO@OLY. The following trend in all of the complexes for $Q_{\text{NBO}}$ transfer is observed, that is, CO@OLY > CO₂@OLY > CH₄@OLY.

**Density of States.** The DOS of the most stable configurations of analyte@OLY complexes were examined to investigate their conductivity and interactions. DOS analysis was performed to get deep insight into the number of states that are occupied by electrons at an energy level. The changes occurred in the region of the HOMO/LUMO, and the available energy states helped to understand the changes in electronic properties and sensing abilities of olympicene after complexation. The partial density of states (PDOS) plots of all analyte@OLY complexes are plotted in Figure 3. The $E_{\text{HOMO}}$ and $E_{\text{LUMO}}$ for pristine olympicene are −5.511 and −1.496 eV, respectively, with an $E_{\text{H-L}}$ gap of 4.015 eV. After the complexation of olympicene with CO₂, the peaks of the HOMO and LUMO shifted to −5.551 and −1.539 eV, respectively. A slight decrease in $E_{\text{H-L}}$ gap was observed due to the shifting of the HOMO toward lower energy during complexation. The appearance of new energy states in PDOS of olympicene represents the interactions between analytes and the olympicene surface. The PDOS of all complexes shows prominent peaks for the analytes (CH₄, CO₂, and CO) far below the Fermi level near −10.0 eV, indicating the adsorption of these toxic gases on olympicene.

**QTAIM Analysis.** The nature of interactions in analyte@OLY complexes was further characterized by a topological analysis called QTAIM. The bond nature between an analyte and complex depends on the bond critical point (BCP). At BCPs, different topological parameters were employed to quantify the nature of interactions such as the total electron energy density [$H(r)$], electron density ($\rho$), and Laplacian of electron density ($\nabla^2 \rho$). At BCPs, the nature of interactions was quantified by the total electron energy density $H(r)$, potential energy density $V(r)$, Laplacian ($\nabla^2 \rho$), and kinetic energy density $G(r)$, whereas the strength of the bond is determined by electron density ($\rho$). In terms of electronic density ($\rho$), the value of $\rho > 0.1$ indicates the presence of electrostatic interactions or hydrogen bonding, whereas the value of $\rho < 0.1$ confirms weak van der Waals interactions. Generally, at BCPs, the values of $V(r)$ and $G(r)$ always remain negative and positive, respectively. $H(r)$ is obtained by the addition of $V(r)$ and $G(r)$, which indicates the presence of covalent and NCIs.

The presence of covalent interactions is indicated by the value of $H(r)$ less than zero, whereas $H(r)$ is greater than zero for NCIs.

$$H(r) = G(r) + V(r)$$

Table 4 and Figure 4 show the results of QTAIM analysis and isosurfaces of analyte@OLY complexes, respectively. For CH₄@OLY and CO₂@OLY, single BCPs were obtained, but the topological parameters were different due to different compositions and nature of analytes. The values of electron density for CH₄@OLY and CO₂@OLY are 0.005 and 0.007, respectively. The Laplacian of electron density of CO₂@OLY (0.020) is greater than that of CH₄@OLY (0.018). The rest of the BCP values are also in accordance with the Laplacian of electron density and electron density, which is a clear indication of noncovalent nature. In case of CO₂@OLY, two BCPs were obtained, and the strongest NCIs were anticipated between C-22 of olympicene and C-18 of the CO₂ due to its highest value of electron density (0.006) and Laplacian of the electron density (0.021). The remaining values of CO₂@OLY $[H(r), G(r), V(r), \text{and } V(r)/G(r)]$ also proclaim the presence...
Figure 3. PDOS spectra of the CH₄@OLY, CO₂@OLY, and CO@OLY complexes.

Table 4. Values of BCPs of the Analyte@OLY Complexes Obtained from the QTAIM Analysis.

| analyte@OLY | OLY-analyte | BCPs | ρ  | V(ρ) | G(r)   | V(r)  | H(r)  | V(r)/G(r) |
|-------------|-------------|------|----|------|--------|-------|-------|-----------|
| CH₄@OLY     | C14–C26     | 63   | 0.005 | 0.018 | 0.003  | -0.002 | 0.0009 | -0.73     |
| CO@OLY      | C17–C1      | 37   | 0.007 | 0.020 | 0.004  | -0.003 | 0.0008 | -0.81     |
| CO₂@OLY     | C22–C18     | 62   | 0.006 | 0.021 | 0.004  | -0.003 | 0.0008 | -0.79     |
|             | H7–O13      | 47   | 0.004 | 0.020 | 0.004  | -0.002 | 0.0012 | -0.60     |
positive values for the total electron density ($H$) and Laplacian ($\nabla^2 \rho$). Moreover, the values of electron density ($\rho$) for all of the complexes are less than 0.1 au, which indicates the existence of weak van der Waals interactions. These findings are consistent with NCI and SAFT+$\alpha$ analysis.

Noncovalent Interactions. NCI analysis comprises 2D RDG graphs and 3D isosurfaces which help to understand the nature of interactions, particularly intermolecular interactions. RDG analysis is one of the most specific visual approaches for NCIs. RDG spectra have three color codes (green, red, and blue). The spikes of green color indicate the existence of weak NCIs such as dispersion forces or dipole–dipole forces. The 2D-RDG graph and 3D isosurfaces for the analyte@OLY complexes are presented in Figure 5. The 3D isosurfaces of all of the analytes (CH$_4$, CO$_2$, and CO) showed the existence of green patches between the olympicene surface and the analytes, which confirm the presence of weak NCIs. The absence of blue spikes between the analytes and olympicene

Figure 4. Isosurfaces of analyte@OLY complexes in QTAIM analysis.

Figure 5. 2D RDG scatter map and 3D isosurfaces of analyte@OLY complexes.
surface in 3D isosurfaces reflects that there is no hydrogen bonding or strong interactions present. For CH₄@OLY, the 3D isosurface reflects that weak dispersive interactions are present, which can be spotted in the 2D-RGD graph. In all three complexes, CH₄@OLY, CO₂@OLY, and CO@OLY, the appearance of green spikes/peaks projecting between −0.01 and 0.01 in the x-axis (δₓᵧ) confirm the presence of dispersive interaction. At the right side of the RDG scatter graph, the red spikes are an indication of repulsive forces between the atoms of aromatic rings of olympicene. In the 3D isosurface of CO₂@OLY, the green patches are wide and dense, which shows stronger interactions between the atoms of CO₂ and olympicene as compared to the rest of the analyte@OLY complexes. The NCI results of CO₂@OLY are persistent, with the interaction energy analysis having the strongest interaction energy and smallest interaction distance with the olympicene surface.

**Recovery Time of Olympicene.** Calculating the recovery time for desorption of analytes is one of main parameters to judge olympicene as an ideal gas sensor. Theoretically, the recovery times (s) for the desorption of CH₄, CO₂, and CO were calculated using transition state theory, which can be expressed as

\[ \tau = e^{-\frac{E_{ad}}{k_B T}} \]

where \( K \) represents the Boltzmann constant (8.62 × 10⁻⁵ eV K⁻¹), \( T \) stands for temperature of the system, and \( \tau \) represents the attempt frequency of the NO₂ molecule (\( \nu = 10^{11} \) s⁻¹). According to the transition theory, increasing adsorption energy \( E_{ad} \) increases the recovery time. Here, we suppose that the attempt frequencies of CH₄, CO₂, and CO are equal to that of NO₂. At room temperature, when the adsorption energy is greater than 1.0 eV, the recovery time increases and the sensor takes more than 12 h to recover. The adsorption energies for CH₄@OLY, CO₂@OLY, and CO@OLY are 0.133, 0.197, and 0.124 eV, respectively. At 300 K, a very good recovery response is observed (Table 5), which indicates that olympicene can serve as a reusable sensing material for CH₄, CO₂, and CO.

**Table 5. Recovery Time of Olympicene at 300 K**

| complex       | adsorption energies \( E_{ad} \) (eV) | recovery time of sensor (s) |
|---------------|--------------------------------------|-------------------------------|
| CH₄@OLY       | 0.133                                 | 1.73 × 10⁻¹⁰                  |
| CO₂@OLY       | 0.197                                 | 2.103 × 10⁻⁹                  |
| CO@OLY        | 0.120                                 | 1.053 × 10⁻¹⁰                  |

**CONCLUSIONS**

Adsorption of CH₄, CO₂, and CO on the olympicene surface were assessed through DFT and DLPNO-CCSD(T) calculations. All possible orientations of the analytes on the olympicene surface were examined to get the most stable geometries of the analyte@OLY. CO₂@OLY was identified as the lowest-energy complex as compared to CH₄@OLY and CO@OLY. The \( E_{H-L} \) gap of olympicene decreased on complexation with CO₂. The obtained results from QTAIM and NCI analysis indicated NCIs between olympicene and the adsorbed gases. Similarly, the values of electron density \( \rho \) for all complexes are less than 0.1 au, which confirms the existence of weak van der Waals interactions. In the 3D isosurface of CO₂@OLY, the green patches are wide and dense, which shows stronger interactions between CO₂ and olympicene as compared to the rest of the analyte@OLY complexes. The result of SAPT2+ analysis is consistent with QTAIM and NCI analysis. The NBO results indicate that olympicene extracted a relatively higher amount of charge (0.0031 e) from carbon monoxide as compared to carbon dioxide (0.0028 e) and methane (0.0008 e). The PDOS of all complexes revealed the generation of new energy states for the analytes (CH₄, CO₂, and CO) far below the Fermi level near −10.0 eV, indicating the sensitivity of these toxic gases on olympicene.

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**Notes**

The authors declare no competing financial interest. The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

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