

## Experimental and Theoretical Study of Cobalt Hemiporphyrzine Behavior in the Gas Phase by Mass Spectrometry

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*The vapor composition and the enthalpy of sublimation of the cobalt(II) hemiporphyrzine (CoHp) complex were determined by the Knudsen effusion method using mass spectrometric MI-1201 modified for high temperature investigations. Electron ionization mass spectra were also simulated using the QCxMS program implemented in the xTB software package. The enthalpy of sublimation for CoHp determined using the Clausius-Clapeyron equation is 212(5) kJ/mol in the temperature range of 481–544 K. The energy of intermolecular interaction was estimated using the criterion proposed by Espinosa for both H<sub>2</sub>Hp and CoHp within the framework of QTAIM theory. The difference between the energies of intermolecular interactions of H<sub>2</sub>Hp and CoHp was about 20 kJ/mol. In the case of experimental values of the enthalpies of sublimation for H<sub>2</sub>Hp and CoHp, the difference was also 20 kJ/mol.*

**Keywords:** Mass spectrometry, quantum chemistry, hemiporphyrzine, QCxMS.

## Экспериментальное и теоретическое исследование гемипорфиразина кобальта в газовой фазе методом масс-спектрометрии

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*Состав пара и энтальпия сублимации комплекса гемипорфиразина кобальта(II) (CoHp) были определены с помощью эффузионного метода Кнудсена с использованием масс-спектрометра МИ-1201, модифицированного для высокотемпературных исследований. Масс-спектры с ионизацией электронами также моделировались с помощью программы QCxMS, реализованной в программном пакете xTB. Энтальпия сублимации определялась по уравнению Клаузиуса-Клапейрона и составила 212(5) кДж/моль в температурном интервале 481–544 К. Энергия межмолекулярного взаимодействия оценивалась с использованием критерия, предложенного Эспинозой, для гемипорфиразина H<sub>2</sub>Hp и его комплекса с кобальтом CoHp в рамках теории QTAIM. Разница между энергиями межмолекулярного взаимодействия H<sub>2</sub>Hp и CoHp составила около 20 кДж/моль. В случае экспериментальных значений энтальпий сублимаций H<sub>2</sub>Hp и CoHp разница также составила 20 кДж/моль.*

**Ключевые слова:** Масс-спектрометрия, квантовая химия, гемипорфиразин, QCxMS.

### Introduction

Hemiporphyrzines are non-aromatic macroheterocycles of the ABAB type. They differ from other similar types of compounds due to their specific structure, which affects their physical and chemical properties.<sup>[1]</sup> In recent

years, this class of compounds has attracted the attention of scientists because of their potential applications and as a platform for extensive structural modifications.<sup>[2]</sup> For example, in the recent paper low-dimensional polymers based on dicarbahemiporphyrzines were synthesized.<sup>[3]</sup>

Hemiporphyrzine (**H<sub>2</sub>Hp**, Figure 1a) was first synthesized by Elvidge and Linstead.<sup>[4]</sup> Practically at the same time Campbell obtained the same and other structural analogues and proposed in calling them “hemiporphyrzine”.<sup>[5]</sup> Later, Attanasio, Collamatic, and Cervone synthesized hemiporphyrzine metal complexes with Ni, Zn, Co, Cu<sup>[6]</sup> by heating a solution of hemiporphyrzine and the corresponding metal acetate in dimethylformamide (DMF), followed by purification by vacuum sublimation. Since their discovery, hemiporphyrzines attracted great attention due to their structure flexibility which allows large core modification by incorporating various carbo and heterocyclic subunits into macrocyclic framework<sup>[7,8]</sup> as well as to get access to macrocycles with enlarge macrocyclic cores bearing six smaller rings.<sup>[9,10]</sup> Hemiporphyrzines and their structural derivatives demonstrate number of intrinsic properties and therefore can be considered as potential functional organic materials for various applications in microelectronics, nonlinear optics, spintronics and medicine.<sup>[8,11]</sup>

Microwave-assisted approach to the synthesis of hemiporphyrzines developed recently<sup>[12]</sup> essentially facilitates preparation of the macrocycles.

A profound understanding of the structure of hemiporphyrzine and their metal complexes is necessary to develop a relationship between the structure and properties of these important compounds and contribute to the development of these promising compounds. By this reason, in this paper, we will discuss the vapor composition and sublimation enthalpy of the cobalt(II) hemiporphyrzine (**CoHp**, Figure 1b) complex and the modeling of **CoHp** mass spectra using the QCxMS program implemented in the xTB software package.<sup>[13,14]</sup>

## Experimental

### Mass-Spectrometric Experiment

The mass spectrometric study of the sublimation process of **CoHp** from a Knudsen cell was carried out using a MI-1201 magnetic mass spectrometer modified for thermodynamic studies. The solid sample was evaporated from a stainless steel effusion cell. The ratio of the evaporation area to the effusion orifice of the cell was about 1000. The cell temperature was measured using a tungsten-rhenium thermocouple W-Re 5/20. The mass spectra were recorded in a vacuum of  $10^{-7}$  Torr at ionizing voltages  $U_{\text{ion}}$  of 35 and 50 V. The accelerating voltage was 5 kV in all cases. The cathode emission current was  $I_{\text{emis}} = 0.5$  mA.

To determine the enthalpy of sublimation  $\Delta_{\text{subl}}H$  of **CoHp**, a temperature dependence of the intensity of the molecular ion  $[M]^+$  in the spectrum was obtained, measured in the temperature range of 481–544 K with gradual heating of the effusion cell. The value of  $\Delta_{\text{subl}}H$  was calculated using the Clapeyron-Clausius relation as:

$$\ln(IT) = -\frac{\Delta_{\text{subl}}H(T)}{RT} + \text{const},$$

where  $I$  is the ion current,  $T$  is the temperature, and  $R$  is the molar gas constant. The errors to the values of  $\Delta_{\text{subl}}H$  were calculated using the equation:  $\Delta = \sqrt{(3\sigma_{LS})^2 + \sigma_T^2}$ , where  $\sigma_{LS}$  is the standard deviation to the enthalpy value and  $\sigma_T = (H_{T_+} - H_{T_-})/2$ ,  $T_+ = T_i + 5$ ,  $T_- = T_i - 5$ , takes into account the inaccuracy of temperature determination.

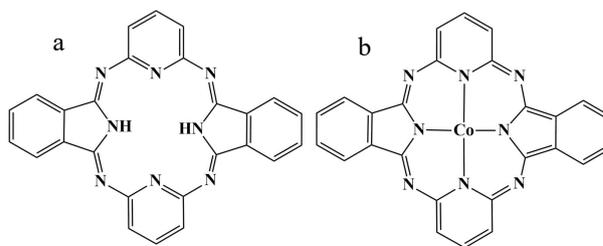


Figure 1. Structural formulas of **H<sub>2</sub>Hp** (a) and **CoHp** (b).

### Computational details

Molecular structures of two electronic states of **CoHp** differ by multiplicity (2 and 4, respectively) were calculated using PBE0/pcseg-2 approach using the Firefly QC package,<sup>[15]</sup> which is partially based on the GAMESS (US)<sup>[16]</sup> source code. It was established, that the ground state is doublet characterized by saddle shape. It should be noted, that complexes of Ca(II), Ni(II), Zn(II) and metal free hemi- and dicarbahemiporphyrzines are also saddle distorted.<sup>[17,18]</sup> Quadruplet state has a significantly higher energy by ~186 kJ/mol and possesses ruffling distortion. No imaginary frequencies were observed for both structures which is evidence that they are minima on potential energy surface. All further calculations were performed for the doublet state.

The QCxMS program was used to obtain the theoretical mass spectra using Born-Oppenheimer molecular dynamics. One of the methods used to model mass spectra and compare them to experimental data is the electron ionization (EI) method,<sup>[19-25]</sup> which increases the internal energy of a molecule, causing bond breakage, fragmentation, etc. Theoretical mass spectra were obtained for temperatures of 540 K and ionization voltages of 35 and 50 V. The excess ionization energy (EIE) per atom was taken by default –0.6 eV/atom; the number of trajectories was calculated using the following formula: number of atoms multiplied by 25. In our case there should have been about 1225 trajectories, but due to limited computing power, the values of 545 and 600 trajectories were utilized for 35 and 50 V, respectively. The maximum sampling time for molecular dynamics (MD) was 10 ps; for low ionization energy (35 V), the Gaussian distribution was applied.

Geometry optimization of **CoHp** (single molecule) along with calculations of the harmonic vibrational frequencies were performed using the PBEh-3c composite method<sup>[26]</sup> implemented in ORCA 5.0 program package<sup>[27]</sup> and recommended in Ref.<sup>[28]</sup> for structure optimizations. For **CoHp** and **H<sub>2</sub>Hp** (dimeric molecules) quantum-chemical calculations were performed by PBEh-3c method. The calculation of **H<sub>2</sub>Hp** dimeric structure was carried out in assumption of singlet state, due to monomeric form is closed-shell system, while **CoHp** has an unpaired electron and its dimer was considered as triplet state. Analysis of the electron density distribution in dimeric molecules by the QTAIM<sup>[29]</sup> method was carried out using the MiltiWFN<sup>[30]</sup> program in order to estimate the energies of intermolecular interactions.

## Results and Discussion

The mass spectrum recorded at  $T = 543$  K with  $U_{\text{ion}} = 50$  V is shown in Figure 2a. The most intense peak in the mass spectrum corresponds to the molecular ion  $[C_{26}H_{14}N_8Co]^+$ . A high relative intensity (18.6%) of the  $[C_5H_3N_3]^+$  in the mass spectrum with  $U_{\text{ion}} = 50$  V is worth noting. However, it is practically absent in the mass spectrum with an ionizing voltage of 35 V. This is an evidence of the fact, that this ion is a fragmentation, and not a decomposition product or an impurity. The intensities of the

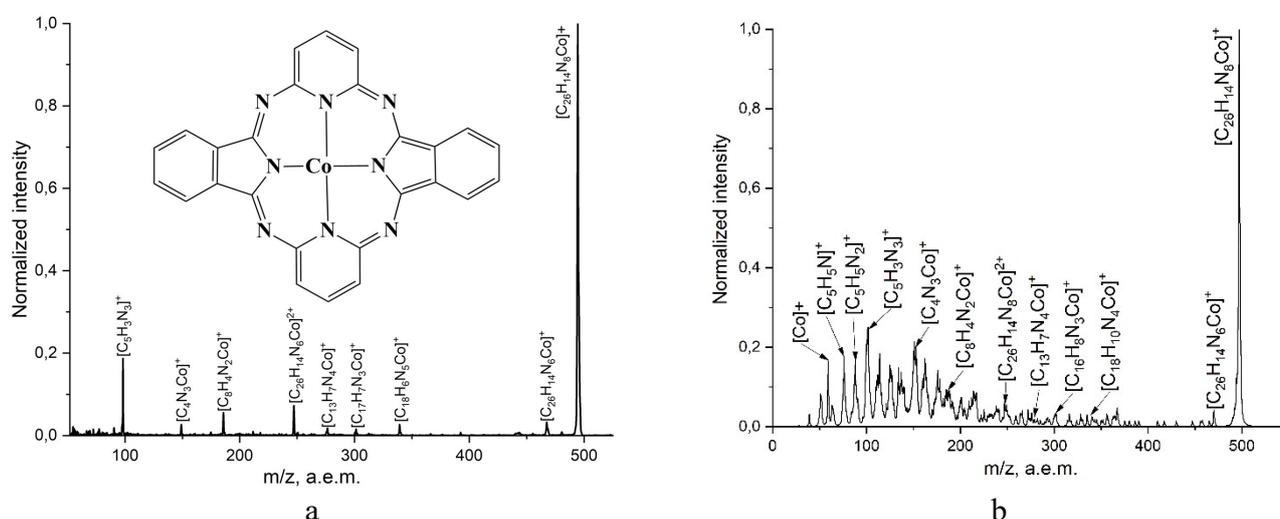
remaining fragmentation ions do not exceed 10%. A peak with  $m/z = 248$  Da corresponding to a  $[C_{26}H_{14}N_8Co]^{2+}$  ion was also detected in the mass spectrum. The general appearance of the mass spectra, namely the presence of an intense molecular ion and a small number of fragmented ions of rather low intensity, can be described as typical for macroheterocyclic compounds.<sup>[31-33]</sup>

In the simulated mass spectra, the intensity of the fragmentation ions also changes of about 2–3 times with increasing ionization voltage (Table 1).

When comparing the recorded and simulated mass spectra at the same ionization voltages, it is noticeable that the intensity of the fragmentation ions is higher in the simulated mass spectra than in the experimental mass spectra. However, the intensity of some ion currents is higher in the experimental mass spectra, namely: ions with  $m/z = 339$  Da at 35 V and 50 V, and a doubly charged molecular ion in the mass spectrum at 50 V. The simulation shows many

ions in the low mass region (up to 200 Da) with high intensities, while the recorded mass spectrum shows only three ion currents in this region. An example of the simulated mass spectrum can be seen in Figure 2b.

Also, temperature dependencies of the molecular ion current were obtained to determine the sublimation enthalpy value. Figure 3 shows the dependence of the logarithm of the ion current/temperature product on the inverse temperature  $\ln(IT) = f(1000/T)$  for a molecular ion. Each point corresponds to the  $IT$  value measured after temperature stabilization. It was found that a congruent transition to the gas phase occurred in this region which is confirmed by both linear dependences  $\ln(IT) = f(1000/T)$  and the same ratio of ions in mass spectra at different temperature. The dependence  $\ln(IT) = f(1000/T)$  is close to a straight line (the correlation coefficient was 0.999). The value of  $\Delta_{\text{subl}}H$  was calculated using the Clapeyron-Clausius equation, 212(5) kJ/mol at  $T = 481\text{--}544$  K.



**Figure 2.** Recorded (a) and simulated (b) mass spectra of **CoHp** at  $U_{\text{ion}} = 50$  V.

**Table 1.** Ion composition of **CoHp** in recorded and simulated mass spectra.

| Ion                        | 35 V  |        | 35 V (theor) |        | 50 V  |         | 50 V (theor) |        |
|----------------------------|-------|--------|--------------|--------|-------|---------|--------------|--------|
|                            | $m/z$ | Int(%) | $m/z$        | Int(%) | $m/z$ | Int (%) | $m/z$        | Int(%) |
| $[C_{26}H_{14}N_8Co]^+$    | 497   | 100    | 497          | 100    | 497   | 100     | 497          | 100    |
| $[C_{26}H_{14}N_6Co]^+$    | 469   | 3.4    | 469          | 8      | 469   | 3.1     | 469          | 4      |
| $[C_{18}H_{10}N_4Co]^+$    | 341   | 3.7    | 341          | 3      | 341   | 2.5     | 341          | 2      |
| $[C_{16}H_8N_3Co]^+$       | 301   | 0.9    | 301          | 3      | 301   | 1.4     | 301          | 3      |
| $[C_{13}H_7N_4Co]^+$       | 278   | 1.1    | 278          | 3      | 278   | 1.6     | 278          | 3      |
| $[C_{26}H_{14}N_8Co]^{2+}$ | 248   | 1.2    | 248          | 2      | 248   | 7.1     | 248          | 6      |
| $[C_8H_4N_2Co]^+$          | 187   | 2.9    | 187          | 4      | 187   | 5.5     | 187          | 9      |
| $[C_4N_3Co]^+$             | 149   | 2.5    | 149          | 11     | 149   | 2.5     | 149          | 21     |
| $[C_5H_3N_3]^+$            | 105   | -      | 105          | 7      | 105   | 18.6    | 105          | 25     |
| $[C_5H_3N_2]^+$            | 93    | -      | 93           | 6      | 93    | 1.7     | 93           | 16     |
| $[C_5H_5N]^+$              | 79    | -      | 79           | 10     | 79    | 1.5     | 79           | 17     |
| $[C_4N_2]^+$               | 76    | 1.4    | -            | -      | 76    | 1.4     | -            | -      |
| $[Co]^+$                   | 58    | 1.1    | 58           | 5      | 58    | 2       | 58           | 16     |

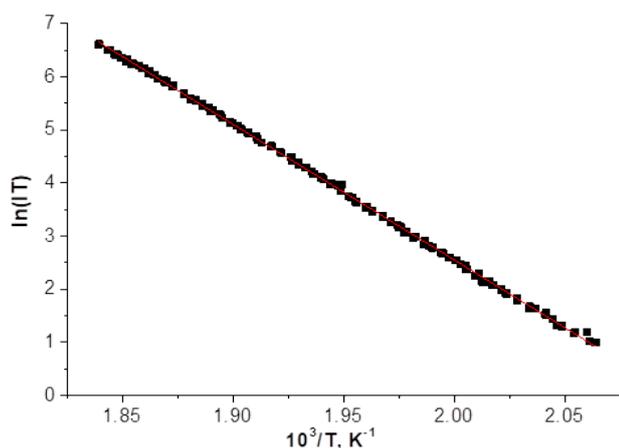


Figure 3. Dependence  $\ln(IT) = f(1000/T)$  for the molecular ion.

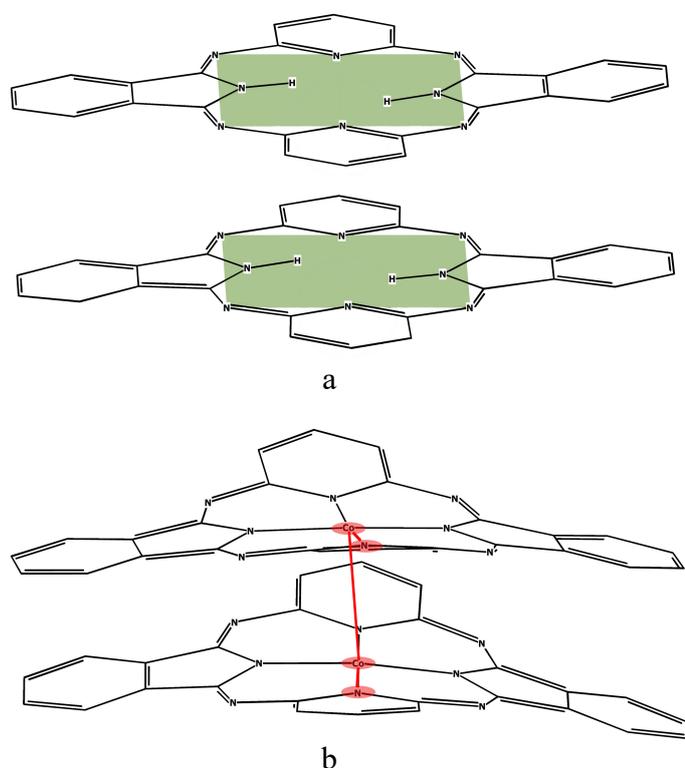


Figure 4. **H<sub>2</sub>Hp** (a) and **CoHp** (b) dimers; the dihedral angle N-Co-Co-N is marked red.

Previously in paper<sup>[32]</sup> an enthalpy of sublimation of hemiporphyrzine (**H<sub>2</sub>Hp**) was found to be 191(1) kJ/mol in a range of 441–531 K.

Also we tried to evaluate the energy of intermolecular interactions which are the main component of sublimation enthalpy values. For this purpose, additional quantum chemical calculations for **H<sub>2</sub>Hp** and **CoHp** dimers were carried out. Starting geometries were taken from Cambridge Crystal Structure Database<sup>[34]</sup> obtained by Yu Wang and coauthors.<sup>[35]</sup> As for **CoHp**, the crystal structure only with axial –OH ligand was observed.<sup>[35]</sup> However, a presence of axial ligand leads to significant changes in crystal structure. For this reason for our calculations a crystal lattice of **NiHp** was used with a substitution of Ni by Co atom. The crystal packing of **H<sub>2</sub>Hp** and **NiHp** is arranged

in such a way that selection of the dimer in the form of a “stack” is possible for further using of this structure as a starting point for optimization of the dimeric structures. In the case of “stack” dimer the maximum number of intermolecular interactions is observed compared to dimers of other configurations. A similar procedure was performed in our recent work.<sup>[36]</sup>

It is worth noting that when optimizing dimeric structures, the relative arrangement of **H<sub>2</sub>Hp** molecules remained unchanged; the value of the  $\angle N_{\text{pyr}}-X_1-X_2-N_{\text{pyr}}$  dihedral angle was 0°, where  $X_1$  and  $X_2$  are dummy atoms centered between  $N_m$  atoms. At the same time optimization of the geometry of **CoHp** dimer results in slightly rotation of the molecules relative to each other. The value of the dihedral angle  $\angle N_{\text{pyr}}-\text{Co}-\text{Co}-N_{\text{pyr}} = 8.1^\circ$  (Figure 4b). Also, a saddle distortion should be mentioned for both dimers as well as for monomer of **CoHp**.

After optimization, bond critical points (BCP) search was performed using the MultiWFN program within QTAIM theory. Total number of intermolecular BCPs is higher for **CoHp**, than for **H<sub>2</sub>Hp**: 18 vs. 12 (Figure 5). This ratio may be related to saddle distortion of the former. In order to estimate the energy of the intermolecular interaction, the criterion proposed by Espinoza<sup>[37]</sup> was used:  $E=1/2V_{\text{BCP}}$ , where  $V_{\text{BCP}}$  is virial value at BCP. Total energies, evaluated in this way, correlate with number of intermolecular BCPs and are 59 and 79 kJ/mol for **H<sub>2</sub>Hp** and **CoHp**, respectively. Previously, the same approach to estimating the intermolecular interactions energy and its correlation with enthalpies of sublimation was used for metal complexes of etioporphyrin-III with Cu and VO.<sup>[36]</sup> In that work, ratio of these energies was similar for two investigated compounds, while in present work the differences are reproducible. So, this approach may be applied for a qualitative prediction of the sublimation enthalpies relation.

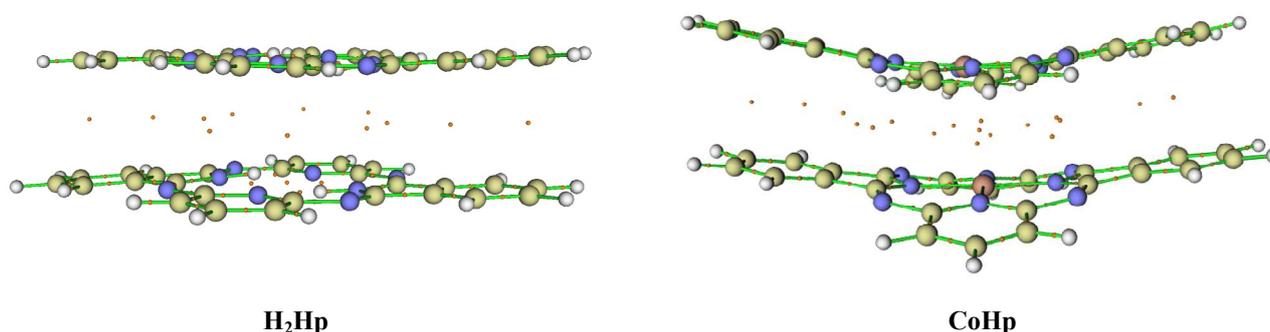
An important factor in determining the enthalpy of sublimation is the distance between two optimized molecules. The closer the molecules are located, the greater the energy of the intermolecular interaction, and the higher the enthalpy of sublimation. In this case, the distance between two molecules was evaluated as the distance between two quadrangles, formed by  $N_m$  atoms of each molecule (Figure 4a). In the case of **H<sub>2</sub>Hp** intermolecular distance is higher, 3.20 Å, while for **CoHp** it was determined to be 3.16 Å. Also, an important factor is that the **CoHp** molecules are saddle distorted and rotated relative to each other at an angle of 8.1°. The combination of these factors determines a stronger intermolecular interaction in the case of **CoHp** compared to **H<sub>2</sub>Hp** and predestinates a higher value of the enthalpy of sublimation.

## Conclusions

The mass spectra of cobalt(II) hemiporphyrzine were recorded at different ionization voltages, analyzed and compared with theoretical mass spectra. Theoretical simulating of the electron ionization mass spectra allowed us to assign the peaks in the experimental one with fragment ions of the studied complex. It was shown for theoretical mass spectra that changing of the ionization voltage results in different ratios of molecular and daughter

ions while it is typical situation for experimental data. The most intensive peak in mass spectra corresponds to molecular ion  $M^+$ .

The enthalpy of sublimation value for **CoHp** was determined using Clausius-Clapeyron relation and is 212(5) kJ/mol at temperature range of 481–544 K. The energy of intermolecular interactions was estimated for **H<sub>2</sub>Hp** and **CoHp** within the framework of QTAIM theory. The difference between these theoretical predictions and experimental enthalpies of sublimation for **H<sub>2</sub>Hp** and **CoHp** was about 20 kJ/mol in both cases. So, it was established that the higher value of enthalpy of sublimation for **CoHp** compared to **H<sub>2</sub>Hp** is related to higher energies of intermolecular interactions.



**Figure 5.** Location of bond critical points between two molecules.

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