contains the results showing the number of water molecules in the system near the first and second positions).

Table 3 (columns 4 and 6) also shows average numbers of water molecules located near the molecules of the dye during the calculations made **(Figures 6-13)**.

Table 3. Estimated number of water molecules in the solvation shells of Ind 1 and Ind 2.

Model	*r*, nm	Number of water molecules (CC-*H* atom)		Average number of water molecules (CC-*H* atom)	Number of water molecules (CC-*O* atom)	Average number of water molecules (CC-*O* atom)	
		position 1	position 2			position 1	position 2
RD	0.24	3/4	0/0	4/4	0/1	0/0	2/2
RDH	0.24	2/3	0/0	2/3	5/4	3/1	8/6
NPh	0.24	5/6	6/4	10/9	0/0	0/0	0/0
NPhH	0.24	2/2	5/4	6/6	1/0	0/0	1/1

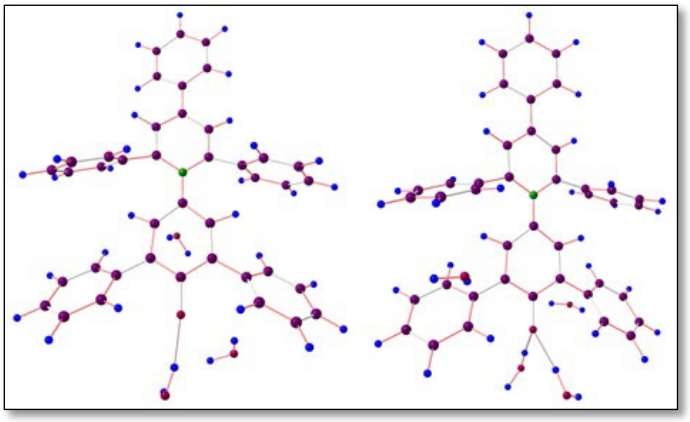

Figure 6. Hydrogen bonds for the RD model with the H water coordination center.

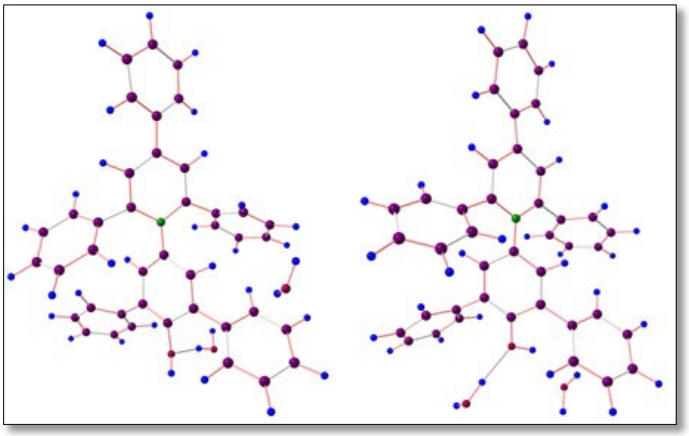

Figure 7. Hydrogen bonds for the RDH model with the H water coordination center.

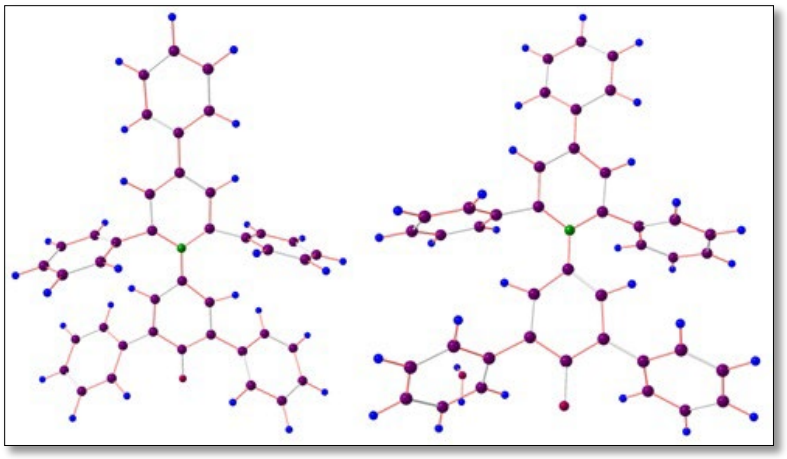

Figure 8. Hydrogen bonds for the RD model with the O water coordination center.

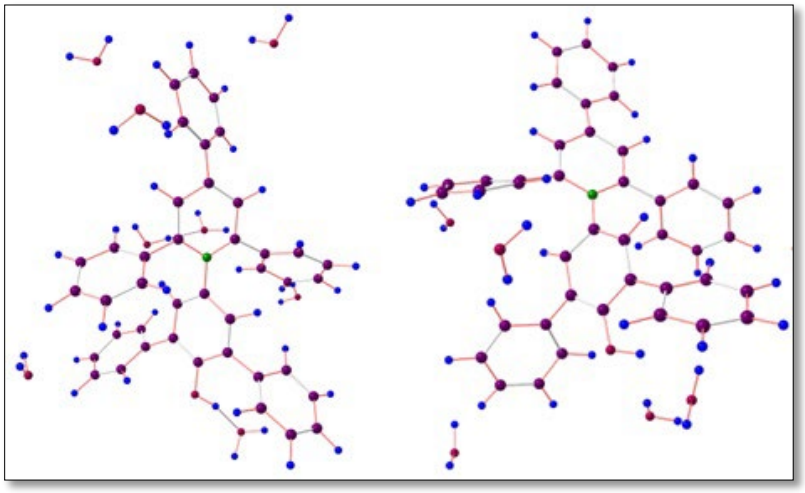

Figure 9. Hydrogen bonds for the RDH model with the O water coordination center.

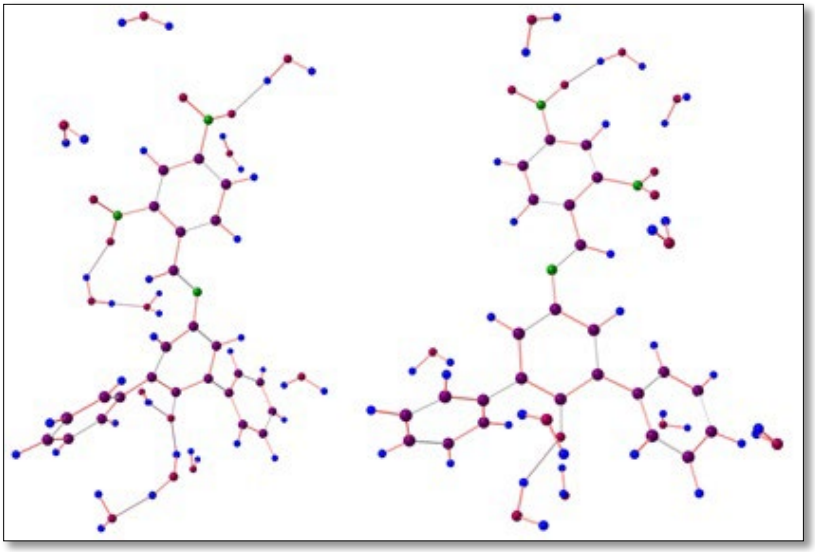

Figure 10. Hydrogen bonds for the NPh model with the H water coordination center.

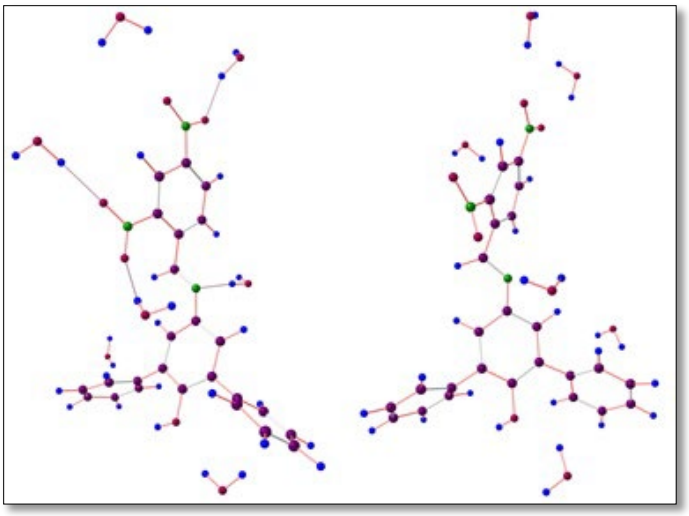

Figure 11. Hydrogen bonds for the NPhH model with the H water coordination center.

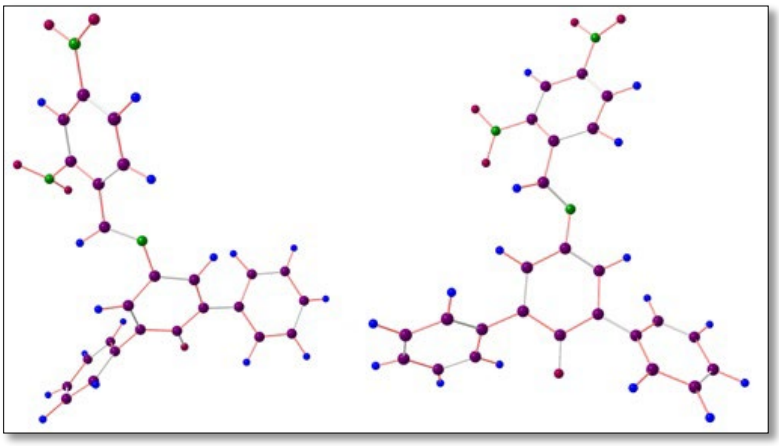

Figure 12. Hydrogen bonds for the NPh model with the O water coordination center.

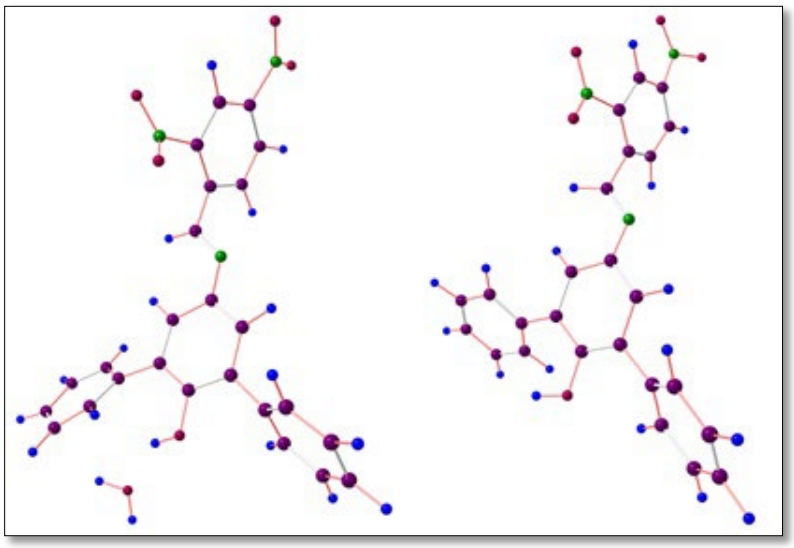

Figure 13. Hydrogen bonds for the NPhH model with the O water coordination center.

The following hydrogen bonds are found according to the results of this study:

1) Between water molecules with the coordination centers H and O atoms of both dyes

2) Between water molecules with the coordination centers H and π-systems of both dyes

3) Between water molecules with the coordination centers O and H atoms of both dyes.

Also, a specific hydrogen bond is found-between the water molecule and the atom N (in the third position) of the model NPhH, which is absent in the Reichardt's dye, probably because of the large loading of the molecule. On the other hand, this bond cannot affect the solvation, since the studied dyes "work" only in the deprotonated state, and no similar bonds are found in the deprotonated models.

Based on the results of simulation, we can state that both models of Ind 2 attract a larger number of water molecules into their solvation shells than the similar models of Ind 1. Also, proceeding from the results of simulation, we can confirm our conclusion about the results of the quantum chemical calculations that in Ind 2, 2 fragments participate in the hydration process during interaction with water-nitrogen-containing and phenol ones. It should be also stated that the molecular dynamics simulation also confirms the assumption that for Ind 2, position 3 does not influence the solvation, since we can observe the full absence of hydrogen bonds with this nitrogen atom in the solvation shell of the deprotonated model of the dye.

CONCLUSION

The influence of solvation of a molecule of the dye Ind 2 on the absorption wavelength is studied by the quantum chemical calculations using the PCM method with water solvent. These studies show that Ind 2 is solvated by water molecules primarily by the nitrogen-containing fragment with the participation of the phenolic fragment, while Ind 1 is solvated by the phenolic fragment only. Due to this, these dyes have different mechanisms of interaction with water.

Hydration in position 1 decreases the absorption wavelength (667.13 => 599.12), and protonation decreases it a lot (to 385.7 nm), which corresponds to experimental observations. Hydration in position 2 increases the absorption wavelength (667.13 => 695.49 for a water molecule). The experimentally determined absorption wavelength corresponds to the hydration by a water molecule of position 1 and four molecules of position 2. In general, the phenol fragment (position 1) is hydrated first as it is seen from the fact that a hydrogen atom in the neutral (protonated) form attaches to it. However, hydration of the dinitrophenol fragment (position 2) has a greater influence on the absorption wavelength. In pure water, the dye is present in the form of an anion hydrated by 5 water molecules: $NPh^{-}+1H_2O(1)+ 4H_2O(2)$, 1 molecule in position 1 and 4 molecules in position 2. The solvation shells of Ind 1 and Ind 2 are studied using the molecular dynamics simulation, which detects specific interactions, namely, hydrogen bonds, between the molecules of the dyes and water. It is also found that Ind 2 attracts water molecules into its solvation shell stronger than Ind 1. The simulation confirms the assumptions made on the basis of the quantum chemical calculations.

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