

## EFFECT OF n-PARAFFINS ON LOW-TEMPERATURE PROPERTIES OF DIESEL FUEL WITH DEPRESSOR ADDITIVES

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According to the data presented in [1, 2], from 2017 to 2021, an increase in the production and consumption of diesel fuel (DF) can be observed. Despite this, the issue of increasing the production of DF with optimal low-temperature properties for the regions of the Far North and Siberia is still relevant. The most economically and technologically advantageous way to obtain cold test DF is the addition of depressor additives (depressors).

There are several theories of the mechanism of depressor additives action, but they are all based on the interaction of the depressor molecule and the n-paraffin crystal. The effectiveness of the depressor depends on how heavy n-paraffins in the composition of DF fall out in the form of the first crystals. The creation of artificial crystallization centers due to the introduction of heavier petroleum n-paraffins activates the action of the additive, thus preventing the growth of crystals of n-paraffins that are part of the fuel.

The paper considers the low-temperature properties of mixtures of straight-run DF with a depressor, as well as an additional concentration of n-paraffins (0.05; 0.10; 0.25; 0.50 % by weight). The determination of the Cloud Point (Cp), Cold Filter Plugging Point and Pour point (Pp) was carried out according to the methods described in [3, 4, 5]. The results are presented in Table 1.

According to the data presented in Table 1, a sample of straight-run DF with an additive corresponds to the off-season brand [6], which indicates the inexpediency of using this fuel at lower temperatures.

It can also be seen that the nature of the effect on the effectiveness of the additive significantly depends on the concentration of additional paraffins. So, when adding n-paraffins in concentrations of 0.10–0.50 % by weight, we can talk about a negative effect on the effectiveness of the additive in relation to all low-temperature properties. However, when the concentration of the added n-paraffins is 0.05 % by weight, there is an improvement in the effectiveness of the additive with respect to Cp ( $\Delta 1$  °C) and CFPP ( $\Delta 2$  °C).

The observed effect can be explained as follows: the addition of 0.05 % by weight of n-paraffins creates the optimal number of additional crystallization centers, which contribute to a more efficient action of the additive. At concentrations of 0.10–0.50 % by weight the number of additional crystallization centers becomes excessive and the depressor molecules do not stop the growth of all n-paraffins crystals, which contributes to a negative effect on the low-temperature properties of the DT/depressor mixture.

**Table 1.** Effect of additional concentrations of n-paraffins on the low-temperature properties of the DT/depressor mixture

Concentration of n-paraffins, % by weight	Cp	$\Delta$ Cp	CFPP	$\Delta$ CFPP	Pp	$\Delta$ Pp
	°C					
<b>0.00</b>	<b>–6</b>		<b>–20</b>		<b>–38</b>	
0.50	–2	4	–3	17	–36	2
0.25	–3	3	–6	14	–35	3
0.10	–5	1	–13	7	–34	4
0.05	–7	1	–22	2	–36	2

### References

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## THEORETICAL STUDY OF THE PHOTOCHEMICAL AND PHOTOPHYSICAL PROPERTIES OF BENZIMIDAZOLE-BASED ESIPT-FLUOROPHORES USING STATE-OF-THE-ART QUANTUM CHEMICAL METHODS

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Molecules featuring short intramolecular hydrogen bonds of the O–H···N, O–H···O and N–H···N types tend to show excited state intramolecular proton transfer (ESIPT), one of the simplest photochemical reactions (Fig. 1). The emission properties associated with excited state intramolecular proton transfer (ESIPT) were theoretically studied in solution and in the solid state for a series of 2-(2'-hydroxyphenyl)benzimidazole-based (HBI) ESIPT-fluorophores **3a** – **3e** having different halogen substituents in the *ortho*- and *para*-positions to the proton-donating hydroxy group (Fig. 2). DFT and TDDFT computations were performed for understanding experimental trends in the absorption and fluorescence spectra on going from a

non-halogenated compound **3a** to monohalogenated compounds **3b**–**3d** and a dihalogenated compound **3e**. Both implicit and explicit solvent models were employed to simulate the photochemistry of **3a**–**3e** in solution, while QM/MM calculations with two-layer ONIOM model were carried out to reveal peculiarities of fluorescence in the solid state. All computations are in excellent agreement with the experimental data, thus validating the chosen level of theory B3LYP/6-31+g(d,p).

Quantum chemical calculations identified an interplay of solvent and halogen atoms as a factor controlling the photophysics and photochemistry of ESIPT-fluorophores **3a**–**3e**. ESIPT and emission from the keto form can be observed in solution if at

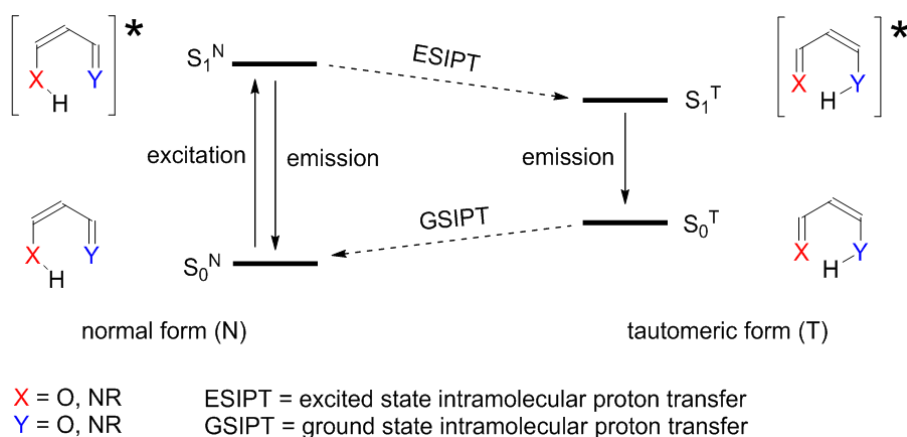


Fig. 1. Typical photocycle in ESIPT-fluorophores