Supporting Information

Optical behavior of conjugated Pt-containing polymetallaynes exposed to gamma-ray radiation doses

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UV absorption and emission characteristics of Pt-DEBP polymer and related molecules

Table 1: UV data

sample	Absorption (nm)	Emission (nm)
DEBP	303	340
trans-$PtCl_2(PBu_3)_2$	250+265	324
Pt_2-DEBP	340	390
Pt-DEBP	375	420

DEBP = H-C≡C-C_6H_4-C_6H_4-C≡C-H

Pt_2-DEBP = Cl-Pt$(PBu_3)_2$-C≡C-C_6H_4-C_6H_4-C≡C- Pt$(PBu_3)_2$Cl

Pt-DEBP = [-Pt$(PBu_3)_2$-C≡C-C_6H_4-C_6H_4-C≡C-]$_n$,

Figure 1: UV-vis absorption and emission in $CHCl_3$ of DEBP and $PtCl_2(PBu_3)_2$

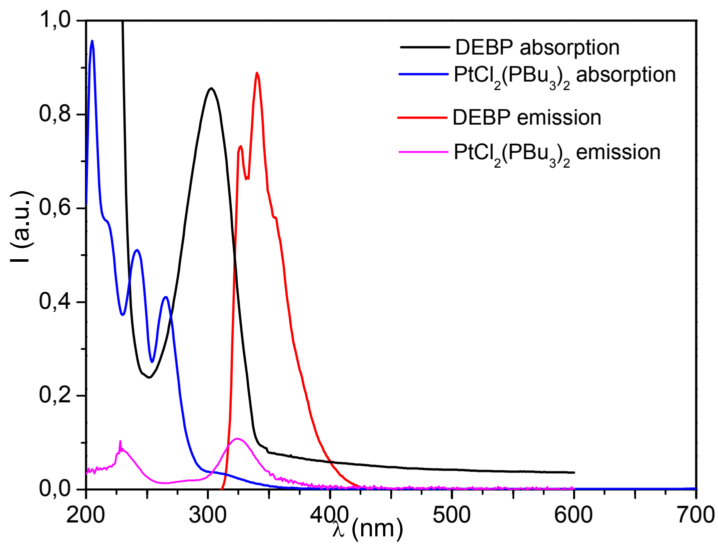


Figure 2: UV-vis absorption and emission of Pt-DEBP in $CHCl_3$

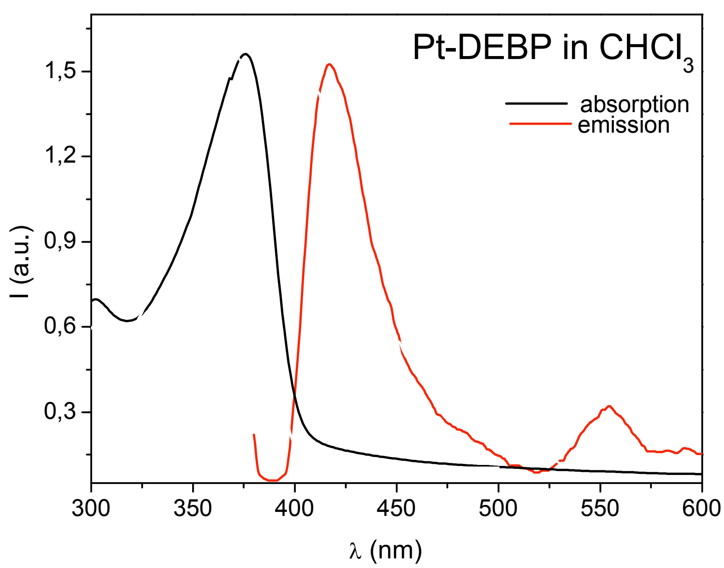


Figure 3: Optical absorption spectra of Pt-DEBP in toluene before and after irradiation with γ rays at different radiation doses (C = 0.0500 mg/mL).

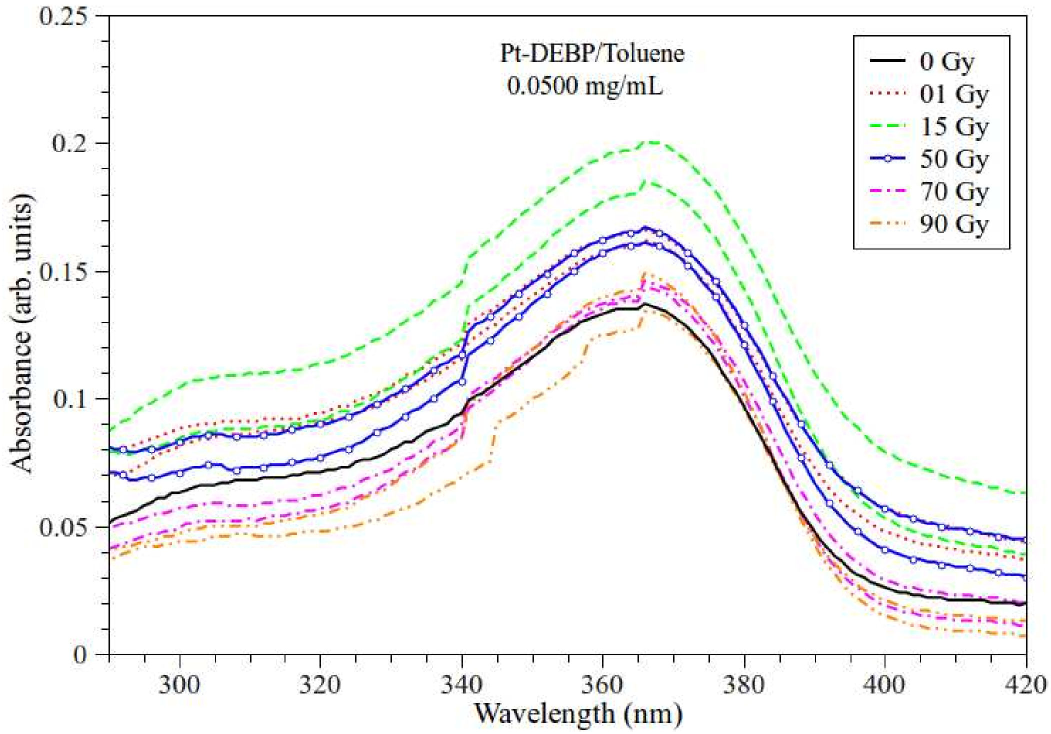


Figure 4: Emission spectra of the samples of Pt-DEBP in toluene before and after irradiation at different doses (C=0.0375 mg/mL).

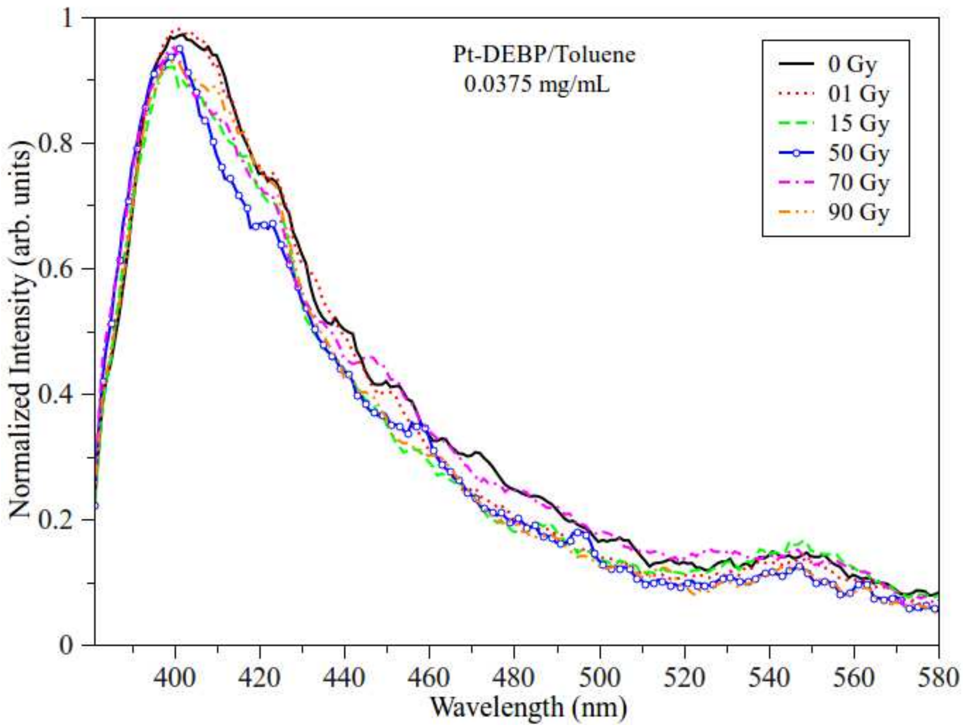
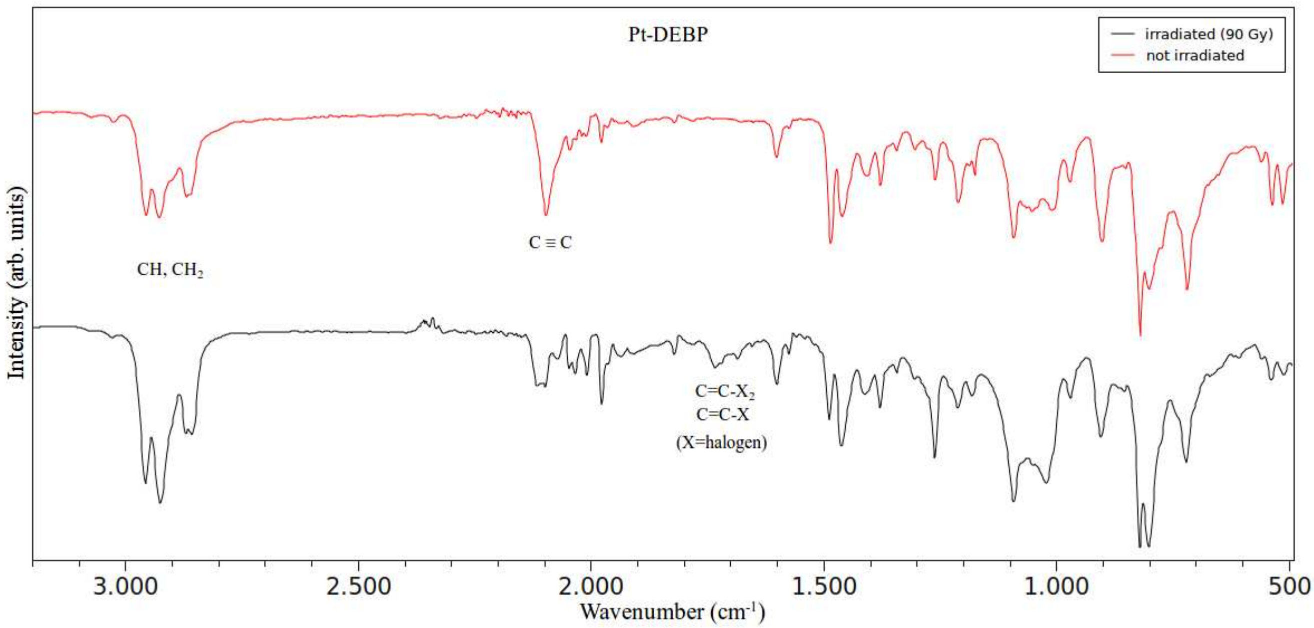


Figure 5: FTIR spectra of gamma ray irradiated and non irradiated Pt-DEBP.



Dosimetry data

Table 1 presents the linear regressions results for each solution concentration. In all cases we obtain a correlation parameter $R^2 \geq 0.969$. The data point related to 90 Gy on samples with 0.0113 mg/mL was disregarded in the regression, since it is apparently related to saturation effects.

$$\lambda_{max} = a_C . D + b \qquad (1)$$

Table 1. Regression results.

Concentration (mg/mL)	Regression Parameters	
	a_C (nm/Gy)	b (nm)
0.0500	-0.319455	374.040
0.0375	-0.377945	372.893
0.0250	-0.436436	373.746
0.0113	-0.506483	373.180

In equation 1, D represents the radiation dose; a_C and b are the angular and linear coefficients, and a_C has a dependency on the solutions concentration (C). A linear relationship between a_C and C are observed (R^2=0.9995) and can be expressed by:

$$a_C = \alpha . C + \beta \qquad (2)$$

where $\alpha = 4.81474 \left(\frac{nm}{Gy(mg/mL)} \right)$ and $\beta = -0.559035\,(nm/Gy)$.

Thus, we can express λ_{max}, in an approximate way, as a function of the dose employed and solutions concentration through:

$$\lambda_{max} = 4.81474(C.D) - 0.559035(D) + \lambda^0_{max} \qquad (3)$$

where $\lambda^0{}_{max}$ = 373.465 (nm), the average value of b parameters presented in Table 1, related to peak position of non-irradiated samples.