

Solid State Double [2+2] Photochemical Reactions in the Co-crystal forms of 1,5-bis(4-pyridyl)-1,4-pentadiene-3-one: Establishing Mechanism Using Single Crystal X-ray, UV and  $^1\text{H}$  NMR.

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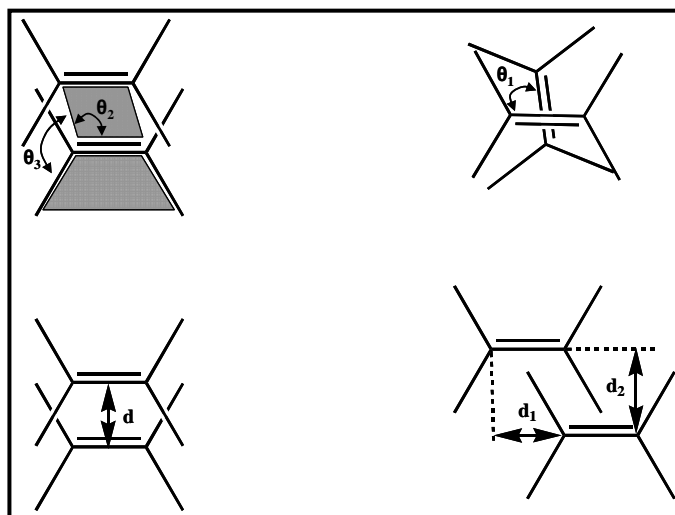
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*Supporting Information*

(Other geometrical parameters for all the reactive double bonds in the co-crystals,  
*IR spectra,  $^1\text{H}$  NMR spectra,  $^{13}\text{C}$  NMR spectra, XRPD patterns*)

Geometrical parameters for illustrating the deviations from ideal overlap of  $p$ -orbitals of reactive double bonds.<sup>1</sup>



**Scheme 1.** Different geometrical parameters for the  $\pi$  orbitals overlap.

**Table 1:** Geometrical parameters for double bond orientation in compounds **1P**, **3-7**.

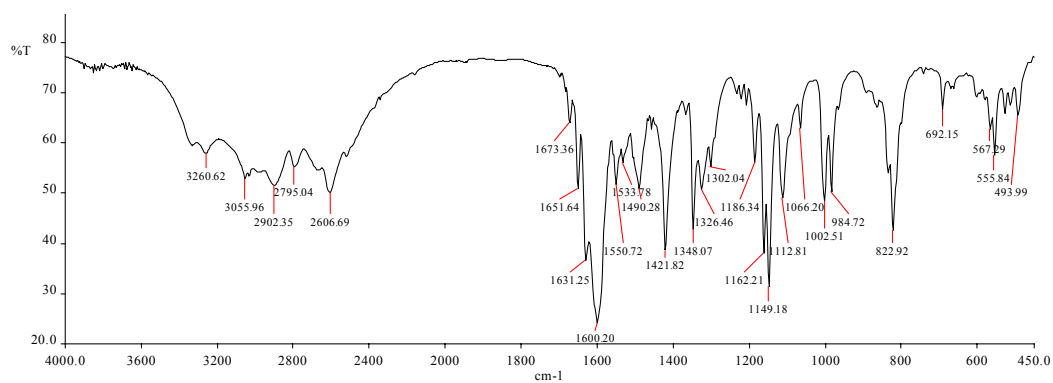
References:

1. K. Gnanaguru, N. Ramasubbu, K. Venkatesan, V. Ramamurthy, *J. Org. Chem.*, 1985, **50**, 2337-2346.

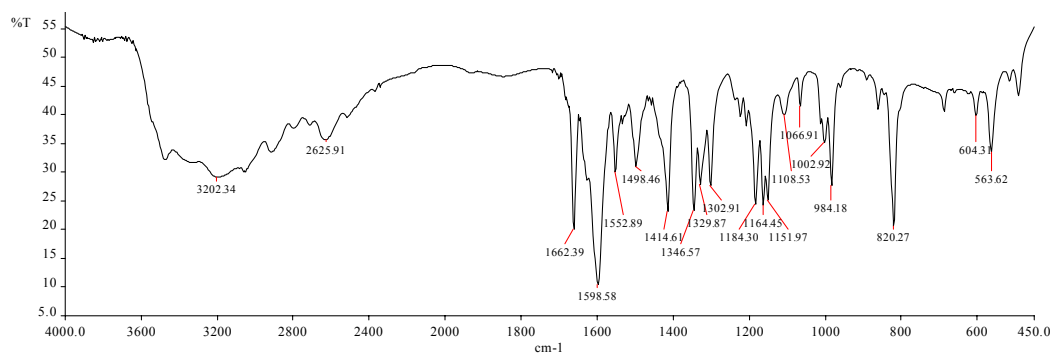
Comp.	Centroid to centroid distance $d$ , Å	$\theta_1$ , deg	$\theta_2$ , deg	$\theta_3$ , deg	Displacement of double bonds upon projection $d_1$ , Å $d_2$ , Å	
<b>1P</b>	3.888	0.00	91.97	67.82	0.306	3.886
<b>3</b>	3.724	3.63	101.6	81.95	0.567	3.853
<b>4</b>	Set-I: 3.622	2.62	113	86.6	1.389	3.65
	Set-II: 3.648	5.42	109.2	80.6	1.16	3.476
	Set-III: 3.672	4.05	107.35	72.45	1.069	3.703
	Set-IV: 3.662	3.69	115.72	88.32	1.676	3.515
<b>5</b>	Set-I: 3.683	3.16	95.88	87.47	1.606	3.499
	Set-II: 3.700	0.52	115.53	69.78	0.43	3.764
<b>6</b>	3.610	0.00	92.70	77.57	0.186	3.601
<b>7</b>	3.692	16.11	111.18	86.71	1.371	3.735

## IR Spectra

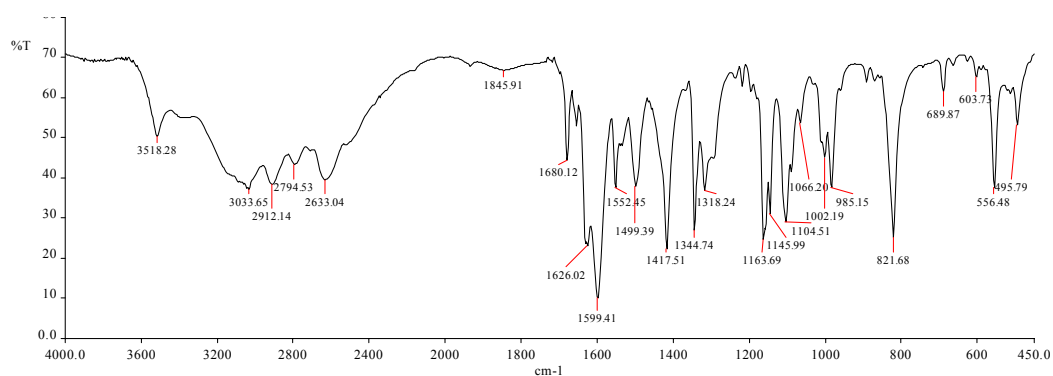
### Co-crystal 4:



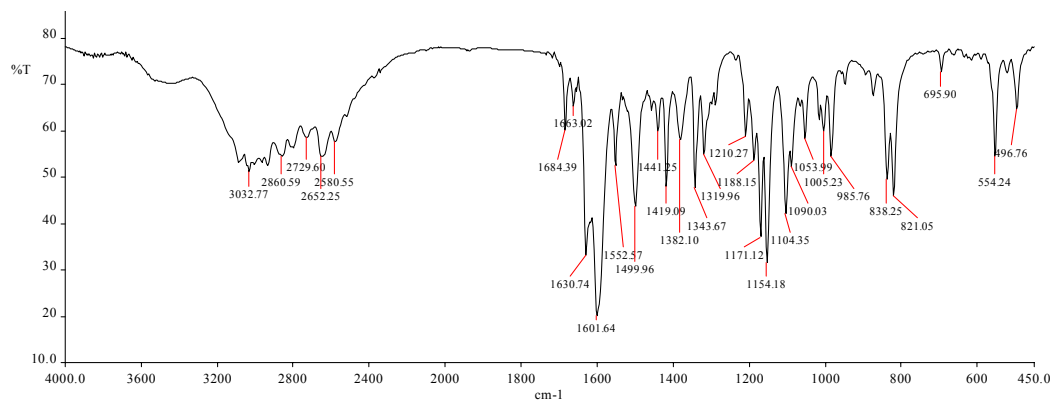
### Co-crystal 5:



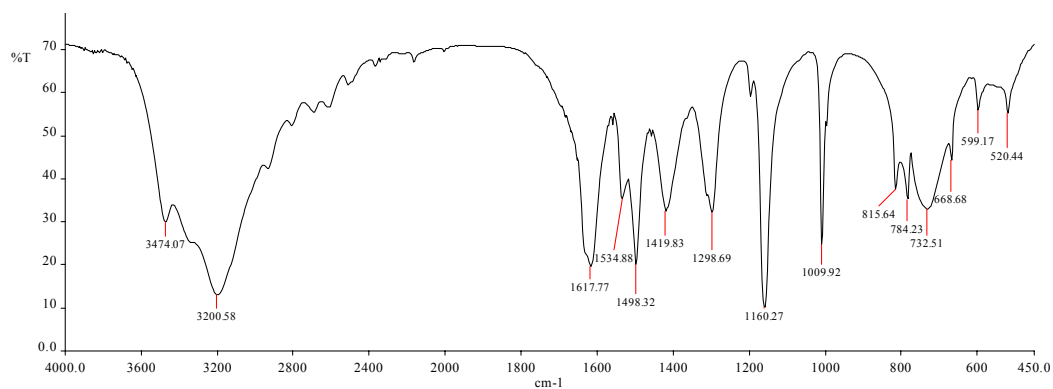
### Co-crystal 6:



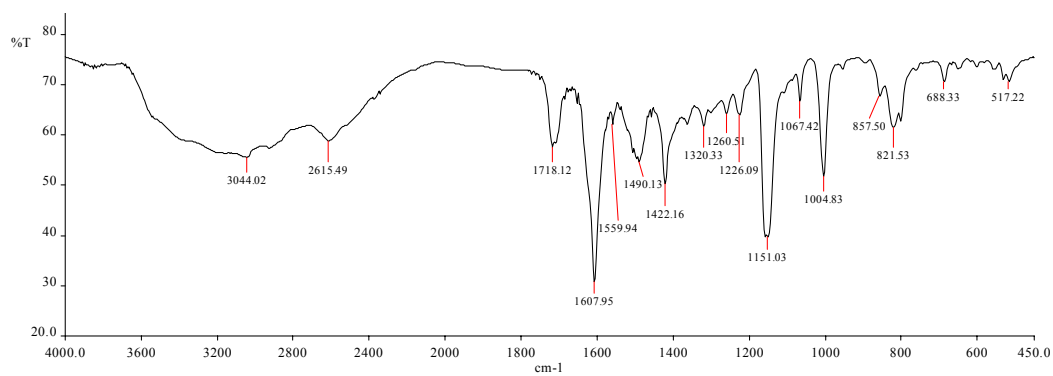
### Co-crystal 7:



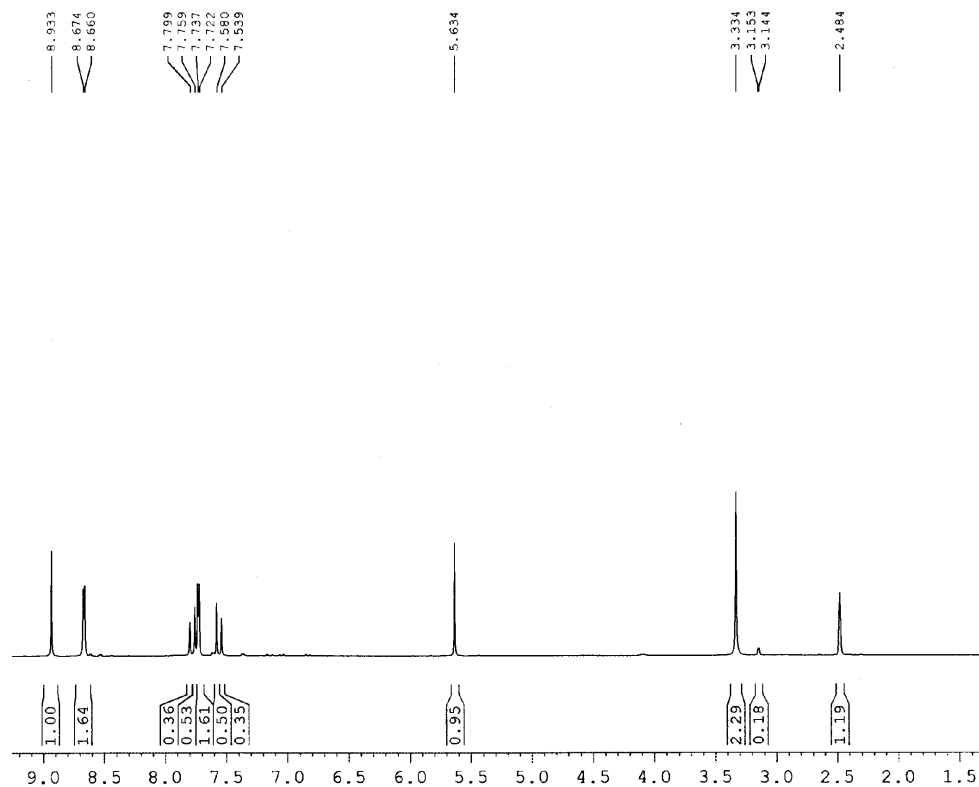
### Compound 8:



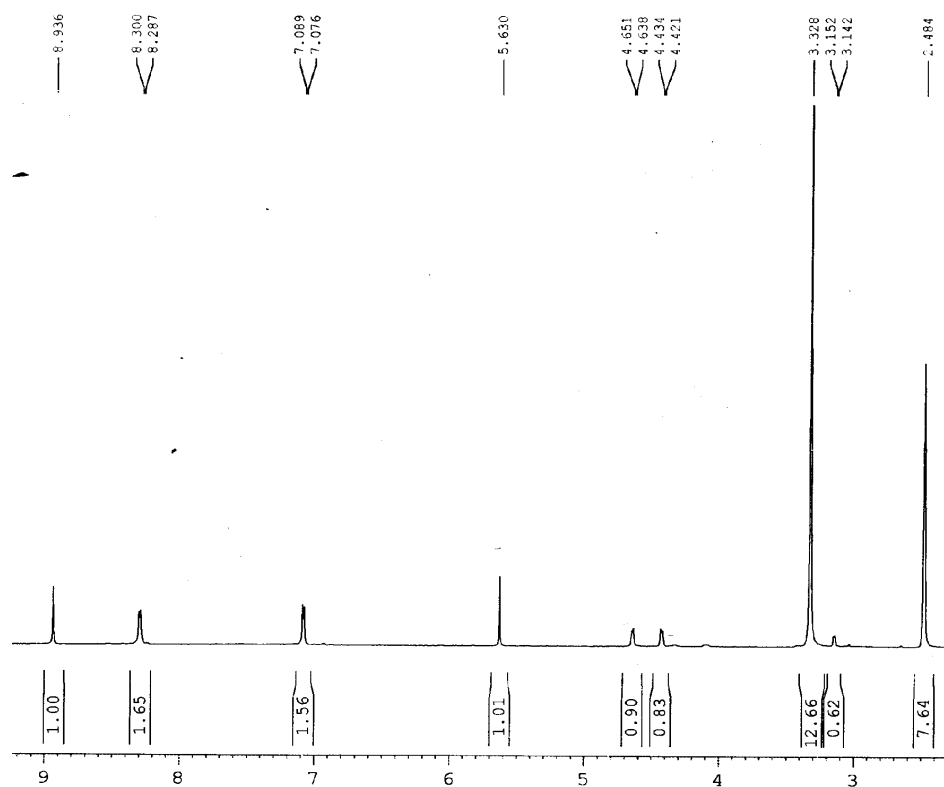
### Compound TCD:



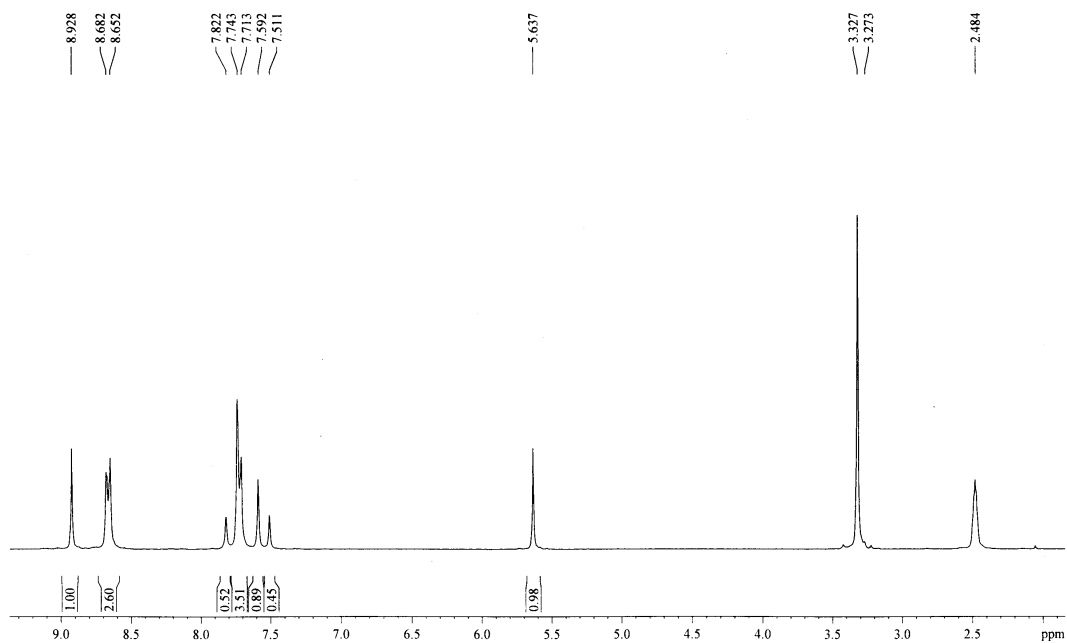
## <sup>1</sup>H NMR Spectra: Co-crystal 4:



## Irradiated co-crystal 4:

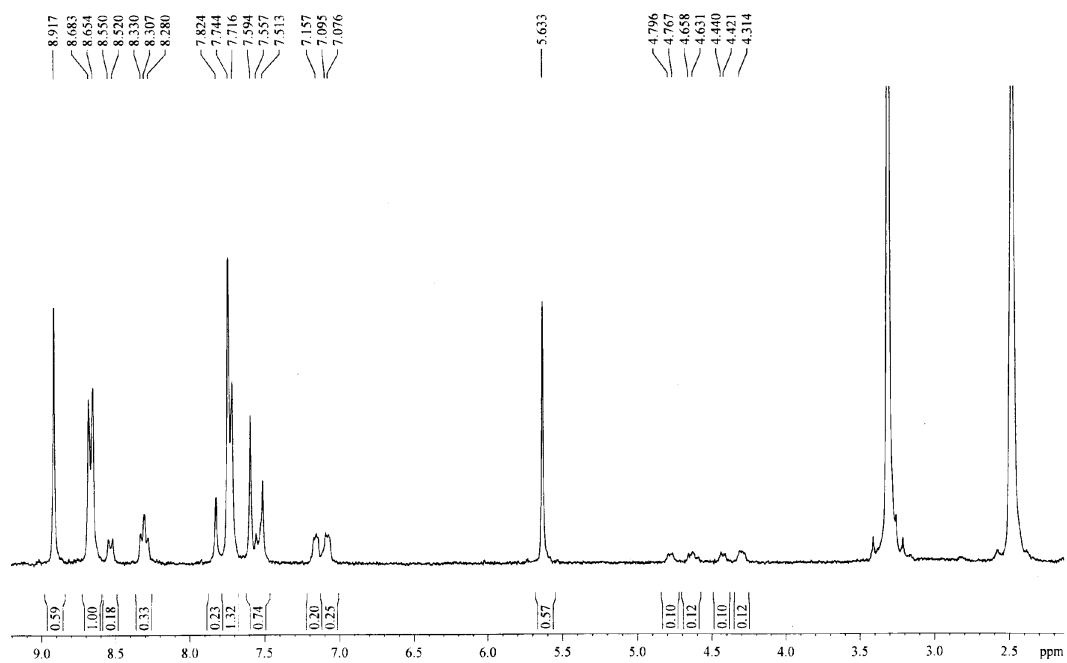


## Co-crystal 5:

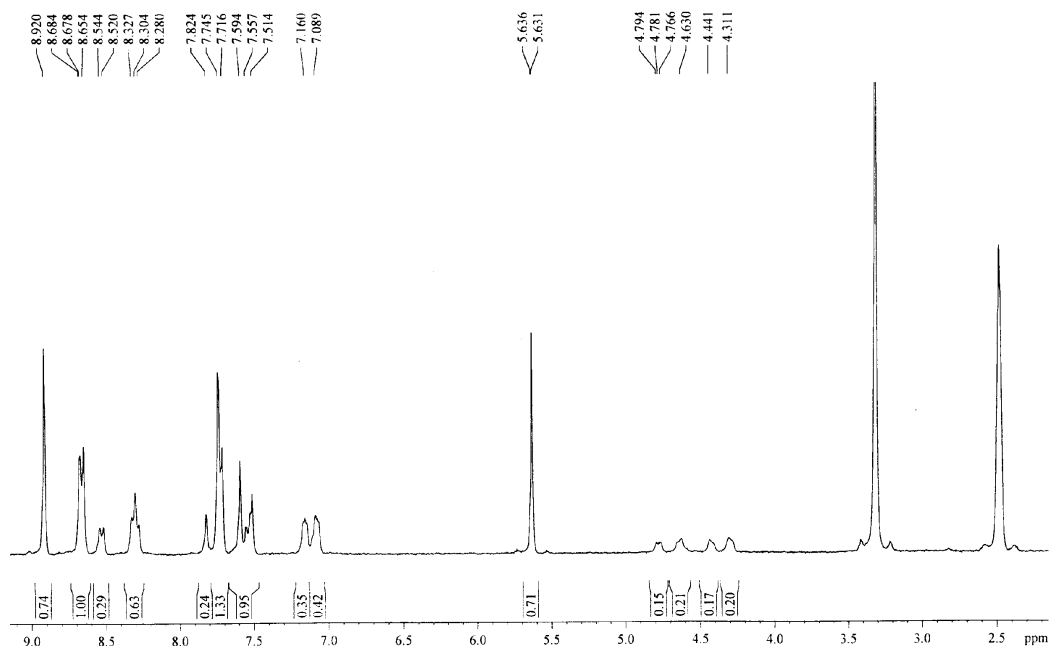


## Partially irradiated co-crystal 5 (b-d):

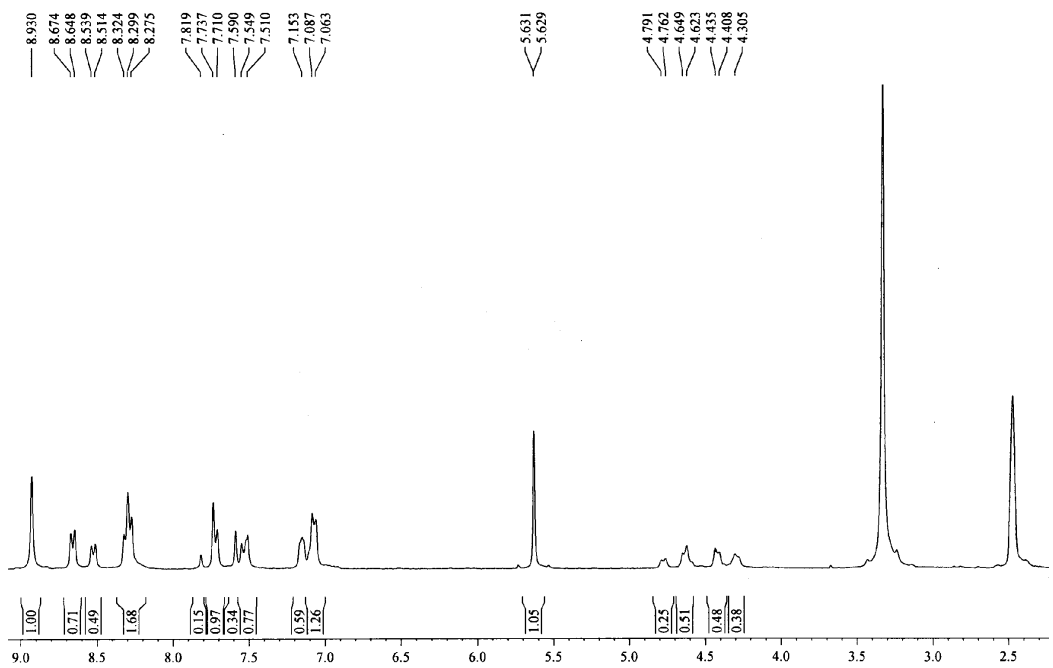
(b)



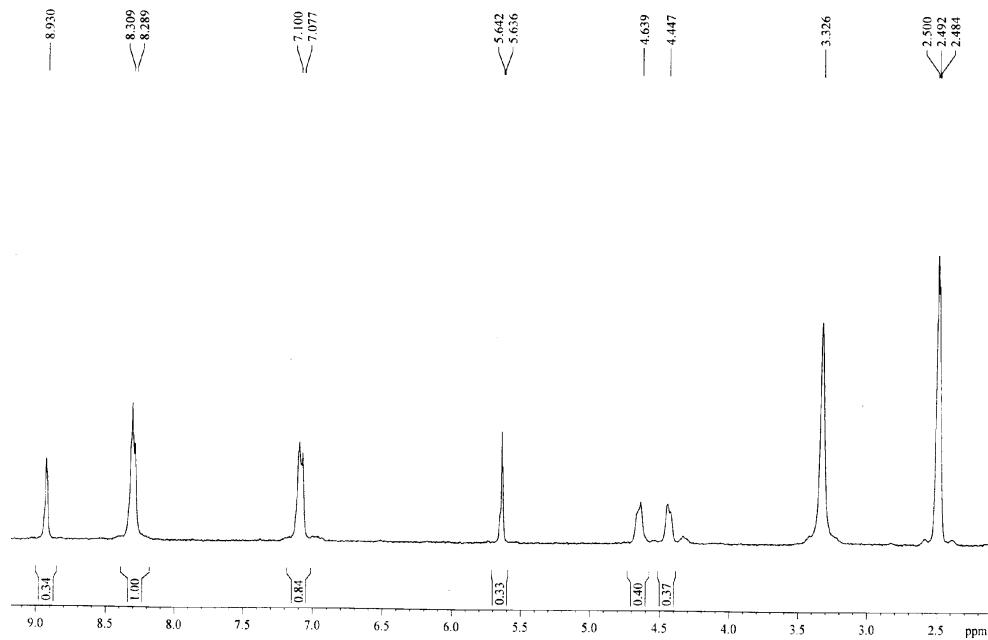
(c)



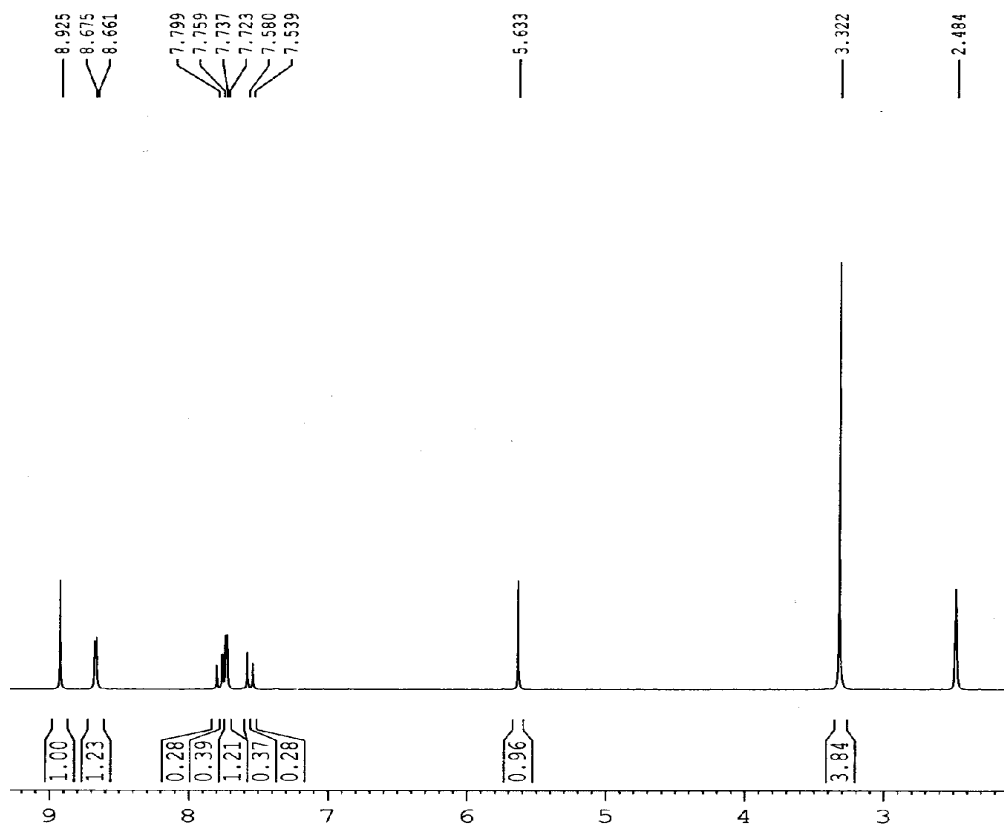
(d)



### Fully irradiated co-crystal 5:

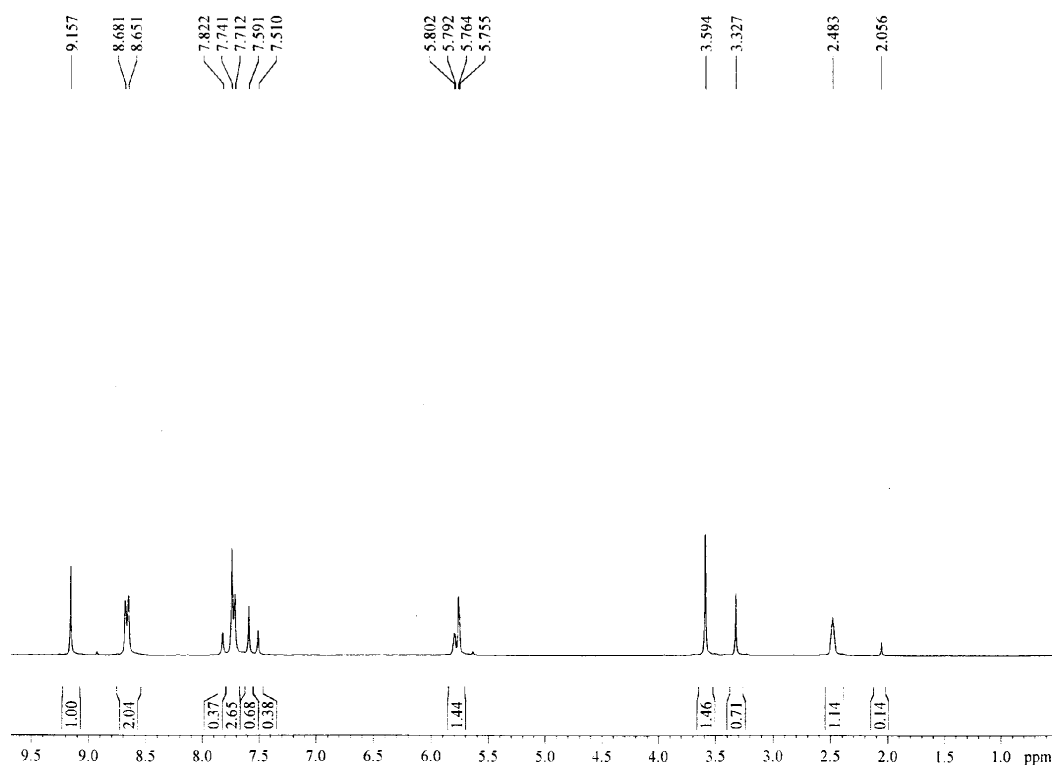


### Co-crystal 6:



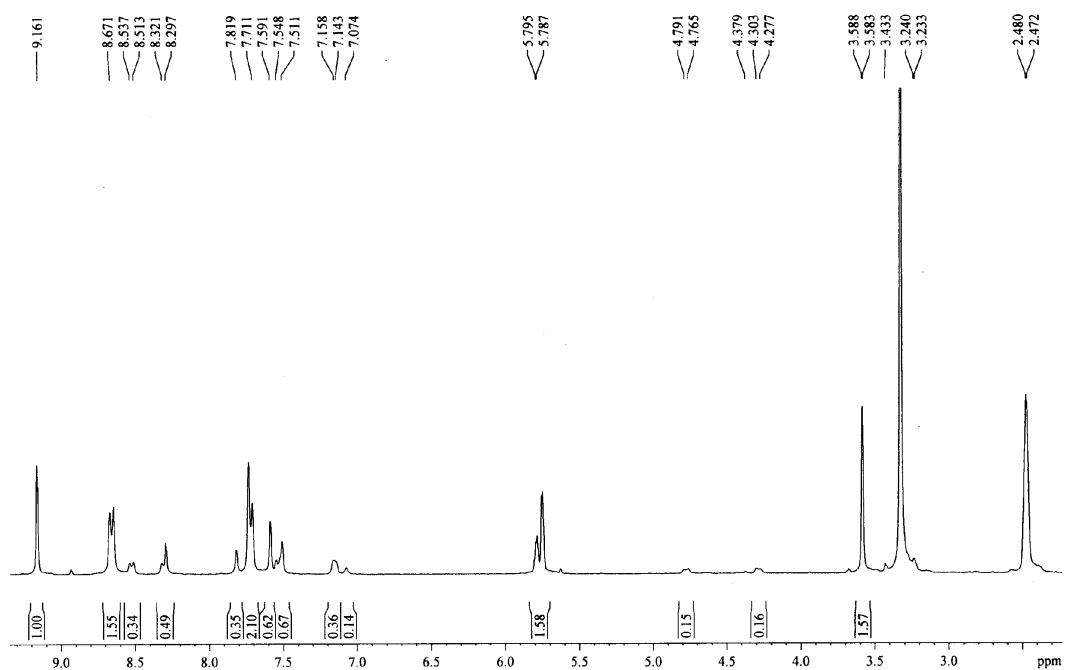


### Co-crystal 7:

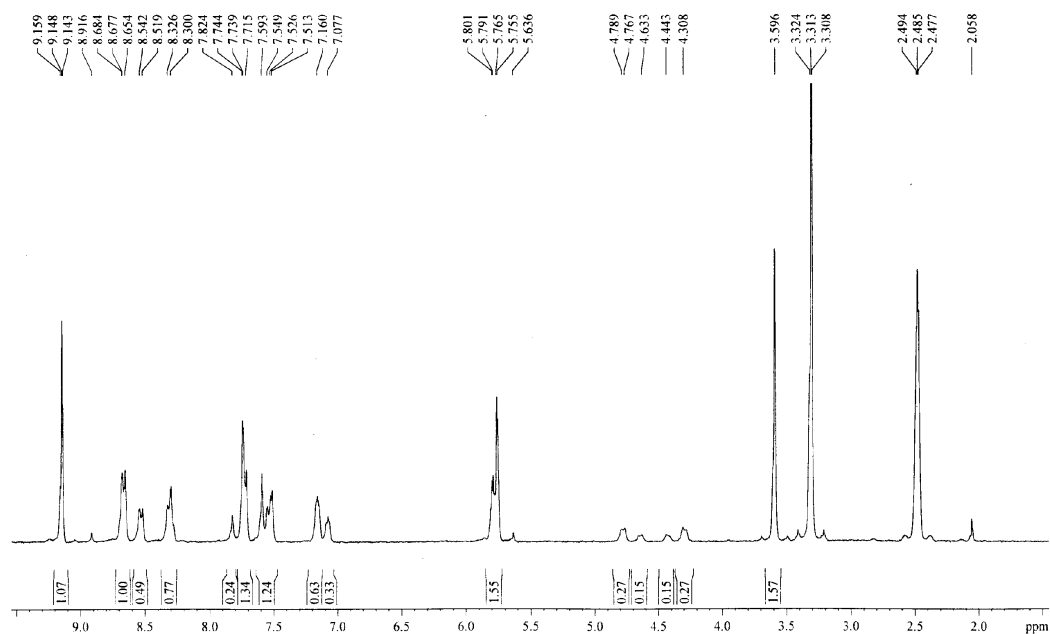


### Partially irradiated co-crystal 7 (b-e):

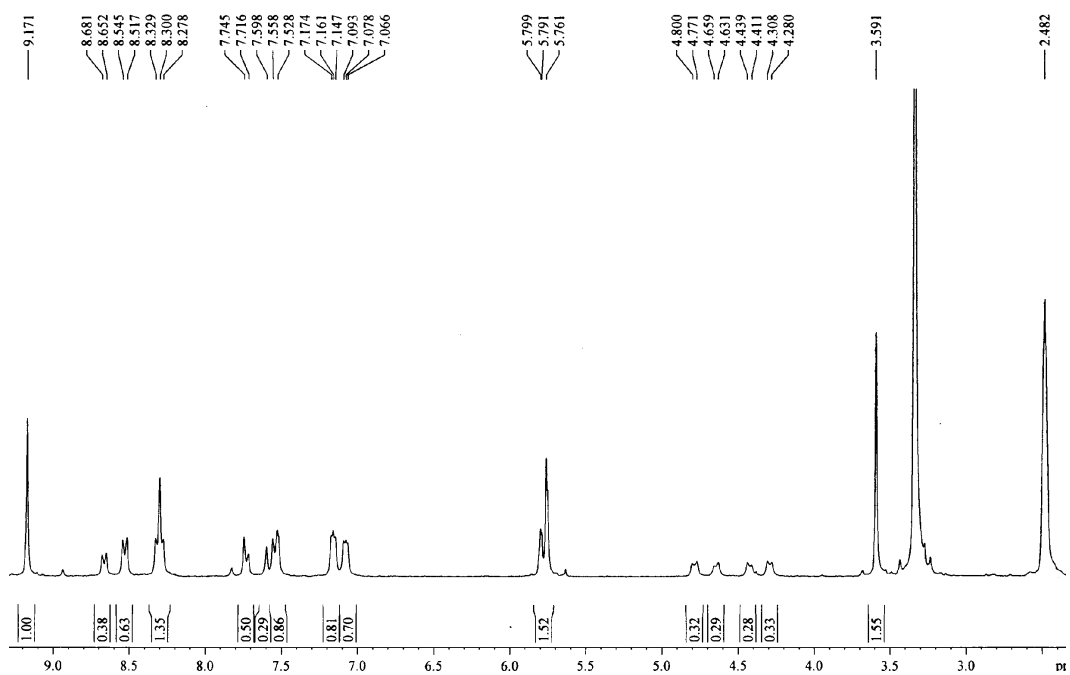
(b)



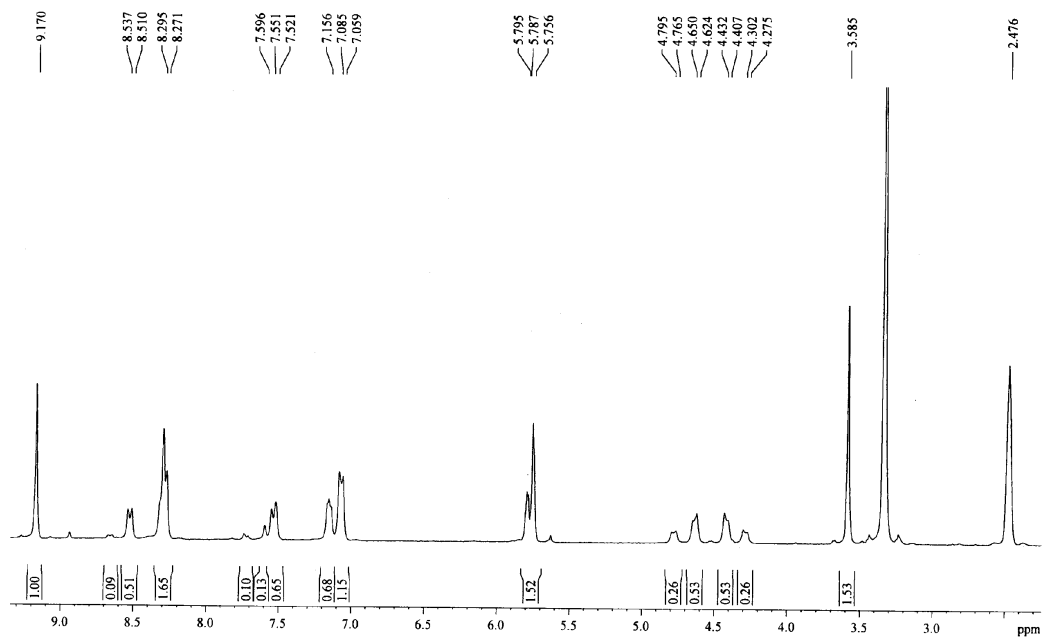
(c)



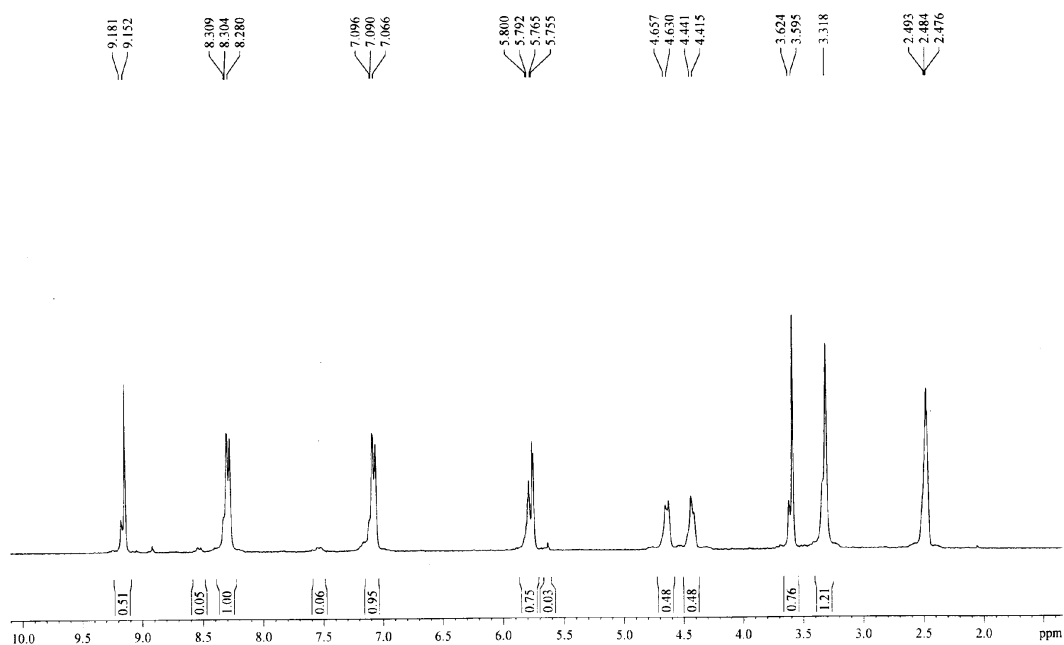
(d)



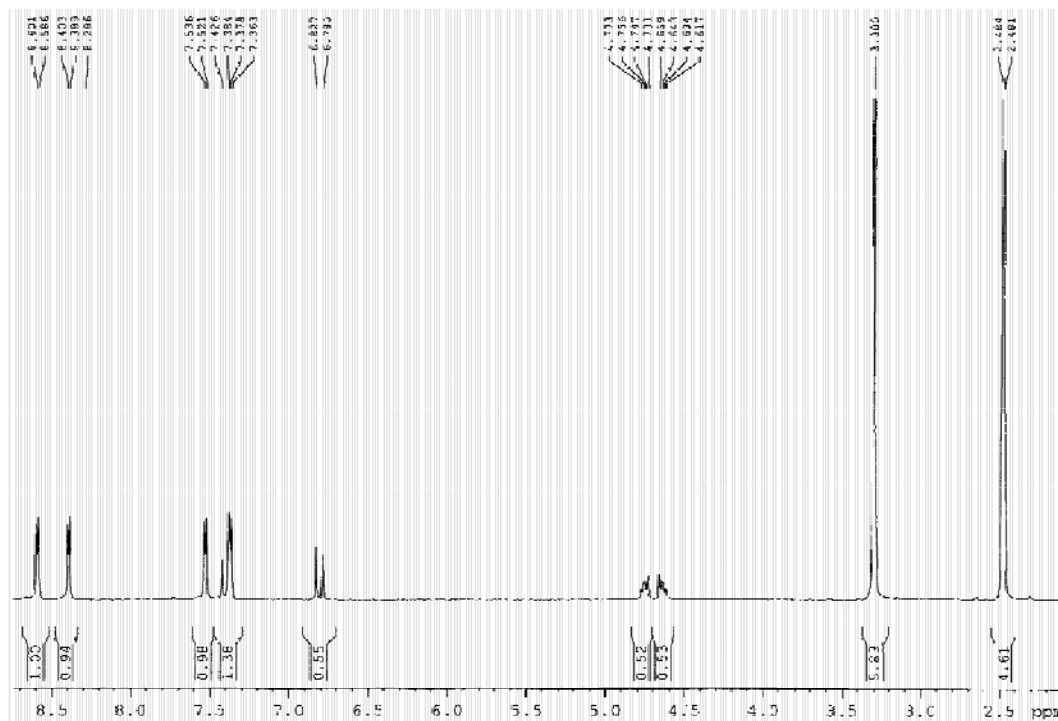
(e)



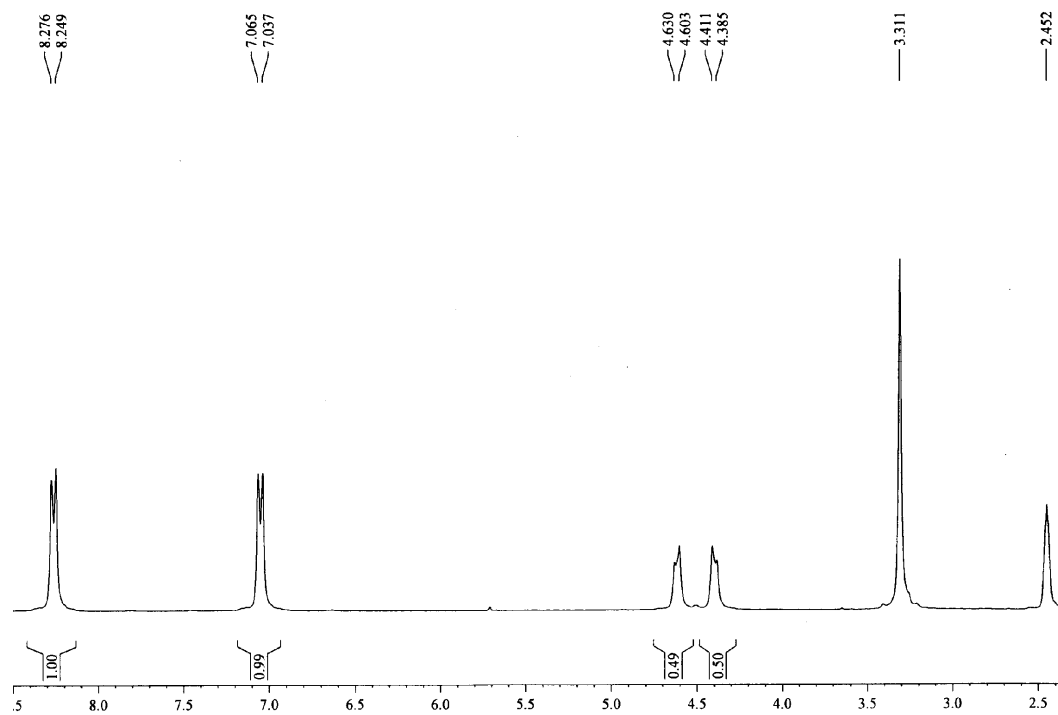
Fully irradiated co-crystal 7:



### Compound 8:

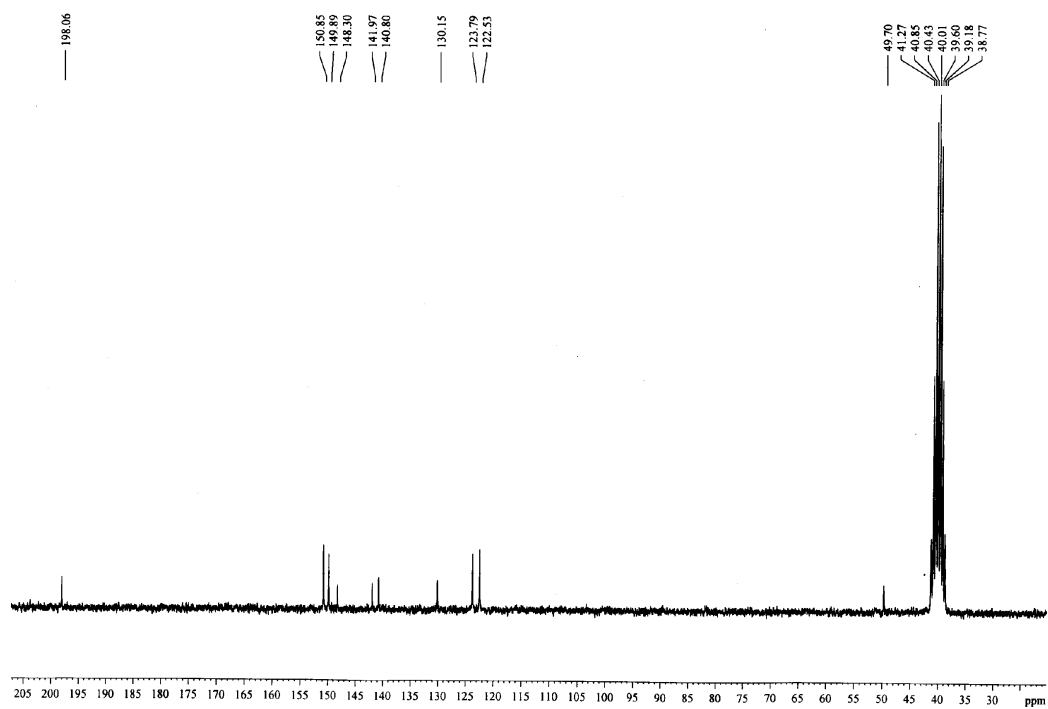


### Compound TCD:

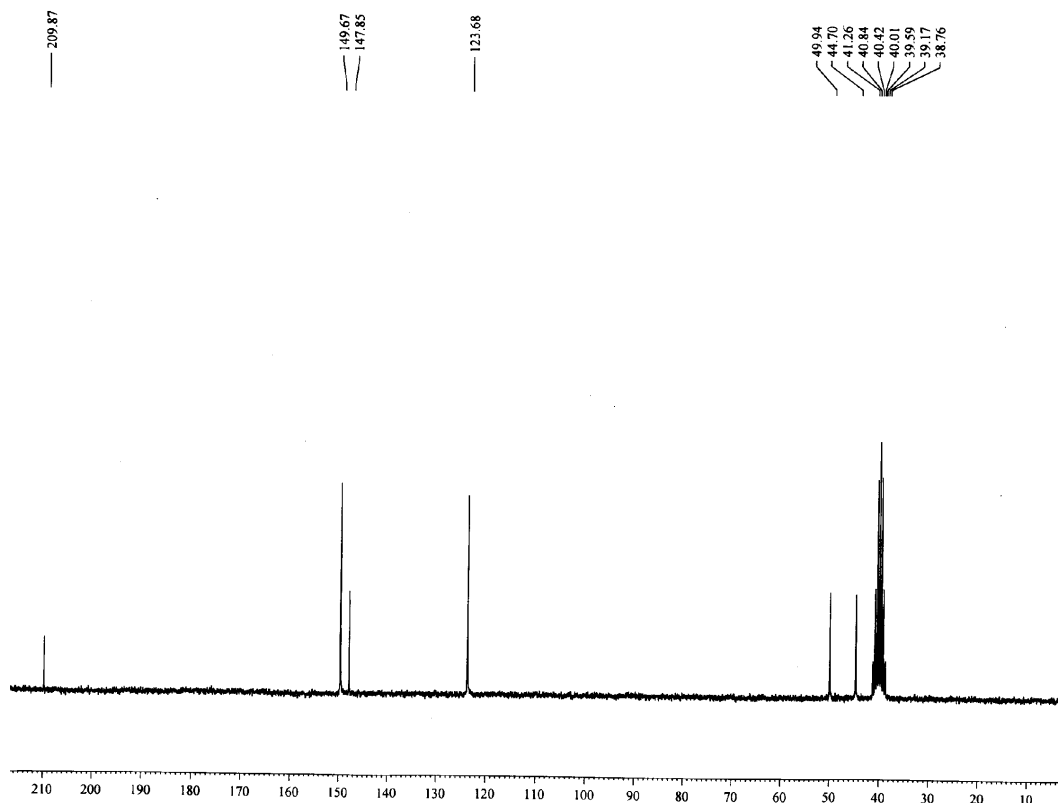


## <sup>13</sup>C NMR Spectra:

### Compound 8:

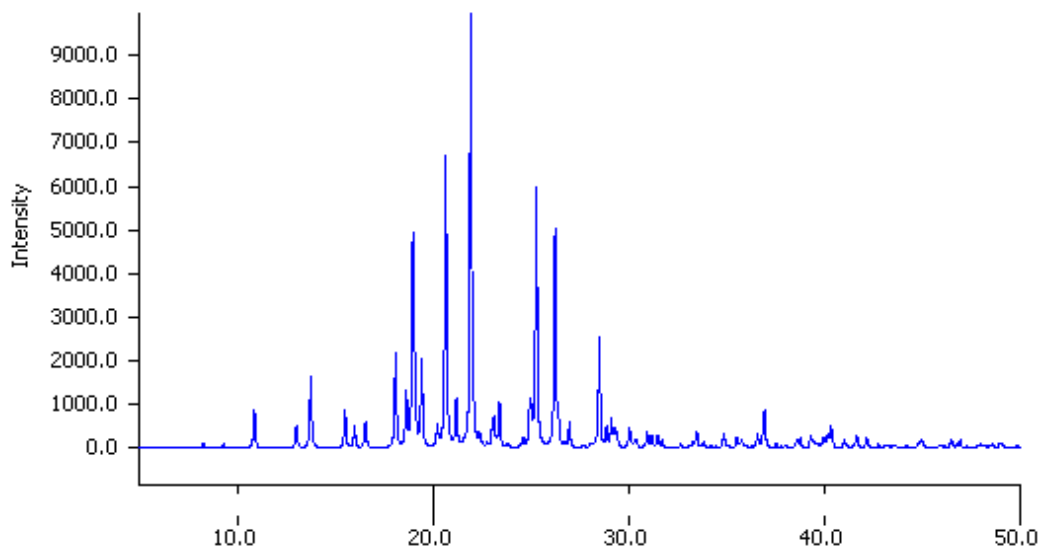


### Compound TCD:

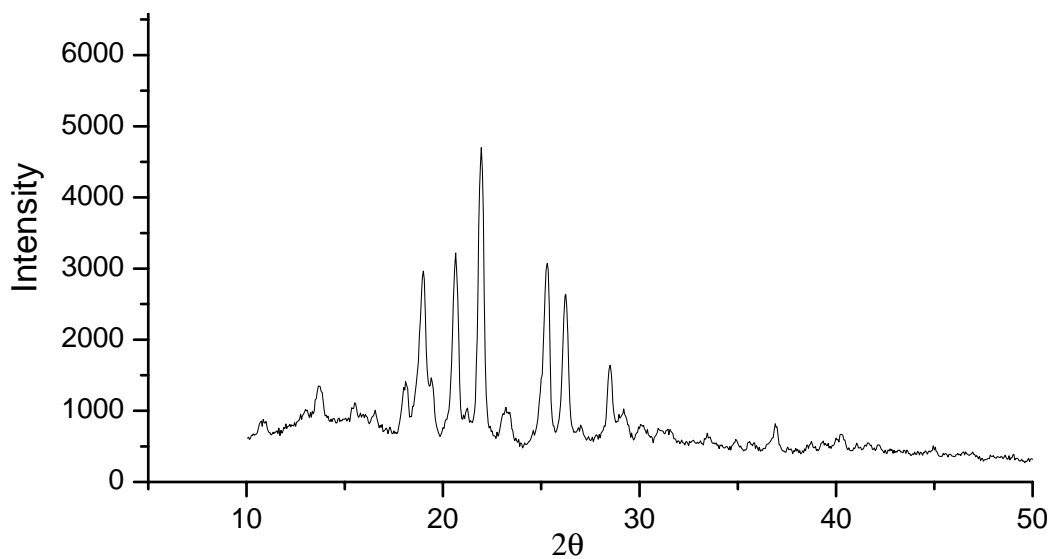


## **XRPD Patterns:**

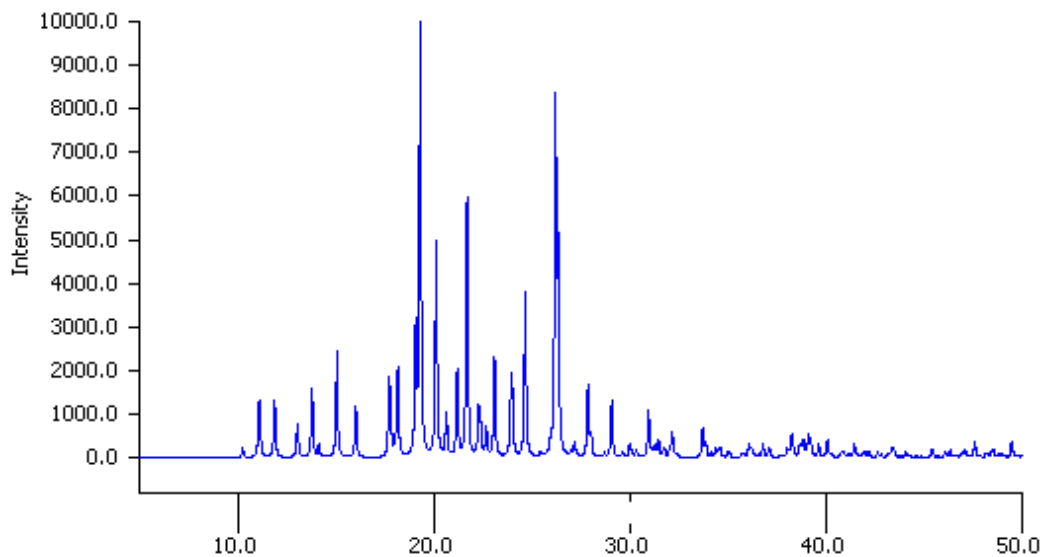
### Calculated XRPD Patterns of **2**:



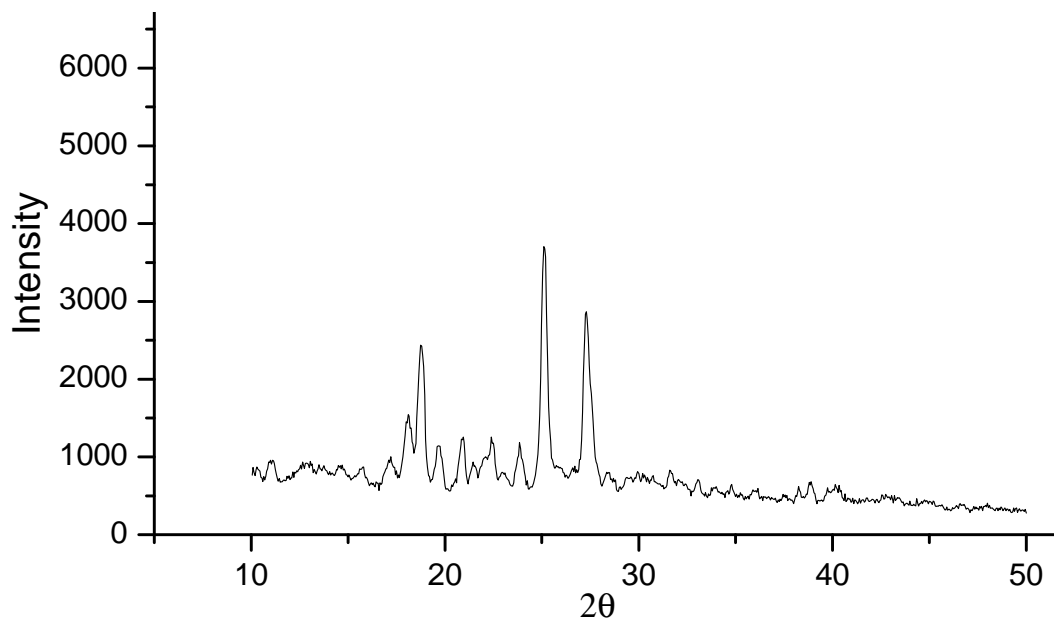
### XRPD Patterns for (1:1) co-grounded solid of **1P** & RN:



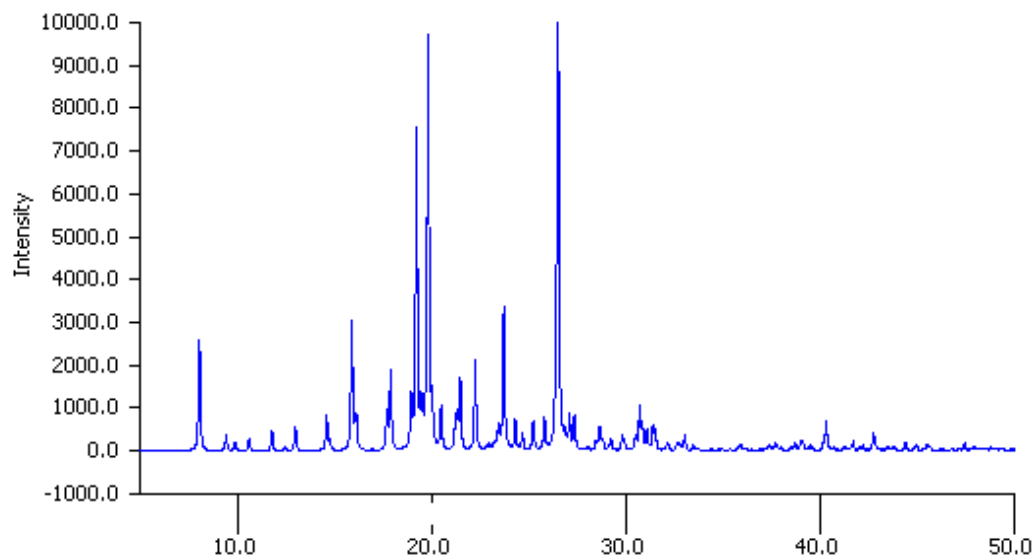
### Calculated XRPD Patterns of 6:



### XRPD Patterns for (1:1) co-grounded solid of 1P & PG:



### Calculated XRPD Patterns of 7:



### XRPD Patterns for (1:1) co-grounded solid of 1P & MR:

