

# Supporting information

## **Puckering behavior in six new phosphoric triamides containing aliphatic six- and seven-membered ring groups and a database survey of analogous ring-containing structures**

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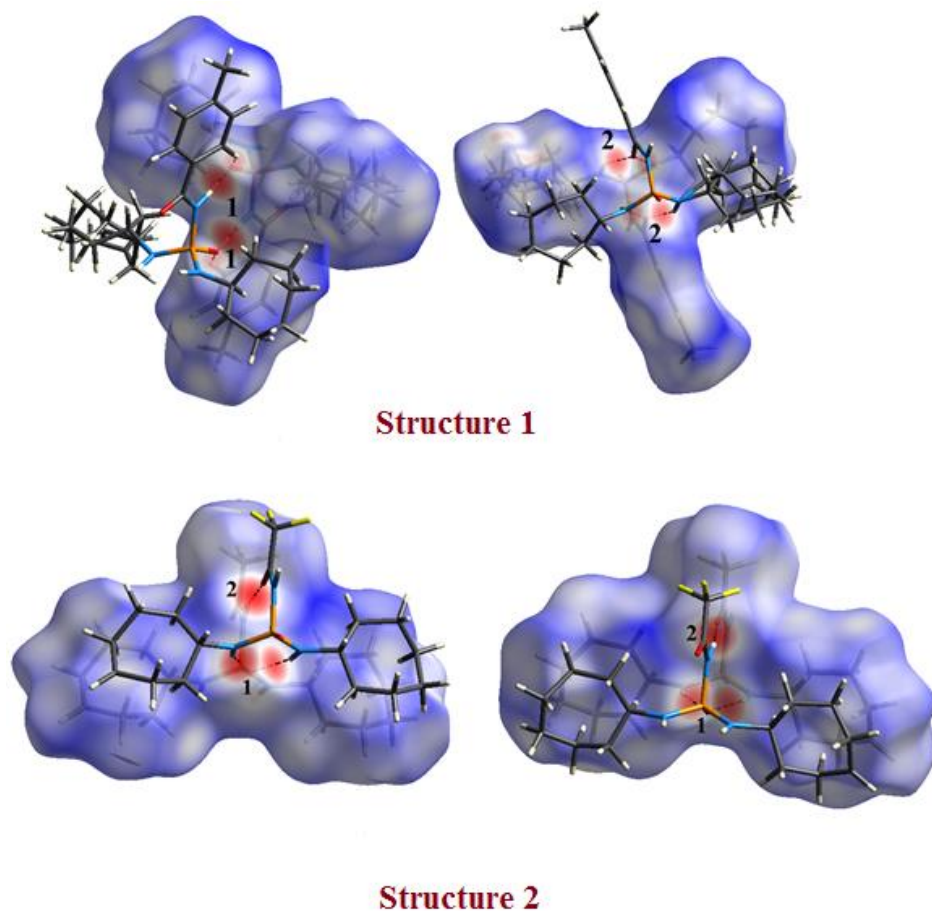
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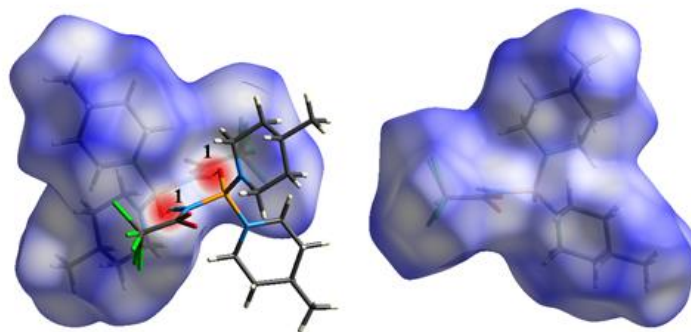
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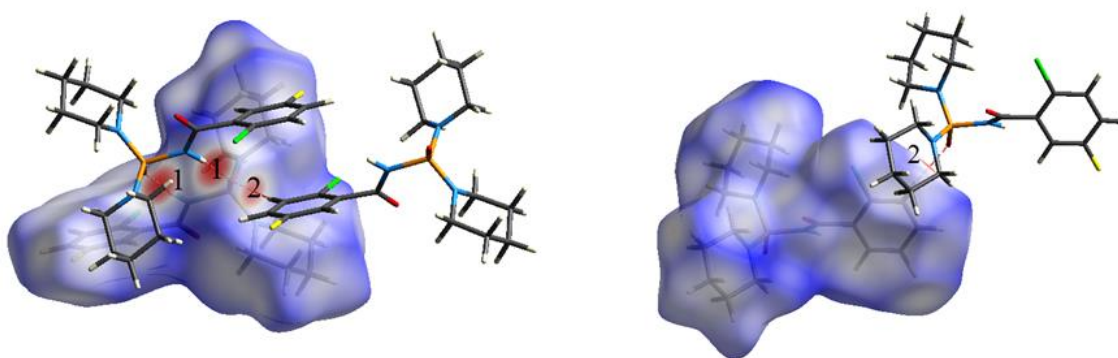
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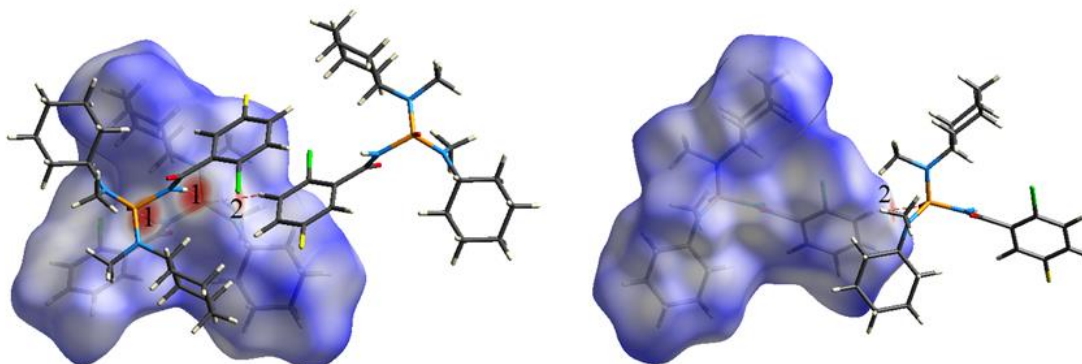
**Fig. S1.** Views of  $d_{\text{norm}}$  Hirshfeld surfaces plotted on the structures **1** and **2**, in two orientations, surrounded by neighboring molecules associated with close contacts. Labels on HSs are as follows: P1-O1[ $\cdots$ H1N-N1][ $\cdots$ H3-C3] (**1**), C1-O2[ $\cdots$ H2N-N2][ $\cdots$ H3N-N3] (**2**) for structure (**1**), P1-O1[ $\cdots$ H1N-N1][ $\cdots$ H2N-N2] (**1**), C15-O2[ $\cdots$ H3N-N3] (**2**) for structure (**2**).



**Structure 4**

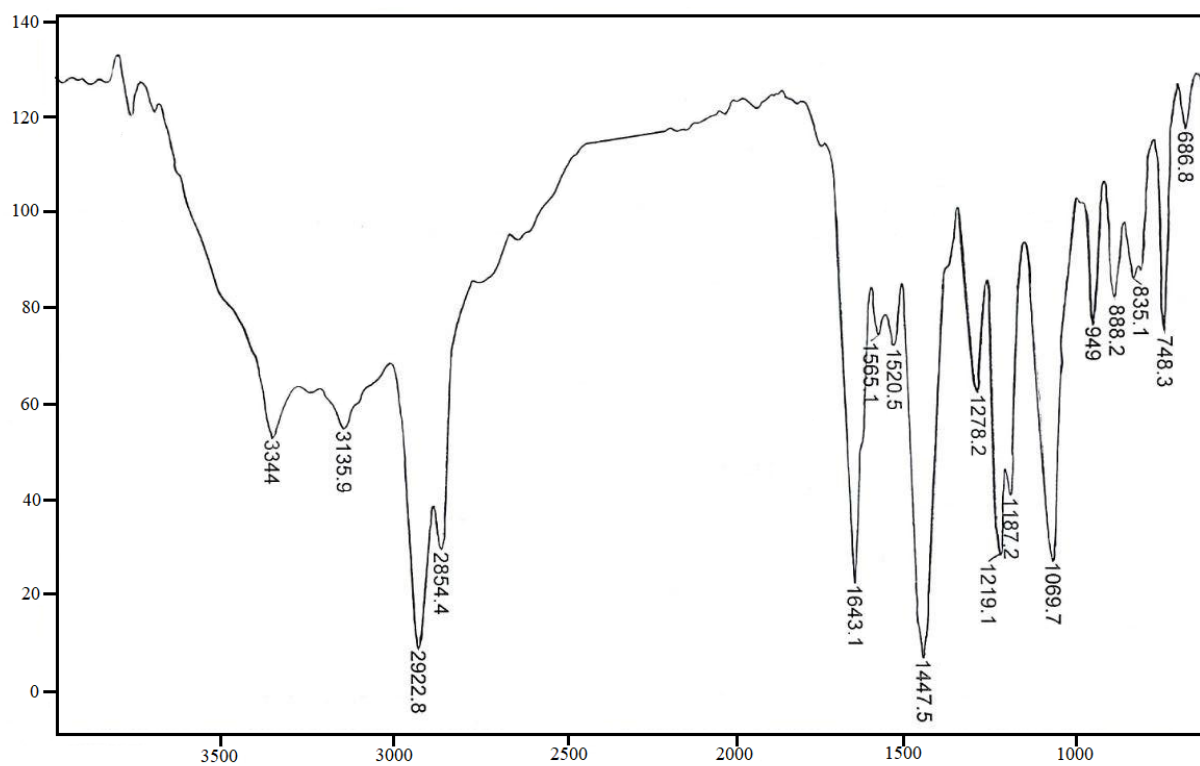


**Structure 5**

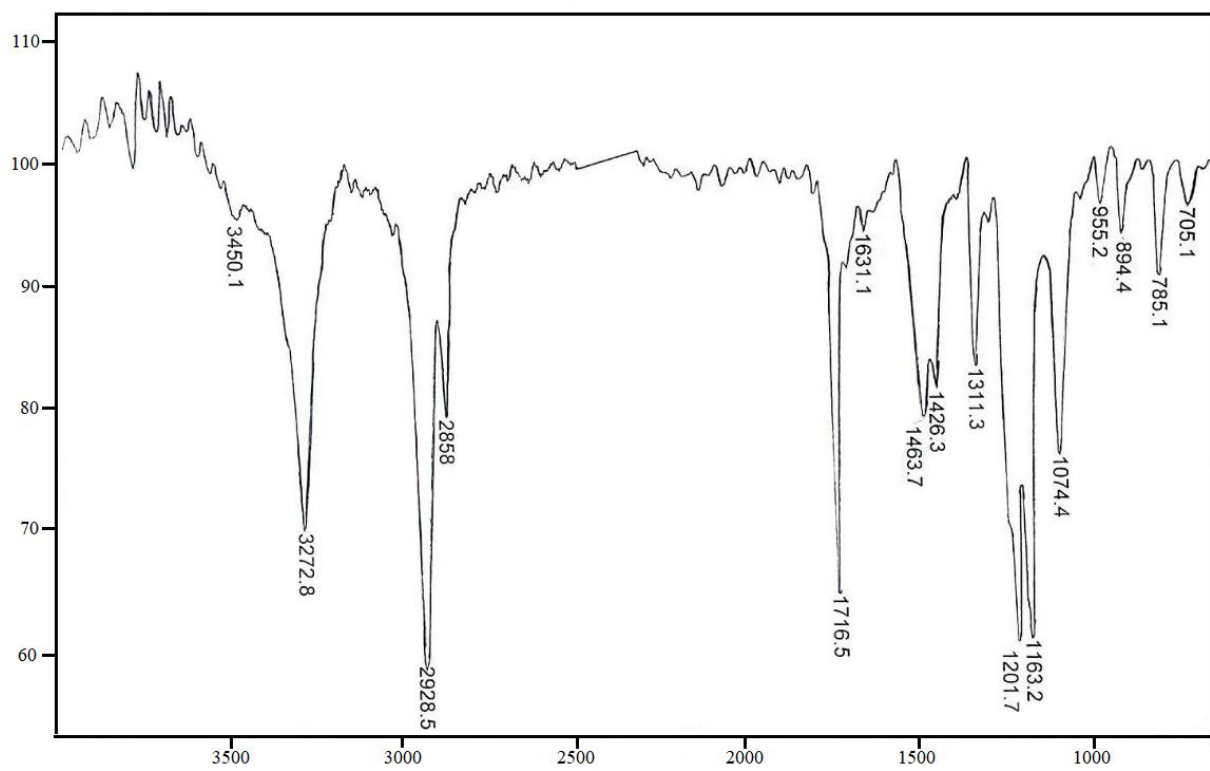


**Structure 6**

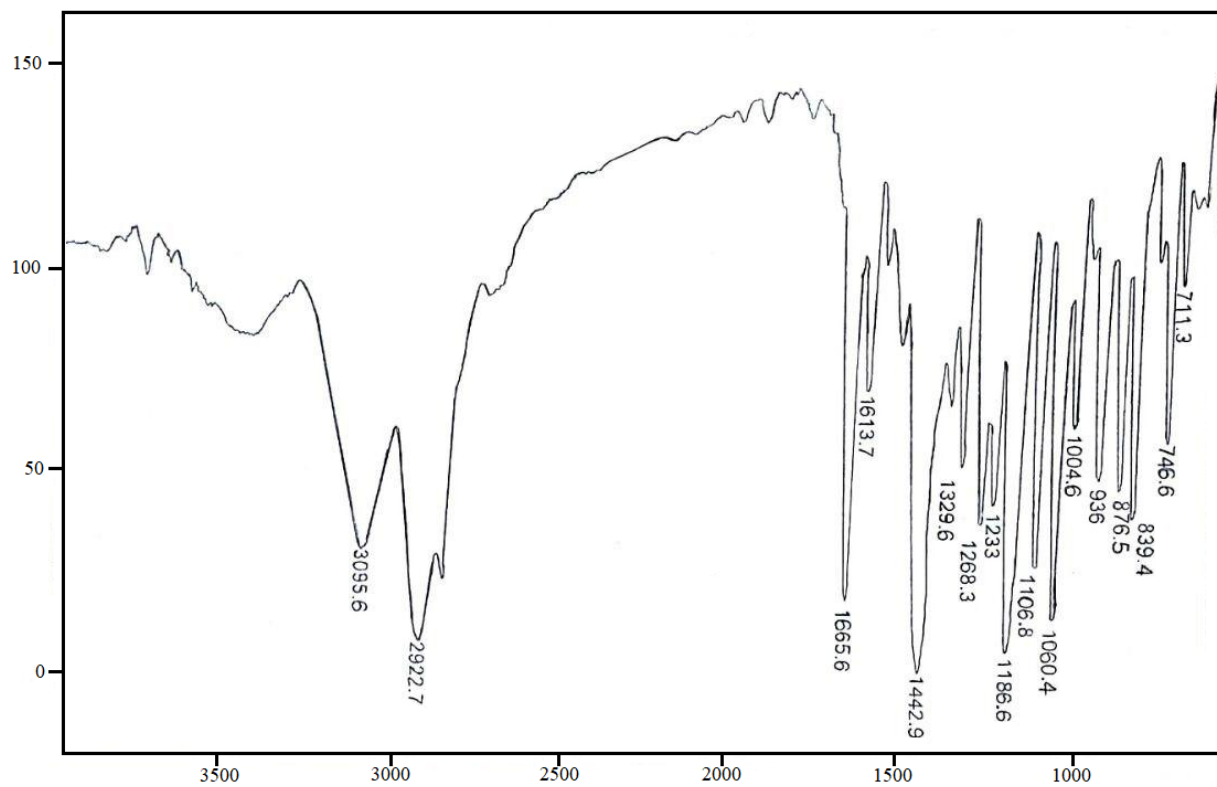
**Fig. S2.** Views of  $d_{\text{norm}}$  Hirshfeld surfaces plotted on the structures 4–6, in two orientations, surrounded by neighboring molecules associated with close contacts. Labels on HSs are as follows: P13-O14···H15-N15 (1) for structure (4), P7-O8···H61-N6 (1), P7-O8···H251-C25 (2) for structure (5), P1-O2···H191-N19 (1), P1-O2···H271-C27 (2) for structure (6).



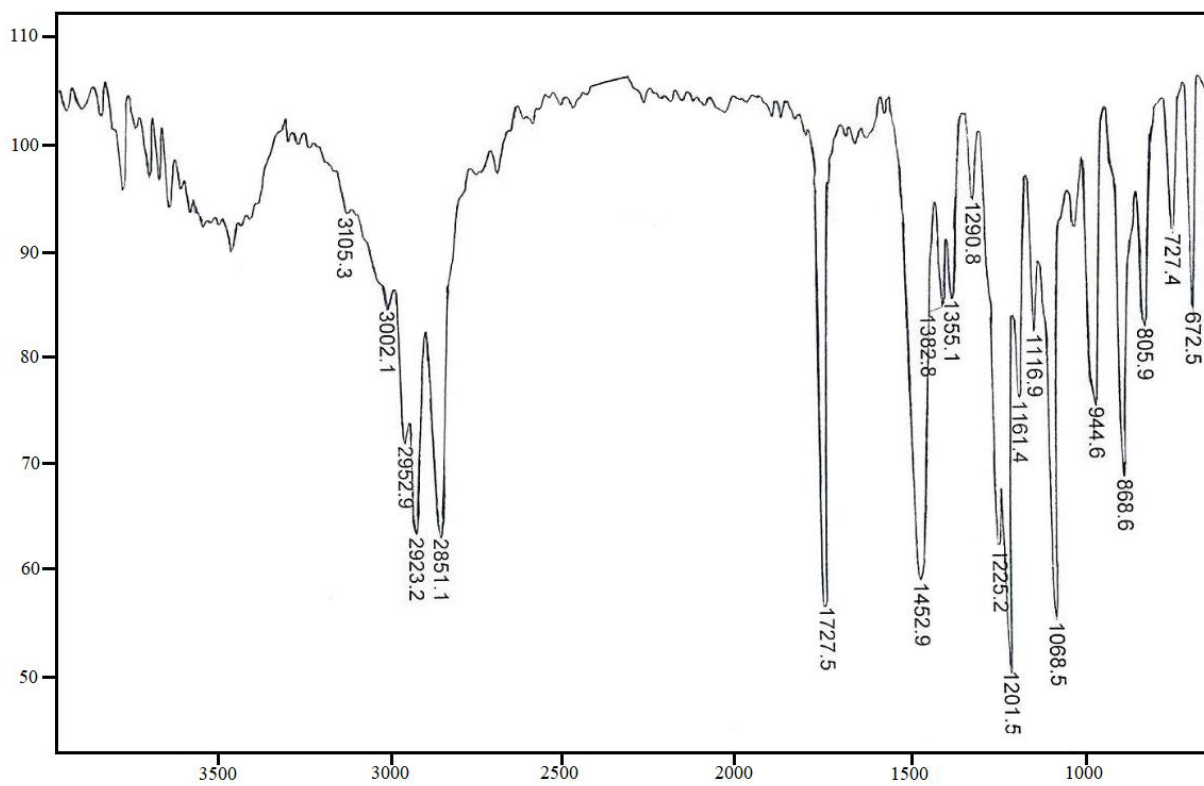
**Fig. S3.** IR spectrum of compound 1.



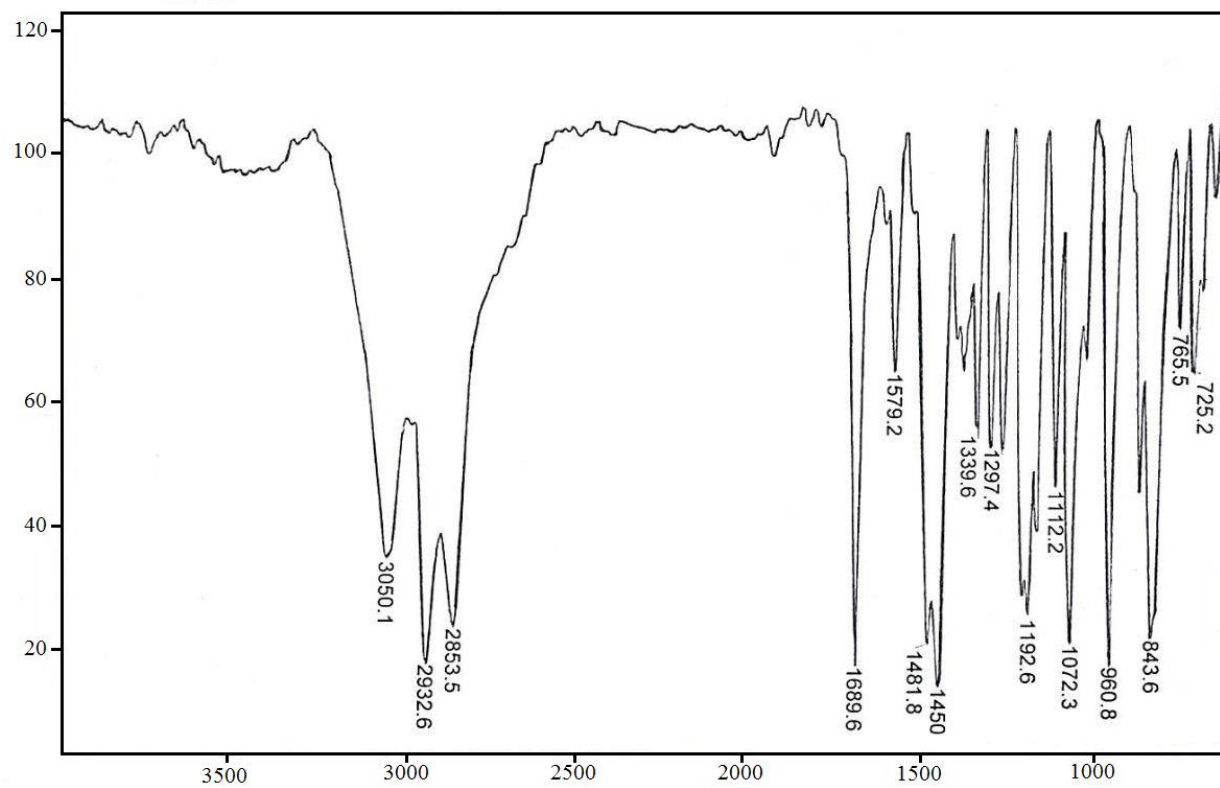
**Fig. S4.** IR spectrum of compound 2.



**Fig. S5.** IR spectrum of compound 3.

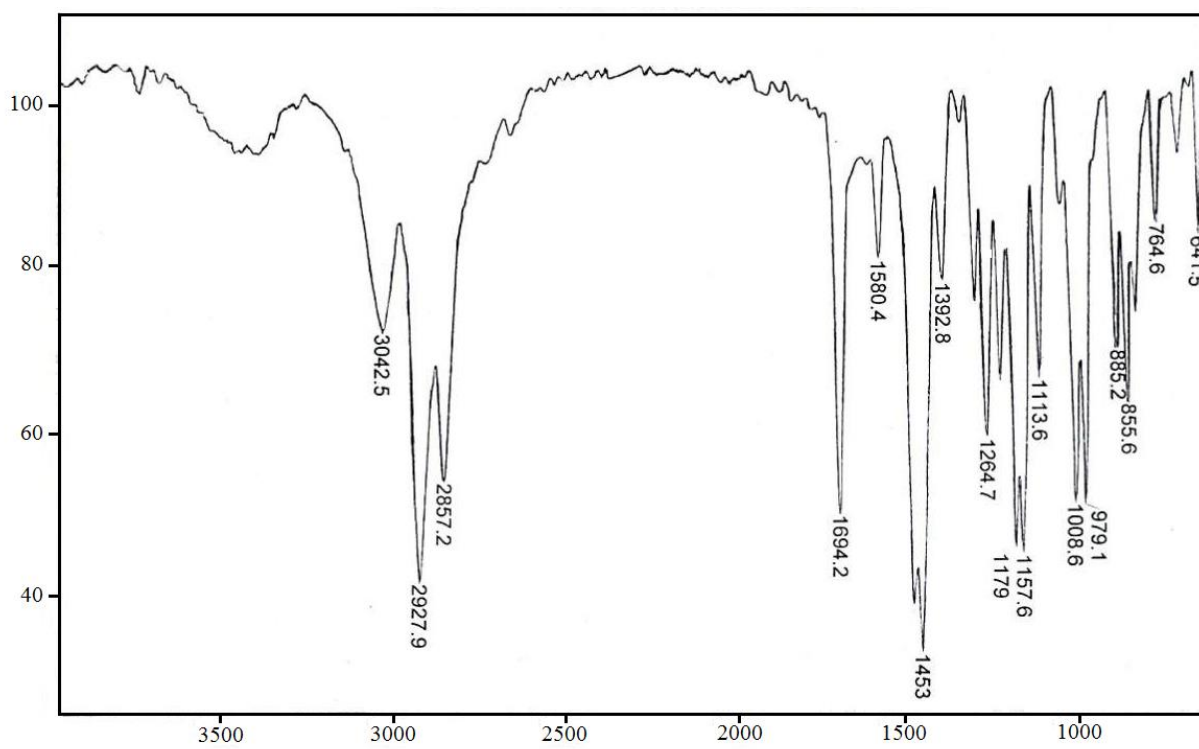


**Fig. S6.** IR spectrum of compound 4.



**Fig. S7.** IR spectrum of compound **5**.





**Fig. S8.** IR spectrum of compound **6**.