

## Pyrolysis characteristic and evolution of char structure during pulverized coal pyrolysis in drop tube furnace: influence of temperature

Qian Li, Zhihua Wang\*, Yong He, Qiang Sun, Yanwei Zhang, Sunel Kumar, Kang Zhang, Kefa Cen

State Key Laboratory of Clean Energy Utilization, Zhejiang University, 310027, Hangzhou, China

\*Corresponding author: Tel.: +86 571 87953162; Fax: +86 571 87951616.

Email address: [wangzh@zju.edu.cn](mailto:wangzh@zju.edu.cn)

### Part I the experimental results for Huainan coal and Babaoshan coal.

Two coals which has been discussed in the manuscript are Shenhua bituminous and Pingzhuang lignite. Besides, the authors also employed two other coals, which are called Huainan (HN) coal and Babaoshan (BBS) coal. Altogether four coals have been used to conduct the DTF pyrolysis experiments in the same working condition. Shenhua coal and Huainan coal are bituminous, Pingzhuang coal and Babaoshan coal are both lignite produced in Inner Mongolia. The pyrolysis temperature rose from 600 to 1000 oC (100 oC increments), coal particle feeding rate was 600 g/h, carrier gas mass flow rate was 5 L/min, the length of reacting zone was 4 meters. The results of proximate and ultimate analysis of raw coal and coal char for HN and BBS are shown in Table S1, the results of pyrolysis gas component are shown in Figure S1.

As shown in Table R1, multiple species have been released from HN and BBS. During this DTF pyrolysis process, volatiles decrease from 27.62% in HN raw coal to 17.49% in HN600 and it decreases to 5.07% in HN1000, for BBS, volatiles decreases from 37.09% in BBS raw coal to 27.01% and only 5.22% in BBS600 and BBS1000, respectively. It can be seen that two bituminous have similar volatiles in raw coal, also have similar pyrolysis behavior in DTF. As for pyrolysis gas component, which is shown in Figure R1, four coals show the same trend when pyrolysis varies. Combustible light gas H<sub>2</sub> and CO increase significantly with the rising of pyrolysis temperature, CO<sub>2</sub> and CH<sub>4</sub> shows an obvious decrease trend. The change mechanism has been discussed in detail in the manuscript.

**Table S1** Proximate and ultimate analysis of coal char

| Sample ID | Proximate Analysis /w <sub>t</sub> ,% |                |                |                 | Q <sub>net,d</sub><br>J/g | Ultimate Analysis /w <sub>t</sub> ,% |                |                |                  |                |
|-----------|---------------------------------------|----------------|----------------|-----------------|---------------------------|--------------------------------------|----------------|----------------|------------------|----------------|
|           | M <sub>ad</sub>                       | A <sub>d</sub> | V <sub>d</sub> | FC <sub>d</sub> |                           | C <sub>d</sub>                       | H <sub>d</sub> | N <sub>d</sub> | S <sub>t,d</sub> | O <sub>d</sub> |
| HNraw     | 1.74                                  | 18.18          | 27.62          | 52.46           | 26598                     | 69.88                                | 4.39           | 1.08           | 0.6              | 4.13           |
| HN600     | 1.98                                  | 25.12          | 17.49          | 55.41           | 24910                     | 63.12                                | 3.3            | 1.02           | 0.61             | 4.85           |

|         |      |       |       |       |       |       |      |      |      |       |
|---------|------|-------|-------|-------|-------|-------|------|------|------|-------|
| HN700   | 2.64 | 21.97 | 12.19 | 63.2  | 26117 | 67.02 | 2.77 | 1.08 | 0.47 | 4.05  |
| HN800   | 2.85 | 24.7  | 9.30  | 63.15 | 25068 | 65.21 | 2.28 | 1.02 | 0.46 | 3.48  |
| HN900   | 2.22 | 25.36 | 8.05  | 64.37 | 26142 | 67.4  | 2.5  | 1.08 | 0.46 | 0.98  |
| HN1000  | 2.03 | 27.88 | 5.07  | 65.02 | 24568 | 65.9  | 1.74 | 1.01 | 0.44 | 1.00  |
| BBSraw  | 4.58 | 15.53 | 37.09 | 42.80 | 21123 | 56.25 | 3.52 | 1.43 | 1.37 | 17.32 |
| BBS600  | 8.11 | 16.38 | 27.01 | 48.50 | 22068 | 57.12 | 2.62 | 1.09 | 1.15 | 13.53 |
| BBS700  | 7.32 | 18.00 | 19.84 | 54.84 | 23284 | 61.15 | 1.93 | 1.07 | 1.16 | 9.37  |
| BBS800  | 6.29 | 20.53 | 16.77 | 56.41 | 23952 | 61.18 | 1.51 | 0.90 | 1.30 | 8.29  |
| BBS900  | 4.60 | 23.26 | 10.24 | 61.90 | 24173 | 64.73 | 0.73 | 1.05 | 1.61 | 4.02  |
| BBS1000 | 1.20 | 28.23 | 5.22  | 65.35 | 24254 | 66.25 | 0    | 0.70 | 1.03 | 2.59  |

**Note:**  $Q_{\text{net}}$ , lower heating value; ad, on air-dried basis; d, on dry basis;  $S_t$ , total sulphur; Oxygen is calculated by difference; coal and char are referenced by their abbreviated name and pyrolysis temperature (e.g. HN600 and BBS600).

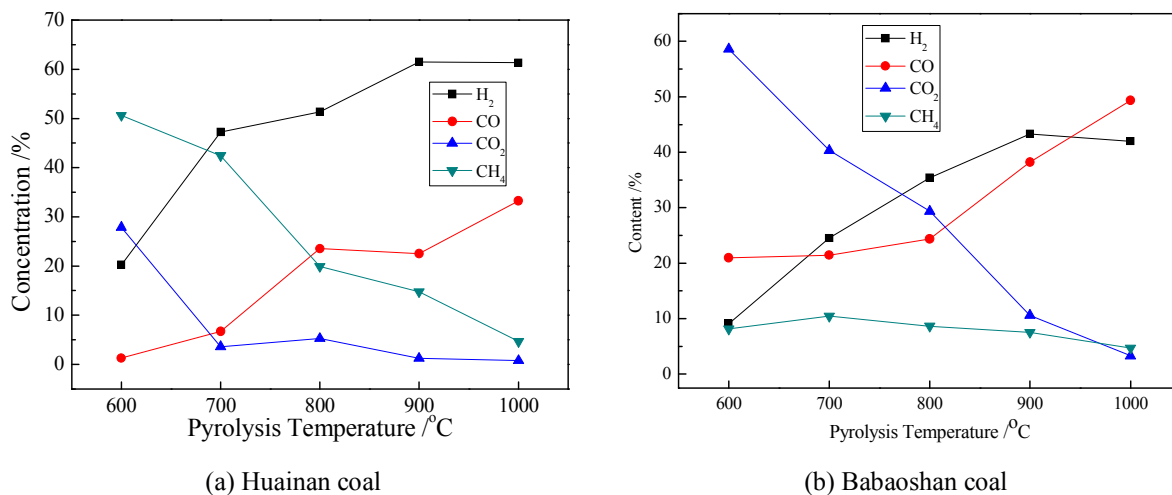
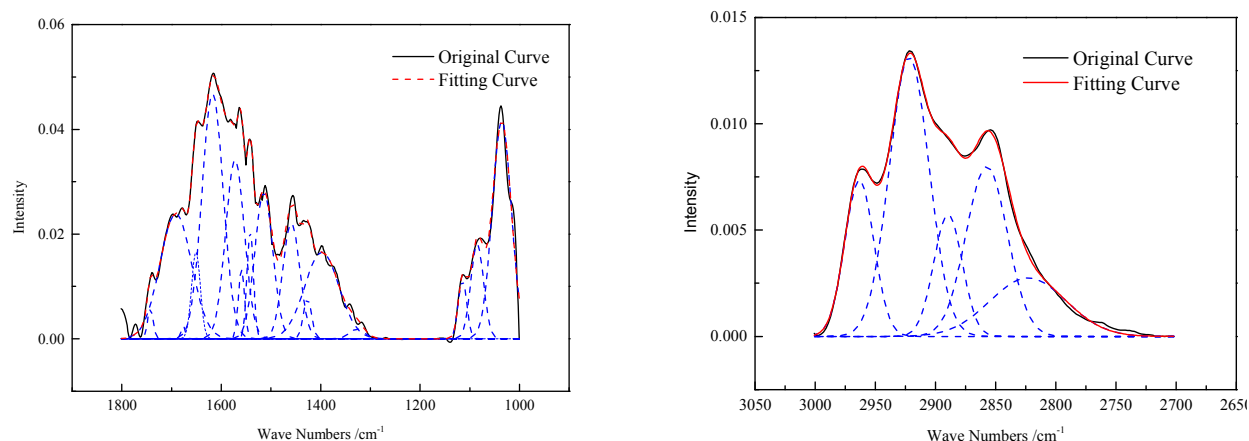


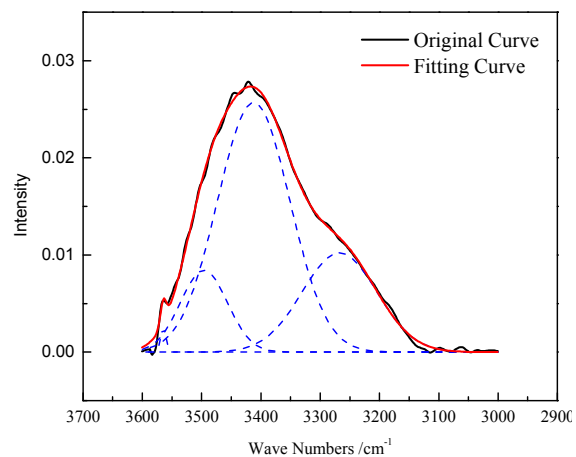
Figure S1 Component of pyrolysis gas of Huainan and Babaoshan coal under different temperature in DTF

## Part II the FTIR spectrum of Shenhua and Pingzhuang Coal

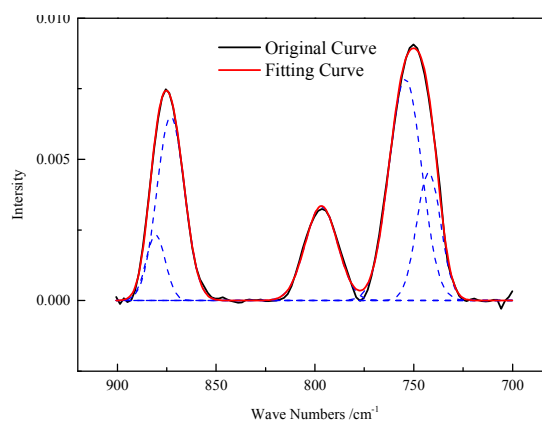
The FTIR spectrum of Shenhua and Pingzhuang Coal are shown in Figure 2 of the paper. The absorption peaks of structures and functional groups in coal can be divided into four sections: hydroxyl (3600~3000 cm<sup>-1</sup>), aliphatic structures (3000~2700 cm<sup>-1</sup>), oxygen-containing functional groups and aromatic structures (1800~1000 cm<sup>-1</sup>) and low-wavenumber aromatic structures and ash (900~700 cm<sup>-1</sup>). The results of peak separation of all samples are listed below.



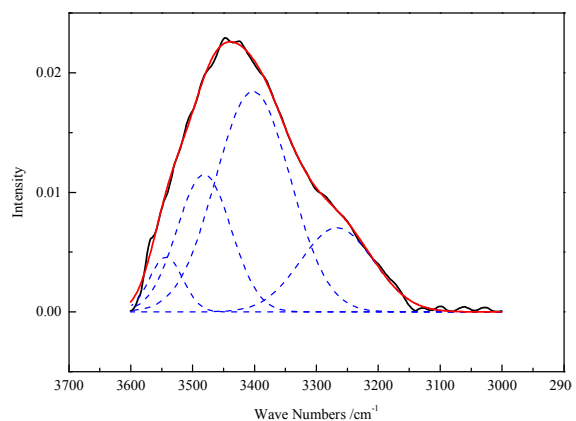
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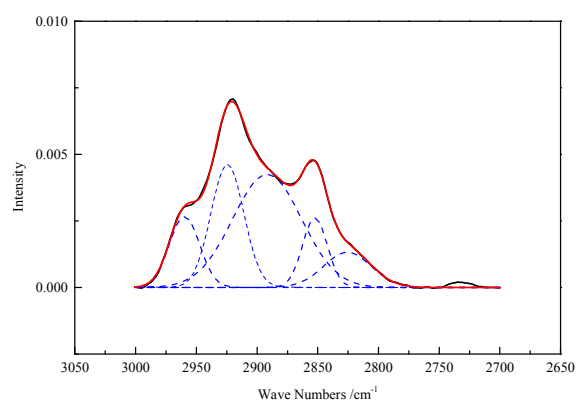
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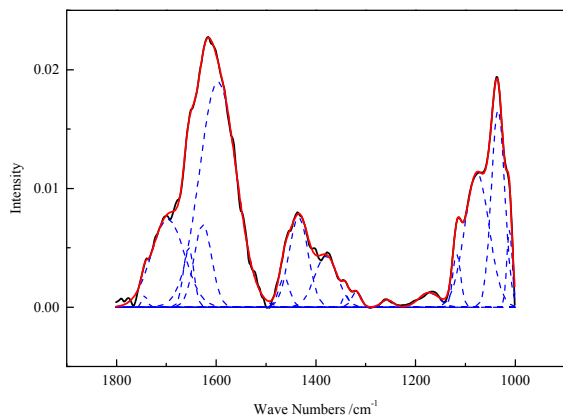
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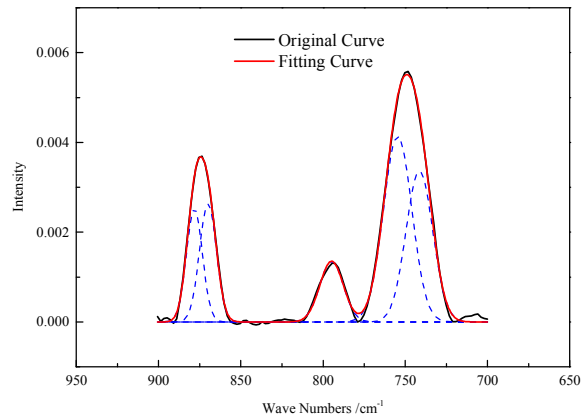
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SH700 3600~3000

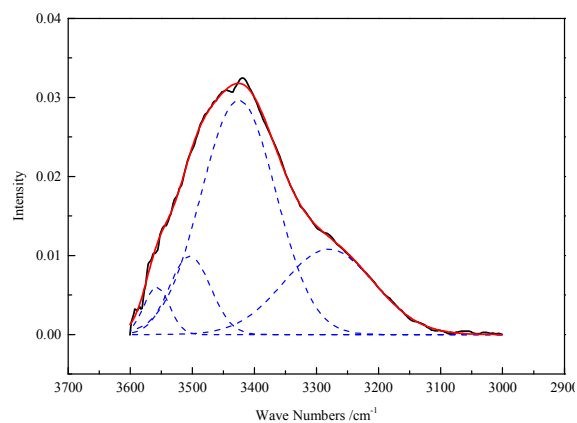


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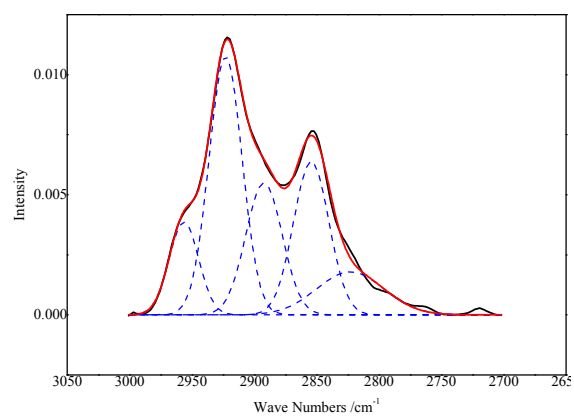


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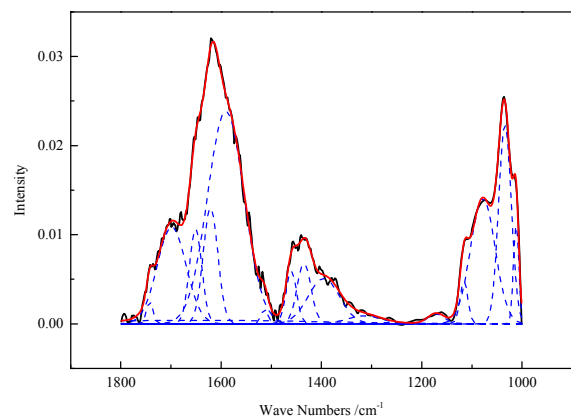
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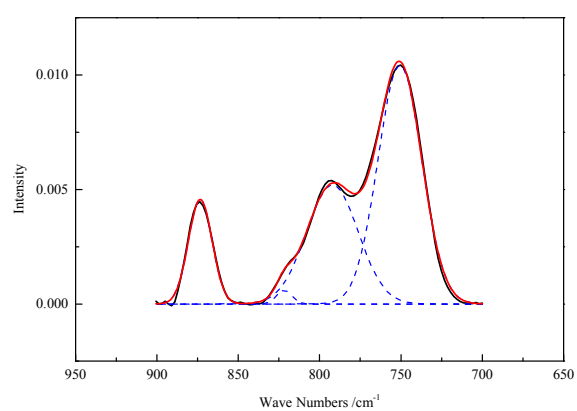
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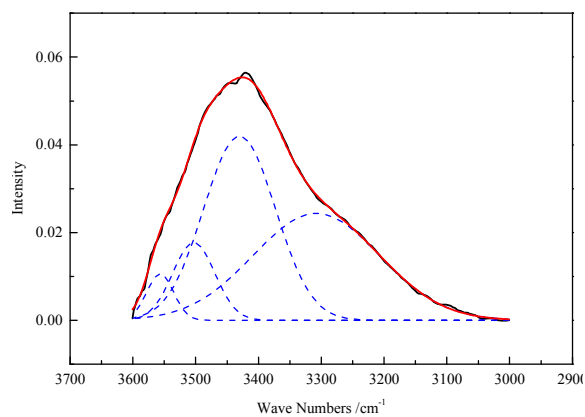
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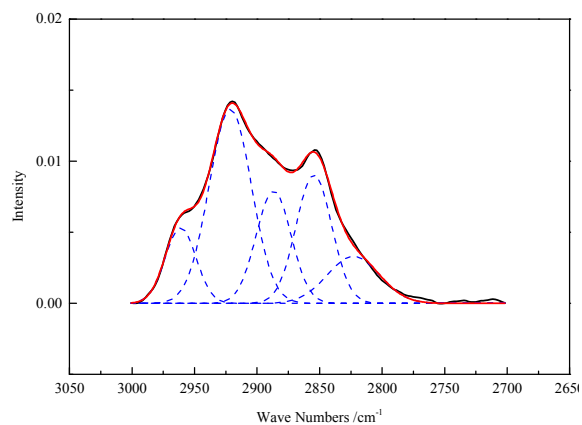
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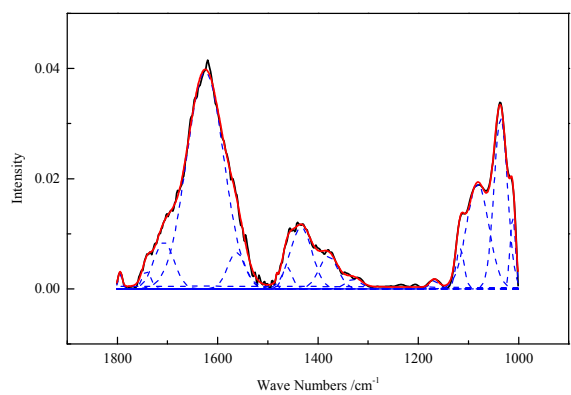
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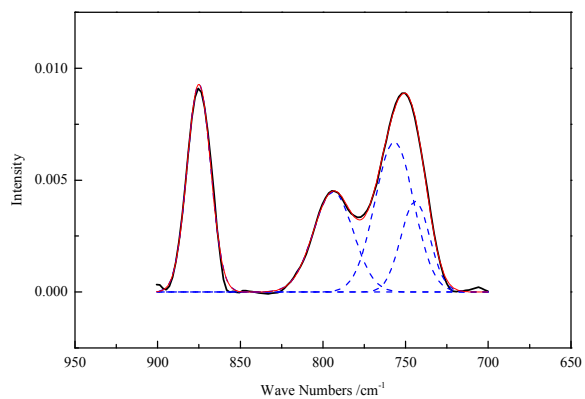
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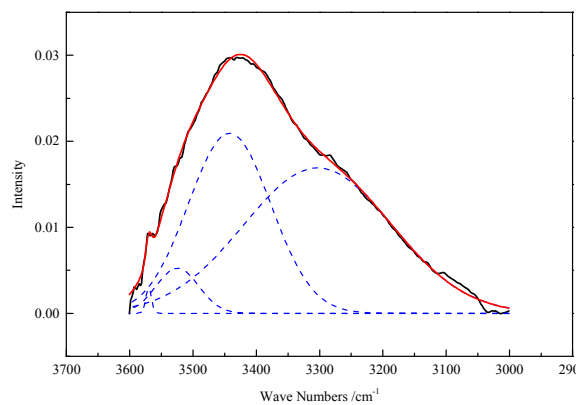
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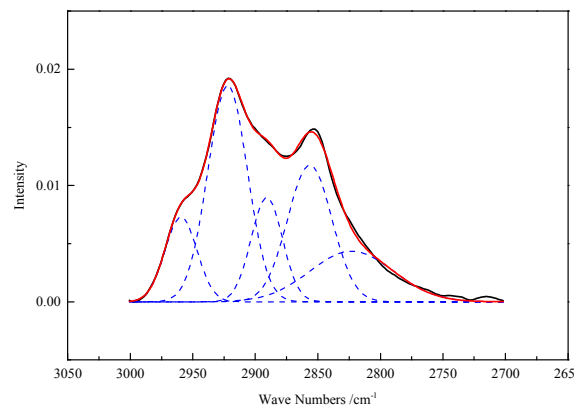
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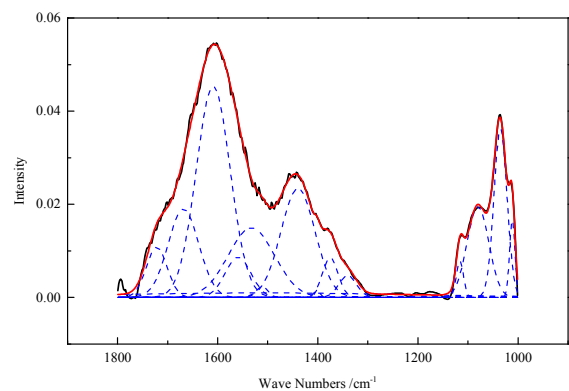
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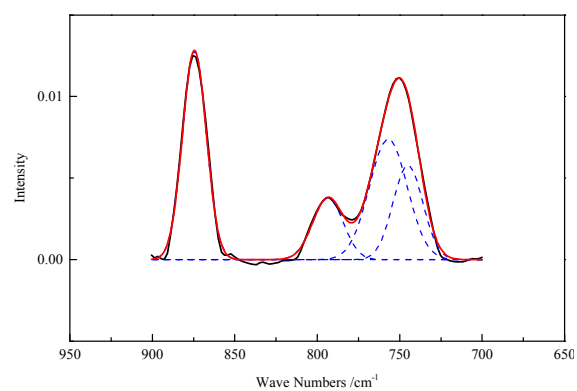
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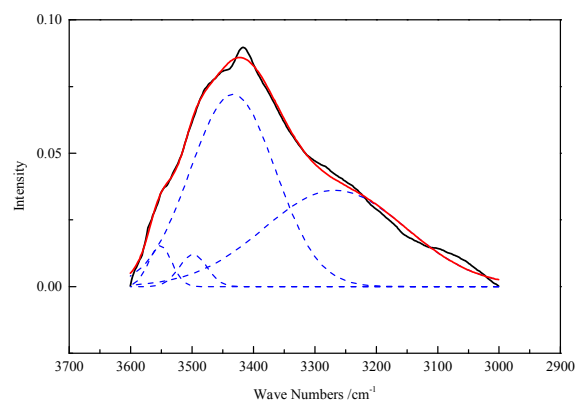
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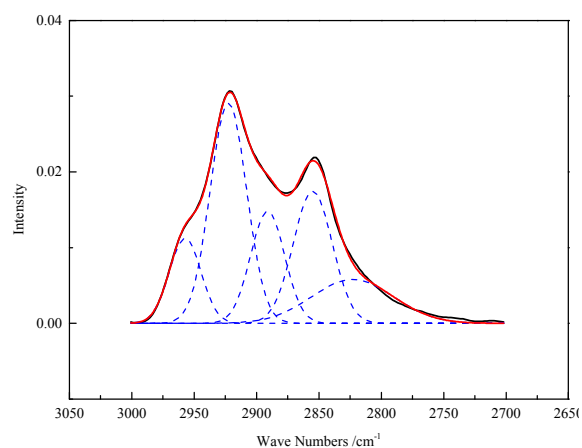
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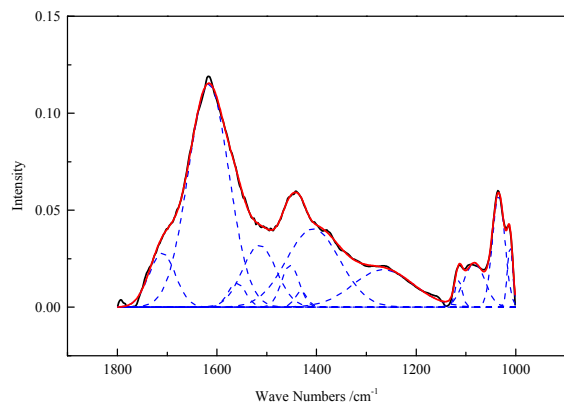
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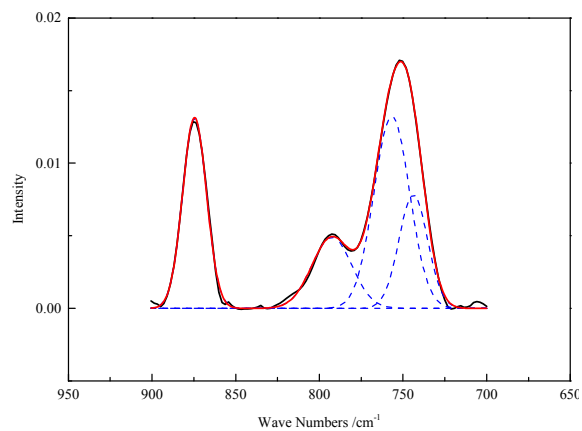
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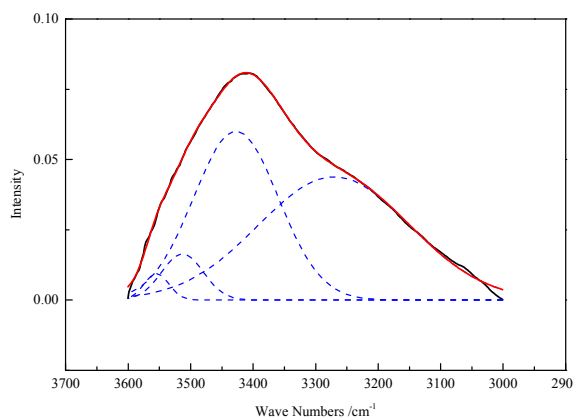
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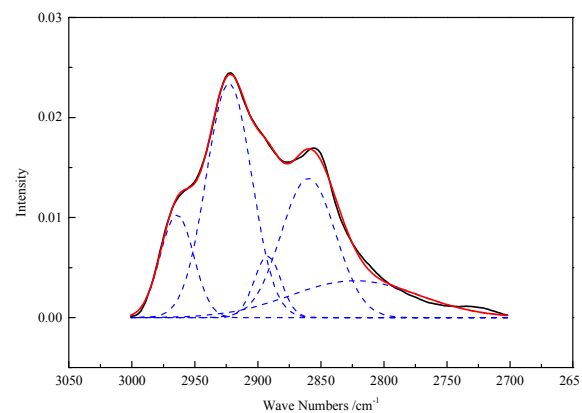
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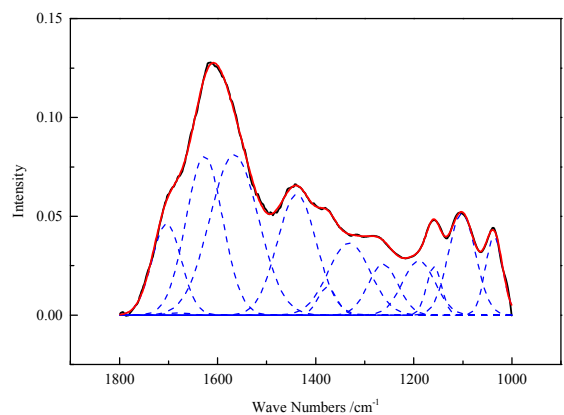
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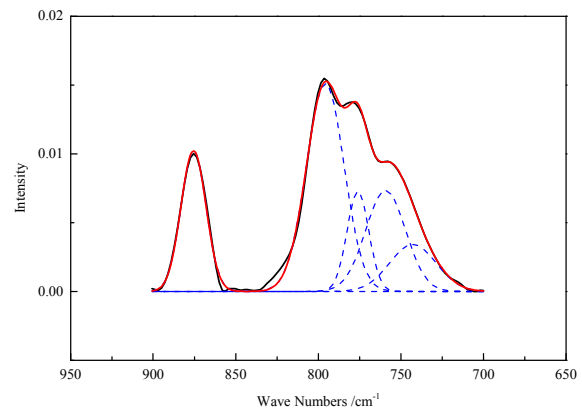
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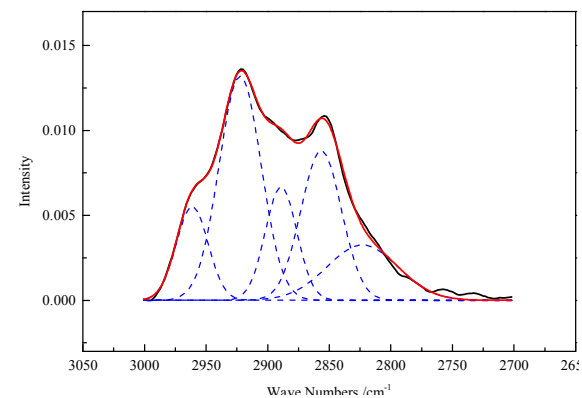
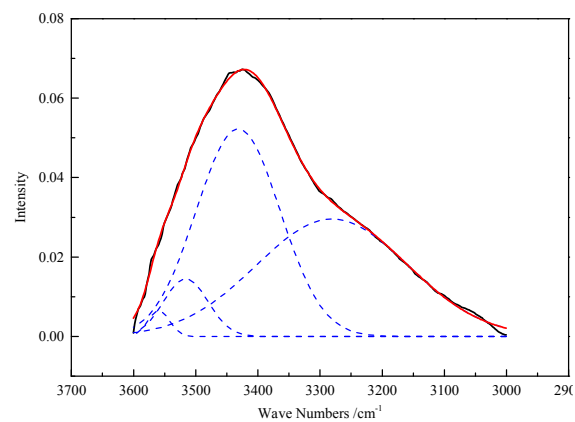
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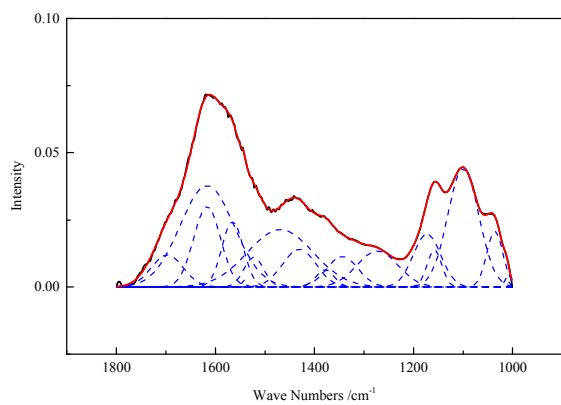
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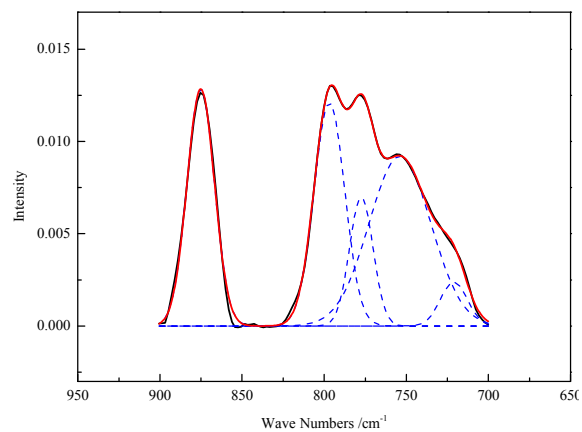
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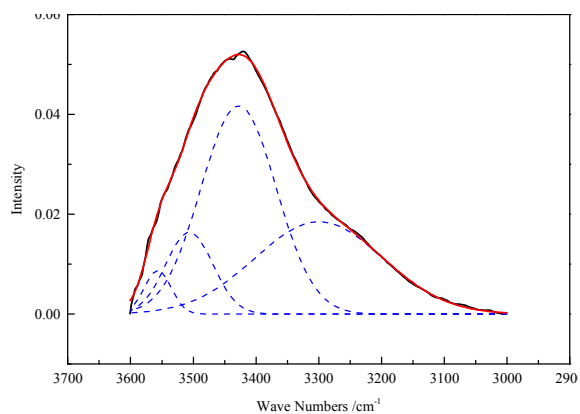
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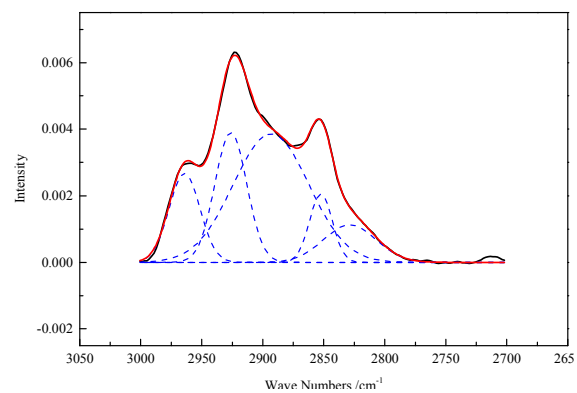
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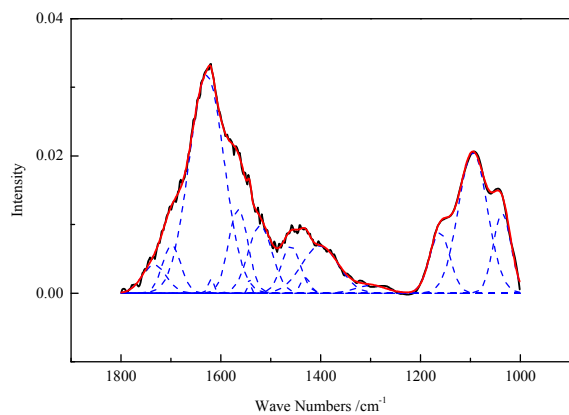
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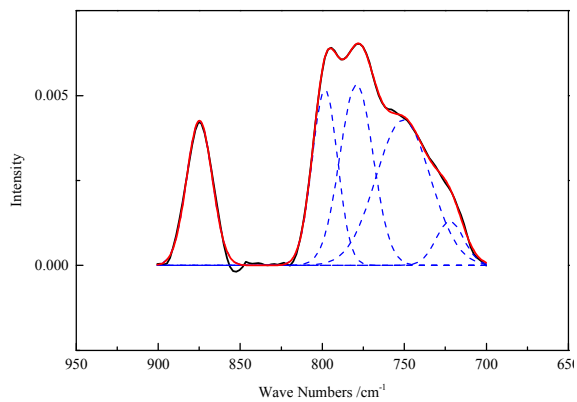
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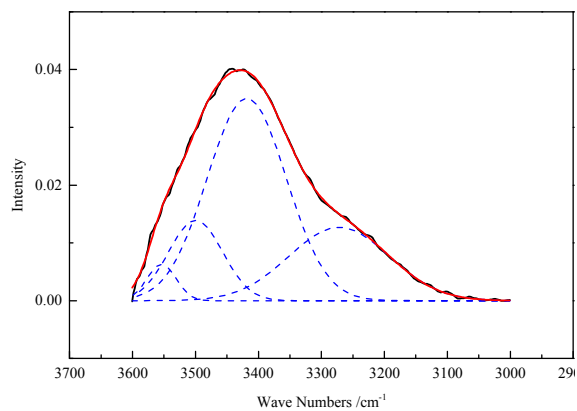


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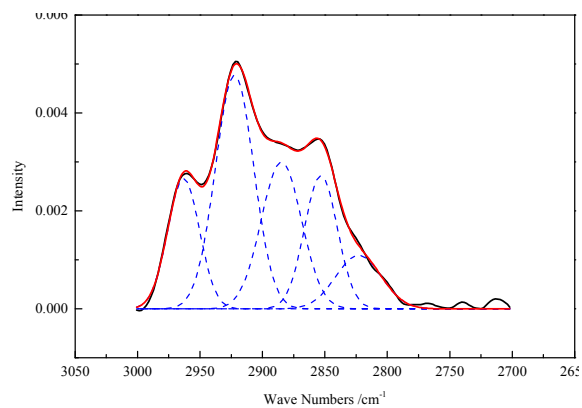


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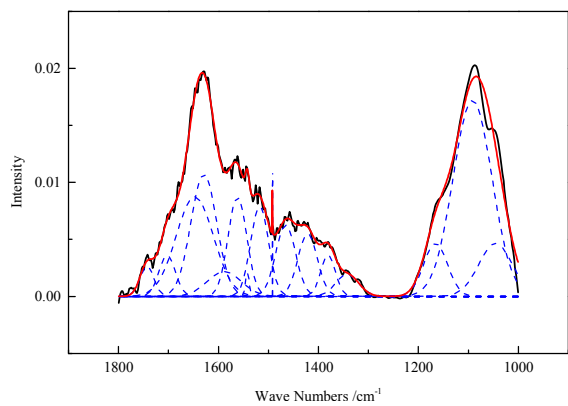
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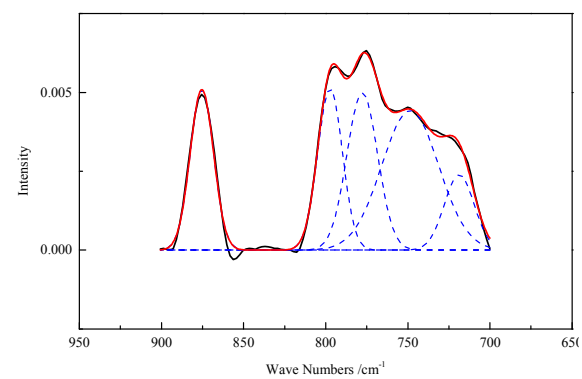
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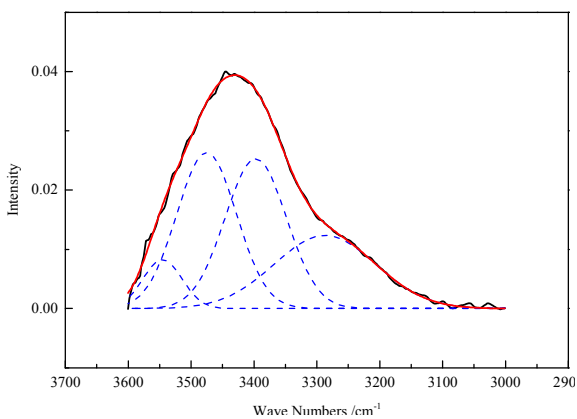
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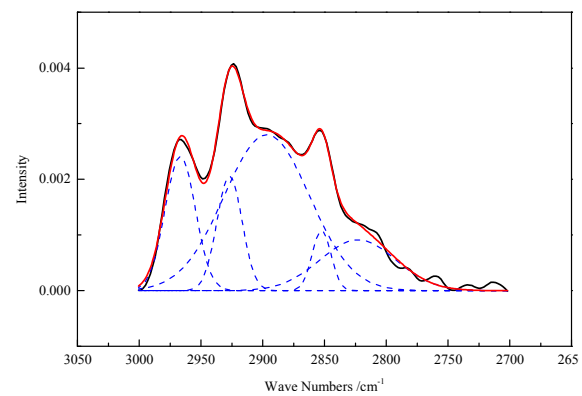
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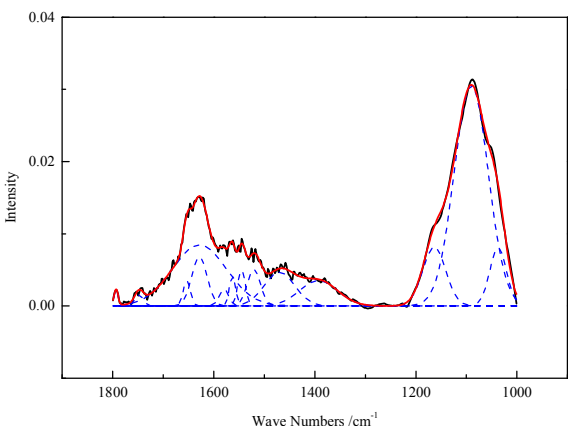
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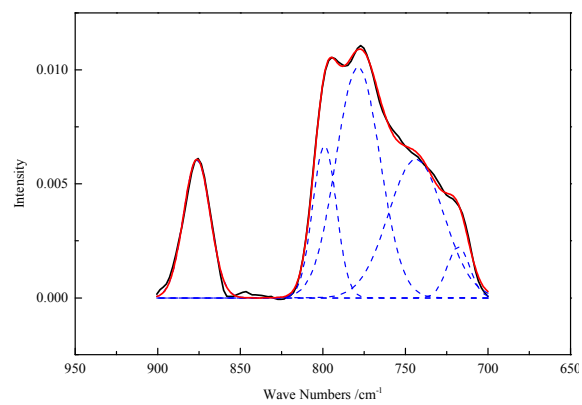
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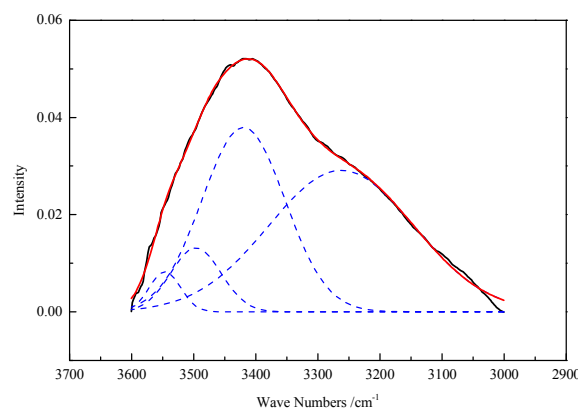
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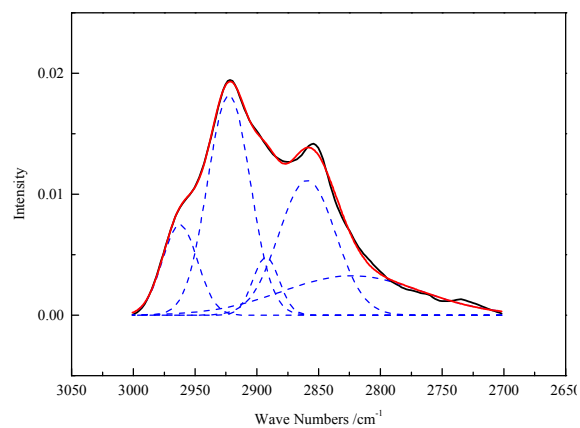
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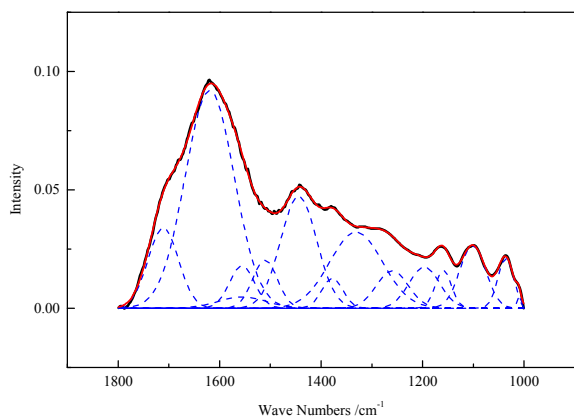
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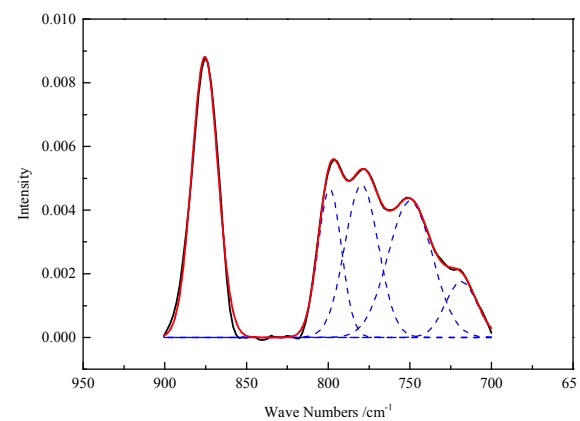
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