Supplementary Materials

Thermal properties and kinetic analysis of pyrolysis products of nicotine salts from e-cigarette using pyrolysis-gas chromatography/mass spectrometry

Ji Yang1\*, Yirong Li1,2, Chunbo Liu1, Shiyun Tang1, Zhengjie Li1, Lihong Jiang2\*

1 Technology Center, China Tobacco Yunnan Industrial Company Limited, Kunming 650231, Yunnan, China.

2 College of Chemistry and Chemical Engineering, Kunming University of Science and Technology, Kunming 650224, Yunnan, China.

\*Correspondence:

yangji052@163.com (J.Y.)

jlh65@163.com (L.J.)

Table S1. Physical properties of nicotine salt samples.

|  |  |  |  |
| --- | --- | --- | --- |
| Sample | Molar ratio of acid to nicotine | Nicotine content  (mg g-1) | Physical form |
| Nicotine benzoate | 1:1 | 306.11 | Orange oily |
| Nicotine tartrate | 2:1 | 303.11 | Orange oily |
| Nicotine citrate | 2:1 | 304.28 | Solid crystals |
| Nicotine malate | 2:1 | 309.75 | Yellow oily |
| Nicotine lactate | 1:1 | 305.32 | Yellow oily |
| Nicotine levulinate | 1:1 | 301.62 | Orange oily |

Table S2. Different reaction models of pyrolysis with various functions of G(α) and f(α).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Reaction model | | *f*(*α*) | *G*(*α*) | Reaction mechanism |
| Chemical reaction | F1 | 1-*α* | -ln(1-*α*) | First-order reaction |
| F1.5 | (1-*α*)3/2 | 2[(1-*α*)-1/2-1] | 1.5-order reaction |
| F2 | (1-*α*)2 | (1-*α*)-1 | Second-order reaction |
| Diffusion-controlled reaction | D1 | 1/2*α* | *α*2 | One-dimensional diffusion |
| D2 | -ln(1-*α*)-1 | (1-*α*)ln(1-*α*)+*α* | Two-dimensional diffusion |
| D3 | 3(1-*α*)3/2 × [1-(1-*α*)1/3]-1/2 | [1-(1-*α*)1/3]2 | Three-dimentional diffusion |

Table S3. Major pyrolysis products of nicotine salts.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Retention time  (min) | Pyrolysis compounds | CAS | nicotine benzoate  (%) | nicotine citrate  (%) | nicotine malate  (%) | nicotine lactate  (%) | nicotine tartrate  (%) | nicotine levulinate  (%) |
| 5.26 | Triethyl borate | 150-46-9 | -\* | 0.13 | - | - | - | - |
| 6.43 | 1-Acetylguanidine | 5699-40-1 | - | - | - | - | 3.46 | - |
| 6.48 | Maleic anhydride | 108-31-6 | - | - | 1.11 | - | - | - |
| 8.26 | Itaconic anhydride | 2170-03-8 | - | 5.31 | - | - | - | - |
| 11.36 | L(+)-Lactic acid | 79-33-4 | - | - | - | 13.60 | - | - |
| 11.64 | L-Lactide | 4511-42-6 | - | - | - | 1.14 | - | - |
| 12.15 | Levulinic acid | 123-76-2 | - | - | - | - | - | 32.35 |
| 12.25 | benzoic acid | 65-85-0 | 46.59 | - | - | - | - | - |
| 14.78 | 3-methyl-2-Pentanol | 565-60-6 | - | - | - | 3.92 | - | - |
| 14.92 | L-Nicotine | 54-11-5 | 51.26 | 91.29 | 95.52 | 78.11 | 95.39 | 65.20 |
| 16.04 | 3-(3,4-dihydro-2H-pyrrol-5-yl)- Pyridine | 532-12-7 | - | - | - | 0.24 | 0.13 | 0.32 |
| 16.66 | 3-(1-methyl-1H-pyrrol-2-yl)-Pyridine | 487-19-4 | 1.96 | 1.51 | - | - | - | - |
| 16.68 | 3-methyl-4-phenyl-1H-Pyrazole | 13788-84-6 | - | - | 3.38 | 1.62 | 0.90 | 0.43 |

\*: no detected

Table S4. Kinetic parameters of different nicotine salts during thermal decomposition process.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Sample** | **Stage** | **Fitting equation** | **EC-R (kJ mol-1)** | **A(min-1)** | **Model** | **R2** | **ΔH**  **(kJ mol-1)** | **ΔG**  **(kJ mol-1)** | **ΔS**  **(kJ mol-1 K-1)** |
| Nicotine benzoate | Ⅰ | y=2557.19x+6.66 | 21.26 | 1.04\*1010 | F 1.5 | 0.957 | 18.21 | 41.38 | -0.06 |
| Ⅱ | y=8913.21x+7.23 | 74.10 | 1.24\*1011 | F 2 | 0.950 | 69.82 | 93.23 | -0.05 |
| Nicotine tartrate | Ⅰ | y=2823.46x-5.93 | 31.67 | 3.84\*108 | F 1.5 | 0.953 | 30.79 | 27.86 | -0.08 |
| Ⅱ | y=8461.39x+7.14 | 50.35 | 1.07\*108 | F 2 | 0.947 | 48.63 | 68.55 | -0.09 |
| Nicotine citrate | Ⅰ | y=4650.85x+1.57 | 38.61 | 2.23\*108 | F 1.5 | 0.978 | 37.73 | 46.73 | -0.08 |
| Ⅱ | y=7109.83x+4.72 | 59.11 | 7.95\*109 | F 2 | 0.973 | 57.56 | 68.72 | -0.06 |
| Nicotine malate | Ⅰ | y=3889.84x+3.27 | 32.34 | 1.03\*109 | F 1.5 | 0.971 | 31.44 | 39.23 | -0.07 |
| Ⅱ | y=5631.59x+1.75 | 46.82 | 3.25\*108 | F 2 | 0.943 | 45.16 | 62.54 | -0.09 |
| Nicotine levulinate | Ⅰ | y=5025.38x+1.45 | 49.78 | 2.14\*108 | F 1.5 | 0.986 | 39.69 | 62.89 | -0.09 |
| Nicotine lactate | Ⅰ | y=6853.11x+0.32 | 65.04 | 9.46\*107 | D 1 | 0.988 | 63.14 | 85.65 | -0.10 |