**Supplementary Material**

**for**

**Kinetic Parameters Underlying Hematite-assisted Decomposition of Tribromophenol**

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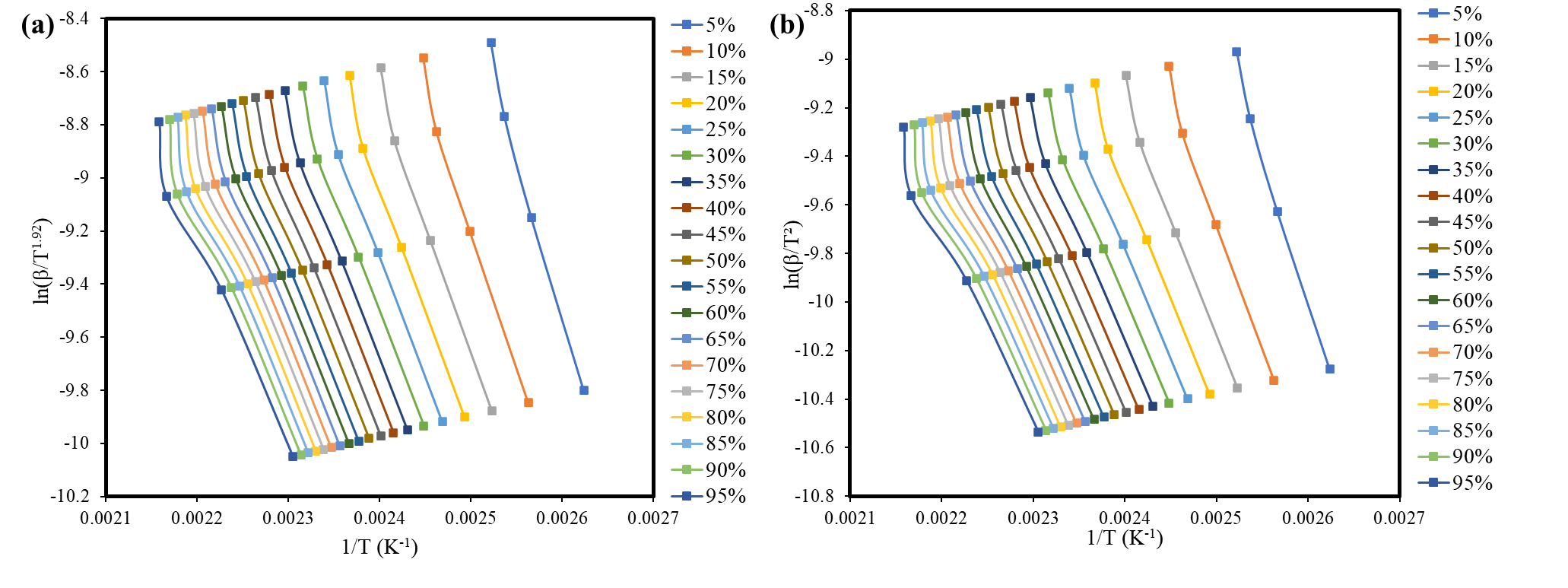
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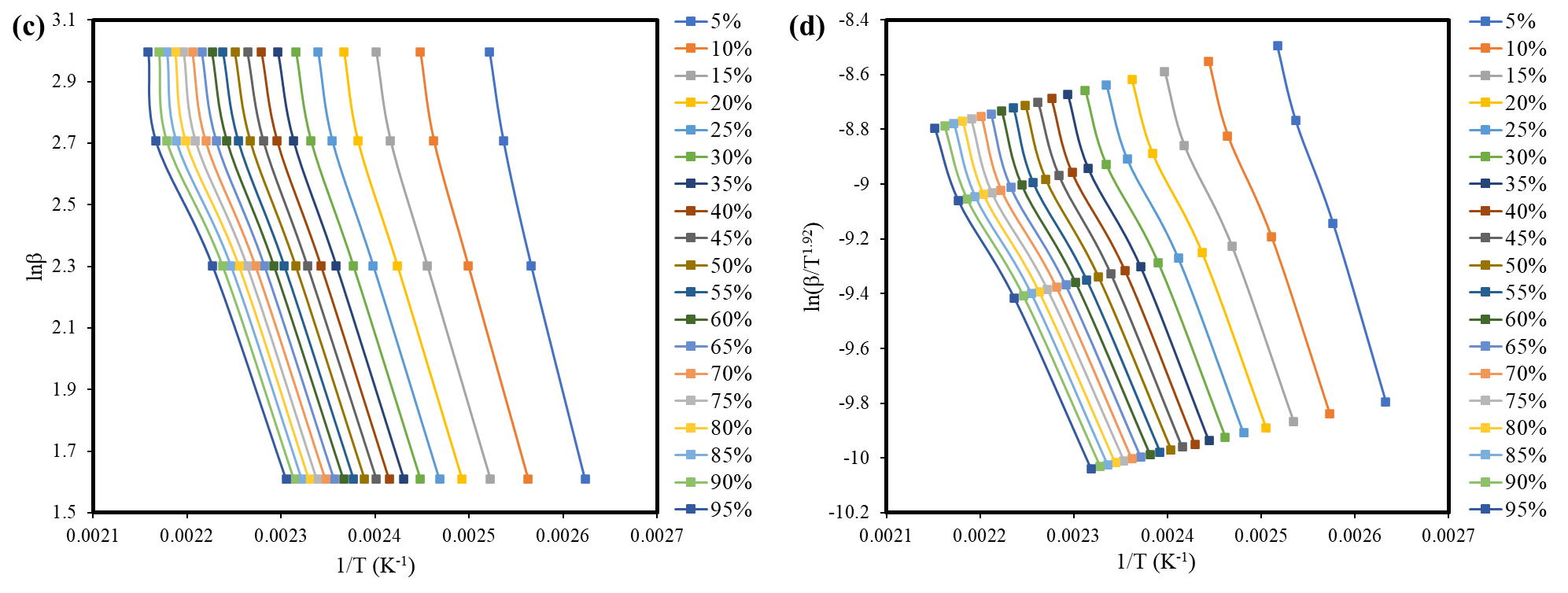
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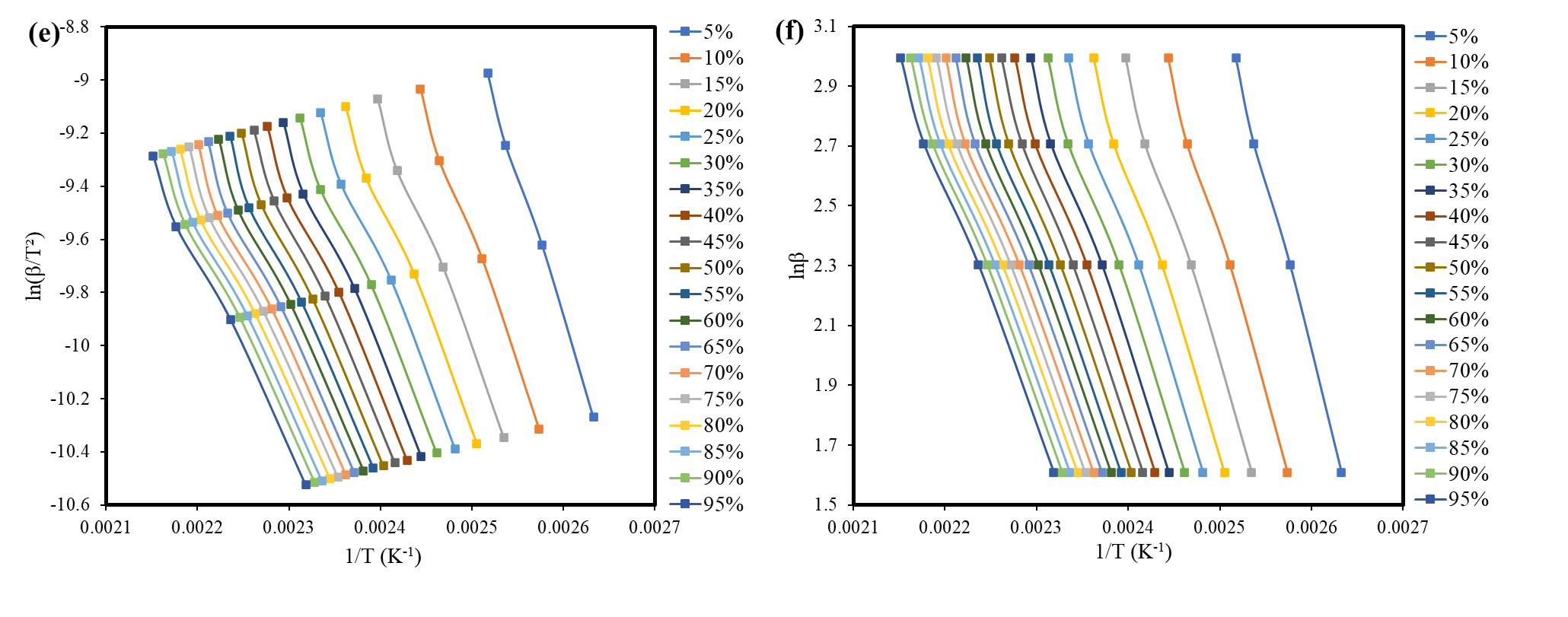
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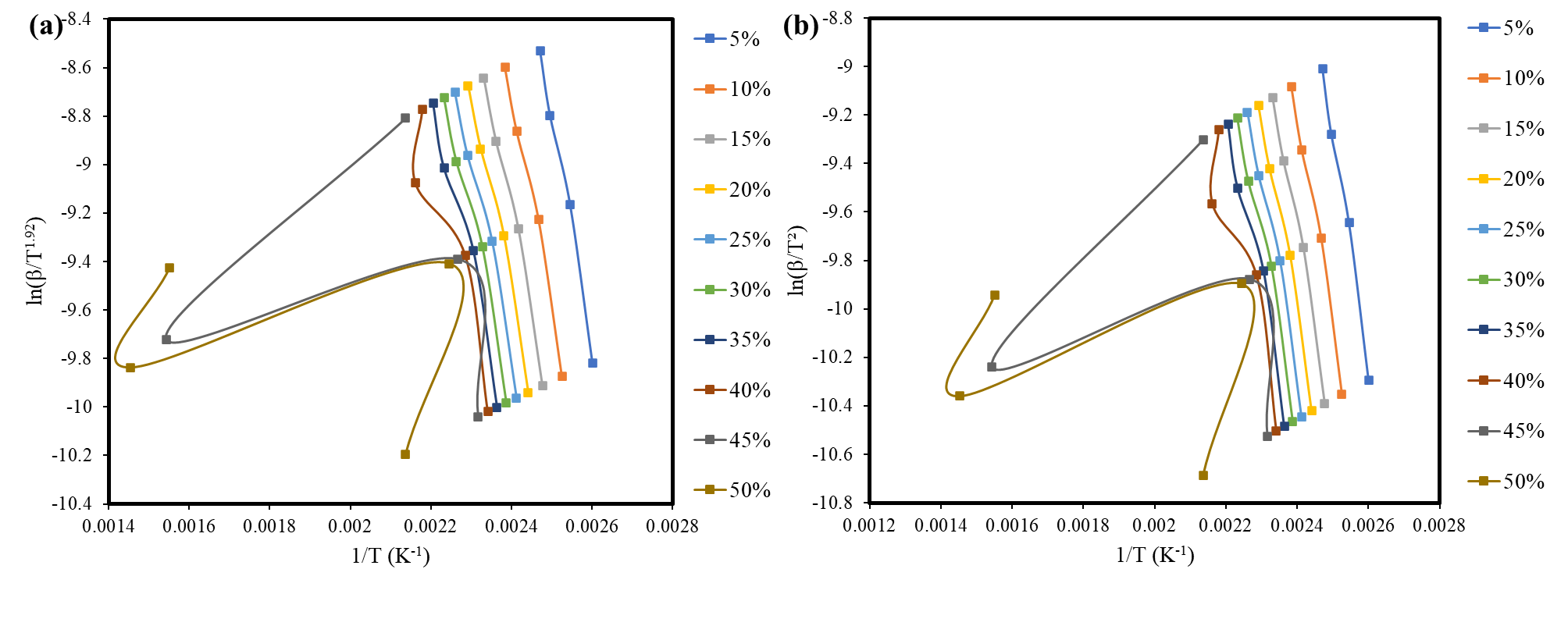
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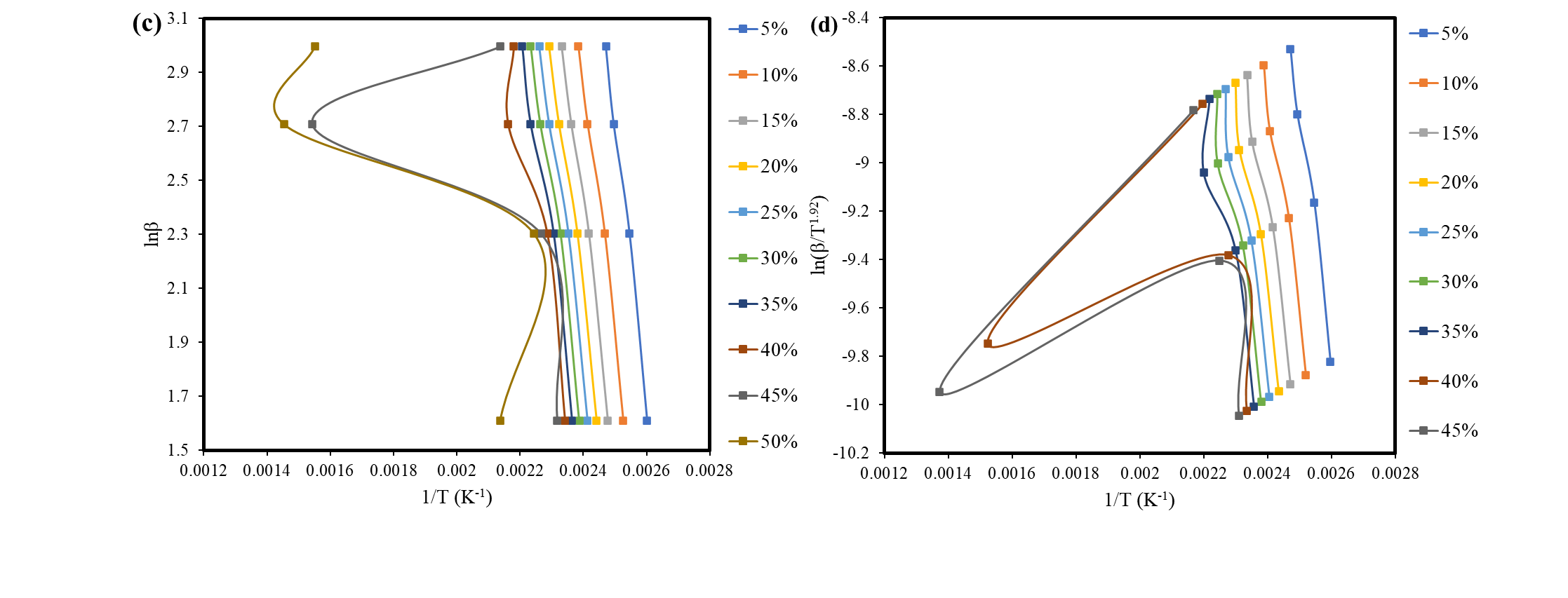
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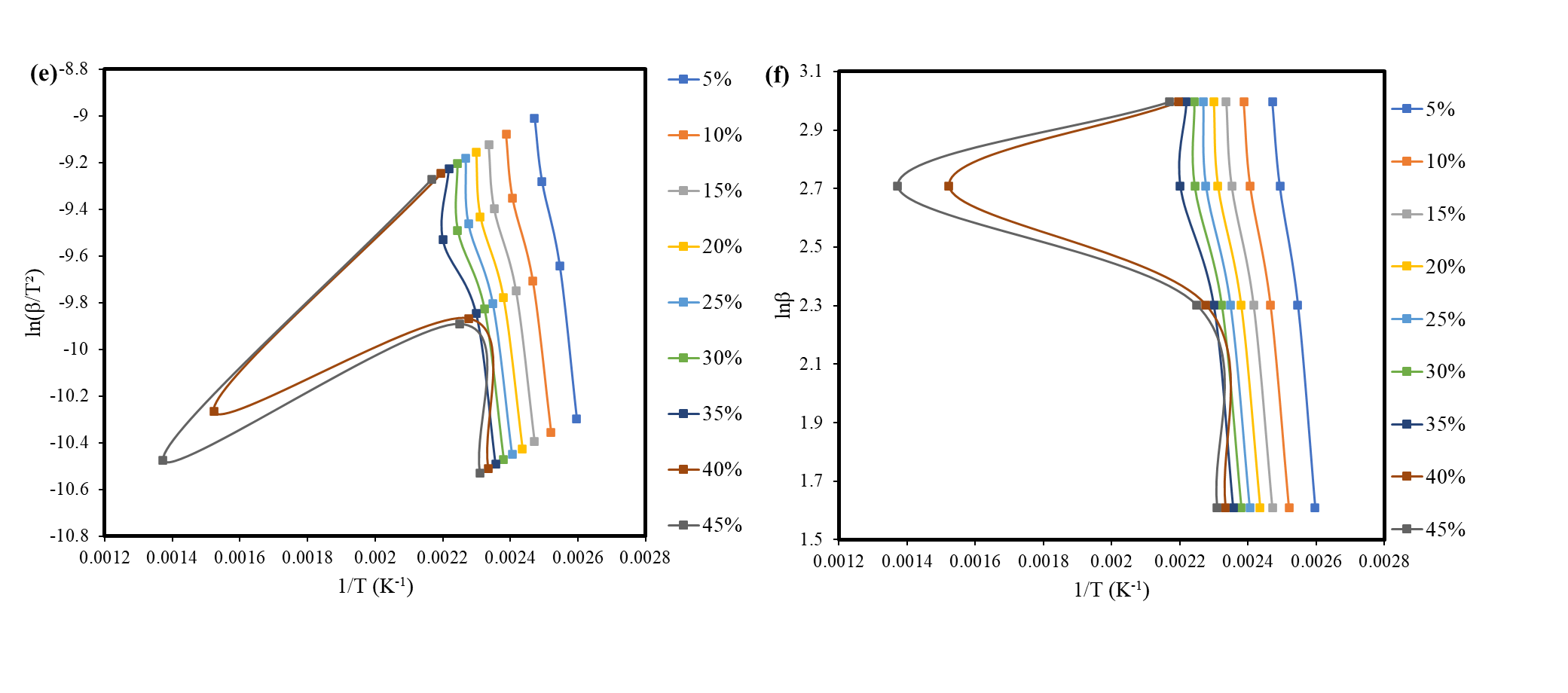
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**Fig. S.1.** Linear regression lines generated for different isoconversional models in combustion of TBP (a) Starink, (b) KAS, (c) FWO, and pyrolysis of TBP (d) Starink, (e) KAS, (f) FWO.

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**Fig. S.2**. Linear regression lines generated for different isoconversional models in the combustion of TBP with Fe2O3 (a) Starink, (b) KAS, (c) FWO, and pyrolysis of TBP (d) Starink, (e) KAS, (f) FWO.

**Table S.1.** *E*a and *A* values calculated for TBP for the combustion reaction using model-free

methods at different conversions

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Conversion  (%) | Straink Model | | | | KAS Model | | | | FWO model | | | |
| R2 | Ea (kJ/mol) | A (min-1) | MSE | R2 | Ea (kJ/mol) | A (min-1) | MSE | R2 | Ea (kJ/mol) | A (min-1) | MSE |
|  |
| 0.05 | 0.99 | 104.28 | 2.73E+13 | 0.0018 | 0.99 | 104.11 | 2.60E+13 | 0.0018 | 0.99 | 105.09 | 3.42E+13 | 0.0018 |  |
| 0.1 | 0.99 | 90.90 | 6.50E+11 | 0.0021 | 0.99 | 90.71 | 6.15E+11 | 0.0021 | 0.99 | 92.53 | 1.02E+12 | 0.0021 |  |
| 0.15 | 0.99 | 85.13 | 1.29E+11 | 0.0021 | 0.99 | 84.92 | 1.21E+11 | 0.0021 | 0.99 | 87.14 | 2.26E+11 | 0.0021 |  |
| 0.2 | 0.99 | 81.82 | 5.08E+10 | 0.0023 | 0.99 | 81.61 | 4.79E+10 | 0.0023 | 0.99 | 84.08 | 9.60E+10 | 0.0023 |  |
| 0.25 | 0.99 | 79.25 | 2.47E+10 | 0.0023 | 0.99 | 79.04 | 2.33E+10 | 0.0023 | 0.99 | 81.71 | 4.93E+10 | 0.0023 |  |
| 0.3 | 0.99 | 77.33 | 1.44E+10 | 0.0021 | 0.99 | 77.11 | 1.35E+10 | 0.0021 | 0.99 | 79.93 | 2.99E+10 | 0.0021 |  |
| 0.35 | 0.99 | 76.18 | 1.04E+10 | 0.0019 | 0.99 | 75.96 | 9.75E+09 | 0.0019 | 0.99 | 78.89 | 2.23E+10 | 0.0020 |  |
| 0.4 | 0.99 | 74.86 | 7.16E+09 | 0.0019 | 0.99 | 74.64 | 6.72E+09 | 0.0019 | 0.99 | 77.68 | 1.59E+10 | 0.0020 |  |
| 0.45 | 0.99 | 74.50 | 6.46E+09 | 0.0019 | 0.99 | 74.27 | 6.06E+09 | 0.0019 | 0.99 | 77.37 | 1.45E+10 | 0.0019 |  |
| 0.5 | 0.99 | 73.65 | 5.08E+09 | 0.0021 | 0.99 | 73.42 | 4.77E+09 | 0.0021 | 0.99 | 76.60 | 1.17E+10 | 0.0021 |  |
| 0.55 | 0.99 | 72.82 | 4.02E+09 | 0.0022 | 0.99 | 72.59 | 3.77E+09 | 0.0022 | 0.99 | 75.85 | 9.46E+09 | 0.0022 |  |
| 0.6 | 0.99 | 72.13 | 3.31E+09 | 0.0024 | 0.99 | 71.90 | 3.10E+09 | 0.0024 | 0.99 | 75.22 | 7.93E+09 | 0.0024 |  |
| 0.65 | 0.99 | 71.44 | 2.72E+09 | 0.0026 | 0.99 | 71.21 | 2.55E+09 | 0.0026 | 0.99 | 74.60 | 6.65E+09 | 0.0026 |  |
| 0.7 | 0.99 | 70.63 | 2.16E+09 | 0.0031 | 0.99 | 70.40 | 2.02E+09 | 0.0031 | 0.99 | 73.86 | 5.39E+09 | 0.0031 |  |
| 0.75 | 0.98 | 69.72 | 1.67E+09 | 0.0037 | 0.98 | 69.48 | 1.56E+09 | 0.0037 | 0.99 | 73.02 | 4.25E+09 | 0.0037 |  |
| 0.8 | 0.98 | 68.96 | 1.35E+09 | 0.0044 | 0.98 | 68.72 | 1.26E+09 | 0.0044 | 0.98 | 72.33 | 3.50E+09 | 0.0044 |  |
| 0.85 | 0.98 | 68.13 | 1.07E+09 | 0.0051 | 0.98 | 67.89 | 9.96E+08 | 0.0051 | 0.98 | 71.56 | 2.82E+09 | 0.0051 |  |
| 0.9 | 0.97 | 67.32 | 8.46E+08 | 0.0058 | 0.97 | 67.07 | 7.89E+08 | 0.0058 | 0.98 | 70.81 | 2.28E+09 | 0.0058 |  |
| 0.95 | 0.97 | 65.57 | 5.15E+08 | 0.0060 | 0.97 | 65.33 | 4.80E+08 | 0.0060 | 0.98 | 69.18 | 1.44E+09 | 0.0060 |  |

Table S.2. Ea and A values calculated for TBP for the pyrolysis reaction using model-free methods at different conversions

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Conversion  (%) | Straink Model | | | | KAS Model | | | | FWO model | | | |
| R2 | Ea (kJ/mol) | A (min-1) | MSE | R2 | Ea (kJ/mol) | A (min-1) | MSE | R2 | Ea (kJ/mol) | A (min-1) | MSE |
|  |
| 0.05 | 0.99 | 91.75 | 8.61E+11 | 0.0006 | 0.99 | 91.56 | 8.18E+11 | 0.0006 | 0.99 | 93.17 | 1.28E+12 | 0.0006 |  |
| 0.1 | 0.99 | 80.24 | 3.39E+10 | 0.0010 | 0.99 | 80.03 | 3.20E+10 | 0.0010 | 0.99 | 82.38 | 6.20E+10 | 0.0010 |  |
| 0.15 | 0.99 | 74.93 | 7.58E+09 | 0.0013 | 0.99 | 74.72 | 7.14E+09 | 0.0013 | 0.99 | 77.44 | 1.54E+10 | 0.0013 |  |
| 0.2 | 0.99 | 71.71 | 3.05E+09 | 0.0013 | 0.99 | 71.50 | 2.86E+09 | 0.0013 | 0.99 | 74.45 | 6.62E+09 | 0.0013 |  |
| 0.25 | 0.99 | 69.55 | 1.65E+09 | 0.0014 | 0.99 | 69.33 | 1.55E+09 | 0.0014 | 0.99 | 72.46 | 3.77E+09 | 0.0014 |  |
| 0.3 | 0.99 | 68.09 | 1.09E+09 | 0.0015 | 0.99 | 67.87 | 1.02E+09 | 0.0015 | 0.99 | 71.13 | 2.58E+09 | 0.0014 |  |
| 0.35 | 0.99 | 67.22 | 8.51E+08 | 0.0015 | 0.99 | 66.99 | 7.98E+08 | 0.0015 | 0.99 | 70.35 | 2.07E+09 | 0.0015 |  |
| 0.4 | 0.99 | 66.18 | 6.34E+08 | 0.0015 | 0.99 | 65.95 | 5.93E+08 | 0.0015 | 0.99 | 69.41 | 1.59E+09 | 0.0015 |  |
| 0.45 | 0.99 | 65.79 | 5.67E+08 | 0.0013 | 0.99 | 65.56 | 5.30E+08 | 0.0013 | 0.99 | 69.07 | 1.44E+09 | 0.0013 |  |
| 0.5 | 0.99 | 64.98 | 4.50E+08 | 0.0015 | 0.99 | 64.74 | 4.21E+08 | 0.0015 | 0.99 | 68.34 | 1.17E+09 | 0.0015 |  |
| 0.55 | 0.99 | 64.25 | 3.65E+08 | 0.0017 | 0.99 | 64.01 | 3.41E+08 | 0.0017 | 0.99 | 67.68 | 9.69E+08 | 0.0017 |  |
| 0.6 | 0.99 | 63.51 | 2.96E+08 | 0.0016 | 0.99 | 63.27 | 2.77E+08 | 0.0016 | 0.99 | 67.01 | 8.02E+08 | 0.0016 |  |
| 0.65 | 0.99 | 62.72 | 2.36E+08 | 0.0017 | 0.99 | 62.48 | 2.20E+08 | 0.0017 | 0.99 | 66.28 | 6.52E+08 | 0.0017 |  |
| 0.7 | 0.99 | 62.11 | 1.99E+08 | 0.0017 | 0.99 | 61.87 | 1.85E+08 | 0.0017 | 0.99 | 65.74 | 5.58E+08 | 0.0017 |  |
| 0.75 | 0.99 | 61.47 | 1.65E+08 | 0.0016 | 0.99 | 61.23 | 1.54E+08 | 0.0016 | 0.99 | 65.16 | 4.73E+08 | 0.0016 |  |
| 0.8 | 0.99 | 61.16 | 1.51E+08 | 0.0015 | 0.99 | 60.92 | 1.41E+08 | 0.0015 | 0.99 | 64.89 | 4.39E+08 | 0.0015 |  |
| 0.85 | 0.99 | 60.75 | 1.35E+08 | 0.0015 | 0.99 | 60.51 | 1.26E+08 | 0.0015 | 0.99 | 64.53 | 3.96E+08 | 0.0015 |  |
| 0.9 | 0.99 | 60.39 | 1.22E+08 | 0.0013 | 0.99 | 60.15 | 1.13E+08 | 0.0013 | 0.99 | 64.21 | 3.62E+08 | 0.0013 |  |
| 0.95 | 0.99 | 59.98 | 1.08E+08 | 0.0011 | 0.99 | 59.73 | 1.01E+08 | 0.0011 | 0.99 | 63.85 | 3.26E+08 | 0.0011 |  |

Table S.3. Thermodynamic parameters for pyrolysis of TBP

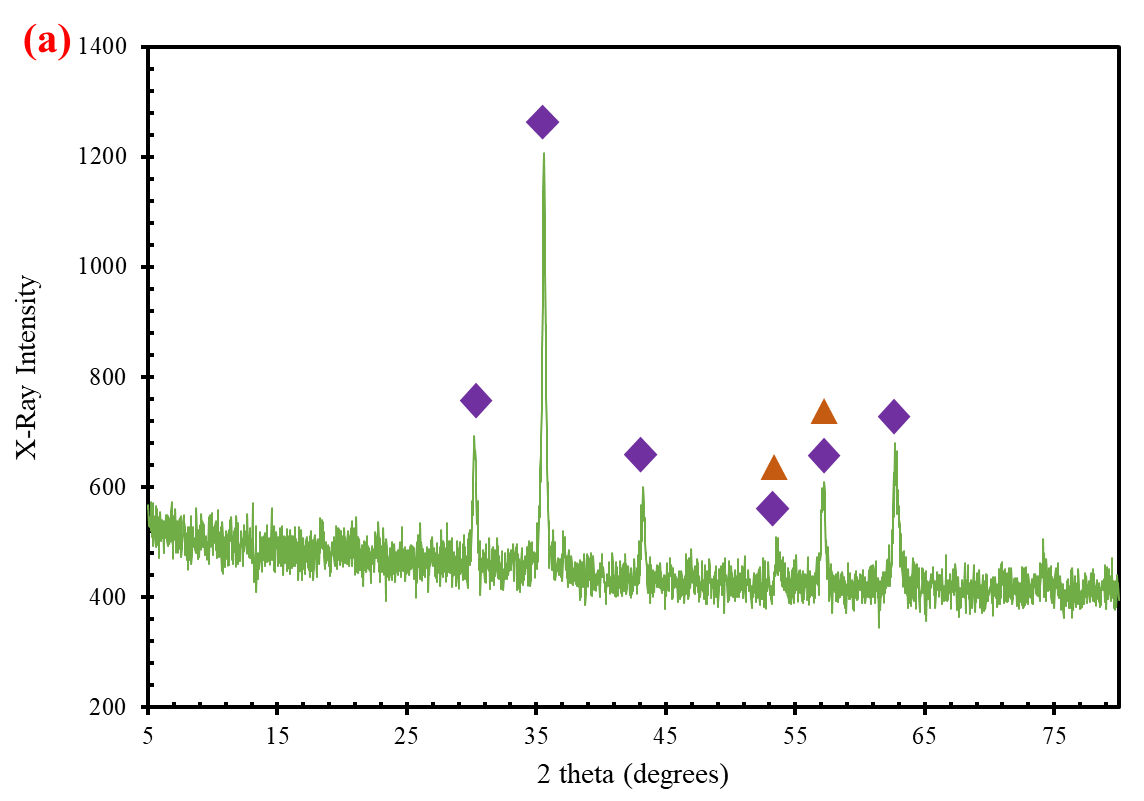
|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Coversion (%) | Straink Model | | | KAS Model | | | FWO model | | |
| ΔH (kJ/mol) | ΔG (kJ/mol) | ΔS (kJ/mol) | ΔH (kJ/mol) | ΔG (kJ/mol) | ΔS (kJ/mol) | ΔH (kJ/mol) | ΔG (kJ/mol) | ΔS (kJ/mol) |
| 0.5 | 88.33 | 100.58 | -0.03 | 88.15 | 100.59 | -0.03 | 89.75 | 83.43 | 0.01 |
| 0.1 | 76.82 | 101.08 | -0.05 | 76.62 | 101.09 | -0.05 | 78.97 | 83.89 | -0.01 |
| 0.15 | 71.52 | 101.33 | -0.07 | 71.31 | 101.34 | -0.07 | 74.02 | 84.12 | -0.02 |
| 0.2 | 68.30 | 101.49 | -0.07 | 68.08 | 101.50 | -0.07 | 71.04 | 84.26 | -0.03 |
| 0.25 | 66.13 | 101.61 | -0.08 | 65.91 | 101.62 | -0.08 | 69.05 | 84.36 | -0.03 |
| 0.3 | 64.68 | 101.69 | -0.08 | 64.45 | 101.70 | -0.08 | 67.72 | 84.43 | -0.04 |
| 0.35 | 63.81 | 101.73 | -0.08 | 63.58 | 101.75 | -0.09 | 66.94 | 84.47 | -0.04 |
| 0.4 | 62.77 | 101.79 | -0.09 | 62.54 | 101.80 | -0.09 | 66.00 | 84.52 | -0.04 |
| 0.45 | 62.38 | 101.81 | -0.09 | 62.14 | 101.83 | -0.09 | 65.66 | 84.54 | -0.04 |
| 0.5 | 61.56 | 101.86 | -0.09 | 61.33 | 101.87 | -0.09 | 64.92 | 84.58 | -0.04 |
| 0.55 | 60.83 | 101.90 | -0.09 | 60.60 | 101.92 | -0.09 | 64.26 | 84.62 | -0.05 |
| 0.6 | 60.10 | 101.94 | -0.09 | 59.86 | 101.96 | -0.09 | 63.59 | 84.65 | -0.05 |
| 0.65 | 59.30 | 101.99 | -0.10 | 59.06 | 102.01 | -0.10 | 62.87 | 84.69 | -0.05 |
| 0.7 | 58.70 | 102.03 | -0.10 | 58.46 | 102.04 | -0.10 | 62.32 | 84.72 | -0.05 |
| 0.75 | 58.06 | 102.07 | -0.10 | 57.81 | 102.08 | -0.10 | 61.74 | 84.76 | -0.05 |
| 0.8 | 57.75 | 102.08 | -0.10 | 57.50 | 102.10 | -0.10 | 61.48 | 84.77 | -0.05 |
| 0.85 | 57.34 | 102.11 | -0.10 | 57.09 | 102.12 | -0.10 | 61.11 | 84.79 | -0.05 |
| 0.9 | 56.98 | 102.13 | -0.10 | 56.73 | 102.15 | -0.10 | 60.80 | 84.81 | -0.05 |
| 0.95 | 56.57 | 102.16 | -0.10 | 56.32 | 102.17 | -0.10 | 60.44 | 84.83 | -0.05 |

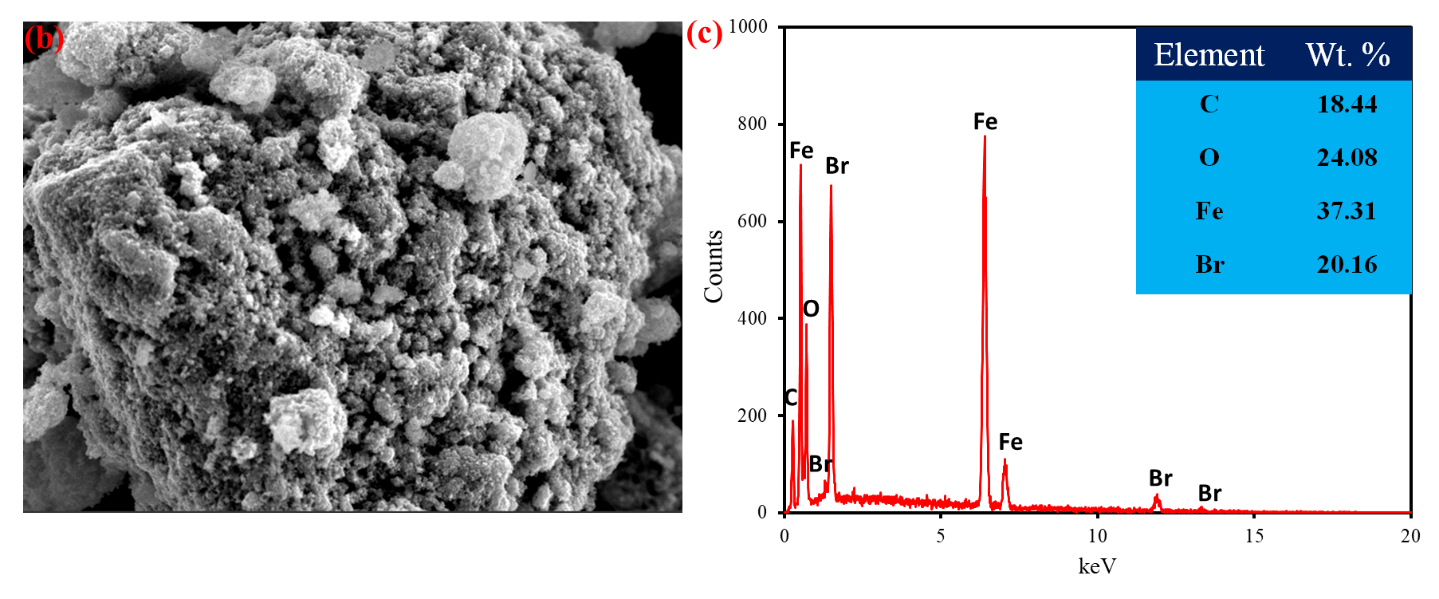
Table S.4. Thermodynamic parameters for catalytic combustion of TBP using Fe2O3

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Coversion (%) | Straink Model | | | KAS Model | | | FWO model | | |
| ΔH (kJ/mol) | ΔG (kJ/mol) | ΔS (kJ/mol) | ΔH (kJ/mol) | ΔG (kJ/mol) | ΔS (kJ/mol) | ΔH (kJ/mol) | ΔG (kJ/mol) | ΔS (kJ/mol) |
| 0.05 | 75.78 | 99.44 | -0.05 | 75.58 | 99.45 | -0.05 | 77.85 | 82.51 | -0.01 |
| 0.1 | 68.71 | 99.78 | -0.07 | 68.50 | 99.79 | -0.07 | 71.33 | 82.81 | -0.03 |
| 0.15 | 66.04 | 99.92 | -0.08 | 65.82 | 99.93 | -0.08 | 68.92 | 82.93 | -0.03 |
| 0.2 | 64.19 | 100.01 | -0.08 | 63.96 | 100.02 | -0.08 | 67.26 | 83.01 | -0.04 |
| 0.25 | 62.36 | 100.11 | -0.09 | 62.13 | 100.12 | -0.09 | 65.60 | 83.10 | -0.04 |
| 0.3 | 60.48 | 100.22 | -0.09 | 60.25 | 100.23 | -0.09 | 63.89 | 83.19 | -0.04 |
| 0.35 | 57.43 | 100.39 | -0.10 | 57.19 | 100.41 | -0.10 | 61.06 | 83.34 | -0.05 |
| 0.4 | 42.73 | 101.38 | -0.13 | 42.47 | 101.40 | -0.13 | 47.18 | 84.21 | -0.08 |
| 0.45 | -3.36 | 115.02 | -0.27 | -3.01 | 114.03 | -0.27 | 2.47 | 91.54 | -0.20 |
| 0.5 | -3.54 | 115.66 | -0.27 | -3.91 | 117.42 | -0.28 | 4.73 | 90.51 | -0.19 |

Table S.5. Thermodynamic parameters for catalytic pyrolysis of TBP using Fe2O3

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Coversion (%) | Straink Model | | | KAS Model | | | FWO model | | |
| ΔH (kJ/mol) | ΔG (kJ/mol) | ΔS (kJ/mol) | ΔH (kJ/mol) | ΔG (kJ/mol) | ΔS (kJ/mol) | ΔH (kJ/mol) | ΔG (kJ/mol) | ΔS (kJ/mol) |
| 0.05 | 77.65 | 99.41 | -0.05 | 77.45 | 99.42 | -0.05 | 79.63 | 82.47 | -0.01 |
| 0.1 | 70.82 | 99.73 | -0.07 | 70.61 | 99.74 | -0.07 | 73.33 | 82.75 | -0.02 |
| 0.15 | 67.82 | 99.87 | -0.07 | 67.60 | 99.89 | -0.07 | 70.61 | 82.88 | -0.03 |
| 0.2 | 65.95 | 99.97 | -0.08 | 65.73 | 99.98 | -0.08 | 68.93 | 82.97 | -0.03 |
| 0.25 | 66.05 | 99.97 | -0.08 | 64.03 | 100.07 | -0.08 | 66.98 | 83.07 | -0.04 |
| 0.3 | 61.13 | 100.23 | -0.09 | 60.89 | 100.24 | -0.09 | 64.50 | 83.19 | -0.04 |
| 0.35 | 53.00 | 100.71 | -0.11 | 52.76 | 100.73 | -0.11 | 56.86 | 83.62 | -0.06 |
| 0.4 | -2.53 | 112.66 | -0.26 | -2.18 | 112.11 | -0.26 | 1.24 | 92.16 | -0.21 |
| 0.45 | -0.99 | 110.72 | -0.25 | -0.61 | 110.37 | -0.25 | 0.22 | 92.84 | -0.21 |





**Fig. S.3.** XRD pattern for the co-pyrolyzed mixture of TBP:Fe2O3 (a), SEM-EDX analysis of (b) co-pyrolyzed TBP: Fe2O3, (b) Elemental composition of the sample.