

Supplementary Materials

***Operando* dual beam FTIR unravels promotional effect of Zn for HZSM-5 in short-chain alkane aromatization**

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Table S1 Catalytic performance of HZSM-5 and Zn/HZSM-5 in *iso*-butane aromatization under different pressures

Cat.	Pressure /kPa	Con. %	Product Selectivity (wt %)		
			Alkanes (C ₁ ⁰ +C ₂ ⁰ + C ₃ ⁰ + <i>n</i> -C ₄ ⁰)	Olefins (C ₂ ⁼ +C ₃ ⁼ +C ₄ ⁼)	Aromatics (BTX)
HZ	101.33	87.51	57.11	13.37	29.52
	91.20	79.06	46.23	36.46	17.31
	81.06	75.01	46.50	39.07	14.43
	60.80	66.13	36.10	54.30	9.60
Zn _{1.03} /HZ	101.33	95.46	40.04	23.02	36.94
	91.20	93.33	46.68	31.85	21.47
	81.06	85.57	36.34	45.02	18.64
	60.80	73.46	26.60	60.42	12.98
Zn _{2.34} /HZ	101.33	97.05	41.42	16.69	41.89
	91.20	96.94	44.83	17.14	38.03
	81.06	94.03	33.73	36.67	29.60
	60.80	90.55	39.82	41.41	19.07
Zn _{8.47} /HZ	101.33	99.32	54.80	6.22	38.98
	91.20	96.03	46.60	22.20	31.20
	81.06	94.27	47.91	23.14	28.95
	60.80	93.54	47.08	32.46	20.16

Reaction conditions: fixed-bed reactor, *T*=560 °C, *WHSV*=0.75h⁻¹, *TOS*=24 h.

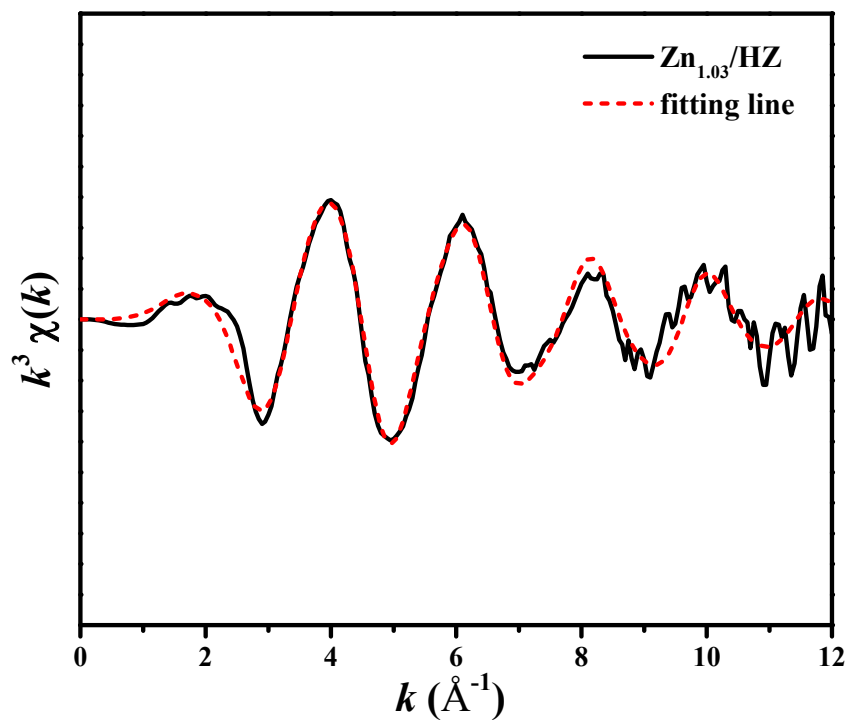


Figure S1 EXAFS functions and the fittings of Zn_{1.03}/HZSM-5 catalyst for the Zn K filtered k^3 -weighted $\chi(k)$ and the Fourier Transform function in the k range of 3-12Å⁻¹.

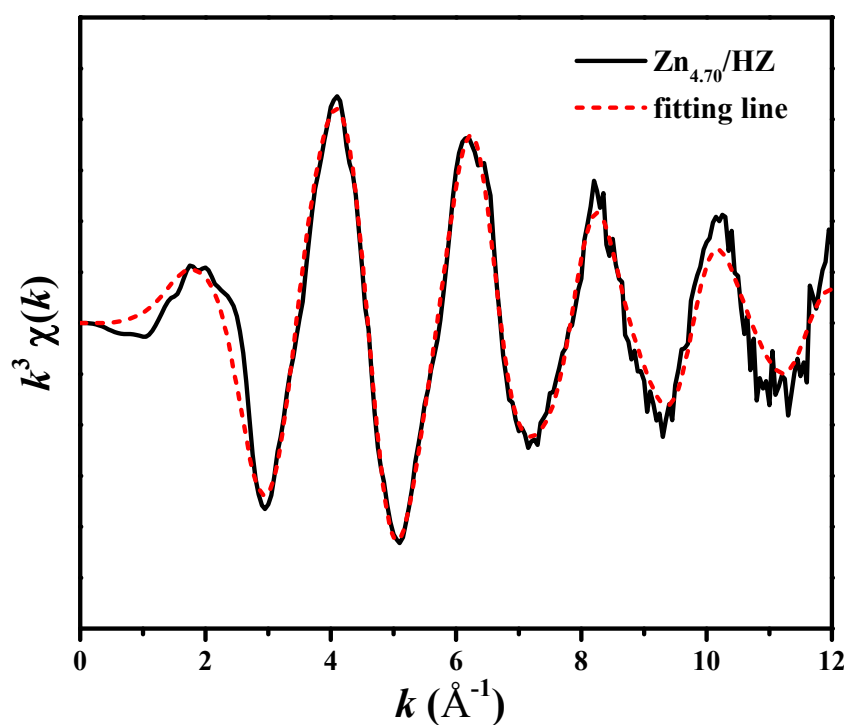


Figure S2 EXAFS functions and the fittings of Zn_{4.70}/HZSM-5 catalyst for the Zn K filtered k^3 -weighted $\chi(k)$ and the Fourier Transform function in the k range of 3-12Å⁻¹.

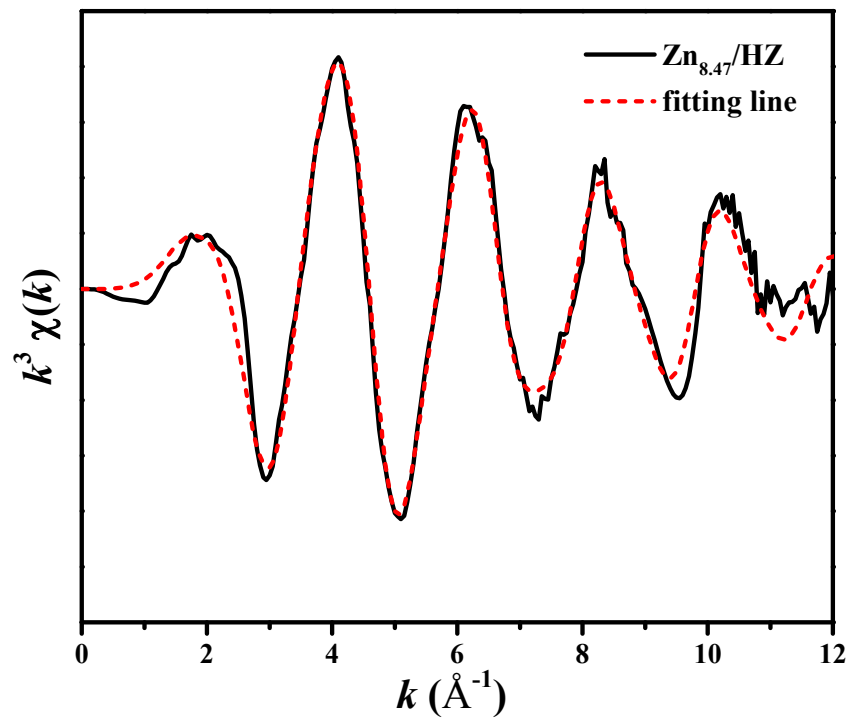


Figure S3 EXAFS functions and the fittings of $\text{Zn}_{8.47}/\text{HZSM-5}$ catalyst for the Zn K filtered k^3 -weighted $\chi(k)$ and the Fourier Transform function in the k range of $3\text{-}12\text{\AA}^{-1}$.

HZSM-5

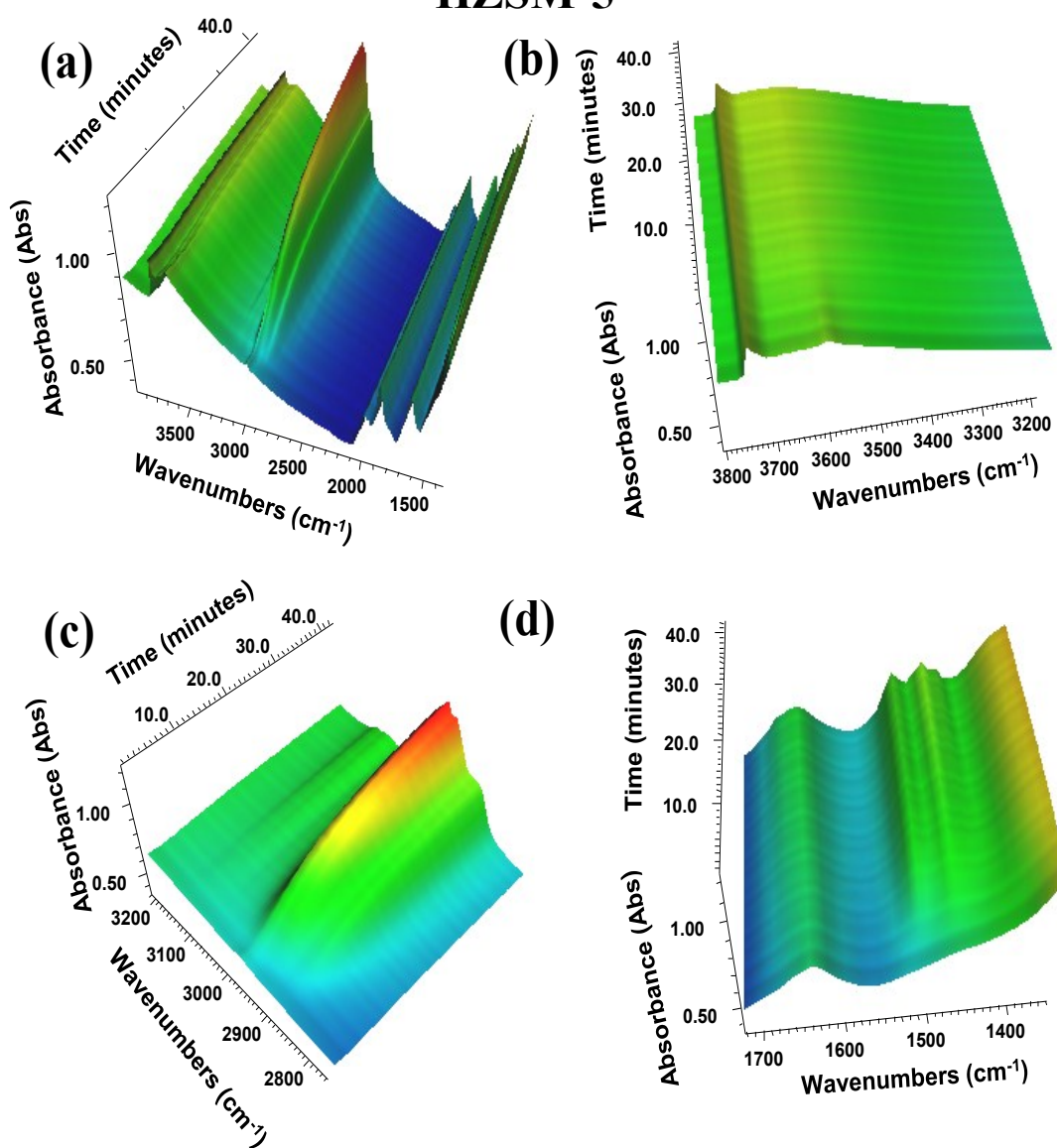


Figure S4 Three-dimensional FTIR profiles of propene aromatization on HZSM-5 at 250°C and 60.80 kPa, obtained using DB-FTIR in a flowing mixture of propene and nitrogen gas (6 % propene - 94 % nitrogen) for 40 minutes, GHSV=1080 h^{-1} (a) 4000-1300 cm^{-1} , (b) 3800-3100 cm^{-1} , (c) 3200-2700 cm^{-1} and (d) 1700-1300 cm^{-1} .

Zn_{1.03}/HZSM-5

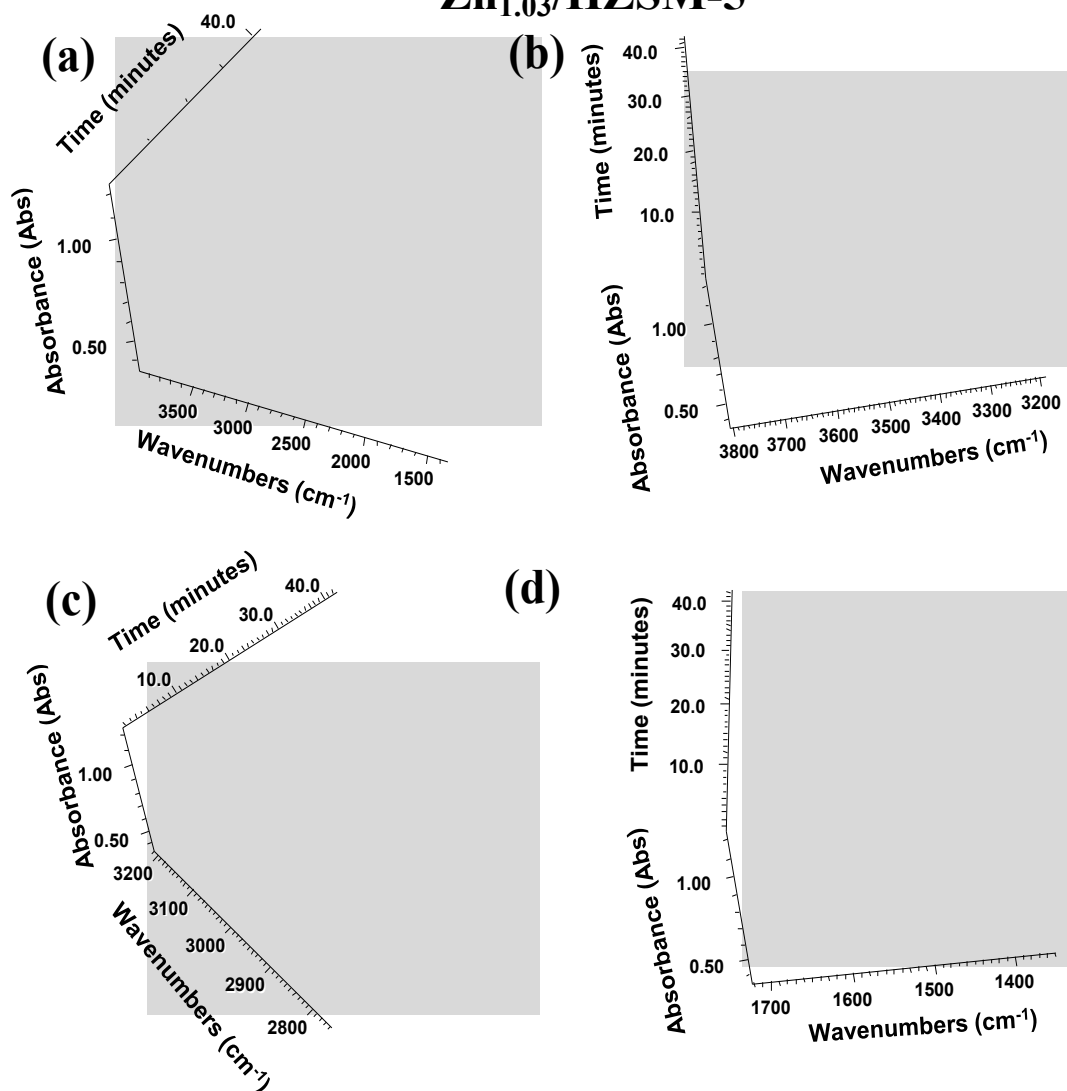


Figure S5 Three-dimensional FTIR profiles of propene aromatization on Zn_{1.03}/HZSM-5 at 250°C and 60.80 kPa, obtained using DB-FTIR in a flowing mixture of propene and nitrogen gas (6 % propene - 94 % nitrogen) for 40 minutes, GHSV=1080 h⁻¹ (a) 4000-1300 cm⁻¹, (b) 3800-3100 cm⁻¹, (c) 3200-2700 cm⁻¹ and (d) 1700-1300 cm⁻¹.

Zn_{2.34}/HZSM-5

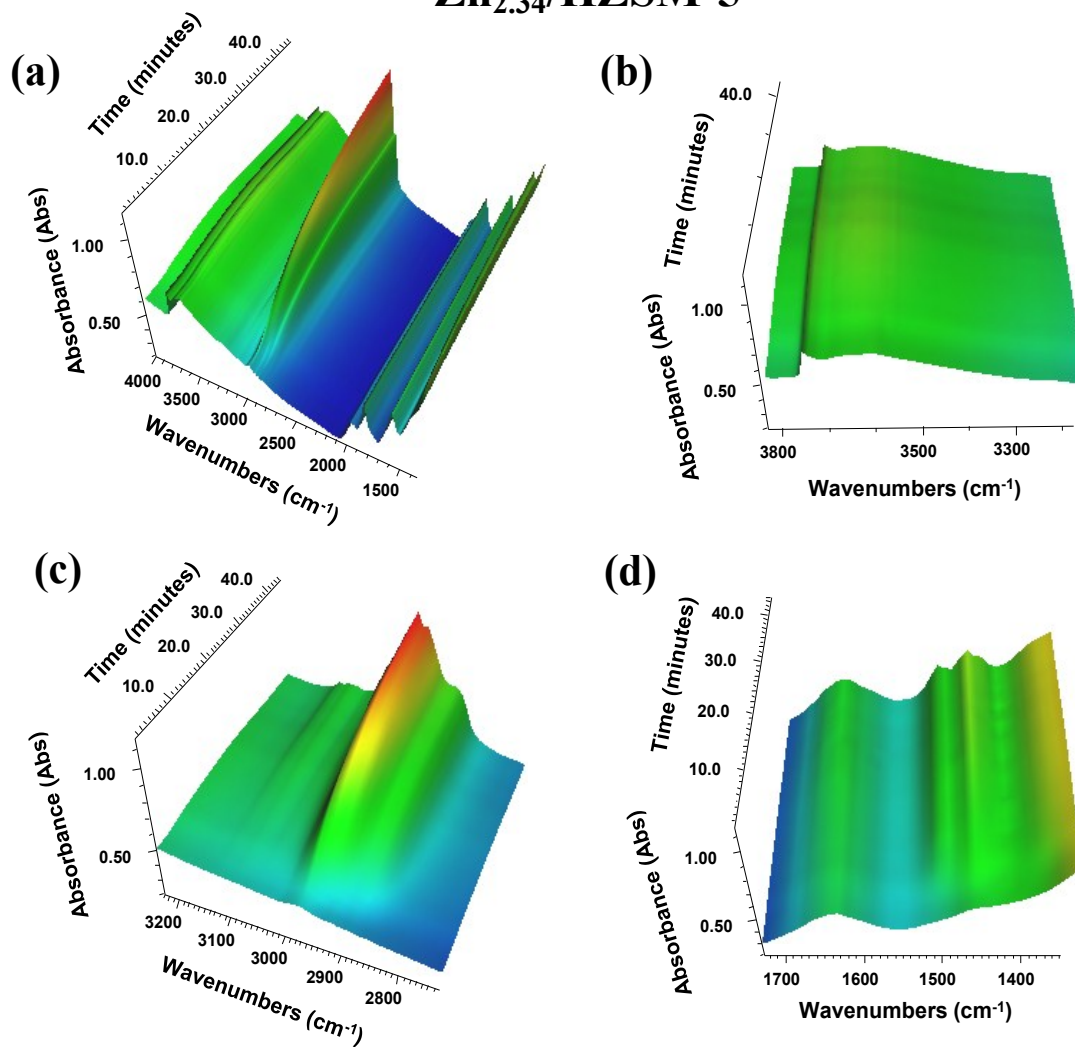


Figure S6 Three-dimensional FTIR profiles of propene aromatization on Zn_{2.34}/HZSM-5 at 250°C and 60.80 kPa, obtained using DB-FTIR in a flowing mixture of propene and nitrogen gas (6 % propene - 94 % nitrogen) for 40 minutes, GHSV=1080 h⁻¹ (a) 4000-1300 cm⁻¹, (b) 3800-3100 cm⁻¹, (c) 3200-2700 cm⁻¹ and (d) 1700-1300 cm⁻¹.

Zn_{8.47}/HZSM-5

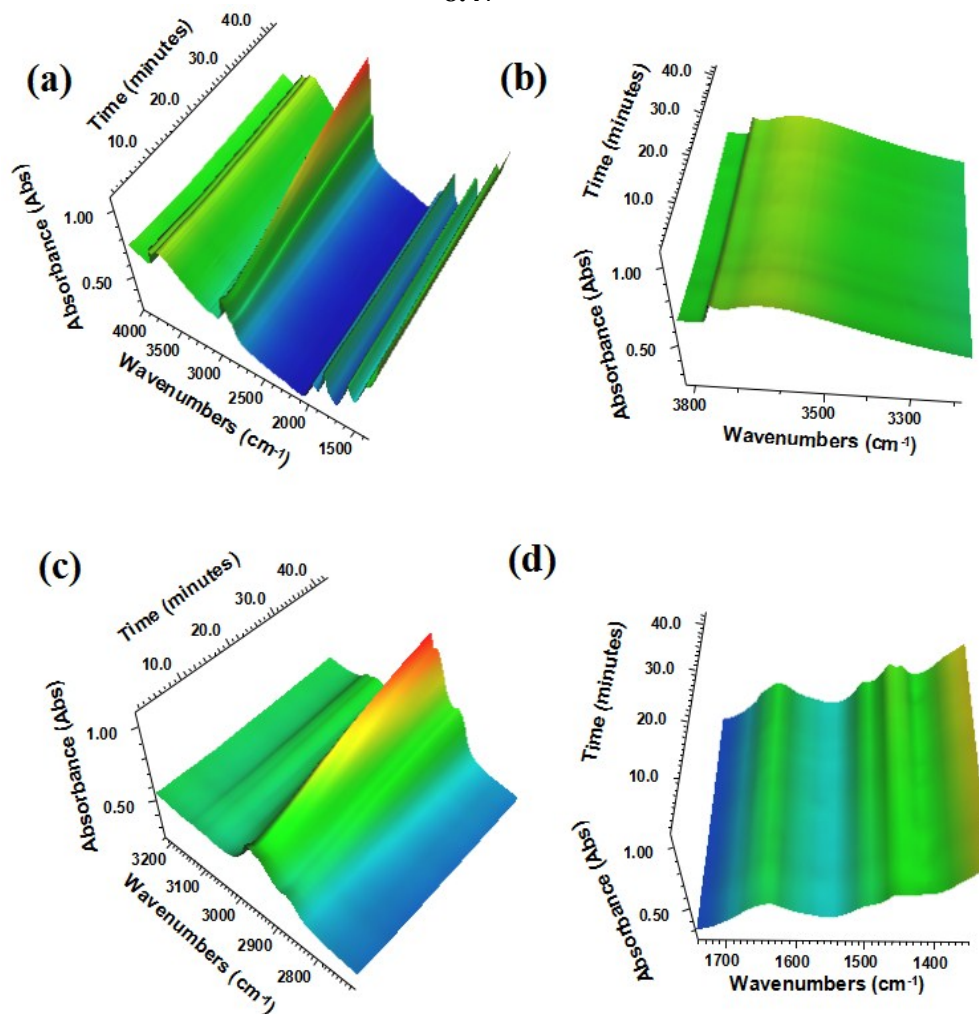


Figure S7 Three-dimensional FTIR profiles of propene aromatization on Zn_{8.47}/HZSM-5 at 250°C and 60.80 kPa, obtained using DB-FTIR in a flowing mixture of propene and nitrogen gas (6 % propene - 94 % nitrogen) for 40 minutes, GHSV=1080 h⁻¹ (a) 4000-1300 cm⁻¹, (b) 3800-3100 cm⁻¹, (c) 3200-2700 cm⁻¹ and (d) 1700-1300 cm⁻¹.