

# Use of the Far Infrared Spectroscopy for NaCl and KCl Minerals Characterization—A Case Study of Halides from Kłodawa in Poland

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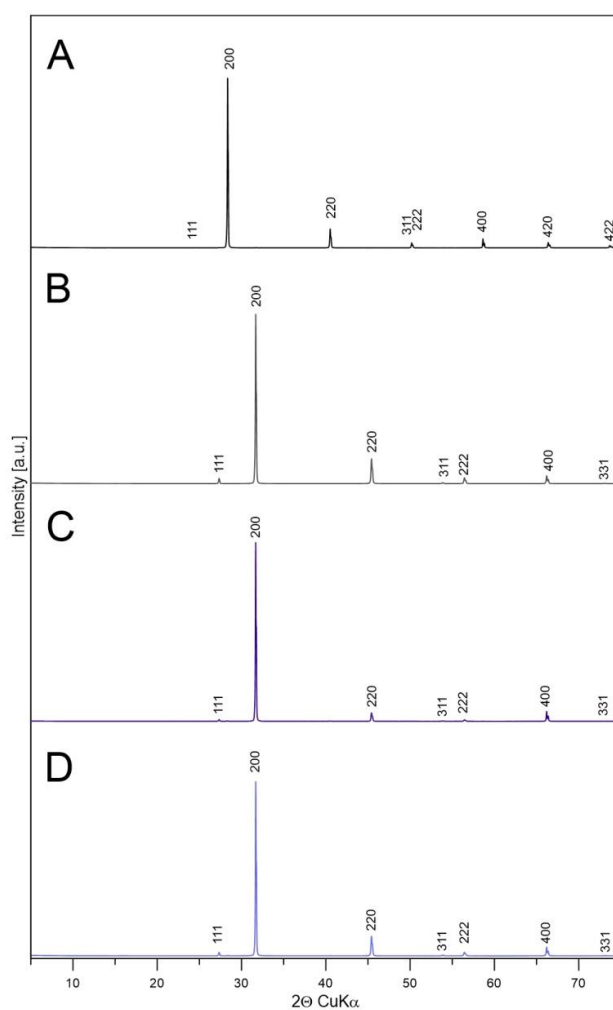
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**Figure S1.** Experimental X-ray diffraction pattern of minerals: colorless sylvite (A), colorless halite (B), purple halite (C) and blue halite (D).

**Table S1.** Calculated IR Frequency and Intensity of T1u vibrational modes for 125-atom NaCl and KCl models (B3LYP/6-31g\*).

	NaCl		KCl	
	Frequency [cm <sup>-1</sup> ]	IR Intensity [KM/Mole]	Frequency [cm <sup>-1</sup> ]	IR Intensity [KM/Mole]
1	48.7375	1.4550	34.8871	0.6111
2	73.6758	0.0072	56.3326	0.3875
3	84.7968	1.0561	60.0623	1.3223
4	88.5842	4.6814	61.5352	1.3009
5	93.1275	1.6429	72.0011	0.1576
6	97.1096	1.4783	73.6195	0.2502
7	106.7581	3.0053	80.1951	0.5836
8	113.6858	9.3078	86.4656	10.0793
9	120.3571	1.7680	91.0570	5.5522
10	123.2576	11.9396	97.1164	1.6023
11	130.2331	7.7507	102.9430	1.4129
12	136.3062	1.0737	106.4910	3.4732
13	140.3303	9.9069	108.0022	1.7009
14	143.1047	5.1626	112.1875	63.1098
15	146.8878	186.3441	113.8818	70.9338
16	153.8113	1.6411	118.4101	30.3330
17	161.8600	51.7630	134.0071	2.3555
18	168.4465	1.0132	137.0255	9.1089
19	171.6719	9.8683	139.4639	13.2024
20	176.3972	22.7052	142.3388	0.4886
21	182.7580	266.1723	143.9887	181.8344
22	186.8098	80.8524	150.1256	11.7897
23	191.9967	18.3741	152.1756	196.8190
24	194.4425	114.9770	154.3016	10.5380
25	197.1484	2.4169	156.6175	1.0833
26	204.1634	96.4358	159.6395	10.0151
27	213.0107	916.0933	163.6259	403.9725
28	225.5459	492.2016	173.6640	735.1937
29	239.3126	503.8864	188.1144	548.701