File: Sample ( 0.939 G HAP) Mohamed Ali Name and formula 04-017-1206 Reference code: Mineral name: Hydroxylapatite Hydrogen Calcium Chloride Carbonate Phosphate Hydroxide Hydrate Compound name: C<sub>0.25</sub>Ca<sub>4.575</sub>Cl<sub>0.05</sub>H<sub>3.55</sub>O<sub>13.7</sub>P<sub>2.75</sub> Empirical formula: Chemical formula:  ${
m H_{0.6}Ca_{4.575}\,(PO_4\,)_{2.75}\,(CO_3\,)_{0.25}Cl_{0.05}\,(OH\,)_{0.95}\,(H_2O\,)}$ Crystallographic parameters Hexagonal P63/m Space group: Space group number: 9.4420 9.4420 6.8770 90.0000 90.0000 120.0000 Subfiles and quality LPF Pattern Mineral Blank (B) <u>Comments</u> 01/01/1970 Modification Date: LPF Collection Code: STARTING MATERIALS: adult human tooth enamel. Significant Warning from the LPF Editor Comment: occupancy of site OH4 was set to unity for standardized data. Sample Source or Locality: human dental enamel. Minor Warning: Density occupancy of site OH4 was set to unity for standardized data. Sample Source or Locality: human dental enamel. Minor Warning: Density occupancy of site OH4 was set to unity for standardized data. Sample Source or Locality: human dental enamel. Minor Warning: Density occupancies or Locality: human dental enamel. Minor Warning: Density occupance or Locality: human dental enamel. Minor Warning: Density occupance or Locality: human dental enamel. Comment: short interatom occupance or Locality: human dental enamel. Minor Warning: Density occupance or Locality: human dental enamel. Comment: short interatom occupance or Locality: human dental enamel. Minor Warning: Density occupance or Locality: human dental enamel. Minor Warning: Density occupance or Locality: human dental enamel. Minor Warning: Density occupance or Locality: human dental enamel. Minor Warning: Density occupance or Locality: human dental enamel. Minor warning: Density occupance or Locality: human dental enamel. Minor warning: Density occupance or Locality: human dental enamel. Minor warning: Density occupance or Locality: human dental enamel. Minor warning: Density occupance or Locality: human dental enamel. Minor warning: Density occupance or Locality: human dental enamel. Minor warning: Density occupance or Locality: human dental enamel. Minor warning: Density occupance or Locality: human dental enamel. Minor warning: Density occupance or Locality: human dental enamel. Minor warning: Density occupance or Locality: human dental enamel. Minor warning: Density occupance or Locality: human dental enamel. Minor warning: Density occupance or Locality: human dental enamel. Minor warning: Density occupance or Locality: human dental enamel. Minor warning: Density occupance or Locality: human dental enamel. Minor warning: Density occu Sample Preparation: <u>References</u> Young R.A., Mackie P.E., *Mater. Res. Bull.*, **15**, 17, (1980) Primary reference: Young R.A., Mackie P.E., *Mater. Res. Bull.*, **15**, 17, (1980) <u>Peak list</u> No. h k l d [A] 2Theta[deg] I [%]
1 1 0 0 8.17700 10.811 12.7 2 1 0 1 5.26310 16.832 23.8 3 1 1 0 4.72100 18.781 1.5 4 2 0 0 4.08850 21.720 2.5 5 1 1 1 3.89210 22.830 4.3 6 2 0 1 3.51430 25.323 3.0 7 0 0 2 3.43850 25.891 18.7 8 1 0 2 3.16970 28.130 4.1 9 1 2 0 3.09060 28.865 21.8 10 2 1 1 2.81900 31.716 97.9 11 1 1 2 2.77940 32.180 39.6 12 3 0 0 2.72570 32.832 100.0 13 2 0 2 2.63160 34.041 14.7 14 3 0 1 2.53390 35.396 4.1 15 2 2 0 2.36050 38.092 1.4 16 1 2 2 2.29860 39.159 6.4 17 1 3 0 2.26790 39.712 28.5 18 2 2 1 2.23260 40.366 2.2 19 1 0 3 2.20720 40.852 0.1 20 1 3 1 2.15380 41.912 5.6 21 3 0 2 2.13600 42.277 2.6 22 1 1 3 2.06210 43.870 6.6 23 4 0 0 2.04420 44.274 1.7 24 2 0 3 1.99950 45.318 3.1 25 4 0 1 1.95950 46.296 1.5 26 2 2 2 1.94610 46.634 24.8 27 3 1 2 1.89320 48.018 11.9 28 2 3 0 1.87590 48.489 5.1 29 2 1 3 1.84120 49.463 21.5 30 2 3 1 1.80980 50.381 21.0 31 4 1 0 1.78440 51.149 18.6 32 4 0 2 1.75720 52.000 9.4 33 4 1 1 1.72720 52.972 0.8 34 0 0 4 1.71920 53.238 13.0 35 1 0 4 1.68250 54.494 1.9 36 3 2 2 1.64680 55.777 3.5 37 5 0 0 1.63540 56.201 0.4 38 3 1 3 1.61220 57.083 3.9 39 5 0 1 1.59100 57.915 0.8 40 4 1 2 1.58380 58.203 2.1 41 3 3 0 1.57370 58.613 2.2 42 2 4 0 1.54530 59.799 1.6 43 3 3 1 1.53400 60.285 1.3 44 4 0 3 1.52570 60.647 0.1 45 2 4 1 1.50770 61.449 2.5 46 2 1 4 1.50240 61.689 5.4 47 5 0 2 1.47690 62.875 5.7 48 1 5 0 1.46860 63.271 2.3 49 3 0 4 1.45410 63.976 5.7 50 3 2 3 1.45180 64.090 4.5 51 5 1 1 1.43620 64.870 8.1 52 3 3 2 1.43090 65.140 1.1 53 4 2 2 1.40950 66.255 2.9 54 2 2 4 1.38970 67.324 0.3 55 3 1 4 1.37010 68.419 0.9 56 6 0 0 1.36280 68.837 0.3 57 1 0 5 1.35640 69.208 0.4 58 5 1 2 1.35060 69.548 2.0 59 3 4 0 1.34430 69.921 0.3 60 6 0 1 1.33680 70.371 0.1 61 5 0 3 1.33130 70.705 0.3 62 4 3 1 1.31930 71.446 3.7 63 5 2 0 1.30940 72.071 3.0 64 2 0 5 1.30360 72.442 0.6

65 3 3 1.29740 72.844 0.2 66 5 2 1 1.28630 73.575 0.7 67 2 4 3 1.28140 73.903 2.4 68 6 0 2 1.26750 74.851 3.2 69 2 3 4 1.26750 74.851 3.2 70 2 1 5 1.25660 75.614 4.2 71 3 4 2 1.25200 75.941 2.2 72 6 1 0 1.24700 76.300 0.5 73 1 4 4 1.23810 76.949 2.7 74 5 1 3 1.23660 77.059 3.3 75 1 6 1 1.22700 77.775 1.5 76 2 5 2 1.22360 78.032 6.8 77 2 2 5 1.18840 80.809 0.4 78 4 4 0 1.18020 81.489 3.6 79 3 1 5 1.17600 81.842 0.8 80 6 0 3 1.17230 82.156 0.7 81 1 6 2 1.17230 82.156 0.7 82 7 0 0 1.16810 82.515 0.5 83 4 4 1 1.16320 82.940 0.4 84 4 3 3 1.15960 83.254 3.2 85 7 0 1 1.15160 83.964 0.3 86 2 4 4 1.14930 84.170 2.9 87 0 0 6 1.14620 84.450 1.0 88 4 0 5 1.14120 84.907 0.4

89 5 2 3 1.13700 85.295 1.0 90 2 6 0 1.13400 85.574 0.2

91 6 2 1 1.11880 87.024 0.3 92 4 4 2 1.11670 87.229 2.6 93 5 1 4 1.11670 87.229 2.6 94 1 1 6 1.11380 87.513 3.0 95 2 3 5 1.10920 87.969 3.6 96 7 0 2 1.10610 88.279 3.7 97 1 6 3 1.09540 89.371 0.4 98 4 1 5 1.08940 89.997 0.1 99 1 7 0 1.08310 90.665 2.5 100 6 2 2 1.07690 91.335 0.8 101 2 1 6 1.07460 91.586 0.2 102 7 1 1 1.06990 92.105 0.1 103 6 0 4 1.06800 92.316 0.1 104 4 3 4 1.05900 93.335 0.4 105 5 0 5 1.05260 94.076 0.4 106 5 4 0 1.04700 94.736 0.3 107 5 2 4 1.04170 95.372 0.5 108 5 3 3 1.04080 95.481 0.7 109 4 5 1 1.03500 96.190 1.1 110 7 1 2 1.03300 96.437 1.8 111 2 2 6 1.03100 96.686 2.1 112 3 6 0 1.03100 96.686 2.1

127 3 2 6 0.97810 103.914 0.5 128 4 4 4 0.97300 104.685 2.2 129 6 0 5 0.96810 105.439 0.1 130 3 5 4 0.96620 105.736 0.1 1 CA1 Ca 0.33333 0.66666 0.00300 0.5000 0.7170 4f

8 05 0 0.00000 0.00000 0.15000 0.5000 1.0000 4e 9 06 0 0.00000 0.00000 0.75000 0.5000 0.2040 2a

100 – Ref. Pattern: Hydrogen Calcium Chloride Carbonate Phosphate Hydroxide Hydrate, 04-01 

Nanotechnolody & Advanced Material Centeral Characterization Lab.