# X-ray powder diffraction data for holmium nitrate pentahydrate

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X-ray powder diffraction data, unit-cell parameters, and space group for the holmium nitrate pentahydrate $Ho(NO_3)_3•5H_2O$ are reported [$a = 6.642(8)$ Å, $b = 9.55(2)$ Å, $c = 10.56(2)$ Å, $\alpha = 63.672(1)°$, $\beta = 84.622(2)°$, $\gamma = 76.085(2)°$, unit-cell volume $V = 582{,}74$ Å$^3$, $Z = 2$, space group $P$-1]. $Ho(NO_3)_3•5H_2O$ is isostructural with ytrium nitrate pentahydrate (PDF 01-75-2104) (ICDD, 2011). All measured lines were indexed and are consistent with the $P$-1 space group. No detectable impurities were observed. © *2012 International Centre for Diffraction Data* [doi:10.1017/S0885715612000334]

Key words: X-ray powder diffraction, holmium nitrate pentahydrate

## I. INTRODUCTION

Holmium (Ho) is an important element from the f-block elements of the periodic table, the so-called lanthanides. Ho has wide use for example in Ho lasers used in medicine (Suardi *et al.*, 2009; Helfand *et al.*, 2010) and in magnetic resonance imaging (MRI) contrast agents (Norek and Peters, 2011). Ho compounds have interesting optical properties, such as changing of colors under different light sources, which could be used, for example, in glasses (Farok *et al.*, 1996). Holmium oxide is used in spectrophotometry such as calibration filter (Macdonald, 1964; Travis *et al.*, 2002).

Holmium nitrate is usually a pale pink or pale yellow substance depending on light source similar to holmium oxide. It is usually in the form of pentahydrate. It is soluble in water and stable in air, and therefore is a suitable precursor for various chemical reactions (Yan and Chen, 2001; Fox *et al.*, 2005).

## II. EXPERIMENTAL

### A. Synthesis

Holmium nitride was prepared by reaction of diluted (20 wt%) nitric acid with an abundant amount of holmium oxide. After reaction the solution has neutral pH. This solution was subsequently evaporated at a temperature of about 50 °C in an evaporator. When crystals started to form, the solution was removed from the evaporator and cooled to room temperature. Crystals obtained from the solution after filtration, were dried in air. The nitric acid used in this study was of

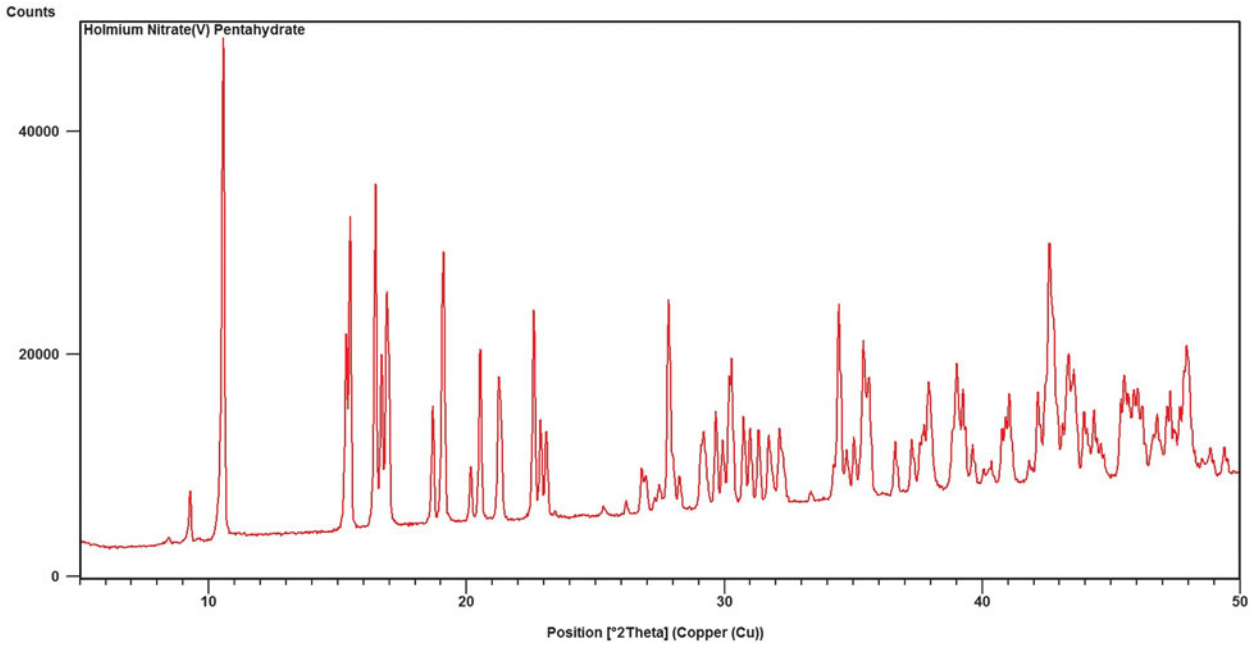


Figure 1. X-ray powder diffraction pattern of the $Ho(NO_3)_3•5H_2O$, using Cu$K\alpha_1$ radiation ($\lambda = 1.5406$ Å).

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p.a. quality, and holmium oxide (99.9% purity) was purchased from LACHEMA. All chemicals were used as received without further purification.

Formation of holmium nitride in the form of pentahydrate was confirmed by its absolute calcination in the furnace. The sample was heated to 1000 °C at 5 °C/min and then cooled spontaneously. Only holmium oxide remained (Balboul, 2000). The rest of the sample (57%) corresponds to absolute calcination of holmium oxide pentahydrate (Balboul, 2000).

### B. Powder data collection

The diffraction pattern for holmium nitrate pentahydrate [$Ho(NO_3)_3$•$5H_2O$] was collected at room temperature using an X'Pert PRO $\theta$–$\theta$ powder diffractometer with parafocusing Bragg–Brentano geometry and Cu$K\alpha_1$ radiation ($\lambda = 1.5406$ Å, generator setting: 40 kV, 30 mA). An ultrafast X'Celerator detector was employed to collect XRD data over the angular range from 4° to 80° 2$\theta$ with a step size of 0.017° 2$\theta$ and a counting time of 81.28 s/step. The software package HighScore Plus V 3.0d (PANalytical, Almelo, Netherlands) was used to analyze the data, to fit the background, and to eliminate the $K\alpha_2$ component. The top of smoothed peak method was used to determine the peak positions and intensities of the diffraction peaks. Automatic indexing of the experimental XRD pattern was performed using DICVOL04 (Boultif and Louër, 2004).

## III. RESULTS

The experimental powder diffraction pattern is depicted in Figure 1. Automatic indexing of results obtained using DICVOL04 show that $Ho(NO_3)_3$•$5H_2O$ is triclinic with space group $P$-1 and unit-cell parameters: $a = 6.642(8)$ Å, $b = 9.55(2)$ Å, $c = 10.56(2)$ Å, $\alpha = 63.672(1)°$, $\beta = 84.622(2)°$, $\gamma = 76.085(2)°$, unit-cell volume $V = 582{,}74$ Å$^3$, $Z = 2$, space group $P$-1 . The figures of merits are $F_{30} = 37.1(0.0165, 49)$ (Smith and Snyder, 1979) and $M_{20} = 12.3$ (de Wolff, 1968). All lines were indexed (Table I) and are consistent with the $P$-1 space group.

TABLE I. Indexed X-ray powder diffraction data for $Ho(NO_3)_3 \cdot 5H_2O$. Only the peaks with $I_{rel}$ of 1 or greater are presented [$a = 6.642(8)$ Å, $b = 9.55(2)$ Å, $c = 10.56(2)$ Å, $\alpha = 63.672(1)°$, $\beta = 84.622(2)°$, $\gamma = 76.085(2)°$, unit-cell volume $V = 582{,}74$ Å$^3$, $Z = 2$, space group $P$-1]. All lines were indexed and are consistent with the $P$-1 space group. The $d$-values were calculated using Cu$K\alpha_1$ radiation ($\lambda = 1.5406$ Å).

| $2\theta_{obs}$ (°) | $d_{obs}$ (Å) | $I_{obs}$ | $H$ | $k$ | $L$ | $2\theta_{cal}$ (°) | $d_{calc}$ (Å) | $\Delta 2\theta$ |
|---|---|---|---|---|---|---|---|---|
| 9.276 | 9.526 | 10 | 0 | 0 | 1 | 9.335 | 9.466 | 0.0591 |
| 10.552 | 8.377 | 100 | 0 | 1 | 0 | 10.595 | 8.343 | 0.0436 |
| 15.324 | 5.778 | 41 | 1 | 1 | 0 | 15.371 | 5.760 | 0.0471 |
| 15.477 | 5.721 | 66 | 1 | 1 | 1 | 15.528 | 5.702 | 0.0509 |
| 16.457 | 5.382 | 73 | 1 | 0 | −1 | 16.509 | 5.365 | 0.0517 |
| 16.689 | 5.308 | 37 | 1 | 0 | 1 | 16.740 | 5.292 | 0.0518 |
| 16.906 | 5.240 | 51 | 0 | 1 | −1 | 16.939 | 5.230 | 0.0333 |
| 16.988 | 5.215 | 30 | 0 | 1 | 2 | 17.029 | 5.203 | 0.0405 |
| 18.683 | 4.746 | 26 | 0 | 0 | 2 | 18.734 | 4.733 | 0.0506 |
| 19.081 | 4.647 | 56 | 1 | −1 | −1 | 19.094 | 4.644 | 0.0130 |
| 20.151 | 4.403 | 12 | 1 | 1 | −1 | 20.203 | 4.392 | 0.0520 |
| 20.516 | 4.326 | 39 | 1 | 1 | 2 | 20.564 | 4.316 | 0.0481 |
| 21.239 | 4.180 | 32 | 0 | 2 | 0 | 21.282 | 4.172 | 0.0432 |
| 21.339 | 4.161 | 21 | 0 | 2 | 2 | 21.378 | 4.153 | 0.0395 |
| 22.596 | 3.932 | 48 | 1 | 2 | 0 | 22.643 | 3.924 | 0.0475 |
| 22.859 | 3.887 | 22 | 1 | 2 | 2 | 22.905 | 3.880 | 0.0456 |
| 23.080 | 3.850 | 20 | 1 | 0 | −2 | 23.129 | 3.842 | 0.0491 |
| 23.413 | 3.796 | 2 | 1 | −1 | 1 | 23.416 | 3.796 | 0.0029 |
| 25.298 | 3.518 | 2 | 0 | 1 | −2 | 25.339 | 3.512 | 0.0414 |
| 26.184 | 3.401 | 3 | 1 | −2 | −1 | 26.222 | 3.396 | 0.0378 |
| 26.790 | 3.325 | 11 | 0 | 2 | −1 | 26.827 | 3.321 | 0.0369 |
| 26.941 | 3.307 | 8 | 0 | 2 | 3 | 26.981 | 3.302 | 0.0400 |
| 27.292 | 3.265 | 3 | 2 | 1 | 0 | 27.328 | 3.261 | 0.0356 |
| 27.459 | 3.246 | 6 | 2 | 1 | 1 | 27.491 | 3.242 | 0.0314 |
| 27.824 | 3.204 | 52 | 1 | −2 | −2 | 27.857 | 3.200 | 0.0329 |
| 28.013 | 3.183 | 11 | 1 | 1 | 3 | 28.046 | 3.179 | 0.0326 |
| 28.244 | 3.157 | 8 | 0 | 0 | 3 | 28.261 | 3.155 | 0.0166 |
| 29.083 | 3.068 | 15 | 2 | 0 | −1 | 29.111 | 3.065 | 0.0278 |
| 29.197 | 3.056 | 15 | 1 | 3 | 1 | 29.195 | 3.056 | −0.0017 |
| 29.282 | 3.048 | 8 | 0 | 3 | 2 | 29.293 | 3.046 | 0.0104 |
| 29.352 | 3.040 | 3 | 2 | 0 | 1 | 29.382 | 3.037 | 0.0301 |
| 29.657 | 3.010 | 24 | 2 | 2 | 1 | 29.692 | 3.006 | 0.0348 |
| 29.924 | 2.984 | 16 | 1 | −1 | −3 | 29.961 | 2.980 | 0.0372 |
| 30.179 | 2.959 | 31 | 1 | −1 | 2 | 30.204 | 2.957 | 0.0256 |
| 30.280 | 2.949 | 28 | 2 | 1 | −1 | 30.321 | 2.945 | 0.0404 |
| 30.732 | 2.907 | 23 | 2 | 1 | 2 | 30.763 | 2.904 | 0.0310 |
| 30.995 | 2.883 | 19 | 2 | 2 | 0 | 31.027 | 2.880 | 0.0321 |
| 31.310 | 2.855 | 19 | 2 | 2 | 2 | 31.351 | 2.851 | 0.0403 |
| 31.711 | 2.819 | 17 | 1 | 0 | 3 | 31.733 | 2.818 | 0.0222 |

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TABLE I. Continued

| $2\theta_{obs}$ (°) | $d_{obs}$ (Å) | $I_{obs}$ | $H$ | $k$ | $L$ | $2\theta_{cal}$ (°) | $d_{calc}$ (Å) | $\Delta 2\theta$ |
|---|---|---|---|---|---|---|---|---|
| 31.860 | 2.807 | 5 | 2 | −1 | 0 | 31.892 | 2.804 | 0.0316 |
| 32.131 | 2.783 | 18 | 0 | 3 | 0 | 32.161 | 2.781 | 0.0293 |
| 32.275 | 2.771 | 10 | 0 | 3 | 3 | 32.308 | 2.769 | 0.0333 |
| 33.336 | 2.686 | 2 | 2 | 0 | −2 | 33.373 | 2.683 | 0.0368 |
| 34.238 | 2.617 | 9 | 0 | 2 | −2 | 34.263 | 2.615 | 0.0249 |
| 34.426 | 2.603 | 48 | 0 | 2 | 4 | 34.449 | 2.601 | 0.0236 |
| 34.523 | 2.596 | 11 | 0 | 1 | 4 | 34.573 | 2.592 | 0.0494 |
| 34.740 | 2.580 | 12 | 2 | −1 | 1 | 34.760 | 2.579 | 0.0193 |
| 35.017 | 2.560 | 16 | 1 | 2 | −2 | 35.042 | 2.559 | 0.0247 |
| 35.258 | 2.543 | 10 | 2 | 3 | 1 | 35.291 | 2.541 | 0.0331 |
| 35.384 | 2.535 | 38 | 1 | −3 | −2 | 35.391 | 2.534 | 0.0073 |
| 35.595 | 2.520 | 27 | 1 | 2 | 4 | 35.567 | 2.522 | −0.0275 |
| 36.620 | 2.452 | 13 | 1 | 1 | 4 | 36.643 | 2.450 | 0.0225 |
| 37.261 | 2.411 | 14 | 1 | 3 | −1 | 37.291 | 2.409 | 0.0294 |
| 37.588 | 2.391 | 13 | 2 | −2 | −1 | 37.597 | 2.390 | 0.0092 |
| 37.753 | 2.381 | 15 | 1 | 3 | 4 | 37.778 | 2.379 | 0.0245 |
| 37.925 | 2.371 | 27 | 1 | −3 | −3 | 37.922 | 2.371 | −0.0029 |
| 38.847 | 2.316 | 15 | 1 | −2 | −4 | 38.857 | 2.316 | 0.0106 |
| 39.012 | 2.307 | 30 | 1 | −2 | 2 | 39.007 | 2.307 | −0.0053 |
| 39.245 | 2.294 | 26 | 1 | 4 | 3 | 39.270 | 2.292 | 0.0245 |
| 39.363 | 2.287 | 5 | 2 | −1 | −3 | 39.413 | 2.284 | 0.0502 |
| 39.616 | 2.273 | 11 | 2 | 0 | −3 | 39.643 | 2.272 | 0.0269 |
| 40.056 | 2.249 | 5 | 0 | 4 | 3 | 40.082 | 2.248 | 0.0265 |
| 40.251 | 2.239 | 5 | 2 | 0 | 3 | 40.262 | 2.238 | 0.0106 |
| 40.349 | 2.234 | 6 | 1 | 0 | −4 | 40.373 | 2.232 | 0.0241 |
| 40.766 | 2.212 | 15 | 1 | 0 | 4 | 40.780 | 2.211 | 0.0145 |
| 40.927 | 2.203 | 15 | 3 | 1 | 0 | 40.936 | 2.203 | 0.0088 |
| 41.055 | 2.197 | 19 | 2 | 2 | −2 | 41.072 | 2.196 | 0.0168 |
| 41.818 | 2.158 | 6 | 2 | 2 | 4 | 41.831 | 2.158 | 0.0130 |
| 42.157 | 2.142 | 24 | 2 | 4 | 2 | 42.172 | 2.141 | 0.0154 |
| 42.444 | 2.128 | 25 | 1 | 4 | 0 | 42.438 | 2.128 | −0.0059 |
| 42.607 | 2.120 | 58 | 1 | −3 | −4 | 42.609 | 2.120 | 0.0015 |
| 42.783 | 2.112 | 28 | 0 | 2 | −3 | 42.773 | 2.112 | −0.0099 |
| 42.936 | 2.105 | 10 | 2 | 3 | 4 | 42.953 | 2.104 | 0.0167 |
| 43.123 | 2.096 | 14 | 3 | 2 | 2 | 43.136 | 2.095 | 0.0133 |
| 43.332 | 2.086 | 30 | 0 | 4 | 0 | 43.346 | 2.086 | 0.0142 |
| 43.549 | 2.077 | 27 | 0 | 4 | 4 | 43.550 | 2.076 | 0.0004 |
| 43.944 | 2.059 | 19 | 1 | 2 | 5 | 43.959 | 2.058 | 0.0150 |
| 44.153 | 2.050 | 8 | 0 | 1 | 5 | 44.168 | 2.049 | 0.0149 |
| 44.342 | 2.041 | 18 | 0 | 3 | −2 | 44.354 | 2.041 | 0.0120 |
| 44.593 | 2.030 | 9 | 1 | −4 | −2 | 44.584 | 2.031 | −0.0093 |
| 45.381 | 1.997 | 22 | 3 | 3 | 1 | 45.383 | 1.997 | 0.0017 |
| 45.540 | 1.990 | 22 | 2 | −3 | −1 | 45.534 | 1.991 | −0.0063 |
| 45.663 | 1.985 | 15 | 1 | −4 | −3 | 45.657 | 1.985 | −0.0056 |
| 45.735 | 1.982 | 14 | 3 | −1 | −1 | 45.733 | 1.982 | −0.0017 |
| 45.894 | 1.976 | 21 | 3 | 2 | −1 | 45.884 | 1.976 | −0.0100 |
| 46.038 | 1.970 | 18 | 2 | −1 | −4 | 46.042 | 1.970 | 0.0046 |
| 46.217 | 1.963 | 16 | 2 | 4 | 0 | 46.237 | 1.962 | 0.0193 |
| 46.535 | 1.950 | 8 | 3 | 2 | 3 | 46.532 | 1.950 | −0.0037 |
| 46.628 | 1.946 | 10 | 3 | 0 | 2 | 46.644 | 1.946 | 0.0161 |
| 46.787 | 1.940 | 14 | 2 | 4 | 4 | 46.795 | 1.940 | 0.0079 |
| 46.997 | 1.932 | 5 | 1 | −1 | −5 | 47.016 | 1.931 | 0.0187 |
| 47.172 | 1.925 | 19 | 3 | 1 | −2 | 47.176 | 1.925 | 0.0043 |
| 47.300 | 1.920 | 17 | 3 | 3 | 0 | 47.307 | 1.920 | 0.0069 |
| 47.505 | 1.912 | 11 | 2 | −3 | −3 | 47.515 | 1.912 | 0.0097 |
| 47.679 | 1.906 | 17 | 2 | −3 | 0 | 47.677 | 1.906 | −0.0020 |
| 47.849 | 1.899 | 25 | 1 | 5 | 2 | 47.841 | 1.900 | −0.0076 |
| 47.921 | 1.897 | 29 | 3 | 1 | 3 | 47.909 | 1.897 | −0.0119 |
| 47.998 | 1.894 | 22 | 2 | 0 | 4 | 47.992 | 1.894 | −0.0055 |
| 48.239 | 1.885 | 7 | 1 | 4 | 5 | 48.253 | 1.885 | 0.0142 |
| 48.536 | 1.874 | 5 | 2 | 3 | −2 | 48.537 | 1.874 | 0.0007 |
| 48.767 | 1.866 | 5 | 1 | −4 | −4 | 48.763 | 1.866 | −0.0047 |
| 48.844 | 1.863 | 8 | 0 | 4 | 5 | 48.857 | 1.863 | 0.0126 |
| 49.393 | 1.844 | 8 | 2 | 3 | 5 | 49.395 | 1.844 | 0.0021 |
| 49.752 | 1.831 | 2 | 1 | 5 | 1 | 49.756 | 1.831 | 0.0039 |

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TABLE I. Continued

| $2\theta_{obs}$ (°) | $d_{obs}$ (Å) | $I_{obs}$ | $H$ | $k$ | $L$ | $2\theta_{cal}$ (°) | $d_{calc}$ (Å) | $\Delta 2\theta$ |
|---|---|---|---|---|---|---|---|---|
| 50.091 | 1.820 | 1 | 1 | 5 | 4 | 50.058 | 1.821 | −0.0338 |
| 50.805 | 1.796 | 9 | 3 | 2 | −2 | 50.807 | 1.796 | 0.0026 |
| 51.153 | 1.784 | 16 | 2 | 4 | −1 | 51.154 | 1.784 | 0.0006 |
| 51.241 | 1.781 | 15 | 0 | 5 | 1 | 51.245 | 1.781 | 0.0044 |
| 51.410 | 1.776 | 11 | 0 | 5 | 4 | 51.413 | 1.776 | 0.0030 |
| 51.600 | 1.770 | 8 | 3 | 4 | 3 | 51.615 | 1.769 | 0.0153 |
| 51.774 | 1.764 | 8 | 3 | −2 | −2 | 51.785 | 1.764 | 0.0104 |
| 51.980 | 1.758 | 14 | 3 | −2 | 0 | 51.993 | 1.757 | 0.0133 |
| 52.164 | 1.752 | 6 | 3 | −1 | 2 | 52.136 | 1.753 | −0.0281 |
| 52.246 | 1.749 | 5 | 1 | 3 | −3 | 52.250 | 1.749 | 0.0033 |
| 52.457 | 1.743 | 5 | 0 | 3 | −3 | 52.444 | 1.743 | −0.0125 |
| 52.898 | 1.729 | 7 | 2 | 5 | 4 | 52.899 | 1.729 | 0.0014 |
| 53.539 | 1.710 | 9 | 1 | 5 | 0 | 53.530 | 1.711 | −0.0095 |
| 53.616 | 1.708 | 10 | 1 | −4 | 1 | 53.621 | 1.708 | 0.0050 |
| 53.981 | 1.697 | 12 | 3 | 4 | 0 | 53.968 | 1.698 | −0.0130 |
| 54.455 | 1.684 | 4 | 1 | 4 | −2 | 54.447 | 1.684 | −0.0081 |
| 54.917 | 1.671 | 5 | 3 | −2 | 1 | 54.929 | 1.670 | 0.0115 |
| 55.112 | 1.665 | 4 | 1 | 4 | 6 | 55.114 | 1.665 | 0.0019 |
| 55.666 | 1.650 | 4 | 4 | 2 | 1 | 55.653 | 1.650 | −0.0132 |
| 55.764 | 1.647 | 6 | 1 | 1 | 6 | 55.770 | 1.647 | 0.0063 |
| 55.913 | 1.643 | 5 | 2 | 0 | −5 | 55.914 | 1.643 | 0.0011 |
| 56.066 | 1.639 | 2 | 2 | 5 | 0 | 56.088 | 1.638 | 0.0217 |
| 56.385 | 1.630 | 2 | 4 | 2 | 0 | 56.387 | 1.630 | 0.0027 |
| 56.651 | 1.623 | 5 | 1 | −3 | 3 | 56.652 | 1.623 | 0.0002 |
| 56.995 | 1.614 | 12 | 2 | 2 | −4 | 56.982 | 1.615 | −0.0132 |
| 57.118 | 1.611 | 9 | 4 | 0 | 0 | 57.107 | 1.612 | −0.0114 |
| 57.221 | 1.609 | 6 | 4 | 1 | −1 | 57.224 | 1.609 | 0.0034 |
| 57.400 | 1.604 | 8 | 3 | 5 | 2 | 57.399 | 1.604 | −0.0014 |
| 57.735 | 1.596 | 6 | 4 | 1 | 2 | 57.727 | 1.596 | −0.0079 |
| 57.986 | 1.589 | 5 | 3 | −3 | −2 | 57.991 | 1.589 | 0.0051 |
| 58.376 | 1.580 | 2 | 3 | 4 | −1 | 58.374 | 1.580 | −0.0019 |
| 58.530 | 1.576 | 3 | 2 | 4 | 6 | 58.523 | 1.576 | −0.0068 |
| 58.699 | 1.572 | 4 | 1 | 6 | 2 | 58.690 | 1.572 | −0.0096 |
| 58.894 | 1.567 | 6 | 1 | 6 | 4 | 58.890 | 1.567 | −0.0045 |
| 59.526 | 1.552 | 7 | 3 | 5 | 4 | 59.516 | 1.552 | −0.0098 |
| 59.792 | 1.545 | 7 | 2 | 6 | 3 | 59.799 | 1.545 | 0.0065 |
| 60.028 | 1.540 | 8 | 4 | 3 | 3 | 60.042 | 1.540 | 0.0134 |
| 60.131 | 1.538 | 8 | 3 | 1 | −4 | 60.125 | 1.538 | −0.0057 |
| 60.326 | 1.533 | 10 | 0 | 5 | −1 | 60.325 | 1.533 | −0.0005 |
| 60.654 | 1.526 | 6 | 0 | 6 | 2 | 60.636 | 1.526 | −0.0187 |
| 60.978 | 1.518 | 6 | 4 | 0 | 2 | 60.957 | 1.519 | −0.0209 |
| 61.265 | 1.512 | 6 | 1 | 3 | −4 | 61.261 | 1.512 | −0.0036 |
| 61.460 | 1.507 | 3 | 0 | 3 | −4 | 61.475 | 1.507 | 0.0147 |
| 61.660 | 1.503 | 4 | 4 | 4 | 2 | 61.652 | 1.503 | −0.0075 |
| 61.834 | 1.499 | 3 | 0 | 3 | 7 | 61.802 | 1.500 | −0.0321 |
| 62.158 | 1.492 | 6 | 2 | 5 | 6 | 62.164 | 1.492 | 0.0068 |
| 62.363 | 1.488 | 9 | 1 | 2 | −5 | 62.368 | 1.488 | 0.0054 |
| 62.782 | 1.479 | 4 | 4 | 3 | −1 | 62.776 | 1.479 | −0.0062 |
| 63.085 | 1.472 | 6 | 4 | 2 | −2 | 63.073 | 1.473 | −0.0119 |
| 63.213 | 1.470 | 4 | 0 | 4 | −3 | 63.198 | 1.470 | −0.0154 |
| 63.516 | 1.464 | 8 | 2 | 6 | 5 | 63.518 | 1.463 | 0.0024 |
| 63.952 | 1.455 | 4 | 2 | −3 | −6 | 63.954 | 1.455 | 0.0018 |
| 64.280 | 1.448 | 5 | 3 | 4 | −2 | 64.278 | 1.448 | −0.0019 |
| 64.773 | 1.438 | 5 | 3 | 3 | 6 | 64.753 | 1.439 | −0.0197 |
| 65.460 | 1.425 | 8 | 3 | 4 | 6 | 65.465 | 1.425 | 0.0052 |
| 65.686 | 1.420 | 6 | 1 | 5 | −2 | 65.690 | 1.420 | 0.0044 |
| 65.953 | 1.415 | 3 | 3 | −4 | −2 | 65.960 | 1.415 | 0.0071 |
| 66.291 | 1.409 | 6 | 2 | 0 | 6 | 66.295 | 1.409 | 0.0032 |
| 68.709 | 1.365 | 5 | 2 | −5 | −5 | 68.707 | 1.365 | −0.0019 |
| 68.996 | 1.360 | 5 | 1 | 7 | 3 | 68.968 | 1.361 | −0.0285 |
| 70.145 | 1.341 | 2 | 2 | 1 | −6 | 70.124 | 1.341 | −0.0214 |
| 70.354 | 1.337 | 1 | 4 | −1 | −4 | 70.343 | 1.337 | −0.0104 |
| 71.264 | 1.322 | 4 | 4 | −1 | 3 | 71.261 | 1.322 | −0.0032 |
| 71.418 | 1.320 | 6 | 1 | 0 | 7 | 71.432 | 1.320 | 0.0147 |
| 71.590 | 1.317 | 3 | 3 | 3 | −4 | 71.579 | 1.317 | −0.0114 |

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TABLE I. Continued

| $2\theta_{obs}$ (°) | $d_{obs}$ (Å) | $I_{obs}$ | $H$ | $k$ | $L$ | $2\theta_{cal}$ (°) | $d_{calc}$ (Å) | $\Delta 2\theta$ |
|---|---|---|---|---|---|---|---|---|
| 72.006 | 1.310 | 6 | 3 | −1 | −6 | 72.026 | 1.310 | 0.0206 |
| 72.262 | 1.306 | 3 | 1 | 4 | 8 | 72.261 | 1.306 | −0.0012 |
| 72.632 | 1.301 | 4 | 0 | 4 | 8 | 72.631 | 1.301 | −0.0001 |
| 72.945 | 1.296 | 4 | 0 | 2 | 8 | 72.924 | 1.296 | −0.0203 |
| 73.099 | 1.294 | 5 | 3 | 6 | 6 | 73.119 | 1.293 | 0.0203 |
| 73.401 | 1.289 | 3 | 5 | 1 | 2 | 73.404 | 1.289 | 0.0032 |
| 73.596 | 1.286 | 6 | 1 | 7 | 1 | 73.577 | 1.286 | −0.0191 |
| 73.755 | 1.284 | 4 | 5 | 2 | −1 | 73.758 | 1.284 | 0.0028 |
| 74.104 | 1.278 | 7 | 2 | −6 | −3 | 74.105 | 1.278 | 0.0005 |
| 74.366 | 1.275 | 3 | 2 | 3 | −5 | 74.357 | 1.275 | −0.0092 |
| 74.633 | 1.271 | 2 | 4 | 6 | 2 | 74.639 | 1.271 | 0.0061 |
| 74.925 | 1.266 | 4 | 2 | −4 | −7 | 74.931 | 1.266 | 0.0060 |
| 75.069 | 1.264 | 4 | 1 | −3 | 5 | 75.042 | 1.265 | −0.0269 |
| 75.238 | 1.262 | 2 | 2 | −4 | 3 | 75.255 | 1.262 | 0.0169 |
| 75.541 | 1.258 | 3 | 0 | 5 | 8 | 75.534 | 1.258 | −0.0071 |
| 75.828 | 1.254 | 2 | 5 | 1 | −2 | 75.829 | 1.254 | 0.0011 |
| 76.434 | 1.245 | 2 | 1 | −4 | −8 | 76.395 | 1.246 | −0.0391 |
| 76.767 | 1.241 | 4 | 2 | 0 | 7 | 76.779 | 1.240 | 0.0123 |
| 77.101 | 1.236 | 5 | 3 | −5 | −1 | 77.106 | 1.236 | 0.0056 |
| 77.562 | 1.230 | 5 | 4 | 6 | 5 | 77.556 | 1.230 | −0.0064 |
| 78.163 | 1.222 | 3 | 1 | 7 | 0 | 78.176 | 1.222 | 0.0135 |
| 78.522 | 1.217 | 3 | 5 | −1 | −2 | 78.533 | 1.217 | 0.0110 |
| 78.717 | 1.215 | 2 | 5 | 4 | 4 | 78.696 | 1.215 | −0.0205 |
| 79.045 | 1.210 | 2 | 5 | −1 | 1 | 79.013 | 1.211 | −0.0325 |
| 79.897 | 1.200 | 3 | 5 | 0 | −3 | 79.891 | 1.200 | −0.0063 |


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Balboul, B. (**2000**). "Physicochemical characterization of the decomposition course of hydrated holmium nitrate. Thermoanalytical studies," Powder Technol. **107**(1–2), 168–174.

Boultif, A. and Louër, D. (**2004**). "Powder pattern indexing with the dichotomy method," J. Appl. Crystallogr. **37**, 724–731.

de Wollf, P. M. (**1968**). "A simplified criterion for the reliability of a powder pattern," J. Appl. Crystallogr. **1**, 108–113.

Farok, H. M., Saunders, G. A., Lambson, W. A., Kruger, R., Senin, H. B., Bartlett, S., and Takel, S. (**1996**). "An 'Alexandrite' effect and optical properties of holmium metaphosphate glass," Phys. Chem. Glasses **37** (3), 125–128.

Fox, R. V., Ball, R. D., Harrington, P. D., Rollins, H. W., and Wai, C. M. (**2005**). "Holmium nitrate complexation with tri-n-butyl phosphate in supercritical carbon dioxide," J. Supercrit. Fluids **36**(2), 137–144.

Helfand, B. T., Manvar, A. M., Auffenberg, G. B., Blackwell, R., Hartman, R. J., and McVary, K. T. (**2010**). "Holmium laser ablation and enucleation of the prostate: a pilot study of the hybrid technique," Can. J. Urol. **17**(3), 5190–5194.

ICDD (**2011**). *Powder Diffraction File*, edited by Frank McClune (International Centre for Diffraction Data, Newtown Square, PA USA)

Macdonald, R. P. (**1964**). "Uses for holmium oxide filter in spectrometry," Clin. Chem. **10**(12), 1117.

Norek, M. and Peters, J. A. (**2011**). "MRI contrast agents based on dysprosium or holmium," Prog. Nucl. Magn. Reson. Spectrosc. **59**(1), 64–82.

Smith, G. S. and Snyder, R. L. (**1979**). "$F_N$: a criterion for rating powder diffraction patterns and evaluating the reliability of powder indexing," J. Appl. Crystallogr. **12**, 60–65.

Suardi, N., Gallina, A., Salonia, A., Briganti, A., Deho, F., Zanni, G., Abdollah, F., Naspro, R., Cestari, A., Guazzoni, G., Rigatti, P., and Montorsi, F. (**2009**). "Holmium laser enucleation of the prostate and holmium laser ablation of the prostate: indications and outcome," Curr. Opin. Urol. **19**(1), 38–43.

Travis, J. C., Zwinkels, J. C., Mercader, F., Ruiz, A., Early, E. A., Smith, M. V., Noel, M., Maley, M., Kramer, G. W., Eckerle, K. L., and Duewer, D.L. (**2002**). "An international evaluation of holmium oxide solution reference materials for wavelength calibration in molecular absorption spectrophotometry," Anal. Chem. **74**(14), 3408–3415.

Yan, B. and Chen, Z. (**2001**). "Cyano-bridged aqua(*N,N*-dimethylacetamide)(cyanoiron) lanthanides from samarium, gadolinium, or holmium nitrate and potassium hexacyanoferrate: crystal structures and magnetochemistry," Helv. Chim. Acta **84**(4), 817–829.