## Supporting Information

# Design, Growth and Characterization of $Y_2Mo_4O_{15}$ Crystal for Raman laser applications

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**Table S1. Crystal Data and Structure Refinement for $Y_2Mo_4O_{15}$**

| Empirical formula | $Y_2Mo_4O_{15}$ |
|---|---|
| Formula weight | 801.58 |
| Temperature | 293 K |
| Wavelength | 0.71073 Å |
| Crystal system | Monoclinic |
| Space group | *P2₁/c* (No. 14) |
| Unit cell dimensions | a = 6.8110(4) Å, α = 90.00°<br>b = 9.5833(5) Å, β = 105.512(7)°<br>c = 10.5124(6) Å, γ = 90° |
| Volume | 661.17(8) $Å^3$ |
| Z | 2 |
| Density (calculated) | 4.026 $g/cm^3$ |
| Absorption coefficient | 12.429 $mm^{-1}$ |
| F(000) | 732 |
| Crystal size | 0.02 × 0.04 × 0.05 $mm^3$ |
| θ range for data collection | 2.903 to 30.323° |
| Index ranges | -8 ≤h ≤8,<br>-11 ≤k ≤10,<br>-13 ≤l ≤13 |
| Reflections collected | 5250 |
| $R_{int}$ | 0.1013 |
| Data / restraints / parameters | 1342 / 0 / 98 |
| Goodness-of-fit | 1.076 |
| Final R indices [>2$\sigma$(I)] | $R_{obs}$ = 0.0531, $wR_{obs}$ = 0.1280 |
| R indices [all data] | $R_{all}$ = 0.0563, $wR_{all}$ = 0.1306 |
| Extinction coefficient | 0.257(11) |
| Largest diff. peak and hole | 2.188 and -2.120 $e.Å^{-3}$ |

$R = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$, $wR = \{\Sigma[w(|F_o|^2 - |F_c|^2)^2] / \Sigma[w(|F_o|^4)]\}^{1/2}$ and calc $w=1/[\sigma^2(Fo^2)+(0.0503P)^2+0.0000P]$ where $P=(Fo^2+2Fc^2)/3$

**Table S2. Selected bond lengths (Å) and angles (deg.) in $Y_2Mo_4O_{15}$**

| | | | |
|---|---|---|---|
| Mo1—O2 | 178.3(7) | Mo1—O6 | 1.735(6) |
| Mo1—O3 | 1.746(6) | Y1—O2$^{iii}$ | 2.316(6) |
| Mo1—O7 | 1.763(7) | Y1—O3$^{iv}$ | 2.268(6) |
| Mo1—O8 | 1.750(6) | Y1—O4$^{v}$ | 2.342(7) |
| Mo2—Y1$^{i}$ | 3.5377(11) | Y1—O5 | 2.301(7) |
| Mo2—O1 | 1.8665(7) | Y1—O6$^{vi}$ | 2.355(7) |
| Mo2—O2$^{ii}$ | 2.508(7) | Y1—O7 | 2.260(6) |
| Mo2—O4 | 1.735(6) | Y1—O8$^{vi}$ | 2.247(6) |
| Mo2—O5 | 1.737(7) | O4$^{v}$—Y1—O6$^{vi}$ | 142.5(2) |
| O3—Mo1—O2 | 110.6(3) | O5—Y1—Mo2$^{v}$ | 90.51(17) |
| O3—Mo1—O7 | 109.1(3) | O5—Y1—O2$^{iii}$ | 131.6(2) |
| O3—Mo1—O8 | 110.0(3) | O5—Y1—O4$^{v}$ | 74.6(2) |
| O7—Mo1—O2 | 110.4(3) | O5—Y1—O6$^{vi}$ | 141.0(2) |
| O8—Mo1—O2 | 109.0(3) | O6$^{vi}$—Y1—Mo2$^{v}$ | 120.83(15) |
| O8—Mo1—O7 | 107.7(3) | O7—Y1—Mo2$^{v}$ | 89.21(18) |
| O1—Mo2—Y1$^{i}$ | 87.35(3) | O7—Y1—O2$^{iii}$ | 83.0(2) |
| O1—Mo2—O2 | 75.14(16) | O7—Y1—O3$^{iv}$ | 96.1(3) |
| O2$^{ii}$—Mo2—Y1 | 40.75(14) | O7—Y1—O4$^{v}$ | 104.4(2) |
| O4—Mo2—Y1$^{i}$ | 35.1(2) | O7—Y1—O5 | 77.5(3) |
| O4—Mo2—O1 | 113.1(2) | O7—Y1—O6 | 80.1(3) |
| O4—Mo2—O2$^{ii}$ | 73.1(3) | O8$^{vi}$—Y1—Mo2$^{v}$ | 96.83(16) |
| O4—Mo2—O5 | 114.1(3) | O8$^{vi}$—Y1—O2$^{iii}$ | 90.1(2) |
| O4—Mo2—O6 | 105.1(3) | O8$^{vi}$—Y1—O3$^{iv}$ | 82.3(2) |
| O5—Mo2—Y1$^{i}$ | 108.7(2) | O8$^{vi}$—Y1—O4$^{v}$ | 87.2(2) |
| O5—Mo2—O1 | 115.6(2) | O8$^{vi}$—Y1—O5 | 118.1(2) |
| O5—Mo2—O2$^{ii}$ | 79.3(3) | O8$^{vi}$—Y1—O6$^{vi}$ | 83.2(2) |
| O6—Mo2—Y1$^{i}$ | 136.7(2) | O8$^{vi}$—Y1—O7 | 163.1(3) |
| O6—Mo2—O1 | 103.5(2) | Mo2$^{vii}$—O1—Mo2 | 180 |
| O6—Mo2—O2$^{ii}$ | 176.8(3) | Mo1—O1—Mo2$^{viii}$ | 130.0(3) |
| O6—Mo2—O5 | 103.9(3) | Mo4—O2—Y1$^{iii}$ | 135.6(4) |
| O2$^{iii}$—Y1—Mo2$^{v}$ | 44.99(18) | Y1$^{iii}$—O2—Mo2$^{viii}$ | 94.3(2) |
| O2$^{iii}$—Y1—O4$^{v}$ | 68.0(2) | Mo1—O3—Y1$^{ix}$ | 164.7(4) |
| O2$^{iii}$—Y1—O6$^{vi}$ | 75.9(2) | Mo2—O4—Y1$^{i}$ | 119.7(3) |
| O3—Y1—Mo2$^{v}$ | 163.98(18) | Mo2—O5—Y1 | 143.6(4) |
| O3—Y1—O2$^{iii}$ | 150.6(3) | Mo2—O6—Y1$^{x}$ | 163.5(4) |
| O3—Y1—O4 | 139.3(2) | Mo1—O7—Y1 | 147.8(4) |
| O3$^{iv}$—Y1—O5 | 76.0(2) | Mo1—O8—Y1$^{x}$ | 144.9(4) |
| O3$^{iv}$—Y1—O6 | 75.1(2) | | |
| O4—Y1—Mo2$^{v}$ | 25.21(16) | | |

(i) 2-x, -0.5+y, 1.5-z; (ii) 1+x, 1.5-y, 0.5+z; (iii) 1-x, 2-y, 1-z; (iv) x, 1.5-y, 0.5+z;
(v) 2-x, 0.5+y, 1.5-z; (vi) 1-x, 0.5+y, 1.5-z; (vii) 2-x, 1-y, 2-z; (viii) -1+x, 1.5-y, -0.5+z;
(ix) x, 1.5-y, -0.5+z; (x) 1-x, -0.5+y, 1.5-z.

**Table S3. Atomic displacement parameters (Å$^2$) for $Y_2Mo_4O_{15}$**

| Atom | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Mo1 | 0.0125(5) | 0.0143(5) | 0.0097(5) | 0.0002(2) | 0.0032(4) | 0.0013(2) |
| Mo2 | 0.0104(5) | 0.0150(5) | 0.0117(5) | 0.0004(2) | 0.0012(4) | 0.0008(3) |
| Y1 | 0.0112(6) | 0.0135(5) | 0.0106(5) | 0.0005(3) | 0.0031(4) | 0.0002(3) |
| O1 | 0.019(6) | 0.029(5) | 0.022(5) | 0.014(4) | -0.003(4) | -0.001(4) |
| O2 | 0.019(4) | 0.019(3) | 0.021(3) | 0.006(2) | 0.008(3) | -0.002(3) |
| O3 | 0.023(4) | 0.023(3) | 0.020(3) | -0.006(2) | 0.010(3) | 0.001(3) |
| O4 | 0.010(3) | 0.031(4) | 0.017(3) | -0.010(3) | 0.005(3) | -0.001(3) |
| O5 | 0.015(4) | 0.021(3) | 0.024(3) | 0.004(2) | 0.003(3) | 0.005(2) |
| O6 | 0.008(3) | 0.032(4) | 0.022(3) | -0.006(3) | 0.008(3) | 0.000(3) |
| O7 | 0.023(4) | 0.026(4) | 0.016(3) | -0.008(3) | 0.002(3) | -0.002(3) |
| O8 | 0.018(4) | 0.028(3) | 0.019(3) | 0.011(3) | 0.010(3) | 0.011(3) |