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Crystal structure and Raman spectrum of a high-pressure Li-rich majoritic garnet, $(\text{Li}_2\text{Mg})\text{Si}_2(\text{SiO}_4)_3$

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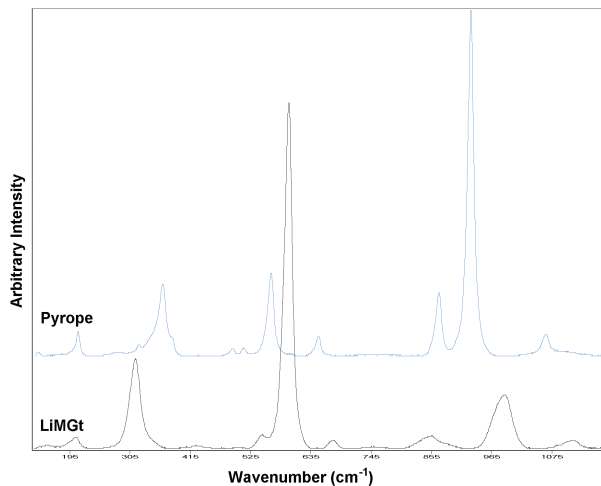


FIGURE 2. Raman spectra of Li-rich majoritic garnet and pyrope.

TABLE 2. Atomic coordinates and displacement parameters in Li-bearing majoritic garnet

Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}	U_{eq}
X	1/8	0	1/4	0.0070(17)	0.0165(6)	$= U_{22}$	0	0	0.0018(4)	0.0133(5)
Y	0	0	0	0.0052(2)	$= U_{11}$	$= U_{11}$	0.0002(1)	$= U_{12}$	$= U_{12}$	0.0052(2)
Si	3/8	0	1/4	0.0056(2)	0.0050(2)	$= U_{22}$	0	0	0	0.0052(1)
O	0.03231(5)	0.04389(5)	0.64800(5)	0.0075(2)	0.0095(2)	0.0061(2)	0.0010(2)	-0.0014(2)	-0.0002(2)	0.0077(2)

Notes: U_{ij} parameters are in unit of Å^2 .