

Appendix A. Supplementary Information - Unit cell indexing of SiD₄

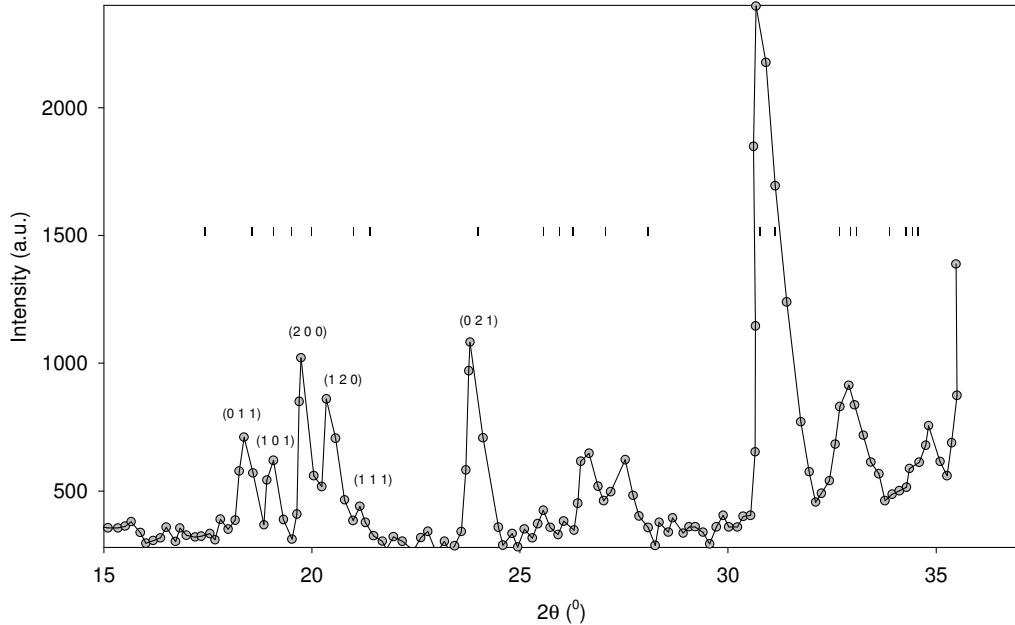


Figure A1 Neutron diffraction pattern of SiD₄ at 26 K ($\lambda=1.263 \text{ \AA}$) reproduced from Fig. 1 of Legrand and Press (1976). The data are indexed (see Table A1 below) based on a cell with lattice constants $a=7.26 \text{ \AA}$, $b=8.21 \text{ \AA}$, $c=4.44 \text{ \AA}$ and unit cell volume of 265 \AA^3 and isostructural with the low-temperature phase of germane.

Table A1 - Observed and calculated peak positions for SiD₄ at 26 K in Figure A1 after Legrand, E. & Press, W. (1976). Solid State Commun. **18**, 1353-1355.

$h \ k \ l$	2θ obs (°)	2θ cal (°)	obs-cal (°)	d obs (Å)	d cal (Å)	obs-cal (Å)
0 1 1	18.51	18.62	-0.11	3.927	3.904	0.022
1 0 1	19.21	19.20	0.01	3.785	3.787	-0.002
2 0 0	19.91	20.03	-0.12	3.653	3.632	0.021
1 2 0	20.43	20.35	0.08	3.561	3.572	-0.014
0 2 1	24.12	24.19	-0.07	3.022	3.014	0.008
2 2 0	26.75	26.84	-0.09	2.730	2.721	0.009
2 1 1	27.63	27.48	0.16	2.645	2.659	-0.015
2 2 1	30.67	31.60	0.07	2.314	2.319	-0.005
1 3 1	33.07	33.07	0.00	2.219	2.219	0.000