

Short explanation of the files

file s001-I_2-D1.xtl

content: Atomic positions of the I:2-D1 configuration of Fig. 2.
(fractional coordinates, XTL format)

file S001-I_2-M1.xtl

content: Atomic positions of the I:2-M1 configuration of Fig. 2.
(fractional coordinates, XTL format)

file s001-I_4-M.xtl

content: Atomic positions of the I:4-M configuration of Fig. 2.
(fractional coordinates, XTL format)

file s001-II_2-D.xtl

content: Atomic positions of the II:2-D configuration of Fig. 2.
(fractional coordinates, XTL format)

file s100_1-Da.xtl

content: Atomic positions of the 1:Da configuration of Fig. 4.
(fractional coordinates, XTL format)

file s010_2-D1.xtl

content: Atomic positions of the 2-D1 configuration of Fig. 6.
(fractional coordinates, XTL format)

file s010_4-X.xtl

content: Atomic positions of the 4-X configuration of Fig. 6.
(fractional coordinates, XTL format)

file s110_1-D1a.xtl

content: Atomic positions of the 1-D1a configuration of Fig. 8.
(fractional coordinates, XTL format)

file s110_2-X.xtl

content: Atomic positions of the 2-X configuration of Fig. 8.
(fractional coordinates, XTL format)

file s-601_4-X1.xtl

content: Atomic positions of the 4-X1 configuration of Fig. 10.
(fractional coordinates, XTL format)