The file si2h2-pot.f is the FORTRAN source code for the fitted Si2H2 potential energy surface reported in

M. M. Law, J. T. Fraser-Smith and C. U. Perotto,
Phys. Chem. Chem. Phys. (2012)

The user must supply as an argument to the subroutine SI2H2POT an array of 6 internuclear distances (in units of angstroms); the potential energy is returned in cm-1 units.

The elements of the R array are numbered such that

R(1)=D13
R(2)=D24
R(3)=D34
R(4)=D14
R(5)=D23
R(6)=D12

where Dij is the internuclear distance between atoms i and j, numbered as follows:

H1, H2, Si3, Si4.

Note that the energy of the dibridged minimum on this surface is +1.6 cm-1.

Also supplied is a file si2h2-test.f which is the source code for a test main program; compile using (something like):

f77 -o si2h2-test si2h2-test.f si2h2-pot.f

si2h2-test.data contains the six internuclear distances for each of the four isomers and the dibridged-monobridged transition state.