1. Supplementary Data

Please refer to the web version of this work for access to the supplementary data. There are four files provided, as listed in Table 1. The column definitions are given in Table 2 for files 1 and 2 (Marvel input files) and Table 2 for files 3 and 4 (Marvel output files).

Table 1: Supplied supplementary data files.

File	Name
1	H2S_ortho_input_transitions.txt
2	H2S_para_input_transitions.txt
3	H2S_ortho_energylevels_output.txt
4	H2S_para_energylevels_output.txt

Table 2: Definition of columns in files 1 and 2.

Column	Label	Description
1	Energy (cm^{-1})	Transition wavenumber
2	Uncertainty (cm^{-1})	Associated uncertainity
	Upper assignments:	
3	v_1	S-H symmetric stretch
4	v_2	Symmetric bending mode
5	v_3	S-H antisymmetric stretch
6	J	Rotational angular momentum
7	K_a	Projection of rotational angular momentum
8	K_c	Projection of rotational angular momentum
9	*ortho/para*	Nuclear spin state
	Lower assignments:	
10	v_1	S-H symmetric stretch
11	v_2	Symmetric bending mode
12	v_3	S-H antisymmetric stretch
13	J	Rotational angular momentum
14	K_a	Projection of rotational angular momentum
15	K_c	Projection of rotational angular momentum
16	*ortho/para*	Nuclear spin state
17	Ref	Unique reference label

Table 3: Definition of columns in files 3 and 4.

Column	Label	Description
1	v_1	S-H symmetric stretch
2	v_2	Symmetric bending mode
3	v_3	S-H antisymmetric stretch
4	J	Rotational angular momentum
5	K_a	Projection of rotational angular momentum
6	K_c	Projection of rotational angular momentum
7	*ortho/para*	Nuclear spin state
8	Energy (cm^{-1})	MARVEL energy assignment
9	Uncertainty (cm^{-1})	MARVEL uncertainty
10	Num Trans	The number of transitions in the dataset which link to this state