FEFF.INP File

```
TITLE  CaSn(OH)6
HOLE 1   1.0     Sn K edge  ( 29.200 keV), s0^2=1.0
*        mphase,mpath,mfeff,mchi
CONTROL  0     0    0    1
PRINT    1     0    0    0
RMAX     6
SIG2 0.0034
CRITERIA     4 2
NLEG        6
CORRECTIONS -3 0.0
POTENTIALS
 *  ipot   z  label
    0   50   Sn
    1    8   O
    2   20   Ca
    3   50   Sn

ATOMS
  0.00000    0.00000    0.00000   0   Sn          0.00000
 -0.63921   -1.87296    0.53850   1   O           2.05098
 -0.53850    0.63921    1.87296   1   O           2.05098
  0.63921    1.87296   -0.53850   1   O           2.05098
  1.87296   -0.53850    0.63921   1   O           2.05098
 -1.87296    0.53850   -0.63921   1   O           2.05098
  0.53850   -0.63921   -1.87296   1   O           2.05098
  0.00000    0.00000    4.06105   2   Ca          4.06105
  0.00000   -4.06105    0.00000   2   Ca          4.06105
 -4.06105    0.00000    0.00000   2   Ca          4.06105
  4.06105    0.00000    0.00000   2   Ca          4.06105
  0.00000    0.00000   -4.06105   2   Ca          4.06105
  0.00000    4.06105    0.00000   2   Ca          4.06105
 -0.53850    3.42184    2.18809   1   O           4.09716
  2.18809   -0.53850    3.42184   1   O           4.09716
 -2.18809    0.53850   -3.42184   1   O           4.09716
  3.42184    2.18809   -0.53850   1   O           4.09716
 -3.42184   -2.18809    0.53850   1   O           4.09716
  0.53850   -3.42184   -2.18809   1   O           4.09716
 -3.52255    0.63921    2.18809   1   O           4.19580
  2.18809   -3.52255    0.63921   1   O           4.19580
  0.63921    2.18809   -3.52255   1   O           4.19580
 -2.18809    3.52255   -0.63921   1   O           4.19580
 -0.63921   -2.18809    3.52255   1   O           4.19580
  3.52255   -0.63921   -2.18809   1   O           4.19580
  2.18809    4.59954    0.63921   1   O           5.13343
  4.59954    0.63921    2.18809   1   O           5.13343
 -0.63921   -2.18809   -4.59955   1   O           5.13344
```

-4.59955	-0.63921	-2.18809	1	O	5.13344
-2.18809	-4.59955	-0.63921	1	O	5.13344
0.63921	2.18809	4.59954	1	O	5.13343
4.70026	-2.18809	0.53850	1	O	5.21250
-2.18809	0.53850	4.70026	1	O	5.21250
-4.70026	2.18809	-0.53850	1	O	5.21250
-0.53850	-4.70026	2.18809	1	O	5.21250
2.18809	-0.53850	-4.70026	1	O	5.21250
0.53850	4.70026	-2.18809	1	O	5.21250
-3.52255	3.42184	1.87296	1	O	5.25598
3.52255	-3.42184	-1.87296	1	O	5.25598
-1.87296	3.52255	-3.42184	1	O	5.25598
3.42184	1.87296	-3.52255	1	O	5.25598
-3.42184	-1.87296	3.52255	1	O	5.25598
1.87296	-3.52255	3.42184	1	O	5.25598
-4.06105	4.06105	0.00000	3	Sn	5.74319
4.06105	0.00000	4.06105	3	Sn	5.74319
0.00000	4.06105	4.06105	3	Sn	5.74319
0.00000	4.06105	-4.06105	3	Sn	5.74319
-4.06105	0.00000	4.06105	3	Sn	5.74319
0.00000	-4.06105	4.06105	3	Sn	5.74319
4.06105	0.00000	-4.06105	3	Sn	5.74319
-4.06105	-4.06105	0.00000	3	Sn	5.74319
4.06105	-4.06105	0.00000	3	Sn	5.74319
-4.06105	0.00000	-4.06105	3	Sn	5.74319
0.00000	-4.06105	-4.06105	3	Sn	5.74319
4.06105	4.06105	0.00000	3	Sn	5.74319

END

LIST.DAT File

```
CaSn(OH)6                                   Feff 7.02m
 Abs  Z=50 Rmt= 1.150 Rnm= 1.493 K  shell
 Pot 1 Z= 8 Rmt= 0.920 Rnm= 1.171
 Pot 2 Z=20 Rmt= 1.401 Rnm= 1.744
 Pot 3 Z=50 Rmt= 1.184 Rnm= 1.598
 Gam_ch=1.000E+01 H-L exch
 Mu=-2.764E+00 kf=1.913E+00 Vint=-1.671E+01 Rs_int= 1.896
 -----------------------------------------------------------------------
```

pathindex	sig2	amp ratio	deg	nlegs	r effective
1	0.00000	100.000	6.000	2	2.0510
2	0.00300	4.065	12.000	3	3.4742
4	0.00600	14.886	6.000	2	4.0610
6	0.00600	6.254	6.000	3	4.1020
7	0.00600	6.798	6.000	4	4.1020
8	0.00600	4.622	6.000	4	4.1020
10	0.00600	6.516	12.000	3	4.2272
18	0.00600	4.901	12.000	3	5.2692
19	0.01200	13.430	12.000	2	5.7432

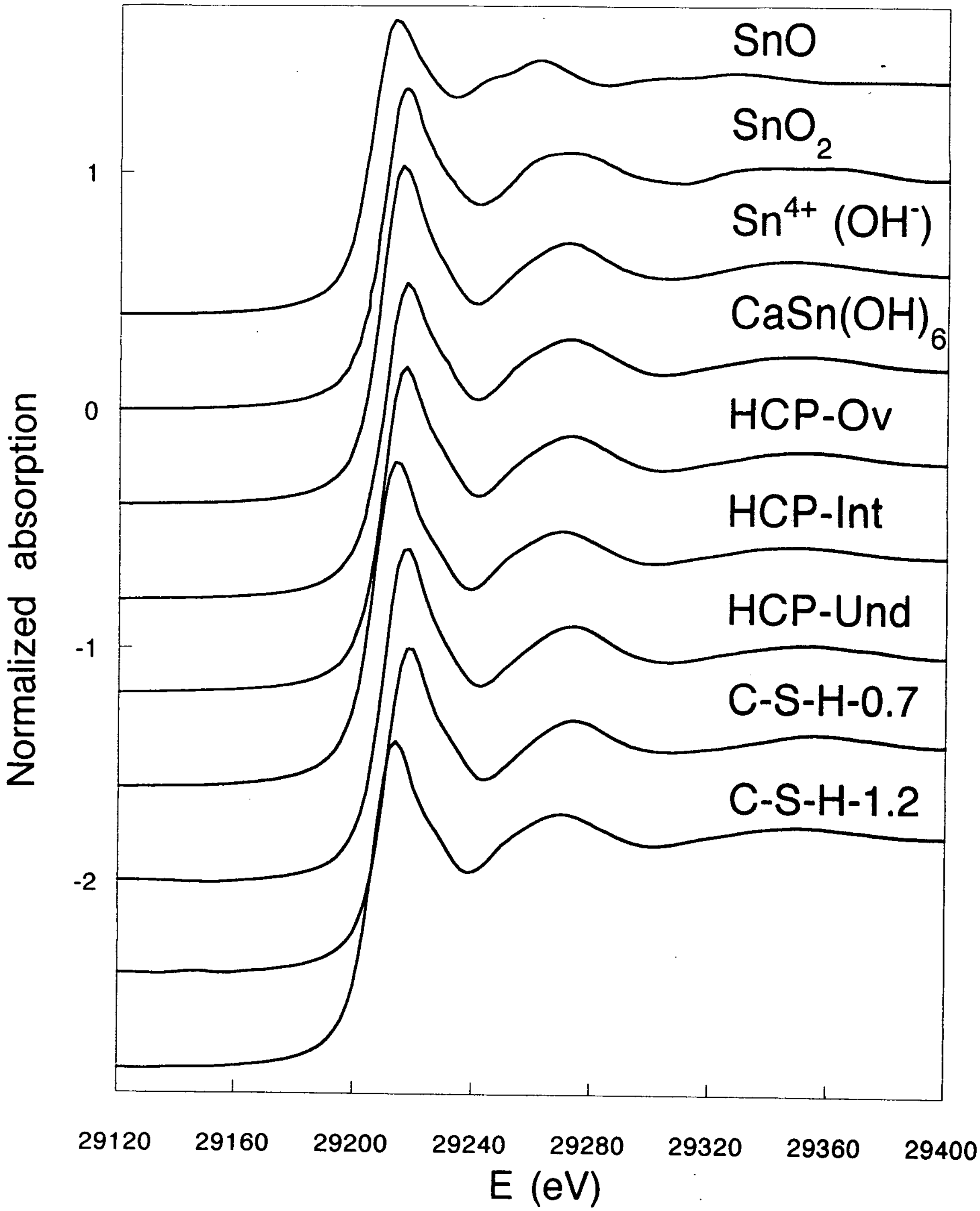

Figure 1 : Sn K-edge XANES spectra for reference compounds (SnO, SnO_2, Sn^{4+} (OH^-) and $CaSn(OH)_6$) and for Sn immobilized on HCP (HCP-Ov/-Int/-Und) and on C-S-H (C-S-H-0.7/1.2).