

Article

# Supplementary Material: On the morphology of group II metal fluoride nanocrystals at finite temperature and partial pressure of HF

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Academic Editor: Arnaud Gautier

Received: 2 February 2017; Accepted: 14 April 2017; Published: date

## 1. Bulk parameters with Hartree-Fock and different DFT functionals

**Table S1.** Optimized bulk parameters for CaF<sub>2</sub>, SrF<sub>2</sub> and BaF<sub>2</sub> using Hartree-Fock and different DFT functionals.

|                  |       | a (Å) | B (GPa) | E <sub>coh</sub> (eV) | E <sub>lat</sub> (eV) |
|------------------|-------|-------|---------|-----------------------|-----------------------|
| CaF <sub>2</sub> | Expt. | 5.463 | 82.71   | -16.08                | -27.46                |
|                  | HF    | 5.509 | 87.01   | -13.94                | -26.83                |
|                  | B3LYP | 5.496 | 85.54   | -16.44                | -26.90                |
|                  | B3PW  | 5.475 | 86.91   | -16.34                | -26.71                |
|                  | LDA   | 5.328 | 85.14   | -18.88                | -28.42                |
|                  | PBE   | 5.501 | 82.23   | -16.88                | -26.89                |
|                  | PWGGA | 5.491 | 84.03   | -17.03                | -26.99                |
| SrF <sub>2</sub> | Expt. | 5.799 | 69      | -15.95                | -26.03                |
|                  | HF    | 5.869 | 65.91   | -14.30                | -25.30                |
|                  | B3LYP | 5.847 | 63.09   | -16.63                | -25.33                |
|                  | B3PW  | 5.814 | 68.08   | -16.51                | -25.20                |
|                  | LDA   | 5.670 | 88.72   | -18.90                | -26.81                |
|                  | PBE   | 5.843 | 61.91   | -17.01                | -25.35                |
|                  | PWGGA | 5.830 | 61.39   | -17.18                | -25.44                |
| BaF <sub>2</sub> | Expt. | 6.20  | 57      | -16.01                | -24.58                |
|                  | HF    | 6.314 | 53.87   | -15.10                | -23.66                |
|                  | B3LYP | 6.260 | 61.25   | -17.53                | -23.79                |
|                  | B3PW  | 6.224 | 64.94   | -17.38                | -23.73                |
|                  | LDA   | 6.061 | 73.34   | -19.73                | -25.31                |
|                  | PBE   | 6.240 | 62.36   | -17.90                | -23.90                |
|                  | PWGGA | 6.230 | 63.49   | -18.07                | -24.00                |

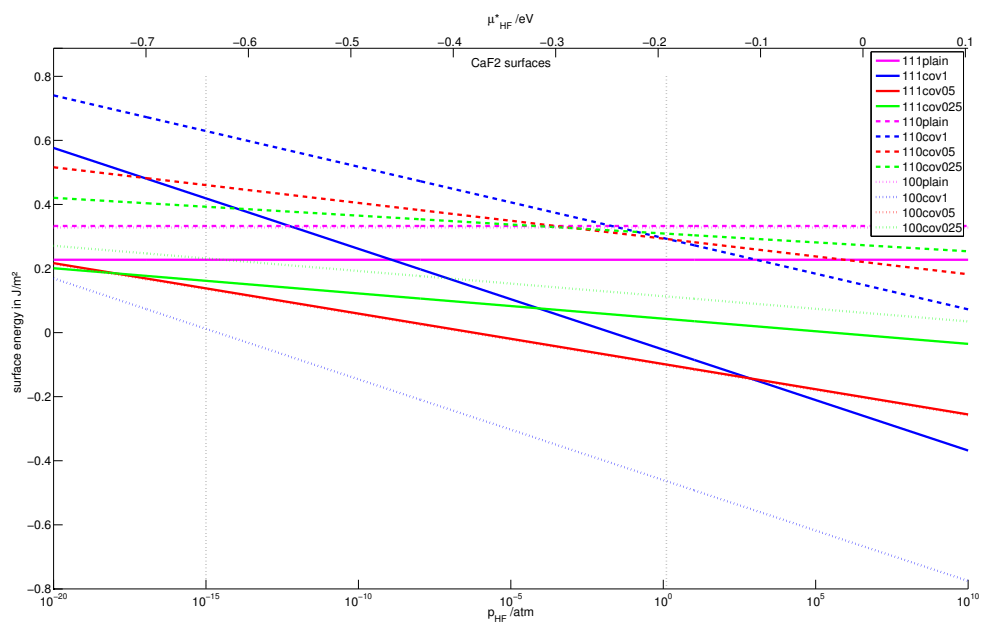
## 2. Convergence of surface energies with slab thickness

Symmetric slabs with a central reflection plane are constructed for each surface. The convergence of the surface energy with the number of layers in the slab is tested and presented in Tab. S2. A layer is defined as different z-coordinate (z axis perpendicular to the surface). For the (111) surface each atom is in its own layer. For the (110) surface a CaF<sub>2</sub>-unit is forming a layer and for the (100) surface Ca has its own layer, whereas two fluorides form one joint layer.

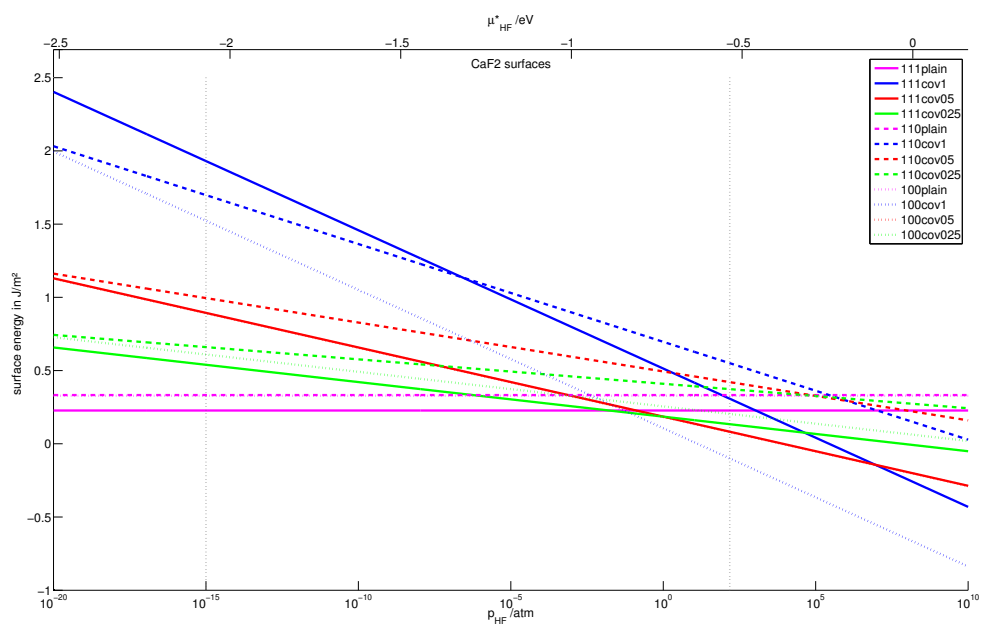
**Table S2.** Surface energies  $\gamma$  (J/m<sup>2</sup>) for the three stable surfaces of CaF<sub>2</sub>, SrF<sub>2</sub> and BaF<sub>2</sub> at different slab thicknesses.

| CaF <sub>2</sub> |              |          | SrF <sub>2</sub> |              |          | BaF <sub>2</sub> |              |          |
|------------------|--------------|----------|------------------|--------------|----------|------------------|--------------|----------|
| (hkl)            | Nb of layers | $\gamma$ | (hkl)            | Nb of layers | $\gamma$ | (hkl)            | Nb of layers | $\gamma$ |
| (111)            | 6            | 0.470    | (111)            | 6            | 0.451    | (111)            | 6            | 0.386    |
|                  | 9            | 0.472    |                  | 9            | 0.454    |                  | 9            | 0.388    |
|                  | 12           | 0.472    |                  | 12           | 0.454    |                  | 12           | 0.388    |
| (110)            | 5            | 0.723    | (110)            | 5            | 0.681    | (110)            | 5            | 0.572    |
|                  | 6            | 0.714    |                  | 6            | 0.675    |                  | 6            | 0.568    |
|                  | 7            | 0.718    |                  | 7            | 0.677    |                  | 7            | 0.569    |
| (100)            | 13           | 0.944    | (100)            | 13           | 0.981    | (100)            | 13           | 0.860    |
|                  | 15           | 0.955    |                  | 15           | 0.984    |                  | 15           | 0.859    |
|                  | 17           | 0.951    |                  | 17           | 0.985    |                  | 17           | 0.859    |

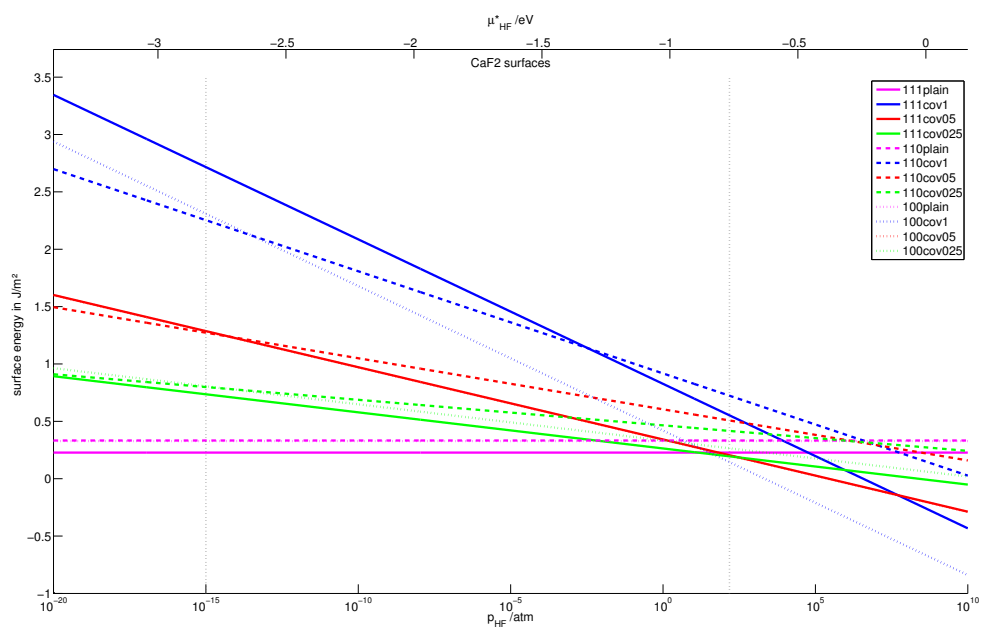
### 3. Surface energies as function of the pressure



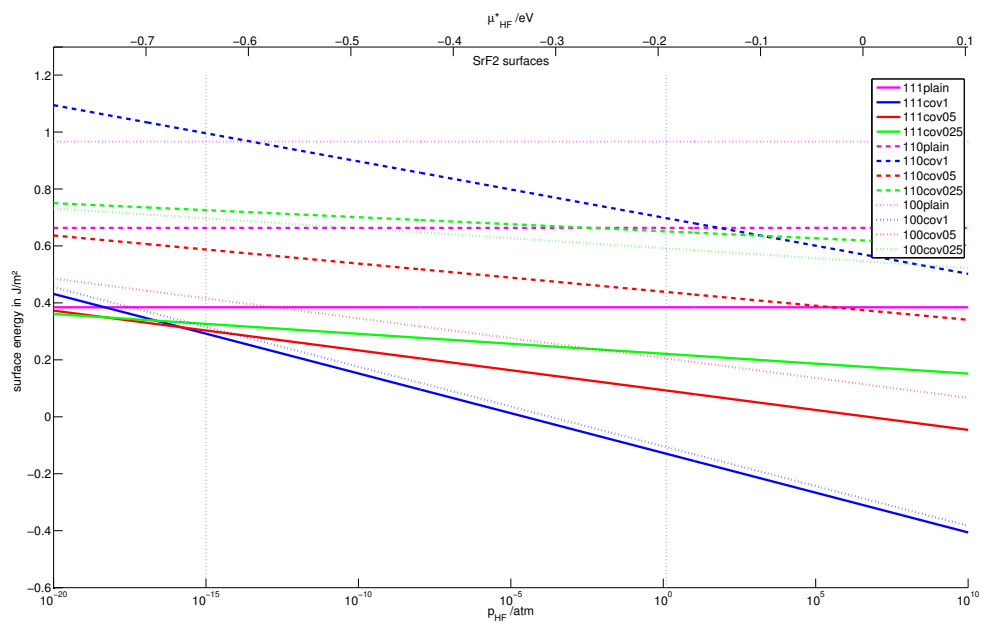
**Figure S1.** Variation of the surface energy as a function of the pressure of HF for the three low index surfaces of CaF<sub>2</sub> at 150 K.



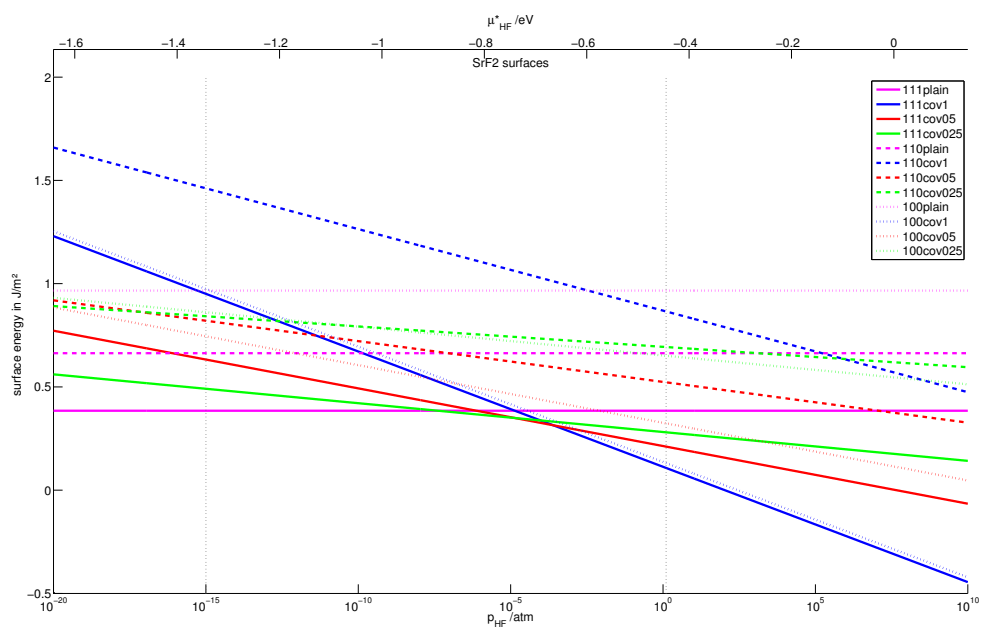
**Figure S2.** Variation of the surface energy as a function of the pressure of HF for the three low index surfaces of CaF<sub>2</sub> at 450 K.



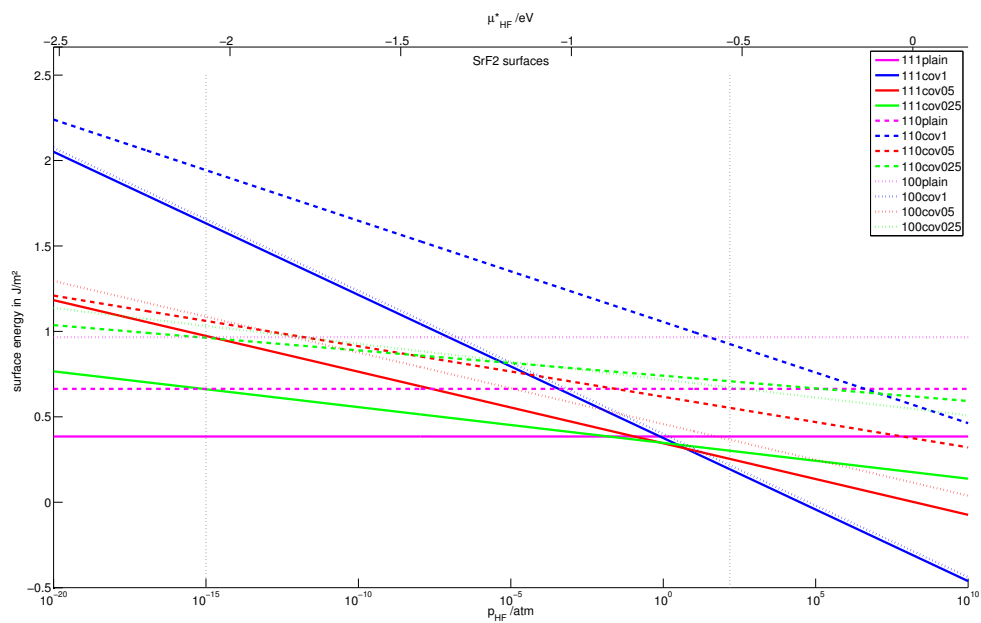
**Figure S3.** Variation of the surface energy as a function of the pressure of HF for the three low index surfaces of  $\text{CaF}_2$  at 600 K.



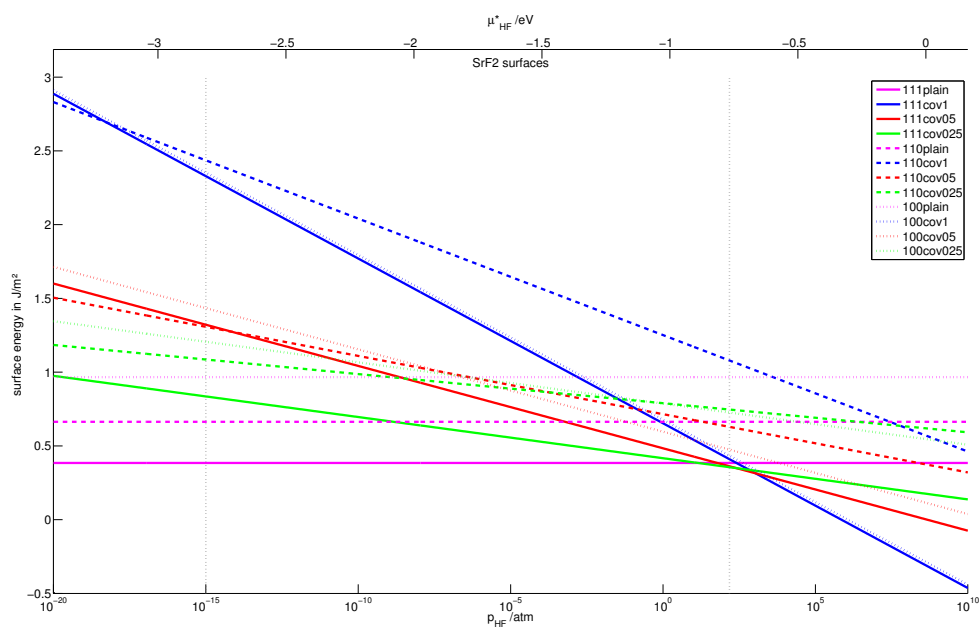
**Figure S4.** Variation of the surface energy as a function of the pressure of HF for the three low index surfaces of  $\text{SrF}_2$  at 150 K.



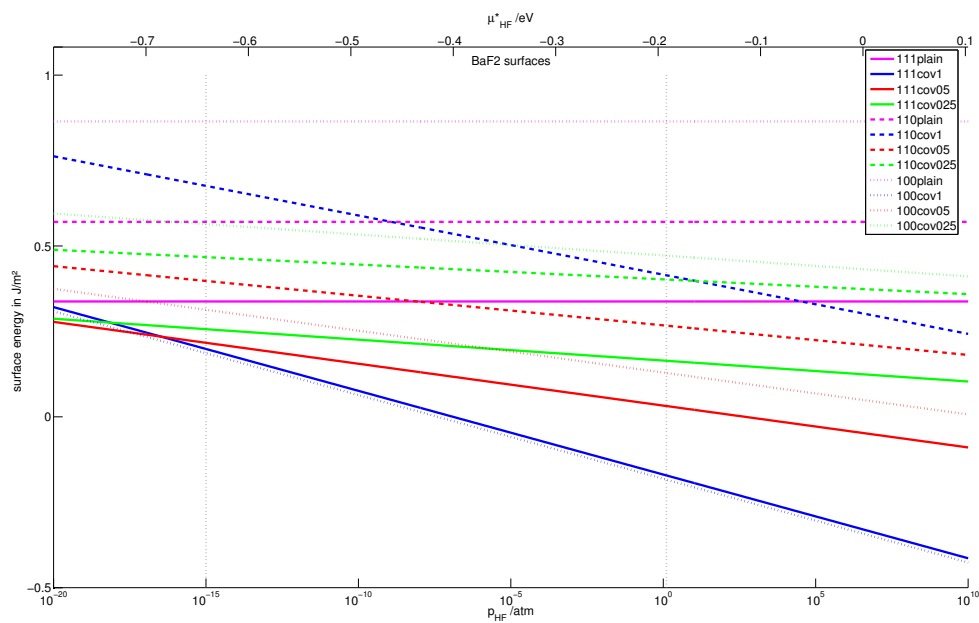
**Figure S5.** Variation of the surface energy as a function of the pressure of HF for the three low index surfaces of  $\text{SrF}_2$  at 300 K.



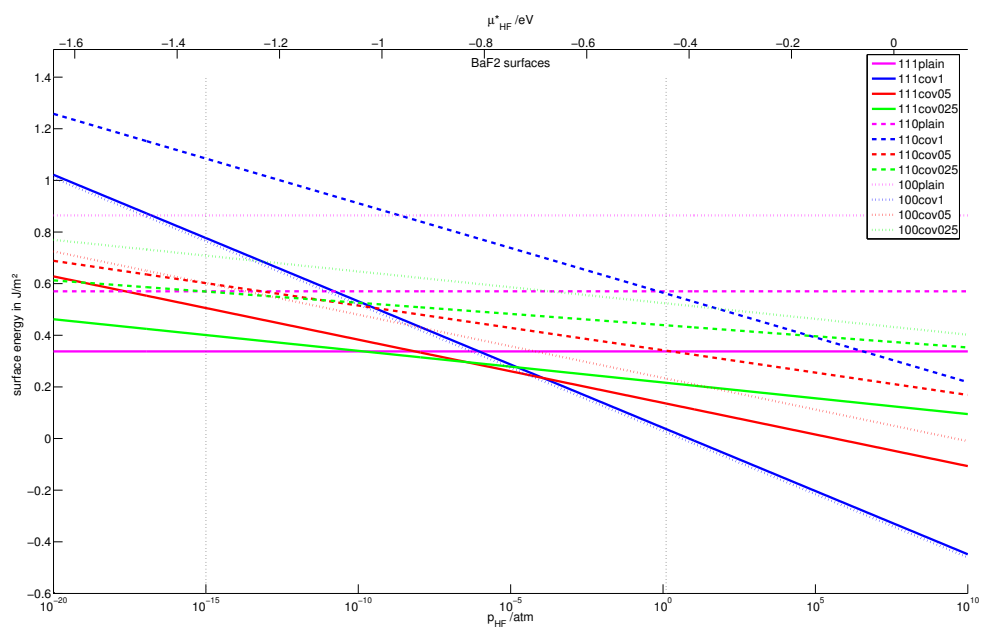
**Figure S6.** Variation of the surface energy as a function of the pressure of HF for the three low index surfaces of  $\text{SrF}_2$  at 450 K.



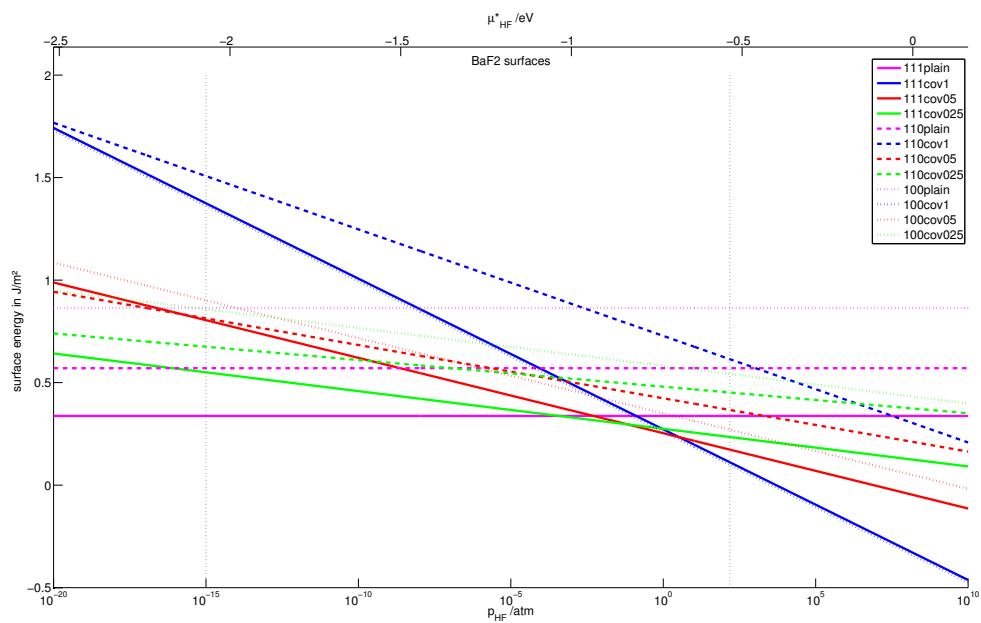
**Figure S7.** Variation of the surface energy as a function of the pressure of HF for the three low index surfaces of  $\text{SrF}_2$  at 600 K.



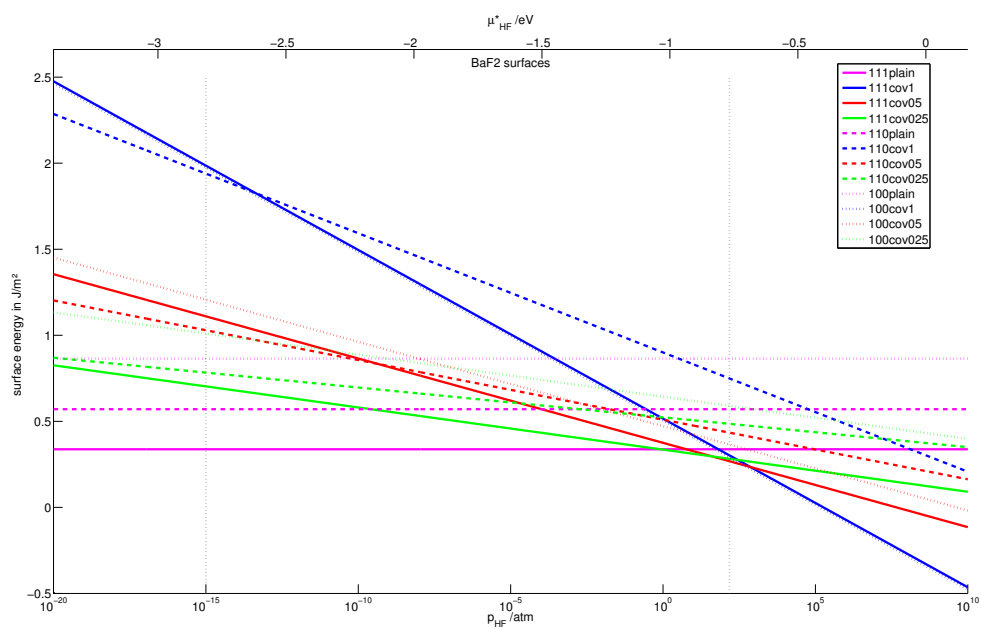
**Figure S8.** Variation of the surface energy as a function of the pressure of HF for the three low index surfaces of  $\text{BaF}_2$  at 150 K.



**Figure S9.** Variation of the surface energy as a function of the pressure of HF for the three low index surfaces of  $\text{BaF}_2$  at 300 K.



**Figure S10.** Variation of the surface energy as a function of the pressure of HF for the three low index surfaces of  $\text{BaF}_2$  at 450 K.



**Figure S11.** Variation of the surface energy as a function of the pressure of HF for the three low index surfaces of BaF<sub>2</sub> at 600 K.

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## 1. CaF<sub>2</sub>:

### (111) surface, 100% coverage

|    |     |    |                     |                     |                     |
|----|-----|----|---------------------|---------------------|---------------------|
| 1  | 9   | F  | 9.728321703337E-01  | -1.690678081025E+00 | 2.370862283267E+00  |
| 2  | 9   | F  | -9.728321703337E-01 | 1.690678081025E+00  | -2.370862283267E+00 |
| 3  | 220 | CA | -9.729787924481E-01 | -5.571628753158E-01 | 1.580004579276E+00  |
| 4  | 220 | CA | 9.729787924481E-01  | 5.571628753158E-01  | -1.580004579276E+00 |
| 5  | 9   | F  | 9.732923590636E-01  | 5.618439802655E-01  | 7.762492940912E-01  |
| 6  | 9   | F  | -9.732923590636E-01 | -5.618439802655E-01 | -7.762492940912E-01 |
| 7  | 109 | F  | -1.254748082362E+00 | -5.604086033089E-01 | 4.242510948587E+00  |
| 8  | 109 | F  | 1.254748082362E+00  | 5.604086033089E-01  | -4.242510948587E+00 |
| 9  | 1   | H  | -1.928638566151E+00 | -1.211670906084E+00 | 4.418132538676E+00  |
| 10 | 1   | H  | 1.928638566151E+00  | 1.211670906084E+00  | -4.418132538676E+00 |

### (111) surface, 50% coverage

|    |     |    |                     |                     |                     |
|----|-----|----|---------------------|---------------------|---------------------|
| 1  | 9   | F  | 7.788128108513E-02  | 6.056354242180E-02  | 2.253572277919E+00  |
| 2  | 9   | F  | -7.788128108513E-02 | -6.056354242179E-02 | -2.253572277919E+00 |
| 3  | 9   | F  | 3.447090306015E+00  | -3.125677040127E-01 | 2.672905786883E+00  |
| 4  | 9   | F  | -3.447090306015E+00 | 3.125677040127E-01  | -2.672905786883E+00 |
| 5  | 220 | CA | 1.376965191417E-01  | -2.154852767347E+00 | 1.683131420072E+00  |
| 6  | 220 | CA | -1.376965191417E-01 | 2.154852767347E+00  | -1.683131420072E+00 |
| 7  | 220 | CA | 1.916592293146E+00  | 1.083902142328E+00  | 1.506088210881E+00  |
| 8  | 220 | CA | -1.916592293146E+00 | -1.083902142328E+00 | -1.506088210881E+00 |
| 9  | 9   | F  | 5.416516341449E-02  | 2.271167064005E+00  | 6.165910509208E-01  |
| 10 | 9   | F  | -5.416516341449E-02 | -2.271167064005E+00 | -6.165910509208E-01 |
| 11 | 9   | F  | -2.010093759969E+00 | -1.158694226407E+00 | 9.546252120016E-01  |
| 12 | 9   | F  | 2.010093759969E+00  | 1.158694226407E+00  | -9.546252120016E-01 |
| 13 | 109 | F  | -8.207154604467E-01 | -2.317288538156E+00 | 3.798872741481E+00  |
| 14 | 109 | F  | 8.207154604467E-01  | 2.317288538156E+00  | -3.798872741481E+00 |
| 15 | 1   | H  | -1.531320705997E+00 | -2.993522574597E+00 | 3.557566505132E+00  |
| 16 | 1   | H  | 1.531320705997E+00  | 2.993522574597E+00  | -3.557566505132E+00 |

### (111) surface, 25% coverage

|    |     |    |                     |                     |                     |
|----|-----|----|---------------------|---------------------|---------------------|
| 1  | 9   | F  | -1.873271718305E+00 | 3.381959753790E+00  | 2.304357097233E+00  |
| 2  | 9   | F  | 1.873271718305E+00  | -3.381959753790E+00 | -2.304357097233E+00 |
| 3  | 9   | F  | 4.496626758716E-02  | 4.959086668690E-02  | 2.325072840907E+00  |
| 4  | 9   | F  | -4.496626758716E-02 | -4.959086668690E-02 | -2.325072840907E+00 |
| 5  | 9   | F  | 1.489324737247E+00  | 3.121221438468E+00  | 2.676034512641E+00  |
| 6  | 9   | F  | -1.489324737247E+00 | -3.121221438468E+00 | -2.676034512641E+00 |
| 7  | 9   | F  | 3.879071634032E+00  | -7.129879534649E-03 | 2.324739139450E+00  |
| 8  | 9   | F  | -3.879071634032E+00 | 7.129879534649E-03  | -2.324739139450E+00 |
| 9  | 220 | CA | -1.947154223848E+00 | 1.118170772731E+00  | 1.662434905485E+00  |
| 10 | 220 | CA | 1.947154223848E+00  | -1.118170772731E+00 | -1.662434905485E+00 |
| 11 | 220 | CA | 1.614525252818E-01  | -2.158952677323E+00 | 1.635193552382E+00  |
| 12 | 220 | CA | -1.614525252818E-01 | 2.158952677323E+00  | -1.635193552382E+00 |
| 13 | 220 | CA | 1.915342301166E+00  | 1.116729940839E+00  | 1.519309430652E+00  |
| 14 | 220 | CA | -1.915342301166E+00 | -1.116729940839E+00 | -1.519309430652E+00 |
| 15 | 220 | CA | 3.869137734866E+00  | -2.261038506821E+00 | 1.512497751215E+00  |

16 220 CA -3.869137734866E+00 2.261038506821E+00 -1.512497751215E+00  
17 9 F -3.009605246447E-02 2.224429836187E+00 6.884592241849E-01  
18 9 F 3.009605246447E-02 -2.224429836187E+00 -6.884592241849E-01  
19 9 F 2.019187395335E+00 -1.075032043640E+00 6.677028754959E-01  
20 9 F -2.019187395335E+00 1.075032043640E+00 -6.677028754959E-01  
21 9 F -1.006997239251E-01 -4.407942603071E+00 8.772482950725E-01  
22 9 F 1.006997239251E-01 4.407942603071E+00 -8.772482950725E-01  
23 9 F -1.916268106365E+00 -1.250515559211E+00 8.815709420667E-01  
24 9 F 1.916268106365E+00 1.250515559211E+00 -8.815709420667E-01  
25 109 F -5.897842029139E-01 -2.683872046182E+00 3.827942351982E+00  
26 109 F 5.897842029139E-01 2.683872046182E+00 -3.827942351982E+00  
27 1 H -1.446452628759E+00 -3.108987474275E+00 3.452169669481E+00  
28 1 H 1.446452628759E+00 3.108987474275E+00 -3.452169669481E+00

(110) surface, 100% coverage

1 220 CA 9.735490505145E-01 1.372463855412E+00 4.691722744229E+00  
2 220 CA -9.735490505145E-01 -1.372463855412E+00 -4.691722744229E+00  
3 9 F -9.726509997281E-01 2.679157105085E+00 4.859659103540E+00  
4 9 F 9.726509997281E-01 -2.679157105085E+00 -4.859659103540E+00  
5 9 F 9.726787106401E-01 -5.785838112376E-02 -4.897179309244E+00  
6 9 F -9.726787106401E-01 5.785838112376E-02 4.897179309244E+00  
7 220 CA -9.724796706846E-01 -1.379327164926E+00 3.012826543947E+00  
8 220 CA 9.724796706846E-01 1.379327164926E+00 -3.012826543947E+00  
9 9 F 9.731808004583E-01 -1.068621726256E-02 2.901298208478E+00  
10 9 F -9.731808004583E-01 1.068621726256E-02 -2.901298208478E+00  
11 9 F -9.731828583123E-01 2.747848419321E+00 -2.892990146600E+00  
12 9 F 9.731828583123E-01 -2.747848419321E+00 2.892990146600E+00  
13 220 CA 9.734171426759E-01 1.375940655502E+00 9.263798947039E-01  
14 220 CA -9.734171426759E-01 -1.375940655502E+00 -9.263798947039E-01  
15 9 F -9.730141800895E-01 2.751129400086E+00 9.859452265408E-01  
16 9 F 9.730141800895E-01 -2.751129400086E+00 -9.859452265408E-01  
17 9 F 9.730148739033E-01 -1.269710934598E-03 -9.887147329187E-01  
18 9 F -9.730148739033E-01 1.269710934598E-03 9.887147329187E-01  
19 109 F 9.694375810767E-01 1.654061806104E+00 7.259856570428E+00  
20 109 F -9.694375810767E-01 -1.654061806104E+00 -7.259856570428E+00  
21 1 H 9.696185066527E-01 1.192756678241E+00 8.076847067926E+00  
22 1 H -9.696185066527E-01 -1.192756678241E+00 -8.076847067926E+00

(110) surface, 50% coverage

1 220 CA 1.868168098976E+00 2.628860947204E+00 4.719206996255E+00  
2 220 CA -2.023659035898E+00 2.633550856576E+00 4.668460780087E+00  
3 220 CA -7.707401761300E-02 -1.173357884546E-01 -4.707255341112E+00  
4 220 CA 3.814368551590E+00 -1.189167721721E-01 -4.660140765075E+00  
5 9 F -9.519750137734E-02 -1.565605733962E+00 4.874193939177E+00  
6 9 F 3.830006933961E+00 -1.565339243394E+00 4.882453087347E+00  
7 9 F 1.877464801614E+00 1.188779260362E+00 -4.885670478810E+00  
8 9 F -2.037998230878E+00 1.189754600473E+00 -4.879820517286E+00  
9 9 F 1.887708262352E+00 -1.422067226255E+00 -4.867815290195E+00  
10 9 F -2.045620531509E+00 -1.421380320963E+00 -4.851308580445E+00  
11 9 F -1.010800631706E-01 1.322983877766E+00 4.877268555520E+00

12 9 F 3.831560310832E+00 1.324131160404E+00 4.892582184157E+00  
13 220 CA -7.757278602693E-02 -1.207643299790E-01 3.017426475194E+00  
14 220 CA 3.810604343845E+00 -1.198669362198E-01 3.024030745120E+00  
15 220 CA 1.864937161406E+00 2.634271042575E+00 -3.012087034156E+00  
16 220 CA -2.023029613507E+00 2.633936908718E+00 -3.010610064270E+00  
17 9 F 1.869528163962E+00 1.248702739671E+00 2.917673745016E+00  
18 9 F -2.029117205086E+00 1.248595099580E+00 2.888039695403E+00  
19 9 F -7.586141140673E-02 -1.499164425964E+00 -2.903565561486E+00  
20 9 F 3.809559982519E+00 -1.502247391074E+00 -2.876103890503E+00  
21 9 F -7.900475328907E-02 1.263718798223E+00 -2.906801372535E+00  
22 9 F 3.812049750422E+00 1.266584811813E+00 -2.883741973229E+00  
23 9 F 1.868081889957E+00 -1.491425983376E+00 2.914407350074E+00  
24 9 F -2.025962211581E+00 -1.486932711307E+00 2.888692496179E+00  
25 220 CA 1.866080386113E+00 2.632711335653E+00 9.352323119676E-01  
26 220 CA -2.024950270219E+00 2.632330821341E+00 9.247067508387E-01  
27 220 CA -7.803811957940E-02 -1.191287006818E-01 -9.252600617087E-01  
28 220 CA 3.810527879802E+00 -1.200176162523E-01 -9.150829354678E-01  
29 9 F -7.688088020963E-02 -1.496886801156E+00 9.914629784166E-01  
30 9 F 3.810219091926E+00 -1.496242298305E+00 9.930810986228E-01  
31 9 F 1.862496956958E+00 1.256530851777E+00 -9.842461299173E-01  
32 9 F -2.021735157880E+00 1.253985495113E+00 -9.830235893005E-01  
33 9 F 1.862855943274E+00 -1.494040360328E+00 -9.801034351711E-01  
34 9 F -2.021648112340E+00 -1.494173199199E+00 -9.836573537735E-01  
35 9 F -7.516619294117E-02 1.257360073742E+00 9.939628768886E-01  
36 9 F 3.807601018276E+00 1.258859583719E+00 9.916726920246E-01  
37 109 F 1.707614952328E+00 2.672748104271E+00 7.251904542102E+00  
38 1 H 1.710888716617E+00 2.201334536519E+00 8.066477738167E+00  
39 109 F -2.850955413314E-01 -5.261953888698E-01 -7.339529567333E+00  
40 1 H -2.803900480376E-01 -5.999967758788E-02 -8.157113096784E+00

(110) surface, 25% coverage

1 220 CA 1.904991178929E+00 2.692588215650E+00 4.723712169654E+00  
2 220 CA 1.902205175726E+00 -2.816933048463E+00 4.679296002876E+00  
3 220 CA -1.987948154055E+00 2.693058102960E+00 4.671130847023E+00  
4 220 CA -1.989170785039E+00 -2.815812798506E+00 4.680500887502E+00  
5 220 CA -4.156164340169E-02 -6.561635012633E-02 -4.719103932795E+00  
6 220 CA -4.326483061395E-02 5.449867384401E+00 -4.675939708122E+00  
7 220 CA 3.849984523384E+00 -6.482839215888E-02 -4.669469033552E+00  
8 220 CA 3.848870130172E+00 5.447091588067E+00 -4.675819079003E+00  
9 9 F -6.136907202490E-02 3.995953903827E+00 4.858874712027E+00  
10 9 F -4.031853387685E-02 -1.513914174357E+00 4.889178769186E+00  
11 9 F 3.867865452040E+00 3.997630330186E+00 4.868289146568E+00  
12 9 F 3.845635944711E+00 -1.513211946511E+00 4.889655246269E+00  
13 9 F 1.912875245559E+00 1.246844208492E+00 -4.888846542447E+00  
14 9 F 1.903206821563E+00 -4.262626109299E+00 -4.872256454209E+00  
15 9 F -2.001467894262E+00 1.247067395801E+00 -4.886012358991E+00  
16 9 F -1.989313910704E+00 -4.263548881823E+00 -4.870878608343E+00  
17 9 F 1.927440796232E+00 -1.365373962731E+00 -4.856813073183E+00  
18 9 F 1.900621576305E+00 4.143976364079E+00 -4.884048900536E+00  
19 9 F -2.012929582297E+00 -1.365616084886E+00 -4.840339426565E+00  
20 9 F -1.986906773686E+00 4.144019682790E+00 -4.886203500071E+00

21 9 F -6.504771705583E-02 1.379698969508E+00 4.871526005853E+00  
22 9 F -4.397565271619E-02 -4.114965164233E+00 4.879303410347E+00  
23 9 F 3.869530396650E+00 1.381822704192E+00 4.881068598908E+00  
24 9 F 3.848550764605E+00 -4.114712579835E+00 4.879338706775E+00  
25 220 CA -4.185727987051E-02 -5.742377157644E-02 3.017789160277E+00  
26 220 CA -4.298165921502E-02 5.438147873560E+00 3.017310364245E+00  
27 220 CA 3.848420838792E+00 -5.734805344550E-02 3.023046822567E+00  
28 220 CA 3.846751748945E+00 5.438677298054E+00 3.017016610434E+00  
29 220 CA 1.900568738821E+00 2.687943099774E+00 -3.021452034524E+00  
30 220 CA 1.903081591491E+00 -2.808289740636E+00 -3.010307953364E+00  
31 220 CA -1.987587973493E+00 2.688158992894E+00 -3.024019140948E+00  
32 220 CA -1.988484733732E+00 -2.809028247148E+00 -3.005552388068E+00  
33 9 F 1.904820807834E+00 1.308568350052E+00 2.916140762026E+00  
34 9 F 1.902193197356E+00 -4.196664123398E+00 2.897595548303E+00  
35 9 F -1.991242919183E+00 1.307212565132E+00 2.884249681599E+00  
36 9 F -1.989792164053E+00 -4.195831680039E+00 2.898134035239E+00  
37 9 F -4.374606884517E-02 4.060857175736E+00 -2.898290612376E+00  
38 9 F -3.960046040579E-02 -1.441269550768E+00 -2.904343088192E+00  
39 9 F 3.848697520675E+00 4.059366134672E+00 -2.901307619697E+00  
40 9 F 3.845817716570E+00 -1.443068598301E+00 -2.872306636035E+00  
41 9 F -4.375408983421E-02 1.320816148221E+00 -2.915367714476E+00  
42 9 F -4.304393894841E-02 -4.181030475369E+00 -2.890365382497E+00  
43 9 F 3.848476057429E+00 1.324397996055E+00 -2.890758237904E+00  
44 9 F 3.848840853892E+00 -4.181986541758E+00 -2.891721807526E+00  
45 9 F 1.902953894540E+00 -1.430942337098E+00 2.900896257832E+00  
46 9 F 1.903995016531E+00 4.072055127551E+00 2.908862974619E+00  
47 9 F -1.989146905950E+00 -1.429744237706E+00 2.905035945957E+00  
48 9 F -1.990392172927E+00 4.074948319208E+00 2.880978657361E+00  
49 220 CA 1.902739254961E+00 2.690267338581E+00 9.324006353900E-01  
50 220 CA 1.901595597577E+00 -2.812425034227E+00 9.260604365350E-01  
51 220 CA -1.989062471655E+00 2.690688021388E+00 9.207667386189E-01  
52 220 CA -1.988685943264E+00 -2.813155702662E+00 9.266598019269E-01  
53 220 CA -4.251004525592E-02 -5.963013012689E-02 -9.302911102857E-01  
54 220 CA -4.247178087633E-02 5.441762440934E+00 -9.211861922921E-01  
55 220 CA 3.847749523114E+00 -5.967224440746E-02 -9.189841517632E-01  
56 220 CA 3.847235928634E+00 5.440950933446E+00 -9.211323538444E-01  
57 9 F -3.987167750928E-02 4.064692441719E+00 9.863713073762E-01  
58 9 F -4.461010210277E-02 -1.437489554626E+00 9.922577706997E-01  
59 9 F 3.845169231081E+00 4.065400176923E+00 9.863112235755E-01  
60 9 F 3.850014026495E+00 -1.437758253666E+00 9.931121618912E-01  
61 9 F 1.899114923419E+00 1.315704322201E+00 -9.895964775416E-01  
62 9 F 1.902525424199E+00 -4.190874464276E+00 -9.841377142624E-01  
63 9 F -1.985755714247E+00 1.313852134255E+00 -9.900129064086E-01  
64 9 F -1.989514087292E+00 -4.191912848361E+00 -9.819830002845E-01  
65 9 F 1.898452836487E+00 -1.434506741960E+00 -9.792595484759E-01  
66 9 F 1.902771257772E+00 4.067273697372E+00 -9.895202693647E-01  
67 9 F -1.984686687178E+00 -1.434964769611E+00 -9.822189077310E-01  
68 9 F -1.989890142945E+00 4.067494439439E+00 -9.905370497122E-01  
69 9 F -3.892563377920E-02 1.315680318176E+00 9.896711756585E-01  
70 9 F -4.285849924881E-02 -4.187784996000E+00 9.899086849931E-01  
71 9 F 3.844104342622E+00 1.316703423105E+00 9.887066022454E-01  
72 9 F 3.847612106974E+00 -4.187297545209E+00 9.897651248247E-01

73 109 F 1.774023769064E+00 2.729956867361E+00 7.256225908960E+00  
74 1 H 1.776122588945E+00 2.266129908405E+00 8.075405437804E+00  
75 109 F -2.208000936005E-01 -5.325107191542E-01 -7.320078074383E+00  
76 1 H -2.165959792483E-01 -7.355453970844E-02 -8.142093344171E+00

(100) surface, 100% coverage

1 9 F -9.194857957268E-02 1.126890121001E+00 9.323782460780E+00  
2 9 F -9.194857957268E-02 1.126890121001E+00 -9.323782460780E+00  
3 220 CA -2.066178277749E+00 1.646283735892E+00 8.271500187187E+00  
4 220 CA -2.066178277749E+00 1.646283735892E+00 -8.271500187187E+00  
5 9 F -1.149777469387E-01 1.716461170971E+00 6.759250533844E+00  
6 9 F -1.149777469387E-01 1.716461170971E+00 -6.759250533844E+00  
7 9 F 1.830686803769E+00 -2.767624588512E-01 7.041342482706E+00  
8 9 F 1.830686803769E+00 -2.767624588512E-01 -7.041342482706E+00  
9 220 CA -1.197078430626E-01 -2.377280741046E-01 5.513631494223E+00  
10 220 CA -1.197078430626E-01 -2.377280741046E-01 -5.513631494223E+00  
11 9 F 1.827288161891E+00 -2.312265177144E-01 4.197026205207E+00  
12 9 F 1.827288161891E+00 -2.312265177144E-01 -4.197026205207E+00  
13 9 F -1.187579113753E-01 1.714525199055E+00 4.071939211503E+00  
14 9 F -1.187579113753E-01 1.714525199055E+00 -4.071939211503E+00  
15 220 CA 1.828514972819E+00 1.715485814622E+00 2.754131967766E+00  
16 220 CA 1.828514972819E+00 1.715485814622E+00 -2.754131967766E+00  
17 9 F -1.165838836517E-01 1.715191214603E+00 1.359682863359E+00  
18 9 F -1.165838836517E-01 1.715191214603E+00 -1.359682863359E+00  
19 9 F 1.829230651667E+00 -2.307107842169E-01 1.394822038544E+00  
20 9 F 1.829230651667E+00 -2.307107842169E-01 -1.394822038544E+00  
21 220 CA -1.161566640852E-01 -2.313154858805E-01 0.000000000000E+00  
22 109 F -1.777512036982E+00 -6.206081450174E-01 1.009033689242E+01  
23 109 F -1.777512036982E+00 -6.206081450174E-01 -1.009033689242E+01  
24 1 H -9.179338405953E-01 -1.502278096491E-01 1.009510869026E+01  
25 1 H -9.179338405953E-01 -1.502278096491E-01 -1.009510869026E+01

(100) surface, 50% coverage

1 9 F 1.466611705386E-01 1.467676319396E+00 9.414898241809E+00  
2 9 F 3.811725355920E+00 1.852353811726E+00 9.342086125234E+00  
3 9 F 1.466611705386E-01 1.467676319396E+00 -9.414898241809E+00  
4 9 F 3.811725355920E+00 1.852353811726E+00 -9.342086125234E+00  
5 220 CA -2.010350237742E+00 1.914072166641E+00 8.351790682410E+00  
6 220 CA 1.973894815571E+00 1.909872326421E+00 8.215139205865E+00  
7 220 CA 1.973894815571E+00 1.909872326421E+00 -8.215139205865E+00  
8 220 CA -2.010350237742E+00 1.914072166641E+00 -8.351790682410E+00  
9 9 F -2.811068675149E-02 1.957177187916E+00 6.780482406509E+00  
10 9 F 3.874600060783E+00 1.925487871535E+00 6.696011015899E+00  
11 9 F -2.811068675149E-02 1.957177187916E+00 -6.780482406509E+00  
12 9 F 3.874600060783E+00 1.925487871535E+00 -6.696011015899E+00  
13 9 F -1.985472203022E+00 -2.289366593966E-02 7.080655697003E+00  
14 9 F 1.940014704322E+00 -2.638009020117E-02 7.077804223582E+00  
15 9 F 1.940014704322E+00 -2.638009020117E-02 -7.077804223582E+00  
16 9 F -1.985472203022E+00 -2.289366593966E-02 -7.080655697003E+00  
17 220 CA -3.888834605959E-02 1.231641730653E-03 5.535965151468E+00

18 220 CA 3.889763239475E+00 -1.968992106257E-02 5.490192959016E+00  
19 220 CA -3.888834605959E-02 1.231641730654E-03 -5.535965151468E+00  
20 220 CA 3.889763239475E+00 -1.968992106257E-02 -5.490192959016E+00  
21 9 F -1.958586457605E+00 -7.003399946217E-03 4.197939701955E+00  
22 9 F 1.919301499129E+00 -7.003044942217E-03 4.218279044914E+00  
23 9 F 1.919301499129E+00 -7.003044942216E-03 -4.218279044914E+00  
24 9 F -1.958586457605E+00 -7.003399946216E-03 -4.197939701955E+00  
25 9 F -2.413629306563E-02 1.940662989913E+00 4.083468123838E+00  
26 9 F 3.876340946343E+00 1.936171554504E+00 4.041202681592E+00  
27 9 F -2.413629306563E-02 1.940662989913E+00 -4.083468123838E+00  
28 9 F 3.876340946343E+00 1.936171554504E+00 -4.041202681592E+00  
29 220 CA -1.960329219409E+00 1.939109411018E+00 2.746444497604E+00  
30 220 CA 1.920996933967E+00 1.938651274496E+00 2.761381673993E+00  
31 220 CA 1.920996933967E+00 1.938651274496E+00 -2.761381673993E+00  
32 220 CA -1.960329219409E+00 1.939109411018E+00 -2.746444497604E+00  
33 9 F -1.750901433957E-02 1.938259216151E+00 1.359042323016E+00  
34 9 F 3.871315149505E+00 1.938519612745E+00 1.352989848611E+00  
35 9 F -1.750901433957E-02 1.938259216151E+00 -1.359042323016E+00  
36 9 F 3.871315149505E+00 1.938519612745E+00 -1.352989848611E+00  
37 9 F -1.962511132480E+00 -7.250723656567E-03 1.394645364338E+00  
38 9 F 1.924000969478E+00 -7.482853700916E-03 1.402216013666E+00  
39 9 F 1.924000969478E+00 -7.482853700916E-03 -1.402216013666E+00  
40 9 F -1.962511132480E+00 -7.250723656567E-03 -1.394645364338E+00  
41 220 CA -1.562129433459E-02 -7.381564506718E-03 2.426260859039E-51  
42 220 CA 3.870058308705E+00 -8.146741120792E-03 2.426260859039E-51  
43 109 F -1.625851470318E+00 -2.177516349320E-01 1.001071085020E+01  
44 1 H -7.539976889285E-01 2.446324902364E-01 1.001444221871E+01  
45 109 F -1.625851470318E+00 -2.177516349320E-01 -1.001071085020E+01  
46 1 H -7.539976889285E-01 2.446324902364E-01 -1.001444221871E+01

(100) surface, 25% coverage

1 9 F 9.720288238013E-02 -2.383583154628E+00 9.327491376968E+00  
2 9 F 3.504141920893E-02 1.672244161700E+00 9.438950736618E+00  
3 9 F 3.896253903706E+00 -2.114462996874E+00 9.343769694216E+00  
4 9 F 3.829616839306E+00 2.030549917822E+00 9.349073986105E+00  
5 9 F 9.720288238012E-02 -2.383583154628E+00 -9.327491376968E+00  
6 9 F 3.504141920893E-02 1.672244161700E+00 -9.438950736618E+00  
7 9 F 3.896253903706E+00 -2.114462996874E+00 -9.343769694216E+00  
8 9 F 3.829616839306E+00 2.030549917822E+00 -9.349073986105E+00  
9 220 CA -1.896498221140E+00 -1.948319221178E+00 8.382853148876E+00  
10 220 CA -2.037003167800E+00 1.903418119356E+00 8.274841906832E+00  
11 220 CA 1.993484649506E+00 -2.006914097733E+00 8.262778130171E+00  
12 220 CA 1.941094894884E+00 1.949333378963E+00 8.263655815976E+00  
13 220 CA 1.993484649506E+00 -2.006914097733E+00 -8.262778130171E+00  
14 220 CA 1.941094894884E+00 1.949333378963E+00 -8.263655815976E+00  
15 220 CA -1.896498221140E+00 -1.948319221178E+00 -8.382853148876E+00  
16 220 CA -2.037003167800E+00 1.903418119356E+00 -8.274841906832E+00  
17 9 F 8.294216473661E-03 -1.925233169128E+00 6.717586097557E+00  
18 9 F -3.130201780992E-02 1.947465832777E+00 6.767406381606E+00  
19 9 F 3.854022349075E+00 -1.956969697854E+00 6.688507541947E+00  
20 9 F 3.895181491674E+00 1.921432618862E+00 6.703537020557E+00

21 9 F 8.294216473660E-03 -1.925233169128E+00 -6.717586097557E+00  
22 9 F -3.130201780992E-02 1.947465832777E+00 -6.767406381606E+00  
23 9 F 3.854022349075E+00 -1.956969697854E+00 -6.688507541947E+00  
24 9 F 3.895181491674E+00 1.921432618862E+00 -6.703537020557E+00  
25 9 F -1.971563347074E+00 -2.883608260150E-02 7.070038885366E+00  
26 9 F -1.959613593804E+00 3.884338241917E+00 7.164878152380E+00  
27 9 F 1.947168098796E+00 -7.204215420688E-03 7.176008032206E+00  
28 9 F 1.943401219719E+00 3.856206036394E+00 7.074193188402E+00  
29 9 F 1.947168098796E+00 -7.204215420688E-03 -7.176008032206E+00  
30 9 F 1.943401219719E+00 3.856206036394E+00 -7.074193188402E+00  
31 9 F -1.971563347074E+00 -2.883608260150E-02 -7.070038885366E+00  
32 9 F -1.959613593804E+00 3.884338241917E+00 -7.164878152380E+00  
33 220 CA -2.130885365670E-02 1.142600697591E-03 5.521221916218E+00  
34 220 CA -1.410576297572E-02 3.899502243540E+00 5.533636514206E+00  
35 220 CA 3.893922472144E+00 -2.644880219981E-02 5.498772591742E+00  
36 220 CA 3.890286709442E+00 3.887207607833E+00 5.508176471257E+00  
37 220 CA -2.130885365670E-02 1.142600697592E-03 -5.521221916218E+00  
38 220 CA -1.410576297572E-02 3.899502243540E+00 -5.533636514206E+00  
39 220 CA 3.893922472144E+00 -2.644880219981E-02 -5.498772591742E+00  
40 220 CA 3.890286709442E+00 3.887207607833E+00 -5.508176471257E+00  
41 9 F -1.951172263584E+00 -1.600915239263E-03 4.199492874880E+00  
42 9 F -1.950257793892E+00 3.887525966755E+00 4.230241625539E+00  
43 9 F 1.932978632811E+00 -4.665145652781E-03 4.236898416242E+00  
44 9 F 1.933996865217E+00 3.891454587371E+00 4.218306259008E+00  
45 9 F 1.932978632811E+00 -4.665145652780E-03 -4.236898416242E+00  
46 9 F 1.933996865217E+00 3.891454587371E+00 -4.218306259008E+00  
47 9 F -1.951172263584E+00 -1.600915239263E-03 -4.199492874880E+00  
48 9 F -1.950257793892E+00 3.887525966755E+00 -4.230241625539E+00  
49 9 F -1.261861413530E-02 -1.949154767818E+00 4.053111446290E+00  
50 9 F -8.520249925752E-03 1.946801903394E+00 4.075281260291E+00  
51 9 F 3.888355201356E+00 -1.953495338396E+00 4.034518341083E+00  
52 9 F 3.883796400229E+00 1.942273206216E+00 4.047077208780E+00  
53 9 F -1.261861413530E-02 -1.949154767818E+00 -4.053111446290E+00  
54 9 F -8.520249925752E-03 1.946801903394E+00 -4.075281260291E+00  
55 9 F 3.888355201356E+00 -1.953495338396E+00 -4.034518341083E+00  
56 9 F 3.883796400229E+00 1.942273206216E+00 -4.047077208780E+00  
57 220 CA -1.950738095630E+00 -1.948646168052E+00 2.746169540042E+00  
58 220 CA -1.953230322859E+00 1.943347680844E+00 2.754075897317E+00  
59 220 CA 1.933805376664E+00 -1.951182090256E+00 2.754950490464E+00  
60 220 CA 1.935279557496E+00 1.945476370290E+00 2.761684115434E+00  
61 220 CA 1.933805376664E+00 -1.951182090256E+00 -2.754950490464E+00  
62 220 CA 1.935279557496E+00 1.945476370290E+00 -2.761684115434E+00  
63 220 CA -1.950738095630E+00 -1.948646168052E+00 -2.746169540042E+00  
64 220 CA -1.953230322859E+00 1.943347680844E+00 -2.754075897317E+00  
65 9 F -7.019353467222E-03 -1.949229378076E+00 1.351611221138E+00  
66 9 F -7.694902067544E-03 1.943320387770E+00 1.359763469368E+00  
67 9 F 3.881983426335E+00 -1.949114185528E+00 1.349694215504E+00  
68 9 F 3.882494711047E+00 1.943617948038E+00 1.35419777746E+00  
69 9 F -7.019353467222E-03 -1.949229378076E+00 -1.351611221138E+00  
70 9 F -7.694902067544E-03 1.943320387770E+00 -1.359763469368E+00  
71 9 F 3.881983426335E+00 -1.949114185528E+00 -1.349694215504E+00  
72 9 F 3.882494711047E+00 1.943617948038E+00 -1.35419777746E+00

73 9 F -1.952718994530E+00 -1.642722427215E-03 1.395394895883E+00  
 74 9 F -1.952919045132E+00 3.887964644217E+00 1.401309288984E+00  
 75 9 F 1.936155080448E+00 -1.363929477809E-03 1.406477200011E+00  
 76 9 F 1.935804957625E+00 3.887615087942E+00 1.401126514871E+00  
 77 9 F 1.936155080448E+00 -1.363929477809E-03 -1.406477200011E+00  
 78 9 F 1.935804957625E+00 3.887615087942E+00 -1.401126514871E+00  
 79 9 F -1.952718994530E+00 -1.642722427214E-03 -1.395394895883E+00  
 80 9 F -1.952919045132E+00 3.887964644217E+00 -1.401309288984E+00  
 81 220 CA -6.209940214104E-03 -1.287068520730E-03 3.074169222090E-50  
 82 220 CA -6.908136979407E-03 3.887616132947E+00 3.074169222090E-50  
 83 220 CA 3.882285815084E+00 -2.315739169832E-03 3.074169222090E-50  
 84 220 CA 3.881609583230E+00 3.887989593421E+00 3.074169222090E-50  
 85 109 F -1.658700276791E+00 -8.496073176892E-02 1.000576528210E+01  
 86 1 H -7.923980572569E-01 3.911923664562E-01 1.001547427735E+01  
 87 109 F -1.658700276791E+00 -8.496073176892E-02 -1.000576528210E+01  
 88 1 H -7.923980572569E-01 3.911923664562E-01 -1.001547427735E+01

## 2. SrF2:

### (111) surface, 100% coverage

1 9 F -1.033363115623E+00 1.833650483242E+00 2.475433147356E+00  
 2 9 F -1.033156452401E+00 1.745666403398E+00 -2.475433147356E+00  
 3 238 SR -1.034453951997E+00 -6.142232169736E-01 1.690581471530E+00  
 4 238 SR 1.034453951996E+00 6.142232169746E-01 -1.690581471530E+00  
 5 9 F 1.033362132472E+00 5.998749233479E-01 8.254826511571E-01  
 6 9 F -1.033362132471E+00 -5.998749233490E-01 -8.254826511571E-01  
 7 109 F -1.025107609167E+00 1.284868673780E-01 4.195398325048E+00  
 8 1 H -1.028565668754E+00 1.025287458947E+00 3.784604538686E+00  
 9 109 F 1.025107609167E+00 -1.284868673780E-01 -4.195398325048E+00  
 10 1 H 1.028565668754E+00 -1.025287458947E+00 -3.784604538686E+00

### (111) surface, 50% coverage

1 9 F 1.129497003163E-01 -2.936491029848E-02 2.571343478637E+00  
 2 9 F 4.104861152949E+00 -6.528096961124E-03 2.371947858710E+00  
 3 9 F -1.129497003196E-01 2.936491029745E-02 -2.571343478637E+00  
 4 9 F 4.161217119131E+00 6.528096960095E-03 -2.371947858710E+00  
 5 238 SR -2.113172541412E+00 1.196976272550E+00 1.686556573533E+00  
 6 238 SR 2.094452557192E+00 1.204902091384E+00 1.676590706341E+00  
 7 238 SR 2.113172541410E+00 -1.196976272549E+00 -1.686556573533E+00  
 8 238 SR -2.094452557193E+00 -1.204902091383E+00 -1.676590706341E+00  
 9 9 F 2.046489169736E+00 -1.231620375690E+00 8.262746182015E-01  
 10 9 F -2.038861949057E+00 -1.159175554748E+00 8.117033467591E-01  
 11 9 F -2.046489169735E+00 1.231620375689E+00 -8.262746182015E-01  
 12 9 F 2.038861949058E+00 1.159175554747E+00 -8.117033467591E-01  
 13 109 F -1.461233543818E+00 7.440034009931E-01 4.189846620105E+00  
 14 1 H -6.704500890947E-01 3.367035866896E-01 3.731656014586E+00  
 15 109 F 1.461233543818E+00 -7.440034009931E-01 -4.189846620105E+00



16 1 H 6.704500890947E-01 -3.367035866896E-01 -3.731656014586E+00

(111) surface, 25% coverage

1 9 F 2.778071642621E-01 -1.598148947422E-01 2.712548327994E+00  
2 9 F -2.094256511543E+00 3.619705320773E+00 2.424672280726E+00  
3 9 F 4.083435727702E+00 3.655233855473E-03 2.423283132556E+00  
4 9 F 2.088591978363E+00 3.567067694687E+00 2.428715395665E+00  
5 9 F -2.038782624501E+00 3.538928452507E+00 -2.424672280726E+00  
6 9 F -2.778071642655E-01 1.598148947412E-01 -2.712548327994E+00  
7 9 F 2.044447157677E+00 3.591566078593E+00 -2.428715395665E+00  
8 9 F 4.182642544378E+00 -3.655233856501E-03 -2.423283132556E+00  
9 238 SR -2.165755480867E+00 1.250142304211E+00 1.719860129789E+00  
10 238 SR 1.673850506991E-02 -2.413788112407E+00 1.625534065949E+00  
11 238 SR 2.098634774100E+00 1.193057330106E+00 1.625023530460E+00  
12 238 SR 4.134213419032E+00 -2.387106238378E+00 1.742469101370E+00  
13 238 SR -1.673850507103E-02 2.413788112408E+00 -1.625534065949E+00  
14 238 SR 2.165755480865E+00 -1.250142304210E+00 -1.719860129789E+00  
15 238 SR -4.134213419033E+00 2.387106238379E+00 -1.742469101370E+00  
16 238 SR -2.098634774101E+00 -1.193057330105E+00 -1.625023530460E+00  
17 9 F -1.487032249573E-02 2.309318951582E+00 8.791687027146E-01  
18 9 F 2.067862288630E+00 -1.193826202602E+00 7.682793801851E-01  
19 9 F -4.160355291012E+00 2.402387152236E+00 7.392995184113E-01  
20 9 F -2.007075169287E+00 -1.142063024584E+00 8.789518946167E-01  
21 9 F -2.067862288629E+00 1.193826202601E+00 -7.682793801851E-01  
22 9 F 1.487032249684E-02 -2.309318951583E+00 -8.791687027146E-01  
23 9 F 2.007075169288E+00 1.142063024583E+00 -8.789518946167E-01  
24 9 F 4.160355291013E+00 -2.402387152237E+00 -7.392995184113E-01  
25 109 F -1.362971176414E+00 7.803585329229E-01 4.125521022111E+00  
26 1 H -5.678497265338E-01 3.246983945571E-01 3.674797064383E+00  
27 109 F 1.362971176414E+00 -7.803585329229E-01 -4.125521022111E+00  
28 1 H 5.678497265338E-01 -3.246983945571E-01 -3.674797064383E+00

(110) surface, 100% coverage

1 238 SR 1.033259784010E+00 1.461250000000E+00 5.003948972420E+00  
2 238 SR -1.033259784010E+00 -1.461250000000E+00 -5.003948972420E+00  
3 9 F -1.033259784010E+00 2.838512608797E+00 5.150386023294E+00  
4 9 F 1.033259784010E+00 -8.398739120270E-02 -5.150386023294E+00  
5 9 F 1.033259784010E+00 -2.838512608797E+00 -5.150386023294E+00  
6 9 F -1.033259784010E+00 8.398739120270E-02 5.150386023294E+00  
7 238 SR -1.033259784010E+00 -1.461250000000E+00 3.178706935499E+00  
8 238 SR 1.033259784010E+00 1.461250000000E+00 -3.178706935499E+00  
9 9 F 1.033259784010E+00 -2.063629581335E-03 3.077019974441E+00  
10 9 F -1.033259784010E+00 2.920436370419E+00 -3.077019974441E+00  
11 9 F -1.033259784010E+00 2.063629581335E-03 -3.077019974441E+00  
12 9 F 1.033259784010E+00 -2.920436370419E+00 3.077019974441E+00  
13 238 SR 1.033259784010E+00 1.461250000000E+00 9.936767255593E-01  
14 238 SR -1.033259784010E+00 -1.461250000000E+00 -9.936767255593E-01  
15 9 F -1.033259784010E+00 2.922331378381E+00 1.048494731519E+00

16 9 F 1.033259784010E+00 -1.686216190769E-04 -1.048494731519E+00  
17 9 F 1.033259784010E+00 -2.922331378381E+00 -1.048494731519E+00  
18 9 F -1.033259784010E+00 1.686216190769E-04 1.048494731519E+00  
19 109 F 1.033259780000E+00 1.461250000000E+00 7.771224162931E+00  
20 109 F -1.033259780000E+00 4.383750000000E+00 -7.771224162931E+00  
21 1 H 1.033259780000E+00 1.461250000000E+00 8.711071486663E+00  
22 1 H -1.033259780000E+00 4.383750000000E+00 -8.711071486663E+00

(110) surface, 50% coverage

1 238 SR 2.177365392789E+00 2.654239455628E+00 5.086363348522E+00  
2 238 SR -2.177365392789E+00 2.654239455628E+00 5.086363348522E+00  
3 238 SR -1.111483713991E-15 -1.608961857570E-01 -5.005677640158E+00  
4 238 SR 4.133039136040E+00 -1.618378215110E-01 -5.002846317691E+00  
5 9 F 1.215039912491E-15 -1.281517686665E+00 5.472053297136E+00  
6 9 F 4.133039136040E+00 -1.855608689962E+00 4.881940914046E+00  
7 9 F 2.068619693836E+00 1.208241369102E+00 -5.145038264131E+00  
8 9 F -2.068619693836E+00 1.208241369102E+00 -5.145038264131E+00  
9 9 F 2.065151074672E+00 -1.530857413093E+00 -5.144740510352E+00  
10 9 F -2.065151074672E+00 -1.530857413093E+00 -5.144740510352E+00  
11 9 F 1.106069855864E-15 1.600816933164E+00 4.981295790714E+00  
12 9 F 4.133039136040E+00 1.253273308939E+00 5.147965958460E+00  
13 238 SR 6.932085857215E-16 -1.118723196690E-01 3.121933928346E+00  
14 238 SR 4.133039136040E+00 -2.135463862520E-01 3.139956414392E+00  
15 238 SR 2.067353740739E+00 2.760886165569E+00 -3.176316926324E+00  
16 238 SR -2.067353740739E+00 2.760886165569E+00 -3.176316926324E+00  
17 9 F 2.110458331824E+00 1.247253092730E+00 3.055119086165E+00  
18 9 F -2.110458331824E+00 1.247253092730E+00 3.055119086165E+00  
19 9 F -6.833961708602E-16 -1.622333909348E+00 -3.077742740433E+00  
20 9 F 4.133039136040E+00 -1.624978684572E+00 -3.081668660393E+00  
21 9 F -6.851473910669E-16 1.303615218881E+00 -3.085629535103E+00  
22 9 F 4.133039136040E+00 1.299058711272E+00 -3.075202838158E+00  
23 9 F 1.941145465895E+00 -1.682404049025E+00 3.139216524109E+00  
24 9 F -1.941145465895E+00 -1.682404049025E+00 3.139216524109E+00  
25 238 SR 2.060762610391E+00 2.758918858293E+00 1.012571020597E+00  
26 238 SR -2.060762610391E+00 2.758918858293E+00 1.012571020597E+00  
27 238 SR -2.239131519676E-16 -1.605923590050E-01 -1.008415187765E+00  
28 238 SR 4.133039136040E+00 -1.607969575940E-01 -9.980912959220E-01  
29 9 F 2.261666014034E-16 -1.601820150053E+00 1.018563821804E+00  
30 9 F 4.133039136040E+00 -1.634737346127E+00 1.073028924942E+00  
31 9 F 2.057582423198E+00 1.299584439404E+00 -1.047601176365E+00  
32 9 F -2.057582423198E+00 1.299584439404E+00 -1.047601176365E+00  
33 9 F 2.075905304989E+00 -1.623495547648E+00 -1.043106851587E+00  
34 9 F -2.075905304989E+00 -1.623495547648E+00 -1.043106851587E+00  
35 9 F 2.326627906883E-16 1.310292003867E+00 1.047820057447E+00  
36 9 F 4.133039136040E+00 1.299524446285E+00 1.016671214089E+00  
37 109 F 1.817729731588E+00 -1.506755523672E+00 7.023717373519E+00  
38 109 F -1.817729731588E+00 -1.506755523672E+00 7.023717373519E+00  
39 1 H -1.021479936875E+00 -1.238098235330E+00 6.479616111871E+00  
40 1 H 1.021479936875E+00 -1.238098235330E+00 6.479616111871E+00

(110) surface, 25% coverage

1 238 SR 2.067058827348E+00 2.922046949538E+00 5.030646307023E+00  
2 238 SR -2.066893436378E+00 -2.922195944289E+00 4.991145405603E+00  
3 238 SR 2.066240332680E+00 -2.922177645841E+00 4.992283868987E+00  
4 238 SR -2.066184965441E+00 2.922265325980E+00 4.990316752474E+00  
5 9 F 2.182504189176E-04 -1.554141429379E+00 5.149892247199E+00  
6 9 F -1.273923181296E-02 1.547563086732E+00 5.141207071980E+00  
7 9 F -1.269561032197E-02 4.297138660940E+00 5.143201053923E+00  
8 9 F 7.462257774853E-05 -4.290413296559E+00 5.151571935282E+00  
9 9 F 4.132414631394E+00 -1.554156045354E+00 5.150508935548E+00  
10 9 F 4.146410770151E+00 1.547231846687E+00 5.142129737972E+00  
11 9 F 4.146143853780E+00 4.297124392119E+00 5.142043949268E+00  
12 9 F 4.132441988487E+00 -4.290559102674E+00 5.150819087832E+00  
13 238 SR 1.273731460994E-03 3.565587962888E-03 3.177616679820E+00  
14 238 SR 9.397547017157E-04 5.841525953691E+00 3.180741751249E+00  
15 238 SR 4.131960857679E+00 3.227134190278E-03 3.178760802683E+00  
16 238 SR 4.131348268383E+00 5.841713842801E+00 3.179168132762E+00  
17 9 F 2.066937019492E+00 1.460857360267E+00 3.087380199294E+00  
18 9 F -2.066398646471E+00 -1.459023594148E+00 3.075595953917E+00  
19 9 F 2.066508276475E+00 -1.459664215100E+00 3.075133933236E+00  
20 9 F -2.066532038862E+00 1.458533228006E+00 3.067706324129E+00  
21 9 F 2.066163924890E+00 -4.385300688146E+00 3.075911449210E+00  
22 9 F -2.066413178252E+00 4.386669024687E+00 3.068416646981E+00  
23 9 F 2.066292574938E+00 4.383893350144E+00 3.087899155481E+00  
24 9 F -2.066588008008E+00 -4.385718415014E+00 3.076064524441E+00  
25 238 SR 2.066752583391E+00 2.921887660857E+00 9.997046391569E-01  
26 238 SR -2.065748296747E+00 -2.921940102885E+00 9.896034520559E-01  
27 238 SR 2.065866628380E+00 -2.921983056538E+00 9.907123139525E-01  
28 238 SR -2.066175582663E+00 2.922119843176E+00 9.916645692466E-01  
29 9 F -1.719693509669E-05 -1.461397084077E+00 1.046563128595E+00  
30 9 F 2.095211051669E-03 1.461315726140E+00 1.047143805439E+00  
31 9 F 2.148231114365E-03 4.383486061484E+00 1.049793299267E+00  
32 9 F 3.000099856660E-04 -4.383227974623E+00 1.049374602513E+00  
33 9 F 4.132944352822E+00 -1.462159638218E+00 1.048374368317E+00  
34 9 F 4.131275502046E+00 1.461510753040E+00 1.048835200068E+00  
35 9 F 4.131350510311E+00 4.383451669120E+00 1.049333163037E+00  
36 9 F 4.132738184473E+00 -4.382956115235E+00 1.048704916820E+00  
37 238 SR -1.576507703459E-04 8.344038842445E-04 -1.000164218493E+00  
38 238 SR 8.244597795109E-04 5.844284435163E+00 -9.899681539110E-01  
39 238 SR 4.132696506565E+00 4.005756126860E-04 -9.913206188134E-01  
40 238 SR 4.132791284819E+00 5.844538054123E+00 -9.907993046935E-01  
41 9 F 2.064451272695E+00 1.461227244728E+00 -1.047478770885E+00  
42 9 F -2.064540632690E+00 -1.460773145190E+00 -1.049891863423E+00  
43 9 F 2.064181150054E+00 -1.460993510575E+00 -1.049397517352E+00  
44 9 F -2.064674757845E+00 1.461097550263E+00 -1.048728623125E+00  
45 9 F 2.066595309320E+00 -4.384337902649E+00 -1.049129148737E+00  
46 9 F -2.066282092807E+00 4.384702434405E+00 -1.048392938498E+00  
47 9 F 2.066846057094E+00 4.384021802442E+00 -1.046670851214E+00  
48 9 F -2.066198252324E+00 -4.384544420823E+00 -1.048966255763E+00  
49 238 SR 2.065444768231E+00 2.919048036085E+00 -3.177960854475E+00

50 238 SR -2.065217771716E+00 -2.919202980198E+00 -3.180357419772E+00  
51 238 SR 2.065045610013E+00 -2.918928902222E+00 -3.179220718936E+00  
52 238 SR -2.065449213152E+00 2.919120193036E+00 -3.178234138687E+00  
53 9 F 3.349359360306E-04 4.382078227750E+00 -3.074623580755E+00  
54 9 F -7.496743102819E-05 -4.382120678695E+00 -3.075225704591E+00  
55 9 F 3.062047432018E-05 -1.461322290184E+00 -3.088341924495E+00  
56 9 F -1.813921984487E-04 1.461655704505E+00 -3.087814516052E+00  
57 9 F 4.132787316000E+00 4.381649111773E+00 -3.076074834181E+00  
58 9 F 4.133243696973E+00 -4.381724034706E+00 -3.076667915732E+00  
59 9 F 4.132881364605E+00 -1.464274925835E+00 -3.067893351265E+00  
60 9 F 4.133133386192E+00 1.464024637287E+00 -3.067369992311E+00  
61 238 SR -9.070462835605E-05 5.315944869594E-04 -5.031230856600E+00  
62 238 SR 3.797427591453E-04 5.844712808759E+00 -4.991655144966E+00  
63 238 SR 4.132864023834E+00 1.252568599269E-04 -4.989927913539E+00  
64 238 SR 4.133323591372E+00 5.844794771371E+00 -4.991674405729E+00  
65 9 F 2.079701522768E+00 1.374824302334E+00 -5.141409786609E+00  
66 9 F -2.079572269198E+00 -1.374538210657E+00 -5.142516929850E+00  
67 9 F 2.079492898503E+00 -1.374818251295E+00 -5.142410894884E+00  
68 9 F -2.079804435929E+00 1.375252359319E+00 -5.141728304599E+00  
69 9 F 2.066140023278E+00 -4.477016696350E+00 -5.151107240106E+00  
70 9 F -2.065916416997E+00 4.476599347570E+00 -5.150275054864E+00  
71 9 F 2.066117403904E+00 4.476472158576E+00 -5.150585998403E+00  
72 9 F -2.065802300325E+00 -4.476895889886E+00 -5.151769662383E+00  
73 109 F 2.067092461087E+00 2.921433349186E+00 7.756948904022E+00  
74 1 H 2.064000738537E+00 2.921184903219E+00 8.699163691211E+00  
75 109 F 9.587256274143E-05 9.551118089181E-04 -7.757342295439E+00  
76 1 H -3.120074942259E-04 9.767407073637E-04 -8.699563877226E+00

(100) surface, 100% coverage

1 9 F 2.516058014189E-02 2.306683037906E+00 1.012206601313E+01  
2 9 F 2.516058014189E-02 2.306683037906E+00 -1.012206601313E+01  
3 238 SR -1.931906488065E+00 1.771045387769E+00 8.768662296077E+00  
4 238 SR -1.931906488065E+00 1.771045387769E+00 -8.768662296077E+00  
5 9 F 1.506605874085E-01 1.712713138510E+00 7.300433195570E+00  
6 9 F 1.506605874085E-01 1.712713138510E+00 -7.300433195570E+00  
7 9 F -1.872854436523E+00 -3.155295666744E-01 7.304295197971E+00  
8 9 F -1.872854436523E+00 -3.155295666744E-01 -7.304295197971E+00  
9 238 SR 1.839196975150E-01 -3.479311804202E-01 5.845419370440E+00  
10 238 SR 1.839196975150E-01 -3.479311804202E-01 -5.845419370440E+00  
11 9 F -1.878771454857E+00 -3.333572433911E-01 4.383044839791E+00  
12 9 F -1.878771454857E+00 -3.333572433911E-01 -4.383044839791E+00  
13 9 F 1.683121910861E-01 1.718829945061E+00 4.384120846256E+00  
14 9 F 1.683121910861E-01 1.718829945061E+00 -4.384120846256E+00  
15 238 SR -1.896746616440E+00 1.736059847794E+00 2.922382182897E+00  
16 238 SR -1.896746616440E+00 1.736059847794E+00 -2.922382182897E+00  
17 9 F 1.680267768859E-01 1.718573857244E+00 1.460018816672E+00  
18 9 F 1.680267768859E-01 1.718573857244E+00 -1.460018816672E+00  
19 9 F -1.878749000336E+00 -3.328981645705E-01 1.462063600945E+00  
20 9 F -1.878749000336E+00 -3.328981645705E-01 -1.462063600945E+00  
21 238 SR 1.854471762091E-01 -3.501984353670E-01 0.000000000000E+00

22 109 F 1.666605389058E+00 -2.203970005955E-01 1.012802649219E+01  
23 109 F 1.666605389058E+00 -2.203970005955E-01 -1.012802649219E+01  
24 1 H 7.466037789832E-01 -9.054899677088E-01 1.026454855101E+01  
25 1 H 7.466037789832E-01 -9.054899677088E-01 -1.026454855101E+01

(100) surface, 50% coverage

1 9 F -1.049817264200E+00 -1.650797494109E-01 9.954726412549E+00  
2 9 F -1.049817264200E+00 -1.650797494109E-01 -9.954726412549E+00  
3 9 F -4.028400953353E+00 9.815020157379E-01 9.688672822697E+00  
4 9 F -4.028400953353E+00 9.815020157379E-01 -9.688672822697E+00  
5 238 SR 2.298322826420E+00 1.920913651168E+00 8.748811658960E+00  
6 238 SR 2.298322826420E+00 1.920913651168E+00 -8.748811658960E+00  
7 238 SR -2.087864456132E+00 1.919211667560E+00 8.747191598466E+00  
8 238 SR -2.087864456132E+00 1.919211667560E+00 -8.747191598466E+00  
9 9 F 1.047219499822E-01 1.942732685330E+00 7.470184510838E+00  
10 9 F 1.047219499822E-01 1.942732685330E+00 -7.470184510838E+00  
11 9 F -4.030245774073E+00 2.045338832487E+00 7.174752685422E+00  
12 9 F -4.030245774073E+00 2.045338832487E+00 -7.174752685422E+00  
13 9 F 2.212024731651E+00 -1.019527193930E-01 7.282078661573E+00  
14 9 F 2.212024731651E+00 -1.019527193930E-01 -7.282078661573E+00  
15 9 F -2.004619109879E+00 -1.047185672337E-01 7.280206945884E+00  
16 9 F -2.004619109879E+00 -1.047185672337E-01 -7.280206945884E+00  
17 238 SR 1.058707848037E-01 -1.030946889478E-01 5.908836322761E+00  
18 238 SR 1.058707848037E-01 -1.030946889478E-01 -5.908836322761E+00  
19 238 SR -4.029104605303E+00 -5.198865585881E-02 5.785953038879E+00  
20 238 SR -4.029104605303E+00 -5.198865585881E-02 -5.785953038879E+00  
21 9 F 2.146283297114E+00 -7.330787656247E-02 4.376620782011E+00  
22 9 F 2.146283297114E+00 -7.330787656247E-02 -4.376620782011E+00  
23 9 F -1.937316277511E+00 -7.244741752878E-02 4.378178725321E+00  
24 9 F -1.937316277511E+00 -7.244741752878E-02 -4.378178725321E+00  
25 9 F 1.048530203180E-01 1.978883558445E+00 4.460786837547E+00  
26 9 F 1.048530203180E-01 1.978883558445E+00 -4.460786837547E+00  
27 9 F -4.029081720905E+00 2.005893136852E+00 4.324503798851E+00  
28 9 F -4.029081720905E+00 2.005893136852E+00 -4.324503798851E+00  
29 238 SR 2.159746693292E+00 1.991919142174E+00 2.921137744225E+00  
30 238 SR 2.159746693292E+00 1.991919142174E+00 -2.921137744225E+00  
31 238 SR -1.950654511401E+00 1.994857066769E+00 2.924305489949E+00  
32 238 SR -1.950654511401E+00 1.994857066769E+00 -2.924305489949E+00  
33 9 F 1.039451336032E-01 1.994095115570E+00 1.468801923260E+00  
34 9 F 1.039451336032E-01 1.994095115570E+00 -1.468801923260E+00  
35 9 F -4.027856124758E+00 1.991790173531E+00 1.456437144811E+00  
36 9 F -4.027856124758E+00 1.991790173531E+00 -1.456437144811E+00  
37 9 F 2.165380634054E+00 -7.390115486362E-02 1.458969709155E+00  
38 9 F 2.165380634054E+00 -7.390115486362E-02 -1.458969709155E+00  
39 9 F -1.956264776473E+00 -7.273703740438E-02 1.460500377484E+00  
40 9 F -1.956264776473E+00 -7.273703740438E-02 -1.460500377484E+00  
41 238 SR 1.033011839527E-01 -7.296763312620E-02 0.000000000000E+00  
42 238 SR -4.026998497965E+00 -7.444446822283E-02 0.000000000000E+00  
43 109 F 1.265700838683E+00 -1.666662891397E-01 9.961590964593E+00  
44 109 F 1.265700838683E+00 -1.666662891397E-01 -9.961590964593E+00

45 1 H 1.077182408945E-01 -1.682281267100E-01 9.999669490545E+00  
46 1 H 1.077182408945E-01 -1.682281267100E-01 -9.999669490545E+00

(100) surface, 25% coverage

1 9 F 5.454421236334E-02 3.199980112350E+00 9.584682513208E+00  
2 9 F 5.454421236334E-02 3.199980112350E+00 -9.584682513208E+00  
3 9 F -1.102467844066E+00 -1.621000242378E-01 9.992793810452E+00  
4 9 F -1.102467844066E+00 -1.621000242378E-01 -9.992793810452E+00  
5 9 F -4.078436770695E+00 2.494074482815E+00 9.818089005248E+00  
6 9 F -4.078436770695E+00 2.494074482815E+00 -9.818089005248E+00  
7 9 F -4.077567644694E+00 -1.947942440879E+00 9.930553379335E+00  
8 9 F -4.077567644694E+00 -1.947942440879E+00 -9.930553379335E+00  
9 238 SR 2.090242608742E+00 2.004675481096E+00 8.797019228036E+00  
10 238 SR 2.090242608742E+00 2.004675481096E+00 -8.797019228036E+00  
11 238 SR 2.233075305019E+00 -2.109537667247E+00 8.705657480934E+00  
12 238 SR 2.233075305019E+00 -2.109537667247E+00 -8.705657480934E+00  
13 238 SR -1.981320513047E+00 2.004311394989E+00 8.796561071937E+00  
14 238 SR -1.981320513047E+00 2.004311394989E+00 -8.796561071937E+00  
15 238 SR -2.122795292718E+00 -2.110254253855E+00 8.705219587890E+00  
16 238 SR -2.122795292718E+00 -2.110254253855E+00 -8.705219587890E+00  
17 9 F 5.478011619649E-02 1.880586865429E+00 7.198833034307E+00  
18 9 F 5.478011619649E-02 1.880586865429E+00 -7.198833034307E+00  
19 9 F 5.541536116979E-02 -2.158750640779E+00 7.444872944844E+00  
20 9 F 5.541536116979E-02 -2.158750640779E+00 -7.444872944844E+00  
21 9 F -4.077254151695E+00 1.931263346542E+00 7.153787756231E+00  
22 9 F -4.077254151695E+00 1.931263346542E+00 -7.153787756231E+00  
23 9 F -4.078544698389E+00 -2.170841733157E+00 7.171663587693E+00  
24 9 F -4.078544698389E+00 -2.170841733157E+00 -7.171663587693E+00  
25 9 F 2.177121264904E+00 -1.061305880343E-01 7.324210737708E+00  
26 9 F 2.177121264904E+00 -1.061305880343E-01 -7.324210737708E+00  
27 9 F 2.163231948348E+00 4.065613465143E+00 7.410105488650E+00  
28 9 F 2.163231948348E+00 4.065613465143E+00 -7.410105488650E+00  
29 9 F -2.067215579517E+00 -1.071669037948E-01 7.323159642355E+00  
30 9 F -2.067215579517E+00 -1.071669037948E-01 -7.323159642355E+00  
31 9 F -2.053062055797E+00 4.065631804315E+00 7.409378450412E+00  
32 9 F -2.053062055797E+00 4.065631804315E+00 -7.409378450412E+00  
33 238 SR 5.510284722403E-02 -1.284519400265E-01 5.852163596466E+00  
34 238 SR 5.510284722403E-02 -1.284519400265E-01 -5.852163596466E+00  
35 238 SR 5.490347222950E-02 3.998350824762E+00 5.924407825727E+00  
36 238 SR 5.490347222949E-02 3.998350824762E+00 -5.924407825727E+00  
37 238 SR -4.077966673107E+00 -8.944894492205E-02 5.783434997412E+00  
38 238 SR -4.077966673107E+00 -8.944894492205E-02 -5.783434997412E+00  
39 238 SR -4.078395192484E+00 3.990236607028E+00 5.828458491541E+00  
40 238 SR -4.078395192484E+00 3.990236607028E+00 -5.828458491541E+00  
41 9 F 2.102520804187E+00 -1.280767468963E-01 4.380869846944E+00  
42 9 F 2.102520804187E+00 -1.280767468963E-01 -4.380869846944E+00  
43 9 F 2.103069180328E+00 4.002301032877E+00 4.432986538652E+00  
44 9 F 2.103069180328E+00 4.002301032877E+00 -4.432986538652E+00  
45 9 F -1.992811758997E+00 -1.278695264454E-01 4.380917785945E+00  
46 9 F -1.992811758997E+00 -1.278695264454E-01 -4.380917785945E+00

47 9 F -1.993725712236E+00 4.002257523461E+00 4.433112089103E+00  
 48 9 F -1.993725712236E+00 4.002257523461E+00 -4.433112089103E+00  
 49 9 F 5.488209154700E-02 1.948853351718E+00 4.369398973991E+00  
 50 9 F 5.488209154700E-02 1.948853351718E+00 -4.369398973991E+00  
 51 9 F 5.460726994478E-02 -2.212672682829E+00 4.438063565080E+00  
 52 9 F 5.460726994477E-02 -2.212672682829E+00 -4.438063565080E+00  
 53 9 F -4.078445598101E+00 1.953362038822E+00 4.307184954773E+00  
 54 9 F -4.078445598101E+00 1.953362038822E+00 -4.307184954773E+00  
 55 9 F -4.078376772027E+00 -2.199598416541E+00 4.335836056900E+00  
 56 9 F -4.078376772027E+00 -2.199598416541E+00 -4.335836056900E+00  
 57 238 SR 2.109648834844E+00 1.943709326492E+00 2.914460457739E+00  
 58 238 SR 2.109648834844E+00 1.943709326492E+00 -2.914460457739E+00  
 59 238 SR 2.115700821867E+00 -2.200798476314E+00 2.930315634187E+00  
 60 238 SR 2.115700821867E+00 -2.200798476314E+00 -2.930315634187E+00  
 61 238 SR -2.000253542070E+00 1.943802818372E+00 2.914942364169E+00  
 62 238 SR -2.000253542070E+00 1.943802818372E+00 -2.914942364169E+00  
 63 238 SR -2.006917620886E+00 -2.201022463412E+00 2.930701911579E+00  
 64 238 SR -2.006917620886E+00 -2.201022463412E+00 -2.930701911579E+00  
 65 9 F 5.450588321454E-02 1.940379704141E+00 1.447780312718E+00  
 66 9 F 5.450588321454E-02 1.940379704141E+00 -1.447780312718E+00  
 67 9 F 5.437792777224E-02 -2.197079858210E+00 1.471063002189E+00  
 68 9 F 5.437792777224E-02 -2.197079858210E+00 -1.471063002189E+00  
 69 9 F -4.078367988631E+00 1.939597246966E+00 1.446280113696E+00  
 70 9 F -4.078367988631E+00 1.939597246966E+00 -1.446280113696E+00  
 71 9 F -4.078469211674E+00 -2.198441165781E+00 1.458371602180E+00  
 72 9 F -4.078469211674E+00 -2.198441165781E+00 -1.458371602180E+00  
 73 9 F 2.117051872637E+00 -1.326981752270E-01 1.464677166365E+00  
 74 9 F 2.117051872637E+00 -1.326981752270E-01 -1.464677166365E+00  
 75 9 F 2.117352655360E+00 4.008308383281E+00 1.468380622260E+00  
 76 9 F 2.117352655360E+00 4.008308383281E+00 -1.468380622260E+00  
 77 9 F -2.008182917661E+00 -1.327074116370E-01 1.464859340116E+00  
 78 9 F -2.008182917661E+00 -1.327074116370E-01 -1.464859340116E+00  
 79 9 F -2.008004834648E+00 4.008304283817E+00 1.468546289397E+00  
 80 9 F -2.008004834648E+00 4.008304283817E+00 -1.468546289397E+00  
 81 238 SR 5.398943507733E-02 -1.319788397406E-01 0.000000000000E+00  
 82 238 SR 5.466949694039E-02 4.008568733090E+00 0.000000000000E+00  
 83 238 SR -4.078484119899E+00 -1.311129026505E-01 0.000000000000E+00  
 84 238 SR -4.078166104932E+00 4.005613688050E+00 0.000000000000E+00  
 85 109 F 1.214185302695E+00 -1.613912087229E-01 9.995533440803E+00  
 86 109 F 1.214185302695E+00 -1.613912087229E-01 -9.995533440803E+00  
 87 1 H 5.603691055607E-02 -1.466989087891E-01 1.004756870274E+01  
 88 1 H 5.603691055606E-02 -1.466989087891E-01 -1.004756870274E+01

### 3. BaF2:

*(111) surface, 100% coverage*

1 9 F -1.100851029793E+00 1.968033605379E+00 2.590045034633E+00  
 2 9 F -1.105322127507E+00 1.853170393361E+00 -2.590045034633E+00  
 3 256 BA -1.101707728632E+00 -6.573687137988E-01 1.797979677704E+00

4 256 BA 1.101707728632E+00 6.573687137979E-01 -1.797979677704E+00  
5 9 F 1.104312026284E+00 6.391801192552E-01 8.683569029906E-01  
6 9 F -1.104312026284E+00 -6.391801192543E-01 -8.683569029906E-01  
7 109 F -1.179407931282E+00 3.542903644477E-01 4.391299057898E+00  
8 1 H -1.142826164168E+00 1.200269061399E+00 3.878280462758E+00  
9 109 F 1.179407931282E+00 -3.542903644477E-01 -4.391299057898E+00  
10 1 H 1.142826164168E+00 -1.200269061399E+00 -3.878280462758E+00

(111) surface, 50% coverage

1 9 F 1.037524630547E-01 -2.980057425011E-02 2.688755388173E+00  
2 9 F 4.392807107747E+00 -2.110687711068E-03 2.463944996884E+00  
3 9 F -1.037524630547E-01 2.980057425103E-02 -2.688755388173E+00  
4 9 F 4.431885521452E+00 2.110687711991E-03 -2.463944996884E+00  
5 256 BA -2.259172144309E+00 1.272793968190E+00 1.776384365513E+00  
6 256 BA 2.237910500168E+00 1.291529221215E+00 1.799487086564E+00  
7 256 BA 2.259172144309E+00 -1.272793968191E+00 -1.776384365513E+00  
8 256 BA -2.237910500168E+00 -1.291529221216E+00 -1.799487086564E+00  
9 9 F 2.183364325081E+00 -1.304324558510E+00 8.774086510950E-01  
10 9 F -2.175503095547E+00 -1.246178488840E+00 8.438395247291E-01  
11 9 F -2.183364325081E+00 1.304324558511E+00 -8.774086510950E-01  
12 9 F 2.175503095547E+00 1.246178488841E+00 -8.438395247291E-01  
13 109 F -1.426912120492E+00 6.384369779164E-01 4.390402140772E+00  
14 1 H -6.623744869218E-01 2.871589539620E-01 3.836965450203E+00  
15 109 F 1.426912120492E+00 -6.384369779164E-01 -4.390402140772E+00  
16 1 H 6.623744869218E-01 -2.871589539620E-01 -3.836965450203E+00

(111) surface, 25% coverage

1 9 F 1.804284958352E-01 -1.039898408531E-01 2.784216664113E+00  
2 9 F -2.228089204028E+00 3.849822958116E+00 2.528946116030E+00  
3 9 F 4.376374427994E+00 4.868998145475E-03 2.529241462721E+00  
4 9 F 2.225599862600E+00 3.810197960955E+00 2.531942739322E+00  
5 9 F -1.804284958353E-01 1.039898408540E-01 -2.784216664113E+00  
6 9 F -2.184257110572E+00 3.792585039364E+00 -2.528946116030E+00  
7 9 F 4.448318201206E+00 -4.868998144552E-03 -2.529241462721E+00  
8 9 F 2.186746452000E+00 3.832210036525E+00 -2.531942739322E+00  
9 256 BA -2.279228099268E+00 1.315772012192E+00 1.815227162144E+00  
10 256 BA 8.970002063244E-03 -2.585176720610E+00 1.740062068210E+00  
11 256 BA 2.243103979112E+00 1.284718576503E+00 1.739842304601E+00  
12 256 BA 4.412267353292E+00 -2.547303666085E+00 1.842880075058E+00  
13 256 BA -8.970002063269E-03 2.585176720609E+00 -1.740062068210E+00  
14 256 BA 2.279228099268E+00 -1.315772012193E+00 -1.815227162144E+00  
15 256 BA -4.412267353292E+00 2.547303666084E+00 -1.842880075058E+00  
16 256 BA -2.243103979112E+00 -1.284718576504E+00 -1.739842304601E+00  
17 9 F -9.575285525426E-03 2.496497930106E+00 8.984832976719E-01  
18 9 F 2.194465635055E+00 -1.266850044744E+00 8.332679671283E-01  
19 9 F -4.421171338974E+00 2.552570720565E+00 7.969940471443E-01  
20 9 F -2.166584565134E+00 -1.239951569455E+00 8.983754139478E-01  
21 9 F -2.194465635055E+00 1.266850044745E+00 -8.332679671283E-01



22 9 F 9.575285525452E-03 -2.496497930105E+00 -8.984832976719E-01  
23 9 F 2.166584565134E+00 1.239951569456E+00 -8.983754139478E-01  
24 9 F 4.421171338974E+00 -2.552570720564E+00 -7.969940471443E-01  
25 109 F -1.321076237587E+00 7.581047343251E-01 4.399430760729E+00  
26 1 H -5.846862068058E-01 3.350133730440E-01 3.831858528597E+00  
27 109 F 1.321076237587E+00 -7.581047343251E-01 -4.399430760729E+00  
28 1 H 5.846862068058E-01 -3.350133730440E-01 -3.831858528597E+00

(110) surface, 100% coverage

1 256 BA 1.123043445416E+00 1.560000000000E+00 5.340088156081E+00  
2 256 BA -1.123043445416E+00 -1.560000000000E+00 -5.340088156081E+00  
3 9 F -1.106414689585E+00 2.971246809785E+00 5.449193386137E+00  
4 9 F 1.106414689585E+00 -1.487531902150E-01 -5.449193386137E+00  
5 9 F 1.106414689585E+00 -2.971246809785E+00 -5.449193386137E+00  
6 9 F -1.106414689585E+00 1.487531902150E-01 5.449193386137E+00  
7 256 BA -1.099645546041E+00 -1.560000000000E+00 3.379306677028E+00  
8 256 BA 1.099645546041E+00 1.560000000000E+00 -3.379306677028E+00  
9 9 F 1.103937955245E+00 -6.799517556000E-03 3.274679071527E+00  
10 9 F -1.103937955245E+00 3.113200482444E+00 -3.274679071527E+00  
11 9 F -1.103937955245E+00 6.799517556000E-03 -3.274679071527E+00  
12 9 F 1.103937955245E+00 -3.113200482444E+00 3.274679071527E+00  
13 256 BA 1.103682149579E+00 1.560000000000E+00 1.063269877411E+00  
14 256 BA -1.103682149579E+00 -1.560000000000E+00 -1.063269877411E+00  
15 9 F -1.102598918396E+00 -3.119157938471E+00 1.120057930961E+00  
16 9 F 1.102598918396E+00 8.420615290001E-04 -1.120057930961E+00  
17 9 F 1.102598918396E+00 3.119157938471E+00 -1.120057930961E+00  
18 9 F -1.102598918396E+00 -8.420615290001E-04 1.120057930961E+00  
19 109 F -1.412631113830E-01 1.560000000000E+00 7.888107155958E+00  
20 109 F 1.412631113830E-01 -1.560000000000E+00 -7.888107155958E+00  
21 1 H -8.565441538480E-01 1.560000000000E+00 7.255776793933E+00  
22 1 H 8.565441538480E-01 -1.560000000000E+00 -7.255776793933E+00

(110) surface, 50% coverage

1 256 BA 2.198796035955E+00 3.198697006867E+00 5.444653609366E+00  
2 256 BA -2.350914035533E+00 3.175154488080E+00 5.370706930429E+00  
3 256 BA -2.202042507059E-01 8.129407982021E-02 -5.447297864787E+00  
4 256 BA 4.335499690927E+00 5.452435971301E-02 -5.369931010326E+00  
5 9 F -8.650882512439E-02 -1.815076392668E+00 5.275900044116E+00  
6 9 F 4.331290211856E+00 -1.604040736728E+00 5.445501882863E+00  
7 9 F 2.068420407171E+00 1.293226648499E+00 -5.268070912655E+00  
8 9 F -2.349342579077E+00 1.519234292597E+00 -5.449003180586E+00  
9 9 F 2.350338553303E+00 -1.726506385395E+00 -5.631741809687E+00  
10 9 F -2.356907575757E+00 -1.387170669468E+00 -5.361163799766E+00  
11 9 F -3.437305830413E-01 1.413436120400E+00 5.620609682799E+00  
12 9 F 4.341159552758E+00 1.731964622441E+00 5.363606089191E+00  
13 256 BA -1.088383231498E-01 -2.946462514503E-02 3.326372715433E+00  
14 256 BA 4.305276578682E+00 4.621347264315E-02 3.368686628677E+00  
15 256 BA 2.093304112565E+00 3.089282905387E+00 -3.327448370085E+00

16 256 BA -2.321661737685E+00 3.166742207605E+00 -3.368425859072E+00  
17 9 F 2.033359894047E+00 1.611488641217E+00 3.368899675221E+00  
18 9 F -2.271112081625E+00 1.604740082065E+00 3.286353800282E+00  
19 9 F -4.614371690151E-02 -1.507245992341E+00 -3.373587699805E+00  
20 9 F 4.255167782186E+00 -1.514648383288E+00 -3.284548194267E+00  
21 9 F -1.542908306646E-01 1.597876936053E+00 -3.280049379922E+00  
22 9 F 4.326521329386E+00 1.586127535537E+00 -3.267878290453E+00  
23 9 F 2.136244299174E+00 -1.523542960126E+00 3.279580462918E+00  
24 9 F -2.340844202883E+00 -1.534533658207E+00 3.268423655524E+00  
25 256 BA 2.093420739578E+00 3.132675909657E+00 1.096826330142E+00  
26 256 BA -2.315840757675E+00 3.129396177947E+00 1.061743286323E+00  
27 256 BA -1.089048951433E-01 1.272435699212E-02 -1.098503238443E+00  
28 256 BA 4.300200205230E+00 9.633059474101E-03 -1.061647254101E+00  
29 9 F -1.132982529764E-01 -1.555145100823E+00 1.103845738648E+00  
30 9 F 4.307084985506E+00 -1.545595327622E+00 1.098413280916E+00  
31 9 F 2.097864655482E+00 1.564136790646E+00 -1.104969027536E+00  
32 9 F -2.322343058481E+00 1.573795768711E+00 -1.098112092075E+00  
33 9 F 2.083665422007E+00 -1.563721150958E+00 -1.098360094508E+00  
34 9 F -2.303691066457E+00 -1.540773569220E+00 -1.132135281894E+00  
35 9 F -9.942036319855E-02 1.557248766472E+00 1.097100319478E+00  
36 9 F 4.288820645182E+00 1.579608953056E+00 1.131650947375E+00  
37 109 F 1.126116400864E+00 1.618156456783E+00 7.438786006610E+00  
38 1 H 4.076125759811E-01 1.421636475491E+00 6.704069078349E+00  
39 109 F 8.593852928759E-01 -1.499118990591E+00 -7.428257394221E+00  
40 1 H 1.585564596766E+00 -1.702432171575E+00 -6.700599410472E+00

(110) surface, 25% coverage

1 256 BA 2.228145984543E+00 3.162233389399E+00 5.430216756431E+00  
2 256 BA 2.151049149818E+00 -3.111805378127E+00 5.361100721464E+00  
3 256 BA -2.301796265647E+00 3.158685979471E+00 5.373069575193E+00  
4 256 BA -2.262564763697E+00 -3.119669982118E+00 5.349450222108E+00  
5 256 BA -1.401470074935E-01 4.694015030061E-02 -5.433906534339E+00  
6 256 BA -6.118808803541E-02 -6.235650155417E+00 -5.356494661307E+00  
7 256 BA 4.391890042581E+00 4.202622002905E-02 -5.367825560203E+00  
8 256 BA 4.352049851185E+00 6.236179695411E+00 -5.353654437620E+00  
9 9 F -4.653003796231E-02 4.469496373932E+00 5.360738556810E+00  
10 9 F -5.775620328966E-02 -1.697402955437E+00 5.372148248810E+00  
11 9 F 4.369655411500E+00 4.607077115611E+00 5.477680813654E+00  
12 9 F 4.359458094616E+00 -1.674528774394E+00 5.414502648093E+00  
13 9 F 2.135836732483E+00 1.349384527713E+00 -5.350334183243E+00  
14 9 F 2.146967833327E+00 -4.820768300575E+00 -5.379871327110E+00  
15 9 F -2.280487820943E+00 1.490993286440E+00 -5.473802183183E+00  
16 9 F -2.269564039777E+00 -4.797322113069E+00 -5.419954398253E+00  
17 9 F 2.313169552565E+00 -1.639624478456E+00 -5.612539460876E+00  
18 9 F 2.144198379458E+00 4.765868035040E+00 -5.442254052723E+00  
19 9 F -2.295758160920E+00 -1.415476623125E+00 -5.391098619917E+00  
20 9 F -2.266121470332E+00 4.797572719098E+00 -5.421928369785E+00  
21 9 F -2.153706441771E-01 1.481666500329E+00 5.601669424619E+00  
22 9 F -5.525539403897E-02 -4.589869502996E+00 5.448996802808E+00  
23 9 F 4.385391917971E+00 1.701539841989E+00 5.388035864915E+00

24 9 F 4.356713260274E+00 -4.559799054434E+00 5.427549894776E+00  
25 256 BA -6.395413550518E-02 -3.621183557939E-02 3.328908807190E+00  
26 256 BA -4.901870503561E-02 6.236090674723E+00 3.378673705886E+00  
27 256 BA 4.352385563638E+00 4.194132684551E-03 3.381960362666E+00  
28 256 BA 4.356861656440E+00 -6.216729943557E+00 3.369238120858E+00  
29 256 BA 2.138502829548E+00 3.115751558562E+00 -3.366663974946E+00  
30 256 BA 2.154211840915E+00 -3.156394129164E+00 -3.341026841360E+00  
31 256 BA -2.267143742317E+00 3.143929095429E+00 -3.363165719970E+00  
32 256 BA -2.262340557724E+00 -3.116996385870E+00 -3.387661477308E+00  
33 9 F 2.094882550615E+00 1.580898479713E+00 3.359722477629E+00  
34 9 F 2.146195433904E+00 -4.664048962779E+00 3.287361387774E+00  
35 9 F -2.228076192619E+00 1.581371635382E+00 3.305731606169E+00  
36 9 F -2.254151693102E+00 -4.668660543770E+00 3.278051107098E+00  
37 9 F -4.125122591711E-03 -1.537678623407E+00 -3.368064131220E+00  
38 9 F -5.559545081311E-02 4.694363580704E+00 -3.279724077754E+00  
39 9 F 4.319145833345E+00 -1.536053814340E+00 -3.303396497328E+00  
40 9 F 4.343014256348E+00 4.688540829207E+00 -3.278981766383E+00  
41 9 F -8.959266934354E-02 1.569904160036E+00 -3.301828366189E+00  
42 9 F -6.210701075006E-02 -4.681250029770E+00 -3.271279969447E+00  
43 9 F 4.370852829626E+00 1.569376052384E+00 -3.285462382216E+00  
44 9 F 4.362385308196E+00 -4.686234813510E+00 -3.273937399959E+00  
45 9 F 2.177918436900E+00 4.688640907859E+00 3.304164055146E+00  
46 9 F 2.152900211860E+00 -1.560230753100E+00 3.270635204161E+00  
47 9 F -2.280528145652E+00 4.687581738232E+00 3.293699588457E+00  
48 9 F -2.272547913410E+00 -1.564118722764E+00 3.265983510838E+00  
49 256 BA 2.144962495961E+00 3.118602085516E+00 1.093513520532E+00  
50 256 BA 2.151023758800E+00 -3.120425683998E+00 1.067067356894E+00  
51 256 BA -2.263028822570E+00 3.117273510443E+00 1.076809787592E+00  
52 256 BA -2.265499830653E+00 -3.121574430724E+00 1.052793739324E+00  
53 256 BA -5.550990537529E-02 3.465178584389E-03 -1.101769506436E+00  
54 256 BA -5.987084007267E-02 6.234612820341E+00 -1.057588525601E+00  
55 256 BA 4.352519016374E+00 5.089711708481E-03 -1.069199523938E+00  
56 256 BA 4.355761204644E+00 6.230578263000E+00 -1.060406063996E+00  
57 9 F -6.050308141756E-02 -1.561592072432E+00 1.095006903508E+00  
58 9 F -5.836487388004E-02 4.672917019886E+00 1.129477683929E+00  
59 9 F 4.356936144942E+00 -1.558326202915E+00 1.102175895341E+00  
60 9 F 4.356052175822E+00 4.675074746605E+00 1.119692351290E+00  
61 9 F 2.148404297333E+00 1.558489505166E+00 -1.110545024833E+00  
62 9 F 2.150757462391E+00 -4.687220992345E+00 -1.113278795607E+00  
63 9 F -2.267994247012E+00 1.559948299707E+00 -1.105920849194E+00  
64 9 F -2.264936345288E+00 -4.683840494692E+00 -1.115485685007E+00  
65 9 F 2.144005593975E+00 4.672279139829E+00 -1.097222196909E+00  
66 9 F 2.143071525830E+00 -1.565712734127E+00 -1.117739341194E+00  
67 9 F -2.262610717595E+00 4.679601657951E+00 -1.104135463856E+00  
68 9 F -2.255850282416E+00 -1.556642563220E+00 -1.143885290048E+00  
69 9 F -5.347839051291E-02 1.547215485403E+00 1.100837446418E+00  
70 9 F -5.394928634786E-02 -4.679715571329E+00 1.114727792180E+00  
71 9 F 4.345345274427E+00 1.559245636467E+00 1.136242636422E+00  
72 9 F 4.353635135724E+00 -4.676241253911E+00 1.111801671827E+00  
73 109 F 1.073179839759E+00 1.738161903348E+00 7.551103986368E+00  
74 1 H 4.291384023987E-01 1.509914233905E+00 6.762993562791E+00  
75 109 F 1.014787234302E+00 -1.370896455363E+00 -7.553026877568E+00

76 1 H 1.662188996778E+00 -1.604061546720E+00 -6.768474261142E+00

(100) surface, 100% coverage

1 9 F 5.064933075265E-02 1.113070620279E+00 1.070494692967E+01  
2 9 F 5.064933075264E-02 1.113070620279E+00 -1.070494692967E+01  
3 256 BA -2.028866473901E+00 1.855008920421E+00 9.346425784753E+00  
4 256 BA -2.028866473901E+00 1.855008920421E+00 -9.346425784753E+00  
5 9 F 1.896220438966E-01 1.899387736260E+00 7.781555695078E+00  
6 9 F 1.896220438966E-01 1.899387736260E+00 -7.781555695078E+00  
7 9 F -1.992313772555E+00 -3.367632422844E-01 7.788833960868E+00  
8 9 F -1.992313772555E+00 -3.367632422844E-01 -7.788833960868E+00  
9 256 BA 2.061021424218E-01 -3.155803893604E-01 6.233104500177E+00  
10 256 BA 2.061021424218E-01 -3.155803893604E-01 -6.233104500177E+00  
11 9 F -1.998571639680E+00 -3.124992599877E-01 4.675552931839E+00  
12 9 F -1.998571639680E+00 -3.124992599877E-01 -4.675552931839E+00  
13 9 F 2.079516475765E-01 1.892833673603E+00 4.673133149700E+00  
14 9 F 2.079516475765E-01 1.892833673603E+00 -4.673133149700E+00  
15 256 BA -1.998528223978E+00 1.893575626654E+00 3.116123542333E+00  
16 256 BA -1.998528223978E+00 1.893575626654E+00 -3.116123542333E+00  
17 9 F 2.075466057193E-01 1.893937904450E+00 1.557731374621E+00  
18 9 F 2.075466057192E-01 1.893937904450E+00 -1.557731374621E+00  
19 9 F -1.998537638644E+00 -3.125114986059E-01 1.558354182157E+00  
20 9 F -1.998537638644E+00 -3.125114986059E-01 -1.558354182157E+00  
21 256 BA 2.075929438837E-01 -3.123414775095E-01 0.000000000000E+00  
22 109 F 1.673494011396E+00 -4.898018934712E-01 1.075111421098E+01  
23 109 F 1.673494011396E+00 -4.898018934712E-01 -1.075111421098E+01  
24 1 H 7.667897085580E-01 2.078588554013E-01 1.084395158471E+01  
25 1 H 7.667897085580E-01 2.078588554013E-01 -1.084395158471E+01

(100) surface, 50% coverage

1 9 F -1.054252235311E+00 7.805383644079E-02 1.055465881159E+01  
2 9 F -1.054252235311E+00 7.805383644079E-02 -1.055465881159E+01  
3 9 F -4.306506739701E+00 1.068544071701E+00 1.014993897612E+01  
4 9 F -4.306506739701E+00 1.068544071701E+00 -1.014993897612E+01  
5 256 BA -2.233265243738E+00 -2.128037168198E+00 9.315162077010E+00  
6 256 BA -2.233265243738E+00 -2.128037168198E+00 -9.315162077010E+00  
7 256 BA 2.445772684330E+00 2.285610916061E+00 9.316312869656E+00  
8 256 BA 2.445772684330E+00 2.285610916061E+00 -9.316312869656E+00  
9 9 F 1.074521490872E-01 -2.103983302322E+00 7.928395030050E+00  
10 9 F 1.074521490872E-01 -2.103983302322E+00 -7.928395030050E+00  
11 9 F -4.305860980127E+00 -1.973450778819E+00 7.667937609231E+00  
12 9 F -4.305860980127E+00 -1.973450778819E+00 -7.667937609231E+00  
13 9 F -2.134547788703E+00 1.300309608740E-01 7.757066137882E+00  
14 9 F -2.134547788703E+00 1.300309608740E-01 -7.757066137882E+00  
15 9 F 2.348223610428E+00 1.305003138832E-01 7.760352423027E+00  
16 9 F 2.348223610428E+00 1.305003138832E-01 -7.760352423027E+00  
17 256 BA 1.059664772940E-01 1.251175989105E-01 6.290982141514E+00  
18 256 BA 1.059664772940E-01 1.251175989105E-01 -6.290982141514E+00

19 256 BA -4.306525960076E+00 1.881120792807E-01 6.179266353554E+00  
20 256 BA -4.306525960076E+00 1.881120792807E-01 -6.179266353554E+00  
21 9 F -2.074985132133E+00 1.605480300800E-01 4.668985841257E+00  
22 9 F -2.074985132133E+00 1.605480300800E-01 -4.668985841257E+00  
23 9 F 2.287386444602E+00 1.601891918977E-01 4.670151907748E+00  
24 9 F 2.287386444602E+00 1.601891918977E-01 -4.670151907748E+00  
25 9 F 1.058381818337E-01 -2.066147465674E+00 4.737404675295E+00  
26 9 F 1.058381818337E-01 -2.066147465674E+00 -4.737404675295E+00  
27 9 F -4.306279174222E+00 -2.025317678112E+00 4.624718219169E+00  
28 9 F -4.306279174222E+00 -2.025317678112E+00 -4.624718219169E+00  
29 256 BA -2.088001957052E+00 -2.045841638272E+00 3.116000914459E+00  
30 256 BA -2.088001957052E+00 -2.045841638272E+00 -3.116000914459E+00  
31 256 BA 2.299466242339E+00 -2.046352787584E+00 3.116802185808E+00  
32 256 BA 2.299466242339E+00 -2.046352787584E+00 -3.116802185808E+00  
33 9 F 1.059527307742E-01 -2.044179734214E+00 1.560786857295E+00  
34 9 F 1.059527307742E-01 -2.044179734214E+00 -1.560786857295E+00  
35 9 F -4.306937875108E+00 -2.048266497013E+00 1.556967886693E+00  
36 9 F -4.306937875108E+00 -2.048266497013E+00 -1.556967886693E+00  
37 9 F -2.095764248119E+00 1.602070490596E-01 1.556908995277E+00  
38 9 F -2.095764248119E+00 1.602070490596E-01 -1.556908995277E+00  
39 9 F 2.307032441334E+00 1.599400122093E-01 1.557690642688E+00  
40 9 F 2.307032441334E+00 1.599400122093E-01 -1.557690642688E+00  
41 256 BA 1.058608241577E-01 1.614944094388E-01 0.000000000000E+00  
42 256 BA -4.306979013011E+00 1.585247574118E-01 0.000000000000E+00  
43 109 F 1.265687541350E+00 7.889890657041E-02 1.056075045411E+01  
44 109 F 1.265687541350E+00 7.889890657041E-02 -1.056075045411E+01  
45 1 H 1.070869149983E-01 7.683251794566E-02 1.058795145598E+01  
46 1 H 1.070869149983E-01 7.683251794566E-02 -1.058795145598E+01

(100) surface, 25% coverage

1 9 F 8.326379382651E-01 -4.321203858982E+00 1.007510886827E+01  
2 9 F 8.326379382651E-01 -4.321203858982E+00 -1.007510886827E+01  
3 9 F -3.817083055741E-02 1.236990446215E+00 1.055676109652E+01  
4 9 F -3.817083055741E-02 1.236990446215E+00 -1.055676109652E+01  
5 9 F -4.327005521525E+00 -3.106543645182E+00 1.029327153662E+01  
6 9 F -4.327005521525E+00 -3.106543645182E+00 -1.029327153662E+01  
7 9 F 4.442323676185E+00 1.683496035560E+00 1.042721874951E+01  
8 9 F 4.442323676185E+00 1.683496035560E+00 -1.042721874951E+01  
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11 256 BA -2.241355667189E+00 2.355421177142E+00 9.315096619323E+00  
12 256 BA -2.241355667189E+00 2.355421177142E+00 -9.315096619323E+00  
13 256 BA 2.221343303444E+00 -2.288365860475E+00 9.343852139859E+00  
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19 9 F -4.448219912403E-03 2.328979652902E+00 7.728697597687E+00  
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21 9 F -4.338485072341E+00 -2.012035233960E+00 7.673766918191E+00  
22 9 F -4.338485072341E+00 -2.012035233960E+00 -7.673766918191E+00  
23 9 F -4.344649164392E+00 2.407718050928E+00 7.660646159934E+00  
24 9 F -4.344649164392E+00 2.407718050928E+00 -7.660646159934E+00  
25 9 F -2.209886139569E+00 1.315840228752E-01 7.967326819790E+00  
26 9 F -2.209886139569E+00 1.315840228752E-01 -7.967326819790E+00  
27 9 F -2.170362754167E+00 -4.290240181648E+00 7.882946590117E+00  
28 9 F -2.170362754167E+00 -4.290240181648E+00 -7.882946590117E+00  
29 9 F 2.235212320964E+00 1.049996599428E-01 7.959429174354E+00  
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31 9 F 2.343532783934E+00 -4.293715506888E+00 7.663365525406E+00  
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33 256 BA 4.938378328713E-02 1.217619406052E-01 6.288020383074E+00  
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39 256 BA -4.347450033485E+00 -4.247469270856E+00 6.168106322111E+00  
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41 9 F -2.161383126520E+00 1.455011566870E-01 4.746711155259E+00  
42 9 F -2.161383126520E+00 1.455011566870E-01 -4.746711155259E+00  
43 9 F -2.127368216161E+00 -4.267979587785E+00 4.680707727114E+00  
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45 9 F 2.238445192832E+00 1.473546875850E-01 4.726913267120E+00  
46 9 F 2.238445192832E+00 1.473546875850E-01 -4.726913267120E+00  
47 9 F 2.250637744533E+00 -4.267201916856E+00 4.642802864344E+00  
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55 9 F -4.365916705035E+00 2.353331203983E+00 4.628924025360E+00  
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61 256 BA 2.249020377954E+00 -2.056085608394E+00 3.111672214695E+00  
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66 9 F 4.618855638471E-02 -2.056438651943E+00 -1.554398831828E+00  
67 9 F 4.613443999393E-02 2.349910218881E+00 1.552592642721E+00  
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69 9 F -4.359622085969E+00 -2.059968072475E+00 1.554106730727E+00  
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71 9 F -4.359466477533E+00 2.347045700955E+00 1.551977710060E+00  
72 9 F -4.359466477533E+00 2.347045700955E+00 -1.551977710060E+00

73 9 F -2.153018217974E+00 1.445007262911E-01 1.568908945020E+00  
74 9 F -2.153018217974E+00 1.445007262911E-01 -1.568908945020E+00  
75 9 F -2.156230282353E+00 -4.266865087859E+00 1.568902567217E+00  
76 9 F -2.156230282353E+00 -4.266865087859E+00 -1.568902567217E+00  
77 9 F 2.254209899147E+00 1.448687199010E-01 1.560089489036E+00  
78 9 F 2.254209899147E+00 1.448687199010E-01 -1.560089489036E+00  
79 9 F 2.252738472373E+00 -4.266386749776E+00 1.553761386581E+00  
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82 256 BA 4.480347370047E-02 -4.265439589451E+00 0.000000000000E+00  
83 256 BA -4.360073867015E+00 1.432240771248E-01 0.000000000000E+00  
84 256 BA -4.360139033330E+00 -4.267634999426E+00 0.000000000000E+00  
85 109 F -3.015086988296E-02 -1.080471970212E+00 1.060412121912E+01  
86 109 F -3.015086988296E-02 -1.080471970212E+00 -1.060412121912E+01  
87 1 H -2.574157731560E-02 7.730070120520E-02 1.061230124660E+01  
88 1 H -2.574157731560E-02 7.730070120520E-02 -1.061230124660E+01

P.S. : The format is according to notations in the CRYSTAL09 code.