

Supporting information for:
The pressure gap for thiols: Methanethiol self-assembly on Au(111)
from vacuum to 1 bar

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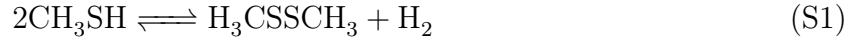
Supporting Information

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S1 Determination of Gas Composition

The thermodynamic description of SAM formation requires the partial pressures of CH_3SH , DMDS and H_2 . These were determined as follows: The UHV dosing pressure of CH_3SH was assumed to be 100 times the chamber pressure. The hydrogen pressure was estimated based on mass spectrometry of the residual gas, assuming uniform hydrogen pressure in the vacuum chamber. For the high-pressure experiments (at 1 bar), a methanethiol-dimethyldisulfide equilibrium was assumed to establish immediately.



Knowledge of the composition of the entering gas (98 Vol% CH_3SH , 2 Vol% DMDS) and the equilibrium reaction allowed the determination of the partial pressures of the different gaseous species. Note that this calculation procedure was necessary due to the low hydrogen pressure, which precluded accurate mass spectroscopic analysis.

The standard free energy change (in eV) of this reaction can be calculated as:

$$\begin{aligned} \Delta G^\circ(T) &\approx \Delta H^\circ(T) - T\Delta S_{298K}^\circ \\ &\approx \Delta H_{298K}^\circ + (T - 298K)\Delta C_{P,298K}^\circ - T\Delta S_{298K}^\circ \\ &= \Delta H_{eff}^\circ - T\Delta S_{eff}^\circ = 0.154 + T \cdot 6.76 \cdot 10^{-4} \end{aligned} \quad (\text{S2})$$

We assumed variations in heat capacity and entropy from their value at 298K to be negligible. At equilibrium, the partial pressures of DMDS, H_2 and CH_3SH are related to ΔG^0 through equation S3:

$$\Delta G^\circ(T) = -k_B T \ln \frac{a_{\text{DMDS}} a_{\text{H}_2}}{a_{\text{CH}_3\text{SH}}^2} \quad (\text{S3})$$

To reach the equilibrium, the gas composition has to move away from the starting conditions determined by the inlet gas, $a_{\text{CH}_3\text{SH}}^0$ and a_{DMDS}^0 , with a^0 the activity P/P_0 . Taking into account the stoichiometry of the reaction, this equilibration results in:

$$a_{\text{H}_2} = \frac{1}{(8K-2)} \left(4K \cdot a_{\text{CH}_3\text{SH}}^0 + a_{\text{DMDS}}^0 - \sqrt{4K \cdot a_{\text{CH}_3\text{SH}}^0 (a_{\text{CH}_3\text{SH}}^0 + 2a_{\text{DMDS}}^0) + a_{\text{DMDS}}^0{}^2} \right) \quad (\text{S4})$$

S2 Supporting Experimental Information

S2.1 Assignment of ultrahigh vacuum saturation structure

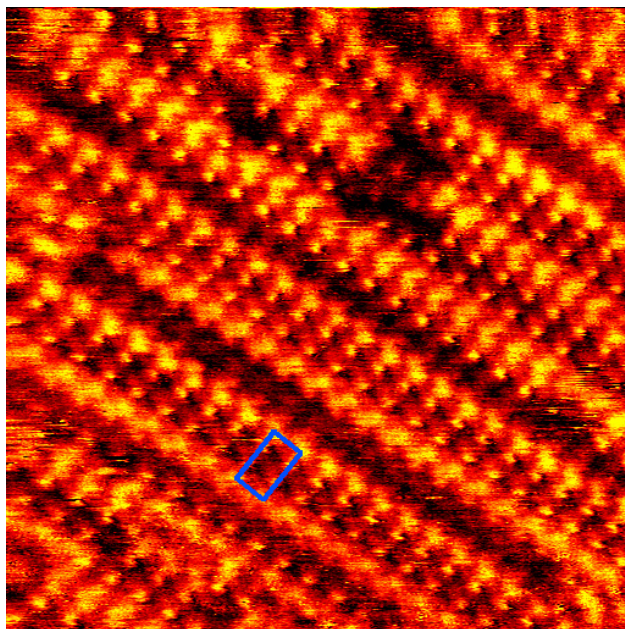


Figure S1: Alternative appearance of methanethiolate SAM at ultrahigh vacuum saturation coverage. A $3 \times \sqrt{3}$ unit cell is indicated in blue. Imaging parameters: $10 \text{ nm} \times 10 \text{ nm}$, $U_s = -0.3 \text{ V}$, $I_t = 520 \text{ pA}$.

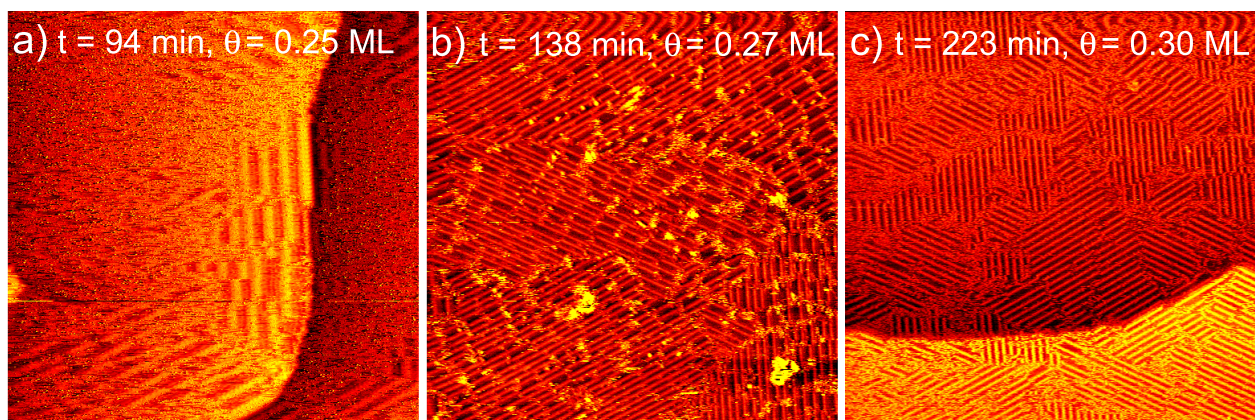


Figure S2: Structural evolution of methylthiolate overlayer formation at room temperature. a) Low coverage structure showing partial self-assembly and partial two-dimensional lattice gas behavior. $40 \text{ nm} \times 40 \text{ nm}$, $U_s = -1 \text{ V}$, $I_t = 160 \text{ pA}$. b) Intermediate stage of self-assembly, showing large $3 \times \sqrt{3}$ areas. $80 \text{ nm} \times 80 \text{ nm}$, $U_s = -1 \text{ V}$, $I_t = 160 \text{ pA}$. c) Close to saturation coverage, where the surface is fully covered with the $3 \times \sqrt{3}$ structure. $80 \text{ nm} \times 80 \text{ nm}$, $U_s = -1 \text{ V}$, $I_t = 160 \text{ pA}$. The indicated coverage was calculated using the S 2p / Au 4f ratio from X-ray photoelectron spectroscopy, calibrated at saturation coverage.

S3 Supporting Theoretical Information

S3.1 Simulated STM images of other $\frac{1}{3}$ ML structures

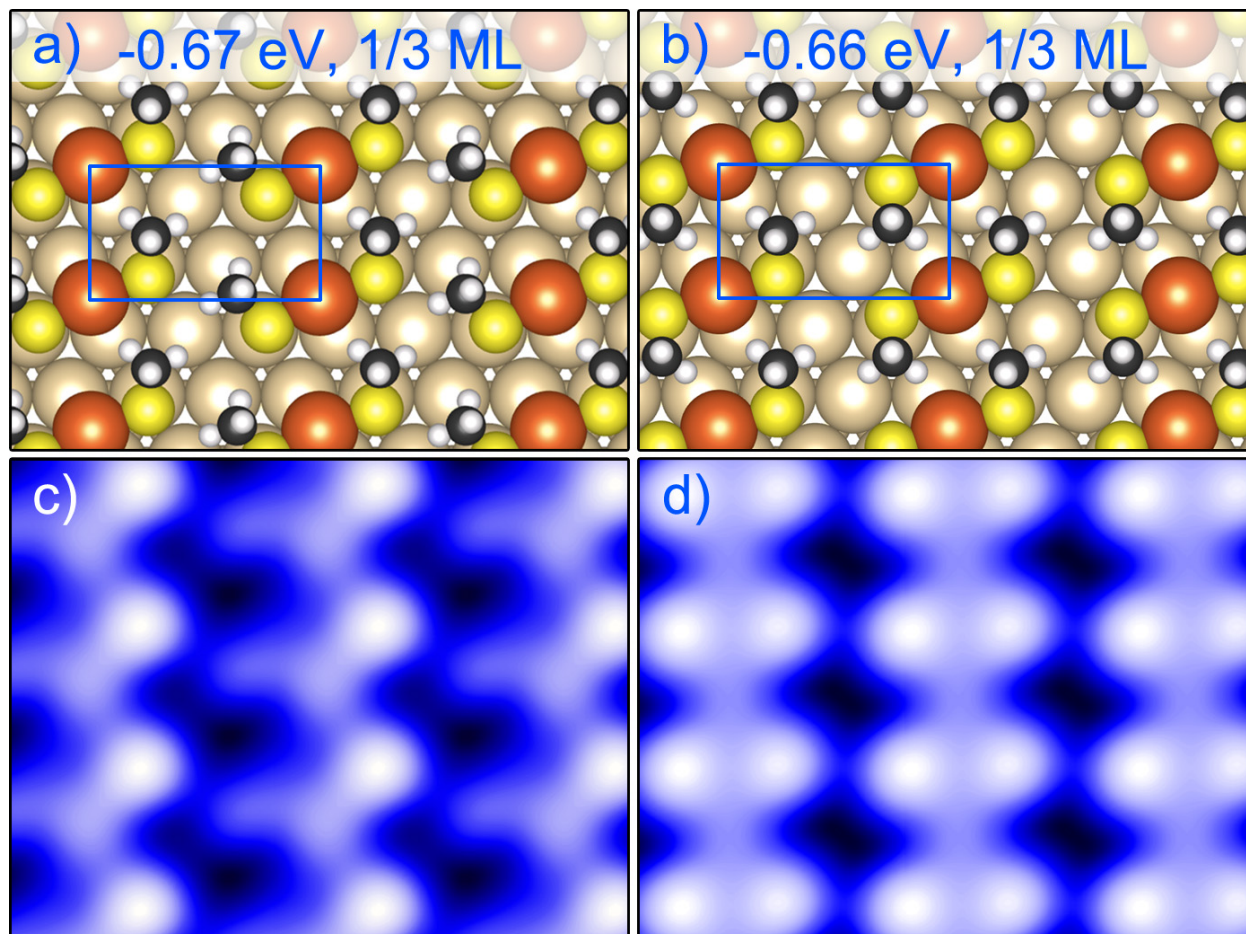


Figure S3: STM computations of other $\frac{1}{3}$ ML methanethiolate SAMs. The simulated STM image in c) corresponds to the structure in a), while d) corresponds to b). Both simulations were conducted for $U_s = -1$ V.

S3.2 Simulated STM images for $3/8$ ML structures

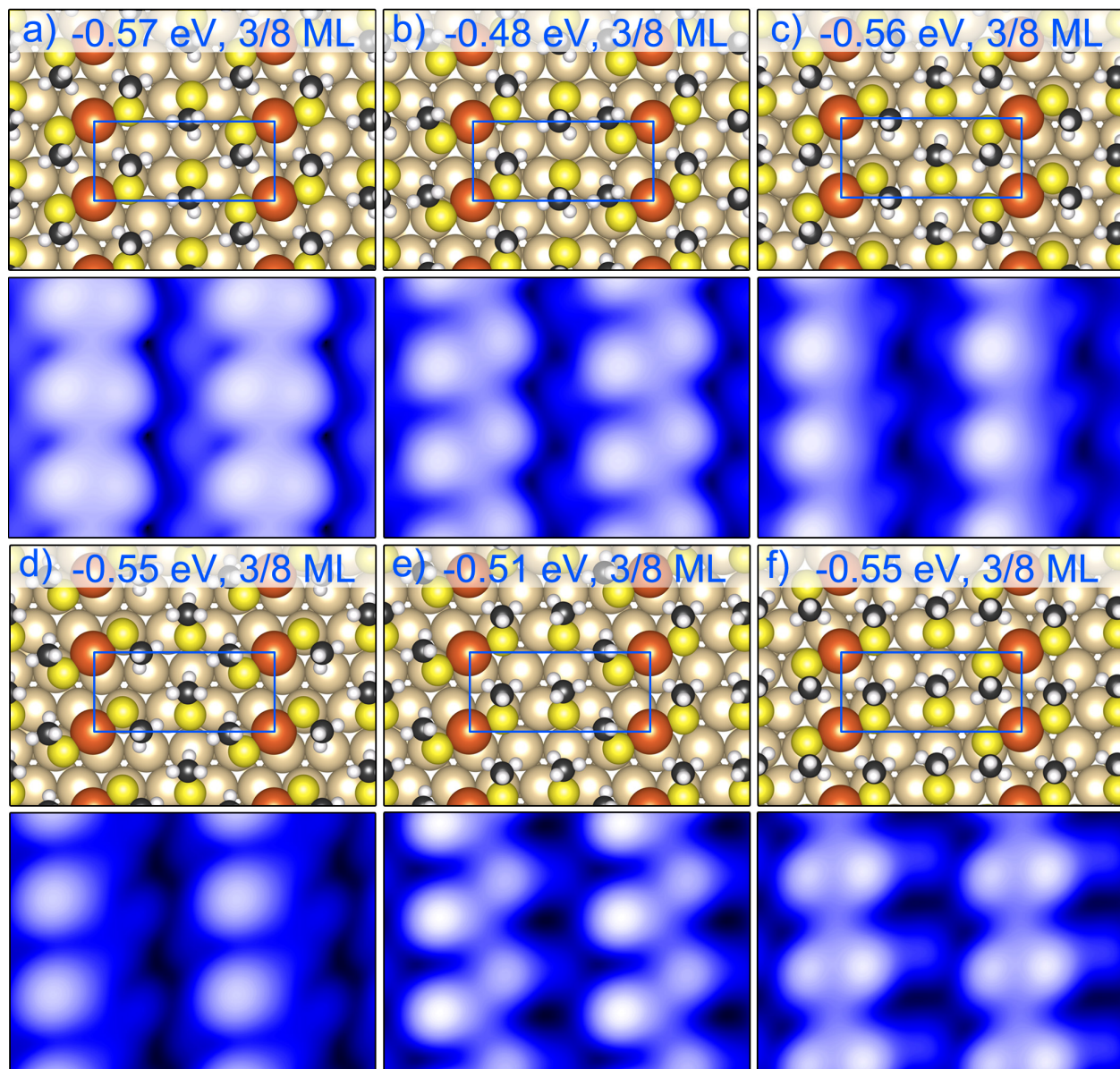


Figure S4: Simulated STM images of the $3/8$ ML structures investigated in this work. The simulations were conducted for $U_s = -0.5$ V.

S3.3 Structural Features Driving Monolayer Configuration

Several isomers have been modeled for the $1/3$ ML structures, starting with the simple adsorption of $-\text{SCH}_3$ units on the unreconstructed Au(111) surface (Fig. S5a). Staple creation strengthens the Au-S interaction (Figs. S5b-e) by simultaneously binding S covalently to an Au-adatom and an atop terrace site. The associated energy gain is larger than the energetic cost to form the adatom. Thiol adsorption hence clearly restructures the surface.^{S1-S4} Figure S5b describes the smallest unit cell ($3 \times \sqrt{3}$) with trans staples. However, the shortest C-C distance is 3.29 Å (compared to 3.6 Å for the methane dimer^{S5,S6}) resulting in steric repulsion. This methyl-methyl repulsion was computationally assessed by comparisons between particular modifications to the surface. For the structure in Figure S5b, for example, half of the vertical columns of staples was removed, yielding a $1/6$ ML coverage surface. The difference in adsorption energy (per thiolate molecule) between this structure and the structure in Figure S5b was taken as the methyl-methyl repulsion. Corroborating this approach, Allinger *et al.* **2000** J. Comput. Chem. 21:1229 showed that this choice of cut allows the full dying out of the methyl-methyl interaction.

The specific staple organization displayed in Fig. S5c, observed experimentally elsewhere,^{S7,S8} yields the most stable isomer, although indistinguishable energetically to the structures in d and e using DFT. Alternatively, the repulsion can be relieved by forming a cis isomer (Fig. S5d) or in a $6 \times \sqrt{3}$ unit cell (Fig. S5e). Only this latter arrangement gives rise to the alternating dark and bright rows in the experimental STM image (Fig. 1 a in the main text).

Relevant $3/8$ ML structures matching the $4 \times \sqrt{3}$ unit cell observed at high pressure and temperature combine a staple and an additional $-\text{SCH}_3$ adsorbate on the terrace (see Fig. S6 and Fig. S4). The structure in Fig. S6a is based on the cis-motif seen above. However, the methyl-methyl repulsion, reflected in the smallest C-C distance of 3.28 Å, renders it energetically less favorable. The more stable isomers (b) and (c) are very close in energy, (c) optimizing the VdW contacts and yielding the best match between theory and experiment

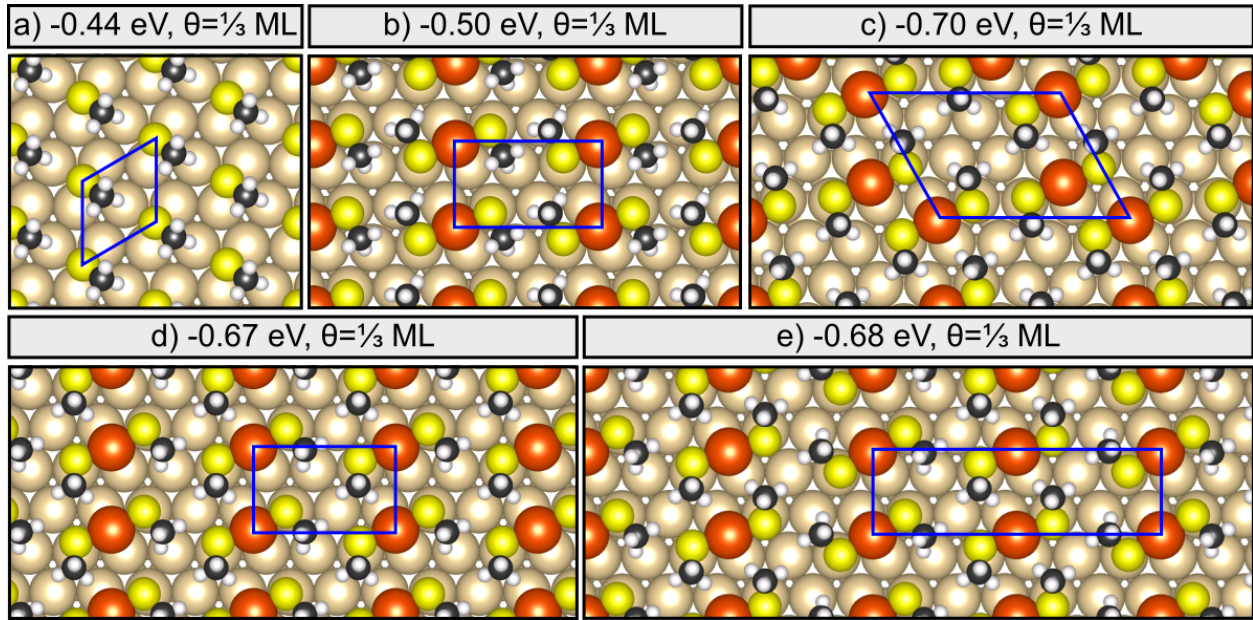


Figure S5: Adsorption energy E_{ads} of relevant methanethiolate adsorption structures with $\vartheta=1/3$ ML, referenced to the clean surface and CH_3SH and H_2 gas. The VdW contributions are included in the adsorption energy shown here, the ZPE and entropic contributions are excluded.

(see main text Figs. 1b, d, f).

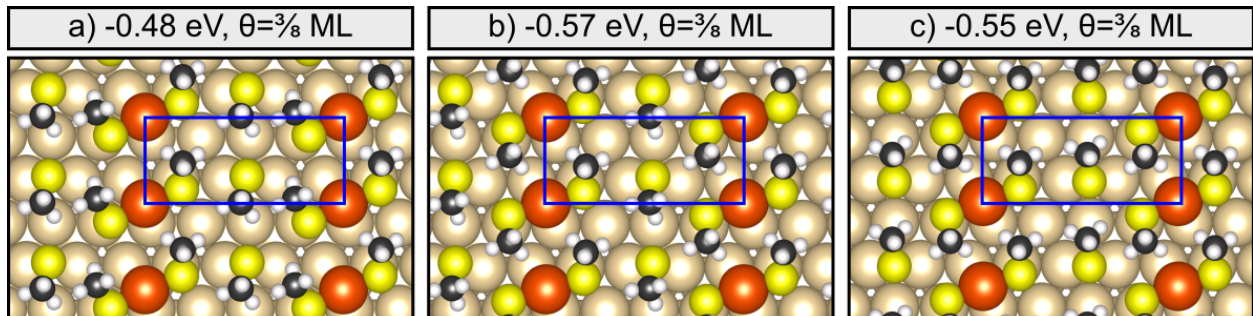


Figure S6: Adsorption energy of various methanethiolate adsorption structures with $\vartheta=3/8$ ML referenced to the clean surface and CH_3SH and H_2 gas.

S3.4 Relative thermodynamic stability of 1/3 ML and 3/8 ML structures

Although Figure 5 in the main text shows that the 1/3 ML and 3/8 ML structures are stable with respect to the gas phase under the conditions where they were experimentally observed, they may not be the most stable structure relative to other adsorbate structures. The transformation from the 1/3 ML to the 3/8 ML structure will occur when the surface free energy (ΔG_{ads} per unit area) is lower for the latter higher coverage than for the lower one. Our modelling does not reproduce such a crossing at any temperature. This could be explained by inaccuracies in both the calculated electronic energy and/or the entropy. A slight overestimation of the ΔE_{ads} (in the order of 0.1 eV) could explain the absence of the phase transition according to our computations. Both the favorability of Au-S bond^{S9,S10} and adatom creation^{S11,S12} seem slightly overestimated by PBE.^{S13} Alternatively, the SAM might not be in equilibrium with an equilibrated gas phase, questioning the use of the gas-phase activities, making the entropy estimate inaccurate.

S3.5 $\sqrt{3}\times\sqrt{3}$, frozen Au coordinates

POSCAR of pure variant

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S3.6 $\sqrt{3}\times\sqrt{3}$, frozen Au coordinates

POSCAR head and tail.

Subdivision 6 times sq 3

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Selective dynamics
Direct

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0.3969955072465875	0.3895707923128772	0.5287194101679401	T	T	T
0.8969955072465876	0.3895707923128772	0.5287194101679401	T	T	T
0.0748439307079807	0.7141282598387461	0.5279387878381313	T	T	T
0.5748439307079808	0.7141282598387461	0.5279387878381313	T	T	T
0.0988308827018300	0.8149691731722218	0.5283916723645083	T	T	T
0.5988308827018299	0.8149691731722218	0.5283916723645083	T	T	T
0.1623826742348645	0.7579554788966897	0.5849218340998295	T	T	T
0.6623826742348644	0.7579554788966897	0.5849218340998295	T	T	T
0.4841452462799647	0.0136891138651673	0.5082869677239338	T	T	T
0.9841452462799647	0.0136891138651673	0.5082869677239338	T	T	T
0.2977817774405785	0.2527886754069360	0.5022260972773614	T	T	T
0.7977817774405784	0.2527886754069360	0.5022260972773614	T	T	T
0.4841452462799647	0.5136886015701645	0.5082869677239338	T	T	T
0.9841452462799647	0.5136886015701645	0.5082869677239338	T	T	T
0.2977817774405785	0.7527886754069361	0.5022260972773614	T	T	T

0.7977817774405784	0.7527886754069361	0.5022260972773614	T	T	T
0.3740045624484393	0.1286504098940192	0.5018011059006044	T	T	T
0.8740045624484393	0.1286504098940192	0.5018011059006044	T	T	T
0.3740045624484393	0.6286504098940192	0.5018011059006044	T	T	T
0.8740045624484393	0.6286504098940192	0.5018011059006044	T	T	T
0.1670125730671347	0.0003320690964954	0.1990284927294078	T	T	T
0.6670125730671347	0.0003320690964954	0.1990284927294078	T	T	T
0.1662694830214176	0.1661412779803366	0.1988345753159920	T	T	T
0.6662694830214175	0.1661412779803366	0.1988345753159920	T	T	T
0.1646972590166939	0.3337790266269460	0.1988860271481278	T	T	T
0.6646972590166940	0.3337790266269460	0.1988860271481278	T	T	T
0.1670125730671347	0.5003320690964954	0.1990284927294078	T	T	T
0.6670125730671347	0.5003320690964954	0.1990284927294078	T	T	T
0.1662694830214176	0.6661412779803366	0.1988345753159920	T	T	T
0.6662694830214175	0.6661412779803366	0.1988345753159920	T	T	T
0.1646972590166939	0.8337790266269460	0.1988860271481278	T	T	T
0.6646972590166940	0.8337790266269460	0.1988860271481278	T	T	T
0.4166551745014894	0.0835879202504281	0.1990677683712270	T	T	T
0.9166551745014894	0.0835879202504281	0.1990677683712270	T	T	T
0.4178365668673850	0.2497119442775377	0.1987631986857664	T	T	T
0.9178365668673850	0.2497119442775377	0.1987631986857664	T	T	T
0.4150691103715078	0.4165000529096246	0.1987729945101486	T	T	T
0.9150691103715078	0.4165000529096246	0.1987729945101486	T	T	T
0.4166551745014894	0.5835879202504354	0.1990677683712270	T	T	T
0.9166551745014894	0.5835879202504354	0.1990677683712270	T	T	T
0.4178365668673850	0.7497119442775376	0.1987631986857664	T	T	T
0.9178365668673850	0.7497119442775376	0.1987631986857664	T	T	T
0.4150691103715078	0.9165000529096246	0.1987729945101486	T	T	T
0.9150691103715078	0.9165000529096246	0.1987729945101486	T	T	T
0.0829651356487159	0.0822336949509783	0.2988921766134200	T	T	T
0.5829651356487159	0.0822336949509783	0.2988921766134200	T	T	T
0.0854356940882206	0.2495648825623680	0.2983254785490071	T	T	T
0.5854356940882206	0.2495648825623680	0.2983254785490071	T	T	T
0.0798509302291455	0.4184742761130926	0.2974482780918645	T	T	T
0.5798509302291454	0.4184742761130926	0.2974482780918645	T	T	T
0.0829651356487159	0.5822336949509782	0.2988921766134200	T	T	T
0.5829651356487159	0.5822336949509782	0.2988921766134200	T	T	T
0.0854356940882206	0.7495648825623680	0.2983254785490071	T	T	T
0.5854356940882206	0.7495648825623680	0.2983254785490071	T	T	T
0.0798509302291455	0.9184742761130925	0.2974482780918645	T	T	T
0.5798509302291454	0.9184742761130925	0.2974482780918645	T	T	T
0.3350754909886117	0.0009367708403595	0.2983297288569958	T	T	T
0.8350754909886117	0.0009367708403595	0.2983297288569958	T	T	T
0.3328983069101621	0.1673998535217860	0.2978273259861109	T	T	T
0.8328983069101622	0.1673998535217860	0.2978273259861109	T	T	T
0.3314067907625432	0.3322568355560913	0.2966109698782500	T	T	T
0.8314067907625432	0.3322568355560913	0.2966109698782500	T	T	T
0.3350754909886117	0.5009367708403595	0.2983297288569958	T	T	T
0.8350754909886117	0.5009367708403595	0.2983297288569958	T	T	T
0.3328983069101621	0.6673998535217860	0.2978273259861109	T	T	T
0.8328983069101622	0.6673998535217860	0.2978273259861109	T	T	T
0.3314067907625432	0.8322568355560913	0.2966109698782500	T	T	T
0.8314067907625432	0.8322568355560913	0.2966109698782500	T	T	T
0.4964577948067979	0.9976902374680152	0.4041174055601485	T	T	T
0.9964577948067979	0.9976902374680152	0.4041174055601485	T	T	T
0.0000626900647323	0.1670068478508143	0.3958473328887873	T	T	T
0.5000626900647323	0.1670068478508143	0.3958473328887873	T	T	T
0.4966061161807511	0.3340208728806379	0.3951844181630156	T	T	T
0.9966061161807510	0.3340208728806379	0.3951844181630156	T	T	T
0.4964577948067979	0.4976902374680152	0.4041174055601485	T	T	T
0.9964577948067979	0.4976902374680152	0.4041174055601485	T	T	T
0.0000626900647323	0.6670068478508142	0.3958473328887873	T	T	T
0.5000626900647323	0.6670068478508142	0.3958473328887873	T	T	T
0.4966061161807511	0.8340208728806379	0.3951844181630156	T	T	T
0.9966061161807510	0.8340208728806379	0.3951844181630156	T	T	T
0.2465503938786731	0.0833648096224768	0.3972696567292840	T	T	T
0.7465503938786732	0.0833648096224768	0.3972696567292840	T	T	T
0.2451556503006862	0.2521682020111427	0.4009216897271186	T	T	T
0.7451556503006863	0.2521682020111427	0.4009216897271186	T	T	T
0.2462516586263788	0.4169793256825901	0.3945015282020700	T	T	T
0.7462516586263789	0.4169793256825901	0.3945015282020700	T	T	T
0.2465503938786731	0.5833648096224768	0.3972696567292840	T	T	T
0.7465503938786732	0.5833648096224768	0.3972696567292840	T	T	T
0.2451556503006862	0.7521682020111427	0.4009216897271186	T	T	T
0.7451556503006863	0.7521682020111427	0.4009216897271186	T	T	T
0.2462516586263788	0.9169793256825901	0.3945015282020700	T	T	T
0.7462516586263789	0.9169793256825901	0.3945015282020700	T	T	T

S3.7 trans, POSCAR center

0.1042461683427902	0.0026580734645378	0.5408003647060440	T	T	T
0.6042461683427902	0.0026580734645378	0.5408003647060440	T	T	T
0.1493569346307524	0.2548097597624661	0.5407949486587000	T	T	T
0.6493569346307524	0.2548097597624661	0.5407949486587000	T	T	T
0.1042461683427902	0.5026580734645378	0.5408003647060440	T	T	T

0.6042461683427902	0.5026580734645378	0.5408003647060440	T	T
0.1493569346307524	0.7548097597624661	0.5407949486587000	T	T
0.6493569346307524	0.7548097597624661	0.5407949486587000	T	T
0.1613599834954940	0.0535799778669457	0.5297088904605829	T	T
0.6613599834954940	0.0535799778669457	0.5297088904605829	T	T
0.0866096619038288	0.0013711317568124	0.5861603212490252	T	T
0.5866096619038288	0.0013711317568124	0.5861603212490252	T	T
0.1607830999469186	0.9521709711900002	0.5279589775026992	T	T
0.6607830999469186	0.9521709711900002	0.5279589775026992	T	T
0.0828851393426220	0.2096504562489514	0.5262318824411949	T	T
0.5828851393426220	0.2096504562489514	0.5262318824411949	T	T
0.1029994604403868	0.3101633342771635	0.5323954002376752	T	T
0.6029994604403868	0.3101633342771635	0.5323954002376752	T	T
0.1682074757753895	0.2483880870156554	0.5857763701639200	T	T
0.6682074757753895	0.2483880870156554	0.5857763701639200	T	T
0.1613599834954940	0.5535799778669457	0.5297088904605829	T	T
0.6613599834954940	0.5535799778669457	0.5297088904605829	T	T
0.0866096619038288	0.5013711317568124	0.5861603212490252	T	T
0.5866096619038288	0.5013711317568124	0.5861603212490252	T	T
0.1607830999469186	0.4521709711900002	0.5279589775026992	T	T
0.6607830999469186	0.4521709711900002	0.5279589775026992	T	T
0.0828851393426220	0.7096504562489514	0.5262318824411949	T	T
0.5828851393426220	0.7096504562489514	0.5262318824411949	T	T
0.1029994604403868	0.8101633342771635	0.5323954002376752	T	T
0.6029994604403868	0.8101633342771635	0.5323954002376752	T	T
0.1682074757753895	0.7483880870156554	0.5857763701639200	T	T
0.6682074757753895	0.7483880870156554	0.5857763701639200	T	T
0.4468381311932603	0.0009640643427389	0.5045331714589665	T	T
0.9468381311932603	0.0009640643427389	0.5045331714589665	T	T
0.3052986980278192	0.2523136760187512	0.5033700362544238	T	T
0.8052986980278192	0.2523136760187512	0.5033700362544238	T	T
0.4468381311932603	0.5009635520477360	0.5045331714589665	T	T
0.9468381311932603	0.5009635520477360	0.5045331714589665	T	T
0.3052986980278192	0.7523136760187441	0.5033700362544238	T	T
0.8052986980278192	0.7523136760187441	0.5033700362544238	T	T
0.3740901596139850	0.1263674693775272	0.5007324960403778	T	T
0.8740901596139850	0.1263674693775272	0.5007324960403778	T	T
0.3740901596139850	0.6263674693775272	0.5007324960403778	T	T
0.8740901596139850	0.6263674693775272	0.5007324960403778	T	T
0.1667395333541393	0.0002414866116283	0.1987848404442758	T	T
0.6667395333541393	0.0002414866116283	0.1987848404442758	T	T
0.1661012106923039	0.1664572735571852	0.1989195828329073	T	T
0.6661012106923039	0.1664572735571852	0.1989195828329073	T	T
0.1650589944240082	0.3336443514546943	0.1991995317527682	T	T
0.6650589944240082	0.3336443514546943	0.1991995317527682	T	T
0.1667395333541393	0.5002414866116283	0.1987848404442758	T	T
0.6667395333541393	0.5002414866116283	0.1987848404442758	T	T
0.1661012106923039	0.6664572735571852	0.1989195828329073	T	T
0.6661012106923039	0.6664572735571852	0.1989195828329073	T	T
0.1650589944240082	0.8336443514546943	0.1991995317527682	T	T
0.6650589944240082	0.8336443514546943	0.1991995317527682	T	T
0.4162164767221626	0.0837902120810341	0.1987747806093267	T	T
0.9162164767221626	0.0837902120810341	0.1987747806093267	T	T
0.4178107981347381	0.2499947298943539	0.1990501375239617	T	T
0.9178107981347381	0.2499947298943539	0.1990501375239617	T	T
0.4152896764840861	0.4163752750174083	0.1988054952434624	T	T
0.9152896764840861	0.4163752750174083	0.1988054952434624	T	T
0.4162164767221626	0.5837902120810341	0.1987747806093267	T	T
0.9162164767221626	0.5837902120810341	0.1987747806093267	T	T
0.4178107981347381	0.7499947298943539	0.1990501375239617	T	T
0.9178107981347381	0.7499947298943539	0.1990501375239617	T	T
0.4152896764840861	0.9163752750174083	0.1988054952434624	T	T
0.9152896764840861	0.9163752750174083	0.1988054952434624	T	T
0.0817171116116242	0.0826140610991217	0.2981217847156188	T	T
0.5817171116116242	0.0826140610991217	0.2981217847156188	T	T
0.0858995970445733	0.2498669021914424	0.2989205557622938	T	T
0.5858995970445733	0.2498669021914424	0.2989205557622938	T	T
0.0803523638631702	0.4185995425479163	0.2974973119107602	T	T
0.5803523638631702	0.4185995425479163	0.2974973119107602	T	T
0.0817171116116242	0.5826140610991217	0.2981217847156188	T	T
0.5817171116116242	0.5826140610991217	0.2981217847156188	T	T
0.0858995970445733	0.7498669021914424	0.2989205557622938	T	T
0.5858995970445733	0.7498669021914424	0.2989205557622938	T	T
0.0803523638631702	0.9185995425479163	0.2974973119107602	T	T
0.5803523638631702	0.9185995425479163	0.2974973119107602	T	T
0.3339763614449822	0.0009576411698689	0.2976286317434429	T	T
0.8339763614449822	0.0009576411698689	0.2976286317434429	T	T
0.3328142930816469	0.1679872671429976	0.2976529881887373	T	T
0.8328142930816469	0.1679872671429976	0.2976529881887373	T	T
0.3320738498202189	0.3326939396734971	0.2972786984294302	T	T
0.8320738498202189	0.3326939396734971	0.2972786984294302	T	T
0.3339763614449822	0.5009576411698689	0.2976286317434429	T	T
0.8339763614449822	0.5009576411698689	0.2976286317434429	T	T
0.3328142930816469	0.6679872671429976	0.2976529881887373	T	T
0.8328142930816469	0.6679872671429976	0.2976529881887373	T	T
0.3320738498202189	0.8326939396734971	0.2972786984294302	T	T
0.8320738498202189	0.8326939396734971	0.2972786984294302	T	T
0.4988436811815191	0.9991367779856617	0.4023281112784147	T	T
0.9988436811815191	0.9991367779856617	0.4023281112784147	T	T
0.0006347446568356	0.1674225554621884	0.3961721881002802	T	T
0.5006347446568356	0.1674225554621884	0.3961721881002802	T	T
0.4986285562585167	0.3345512326440314	0.3957009573999457	T	T

0.9986285562585167	0.3345512326440314	0.3957009573999457	T	T
0.4988436811815191	0.4991367779856617	0.4023281112784147	T	T
0.9988436811815191	0.4991367779856617	0.4023281112784147	T	T
0.0006347446568356	0.6674225554621884	0.3961721881002802	T	T
0.5006347446568356	0.6674225554621884	0.3961721881002802	T	T
0.4986285562585167	0.8345512326440314	0.3957009573999457	T	T
0.9986285562585167	0.8345512326440314	0.3957009573999457	T	T
0.2464773919879022	0.0843376891213339	0.3957881334683790	T	T
0.7464773919879022	0.0843376891213339	0.3957881334683790	T	T
0.2472117410951924	0.2529257352601633	0.4018663838032595	T	T
0.7472117410951924	0.2529257352601633	0.4018663838032595	T	T
0.2474768072181845	0.4176280381870967	0.3951126907024971	T	T
0.7474768072181845	0.4176280381870967	0.3951126907024971	T	T
0.2464773919879022	0.5843376891213339	0.3957881334683790	T	T
0.7464773919879022	0.5843376891213339	0.3957881334683790	T	T
0.2472117410951924	0.7529257352601633	0.4018663838032595	T	T
0.7472117410951924	0.7529257352601633	0.4018663838032595	T	T
0.2474768072181845	0.9176280381870967	0.3951126907024971	T	T
0.7474768072181845	0.9176280381870967	0.3951126907024971	T	T

S3.8 tc, POSCAR center

0.0940910129503646	0.9946130329697714	0.5404535479063851	T	T
0.5940910129503646	0.9946130329697714	0.5404535479063851	T	T
0.1474395600354627	0.2508950453481675	0.5432671014773188	T	T
0.6474395600354628	0.2508950453481675	0.5432671014773188	T	T
0.3680710627963125	0.4456806335075898	0.5322486666991929	T	T
0.8680710627963125	0.4456806335075898	0.5322486666991929	T	T
0.3778725865368026	0.8033333840942137	0.5342573337733219	T	T
0.8778725865368026	0.8033333840942137	0.5342573337733219	T	T
0.1602381566224454	0.0408496913075966	0.5276134005905869	T	T
0.6602381566224453	0.0408496913075966	0.5276134005905869	T	T
0.0734206597183532	0.9983550028810609	0.5854371810131256	T	T
0.5734206597183461	0.9983550028810609	0.5854371810131256	T	T
0.1406483780006290	0.9397488974685920	0.5305411316990923	T	T
0.6406483780006290	0.9397488974685920	0.5305411316990923	T	T
0.0825555137111122	0.2040457457056815	0.5304095769415640	T	T
0.5825555137111122	0.2040457457056815	0.5304095769415640	T	T
0.0982820830266120	0.3052998656024823	0.5343788572446794	T	T
0.5982820830266120	0.3052998656024823	0.5343788572446794	T	T
0.1697366211236436	0.2465468215149592	0.5881133260971562	T	T
0.6697366211236436	0.2465468215149592	0.5881133260971562	T	T
0.2733790818773095	0.4521939918716095	0.5104925698884349	T	T
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0.8367048776699283	0.8610829349138438	0.5328913988711735	T	T
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0.9000200988559192	0.7871849991993636	0.5776255363433438	T	T
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0.8010391046660944	0.2493384423470944	0.5042130532549762	T	T
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S3.9 hybrid, POSCAR center

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S3.9.1 pure cis, POSCAR center

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0.8316008919006391 0.6679239903136940 0.2982876324450794 T T T
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0.9888781038483919	0.9981913829456779	0.4010119767408663	T	T
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0.5015452722325783	0.1690511082600525	0.3970459130110148	T	T
0.9990586356893452	0.3344255341653952	0.3938597070259338	T	T
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S3.9.2 pure trans, POSCAR center

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0.6613599834954940	0.0535799778669457	0.5297088904605829	T	T
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0.5866096619038288	0.0013711317568124	0.5861603212490252	T	T
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S3.10 $4\times\sqrt{3}$, frozen Au coordinates

POSCAR head and tail.

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C H S Au
2.928000000000000
3.4641016151400001 0.0000000000000000 0.0000000000000000
0.0000000000000000 4.0000619999999998 0.0000000000000000
0.0000000000000000 0.0000000000000000 8.1649658092772608
C H S Au
6 18 6 82
Selective dynamics
Direct

INSERT POSCAR CENTER HERE WITHOUT LEAVING BLANK SPACES

0.4166666666666714 0.3750000000000000 0.2000000000000028 F F F
0.9166666666666714 0.3750000000000000 0.2000000000000028 F F F
0.4166666666666714 0.1250000000000000 0.2000000000000028 F F F
0.9166666666666714 0.1250000000000000 0.2000000000000028 F F F
0.1666666666666714 0.2500000000000000 0.2000000000000028 F F F
0.6666666666666714 0.2500000000000000 0.2000000000000028 F F F
0.1666666666666714 0.0000000000000000 0.2000000000000028 F F F

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0.6666666666666714	0.0000000000000000	0.2000000000000028	F	F	F
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0.6666666666666714	0.5000000000000000	0.2000000000000028	F	F	F
0.4166666666666714	0.8750000000000000	0.2000000000000028	F	F	F
0.9166666666666714	0.8750000000000000	0.2000000000000028	F	F	F
0.4166666666666714	0.6250000000000000	0.2000000000000028	F	F	F
0.9166666666666714	0.6250000000000000	0.2000000000000028	F	F	F
0.1666666666666714	0.7500000000000000	0.2000000000000028	F	F	F
0.6666666666666714	0.7500000000000000	0.2000000000000028	F	F	F
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0.7500000000000000	0.1250000000000000	0.1000000000000014	F	F	F
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0.5000000000000000	0.0000000000000000	0.1000000000000014	F	F	F
0.0000000000000000	0.2500000000000000	0.1000000000000014	F	F	F
0.5000000000000000	0.2500000000000000	0.1000000000000014	F	F	F
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0.7500000000000000	0.6250000000000000	0.1000000000000014	F	F	F
0.2500000000000000	0.3750000000000000	0.1000000000000014	F	F	F
0.7500000000000000	0.3750000000000000	0.1000000000000014	F	F	F
0.0000000000000000	0.5000000000000000	0.1000000000000014	F	F	F
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0.0000000000000000	0.7500000000000000	0.1000000000000014	F	F	F
0.5000000000000000	0.7500000000000000	0.1000000000000014	F	F	F
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0.7500000000000000	0.8750000000000000	0.1000000000000014	F	F	F
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0.583333333333286	0.3750000000000000	0.0000000000000000	F	F	F
0.083333333333286	0.1250000000000000	0.0000000000000000	F	F	F
0.583333333333286	0.1250000000000000	0.0000000000000000	F	F	F
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S3.10.1 iso1, POSCAR center

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0.5988982958386160	0.0153694773349500	0.5465911952484817	T	T	T
0.1640310869629147	0.4019695488949040	0.5421415536747247	T	T	T
0.6640310869629147	0.4019695488949040	0.5421415536747247	T	T	T
0.3728494224661603	0.7245662661570762	0.5256703038819666	T	T	T
0.8728494224661603	0.7245662661570762	0.5256703038819666	T	T	T
0.0736114259968943	0.0382404571091115	0.5898345393373106	T	T	T
0.5736114259968943	0.0382404571091115	0.5898345393373106	T	T	T
0.1415190514404969	0.9291162695781807	0.5451838637632562	T	T	T
0.6415190514404969	0.9291162695781807	0.5451838637632562	T	T	T
0.1706934924478745	0.0761144832005982	0.5295146352679012	T	T	T
0.6706934924478745	0.0761144832005982	0.5295146352679012	T	T	T
0.1219193294491063	0.4864103206533485	0.5331647065046283	T	T	T
0.6219193294491063	0.4864103206533485	0.5331647065046283	T	T	T
0.0927471839356784	0.3356005116954535	0.5304850340312512	T	T	T
0.5927471839356784	0.3356005116954535	0.5304850340312512	T	T	T
0.1889533403360559	0.3957186257247542	0.5867347728355412	T	T	T
0.6889533403360559	0.3957186257247542	0.5867347728355412	T	T	T
0.3588424323398058	0.7755012956578611	0.5638060427693787	T	T	T
0.8588424323398058	0.7755012956578611	0.5638060427693787	T	T	T
0.3840256538632758	0.6339050495471596	0.5363205279321761	T	T	T
0.8840256538632758	0.6339050495471596	0.5363205279321761	T	T	T
0.4618030154698332	0.7539243420163828	0.5037447159777741	T	T	T
0.9618030154698332	0.7539243420163828	0.5037447159777741	T	T	T
0.4486771724601368	0.0120395022282054	0.5053093929361268	T	T	T
0.9486771724601368	0.0120395022282054	0.5053093929361268	T	T	T
0.3146806316443858	0.3899618868096510	0.5014493510486417	T	T	T
0.8146806316443858	0.3899618868096510	0.5014493510486417	T	T	T
0.2256753673880354	0.7406904025540513	0.4825929678711702	T	T	T
0.7256753673880354	0.7406904025540513	0.4825929678711702	T	T	T
0.3785073931961449	0.1999033724636803	0.5007015742774001	T	T	T
0.8785073931961449	0.1999033724636803	0.5007015742774001	T	T	T
0.2499300873818413	0.1265249890705960	0.3960843127637972	T	T	T
0.7499300873818413	0.1265249890705960	0.3960843127637972	T	T	T
0.0053827237040522	0.9988887908483619	0.4034879086964978	T	T	T
0.5053827237040522	0.9988887908483619	0.4034879086964978	T	T	T
0.0023941313753824	0.2504022224471072	0.3957332217889089	T	T	T
0.5023941313753824	0.2504022224471072	0.3957332217889089	T	T	T
0.2516190618700165	0.6191394017748522	0.3997127148283823	T	T	T
0.7516190618700165	0.6191394017748522	0.3997127148283823	T	T	T
0.2489806486399644	0.3732745560698305	0.4005081834315405	T	T	T
0.7489806486399644	0.3732745560698305	0.4005081834315405	T	T	T

0.0028893548122042	0.5002193935646133	0.3952619124948455	T	T
0.5028893548122042	0.5002193935646133	0.3952619124948455	T	T
0.9974089563281581	0.7468076216934492	0.3906969123880444	T	T
0.4974089563281581	0.7468076216934492	0.3906969123880444	T	T
0.2542576966506900	0.8782421653296879	0.4025112628183223	T	T
0.7542576966506900	0.8782421653296879	0.4025112628183223	T	T
0.3332297808276294	0.9967051389864139	0.3012828159590129	T	T
0.8332297808276294	0.9967051389864139	0.3012828159590129	T	T
0.0848709516064687	0.3731782289206294	0.2987717374368444	T	T
0.5848709516064687	0.3731782289206294	0.2987717374368444	T	T
0.0809074349502055	0.1226797713159442	0.2987470805260202	T	T
0.5809074349502055	0.1226797713159442	0.2987470805260202	T	T
0.3308004510293330	0.5013319503926397	0.2995516459948107	T	T
0.8308004510293330	0.5013319503926397	0.2995516459948107	T	T
0.3325213754287333	0.2508172760371750	0.2975777077478696	T	T
0.8325213754287333	0.2508172760371750	0.2975777077478696	T	T
0.0834171534649641	0.8790871740637343	0.2998018289374045	T	T
0.5834171534649641	0.8790871740637343	0.2998018289374045	T	T
0.0835430976897342	0.6242770420823689	0.2965898926483348	T	T
0.5835430976897342	0.6242770420823689	0.2965898926483348	T	T
0.3288541574971475	0.7504496850801416	0.2970354410974778	T	T
0.8288541574971475	0.7504496850801416	0.2970354410974778	T	T

S3.10.2 iso2, POSCAR center

0.3572658174578791	0.9737849084772563	0.5511503629911303	T	T
0.8572658174578791	0.9737849084772563	0.5511503629911303	T	T
0.1524201986256344	0.4073204224602165	0.5401591080513271	T	T
0.6524201986256344	0.4073204224602165	0.5401591080513271	T	T
0.3774311207381089	0.7002117255796065	0.5213185573594075	T	T
0.8774311207381089	0.7002117255796065	0.5213185573594075	T	T
0.2685583679651842	0.9617525211807276	0.5256558833358937	T	T
0.7685583679651842	0.9617525211807276	0.5256558833358937	T	T
0.3943628918315554	0.8913210523022030	0.5657163663764493	T	T
0.8943628918315483	0.8913210523022030	0.5657163663764493	T	T
0.3339563662887883	0.0275238071426145	0.5874139852666360	T	T
0.8339563662887883	0.0275238071426145	0.5874139852666360	T	T
0.0982093134282565	0.4841846287735549	0.5274622062339489	T	T
0.5982093134282565	0.4841846287735549	0.5274622062339489	T	T
0.0906236299646750	0.3316874212185681	0.5331807402384214	T	T
0.5906236299646750	0.3316874212185681	0.5331807402384214	T	T
0.1803060819307021	0.4133466556567953	0.5843868248544126	T	T
0.6803060819307021	0.4133466556567953	0.5843868248544126	T	T
0.9568072709725541	0.7594555196933825	0.5099981076366618	T	T
0.4568072709725541	0.7594555196933825	0.5099981076366618	T	T
0.3557056341684017	0.7071813412779875	0.5662567848445761	T	T
0.8557056341684017	0.7071813412779875	0.5662567848445761	T	T
0.4081688350771273	0.6126517018653672	0.5118434013348931	T	T
0.9081688350771273	0.6126517018653672	0.5118434013348931	T	T
0.4881700584301143	0.0440707413841182	0.5115192224838196	T	T
0.9881700584301143	0.0440707413841182	0.5115192224838196	T	T
0.3017784685015599	0.4017460730491393	0.4985914481457243	T	T
0.8017784685015599	0.4017460730491393	0.4985914481457243	T	T
0.2249628358371609	0.7316662031451386	0.4835672032013960	T	T
0.7249628358371609	0.7316662031451386	0.4835672032013960	T	T
0.3845447681010654	0.2180361313474108	0.5006300128066457	T	T
0.8845447681010654	0.2180361313474108	0.5006300128066457	T	T
0.2458099313214106	0.1239284475381695	0.3984014075624458	T	T
0.7458099313214106	0.1239284475381695	0.3984014075624458	T	T
0.9958271922120048	0.9958956274718247	0.4074523519586606	T	T
0.4958271922120048	0.9958956274718247	0.4074523519586606	T	T
0.9983325279534654	0.2487367485502077	0.3939748634934617	T	T
0.4983325279534654	0.2487367485502077	0.3939748634934617	T	T
0.2433920805685545	0.6198471569597857	0.3973873335519897	T	T
0.7433920805685545	0.6198471569597857	0.3973873335519897	T	T
0.2421259825872468	0.3723321771769790	0.3989510305323165	T	T
0.7421259825872468	0.3723321771769790	0.3989510305323165	T	T
0.9960711990995321	0.4998480213166729	0.3938891744225472	T	T
0.4960711990995321	0.4998480213166729	0.3938891744225472	T	T
0.9908156146810683	0.7477356750826019	0.3911889400225448	T	T
0.4908156146810683	0.7477356750826019	0.3911889400225448	T	T
0.2465871682851528	0.8764450156199857	0.4041418787547642	T	T
0.7465871682851528	0.8764450156199857	0.4041418787547642	T	T
0.3322215799492554	0.9964459578470795	0.3027043069218180	T	T
0.8322215799492554	0.9964459578470795	0.3027043069218180	T	T
0.0817229910606230	0.3726682042227765	0.2978996920862258	T	T
0.5817229910606230	0.3726682042227765	0.2978996920862258	T	T
0.079922856388369	0.1216207479216749	0.2991048113530113	T	T
0.579922856388369	0.1216207479216749	0.2991048113530113	T	T
0.3271153363210928	0.5012170163889067	0.2987073319288882	T	T
0.8271153363210928	0.5012170163889067	0.2987073319288882	T	T
0.3292413865499171	0.2489947005904725	0.2976602588964283	T	T
0.8292413865499171	0.2489947005904725	0.2976602588964283	T	T
0.0815058526770827	0.8798096391930059	0.3007782289105094	T	T
0.5815058526770827	0.8798096391930059	0.3007782289105094	T	T
0.0793722429673736	0.6250422357965633	0.2962756823069341	T	T

0.5793722429673736	0.6250422357965633	0.2962756823069341	T	T
0.3261897174327970	0.7512604547779134	0.2967967744929467	T	T
0.8261897174327970	0.7512604547779134	0.2967967744929467	T	T

S3.10.3 iso3, POSCAR center

0.1114083377024926	0.0217619425861457	0.5433547546211486	T	T
0.6114083377024926	0.0217619425861457	0.5433547546211486	T	T
0.3891514633554252	0.4639424836714241	0.5308811676319820	T	T
0.8891514633554252	0.4639424836714241	0.5308811676319820	T	T
0.1145729110815452	0.7219489357256137	0.5242710113931466	T	T
0.6145729110815452	0.7219489357256137	0.5242710113931466	T	T
0.1556171819725165	0.1065757337825772	0.5381375985625212	T	T
0.6556171819725165	0.1065757337825772	0.5381375985625212	T	T
0.0886319299705036	0.0072673179655425	0.5877322162265060	T	T
0.5886319299705036	0.0072673179655425	0.5877322162265060	T	T
0.1812145219067958	0.9571093036386955	0.5282274535966849	T	T
0.6812145219067958	0.9571093036386955	0.5282274535966849	T	T
0.3537442131756379	0.5512632800086692	0.5232044579083919	T	T
0.8537442131756379	0.5512632800086692	0.5232044579083919	T	T
0.4044815028705173	0.4499825656377539	0.5758275028270958	T	T
0.9044815028705173	0.4499825656377539	0.5758275028270958	T	T
0.9821459122721379	0.4505065017505103	0.5082796682333921	T	T
0.4821459122721379	0.4505065017505103	0.5082796682333921	T	T
0.1210570303029854	0.7729010301701607	0.5627491608202959	T	T
0.6210570303029854	0.7729010301701607	0.5627491608202959	T	T
0.0253641461566403	0.7462276212111689	0.5011740147221317	T	T
0.5253641461566403	0.7462276212111689	0.5011740147221317	T	T
0.1090283312570719	0.6309343257784334	0.5350333828125287	T	T
0.6090283312570719	0.6309343257784334	0.5350333828125287	T	T
0.4587733060247885	0.0082665941473223	0.5041907806188419	T	T
0.9587733060247885	0.0082665941473223	0.5041907806188419	T	T
0.2629825775723802	0.3646525436141843	0.5068970626592844	T	T
0.7629825775723802	0.3646525436141843	0.5068970626592844	T	T
0.2642024584761913	0.7465997318176534	0.4839603986861789	T	T
0.7642024584761913	0.7465997318176534	0.4839603986861789	T	T
0.3718813472377533	0.1912135140090285	0.5008453644697326	T	T
0.8718813472377533	0.1912135140090285	0.5008453644697326	T	T
0.2460456516754519	0.1283364644769804	0.3956467114672364	T	T
0.7460456516754519	0.1283364644769804	0.3956467114672364	T	T
0.0007405082486969	0.0024131910443401	0.4020288244124757	T	T
0.5007405082486969	0.0024131910443401	0.4020288244124757	T	T
0.0000305644132439	0.2540470872185594	0.3972433051124327	T	T
0.5000305644132439	0.2540470872185594	0.3972433051124327	T	T
0.2511491499942196	0.6235289476970607	0.4003426386563262	T	T
0.7511491499942196	0.6235289476970607	0.4003426386563262	T	T
0.2505034073821477	0.3781975768894839	0.4025109423255131	T	T
0.7505034073821477	0.3781975768894839	0.4025109423255131	T	T
0.0036681060222676	0.5026298144745951	0.3949825808831164	T	T
0.5036681060222676	0.5026298144745951	0.3949825808831164	T	T
0.9986414052561017	0.7495883038211559	0.3900530448538717	T	T
0.4986414052561017	0.7495883038211559	0.3900530448538717	T	T
0.2472212959053977	0.8797444113776720	0.4011893027124813	T	T
0.7472212959053977	0.8797444113776720	0.4011893027124813	T	T
0.3332928028110089	0.9981187998081538	0.3010121383389190	T	T
0.8332928028110089	0.9981187998081538	0.3010121383389190	T	T
0.0845696524793453	0.3731856775276938	0.2989508853035616	T	T
0.5845696524793453	0.3731856775276938	0.2989508853035616	T	T
0.0804390131856465	0.1245986262303234	0.2987136538314488	T	T
0.5804390131856465	0.1245986262303234	0.2987136538314488	T	T
0.3296602109668214	0.5006758269846543	0.3005975502844223	T	T
0.8296602109668214	0.5006758269846543	0.3005975502844223	T	T
0.3326963067435358	0.2519405690478536	0.2980370001000381	T	T
0.8326963067435358	0.2519405690478536	0.2980370001000381	T	T
0.0836772770997953	0.8798936664865096	0.2985525930318929	T	T
0.5836772770997953	0.8798936664865096	0.2985525930318929	T	T
0.0837965641262457	0.6242401570668790	0.2962806057451886	T	T
0.5837965641262457	0.6242401570668790	0.2962806057451886	T	T
0.3293893524619804	0.7508308857550716	0.2971363335501422	T	T
0.8293893524619804	0.7508308857550716	0.2971363335501422	T	T

S3.10.4 iso4, POSCAR center

0.3724585444176327	0.9045622991197391	0.5322343301898940	T	T
0.8724585444176327	0.9045622991197391	0.5322343301898940	T	T
0.3582671256526595	0.4166255861082107	0.5518001998730213	T	T
0.8582671256526595	0.4166255861082107	0.5518001998730213	T	T
0.1199907590264715	0.6458107629933565	0.5260960575645441	T	T
0.6199907590264715	0.6458107629933565	0.5260960575645441	T	T
0.4104620246749349	0.8178804112024025	0.5252880083677596	T	T

0.9104620246749349	0.8178804112024025	0.5252880083677596	T	T
0.3560783355550612	0.9199069738756620	0.5770198122732353	T	T
0.8560783355550612	0.9199069738756620	0.5770198122732353	T	T
0.2792666003817246	0.9143092193168485	0.5093304304633577	T	T
0.7792666003817246	0.9143092193168485	0.5093304304633577	T	T
0.9584496294171956	0.4126608533389700	0.5347699346068708	T	T
0.4584496294171956	0.4126608533389700	0.5347699346068708	T	T
0.3257281967520953	0.5057297020701270	0.5533048510206910	T	T
0.8257281967520953	0.5057297020701270	0.5533048510206910	T	T
0.3562420819055916	0.3790647774499405	0.5938565779649707	T	T
0.8562420819055916	0.3790647774499405	0.5938565779649707	T	T
0.2134734000310843	0.6392583656701873	0.5031903472455213	T	T
0.7134734000310843	0.6392583656701873	0.5031903472455213	T	T
0.1157011303980369	0.7289529551699445	0.5473662710583653	T	T
0.6157011303980369	0.7289529551699445	0.5473662710583653	T	T
0.1128799060379677	0.5767711527327108	0.5570922322417005	T	T
0.6128799060379677	0.5767711527327108	0.5570922322417005	T	T
0.4948360008073820	0.0069740739391335	0.5074396269861339	T	T
0.9948360008073820	0.0069740739391335	0.5074396269861339	T	T
0.2443157315925291	0.3350853674227494	0.5082479479966651	T	T
0.7443157315925291	0.3350853674227494	0.5082479479966651	T	T
0.9786144059143922	0.6335409708430078	0.4794587518494069	T	T
0.4786144059143922	0.6335409708430078	0.4794587518494069	T	T
0.3691645981755940	0.1707481583190429	0.5008174503415006	T	T
0.8691645981755940	0.1707481583190429	0.5008174503415006	T	T
0.2506893011996638	0.1228566485354037	0.3955293454062883	T	T
0.7506893011996638	0.1228566485354037	0.3955293454062883	T	T
0.0032690720365522	0.0002028094041293	0.4027144829401408	T	T
0.5032690720365522	0.0002028094041293	0.4027144829401408	T	T
0.0051427385828120	0.2482894012762245	0.3980892721320473	T	T
0.5051427385828120	0.2482894012762245	0.3980892721320473	T	T
0.2528712809773239	0.6269727423778804	0.3899623299400901	T	T
0.7528712809773239	0.6269727423778804	0.3899623299400901	T	T
0.2621072022712312	0.3772138455496687	0.4048842218015452	T	T
0.7621072022712312	0.3772138455496687	0.4048842218015452	T	T
0.0129119802120670	0.4944397655303234	0.4019539282050317	T	T
0.5129119802120670	0.4944397655303234	0.4019539282050317	T	T
0.0080186065368935	0.7569271326777383	0.3983762918619576	T	T
0.5080186065368935	0.7569271326777383	0.3983762918619576	T	T
0.2558122580750393	0.8749030903774795	0.3943314369183284	T	T
0.7558122580750393	0.8749030903774795	0.3943314369183284	T	T
0.3359482028028253	0.0015196939329627	0.2977981699314043	T	T
0.8359482028028253	0.0015196939329627	0.2977981699314043	T	T
0.0871777791554464	0.3755060615410528	0.3023275460526236	T	T
0.5871777791554464	0.3755060615410528	0.3023275460526236	T	T
0.0832996830954116	0.1238290879049515	0.2990776866452265	T	T
0.5832996830954116	0.1238290879049515	0.2990776866452265	T	T
0.3364519540534587	0.4940540741185018	0.2996556739589309	T	T
0.8364519540534587	0.4940540741185018	0.2996556739589309	T	T
0.3338100279263543	0.2508899459321370	0.2986678748105902	T	T
0.8338100279263543	0.2508899459321370	0.2986678748105902	T	T
0.0811721373995127	0.8748603384174416	0.2997105091135808	T	T
0.5811721373995127	0.8748603384174416	0.2997105091135808	T	T
0.0803115258997877	0.6232617835470862	0.2970290929175832	T	T
0.5803115258997877	0.6232617835470862	0.2970290929175832	T	T
0.3346282615725542	0.7502688892622089	0.2961508978458411	T	T
0.8346282615725542	0.7502688892622089	0.2961508978458411	T	T

S3.10.5 iso5, POSCAR center

0.0925740731326599	0.9822597975985019	0.5415644761186584	T	T
0.5925740731326599	0.9822597975985019	0.5415644761186584	T	T
0.3741565333963806	0.4164865835933043	0.5510501324604888	T	T
0.8741565333963806	0.4164865835933043	0.5510501324604888	T	T
0.1140918100166601	0.6446275153248493	0.5255420108713054	T	T
0.6140918100166601	0.6446275153248493	0.5255420108713054	T	T
0.1515722672308470	0.0588941734938473	0.5329936924061016	T	T
0.6515722672308470	0.0588941734938473	0.5329936924061016	T	T
0.0661767555627577	0.9792355433640765	0.5860926096491852	T	T
0.5661767555627577	0.9792355433640765	0.5860926096491852	T	T
0.1503345480369447	0.9065370292978372	0.5300420101486338	T	T
0.6503345480369447	0.9065370292978372	0.5300420101486338	T	T
0.9726245942217915	0.4077077783433367	0.5326822231743691	T	T
0.4726245942217915	0.4077077783433367	0.5326822231743691	T	T
0.3467813277326570	0.5070455635184743	0.5521372383431924	T	T
0.8467813277326570	0.5070455635184743	0.5521372383431924	T	T
0.3733572768778899	0.3808023148973447	0.5935244541859817	T	T
0.8733572768778899	0.3808023148973447	0.5935244541859817	T	T
0.1936227717731285	0.6969908727278096	0.5079737526710630	T	T
0.6936227717731285	0.6969908727278096	0.5079737526710630	T	T
0.0819540298054093	0.6799875773462603	0.5658860482032395	T	T
0.5819540298054093	0.6799875773462603	0.5658860482032395	T	T
0.1493810371611204	0.5569405275628014	0.5314372634506128	T	T
0.6493810371611204	0.5569405275628014	0.5314372634506128	T	T
0.4418183500811637	0.9812239521749078	0.5006492547791552	T	T
0.9418183500811637	0.9812239521749078	0.5006492547791552	T	T

0.2517473708965738	0.3390162057554562	0.5100047796002798	T	T	T
0.7517473708965738	0.3390162057554562	0.5100047796002798	T	T	T
0.9705749633008267	0.6415825560981716	0.4794129907030467	T	T	T
0.4705749633008267	0.6415825560981716	0.4794129907030467	T	T	T
0.3583425057326721	0.1651722232773096	0.5015122656917796	T	T	T
0.8583425057326721	0.1651722232773096	0.5015122656917796	T	T	T
0.2466935245699986	0.1285582472742348	0.3941196846696755	T	T	T
0.7466935245699986	0.1285582472742348	0.3941196846696755	T	T	T
0.0028397350849332	0.0069893020911493	0.4003578249912678	T	T	T
0.5028397350849332	0.0069893020911493	0.4003578249912678	T	T	T
0.9997310368764758	0.2530396370578600	0.3991012515651278	T	T	T
0.4997310368764758	0.2530396370578600	0.3991012515651278	T	T	T
0.2468335530391101	0.6297265616404175	0.3904256601156533	T	T	T
0.7468335530391101	0.6297265616404175	0.3904256601156533	T	T	T
0.2551328188836592	0.3809363939832551	0.4057960838340051	T	T	T
0.7551328188836592	0.3809363939832551	0.4057960838340051	T	T	T
0.0054862229845796	0.4996980633333834	0.4029976559932962	T	T	T
0.5054862229845867	0.4996980633333834	0.4029976559932962	T	T	T
0.0043815510438847	0.7622518488709034	0.3980046236791708	T	T	T
0.5043815510438847	0.7622518488709034	0.3980046236791708	T	T	T
0.2526089679193646	0.8786669192362098	0.3942532922319302	T	T	T
0.7526089679193646	0.8786669192362098	0.3942532922319302	T	T	T
0.3338285779832901	0.0031076256392097	0.2973320385780340	T	T	T
0.8338285779832901	0.0031076256392097	0.2973320385780340	T	T	T
0.0861144962716551	0.3782735238225214	0.3033380159423729	T	T	T
0.5861144962716551	0.3782735238225214	0.3033380159423729	T	T	T
0.0808032036493387	0.1262579267765531	0.2984834336399942	T	T	T
0.5808032036493387	0.1262579267765531	0.2984834336399942	T	T	T
0.3349794730061859	0.4966330957679261	0.2999495412181474	T	T	T
0.8349794730061859	0.4966330957679261	0.2999495412181474	T	T	T
0.3329013215321623	0.2536881761354195	0.2983173410444238	T	T	T
0.8329013215321623	0.2536881761354195	0.2983173410444238	T	T	T
0.0803805410852902	0.8761823066975722	0.2990620243258491	T	T	T
0.5803805410852902	0.8761823066975722	0.2990620243258491	T	T	T
0.0788464709175400	0.6250114047778652	0.2969954379219431	T	T	T
0.5788464709175400	0.6250114047778652	0.2969954379219431	T	T	T
0.3334215923680262	0.7517493807104572	0.2964808368177287	T	T	T
0.8334215923680262	0.7517493807104572	0.2964808368177287	T	T	T

S3.10.6 iso6, POSCAR center

0.1141917151705529	0.0290708730235980	0.5432378083376098	T	T	T
0.6144278179470637	0.0286212216769079	0.5431828548251593	T	T	T
0.1541811008483605	0.3864687145788975	0.5415556096589254	T	T	T
0.6539831734191121	0.3865349292573333	0.5414752111928466	T	T	T
0.1036135424963774	0.7326954276408385	0.5203491109209190	T	T	T
0.6041630984296683	0.7332944776659728	0.5204760602433700	T	T	T
0.0928258131814020	0.0302610253678945	0.5882491335946197	T	T	T
0.5931843473753995	0.0285961889027470	0.5882169549659521	T	T	T
0.1778552332856518	0.9562782866592711	0.5329244235157985	T	T	T
0.6783204147820332	0.9562852344635132	0.5323928434241716	T	T	T
0.1659103059048064	0.1077831983757759	0.5312781030373078	T	T	T
0.6657288661713513	0.1077883434380412	0.5316631972924521	T	T	T
0.1018179431600291	0.4662376692631610	0.5322330267955373	T	T	T
0.6011441679679922	0.4659528825322431	0.5318263049310119	T	T	T
0.0908393802805634	0.3144471250511667	0.5296128654989946	T	T	T
0.5909893900030097	0.3140792253531834	0.5297768261337933	T	T	T
0.1776167147517078	0.3820021520356965	0.5863375642718306	T	T	T
0.6772638641301096	0.3828585824582991	0.5863066244200630	T	T	T
0.1244915166898600	0.7438585658477349	0.5651744137369996	T	T	T
0.6248635988776446	0.7473138244097701	0.5651148929022241	T	T	T
0.0577081133668089	0.6492575007916022	0.5131713034227842	T	T	T
0.5594770017965042	0.6489535613282837	0.5144803242670843	T	T	T
0.0349642343674408	0.7994502298995750	0.5065667698423787	T	T	T
0.5344924450476741	0.7984741876334230	0.5057904874052914	T	T	T
0.4599476724695630	0.0139489566678052	0.5055206393953554	T	T	T
0.9599188450327457	0.0140222327233860	0.5055570242559272	T	T	T
0.3070467632860354	0.3863818020648504	0.5020809435117768	T	T	T
0.8069461610948567	0.3864052733348401	0.5020914455781459	T	T	T
0.2611106702537927	0.7430652545048619	0.4838702806331509	T	T	T
0.7614676130474285	0.7431165217165082	0.4838443600543936	T	T	T
0.3797662065917435	0.1989628238430714	0.5003888882093913	T	T	T
0.8796225729675574	0.1990746481706140	0.5003913304398866	T	T	T
0.2500479352462776	0.1260210751913688	0.3962298643690707	T	T	T
0.7500390309861845	0.1260274775143308	0.3962298412359573	T	T	T
0.0048898960184868	0.9998140965075969	0.4030391869072903	T	T	T
0.5048779998653339	0.9997946038441672	0.4030276061116488	T	T	T
0.0025361143217428	0.2508484624554921	0.3955894307740019	T	T	T
0.5025447625740744	0.2508534628109861	0.3955812706421429	T	T	T
0.2507786225388960	0.6203420076965730	0.4002611470109921	T	T	T
0.7506717220389035	0.6203668412943019	0.4002829256942088	T	T	T
0.2480507708073800	0.3742555243938909	0.4006516322164704	T	T	T
0.7480732147226276	0.3742551733320825	0.4006455633526641	T	T	T
0.0028827069276328	0.4998290340592592	0.3952650227488782	T	T	T
0.5028936262235598	0.4998236407423186	0.3952734767952943	T	T	T
0.9998660394998847	0.7466392019460728	0.3902175790028296	T	T	T

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0.4998337632279820 0.7466158861054968 0.3902385776531015 T T T
0.2513527495121127 0.8777037907769666 0.4022983148247709 T T T
0.7514408168759686 0.8777417458658323 0.4022644938537996 T T T
0.3339241437465862 0.9969472848082700 0.3014719263350484 T T T
0.8339307556690825 0.9969623216739854 0.3014628295471688 T T T
0.0849236726503329 0.3729841146213695 0.2984047049706966 T T T
0.5849184126295064 0.3729931359761575 0.2984068698700971 T T T
0.0814817038016206 0.1229353904196653 0.2985119433110938 T T T
0.5814819498198307 0.1229390811245818 0.2985056747936300 T T T
0.3305218179990608 0.5007224756712187 0.2999760908279323 T T T
0.8305120440736690 0.5007247502512890 0.2999804131769772 T T T
0.3328469683115987 0.2507255809338254 0.2977794961284600 T T T
0.8328468997210934 0.2507285689525066 0.2977801225542593 T T T
0.0839111843832892 0.8791670332142280 0.2991946254939345 T T T
0.5839155172261059 0.8791506463478166 0.2992055041027563 T T T
0.0839253359701665 0.6235059955365875 0.2962582273378584 T T T
0.5839262745190842 0.6235147835287626 0.2962568699650477 T T T
0.3295905631433221 0.7505019768575031 0.2974647364547629 T T T
0.8295909048089084 0.7504867139818800 0.2974673070139922 T T T

```

S3.11 $5\times\sqrt{3}$, frozen Au coordinates

POSCAR head and tail.

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POSCAR_MOM_Au_PURE_CARTESIAN_16A_VOID_5L
2.928000000000000
3.4641016151400001 0.0000000000000000 0.0000000000000000
0.0000000000000000 5.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 8.1649658092772608
C H S Au
8 24 8 102
Selective dynamics
Direct

INSERT POSCAR CENTER HERE WITHOUT LEAVING BLANK SPACES

0.4166666664999994 0.2999999999999972 0.20000000000000028 F F F
0.9166666664999994 0.2999999999999972 0.20000000000000028 F F F
0.4166666664999994 0.10000000000000014 0.20000000000000028 F F F
0.9166666664999994 0.10000000000000014 0.20000000000000028 F F F
0.1666666664999994 0.20000000000000028 0.20000000000000028 F F F
0.6666666664999994 0.20000000000000028 0.20000000000000028 F F F
0.1666666664999994 0.0000000000000000 0.20000000000000028 F F F
0.6666666664999994 0.0000000000000000 0.20000000000000028 F F F
0.1666666664999994 0.3999999999999986 0.20000000000000028 F F F
0.6666666664999994 0.3999999999999986 0.20000000000000028 F F F
0.4166666664999994 0.70000000000000028 0.20000000000000028 F F F
0.9166666664999994 0.70000000000000028 0.20000000000000028 F F F
0.4166666664999994 0.5000000000000000 0.20000000000000028 F F F
0.9166666664999994 0.5000000000000000 0.20000000000000028 F F F
0.1666666664999994 0.60000000000000014 0.20000000000000028 F F F
0.6666666664999994 0.60000000000000014 0.20000000000000028 F F F
0.2500000000000000 0.10000000000000014 0.10000000000000014 F F F
0.7500000000000000 0.10000000000000014 0.10000000000000014 F F F
0.0000000000000000 0.0000000000000000 0.10000000000000014 F F F
0.5000000000000000 0.0000000000000000 0.10000000000000014 F F F
0.0000000000000000 0.20000000000000028 0.10000000000000014 F F F
0.5000000000000000 0.20000000000000028 0.10000000000000014 F F F
0.2500000000000000 0.5000000000000000 0.10000000000000014 F F F
0.7500000000000000 0.5000000000000000 0.10000000000000014 F F F
0.2500000000000000 0.2999999999999972 0.10000000000000014 F F F
0.7500000000000000 0.2999999999999972 0.10000000000000014 F F F
0.0000000000000000 0.3999999999999986 0.10000000000000014 F F F
0.5000000000000000 0.3999999999999986 0.10000000000000014 F F F
0.0000000000000000 0.60000000000000014 0.10000000000000014 F F F
0.5000000000000000 0.60000000000000014 0.10000000000000014 F F F
0.2500000000000000 0.70000000000000028 0.10000000000000014 F F F
0.7500000000000000 0.70000000000000028 0.10000000000000014 F F F
0.3333333335000006 0.0000000000000000 0.0000000000000000 F F F
0.8333333335000006 0.0000000000000000 0.0000000000000000 F F F
0.0833333335000006 0.2999999999999972 0.0000000000000000 F F F
0.5833333335000006 0.2999999999999972 0.0000000000000000 F F F
0.0833333335000006 0.10000000000000014 0.0000000000000000 F F F
0.5833333335000006 0.10000000000000014 0.0000000000000000 F F F
0.3333333335000006 0.3999999999999986 0.0000000000000000 F F F
0.8333333335000006 0.3999999999999986 0.0000000000000000 F F F
0.3333333335000006 0.20000000000000028 0.0000000000000000 F F F
0.8333333335000006 0.20000000000000028 0.0000000000000000 F F F
0.0833333335000006 0.70000000000000028 0.0000000000000000 F F F
0.5833333335000006 0.70000000000000028 0.0000000000000000 F F F
0.0833333335000006 0.5000000000000000 0.0000000000000000 F F F
0.5833333335000006 0.5000000000000000 0.0000000000000000 F F F
0.3333333335000006 0.60000000000000014 0.0000000000000000 F F F

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0.8333333335000006	0.60000000000000014	0.0000000000000000	F	F	F
0.4166666664999994	0.8999999999999986	0.20000000000000028	F	F	F
0.9166666664999994	0.8999999999999986	0.20000000000000028	F	F	F
0.25000000000000000	0.8999999999999986	0.10000000000000014	F	F	F
0.75000000000000000	0.8999999999999986	0.10000000000000014	F	F	F
0.0833333335000006	0.8999999999999986	0.0000000000000000	F	F	F
0.5833333335000006	0.8999999999999986	0.0000000000000000	F	F	F
0.1666666664999994	0.7999999999999972	0.20000000000000028	F	F	F
0.6666666664999994	0.7999999999999972	0.20000000000000028	F	F	F
0.00000000000000000	0.7999999999999972	0.10000000000000014	F	F	F
0.50000000000000000	0.7999999999999972	0.10000000000000014	F	F	F
0.3333333335000006	0.7999999999999972	0.0000000000000000	F	F	F
0.8333333335000006	0.7999999999999972	0.0000000000000000	F	F	F

S3.11.1 iso1, POSCAR center

0.1025473080349641	0.0021115290425087	0.5450482941047952	T	T	T
0.6025473080349641	0.0021115290425087	0.5450482941047952	T	T	T
0.3733806883564554	0.3373140079040411	0.5525084928513806	T	T	T
0.8733806883564554	0.3373140079040411	0.5525084928513806	T	T	T
0.1205499273938599	0.5329184310245907	0.5253535456567491	T	T	T
0.6205499273938599	0.5329184310245907	0.5253535456567491	T	T	T
0.3663229401527275	0.7619296121908690	0.5300314403882354	T	T	T
0.8663229401527275	0.7619296121908690	0.5300314403882354	T	T	T
0.1611360761453753	0.0621538575981475	0.5332124514173699	T	T	T
0.6611360761453753	0.0621538575981475	0.5332124514173699	T	T	T
0.0746454652255721	0.0066172038192818	0.5893427691914610	T	T	T
0.5746454652255721	0.0066172038192818	0.5893427691914610	T	T	T
0.1608382774552766	0.9400836767633081	0.5373205614543934	T	T	T
0.6608382774552766	0.9400836767633081	0.5373205614543934	T	T	T
0.9714411540233741	0.3336611736823798	0.5333656512832121	T	T	T
0.4714411540233741	0.3336611736823798	0.5333656512832121	T	T	T
0.3433268389600102	0.4090146585568988	0.5559094590281646	T	T	T
0.8433268389600173	0.4090146585568988	0.5559094590281646	T	T	T
0.3752793252320146	0.3057750719855719	0.5941644805809574	T	T	T
0.8752793252320146	0.3057750719855719	0.5941644805809574	T	T	T
0.1755839382103090	0.5937631514094974	0.5121402677670304	T	T	T
0.6755839382103090	0.5937631514094974	0.5121402677670304	T	T	T
0.0850384259512325	0.5420375560728132	0.5684435732909989	T	T	T
0.5850384259512325	0.5420375560728132	0.5684435732909989	T	T	T
0.1844140579127256	0.4727676692201328	0.5228647911400444	T	T	T
0.6844140579127256	0.4727676692201328	0.5228647911400444	T	T	T
0.9296391643029693	0.7082403870135252	0.5126964873955231	T	T	T
0.4296391643029693	0.7082403870135252	0.5126964873955231	T	T	T
0.4234385395184290	0.8247697087502317	0.5360201712727601	T	T	T
0.9234385395184290	0.8247697087502317	0.5360201712727601	T	T	T
0.3255231040046951	0.7394036024398289	0.5703800658041942	T	T	T
0.8255231040046951	0.7394036024398289	0.5703800658041942	T	T	T
0.4538065742427193	0.9936609444476119	0.5035646172019952	T	T	T
0.9538065742427193	0.9936609444476119	0.5035646172019952	T	T	T
0.2516589075962088	0.2755215465667504	0.5107931631238998	T	T	T
0.7516589075962088	0.2755215465667504	0.5107931631238998	T	T	T
0.9764175048141368	0.5171315966651520	0.4805897002529633	T	T	T
0.4764175048141368	0.5171315966651520	0.4805897002529633	T	T	T
0.2260263671467726	0.7840878635537294	0.4839151675165922	T	T	T
0.7260263671467726	0.7840878635537294	0.4839151675165922	T	T	T
0.3636468700716264	0.1387407584602371	0.5013563144730213	T	T	T
0.8636468700716264	0.1387407584602371	0.5013563144730213	T	T	T
0.2477225327715900	0.1004578498483610	0.3951654608400332	T	T	T
0.7477225327715900	0.1004578498483610	0.3951654608400332	T	T	T
0.0059501615814668	0.9998853552437552	0.4022576169413270	T	T	T
0.5059501615814668	0.9998853552437552	0.4022576169413270	T	T	T
0.0015305349531474	0.1995774438493072	0.3993044570847673	T	T	T
0.5015305349531474	0.1995774438493072	0.3993044570847673	T	T	T
0.2494751758171532	0.4972409520684522	0.3912421277782769	T	T	T
0.7494751758171532	0.4972409520684522	0.3912421277782769	T	T	T
0.2572066186898496	0.3019477934404122	0.4058442346589004	T	T	T
0.7572066186898496	0.3019477934404122	0.4058442346589004	T	T	T
0.0069543937272201	0.3982440073832834	0.4037817798516556	T	T	T
0.5069543937272201	0.3982440073832834	0.4037817798516556	T	T	T
0.0093900029018172	0.6067973198130971	0.3969559904187747	T	T	T
0.5093900029018172	0.6067973198130971	0.3969559904187747	T	T	T
0.2585149645808329	0.6947953849854187	0.3989076405092788	T	T	T
0.7585149645808329	0.6947953849854187	0.3989076405092788	T	T	T
0.9981469886360941	0.8028149123235906	0.3917359136824530	T	T	T
0.4981469886360941	0.8028149123235906	0.3917359136824530	T	T	T
0.2536107545919393	0.8999448086526911	0.4026344800754131	T	T	T
0.7536107545919393	0.8999448086526911	0.4026344800754131	T	T	T
0.0856226609116888	0.9032469191358743	0.2989577751104306	T	T	T
0.5856226609116888	0.9032469191358743	0.2989577751104306	T	T	T
0.3304044550969820	0.8008469674836292	0.2973151673139753	T	T	T
0.8304044550969820	0.8008469674836292	0.2973151673139753	T	T	T
0.3354781193592231	0.9977190241503990	0.3013053904147753	T	T	T
0.8354781193592231	0.9977190241503990	0.3013053904147753	T	T	T
0.0871522161220639	0.3006170439179527	0.3037472215488393	T	T	T
0.5871522161220639	0.3006170439179527	0.3037472215488393	T	T	T

0.0802132853073800	0.1001642321385035	0.2988538332582849	T	T
0.5802132853073800	0.1001642321385035	0.2988538332582849	T	T
0.3368354372559850	0.3954332117583377	0.2995677689213636	T	T
0.8368354372559850	0.3954332117583377	0.2995677689213636	T	T
0.3331266689960088	0.2002696413085729	0.2987070013866600	T	T
0.8331266689960088	0.2002696413085729	0.2987070013866600	T	T
0.0837218350980962	0.6984511166848577	0.2983150127366585	T	T
0.5837218350980962	0.6984511166848577	0.2983150127366585	T	T
0.0803557838752198	0.4979747045177731	0.2970074025458587	T	T
0.5803557838752198	0.4979747045177731	0.2970074025458587	T	T
0.3338611696659015	0.6015501383465462	0.2986659215943277	T	T
0.8338611696659015	0.6015501383465462	0.2986659215943277	T	T

S3.11.2 iso2, POSCAR center

0.0977672900155184	0.0047577605816471	0.5465438768955835	T	T
0.5977672900155184	0.0047577605816471	0.5465438768955835	T	T
0.3828595648493263	0.3595516565321475	0.5375387754019059	T	T
0.8828595648493263	0.3595516565321475	0.5375387754019059	T	T
0.1084205011941535	0.5457834507077735	0.5304888468863993	T	T
0.6084205011941535	0.5457834507077735	0.5304888468863993	T	T
0.3406498662237141	0.7922244139933952	0.5309317945334087	T	T
0.8406498662237141	0.7922244139933952	0.5309317945334087	T	T
0.1746836186216285	0.0491237761475816	0.5291428025898526	T	T
0.6746836186216285	0.0491237761475816	0.5291428025898526	T	T
0.0692955433597717	0.0288955014263408	0.5882500384246470	T	T
0.5692955433597717	0.0288955014263408	0.5882500384246470	T	T
0.1345436823596700	0.9343777975888159	0.5488680526418648	T	T
0.6345436823596700	0.9343777975888159	0.5488680526418648	T	T
0.9785863209456451	0.3464385206186407	0.5178116532309645	T	T
0.4785863209456522	0.3464385206186407	0.5178116532309645	T	T
0.3549137106712905	0.4309524611585047	0.5298983286162695	T	T
0.8549137106712905	0.4309524611585047	0.5298983286162695	T	T
0.3892685274344885	0.3459586238531145	0.5826138994746159	T	T
0.8892685274344885	0.3459586238531145	0.5826138994746159	T	T
0.1889012411405204	0.5935392485405728	0.5210456003035091	T	T
0.6889012411405204	0.5935392485405728	0.5210456003035091	T	T
0.0885615536497255	0.5467451980297184	0.5756972541502563	T	T
0.5885615536497255	0.5467451980297184	0.5756972541502563	T	T
0.1384448131087765	0.4765847318627792	0.5180471215368740	T	T
0.6384448131087836	0.4765847318627792	0.5180471215368740	T	T
0.4392251815480748	0.7921540941172722	0.5120737971426053	T	T
0.9392251815480748	0.7921540941172722	0.5120737971426053	T	T
0.3289464741531773	0.8522327313241220	0.5580199639990937	T	T
0.8289464741531773	0.8522327313241220	0.5580199639990937	T	T
0.3272330027163548	0.7287554713051208	0.5546866375361290	T	T
0.8272330027163548	0.7287554713051208	0.5546866375361290	T	T
0.4527214867733917	0.0022560781465728	0.5024358816373180	T	T
0.9527214867733917	0.0022560781465728	0.5024358816373180	T	T
0.2563344832484589	0.285355541159949	0.5085168632429102	T	T
0.7563344832484589	0.285355541159949	0.5085168632429102	T	T
0.9577764514629763	0.5797689466097324	0.4952874627120494	T	T
0.4577764514629763	0.5797689466097324	0.4952874627120494	T	T
0.2111521058177246	0.7961722850849924	0.4781420582743934	T	T
0.7111521058177246	0.7961722850849924	0.4781420582743934	T	T
0.3667997051540723	0.1482400246325142	0.5012569720958666	T	T
0.8667997051540723	0.1482400246325142	0.5012569720958666	T	T
0.2484499704053746	0.1038126935908537	0.395433339165785	T	T
0.7484499704053746	0.1038126935908537	0.395433339165785	T	T
0.0078253298424755	0.0014496649039373	0.4015321245376242	T	T
0.5078253298424755	0.0014496649039373	0.4015321245376242	T	T
0.0015323257615734	0.2022141344533281	0.3984748569017071	T	T
0.5015323257615734	0.2022141344533281	0.3984748569017071	T	T
0.2561060213807735	0.4958684391861894	0.3961156109185282	T	T
0.7561060213807735	0.4958684391861894	0.3961156109185282	T	T
0.2526542461542718	0.3028243571770517	0.4040579878878603	T	T
0.7526542461542718	0.3028243571770517	0.4040579878878603	T	T
0.0042864770301065	0.3989776828866027	0.3969412202647646	T	T
0.5042864770301065	0.3989776828866027	0.3969412202647646	T	T
0.0113033914010003	0.5963919710356365	0.3993994119095348	T	T
0.5113033914010003	0.5963919710356365	0.3993994119095348	T	T
0.2596187699306611	0.6926297585604289	0.3998631739301359	T	T
0.7596187699306611	0.6926297585604289	0.3998631739301359	T	T
0.9956572054061894	0.7998577819058994	0.3904841360024207	T	T
0.4956572054061894	0.7998577819058994	0.3904841360024207	T	T
0.2562145427628053	0.9041928142808189	0.4008974215220178	T	T
0.7562145427628053	0.9041928142808189	0.4008974215220178	T	T
0.0841720382657059	0.9022817560002565	0.2989654542534552	T	T
0.5841720382657059	0.9022817560002565	0.2989654542534552	T	T
0.3289426839883447	0.7995731877056116	0.2972687893942165	T	T
0.8289426839883447	0.7995731877056116	0.2972687893942165	T	T
0.3338783451734244	0.9982262552117476	0.3012588739384086	T	T
0.8338783451734244	0.9982262552117476	0.3012588739384086	T	T
0.0875976081883323	0.2982188472300251	0.2999279940049746	T	T
0.5875976081883323	0.2982188472300251	0.2999279940049746	T	T
0.0812440209298728	0.0990799784713801	0.2990158226049360	T	T

0.5812440209298728	0.0990799784713801	0.2990158226049360	T	T	T
0.3346625981235292	0.3973224093663319	0.2986034583371833	T	T	T
0.8346625981235292	0.3973224093663319	0.2986034583371833	T	T	T
0.3345701608433842	0.2005786162319154	0.2982428448440473	T	T	T
0.8345701608433842	0.2005786162319154	0.2982428448440473	T	T	T
0.0844918383518802	0.6969299416961618	0.2989236470485395	T	T	T
0.5844918383518802	0.6969299416961618	0.2989236470485395	T	T	T
0.0841541947664268	0.4995016186554011	0.2979054485469206	T	T	T
0.5841541947664268	0.4995016186554011	0.2979054485469206	T	T	T
0.3346702237487520	0.6006846161081540	0.2997037351184133	T	T	T
0.8346702237487520	0.6006846161081540	0.2997037351184133	T	T	T

S3.11.3 iso3, POSCAR center

0.1044408773280003	0.9885758250348905	0.5409833620368055	T	T	T
0.6044408773280000	0.9885758250348905	0.5409833620368055	T	T	T
0.3763105344505499	0.3648143332595383	0.5332175463946763	T	T	T
0.8763105344505501	0.3648143332595383	0.5332175463946763	T	T	T
0.2173800419577197	0.6201468018693252	0.5263116792710796	T	T	T
0.7173800419577196	0.6201468018693252	0.5263116792710796	T	T	T
0.1679392104063602	0.0468911176915741	0.5308548780222325	T	T	T
0.6679392104063601	0.0468911176915741	0.5308548780222325	T	T	T
0.0836518272910781	0.9872821857497888	0.5860344251360834	T	T	T
0.5836518272910780	0.9872821857497888	0.5860344251360834	T	T	T
0.1543626084736420	0.9253285318131472	0.5282778201491760	T	T	T
0.6543626084736419	0.9253285318131472	0.5282778201491760	T	T	T
0.9747988990039457	0.3555297026670220	0.5152577275145916	T	T	T
0.4747988990039526	0.3555297026670220	0.5152577275145916	T	T	T
0.3381361223976796	0.4325478542323345	0.5220368292756055	T	T	T
0.8381361223976794	0.4325478542323345	0.5220368292756055	T	T	T
0.3806701477371204	0.3576513887136313	0.5789437025273456	T	T	T
0.8806701477371206	0.3576513887136313	0.5789437025273456	T	T	T
0.1773472268477218	0.6893555310982161	0.5215284407268740	T	T	T
0.6773472268477221	0.6893555310982161	0.5215284407268740	T	T	T
0.2099244380952980	0.5986149642241380	0.5702510439233193	T	T	T
0.7099244380952978	0.5986149642241380	0.5702510439233193	T	T	T
0.3210717375732408	0.6192837222184834	0.5132104529557227	T	T	T
0.8210717375732405	0.6192837222184834	0.5132104529557227	T	T	T
0.4492136078107433	0.9937921915606986	0.5034850009884764	T	T	T
0.9492136078107433	0.9937921915606986	0.5034850009884764	T	T	T
0.2598797728087928	0.2808460742417280	0.5064384121974128	T	T	T
0.7598797728087930	0.2808460742417280	0.5064384121974128	T	T	T
0.1218447607343554	0.5376017944854938	0.4854321773735795	T	T	T
0.6218447607343556	0.5376017944854938	0.4854321773735795	T	T	T
0.3725315792233858	0.1434462451941030	0.5020158979936762	T	T	T
0.8725315792233858	0.1434462451941030	0.5020158979936762	T	T	T
0.2468134073717714	0.0973697405533576	0.3960403823298942	T	T	T
0.7468134073717715	0.0973697405533576	0.3960403823298942	T	T	T
0.0011745866781461	-0.0038105550409170	0.4021261215115396	T	T	T
0.5011745866781462	-0.0038105550409170	0.4021261215115396	T	T	T
0.0002087686855907	0.1979647098635579	0.3978384443704704	T	T	T
0.5002087686855909	0.1979647098635579	0.3978384443704704	T	T	T
0.2539261668580502	0.5007359504508268	0.4014346634010649	T	T	T
0.7539261668580503	0.5007359504508268	0.4014346634010649	T	T	T
0.2480708845952069	0.2992910492119736	0.4031557570696894	T	T	T
0.7480708845952068	0.2992910492119736	0.4031557570696894	T	T	T
-0.0016248061624173	0.3978071100222230	0.3934873108248879	T	T	T
0.4983751938375827	0.3978071100222230	0.3934873108248879	T	T	T
-0.0012672458707767	0.6051485308292818	0.4045238920681465	T	T	T
0.4987327541292232	0.6051485308292818	0.4045238920681465	T	T	T
0.2538072223083088	0.7060748310495658	0.3958600153120500	T	T	T
0.7538072223083089	0.7060748310495658	0.3958600153120500	T	T	T
0.2498357868405319	0.8983133649406694	0.3969975712408269	T	T	T
0.7498357868405321	0.8983133649406694	0.3969975712408269	T	T	T
0.0017186652323520	0.7995548563308296	0.3978624709542346	T	T	T
0.5017186652323519	0.7995548563308296	0.3978624709542346	T	T	T
0.3338233625532673	0.8004121995941950	0.2969017882517675	T	T	T
0.8338233625532673	0.8004121995941950	0.2969017882517675	T	T	T
0.0821375122117134	0.9010018566923389	0.2988832845228772	T	T	T
0.5821375122117136	0.9010018566923389	0.2988832845228772	T	T	T
0.3349351149003312	0.0007245300803231	0.2986873045492326	T	T	T
0.8349351149003309	0.0007245300803231	0.2986873045492326	T	T	T
0.0852475561498397	0.2979218114282616	0.2991462339986408	T	T	T
0.5852475561498395	0.2979218114282616	0.2991462339986408	T	T	T
0.0819109841033711	0.0981441739694983	0.2992869096986814	T	T	T
0.5819109841033708	0.0981441739694983	0.2992869096986814	T	T	T
0.3280355071237046	0.4005984161114814	0.3004408103483644	T	T	T
0.8280355071237046	0.4005984161114814	0.3004408103483644	T	T	T
0.3333579084958873	0.2018386613558593	0.2990164009506991	T	T	T
0.8333579084958874	0.2018386613558593	0.2990164009506991	T	T	T
0.0831402577678127	0.6987430312504339	0.2985046411982480	T	T	T
0.5831402577678126	0.6987430312504339	0.2985046411982480	T	T	T
0.0838901167528957	0.5015253173511942	0.2988070230496070	T	T	T
0.5838901167528955	0.5015253173511942	0.2988070230496070	T	T	T
0.3375789287569274	0.5981506954428589	0.3013941710557806	T	T	T

S3.12 Energies from DFT calculations

Table S1: Reference calculations. The entropic data at 298.15 K, obtained from the NIST Computational Chemistry Comparison and Benchmark Database, is reported for comparison with the values calculated by statistical mechanics (see Table S3).

Structure	K-points	E_{tot} (eV)	E_{vdW} (eV)	ZPE (eV)	Entropy (eV/K)
H ₂	$1 \times 1 \times 1$	-6.7512	0	0.267295435	0.00134736
CH ₃ SH	$1 \times 1 \times 1$	-27.6341	-0.01408	1.215940302	0.00264435
CH ₃ SSCH ₃	$1 \times 1 \times 1$	-48.3034	-0.07111	2.036793284	0.00349070
Au atom in bulk	$19 \times 19 \times 19$	-3.61	-0.38867		

Table S2: Computed adsorbate structures. The structures are identified by their unit cell and their label in Figure S(3a), 5b), c) etc).

Structure	K-points	Supercell	Adsorbates	E_{tot} (eV)	E_{vdW} (eV)	ZPE (eV)
$\sqrt{3} \times 6$ (blank)	$3 \times 3 \times 1$	$6 \times 2\sqrt{3}$	n.a.	-407.1148	-36.24785	
$3 \times \sqrt{3}$, 3a), 5d)	$3 \times 3 \times 1$	$6 \times 2\sqrt{3}$	$8 \times \text{CH}_3\text{S} +$ $4 \times \text{Au adatom}$	-620.9514	-40.82033	1.038
$3 \times \sqrt{3}$, 5b)	$3 \times 3 \times 1$	$6 \times 2\sqrt{3}$	$8 \times \text{CH}_3\text{S} +$ $4 \times \text{Au adatom}$	-619.5774	-40.91909	
$3 \times \sqrt{3}$, 3b)	$3 \times 3 \times 1$	$6 \times 2\sqrt{3}$	$8 \times \text{CH}_3\text{S} +$ $4 \times \text{Au adatom}$	-620.9188	-40.79112	
$6 \times \sqrt{3}$, 5e)	$3 \times 3 \times 1$	$6 \times 2\sqrt{3}$	$8 \times \text{CH}_3\text{S} +$ $4 \times \text{Au adatom}$	-621.0931	-40.83528	1.039
p(4×3)	$5 \times 5 \times 1$	p(4×3)	n.a.	-203.621	-18.18783	

Structure	K-points	Supercell	Adsorbates	E_{tot} (eV)	E_{vdW} (eV)	ZPE (eV)
p(4×3), 5c)	$5 \times 5 \times 1$	p(4×3)	$4 \times \text{CH}_3\text{S}$ $2 \times \text{Au adatom}$	-310.6798	-20.52851	1.042
$\sqrt{3} \times \sqrt{3}$	$5 \times 5 \times 1$	$2\sqrt{3} \times 2\sqrt{3}$	$4 \times \text{CH}_3\text{S}$	-203.6188	-18.0865	
$\sqrt{3} \times \sqrt{3}$, 5a)	$5 \times 5 \times 1$	$2\sqrt{3} \times 2\sqrt{3}$	$4 \times \text{CH}_3\text{S}$	-302.4244	-19.6084	
$4 \times \sqrt{3}$	$3 \times 3 \times 1$	$4 \times 2\sqrt{3}$	n.a.	-271.5505	-24.19936	
$4 \times \sqrt{3}$, NoAA	$3 \times 3 \times 1$	$4 \times 2\sqrt{3}$	$6 \times \text{CH}_3\text{S}$	-419.4276	-26.70939	
$4 \times \sqrt{3}$, 4a)	$3 \times 3 \times 1$	$4 \times 2\sqrt{3}$	$6 \times \text{CH}_3\text{S} +$ $2 \times \text{Au adatom}$	-427.7557	-27.34053	1.033
$4 \times \sqrt{3}$, 4b)	$3 \times 3 \times 1$	$4 \times 2\sqrt{3}$	$6 \times \text{CH}_3\text{S} +$ $2 \times \text{Au adatom}$	-427.1847	-27.34034	
$4 \times \sqrt{3}$, 4c)	$3 \times 3 \times 1$	$4 \times 2\sqrt{3}$	$6 \times \text{CH}_3\text{S}$ $2 \times \text{Au adatom}$	-427.6809	-27.41898	
$4 \times \sqrt{3}$, 4d)	$3 \times 3 \times 1$	$4 \times 2\sqrt{3}$	$6 \times \text{CH}_3\text{S}$ $2 \times \text{Au adatom}$	-427.5942	-27.36991	
$4 \times \sqrt{3}$, 4e)	$3 \times 3 \times 1$	$4 \times 2\sqrt{3}$	$6 \times \text{CH}_3\text{S}$ $2 \times \text{Au adatom}$	-427.3963	-27.34991	
$4 \times \sqrt{3}$, 4f)	$3 \times 3 \times 1$	$4 \times 2\sqrt{3}$	$6 \times \text{CH}_3\text{S}$ $2 \times \text{Au adatom}$	-427.5925	-27.40243	1.037

Table S3: Temperature dependent corrections (in kJ/mol) to be added to E_{tot} to obtain $G_{\text{tot}}(T)$ at 1 bar (for gases). For the surfaces, the actual correction is twice the value noted, since the frequencies have been computed for the "structure" and not for the "supercell" (see Table S2).

T/K	H ₂	CH ₃ SH	CH ₃ SSCH ₃	$6 \times \sqrt{3}$, d)	$4 \times \sqrt{3}$, l)
0	25.79	117.32	196.52	401.16	300.03
100	18.82	99.95	175.52	397.96	297.8
200	7.82	77.66	147.68	383.55	287.13
298.15	-4.46	53.62	116.46	360.34	269.78
300	-4.7	53.15	115.84	359.83	269.39
383	-15.85	31.46	86.95	334.38	250.34
400	-18.21	26.88	80.78	328.59	246
500	-32.45	-0.92	42.88	290.85	217.7
600	-47.28	-30.12	2.4	247.31	185.04
700	-62.6	-60.6	-40.43	198.5	148.42
800	-78.34	-92.27	-85.43	144.88	108.18
900	-94.45	-125.06	-132.44	86.82	64.62
1000	-110.88	-158.88	-181.32	24.64	17.96

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