

Supporting Information

Imaging Dihydrogen Bond-Driven Assembly of Borazine on Au(111)

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Experimental Procedures

STM/STS experiments have been conducted using a commercial low-temperature STM (Infinity SPM, Scienta Omicron GmbH) in ultrahigh vacuum ($p \approx 5 \times 10^{-10}$ mbar) and at a temperature of ≈ 8.5 K. Bias voltage (V) is given as sample bias with respect to the tip. dI/dV spectroscopy has been performed using lock-in detection of the tunneling current I by adding a sinusoidal voltage modulation ($V_{\text{mod}} = 20$ mV_{rms}) at 759 Hz to the sample bias voltage V . The d^2I/dV^2 spectra have been obtained by numerically differentiation of the dI/dV ones. STM feedback was used for adjusting the tip-sample distance at each location.

STM images have been processed with Gwyddion.^[1] A 2D Fast Fourier Transform (FFT) filter to remove high-frequency noise components.

Mass spectra were measured by a quadrupole mass spectrometer (PrismaPro QMG 250, Pfeiffer Vacuum GmbH).

Borazine was purchased from Katchem. In order to minimize the polymerization of borazine to polyborazylene, borazine was not stored as a liquid, but instead a minican was filled with borazine vapor (at room temperature the vapor pressure of borazine is approximately 270 mbar). The minican was connected to a leak valve by a stainless-steel pipe. Borazine is known to decompose into diborane at room temperature. To avoid contamination with diborane, borazine was cleaned using a modified version of the borazine purification protocol developed by Cuxart et al.^[2] The procedure for purification was as follows:

- Pump gas line for 2 minutes with a scroll pump ($p = 3 \times 10^{-2}$ mbar).
- Install cooling trap filled with a mixture of Ethanol and LN₂ (constant temperature of the mixture is -116°C) and wait 5 minutes for line to cool down.
- Fill line with borazine from the minican for 20 seconds, borazine will condense in the line.
- Pump down line for 2 minutes with scroll pump in order to remove diborane.
- Let line (and borazine) warm to room temperature, the line is now filled with pure borazine.

Borazine molecules have been deposited on the Au(111) substrate kept at a temperature $T \approx 22$ K inside the microscope ($p \approx 5 \times 10^{-7}$ mbar, $t = 10$ minutes) and subsequently cooled down to ≈ 8.5 K for characterization.

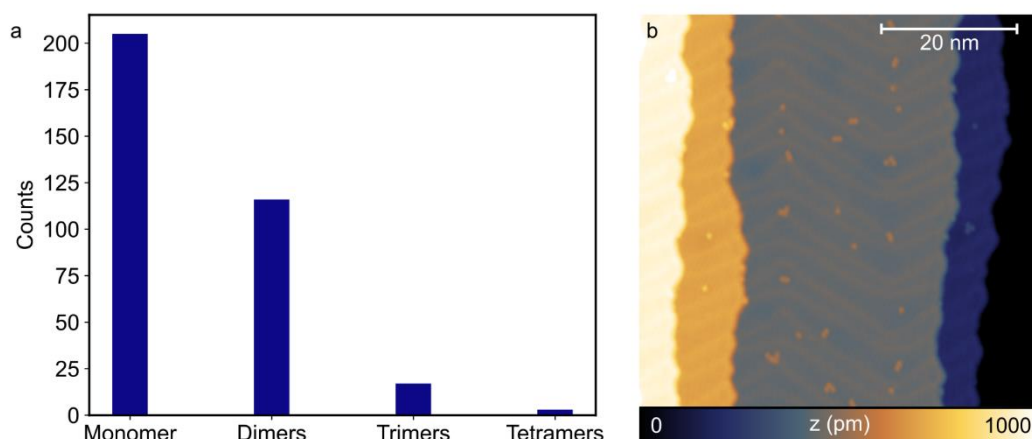


Figure S1. (a) Histogram of monomers, dimers, trimers and tetramers identified upon dosing borazine on the Au(111) kept at $T \approx 22$ K. Out of 14 total dimers resolved with sufficient resolution, 2 correspond to dimer I, 9 to dimer II, and 3 to dimer III. (b) Large scale STM image showing several step edges of the gold surfaces. Individual molecules, as well as small clusters can be observed on the terraces, while no evident decoration of the step edge site is visible.

Details on the analysis of the STM images of the dimers

A total of 12 dimers were selected for determining the centroid distances (d_{cc}) of the three dimer structures. While over 100 dimers were imaged (see Figure S1a), the analysis focused on this subset because these images exhibited the high resolution required to precisely and reliably identify the positions of individual molecules.

The following procedure was applied to all of the detail images:

1. Scaled models of borazine have been superimposed to the high-resolution STM images of the dimers, aligning the bright protrusions with the positions of boron atoms.
2. Center-to-center distances in the models have been measured.

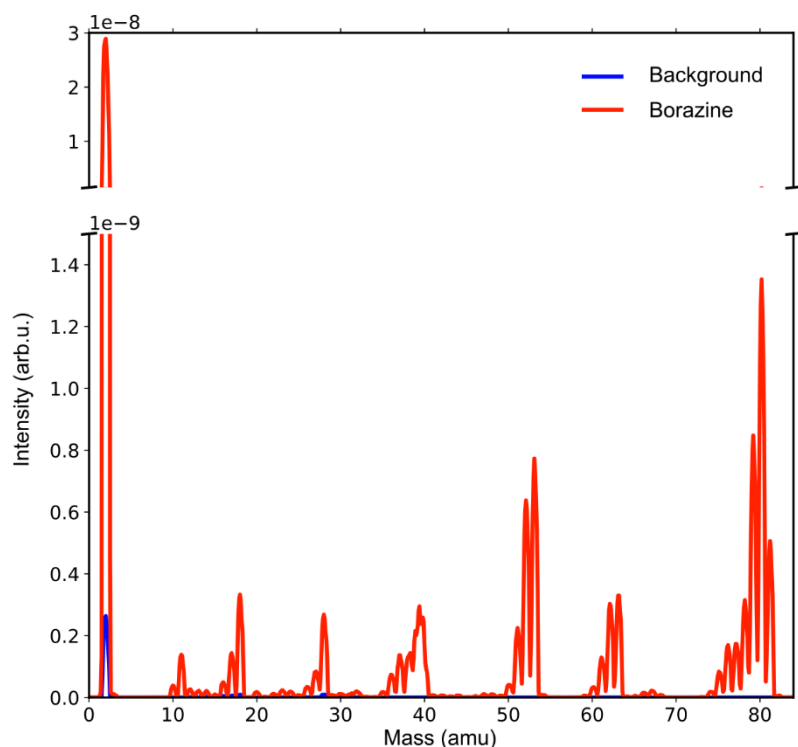


Figure S2. Mass spectra of the chamber background and the purified borazine. The latter has been measured at a partial pressure $p = 5 \times 10^{-7}$ mbar.

Borazine- H_2 structures

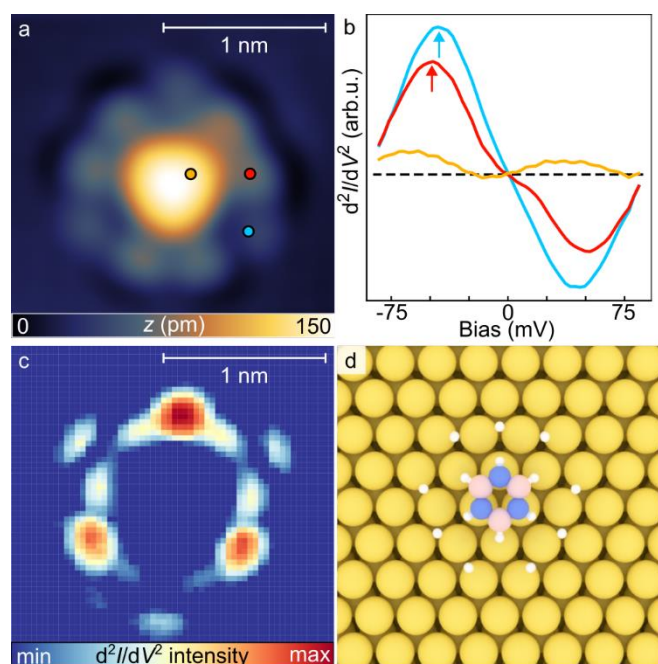


Figure S3. (a) STM image of an individual borazine surrounded by H_2 molecules (a, $V = 100$ mV; $I = 200$ pA), (b) IET spectra recorded at the positions marked in (a). The zero-signal level is indicated by a dashed line. (c) IETS intensity map. STM feedback was used for adjusting the tip-sample distance at each pixel. A slight image distortion is given due to residual drift. (d) Relaxed geometry of borazine with nine H_2 . Pink, blue and white spheres represent boron, nitrogen and hydrogen, respectively.

Figure S3a shows an STM image of a borazine molecule surrounded by a rim of several protrusions. These additional lobes are attributed to adsorbed H_2 , arising from the deposition process (see Figure S2). To unambiguously assign those features to H_2 we performed inelastic electron tunneling spectroscopy (IETS) for a borazine monomer. Spatially resolved IET spectra are shown in Figure S3b. While the spectrum acquired above the center of the borazine is featureless, the line shapes of the d^2I/dV^2 spectra on the rim are characterized by an asymmetric dip. Similar spectral features have been reported for $H_2/Au(110)$.^[3] Hydrogen vibrational motion bouncing between the tip and substrate ($\nu = 0 \rightarrow 1$) has been identified around 11.4 mV on a clean Au(110) surface, while rotational

excitation of para H_2 ($j = 0 \rightarrow 2$) gives rise to a feature at 42.0 mV. The IETS excitation energies have been shown to increase upon tip approach towards the surface.^[3–7] Further changes of the excitation energies occur due to the spatial distribution of the interaction potential within an adsorbed molecule.^[8] As the vibrational excitation is typically characterized by a larger intensity in the IET spectra compared to the rotational one, the features observed in Figure S3b are attributed to H_2 vibrations. We performed d^2I/dV^2 spectroscopic mapping, acquiring a grid of 64×64 spectra over an individual borazine molecule surrounded by adsorbed H_2 . Figure S3c shows a map of the IETS intensities extracted from each spectrum. Notably, as no feature of an IET excitation is observed upon acquisition of a spectrum above the borazine, we conclude that for this tip termination the H_2 is not constantly trapped in the junction.^[3,7] Therefore, the corresponding IETS map allows precisely locating the adsorption sites of the H_2 molecules around the borazine.

Three main features are located in front of the N-H bonds, while groups of three protrusions are located nearby the B-H one. Figure S3d shows the DFT relaxed structure of a borazine monomer surrounded by nine hydrogen molecules. The adsorption sites of the H_2 molecules match the position of the main features in IETS map (Figure S3c). The adsorption energy is about 0.09 eV per H_2 molecule.

Computational details

The calculations were performed on a surface Au(111) model including five Au layers, with the initial closest Au–Au separation of 2.884 Å, each Au layer containing 64 Au atoms (see Figure S4). During the course of optimization, the three lower layers were kept fixed to mimic interactions with bulk. In the z direction, the size of the cell was 30 Å, thus providing more than 15 Å of a vacuum layer between periodic images in this direction. We performed calculations employing density functional theory (DFT) with the PBE functional and the energy cut-off of 350 eV. To obtain more precise energies, the final structures were single-point recalculated using the cut-off of 500 eV, leading to a very slight decrease in adsorption energies below 2%. The smearing method of Methfessel-Paxton, second order, was employed. Only the gamma point was considered in the reciprocal space. Empirical dispersion was included employing the vdW^{surf} correction.^[9] The energy convergence criterion was set to 10^{-6} eV for stopping the electronic self-consistent loop and 10^{-5} eV for structure optimization. We sampled various positions of the borazine monomer and dimer on the Au(111) surface, i.e., *fcc*, *hcp* and with a gold atom of the first layer below in the ring center, with either boron or nitrogen atoms of borazines interacting with surface gold atoms, i.e. structures differing by 60° rotation. The adsorption energy (ΔE) was calculated as the difference of the energy of the whole system compared of the energy of a neat Au(111) layer and the energy of a borazine molecule as calculated alone in a cell of the same shape. Borazine molecules remain almost flat upon adsorption (within dihedral angle of 2°), with only a slight distortion due to molecule-surface interactions. When modeling adsorption of hydrogen molecules, H_2 molecules were added next to the hydrogen atoms of borazine either horizontally or vertically with respect to the surface (for the horizontal position, both along the B-H/N-H bond and perpendicular to it).

For comparison, the dimer binding energy in the gas phase is calculated here to be 0.13 eV, the difference to the CCSD(T)/CBS value of 0.104 eV^[10] can be accounted for the fact that the zero-point correction (0.03 eV) is not included in our calculations.

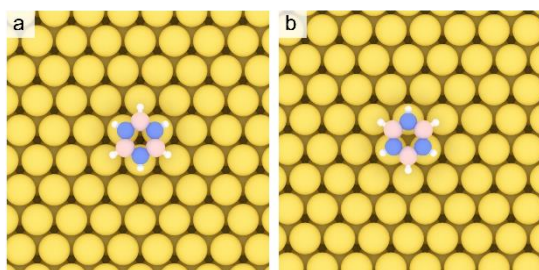


Figure S4. Optimized structures of the borazine monomer adsorbed on a Au(111) surface in *hcp* (a) and *fcc* (b) conformation, as obtained through PBE calculations.

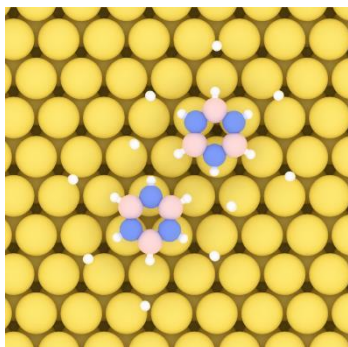


Figure S5. Optimized structures of dimer II in presence of eight H_2 , as obtained through PBE calculations.

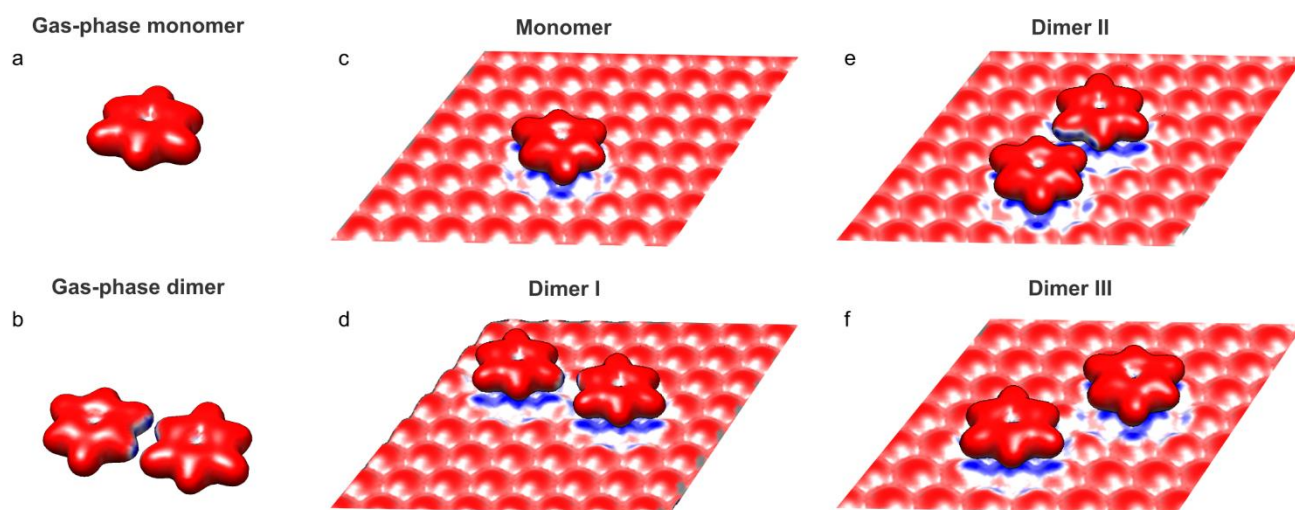


Figure S6. Calculated charge densities for the gas-phase monomer (a) and dimer (b), as well as the monomer (c), dimer I (d), dimer II (e), and dimer III (f) adsorbed on the Au(111) surface, obtained through PBE calculations. The isosurface is set at $\rho = 0.044$ au, with red regions indicating areas of lower negative charge, and blue regions indicating areas of higher negative charge.

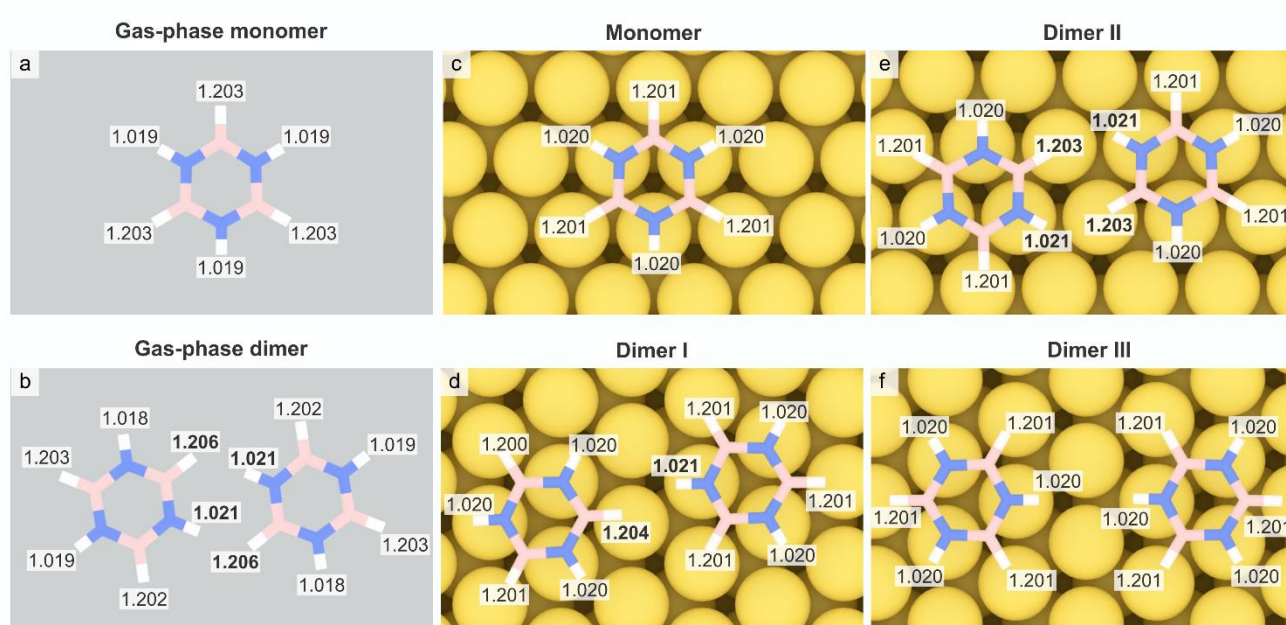


Figure S7. Optimized structures of the gas-phase monomer (a) and dimer (b), along with the monomer (c), dimer I (d), dimer II (e), and dimer III (f) adsorbed on the Au(111) surface, obtained from PBE calculations. The N-H and B-H bond lengths are shown in Å, with bond lengths involving H atoms participating in dihydrogen bonding (DHB) highlighted in bold for clarity.

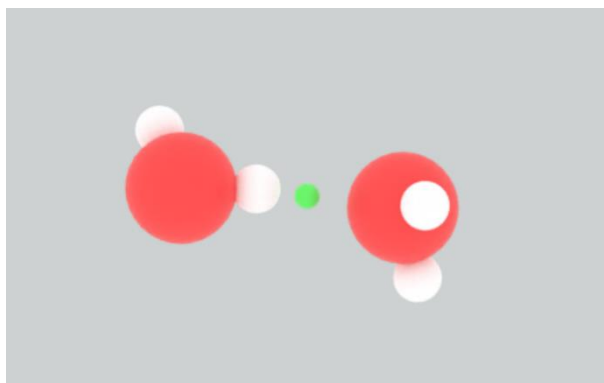


Figure S8. Calculated bond critical point (green) for the gas-phase water dimer. Red and white spheres represent oxygen and hydrogen, respectively.

References

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Coordinates (in Å and fractional coordinates, VASP format) of DFT optimized structures

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0.3750000784427954	0.2499997876146764	0.2386017402791817	T	T	T
0.4166667931327623	0.3333332169946104	0.3224147603230061	T	T	T
0.3749997792182995	0.3749999316845773	0.0000000000000000	F	F	F
0.4166664939082665	0.4583333610645113	0.0784850000000000	F	F	F
0.4583335078227293	0.4166666463745443	0.1569700000000001	F	F	F
0.3749997792182995	0.3749999316845773	0.2386017402791817	T	T	T
0.4166664939082665	0.4583333610645113	0.3224147603230061	T	T	T
0.3749999134612452	0.5000000757544782	0.0000000000000000	F	F	F
0.4166666281512121	0.5833335051344122	0.0784850000000000	F	F	F
0.4583332085982335	0.5416667904444452	0.1569700000000001	F	F	F
0.3749999134612452	0.5000000757544782	0.2386017402791817	T	T	T
0.4166666281512121	0.5833335051344122	0.3224147603230061	T	T	T
0.3750000477041908	0.6250002198243791	0.0000000000000000	F	F	F
0.4166665121315987	0.7083331486791877	0.0784850000000000	F	F	F
0.4583330925786129	0.6666664339892208	0.1569700000000001	F	F	F
0.3750000477041908	0.6250002198243791	0.2386017402791817	T	T	T
0.4166665121315987	0.7083331486791877	0.3224147603230061	T	T	T
0.3749999316845773	0.7499998633691547	0.0000000000000000	F	F	F
0.4166666463745443	0.8333332927490886	0.0784850000000000	F	F	F
0.4583332268215656	0.7916665780591217	0.1569700000000001	F	F	F
0.3749999316845773	0.7499998633691547	0.2386017402791817	T	T	T
0.4166666463745443	0.8333332927490886	0.3224147603230061	T	T	T
0.3750000659275230	0.8750000074390556	0.0000000000000000	F	F	F
0.4166667806174900	0.9583334368189895	0.0784850000000000	F	F	F
0.4583333610645113	0.9166667221290226	0.1569700000000001	F	F	F
0.3750000659275230	0.8750000074390556	0.2386017402791817	T	T	T
0.4166667806174900	0.9583334368189895	0.3224147603230061	T	T	T
0.4999999358034728	0.0000000000000000	0.0000000000000000	F	F	F
0.5416666504934398	0.0833334293799339	0.0784850000000000	F	F	F
0.5833332309404540	0.0416667146899670	0.1569700000000001	F	F	F
0.4999999358034728	-0.0000000000000000	0.2386017402791817	T	T	T
0.5416666504934398	0.0833334293799339	0.3224147603230061	T	T	T
0.5000000700464184	0.1250001440699009	0.0000000000000000	F	F	F
0.5416667847363854	0.2083335734498348	0.0784850000000000	F	F	F
0.5833333651834067	0.1666668587598679	0.1569700000000001	F	F	F
0.5000000700464184	0.1250001440699009	0.2386017402791817	T	T	T
0.5416667847363854	0.2083335734498348	0.3224147603230061	T	T	T
0.4999999540268050	0.2499997876146764	0.0000000000000000	F	F	F
0.5416666687167719	0.3333332169946104	0.0784850000000000	F	F	F
0.5833332491637861	0.2916665023046434	0.1569700000000001	F	F	F
0.4999999540268050	0.2499997876146764	0.2386017402791817	T	T	T
0.5416666687167719	0.3333332169946104	0.3224147603230061	T	T	T
0.5000000882697506	0.3749999316845773	0.0000000000000000	F	F	F
0.5416668029597176	0.4583333610645113	0.0784850000000000	F	F	F
0.5833333834067389	0.4166666463745443	0.1569700000000001	F	F	F
0.5000000882697506	0.3749999316845773	0.2386017402791817	T	T	T
0.5416668029597176	0.4583333610645113	0.3224147603230061	T	T	T
0.5000002225126963	0.5000000757544782	0.0000000000000000	F	F	F
0.5416669372026632	0.5833335051344122	0.0784850000000000	F	F	F
0.5833335176496846	0.5416667904444452	0.1569700000000001	F	F	F

0.50000002225126963	0.5000000757544782	0.2386017402791817	T	T	T
0.5416669372026632	0.5833335051344122	0.3224147603230061	T	T	T
0.4999999232882004	0.6250002198243791	0.0000000000000000	F	F	F
0.5416663877156012	0.7083331486791877	0.0784850000000006	F	F	F
0.5833334016300711	0.6666664339892208	0.1569700000000012	F	F	F
0.4999999232882004	0.6250002198243791	0.2386017402791817	T	T	T
0.5416663877156012	0.7083331486791877	0.3224147603230061	T	T	T
0.4999998072685798	0.7499998633691547	0.0000000000000000	F	F	F
0.5416665219585468	0.8333332927490886	0.0784850000000006	F	F	F
0.5833331024055681	0.7916665780591217	0.1569700000000012	F	F	F
0.4999998072685798	0.7499998633691547	0.2386017402791817	T	T	T
0.5416665219585468	0.8333332927490886	0.3224147603230061	T	T	T
0.4999999415115326	0.8750000074390556	0.0000000000000000	F	F	F
0.5416666562014996	0.9583334368189895	0.0784850000000006	F	F	F
0.5833332366485138	0.9166667221290226	0.1569700000000012	F	F	F
0.4999999415115326	0.8750000074390556	0.2386017402791817	T	T	T
0.5416666562014996	0.9583334368189895	0.3224147603230061	T	T	T
0.6249998113874753	0.0000000000000000	0.0000000000000000	F	F	F
0.6666665260774423	0.0833334293799339	0.0784850000000006	F	F	F
0.7083335399919122	0.0416667146899670	0.1569700000000012	F	F	F
0.6249998113874753	-0.0000000000000000	0.2386017402791817	T	T	T
0.6666665260774423	0.0833334293799339	0.3224147603230061	T	T	T
0.6249999456304209	0.1250001440699009	0.0000000000000000	F	F	F
0.666666603203879	0.2083335734498348	0.0784850000000006	F	F	F
0.7083332407674092	0.1666668587598679	0.1569700000000012	F	F	F
0.6249999456304209	0.1250001440699009	0.2386017402791817	T	T	T
0.666666603203879	0.2083335734498348	0.3224147603230061	T	T	T
0.6249998296108075	0.2499997876146764	0.0000000000000000	F	F	F
0.6666665443007744	0.3333332169946104	0.0784850000000006	F	F	F
0.7083331247477958	0.2916665023046434	0.1569700000000012	F	F	F
0.6249998296108075	0.2499997876146764	0.2386017402791817	T	T	T
0.6666665443007744	0.3333332169946104	0.3224147603230061	T	T	T
0.6249999638537531	0.3749999316845773	0.0000000000000000	F	F	F
0.6666666785437201	0.4583333610645113	0.0784850000000006	F	F	F
0.7083332589907414	0.4166666463745443	0.1569700000000012	F	F	F
0.6249999638537531	0.3749999316845773	0.2386017402791817	T	T	T
0.6666666785437201	0.4583333610645113	0.3224147603230061	T	T	T
0.6250000980967059	0.5000000757544782	0.0000000000000000	F	F	F
0.6666668127866728	0.5833335051344122	0.0784850000000006	F	F	F
0.7083333932336870	0.5416667904444452	0.1569700000000012	F	F	F
0.6250000980967059	0.5000000757544782	0.2386017402791817	T	T	T
0.6666668127866728	0.5833335051344122	0.3224147603230061	T	T	T
0.6250002323396515	0.6250002198243791	0.0000000000000000	F	F	F
0.666666967670594	0.7083331486791877	0.0784850000000006	F	F	F
0.7083332772140736	0.6666664339892208	0.1569700000000012	F	F	F
0.6250002323396515	0.6250002198243791	0.2386017402791817	T	T	T
0.666666967670594	0.7083331486791877	0.3224147603230061	T	T	T
0.6250001163200380	0.7499998633691547	0.0000000000000000	F	F	F
0.6666668310100050	0.8333332927490886	0.0784850000000006	F	F	F
0.7083334114570263	0.7916665780591217	0.1569700000000012	F	F	F
0.6250001163200380	0.7499998633691547	0.2386017402791817	T	T	T
0.6666668310100050	0.8333332927490886	0.3224147603230061	T	T	T
0.6249998170955351	0.8750000074390556	0.0000000000000000	F	F	F
0.6666665317855021	0.9583334368189895	0.0784850000000006	F	F	F
0.7083335456999720	0.9166667221290226	0.1569700000000012	F	F	F
0.6249998170955351	0.8750000074390556	0.2386017402791817	T	T	T
0.6666665317855021	0.9583334368189895	0.3224147603230061	T	T	T
0.7500001204389335	0.0000000000000000	0.0000000000000000	F	F	F
0.7916668351289005	0.0833334293799339	0.0784850000000006	F	F	F
0.8333334155759147	0.0416667146899670	0.1569700000000012	F	F	F
0.7500001204389335	0.0000000000000000	0.2386017402791817	T	T	T
0.7916668351289005	0.0833334293799339	0.3224147603230061	T	T	T
0.7500002546818791	0.1250001440699009	0.0000000000000000	F	F	F
0.7916669693718461	0.2083335734498348	0.0784850000000006	F	F	F
0.8333335498188674	0.1666668587598679	0.1569700000000012	F	F	F
0.7500002546818791	0.1250001440699009	0.2386017402791817	T	T	T
0.7916669693718461	0.2083335734498348	0.3224147603230061	T	T	T
0.7499997051948100	0.2499997876146764	0.0000000000000000	F	F	F
0.7916664198847769	0.3333332169946104	0.0784850000000006	F	F	F
0.8333334337992468	0.2916665023046434	0.1569700000000012	F	F	F
0.7499997051948100	0.2499997876146764	0.2386017402791817	T	T	T
0.7916664198847769	0.3333332169946104	0.3224147603230061	T	T	T
0.7499998394377627	0.3749999316845773	0.0000000000000000	F	F	F
0.7916665541277297	0.4583333610645113	0.0784850000000006	F	F	F
0.8333331345747439	0.4166666463745443	0.1569700000000012	F	F	F
0.7499998394377627	0.3749999316845773	0.2386017402791817	T	T	T
0.7916665541277297	0.4583333610645113	0.3224147603230061	T	T	T
0.7499999736807084	0.5000000757544782	0.0000000000000000	F	F	F

0.7916666883706753	0.5833335051344122	0.0784850000000006	F	F	F
0.8333332688176966	0.5416667904444452	0.1569700000000012	F	F	F
0.7499999736807084	0.5000000757544782	0.2386017402791817	T	T	T
0.7916666883706753	0.5833335051344122	0.3224147603230061	T	T	T
0.7500001079236540	0.6250002198243791	0.0000000000000000	F	F	F
0.7916665723510619	0.7083331486791877	0.0784850000000006	F	F	F
0.8333331527980832	0.6666664339892208	0.1569700000000012	F	F	F
0.7500001079236540	0.6250002198243791	0.2386017402791817	T	T	T
0.7916665723510619	0.7083331486791877	0.3224147603230061	T	T	T
0.7499999919040405	0.7499998633691547	0.0000000000000000	F	F	F
0.7916667065940075	0.8333332927490886	0.0784850000000006	F	F	F
0.8333332870410288	0.7916665780591217	0.1569700000000012	F	F	F
0.7499999919040405	0.7499998633691547	0.2386017402791817	T	T	T
0.7916667065940075	0.8333332927490886	0.3224147603230061	T	T	T
0.7500001261469933	0.8750000074390556	0.0000000000000000	F	F	F
0.7916668408369603	0.9583334368189895	0.0784850000000006	F	F	F
0.8333334212839745	0.9166667221290226	0.1569700000000012	F	F	F
0.7500001261469933	0.8750000074390556	0.2386017402791817	T	T	T
0.7916668408369603	0.9583334368189895	0.3224147603230061	T	T	T
0.8749999960229360	0.0000000000000000	0.0000000000000000	F	F	F
0.9166667107129030	0.0833334293799339	0.0784850000000006	F	F	F
0.9583332911599243	0.0416667146899670	0.1569700000000012	F	F	F
0.8749999960229360	0.0000000000000000	0.2386017402791817	T	T	T
0.9166667107129030	0.0833334293799339	0.3224147603230061	T	T	T
0.8750001302658816	0.1250001440699009	0.0000000000000000	F	F	F
0.9166668449558486	0.2083335734498348	0.0784850000000006	F	F	F
0.9583334254028699	0.1666668587598679	0.1569700000000012	F	F	F
0.8750001302658816	0.1250001440699009	0.2386017402791817	T	T	T
0.9166668449558486	0.2083335734498348	0.3224147603230061	T	T	T
0.8750000142462682	0.2499997876146764	0.0000000000000000	F	F	F
0.9166667289362351	0.3333332169946104	0.0784850000000006	F	F	F
0.9583333093832564	0.2916665023046434	0.1569700000000012	F	F	F
0.8750000142462682	0.2499997876146764	0.2386017402791817	T	T	T
0.9166667289362351	0.3333332169946104	0.3224147603230061	T	T	T
0.8750001484892138	0.3749999316845773	0.0000000000000000	F	F	F
0.9166668631791808	0.4583333610645113	0.0784850000000006	F	F	F
0.9583334436262021	0.4166666463745443	0.1569700000000012	F	F	F
0.8750001484892138	0.3749999316845773	0.2386017402791817	T	T	T
0.9166668631791808	0.4583333610645113	0.3224147603230061	T	T	T
0.8749998492647180	0.5000000757544782	0.0000000000000000	F	F	F
0.9166665639546849	0.5833335051344122	0.0784850000000006	F	F	F
0.9583335778691477	0.5416667904444452	0.1569700000000012	F	F	F
0.8749998492647180	0.5000000757544782	0.2386017402791817	T	T	T
0.9166665639546849	0.5833335051344122	0.3224147603230061	T	T	T
0.8749999835076636	0.6250002198243791	0.0000000000000000	F	F	F
0.9166664479350644	0.7083331486791877	0.0784850000000006	F	F	F
0.9583330283820857	0.6666664339892208	0.1569700000000012	F	F	F
0.8749999835076636	0.6250002198243791	0.2386017402791817	T	T	T
0.9166664479350644	0.7083331486791877	0.3224147603230061	T	T	T
0.8749998674880501	0.7499998633691547	0.0000000000000000	F	F	F
0.9166665821780171	0.8333332927490886	0.0784850000000006	F	F	F
0.9583331626250313	0.7916665780591217	0.1569700000000012	F	F	F
0.8749998674880501	0.7499998633691547	0.2386017402791817	T	T	T
0.9166665821780171	0.8333332927490886	0.3224147603230061	T	T	T
0.8750000017309958	0.8750000074390556	0.0000000000000000	F	F	F
0.9166667164209628	0.9583334368189895	0.0784850000000006	F	F	F
0.9583332968679841	0.9166667221290226	0.1569700000000012	F	F	F
0.8750000017309958	0.8750000074390556	0.2386017402791817	T	T	T
0.9166667164209628	0.9583334368189895	0.3224147603230061	T	T	T

Borazine adsorbed on Au(111), fcc

23.0697829620000014	0.0000000000000000	0.0000000000000000
-11.5348914810000007	19.9790169730000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.0000000000000000

Au B N H

320 3 3 6

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0416667146899670	0.0833334293799339	0.0784850000000006	F	F	F
0.0833332951369883	0.0416667146899670	0.1569700000000012	F	F	F
0.0000160592660004	0.0000824101868994	0.2385903343651345	T	T	T
0.0416890688594192	0.0834359121303156	0.3224531366555959	T	T	T
0.0000001342429456	0.1250001440699009	0.0000000000000000	F	F	F
0.0416668489329126	0.2083335734498348	0.0784850000000006	F	F	F
0.0833334293799339	0.1666668587598679	0.1569700000000012	F	F	F
0.0000214474884563	0.1250725875698087	0.2385955806855374	T	T	T
0.0417019989709336	0.2084313455404652	0.3224667396325719	T	T	T

0.0000000182233322	0.2499997876146764	0.0000000000000000	F	F	F
0.0416667329132991	0.3333332169946104	0.0784850000000000	F	F	F
0.0833333133603205	0.2916665023046434	0.1569700000000012	F	F	F
0.0000670478711396	0.2500812913532237	0.2385948821470338	T	T	T
0.0417376009516099	0.3334464581765001	0.3223702263568261	T	T	T
0.0000001524662778	0.3749999316845773	0.0000000000000000	F	F	F
0.0416668671562448	0.4583333610645113	0.0784850000000000	F	F	F
0.0833334476032661	0.4166666463745443	0.1569700000000012	F	F	F
0.0000756922583793	0.3750812274772664	0.2385949940338609	T	T	T
0.0417210373874813	0.4584503263573055	0.3224602539217810	T	T	T
0.9999997248487205	0.5000000757544782	0.0000000000000000	F	F	F
0.0416665679317489	0.5833335051344122	0.0784850000000000	F	F	F
0.0833335818462118	0.5416667904444452	0.1569700000000012	F	F	F
0.0000405775900372	0.5000518181521261	0.2385968409436032	T	T	T
0.0417189455599258	0.5834382342356161	0.3224641974791492	T	T	T
0.9999998590916661	0.6250002198243791	0.0000000000000000	F	F	F
0.0416664519121284	0.7083331486791877	0.0784850000000000	F	F	F
0.0833330323591497	0.6666664339892208	0.1569700000000012	F	F	F
0.0000321281835850	0.6250326016413928	0.2385955140630000	T	T	T
0.0417522210116292	0.7084507720982216	0.3223808930586209	T	T	T
0.9999997430720526	0.7499998633691547	0.0000000000000000	F	F	F
0.0416665861550811	0.8333332927490886	0.0784850000000000	F	F	F
0.0833331666020953	0.7916665780591217	0.1569700000000012	F	F	F
0.0000315831670588	0.7500363508826305	0.2385638802277331	T	T	T
0.0417479253808527	0.8334588296609430	0.3223406152667365	T	T	T
0.000000057080598	0.8750000074390556	0.0000000000000000	F	F	F
0.0416667203980268	0.9583334368189895	0.0784850000000000	F	F	F
0.0833333008450481	0.9166667221290226	0.1569700000000012	F	F	F
0.0000224060605926	0.8750733623661942	0.2385610529994890	T	T	T
0.0417252749714718	0.9584619671563017	0.3223750103233236	T	T	T
0.1249998755840025	0.0000000000000000	0.0000000000000000	F	F	F
0.1666665902739695	0.0833334293799339	0.0784850000000000	F	F	F
0.2083331707209908	0.0416667146899670	0.1569700000000012	F	F	F
0.1250254457972090	0.0000913385810211	0.2385652099847558	T	T	T
0.1667085419147076	0.0834667517801443	0.3223782345101731	T	T	T
0.1250000098269552	0.1250001440699009	0.0000000000000000	F	F	F
0.1666667245169222	0.2083335734498348	0.0784850000000000	F	F	F
0.2083333049639364	0.1666668587598679	0.1569700000000012	F	F	F
0.1249863516850996	0.1250792665822608	0.2386063318682305	T	T	T
0.1666607678831198	0.2084196106345914	0.3225469426173825	T	T	T
0.1249998938073347	0.2499997876146764	0.0000000000000000	F	F	F
0.1666666084973016	0.3333332169946104	0.0784850000000000	F	F	F
0.2083331889443230	0.2916665023046434	0.1569700000000012	F	F	F
0.1250195141349813	0.2500665478818964	0.2386466328045715	T	T	T
0.1667166587328592	0.3334013807074748	0.3225920198056800	T	T	T
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0.208333231872686	0.4166666463745443	0.1569700000000012	F	F	F
0.1251004037214080	0.3750862444042685	0.2386634885152906	T	T	T
0.1667162845318813	0.4584565942549095	0.3225764301066594	T	T	T
0.1250001622932331	0.5000000757544782	0.0000000000000000	F	F	F
0.1666668769832000	0.5833335051344122	0.0784850000000000	F	F	F
0.2083334574302214	0.5416667904444452	0.1569700000000012	F	F	F
0.1250377096995188	0.5000483897081603	0.2386500565167810	T	T	T
0.1666622786099144	0.5834091161193248	0.3225665458467867	T	T	T
0.1250002965361787	0.6250002198243791	0.0000000000000000	F	F	F
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0.2083333414106079	0.6666664339892208	0.1569700000000012	F	F	F
0.1249943595774436	0.6249981253952990	0.2386144169597353	T	T	T
0.1667351874562576	0.7084305534913176	0.3223901020765795	T	T	T
0.1249997470491166	0.7499998633691547	0.0000000000000000	F	F	F
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0.2083334756535535	0.7916665780591217	0.1569700000000012	F	F	F
0.1250380591481481	0.7500353245148468	0.2385645376315103	T	T	T
0.1667424965866857	0.8334571280175492	0.3223399068847111	T	T	T
0.1249998812920623	0.8750000074390556	0.0000000000000000	F	F	F
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0.2083331764290506	0.9166667221290226	0.1569700000000012	F	F	F
0.1250438912977013	0.8750655773678333	0.2385611201610541	T	T	T
0.1667274768319637	0.9584597603259936	0.3223422800582594	T	T	T
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0.3333334797724490	0.0416667146899670	0.1569700000000012	F	F	F
0.2500620480726536	0.0000874602041673	0.2385642293819977	T	T	T
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0.3333330645283255	0.2916665023046434	0.1569700000000012	F	F	F
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0.2499341453860379	0.3749426527557844	0.2387037518139811	T	T	T
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0.2499475985689924	0.5000555060911974	0.2387016684525545	T	T	T
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0.2498872818709465	0.6250583631379508	0.2386531146874909	T	T	T
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0.4583330925786129	0.6666664339892208	0.1569700000000012	F	F	F
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0.9167135268835643	0.2084351439003534	0.3223878580571163	T	T	T
0.8750000142462682	0.2499997876146764	0.0000000000000000	F	F	F
0.9166667289362351	0.3333332169946104	0.0784850000000006	F	F	F
0.9583333093832564	0.2916665023046434	0.1569700000000012	F	F	F
0.8750300067868249	0.2500629666928998	0.2385872493126994	T	T	T
0.9167256503728450	0.3334541066728871	0.3223780901760834	T	T	T
0.8750001484892138	0.3749999316845773	0.0000000000000000	F	F	F
0.9166668631791808	0.4583333610645113	0.0784850000000006	F	F	F
0.9583334436262021	0.4166666463745443	0.1569700000000012	F	F	F
0.8750352524048489	0.3750687855549502	0.2385885024206458	T	T	T
0.9167388334578909	0.4584419643648290	0.3224233838713951	T	T	T
0.8749998492647180	0.5000000757544782	0.0000000000000000	F	F	F
0.9166665639546849	0.5833335051344122	0.0784850000000006	F	F	F
0.9583335778691477	0.5416667904444452	0.1569700000000012	F	F	F
0.8750283100469880	0.5000490571017728	0.2385949962456681	T	T	T
0.9167708219544763	0.5834343643495539	0.3224633196973464	T	T	T
0.8749999835076636	0.6250002198243791	0.0000000000000000	F	F	F
0.9166664479350644	0.7083331486791877	0.0784850000000006	F	F	F
0.9583330283820857	0.6666664339892208	0.1569700000000012	F	F	F
0.8750390715792831	0.6249970908259023	0.2386144114820282	T	T	T
0.9167507455302246	0.7084283412100667	0.3223847279345599	T	T	T
0.8749998674880501	0.7499998633691547	0.0000000000000000	F	F	F
0.9166665821780171	0.8333332927490886	0.0784850000000006	F	F	F
0.9583331626250313	0.7916665780591217	0.1569700000000012	F	F	F
0.8750475547198707	0.7500510981514640	0.2386489455462041	T	T	T
0.9167381354041818	0.8334531816386493	0.3223726990932861	T	T	T
0.8750000017309958	0.8750000074390556	0.0000000000000000	F	F	F
0.9166667164209628	0.9583334368189895	0.0784850000000006	F	F	F
0.9583332968679841	0.9166667221290226	0.1569700000000012	F	F	F
0.8750357837611958	0.8751101760139146	0.2386153265545460	T	T	T
0.9167439085418626	0.9584762141790304	0.3224613228991354	T	T	T
0.4985231317624903	0.5111316541796056	0.4249580864249467	T	T	T
0.4980725323787391	0.6205597256357003	0.4240104380912588	T	T	T

0.3886593248302897	0.5106751784241700	0.4250994431084564	T	T	T
0.5324360415664221	0.5830292854121019	0.4243391102527191	T	T	T
0.4266493037913939	0.4768038295975132	0.4255281683221306	T	T	T
0.4262021215962384	0.5825864727810881	0.4244902106737157	T	T	T
0.5288002721647466	0.4812991964917966	0.4251325313109072	T	T	T
0.4012886911705003	0.4257494645840658	0.4256950051748943	T	T	T
0.3285616978319402	0.4804680057094995	0.4253690661946297	T	T	T
0.4005179583423151	0.6079608839532756	0.4238438536830658	T	T	T
0.5279444898522178	0.6806768102135600	0.4235244686184481	T	T	T
0.5834934761620081	0.6087239433834507	0.4235830982453749	T	T	T

Borazine adsorbed on Au(111), hpc

23.0697829620000014	0.0000000000000000	0.0000000000000000
-11.5348914810000007	19.9790169730000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.0000000000000000

Au B N H
320 3 3 6

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0416667146899670	0.0833334293799339	0.0784850000000006	F	F	F
0.0833332951369883	0.0416667146899670	0.1569700000000012	F	F	F
0.0000431922751564	0.0000488501489646	0.2385889258787894	T	T	T
0.0416994886856237	0.0833846717342028	0.3224109774406589	T	T	T
0.0000001342429456	0.1250001440699009	0.0000000000000000	F	F	F
0.0416668489329126	0.2083335734498348	0.0784850000000006	F	F	F
0.0833334293799339	0.1666668587598679	0.1569700000000012	F	F	F
0.0000748330865545	0.1250657926988245	0.2385816417791171	T	T	T
0.0416979042769607	0.2084150155376130	0.3224000013429126	T	T	T
0.0000000182233322	0.2499997876146764	0.0000000000000000	F	F	F
0.0416667329132991	0.3333332169946104	0.0784850000000006	F	F	F
0.0833333133603205	0.2916665023046434	0.1569700000000012	F	F	F
0.0000416220571696	0.2500534495710319	0.2385850505461532	T	T	T
0.0416970651711471	0.3334231174689254	0.3224587094286327	T	T	T
0.0000001524662778	0.3749999316845773	0.0000000000000000	F	F	F
0.0416668671562448	0.4583333610645113	0.0784850000000006	F	F	F
0.0833334476032661	0.4166666463745443	0.1569700000000012	F	F	F
0.0000162219827141	0.3750239577851716	0.2386002703718936	T	T	T
0.0417212092289550	0.4584224961160807	0.3224212106111984	T	T	T
0.9999997248487205	0.5000000757544782	0.0000000000000000	F	F	F
0.0416665679317489	0.5833335051344122	0.0784850000000006	F	F	F
0.0833335818462118	0.5416667904444452	0.1569700000000012	F	F	F
0.0000075982423941	0.5000023201163305	0.2385825334536233	T	T	T
0.0417103043445149	0.5834019626535690	0.3223676924601968	T	T	T
0.9999998590916661	0.6250002198243791	0.0000000000000000	F	F	F
0.0416664519121284	0.7083331486791877	0.0784850000000006	F	F	F
0.0833330323591497	0.6666664339892208	0.1569700000000012	F	F	F
0.0000055704891762	0.6250310381774022	0.2385802067194648	T	T	T
0.0417161726169642	0.7084174006638587	0.3223682987100818	T	T	T
0.9999997430720526	0.7499998633691547	0.0000000000000000	F	F	F
0.0416665861550811	0.8333332927490886	0.0784850000000006	F	F	F
0.0833331666020953	0.7916665780591217	0.1569700000000012	F	F	F
0.0000184604111414	0.7500684765157528	0.2385812719905820	T	T	T
0.0417357107506200	0.8334115215596268	0.3224206927582515	T	T	T
0.0000000057080598	0.8750000074390556	0.0000000000000000	F	F	F
0.0416667203980268	0.9583334368189895	0.0784850000000006	F	F	F
0.0833333008450481	0.9166667221290226	0.1569700000000012	F	F	F
0.0000245485176897	0.8750544638390946	0.2386009430498119	T	T	T
0.0417049874061355	0.9583857197262186	0.3224560916523718	T	T	T
0.1249998755840025	0.0000000000000000	0.0000000000000000	F	F	F
0.1666665902739695	0.0833334293799339	0.0784850000000006	F	F	F
0.2083331707209908	0.0416667146899670	0.1569700000000012	F	F	F
0.1250073409330755	0.0000567468266876	0.2386176337874436	T	T	T
0.1666590268323807	0.0833340587178628	0.3225599846902216	T	T	T
0.1250000098269552	0.1250001440699009	0.0000000000000000	F	F	F
0.1666667245169222	0.2083335734498348	0.0784850000000006	F	F	F
0.2083333049639364	0.1666668587598679	0.1569700000000012	F	F	F
0.1250607033470136	0.1250594018683979	0.2386557948401141	T	T	T
0.1666672506476239	0.2083829849359325	0.3225380617768382	T	T	T
0.1249998938073347	0.2499997876146764	0.0000000000000000	F	F	F
0.1666666084973016	0.3333332169946104	0.0784850000000006	F	F	F
0.2083331889443230	0.2916665023046434	0.1569700000000012	F	F	F
0.1250649997100298	0.2500592673913216	0.2386539351381108	T	T	T
0.1666498611542742	0.3334277942226134	0.3225567677382124	T	T	T
0.1250000280502874	0.3749999316845773	0.0000000000000000	F	F	F
0.1666667427402544	0.4583333610645113	0.0784850000000006	F	F	F
0.2083333231872686	0.4166666463745443	0.1569700000000012	F	F	F
0.1250031405516100	0.3750083584451595	0.2386172085944941	T	T	T

0.1667067547052360	0.4584041400412969	0.3224670302262484	T	T	T
0.1250001622932331	0.5000000757544782	0.0000000000000000	F	F	F
0.1666668769832000	0.5833335051344122	0.0784850000000006	F	F	F
0.2083334574302214	0.5416667904444452	0.1569700000000012	F	F	F
0.1250012977972416	0.5000028511279840	0.2385815577284869	T	T	T
0.1667111595781666	0.5834023949350146	0.3223691116008435	T	T	T
0.1250002965361787	0.6250002198243791	0.0000000000000000	F	F	F
0.1666667609635866	0.7083331486791877	0.0784850000000006	F	F	F
0.2083333414106079	0.6666664339892208	0.1569700000000012	F	F	F
0.1250164284477538	0.6250227965433730	0.2385734875208912	T	T	T
0.1667198445962390	0.7084156648814744	0.3223495205257267	T	T	T
0.1249997470491166	0.7499998633691547	0.0000000000000000	F	F	F
0.1666664617390836	0.8333332927490886	0.0784850000000006	F	F	F
0.2083334756535535	0.7916665780591217	0.1569700000000012	F	F	F
0.1250212606022741	0.7500581268347950	0.2385758774610647	T	T	T
0.1667198779067986	0.8334278388292865	0.3223706707974988	T	T	T
0.1249998812920623	0.8750000074390556	0.0000000000000000	F	F	F
0.1666665959820293	0.9583334368189895	0.0784850000000006	F	F	F
0.2083331764290506	0.9166667221290226	0.1569700000000012	F	F	F
0.1250141630341869	0.8750669900920603	0.2385827791044766	T	T	T
0.1667212193132796	0.9584256199133049	0.3224598403943924	T	T	T
0.2500001846354607	0.0000000000000000	0.0000000000000000	F	F	F
0.2916668993254277	0.0833334293799339	0.0784850000000006	F	F	F
0.3333334797724490	0.0416667146899670	0.1569700000000012	F	F	F
0.2499835363830695	0.0000507943561997	0.2386435434117689	T	T	T
0.2917271985191473	0.0834905183991432	0.3225607269333585	T	T	T
0.2499998854109577	0.1250001440699009	0.0000000000000000	F	F	F
0.2916666001009247	0.2083335734498348	0.0784850000000006	F	F	F
0.3333336140153946	0.1666668587598679	0.1569700000000012	F	F	F
0.2499219120466561	0.1249679126704150	0.2386611543870320	T	T	T
0.2914796926259589	0.2082652094152430	0.3226390214749397	T	T	T
0.2499997693913443	0.2499997876146764	0.0000000000000000	F	F	F
0.2916664840813112	0.3333332169946104	0.0784850000000006	F	F	F
0.3333330645283255	0.2916665023046434	0.1569700000000012	F	F	F
0.2499841231861859	0.2500153843809870	0.2386723597343582	T	T	T
0.2914616958986291	0.3333261077549077	0.3226176411682144	T	T	T
0.2499999036342899	0.3749999316845773	0.0000000000000000	F	F	F
0.2916666183242569	0.4583333610645113	0.0784850000000006	F	F	F
0.3333331987712782	0.4166666463745443	0.1569700000000012	F	F	F
0.2499166765091319	0.3750142806003528	0.2386522446643545	T	T	T
0.2917054822715700	0.4583509766002090	0.3225653710111527	T	T	T
0.2500000378772356	0.5000000757544782	0.0000000000000000	F	F	F
0.2916667525672025	0.5833335051344122	0.0784850000000006	F	F	F
0.333333330142239	0.5416667904444452	0.1569700000000012	F	F	F
0.2499656562573671	0.4999950817417154	0.2386463849657386	T	T	T
0.2917348023414235	0.5833828833850240	0.3223701840863876	T	T	T
0.2500001721201883	0.6250002198243791	0.0000000000000000	F	F	F
0.2916666365475891	0.7083331486791877	0.0784850000000006	F	F	F
0.3333332169946104	0.6666664339892208	0.1569700000000012	F	F	F
0.2500338370548463	0.6250263306619017	0.2385804189386988	T	T	T
0.2917214537106873	0.7084158694792860	0.3223673293819338	T	T	T
0.2500000561005749	0.7499998633691547	0.0000000000000000	F	F	F
0.2916667707905418	0.8333332927490886	0.0784850000000006	F	F	F
0.3333333512375560	0.7916665780591217	0.1569700000000012	F	F	F
0.2500477858864210	0.7500546817913447	0.2385728052151030	T	T	T
0.2917281659287926	0.8334293595254556	0.3223577292759690	T	T	T
0.2500001903435205	0.8750000074390556	0.0000000000000000	F	F	F
0.2916669050334875	0.9583334368189895	0.0784850000000006	F	F	F
0.3333334854805088	0.9166667221290226	0.1569700000000012	F	F	F
0.2500394334009555	0.8750767805340293	0.2385750378847285	T	T	T
0.2917465884405477	0.9584769394015821	0.3223580451441161	T	T	T
0.3750000602194632	0.0000000000000000	0.0000000000000000	F	F	F
0.4166667749094302	0.0833334293799339	0.0784850000000006	F	F	F
0.4583333553564515	0.0416667146899670	0.1569700000000012	F	F	F
0.3750655904632578	0.0000471041166120	0.2386384040943304	T	T	T
0.4167786526375494	0.0834937604821266	0.3225496365301242	T	T	T
0.3750001944624159	0.1250001440699009	0.0000000000000000	F	F	F
0.4166669091523829	0.2083335734498348	0.0784850000000006	F	F	F
0.4583334895993971	0.1666668587598679	0.1569700000000012	F	F	F
0.3749118140784740	0.1248257158966613	0.2386778683339228	T	T	T
0.4166760118672473	0.2083273318110385	0.3224941599944781	T	T	T
0.3750000784427954	0.2499997876146764	0.0000000000000000	F	F	F
0.4166667931327623	0.3333332169946104	0.0784850000000006	F	F	F
0.4583333735797837	0.2916665023046434	0.1569700000000012	F	F	F
0.3747771626736816	0.2496697398814658	0.2385171953151829	T	T	T
0.4162133900803770	0.3331806798279605	0.3210176412476629	T	T	T
0.3749997792182995	0.3749999316845773	0.0000000000000000	F	F	F
0.4166664939082665	0.4583333610645113	0.0784850000000006	F	F	F

0.4583335078227293	0.4166666463745443	0.1569700000000012	F	F	F
0.3747737130882079	0.3751522052831085	0.2384957823945500	T	T	T
0.4166413466319109	0.4585187559315705	0.3223457767952304	T	T	T
0.3749999134612452	0.5000000757544782	0.0000000000000000	F	F	F
0.4166666281512121	0.5833335051344122	0.0784850000000006	F	F	F
0.4583332085982335	0.5416667904444452	0.1569700000000012	F	F	F
0.3748813521822366	0.5001686706018749	0.2386487561975986	T	T	T
0.4167731356373290	0.5834288110422339	0.3225429785738348	T	T	T
0.3750000477041908	0.6250002198243791	0.0000000000000000	F	F	F
0.4166665121315987	0.7083331486791877	0.0784850000000006	F	F	F
0.4583330925786129	0.6666664339892208	0.1569700000000012	F	F	F
0.3750554181955329	0.6250979941619889	0.2386475225609768	T	T	T
0.4167150841019379	0.7084238209638575	0.3224668119947934	T	T	T
0.3749999316845773	0.7499998633691547	0.0000000000000000	F	F	F
0.4166666463745443	0.8333332927490886	0.0784850000000006	F	F	F
0.4583332268215656	0.7916665780591217	0.1569700000000012	F	F	F
0.3750617240613495	0.7500654783870117	0.2385833212900069	T	T	T
0.4166962966921063	0.8334117130599068	0.3224198434773448	T	T	T
0.3750000659275230	0.8750000074390556	0.0000000000000000	F	F	F
0.4166667806174900	0.9583334368189895	0.0784850000000006	F	F	F
0.4583333610645113	0.9166667221290226	0.1569700000000012	F	F	F
0.3750626129271483	0.8750645140697232	0.2385774681573733	T	T	T
0.4167222169545299	0.9584260748675310	0.3224531231169689	T	T	T
0.4999999358034728	0.0000000000000000	0.0000000000000000	F	F	F
0.5416666504934398	0.0833334293799339	0.0784850000000006	F	F	F
0.5833332309404540	0.0416667146899670	0.1569700000000012	F	F	F
0.5000548215453933	0.0000564363697229	0.2386154025166596	T	T	T
0.5416978722794368	0.0833325492797155	0.3225649387571113	T	T	T
0.5000000700464184	0.1250001440699009	0.0000000000000000	F	F	F
0.5416667847363854	0.2083335734498348	0.0784850000000006	F	F	F
0.5833333651834067	0.1666668587598679	0.1569700000000012	F	F	F
0.5000497032242821	0.1249608384359570	0.2386580390745248	T	T	T
0.5418090806546200	0.2082568427158436	0.3226373312374159	T	T	T
0.4999999540268050	0.2499997876146764	0.0000000000000000	F	F	F
0.5416666687167719	0.3333332169946104	0.0784850000000006	F	F	F
0.5833332491637861	0.2916665023046434	0.1569700000000012	F	F	F
0.4998956471906179	0.2496558980813096	0.2385105994995380	T	T	T
0.5419958102908581	0.3331706180262211	0.3209794895440694	T	T	T
0.5000000882697506	0.3749999316845773	0.0000000000000000	F	F	F
0.5416668029597176	0.4583333610645113	0.0784850000000006	F	F	F
0.5833333834067389	0.4166666463745443	0.1569700000000012	F	F	F
0.5000126216538100	0.3750185756178682	0.2384149800764902	T	T	T
0.5420291530239248	0.4590167831615598	0.3207401616168774	T	T	T
0.5000002225126963	0.5000000757544782	0.0000000000000000	F	F	F
0.5416669372026632	0.5833335051344122	0.0784850000000006	F	F	F
0.5833335176496846	0.5416667904444452	0.1569700000000012	F	F	F
0.4998933703695531	0.5003284270240798	0.2384500520028452	T	T	T
0.5418352868026564	0.5837422876018240	0.3225730040665205	T	T	T
0.4999999232882004	0.6250002198243791	0.0000000000000000	F	F	F
0.5416663877156012	0.7083331486791877	0.0784850000000006	F	F	F
0.5833334016300711	0.6666664339892208	0.1569700000000012	F	F	F
0.5000422471588180	0.6251771938556332	0.2386485239787164	T	T	T
0.5416927278675615	0.7084989813973986	0.3225780344841722	T	T	T
0.4999998072685798	0.7499998633691547	0.0000000000000000	F	F	F
0.5416665219585468	0.8333332927490886	0.0784850000000006	F	F	F
0.5833331024055681	0.7916665780591217	0.1569700000000012	F	F	F
0.5000567863010532	0.7500704671816846	0.2386265993299221	T	T	T
0.5416961314686218	0.8334404113711529	0.3224664116594329	T	T	T
0.4999999415115326	0.8750000074390556	0.0000000000000000	F	F	F
0.5416666562014996	0.9583334368189895	0.0784850000000006	F	F	F
0.5833332366485138	0.9166667221290226	0.1569700000000012	F	F	F
0.5000387271072305	0.8750512640378777	0.2386012201768689	T	T	T
0.5417014178653047	0.9583859394091622	0.3224534579534868	T	T	T
0.6249998113874753	0.0000000000000000	0.0000000000000000	F	F	F
0.6666665260774423	0.0833334293799339	0.0784850000000006	F	F	F
0.7083335399919122	0.0416667146899670	0.1569700000000012	F	F	F
0.6250121084495712	0.0000486058320117	0.2385856876372890	T	T	T
0.6667091313970448	0.0833862633889639	0.3224116667846010	T	T	T
0.6249999456304209	0.1250001440699009	0.0000000000000000	F	F	F
0.666666603203879	0.2083335734498348	0.0784850000000006	F	F	F
0.7083332407674092	0.1666668587598679	0.1569700000000012	F	F	F
0.6250074109362467	0.1250609929862671	0.2386584845002565	T	T	T
0.6667381654481310	0.2083792797384931	0.3225456252559366	T	T	T
0.6249998296108075	0.2499997876146764	0.0000000000000000	F	F	F
0.6666665443007744	0.3333332169946104	0.0784850000000006	F	F	F
0.7083331247477958	0.2916665023046434	0.1569700000000012	F	F	F
0.6250414930256170	0.2500124401920964	0.2386748143914357	T	T	T
0.6668931576551761	0.3333170922153600	0.3226147473914427	T	T	T

0.6249999638537531	0.3749999316845773	0.0000000000000000	F	F	F
0.6666666785437201	0.4583333610645113	0.0784850000000000	F	F	F
0.70833332589907414	0.4166666463745443	0.1569700000000001	F	F	F
0.6253948674891887	0.3751475795663758	0.2384870947631675	T	T	T
0.6669177955156662	0.4585176763082494	0.3223218302745967	T	T	T
0.6250000980967059	0.5000000757544782	0.0000000000000000	F	F	F
0.6666668127866728	0.5833335051344122	0.0784850000000000	F	F	F
0.7083333932336870	0.5416667904444452	0.1569700000000001	F	F	F
0.6254461036805042	0.5003269123882399	0.2384463269976074	T	T	T
0.6669392060082396	0.5837436068126916	0.3225727137869382	T	T	T
0.6250002323396515	0.6250002198243791	0.0000000000000000	F	F	F
0.6666666967670594	0.7083331486791877	0.0784850000000000	F	F	F
0.7083332772140736	0.6666664339892208	0.1569700000000001	F	F	F
0.6250645375694737	0.6251131592989387	0.2386523426577982	T	T	T
0.6667551743502035	0.7084878462936798	0.3225543404396724	T	T	T
0.6250001163200380	0.7499998633691547	0.0000000000000000	F	F	F
0.6666668310100050	0.8333332927490886	0.0784850000000000	F	F	F
0.7083334114570263	0.7916665780591217	0.1569700000000001	F	F	F
0.6250062821341069	0.7500090463144864	0.2386618271878822	T	T	T
0.6667081045199537	0.8334431776851798	0.3224013404418321	T	T	T
0.6249998170955351	0.8750000074390556	0.0000000000000000	F	F	F
0.6666665317855021	0.9583334368189895	0.0784850000000000	F	F	F
0.7083335456999720	0.9166667221290226	0.1569700000000001	F	F	F
0.6250076881419636	0.8750244664432950	0.2385856837772644	T	T	T
0.6667031486168549	0.9584135121003947	0.3223838232620693	T	T	T
0.7500001204389335	0.0000000000000000	0.0000000000000000	F	F	F
0.7916668351289005	0.0833334293799339	0.0784850000000000	F	F	F
0.8333334155759147	0.0416667146899670	0.1569700000000001	F	F	F
0.7500104890530436	0.0000372991528224	0.2385765932020248	T	T	T
0.7917182894556117	0.0834146910583732	0.3223604719478028	T	T	T
0.7500002546818791	0.1250001440699009	0.0000000000000000	F	F	F
0.7916669693718461	0.2083335734498348	0.0784850000000000	F	F	F
0.8333335498188674	0.1666668587598679	0.1569700000000001	F	F	F
0.7499993075590727	0.1250647952084359	0.2385835652622705	T	T	T
0.7917416160585291	0.2084145661532830	0.3224003148739057	T	T	T
0.7499997051948100	0.2499997876146764	0.0000000000000000	F	F	F
0.7916664198847769	0.3333332169946104	0.0784850000000000	F	F	F
0.8333334337992468	0.2916665023046434	0.1569700000000001	F	F	F
0.7500020334582160	0.2500551034789967	0.2386579059838254	T	T	T
0.7918016492877835	0.3334214480153974	0.3225603838202414	T	T	T
0.7499998394377627	0.3749999316845773	0.0000000000000000	F	F	F
0.7916665541277297	0.4583333610645113	0.0784850000000000	F	F	F
0.8333331345747439	0.4166666463745443	0.1569700000000001	F	F	F
0.7501103582477172	0.3750113816284933	0.2386538097005707	T	T	T
0.7916751140020449	0.4583457643333030	0.3225621356681493	T	T	T
0.7499999736807084	0.5000000757544782	0.0000000000000000	F	F	F
0.7916666883706753	0.5833335051344122	0.0784850000000000	F	F	F
0.8333332688176966	0.5416667904444452	0.1569700000000001	F	F	F
0.7503098333914666	0.5001728027948098	0.2386447668905023	T	T	T
0.7916830691535763	0.5834281644381160	0.3225512549036087	T	T	T
0.7500001079236540	0.6250002198243791	0.0000000000000000	F	F	F
0.7916665723510619	0.7083331486791877	0.0784850000000000	F	F	F
0.8333331527980832	0.6666664339892208	0.1569700000000001	F	F	F
0.7501505022131713	0.6251757467346082	0.2386453594802413	T	T	T
0.7918274751837078	0.7085003315334447	0.3225657042104980	T	T	T
0.749999919040405	0.7499998633691547	0.0000000000000000	F	F	F
0.7916667065940075	0.8333332927490886	0.0784850000000000	F	F	F
0.8333332870410288	0.7916665780591217	0.1569700000000001	F	F	F
0.7500103937773035	0.7500087912333996	0.2386584874752268	T	T	T
0.7917498625658729	0.8334434586509063	0.3223953975627892	T	T	T
0.7500001261469933	0.8750000074390556	0.0000000000000000	F	F	F
0.7916668408369603	0.9583334368189895	0.0784850000000000	F	F	F
0.8333334212839745	0.9166667221290226	0.1569700000000001	F	F	F
0.7499973095978275	0.8749923981448675	0.2385799108484575	T	T	T
0.7917195452509219	0.9584208823658433	0.3223518655690892	T	T	T
0.874999960229360	0.0000000000000000	0.0000000000000000	F	F	F
0.9166667107129030	0.0833334293799339	0.0784850000000000	F	F	F
0.9583332911599243	0.0416667146899670	0.1569700000000001	F	F	F
0.8750354866708661	0.0000357206535356	0.2385785257923624	T	T	T
0.9167190912683238	0.0834128951503190	0.3223607416380690	T	T	T
0.8750001302658816	0.1250001440699009	0.0000000000000000	F	F	F
0.9166668449558486	0.2083335734498348	0.0784850000000000	F	F	F
0.9583334254028699	0.1666668587598679	0.1569700000000001	F	F	F
0.8750353933790356	0.1250582888056386	0.2385806116766890	T	T	T
0.9167253029860166	0.2084232279873291	0.3223903601020432	T	T	T
0.8750000142462682	0.2499997876146764	0.0000000000000000	F	F	F
0.9166667289362351	0.3333332169946104	0.0784850000000000	F	F	F
0.9583333093832564	0.2916665023046434	0.1569700000000001	F	F	F

0.8750219270710047	0.2500537050906462	0.2385878750988218	T	T	T
0.9167485619789226	0.3334193590341606	0.3224608077167541	T	T	T
0.8750001484892138	0.3749999316845773	0.0000000000000000	F	F	F
0.9166668631791808	0.4583333610645113	0.0784850000000006	F	F	F
0.9583334436262021	0.4166666463745443	0.1569700000000012	F	F	F
0.8750145970571515	0.3750062412467143	0.2386210838480654	T	T	T
0.9167189288692561	0.4584003049792973	0.3224764656197019	T	T	T
0.8749998492647180	0.5000000757544782	0.0000000000000000	F	F	F
0.9166665639546849	0.5833335051344122	0.0784850000000006	F	F	F
0.9583335778691477	0.5416667904444452	0.1569700000000012	F	F	F
0.8750454426979284	0.4999957328114930	0.2386479473914358	T	T	T
0.9166716870227114	0.5833833075345108	0.3223718874881867	T	T	T
0.8749999835076636	0.6250002198243791	0.0000000000000000	F	F	F
0.9166664479350644	0.7083331486791877	0.0784850000000006	F	F	F
0.9583330283820857	0.6666664339892208	0.1569700000000012	F	F	F
0.8750579592647515	0.6251008108651238	0.2386475367561453	T	T	T
0.9167310051529433	0.7084250937825805	0.3224641199402443	T	T	T
0.8749998674880501	0.7499998633691547	0.0000000000000000	F	F	F
0.9166665821780171	0.8333332927490886	0.0784850000000006	F	F	F
0.9583331626250313	0.7916665780591217	0.1569700000000012	F	F	F
0.8750300491038828	0.7500769632137582	0.2386216580918650	T	T	T
0.9167624718057445	0.8334417115570288	0.3224663509609216	T	T	T
0.8750000017309958	0.8750000074390556	0.0000000000000000	F	F	F
0.9166667164209628	0.9583334368189895	0.0784850000000006	F	F	F
0.9583332968679841	0.9166667221290226	0.1569700000000012	F	F	F
0.8750274527175103	0.8750300757441655	0.2385855974546473	T	T	T
0.9167278688074065	0.9584111427115058	0.3223946449319174	T	T	T
0.5753796638917655	0.4151425064756368	0.4242899063343946	T	T	T
0.4658655149007977	0.4154431669915506	0.4243564219407636	T	T	T
0.4655687469489420	0.3056431138369070	0.4250034725380502	T	T	T
0.5377598670140127	0.4494258656768019	0.4241470527368331	T	T	T
0.5374697109504183	0.3432701509435259	0.4248318066987057	T	T	T
0.4316008321722401	0.3435633707596037	0.4249221373388460	T	T	T
0.6354953815764925	0.4450897675497759	0.4241434286055407	T	T	T
0.5629003654601088	0.3176365638763913	0.4246064640978772	T	T	T
0.4353968503009434	0.2455468669567303	0.4253639183902407	T	T	T
0.3805393664323758	0.3181470816204967	0.4247642333271714	T	T	T
0.4359532640089918	0.4456456740628821	0.4242367572894408	T	T	T
0.5633974066482309	0.5004816521534471	0.4233725718282645	T	T	T

Borazine dimer adsorbed on Au(111), dimer I

23.0697829620000014	0.0000000000000000	0.0000000000000000
-11.5348914810000007	19.9790169730000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.0000000000000000

Au B N H

320 6 6 12

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0416667146899670	0.0833334293799339	0.0784850000000006	F	F	F
0.0833332951369883	0.0416667146899670	0.1569700000000012	F	F	F
0.9999634263423139	-0.0000122133656657	0.2386171706224730	T	T	T
0.0415513703153966	0.0831715004241697	0.3224476161333843	T	T	T
0.0000001342429456	0.1250001440699009	0.0000000000000000	F	F	F
0.0416668489329126	0.2083335734498348	0.0784850000000006	F	F	F
0.0833334293799339	0.1666668587598679	0.1569700000000012	F	F	F
-0.0000079505279927	0.1249619856191353	0.2385898618898550	T	T	T
0.0415661315594105	0.208222434575048	0.3224182863792385	T	T	T
0.0000000182233322	0.2499997876146764	0.0000000000000000	F	F	F
0.0416667329132991	0.3333332169946104	0.0784850000000006	F	F	F
0.0833333133603205	0.2916665023046434	0.1569700000000012	F	F	F
-0.0000231169765436	0.2499435946088535	0.2385650813097671	T	T	T
0.0415516318805026	0.3332462532979221	0.3224264334460157	T	T	T
0.0000001524662778	0.3749999316845773	0.0000000000000000	F	F	F
0.0416668671562448	0.4583333610645113	0.0784850000000006	F	F	F
0.0833334476032661	0.4166666463745443	0.1569700000000012	F	F	F
-0.0000354301934321	0.3749583860088558	0.2385827247109530	T	T	T
0.0416034061666337	0.4583038451938021	0.3223717303944743	T	T	T
0.9999997248487205	0.5000000757544782	0.0000000000000000	F	F	F
0.0416665679317489	0.5833335051344122	0.0784850000000006	F	F	F
0.0833335818462118	0.5416667904444452	0.1569700000000012	F	F	F
0.9999711206234684	0.4999742802493763	0.2385610477467986	T	T	T
0.0416310226680852	0.5833099399307213	0.3223553270052462	T	T	T
0.9999998590916661	0.6250002198243791	0.0000000000000000	F	F	F
0.0416664519121284	0.7083331486791877	0.0784850000000006	F	F	F
0.0833330323591497	0.6666664339892208	0.1569700000000012	F	F	F
0.9999622963432535	0.6249853436852113	0.2385630969864414	T	T	T
0.0417011893785167	0.7083303685983533	0.3224125231675604	T	T	T

0.9999997430720526	0.7499998633691547	0.0000000000000000	F	F	F
0.0416665861550811	0.8333332927490886	0.0784850000000000	F	F	F
0.0833331666020953	0.7916665780591217	0.1569700000000000	F	F	F
0.9999663589929429	0.7499454663824258	0.2385994772483172	T	T	T
0.0416748511993528	0.8332855208180495	0.3224407897639216	T	T	T
0.0000000057080598	0.8750000074390556	0.0000000000000000	F	F	F
0.0416667203980268	0.9583334368189895	0.0784850000000000	F	F	F
0.0833333008450481	0.9166667221290226	0.1569700000000000	F	F	F
0.9999744929389695	0.8749262160918599	0.2386344853130896	T	T	T
0.0415439992375322	0.9581796876084407	0.3224006756568411	T	T	T
0.1249998755840025	0.0000000000000000	0.0000000000000000	F	F	F
0.1666665902739695	0.0833334293799339	0.0784850000000000	F	F	F
0.2083331707209908	0.0416667146899670	0.1569700000000000	F	F	F
0.1249255427498045	-0.0000390419301642	0.2385992182752396	T	T	T
0.1665351583715427	0.0831510608023622	0.3225396829962296	T	T	T
0.1250000098269552	0.1250001440699009	0.0000000000000000	F	F	F
0.1666667245169222	0.2083335734498348	0.0784850000000000	F	F	F
0.2083333049639364	0.1666668587598679	0.1569700000000000	F	F	F
0.1249699883296576	0.1249638358836705	0.2386396279766422	T	T	T
0.1664958211722642	0.2081638751153918	0.3225495190381326	T	T	T
0.1249998938073347	0.2499997876146764	0.0000000000000000	F	F	F
0.1666666084973016	0.3333332169946104	0.0784850000000000	F	F	F
0.2083331889443230	0.2916665023046434	0.1569700000000000	F	F	F
0.1249782183568886	0.2499542038436312	0.2386516007677137	T	T	T
0.1664555471260750	0.3332158459953336	0.3226024718339743	T	T	T
0.1250000280502874	0.3749999316845773	0.0000000000000000	F	F	F
0.1666667427402544	0.4583333610645113	0.0784850000000000	F	F	F
0.2083333231872686	0.4166666463745443	0.1569700000000000	F	F	F
0.1249398612383777	0.3749298870085053	0.2386043481214850	T	T	T
0.1665332116785349	0.4582333459659587	0.3224424434746835	T	T	T
0.1250001622932331	0.5000000757544782	0.0000000000000000	F	F	F
0.1666668769832000	0.5833335051344122	0.0784850000000000	F	F	F
0.2083334574302214	0.5416667904444452	0.1569700000000000	F	F	F
0.1249858285273305	0.4999685726901013	0.2385580322079655	T	T	T
0.1665980694596580	0.5832950575608477	0.3223598869451025	T	T	T
0.1250002965361787	0.6250002198243791	0.0000000000000000	F	F	F
0.1666667609635866	0.7083331486791877	0.0784850000000000	F	F	F
0.2083333414106079	0.6666664339892208	0.1569700000000000	F	F	F
0.1249823655521063	0.6249864722656207	0.2385573425045146	T	T	T
0.1666555970551839	0.7083264827390999	0.3223752774739835	T	T	T
0.1249997470491166	0.7499998633691547	0.0000000000000000	F	F	F
0.1666664617390836	0.8333332927490886	0.0784850000000000	F	F	F
0.2083334756535535	0.7916665780591217	0.1569700000000000	F	F	F
0.1249835743021611	0.7499839632815112	0.2385633176311925	T	T	T
0.1667157096334090	0.8333570388292068	0.3223519198531133	T	T	T
0.1249998812920623	0.8750000074390556	0.0000000000000000	F	F	F
0.1666665959820293	0.9583334368189895	0.0784850000000000	F	F	F
0.2083331764290506	0.9166667221290226	0.1569700000000000	F	F	F
0.1249664726373983	0.8749624233391324	0.2385591139615433	T	T	T
0.1666672147511054	0.9582905724973135	0.3224124869717306	T	T	T
0.2500001846354607	0.0000000000000000	0.0000000000000000	F	F	F
0.2916668993254277	0.0833334293799339	0.0784850000000000	F	F	F
0.3333334797724490	0.0416667146899670	0.1569700000000000	F	F	F
0.2499514053899252	0.9999541779942824	0.2386238060576498	T	T	T
0.2916781281840444	0.0833540030931566	0.3225187948825120	T	T	T
0.2499998854109577	0.1250001440699009	0.0000000000000000	F	F	F
0.2916666001009247	0.2083335734498348	0.0784850000000000	F	F	F
0.3333336140153946	0.1666668587598679	0.1569700000000000	F	F	F
0.2498290521810950	0.1248413402520080	0.2386386273748198	T	T	T
0.2913212813871484	0.2080588453932765	0.3225841592626696	T	T	T
0.2499997693913443	0.2499997876146764	0.0000000000000000	F	F	F
0.2916664840813112	0.3333332169946104	0.0784850000000000	F	F	F
0.3333330645283255	0.2916665023046434	0.1569700000000000	F	F	F
0.2498487864532039	0.2498840867343047	0.2386492470758152	T	T	T
0.2912366178544199	0.3330877034474294	0.3226574898523127	T	T	T
0.2499999036342899	0.3749999316845773	0.0000000000000000	F	F	F
0.2916666183242569	0.4583333610645113	0.0784850000000000	F	F	F
0.3333331987712782	0.4166666463745443	0.1569700000000000	F	F	F
0.2497770427726008	0.3748974227241433	0.2386729375899876	T	T	T
0.2914511815090920	0.4580667819035447	0.3226900550808574	T	T	T
0.2500000378772356	0.5000000757544782	0.0000000000000000	F	F	F
0.2916667525672025	0.5833335051344122	0.0784850000000000	F	F	F
0.333333330142239	0.5416667904444452	0.1569700000000000	F	F	F
0.2499176613231413	0.4999231152047397	0.2387034007790621	T	T	T
0.2915560094817997	0.5832037290876393	0.3224859518573689	T	T	T
0.2500001721201883	0.6250002198243791	0.0000000000000000	F	F	F
0.2916666365475891	0.7083331486791877	0.0784850000000000	F	F	F
0.3333332169946104	0.6666664339892208	0.1569700000000000	F	F	F

0.2500006307467730	0.6249637778098653	0.2386173419722383	T	T	T
0.2916119185932042	0.7082995478457965	0.3225053773264849	T	T	T
0.2500000561005749	0.7499998633691547	0.0000000000000000	F	F	F
0.2916667707905418	0.8333332927490886	0.0784850000000006	F	F	F
0.3333333512375560	0.7916665780591217	0.1569700000000012	F	F	F
0.2499948478536138	0.7499536695966967	0.2385793303129294	T	T	T
0.2917200717681311	0.8333065100964313	0.3223790994959458	T	T	T
0.2500001903435205	0.8750000074390556	0.0000000000000000	F	F	F
0.2916669050334875	0.9583334368189895	0.0784850000000006	F	F	F
0.3333334854805088	0.9166667221290226	0.1569700000000012	F	F	F
0.2500196044200988	0.8749782752523494	0.2385518798125005	T	T	T
0.2917490672293696	0.9583595608015015	0.3223114200509578	T	T	T
0.3750000602194632	0.0000000000000000	0.0000000000000000	F	F	F
0.4166667749094302	0.0833334293799339	0.0784850000000006	F	F	F
0.4583333553564515	0.0416667146899670	0.1569700000000012	F	F	F
0.3750933710460659	0.9999388741267555	0.2386161774934504	T	T	T
0.4167803629495025	0.0833286824640579	0.3225172854512690	T	T	T
0.3750001944624159	0.1250001440699009	0.0000000000000000	F	F	F
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0.4583334895993971	0.1666668587598679	0.1569700000000012	F	F	F
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0.3746805120188104	0.2495252958130169	0.2384602014340279	T	T	T
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0.4583335078227293	0.4166666463745443	0.1569700000000012	F	F	F
0.3745661492158231	0.3749940255493442	0.2385006483150995	T	T	T
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0.4583332085982335	0.5416667904444452	0.1569700000000012	F	F	F
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0.4163351808655691	0.5830139340483020	0.3227796467078242	T	T	T
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0.4583330925786129	0.6666664339892208	0.1569700000000012	F	F	F
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0.5645156616039663	0.6046895049740046	0.4246511321905811	T	T	T
0.5048148121031450	0.6725653473217027	0.4262216700461778	T	T	T
0.5551797657392176	0.7994855087088044	0.4278876245714536	T	T	T
0.6829371798863197	0.8593418611802759	0.4269920840849530	T	T	T
0.7595271072569304	0.8089970266785543	0.4245896818103122	T	T	T
0.5619405149252060	0.3187647756047928	0.4243231591774929	T	T	T
0.4346000554511448	0.2451874743747922	0.4238783957326131	T	T	T
0.3780987758416799	0.3162844038636561	0.4235642412858199	T	T	T
0.4319501731491018	0.4436962598564295	0.4245804019139115	T	T	T

0.5592591459657918	0.5001466673767569	0.4246313084022399	T	T	T
0.6330294623487451	0.4463215410586702	0.4250868661538686	T	T	T

Borazine dimer adsorbed on Au(111), dimer II

23.0697829620000014	0.0000000000000000	0.0000000000000000
-11.5348914810000007	19.9790169730000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.0000000000000000

Au	B	N	H
320	6	6	12

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0416667146899670	0.0833334293799339	0.0784850000000006	F	F	F
0.0833332951369883	0.0416667146899670	0.1569700000000012	F	F	F
0.0000386306477370	0.0000170664558566	0.2385698720846657	T	T	T
0.0416089149678961	0.0832871233435406	0.3224293160256608	T	T	T
0.0000001342429456	0.1250001440699009	0.0000000000000000	F	F	F
0.0416668489329126	0.2083335734498348	0.0784850000000006	F	F	F
0.0833334293799339	0.1666668587598679	0.1569700000000012	F	F	F
0.0000053299204368	0.1250060024355980	0.2385712140527525	T	T	T
0.0416077587701288	0.2082943639849962	0.3224914544374957	T	T	T
0.0000000182233322	0.2499997876146764	0.0000000000000000	F	F	F
0.0416667329132991	0.3333332169946104	0.0784850000000006	F	F	F
0.0833333133603205	0.2916665023046434	0.1569700000000012	F	F	F
0.0000316525286784	0.2500000010223495	0.2385906300893831	T	T	T
0.0416926258513331	0.3333381824644399	0.3223842374239829	T	T	T
0.0000001524662778	0.3749999316845773	0.0000000000000000	F	F	F
0.0416668671562448	0.4583333610645113	0.0784850000000006	F	F	F
0.0833334476032661	0.4166666463745443	0.1569700000000012	F	F	F
0.0000299193156970	0.3749757588448215	0.2385778313843589	T	T	T
0.0417015115858202	0.4583108135257001	0.3224323782192487	T	T	T
0.9999997248487205	0.5000000757544782	0.0000000000000000	F	F	F
0.0416665679317489	0.5833335051344122	0.0784850000000006	F	F	F
0.0833335818462118	0.5416667904444452	0.1569700000000012	F	F	F
0.0000119841974980	0.4999605717836347	0.2385700617341981	T	T	T
0.0417206905179474	0.5833120037157682	0.3223959633162752	T	T	T
0.9999998590916661	0.6250002198243791	0.0000000000000000	F	F	F
0.0416664519121284	0.7083331486791877	0.0784850000000006	F	F	F
0.0833330323591497	0.6666664339892208	0.1569700000000012	F	F	F
0.0000280631453650	0.6249844706761615	0.2385645502352554	T	T	T
0.0417687498490671	0.7083161238885606	0.3223647164686804	T	T	T
0.9999997430720526	0.7499998633691547	0.0000000000000000	F	F	F
0.0416665861550811	0.8333332927490886	0.0784850000000006	F	F	F
0.0833331666020953	0.7916665780591217	0.1569700000000012	F	F	F
0.0000294896976386	0.7499784121932516	0.2385531422718649	T	T	T
0.0417188364327587	0.8332952603734188	0.3223843597845815	T	T	T
0.000000057080598	0.8750000074390556	0.0000000000000000	F	F	F
0.0416667203980268	0.9583334368189895	0.0784850000000006	F	F	F
0.0833333008450481	0.9166667221290226	0.1569700000000012	F	F	F
0.0000259973922884	0.8750021844097797	0.2385491288807623	T	T	T
0.0416700562060952	0.9582855675970581	0.3223783453548144	T	T	T
0.1249998755840025	0.0000000000000000	0.0000000000000000	F	F	F
0.1666665902739695	0.0833334293799339	0.0784850000000006	F	F	F
0.2083331707209908	0.0416667146899670	0.1569700000000012	F	F	F
0.1250334116036166	0.0000189631215267	0.2386194317910958	T	T	T
0.1665971494415941	0.0832730008639330	0.3225319629464752	T	T	T
0.1250000098269552	0.1250001440699009	0.0000000000000000	F	F	F
0.1666667245169222	0.2083335734498348	0.0784850000000006	F	F	F
0.2083333049639364	0.1666668587598679	0.1569700000000012	F	F	F
0.1249837080829655	0.1250067051670186	0.2386720812904533	T	T	T
0.1665063586988086	0.2082690912798515	0.3227145088917939	T	T	T
0.1249998938073347	0.2499997876146764	0.0000000000000000	F	F	F
0.1666666084973016	0.3333332169946104	0.0784850000000006	F	F	F
0.2083331889443230	0.2916665023046434	0.1569700000000012	F	F	F
0.1249679512871026	0.2499575007549049	0.2386699683677998	T	T	T
0.1666283972666576	0.3332568399588361	0.3226235561515183	T	T	T
0.1250000280502874	0.3749999316845773	0.0000000000000000	F	F	F
0.1666667427402544	0.4583333610645113	0.0784850000000006	F	F	F
0.208333231872686	0.4166666463745443	0.1569700000000012	F	F	F
0.1250424893280548	0.3749888731953435	0.2386423836951643	T	T	T
0.1667069546605455	0.4583302036865209	0.3225603734168396	T	T	T
0.1250001622932331	0.5000000757544782	0.0000000000000000	F	F	F
0.1666668769832000	0.5833335051344122	0.0784850000000006	F	F	F
0.2083334574302214	0.5416667904444452	0.1569700000000012	F	F	F
0.1250120125607395	0.4999620972842820	0.2386259581571761	T	T	T
0.1666978097188219	0.5832850262588114	0.3225014007627608	T	T	T
0.1250002965361787	0.6250002198243791	0.0000000000000000	F	F	F
0.1666667609635866	0.7083331486791877	0.0784850000000006	F	F	F

0.2083333414106079	0.6666664339892208	0.1569700000000012	F	F	F
0.1250125592279338	0.6249506365925894	0.2385838889371117	T	T	T
0.1667546443486833	0.7083194613480004	0.3223326642468579	T	T	T
0.1249997470491166	0.7499998633691547	0.0000000000000000	F	F	F
0.1666664617390836	0.8333332927490886	0.0784850000000006	F	F	F
0.2083334756535535	0.7916665780591217	0.1569700000000012	F	F	F
0.1250409215678483	0.7499920633952669	0.2385417470750013	T	T	T
0.1667522824035617	0.8333409713956782	0.3223842749047085	T	T	T
0.1249998812920623	0.8750000074390556	0.0000000000000000	F	F	F
0.1666665959820293	0.9583334368189895	0.0784850000000006	F	F	F
0.2083331764290506	0.9166667221290226	0.1569700000000012	F	F	F
0.1250149090552297	0.8750053335207481	0.2385780157821667	T	T	T
0.1666412814433432	0.9582347689561923	0.3225028075938766	T	T	T
0.2500001846354607	0.0000000000000000	0.0000000000000000	F	F	F
0.2916668993254277	0.0833334293799339	0.0784850000000006	F	F	F
0.3333334797724490	0.0416667146899670	0.1569700000000012	F	F	F
0.2499268574692073	0.9999143228824598	0.2386198681116336	T	T	T
0.2914430055348309	0.0831744392261397	0.3225906187481656	T	T	T
0.2499998854109577	0.1250001440699009	0.0000000000000000	F	F	F
0.2916666001009247	0.2083335734498348	0.0784850000000006	F	F	F
0.3333336140153946	0.1666668587598679	0.1569700000000012	F	F	F
0.2499215074531732	0.1249303344762971	0.2387173928739616	T	T	T
0.2913737839401276	0.2082334734746714	0.3227237737901724	T	T	T
0.2499997693913443	0.2499997876146764	0.0000000000000000	F	F	F
0.2916664840813112	0.3333332169946104	0.0784850000000006	F	F	F
0.3333330645283255	0.2916665023046434	0.1569700000000012	F	F	F
0.2497088614630870	0.2497808944079073	0.2386839635148557	T	T	T
0.2914501518127459	0.3330250020788116	0.3226905727418584	T	T	T
0.2499999036342899	0.3749999316845773	0.0000000000000000	F	F	F
0.2916666183242569	0.4583333610645113	0.0784850000000006	F	F	F
0.3333331987712782	0.4166666463745443	0.1569700000000012	F	F	F
0.2498309607335171	0.3748623572484606	0.2387326396403029	T	T	T
0.2915035765850779	0.4581506522743228	0.3224667713013010	T	T	T
0.2500000378772356	0.5000000757544782	0.0000000000000000	F	F	F
0.2916667525672025	0.5833335051344122	0.0784850000000006	F	F	F
0.3333333330142239	0.5416667904444452	0.1569700000000012	F	F	F
0.2499189335101808	0.5000003862750636	0.2386772993148299	T	T	T
0.2916523489491263	0.5833128775006903	0.3226314537800222	T	T	T
0.2500001721201883	0.6250002198243791	0.0000000000000000	F	F	F
0.2916666365475891	0.7083331486791877	0.0784850000000006	F	F	F
0.3333332169946104	0.6666664339892208	0.1569700000000012	F	F	F
0.2499505659194408	0.6250052609075997	0.2386527449488306	T	T	T
0.2917750178437022	0.7083057406662621	0.3224770819204379	T	T	T
0.2500000561005749	0.7499998633691547	0.0000000000000000	F	F	F
0.2916667707905418	0.8333332927490886	0.0784850000000006	F	F	F
0.3333333512375560	0.7916665780591217	0.1569700000000012	F	F	F
0.2500802039896866	0.7500166169403738	0.2386063406710545	T	T	T
0.2917928862614041	0.8334005587513509	0.3223238902957940	T	T	T
0.2500001903435205	0.8750000074390556	0.0000000000000000	F	F	F
0.2916669050334875	0.9583334368189895	0.0784850000000006	F	F	F
0.3333334854805088	0.9166667221290226	0.1569700000000012	F	F	F
0.2500380329671115	0.8750135476199568	0.2386066440277506	T	T	T
0.2917488355026619	0.9584295483299539	0.3225025965144908	T	T	T
0.3750000602194632	0.0000000000000000	0.0000000000000000	F	F	F
0.4166667749094302	0.0833334293799339	0.0784850000000006	F	F	F
0.458333353564515	0.0416667146899670	0.1569700000000012	F	F	F
0.3749739829941486	0.9998302925824951	0.2386718633916579	T	T	T
0.4166678465537314	0.0832958832306069	0.3226042296244139	T	T	T
0.3750001944624159	0.1250001440699009	0.0000000000000000	F	F	F
0.4166669091523829	0.2083335734498348	0.0784850000000006	F	F	F
0.4583334895993971	0.1666668587598679	0.1569700000000012	F	F	F
0.3747975445011513	0.1245845574016428	0.2385143282130386	T	T	T
0.4161647310559586	0.2080513798335012	0.3210451462938438	T	T	T
0.3750000784427954	0.2499997876146764	0.0000000000000000	F	F	F
0.4166667931327623	0.3333332169946104	0.0784850000000006	F	F	F
0.4583333735797837	0.2916665023046434	0.1569700000000012	F	F	F
0.3746596958675752	0.2498507677613118	0.2384579990515392	T	T	T
0.4164943741635561	0.3331910729200613	0.3222056588523463	T	T	T
0.3749997792182995	0.3749999316845773	0.0000000000000000	F	F	F
0.4166664939082665	0.4583333610645113	0.0784850000000006	F	F	F
0.4583335078227293	0.4166666463745443	0.1569700000000012	F	F	F
0.3745382088351126	0.3745855656443224	0.2383688769931345	T	T	T
0.4164994236038203	0.4578031854113007	0.3207924367968201	T	T	T
0.3749999134612452	0.5000000757544782	0.0000000000000000	F	F	F
0.4166666281512121	0.5833335051344122	0.0784850000000006	F	F	F
0.4583332085982335	0.5416667904444452	0.1569700000000012	F	F	F
0.3747966707555253	0.5000156742285465	0.2384812165172307	T	T	T
0.4165441751779467	0.5834790143240285	0.3213880453874596	T	T	T

0.3750000477041908	0.6250002198243791	0.0000000000000000	F	F	F
0.4166665121315987	0.7083331486791877	0.0784850000000000	F	F	F
0.4583330925786129	0.6666664339892208	0.1569700000000001	F	F	F
0.3748331232227297	0.6252459379712622	0.2385186767543628	T	T	T
0.4167010890590344	0.7083806334779514	0.3226703739535460	T	T	T
0.3749999316845773	0.7499998633691547	0.0000000000000000	F	F	F
0.4166666463745443	0.8333332927490886	0.0784850000000000	F	F	F
0.4583332268215656	0.7916665780591217	0.1569700000000001	F	F	F
0.3750723793266703	0.7501217265705500	0.2386529089926613	T	T	T
0.4167520771038326	0.8333828271924597	0.3225804277385302	T	T	T
0.3750000659275230	0.8750000074390556	0.0000000000000000	F	F	F
0.4166667806174900	0.9583334368189895	0.0784850000000000	F	F	F
0.4583333610645113	0.9166667221290226	0.1569700000000001	F	F	F
0.3751415738148672	0.8750525403381236	0.2386383877229107	T	T	T
0.4167807425538155	0.9584594499890401	0.3225765167687088	T	T	T
0.4999999358034728	0.0000000000000000	0.0000000000000000	F	F	F
0.5416666504934398	0.0833334293799339	0.0784850000000000	F	F	F
0.5833332309404540	0.0416667146899670	0.1569700000000001	F	F	F
0.5000749452103553	0.9999719838172234	0.2386561661266043	T	T	T
0.5417459826375985	0.0832801594229138	0.3226806311673485	T	T	T
0.5000000700464184	0.1250001440699009	0.0000000000000000	F	F	F
0.5416667847363854	0.2083335734498348	0.0784850000000000	F	F	F
0.5833333651834067	0.1666668587598679	0.1569700000000001	F	F	F
0.4999243790043509	0.1246983204766150	0.2385633138134714	T	T	T
0.5418808776702470	0.2081875671301957	0.3213455627207822	T	T	T
0.4999999540268050	0.2499997876146764	0.0000000000000000	F	F	F
0.541666687167719	0.3333332169946104	0.0784850000000000	F	F	F
0.5833332491637861	0.2916665023046434	0.1569700000000001	F	F	F
0.5000184699329721	0.2499415007501548	0.2384492930543220	T	T	T
0.5419514779386441	0.3339026649559689	0.3208336089399638	T	T	T
0.5000000882697506	0.3749999316845773	0.0000000000000000	F	F	F
0.5416668029597176	0.4583333610645113	0.0784850000000000	F	F	F
0.5833333834067389	0.4166666463745443	0.1569700000000001	F	F	F
0.4998700544234019	0.3751165880308315	0.2383855357527797	T	T	T
0.5420197431461096	0.4585323675802094	0.3222222461944327	T	T	T
0.5000002225126963	0.5000000757544782	0.0000000000000000	F	F	F
0.5416669372026632	0.5833335051344122	0.0784850000000000	F	F	F
0.5833335176496846	0.5416667904444452	0.1569700000000001	F	F	F
0.5001735879922100	0.5000621035683579	0.2383546924752446	T	T	T
0.5422064025833808	0.5836771291369420	0.3209809369314753	T	T	T
0.4999999232882004	0.6250002198243791	0.0000000000000000	F	F	F
0.5416663877156012	0.7083331486791877	0.0784850000000000	F	F	F
0.5833334016300711	0.6666664339892208	0.1569700000000001	F	F	F
0.5001167685780299	0.6252672882191270	0.2384838381082223	T	T	T
0.5417968496850445	0.7085176223528915	0.3226213521347526	T	T	T
0.4999998072685798	0.7499998633691547	0.0000000000000000	F	F	F
0.5416665219585468	0.8333332927490886	0.0784850000000000	F	F	F
0.5833331024055681	0.7916665780591217	0.1569700000000001	F	F	F
0.5000263039564392	0.7500932450481249	0.2387012744504634	T	T	T
0.5416525021114263	0.8332953190698629	0.3226068167340549	T	T	T
0.4999999415115326	0.8750000074390556	0.0000000000000000	F	F	F
0.5416666562014996	0.9583334368189895	0.0784850000000000	F	F	F
0.5833332366485138	0.9166667221290226	0.1569700000000001	F	F	F
0.5000611393584641	0.8750222962984099	0.2386554728319292	T	T	T
0.5416543908636311	0.9582954227085931	0.3225923528339276	T	T	T
0.6249998113874753	0.0000000000000000	0.0000000000000000	F	F	F
0.6666665260774423	0.0833334293799339	0.0784850000000000	F	F	F
0.7083335399919122	0.0416667146899670	0.1569700000000001	F	F	F
0.6249761768348793	0.9999881425351970	0.2386461811762942	T	T	T
0.6666569844973881	0.0833309779446537	0.3224993838677677	T	T	T
0.6249999456304209	0.1250001440699009	0.0000000000000000	F	F	F
0.666666603203879	0.2083335734498348	0.0784850000000000	F	F	F
0.7083332407674092	0.1666668587598679	0.1569700000000001	F	F	F
0.6250155090984976	0.1249998599663626	0.2386750213897391	T	T	T
0.6667668015526491	0.2082911263691476	0.3226495647150775	T	T	T
0.6249998296108075	0.2499997876146764	0.0000000000000000	F	F	F
0.6666665443007744	0.3333332169946104	0.0784850000000000	F	F	F
0.7083331247477958	0.2916665023046434	0.1569700000000001	F	F	F
0.6253027007805015	0.2501306456836418	0.2385539243080913	T	T	T
0.6668223559793783	0.3334660628669788	0.3224165974145379	T	T	T
0.6249999638537531	0.3749999316845773	0.0000000000000000	F	F	F
0.6666666785437201	0.4583333610645113	0.0784850000000000	F	F	F
0.7083332589907414	0.4166666463745443	0.1569700000000001	F	F	F
0.6254433880073987	0.3753290164759124	0.2385041148961546	T	T	T
0.6670133615967371	0.4587095157677564	0.3227272068619101	T	T	T
0.6250000980967059	0.5000000757544782	0.0000000000000000	F	F	F
0.6666668127866728	0.5833335051344122	0.0784850000000000	F	F	F
0.7083333932336870	0.5416667904444452	0.1569700000000001	F	F	F

0.6252957765683381	0.5001466602282129	0.2386491593165870	T	T	T
0.6669947500305841	0.5834698308017335	0.3227025792763917	T	T	T
0.6250002323396515	0.6250002198243791	0.0000000000000000	F	F	F
0.6666666967670594	0.7083331486791877	0.0784850000000000	F	F	F
0.7083332772140736	0.6666664339892208	0.1569700000000012	F	F	F
0.6255611962235981	0.6252596226729162	0.2384857939010777	T	T	T
0.6669188328967058	0.7085318859783961	0.3225801858097385	T	T	T
0.6250001163200380	0.7499998633691547	0.0000000000000000	F	F	F
0.6666668310100050	0.8333332927490886	0.0784850000000000	F	F	F
0.7083334114570263	0.7916665780591217	0.1569700000000012	F	F	F
0.6250858861526419	0.7500658312957227	0.2386864138004693	T	T	T
0.6667072996476834	0.8333331480377165	0.3225429841602457	T	T	T
0.6249998170955351	0.8750000074390556	0.0000000000000000	F	F	F
0.6666665317855021	0.9583334368189895	0.0784850000000000	F	F	F
0.7083335456999720	0.9166667221290226	0.1569700000000012	F	F	F
0.6249711934953646	0.8749404594102754	0.2386454490913155	T	T	T
0.6666471649255907	0.9582956311162443	0.3223739685376169	T	T	T
0.7500001204389335	0.0000000000000000	0.0000000000000000	F	F	F
0.7916668351289005	0.0833334293799339	0.0784850000000000	F	F	F
0.8333334155759147	0.0416667146899670	0.1569700000000012	F	F	F
0.7499570168003625	0.9999731393906468	0.2385798093895336	T	T	T
0.7916787872914868	0.0833336096048046	0.3223733936540477	T	T	T
0.7500002546818791	0.1250001440699009	0.0000000000000000	F	F	F
0.7916669693718461	0.2083335734498348	0.0784850000000000	F	F	F
0.8333335498188674	0.1666668587598679	0.1569700000000012	F	F	F
0.7499751279881895	0.1250137483890346	0.2386407471998124	T	T	T
0.7917129498835961	0.2083538748034177	0.3225376602763446	T	T	T
0.7499997051948100	0.2499997876146764	0.0000000000000000	F	F	F
0.7916664198847769	0.3333332169946104	0.0784850000000000	F	F	F
0.8333334337992468	0.2916665023046434	0.1569700000000012	F	F	F
0.7500444590014702	0.2499729265819828	0.2386536277342459	T	T	T
0.7916264429300607	0.3332860701867816	0.3225510474765942	T	T	T
0.7499998394377627	0.3749999316845773	0.0000000000000000	F	F	F
0.7916665541277297	0.4583333610645113	0.0784850000000000	F	F	F
0.8333331345747439	0.4166666463745443	0.1569700000000012	F	F	F
0.7502350909372982	0.3751273005716033	0.2386677601309950	T	T	T
0.7917031196036455	0.4583594718488516	0.3226089285413223	T	T	T
0.7499999736807084	0.5000000757544782	0.0000000000000000	F	F	F
0.791666883706753	0.5833335051344122	0.0784850000000000	F	F	F
0.8333332688176966	0.5416667904444452	0.1569700000000012	F	F	F
0.7502009377874564	0.5001429546571122	0.2386924350830632	T	T	T
0.7918908093212385	0.5834115307399731	0.3227292083333799	T	T	T
0.7500001079236540	0.6250002198243791	0.0000000000000000	F	F	F
0.7916665723510619	0.7083331486791877	0.0784850000000000	F	F	F
0.8333331527980832	0.6666664339892208	0.1569700000000012	F	F	F
0.7502370595777971	0.6250353811246343	0.2387101600861512	T	T	T
0.7917474118448931	0.7083714326250881	0.3225402951935143	T	T	T
0.7499999919040405	0.7499998633691547	0.0000000000000000	F	F	F
0.7916667065940075	0.8333332927490886	0.0784850000000000	F	F	F
0.8333332870410288	0.7916665780591217	0.1569700000000012	F	F	F
0.7501611736359571	0.7501037605785619	0.2386308619138324	T	T	T
0.7917569597742334	0.8334107355110630	0.3225168917883461	T	T	T
0.7500001261469933	0.8750000074390556	0.0000000000000000	F	F	F
0.7916668408369603	0.9583334368189895	0.0784850000000000	F	F	F
0.8333334212839745	0.9166667221290226	0.1569700000000012	F	F	F
0.7499916878155437	0.8749849635228457	0.2386305989146958	T	T	T
0.7916835696663427	0.9583351133900730	0.3224133703857353	T	T	T
0.874999960229360	0.0000000000000000	0.0000000000000000	F	F	F
0.9166667107129030	0.0833334293799339	0.0784850000000000	F	F	F
0.9583332911599243	0.0416667146899670	0.1569700000000012	F	F	F
0.8749964664992891	0.9999975721163394	0.2385772136852126	T	T	T
0.9166551778834086	0.0833266192105344	0.3223931917645034	T	T	T
0.8750001302658816	0.1250001440699009	0.0000000000000000	F	F	F
0.9166668449558486	0.2083335734498348	0.0784850000000000	F	F	F
0.9583334254028699	0.1666668587598679	0.1569700000000012	F	F	F
0.8749951719431653	0.1249963245445485	0.2385729441597407	T	T	T
0.9166778513127318	0.2083225803430096	0.3224144741286931	T	T	T
0.8750000142462682	0.2499997876146764	0.0000000000000000	F	F	F
0.9166667289362351	0.3333332169946104	0.0784850000000000	F	F	F
0.9583333093832564	0.2916665023046434	0.1569700000000012	F	F	F
0.8749849293914499	0.2499678377799479	0.2386036810400413	T	T	T
0.9166697622440636	0.3333216348962348	0.3224371032879965	T	T	T
0.750001484892138	0.3749999316845773	0.0000000000000000	F	F	F
0.9166668631791808	0.4583333610645113	0.0784850000000000	F	F	F
0.9583334436262021	0.4166666463745443	0.1569700000000012	F	F	F
0.8750084390787186	0.3749450945460523	0.2386267359793159	T	T	T
0.9166704760287457	0.4582885625565627	0.3223685035792473	T	T	T
0.8749998492647180	0.5000000757544782	0.0000000000000000	F	F	F

0.9166665639546849	0.5833335051344122	0.0784850000000006	F	F	F
0.9583335778691477	0.5416667904444452	0.1569700000000012	F	F	F
0.8750517844500681	0.5000303728996032	0.2386355075958893	T	T	T
0.9167713232921944	0.5833291632498445	0.3224958068933951	T	T	T
0.8749999835076636	0.6250002198243791	0.0000000000000000	F	F	F
0.9166664479350644	0.7083331486791877	0.0784850000000006	F	F	F
0.9583330283820857	0.6666664339892208	0.1569700000000012	F	F	F
0.8750441774928925	0.6249802277573251	0.2386373694249301	T	T	T
0.9167846205962739	0.7083495676668895	0.3224140148825805	T	T	T
0.8749998674880501	0.7499998633691547	0.0000000000000000	F	F	F
0.9166665821780171	0.8333332927490886	0.0784850000000006	F	F	F
0.9583331626250313	0.7916665780591217	0.1569700000000012	F	F	F
0.8750384824755867	0.7499965188553219	0.2386272115855010	T	T	T
0.9167261617417881	0.8333375840403283	0.3223724586049072	T	T	T
0.8750000017309958	0.8750000074390556	0.0000000000000000	F	F	F
0.9166667164209628	0.9583334368189895	0.0784850000000006	F	F	F
0.9583332968679841	0.9166667221290226	0.1569700000000012	F	F	F
0.8750182944727136	0.8750275034557626	0.2385929264848662	T	T	T
0.9166965290207343	0.9583415309981868	0.3224091208450008	T	T	T
0.4981397374443788	0.4987444541542301	0.4246930632026708	T	T	T
0.4968813220529382	0.6076642187741228	0.4258197791067935	T	T	T
0.3879252849572198	0.4973768629432142	0.4253588701653682	T	T	T
0.4631480242462623	0.1843243431841038	0.4257074342266295	T	T	T
0.5723159653649948	0.2944262930679252	0.4251541764544037	T	T	T
0.4622819694161499	0.2934446144133709	0.4247082831314418	T	T	T
0.5317060434364665	0.5705330505613534	0.4252952447954559	T	T	T
0.4263160618357206	0.4638516050405172	0.4248458913559977	T	T	T
0.4250569155416224	0.5692419082517572	0.4261918340764884	T	T	T
0.5349881854894891	0.2225632725998618	0.4258724963261889	T	T	T
0.4285246728523127	0.2216471737090494	0.4253404663770769	T	T	T
0.53411115872587792	0.3281452682298924	0.4247846394638051	T	T	T
0.5288091360780905	0.4692259048700862	0.4243455084725177	T	T	T
0.4013822734623937	0.4127990324571206	0.4238653398366077	T	T	T
0.3278282607604190	0.4667651142037434	0.4252653115077730	T	T	T
0.3990633556135978	0.5943025580860098	0.4262954034941833	T	T	T
0.5264348915979777	0.6677542920134044	0.4260881345626407	T	T	T
0.5827508530133764	0.5965495841940732	0.4245601282561782	T	T	T
0.4334335617746649	0.1242360535708535	0.4260441247530231	T	T	T
0.3774703106067069	0.1957732194706159	0.4247633453162271	T	T	T
0.4317721075422573	0.3231328908854648	0.4243919669181742	T	T	T
0.5591818101280515	0.3792072598565570	0.4238446268961418	T	T	T
0.6324058166340905	0.3248778638518003	0.4250654001681876	T	T	T
0.5608437957339083	0.1973625554101314	0.4258380484305509	T	T	T

Borazine dimer adsorbed on Au(111), dimer III

23.0697829620000014	0.0000000000000000	0.0000000000000000
-11.5348914810000007	19.9790169730000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.0000000000000000

Au B N H
320 6 6 12

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0416667146899670	0.0833334293799339	0.0784850000000006	F	F	F
0.0833332951369883	0.0416667146899670	0.1569700000000012	F	F	F
0.0000233846025924	0.0000642879887868	0.2385558817829553	T	T	T
0.0417300320156494	0.0834165798544141	0.3224134215432239	T	T	T
0.0000001342429456	0.1250001440699009	0.0000000000000000	F	F	F
0.0416668489329126	0.2083335734498348	0.0784850000000006	F	F	F
0.0833334293799339	0.1666668587598679	0.1569700000000012	F	F	F
0.0000150135670388	0.1250643605292474	0.2385952416486378	T	T	T
0.0416649455323064	0.2083072856569265	0.3225654114919818	T	T	T
0.0000000182233322	0.2499997876146764	0.0000000000000000	F	F	F
0.0416667329132991	0.3333332169946104	0.0784850000000006	F	F	F
0.0833333133603205	0.2916665023046434	0.1569700000000012	F	F	F
0.0000538879464192	0.2500460820767986	0.2386442595630266	T	T	T
0.0416953429372030	0.3333519609818880	0.3225849703976383	T	T	T
0.0000001524662778	0.3749999316845773	0.0000000000000000	F	F	F
0.0416668671562448	0.4583333610645113	0.0784850000000006	F	F	F
0.0833334476032661	0.4166666463745443	0.1569700000000012	F	F	F
0.0000550864278484	0.3749908507246652	0.2386687645739650	T	T	T
0.0416478587307502	0.4583890359421265	0.3225353453872649	T	T	T
0.9999997248487205	0.5000000757544782	0.0000000000000000	F	F	F
0.0416665679317489	0.5833335051344122	0.0784850000000006	F	F	F
0.0833335818462118	0.5416667904444452	0.1569700000000012	F	F	F
0.0000053826752811	0.4999872734682401	0.2386635222500383	T	T	T
0.0417028299644144	0.5833899535424677	0.3224237312614061	T	T	T
0.9999998590916661	0.6250002198243791	0.0000000000000000	F	F	F

0.0416664519121284	0.7083331486791877	0.0784850000000006	F	F	F
0.0833330323591497	0.6666664339892208	0.1569700000000012	F	F	F
0.0000105932138192	0.6250450810278344	0.2385907676963402	T	T	T
0.0417360921604853	0.7084166093344140	0.3223996977509136	T	T	T
0.9999997430720526	0.7499998633691547	0.0000000000000000	F	F	F
0.0416665861550811	0.8333332927490886	0.0784850000000006	F	F	F
0.0833331666020953	0.7916665780591217	0.1569700000000012	F	F	F
0.0000099640301950	0.7500194949920723	0.2385623918961584	T	T	T
0.0417225916507261	0.8334047155184847	0.3223491397313870	T	T	T
0.0000000057080598	0.8750000074390556	0.0000000000000000	F	F	F
0.0416667203980268	0.9583334368189895	0.0784850000000006	F	F	F
0.0833333008450481	0.9166667221290226	0.1569700000000012	F	F	F
0.0000238369059837	0.8750428765296332	0.2385546913277655	T	T	T
0.0417324923432849	0.9584054975803984	0.3223203340567637	T	T	T
0.1249998755840025	0.0000000000000000	0.0000000000000000	F	F	F
0.1666665902739695	0.0833334293799339	0.0784850000000006	F	F	F
0.2083331707209908	0.0416667146899670	0.1569700000000012	F	F	F
0.1250961775849452	0.0000967272603280	0.2385630796819530	T	T	T
0.1667769946250385	0.0834770519940713	0.3223033318052567	T	T	T
0.1250000098269552	0.1250001440699009	0.0000000000000000	F	F	F
0.1666667245169222	0.2083335734498348	0.0784850000000006	F	F	F
0.2083333049639364	0.1666668587598679	0.1569700000000012	F	F	F
0.1250334381457862	0.1250691839734687	0.2386287747223968	T	T	T
0.1667260025949811	0.2084841862593496	0.3226010890499597	T	T	T
0.1249998938073347	0.2499997876146764	0.0000000000000000	F	F	F
0.1666666084973016	0.3333332169946104	0.0784850000000006	F	F	F
0.2083331889443230	0.2916665023046434	0.1569700000000012	F	F	F
0.1249222673226721	0.2499559674501279	0.2386484564152780	T	T	T
0.1664556333982952	0.3332336087526890	0.3226792814893880	T	T	T
0.1250000280502874	0.3749999316845773	0.0000000000000000	F	F	F
0.1666667427402544	0.4583333610645113	0.0784850000000006	F	F	F
0.2083333231872686	0.4166666463745443	0.1569700000000012	F	F	F
0.1249715743901620	0.3749869484997365	0.2386634820173371	T	T	T
0.1664532120802151	0.4582976832429033	0.3225932679665452	T	T	T
0.1250001622932331	0.5000000757544782	0.0000000000000000	F	F	F
0.1666668769832000	0.5833335051344122	0.0784850000000006	F	F	F
0.2083334574302214	0.5416667904444452	0.1569700000000012	F	F	F
0.1248981083898756	0.4999761248091802	0.2386183315549434	T	T	T
0.1667068758812289	0.5833335420675498	0.3224893359289267	T	T	T
0.1250002965361787	0.6250002198243791	0.0000000000000000	F	F	F
0.1666667609635866	0.7083331486791877	0.0784850000000006	F	F	F
0.2083333414106079	0.6666664339892208	0.1569700000000012	F	F	F
0.1249534453323258	0.6249908684832621	0.2386005610915538	T	T	T
0.1667413248116235	0.7083750063626919	0.3223061138578917	T	T	T
0.1249997470491166	0.7499998633691547	0.0000000000000000	F	F	F
0.1666664617390836	0.8333332927490886	0.0784850000000006	F	F	F
0.2083334756535535	0.7916665780591217	0.1569700000000012	F	F	F
0.1250308063353009	0.7500415374536528	0.2385595458915317	T	T	T
0.1667057136045217	0.8333906076377759	0.3223912196597256	T	T	T
0.1249998812920623	0.8750000074390556	0.0000000000000000	F	F	F
0.1666665959820293	0.9583334368189895	0.0784850000000006	F	F	F
0.2083331764290506	0.9166667221290226	0.1569700000000012	F	F	F
0.1250498750163951	0.8750633479391030	0.2385615947604466	T	T	T
0.1667247163143750	0.9584000426326696	0.3224125317086035	T	T	T
0.2500001846354607	0.0000000000000000	0.0000000000000000	F	F	F
0.2916668993254277	0.0833334293799339	0.0784850000000006	F	F	F
0.3333334797724490	0.0416667146899670	0.1569700000000012	F	F	F
0.2500626951838249	0.0000624199954261	0.2386198693760461	T	T	T
0.2917151876054451	0.08337261411176046	0.3226252674668892	T	T	T
0.2499998854109577	0.1250001440699009	0.0000000000000000	F	F	F
0.2916666001009247	0.2083335734498348	0.0784850000000006	F	F	F
0.33333336140153946	0.1666668587598679	0.1569700000000012	F	F	F
0.2501533197990778	0.1250799611266618	0.2387005588497034	T	T	T
0.2917783383321356	0.2085076974618344	0.3227143907386500	T	T	T
0.2499997693913443	0.2499997876146764	0.0000000000000000	F	F	F
0.2916664840813112	0.3333332169946104	0.0784850000000006	F	F	F
0.33333330645283255	0.2916665023046434	0.1569700000000012	F	F	F
0.2499106186871198	0.2498057076173291	0.2387175877320547	T	T	T
0.2916138131212990	0.3332827061300385	0.3225966405898361	T	T	T
0.2499999036342899	0.3749999316845773	0.0000000000000000	F	F	F
0.2916666183242569	0.4583333610645113	0.0784850000000006	F	F	F
0.3333331987712782	0.4166666463745443	0.1569700000000012	F	F	F
0.2497330572733095	0.3746138843487397	0.2385211339855970	T	T	T
0.2911880015950265	0.4581475752990062	0.3209768471151556	T	T	T
0.2500000378772356	0.5000000757544782	0.0000000000000000	F	F	F
0.2916667525672025	0.5833335051344122	0.0784850000000006	F	F	F
0.333333330142239	0.5416667904444452	0.1569700000000012	F	F	F
0.2497585470118207	0.5001269893968963	0.2384596069399649	T	T	T

0.2916296898967538	0.5834892263286263	0.3223064498787586	T	T	T
0.2500001721201883	0.6250002198243791	0.0000000000000000	F	F	F
0.2916666365475891	0.7083331486791877	0.0784850000000006	F	F	F
0.3333332169946104	0.6666664339892208	0.1569700000000012	F	F	F
0.2498852000698277	0.6251612476309116	0.2386142088834952	T	T	T
0.2917784981569413	0.7084125217423611	0.3224803126280144	T	T	T
0.2500000561005749	0.7499998633691547	0.0000000000000000	F	F	F
0.2916667707905418	0.8333332927490886	0.0784850000000006	F	F	F
0.3333333512375560	0.7916665780591217	0.1569700000000012	F	F	F
0.2500636566583245	0.7501117683484234	0.2386013606417360	T	T	T
0.2917175620083504	0.8334244341784436	0.3224192153050907	T	T	T
0.2500001903435205	0.8750000074390556	0.0000000000000000	F	F	F
0.2916669050334875	0.9583334368189895	0.0784850000000006	F	F	F
0.3333334854805088	0.9166667221290226	0.1569700000000012	F	F	F
0.2500316306099796	0.8750767516647528	0.2385830270649606	T	T	T
0.2916422968151040	0.9583706821636939	0.3225529562827286	T	T	T
0.3750000602194632	0.0000000000000000	0.0000000000000000	F	F	F
0.4166667749094302	0.0833334293799339	0.0784850000000006	F	F	F
0.4583333553564515	0.0416667146899670	0.1569700000000012	F	F	F
0.3749133889799197	0.9999059262188816	0.2386560796522110	T	T	T
0.4165704002393165	0.0832204379033466	0.3226778590915982	T	T	T
0.3750001944624159	0.1250001440699009	0.0000000000000000	F	F	F
0.4166669091523829	0.2083335734498348	0.0784850000000006	F	F	F
0.4583334895993971	0.1666668587598679	0.1569700000000012	F	F	F
0.3749641945940974	0.1249375603018947	0.2387055017568931	T	T	T
0.4164815069669426	0.2082196941612656	0.3226144884716660	T	T	T
0.3750000784427954	0.2499997876146764	0.0000000000000000	F	F	F
0.4166667931327623	0.3333332169946104	0.0784850000000006	F	F	F
0.4583333735797837	0.2916665023046434	0.1569700000000012	F	F	F
0.3749750729856646	0.2499889665097801	0.2387619122318374	T	T	T
0.4166870044788240	0.3333030522027727	0.3229209427121424	T	T	T
0.3749997792182995	0.3749999316845773	0.0000000000000000	F	F	F
0.4166664939082665	0.4583333610645113	0.0784850000000006	F	F	F
0.4583335078227293	0.4166666463745443	0.1569700000000012	F	F	F
0.3747593367096564	0.3746522497737458	0.2385623600697536	T	T	T
0.4169857438066449	0.4581530955833156	0.3210191178635848	T	T	T
0.3749999134612452	0.5000000757544782	0.0000000000000000	F	F	F
0.4166666281512121	0.5833335051344122	0.0784850000000006	F	F	F
0.4583332085982335	0.5416667904444452	0.1569700000000012	F	F	F
0.3750090994151430	0.5000163757243055	0.2384415641435852	T	T	T
0.4169907028751148	0.5839708455410801	0.3207945019592068	T	T	T
0.3750000477041908	0.6250002198243791	0.0000000000000000	F	F	F
0.4166665121315987	0.7083331486791877	0.0784850000000006	F	F	F
0.4583330925786129	0.6666664339892208	0.1569700000000012	F	F	F
0.3749110026384909	0.6253193412346694	0.2384262073709024	T	T	T
0.4168226693627944	0.7086956353535112	0.3225633591713734	T	T	T
0.3749999316845773	0.7499998633691547	0.0000000000000000	F	F	F
0.4166666463745443	0.8333332927490886	0.0784850000000006	F	F	F
0.4583332268215656	0.7916665780591217	0.1569700000000012	F	F	F
0.3750713465445444	0.7501800467539258	0.2386131912210802	T	T	T
0.4167133611792885	0.8334837208474597	0.3225340989237542	T	T	T
0.3750000659275230	0.8750000074390556	0.0000000000000000	F	F	F
0.4166667806174900	0.9583334368189895	0.0784850000000006	F	F	F
0.4583333610645113	0.9166667221290226	0.1569700000000012	F	F	F
0.3750703998803589	0.8750743270552325	0.2386545759688683	T	T	T
0.4167198433242056	0.9584630726498414	0.3225636426372507	T	T	T
0.4999999358034728	0.0000000000000000	0.0000000000000000	F	F	F
0.5416666504934398	0.0833334293799339	0.0784850000000006	F	F	F
0.5833332309404540	0.0416667146899670	0.1569700000000012	F	F	F
0.5000028907970417	0.9998751701942211	0.2386412283771119	T	T	T
0.5416774248711224	0.0832265375823280	0.3226038785250072	T	T	T
0.5000000700464184	0.1250001440699009	0.0000000000000000	F	F	F
0.5416667847363854	0.2083335734498348	0.0784850000000006	F	F	F
0.5833333651834067	0.1666668587598679	0.1569700000000012	F	F	F
0.4997561069162016	0.1245163434831415	0.2384625183618310	T	T	T
0.5414866054403997	0.2079090984408539	0.3210197760231863	T	T	T
0.4999999540268050	0.2499997876146764	0.0000000000000000	F	F	F
0.5416666687167719	0.3333332169946104	0.0784850000000006	F	F	F
0.5833332491637861	0.2916665023046434	0.1569700000000012	F	F	F
0.4997766863942701	0.2499166009461697	0.2384756656778601	T	T	T
0.5415257997524572	0.3336141789709990	0.3209534292073297	T	T	T
0.5000000882697506	0.3749999316845773	0.0000000000000000	F	F	F
0.5416668029597176	0.4583333610645113	0.0784850000000006	F	F	F
0.5833333834067389	0.4166666463745443	0.1569700000000012	F	F	F
0.4997746301012423	0.3752808398873630	0.2385313341635055	T	T	T
0.5418310884658060	0.4584387023654262	0.3229182272052225	T	T	T
0.5000002225126963	0.5000000757544782	0.0000000000000000	F	F	F
0.5416669372026632	0.5833335051344122	0.0784850000000006	F	F	F

0.5833335176496846	0.5416667904444452	0.1569700000000012	F	F	F
0.5003876340817768	0.5002883214027111	0.2385466687560416	T	T	T
0.5419003444124501	0.5835445484812943	0.3224853693475074	T	T	T
0.4999999232882004	0.6250002198243791	0.0000000000000000	F	F	F
0.5416663877156012	0.7083331486791877	0.0784850000000006	F	F	F
0.5833334016300711	0.6666664339892208	0.1569700000000012	F	F	F
0.5004699631856934	0.6253469770693467	0.2384747002606606	T	T	T
0.5419108959476712	0.7087124160427060	0.3226236234368873	T	T	T
0.4999998072685798	0.7499998633691547	0.0000000000000000	F	F	F
0.5416665219585468	0.8333332927490886	0.0784850000000006	F	F	F
0.5833331024055681	0.7916665780591217	0.1569700000000012	F	F	F
0.5000730400557319	0.7501042690574470	0.2386440399135485	T	T	T
0.5417512836278329	0.8334339195271334	0.3225814964656637	T	T	T
0.4999999415115326	0.8750000074390556	0.0000000000000000	F	F	F
0.541666562014996	0.9583334368189895	0.0784850000000006	F	F	F
0.5833332366485138	0.9166667221290226	0.1569700000000012	F	F	F
0.5000606097010258	0.8750119432175464	0.2386650744876862	T	T	T
0.5417376712366540	0.9583846206325884	0.3225381376784260	T	T	T
0.6249998113874753	0.0000000000000000	0.0000000000000000	F	F	F
0.6666665260774423	0.0833334293799339	0.0784850000000006	F	F	F
0.7083335399919122	0.0416667146899670	0.1569700000000012	F	F	F
0.6250071015504314	0.9999830204724355	0.2386240156645407	T	T	T
0.6666903685677387	0.0833394200119989	0.3225368295400738	T	T	T
0.6249999456304209	0.1250001440699009	0.0000000000000000	F	F	F
0.666666603203879	0.2083335734498348	0.0784850000000006	F	F	F
0.7083332407674092	0.1666668587598679	0.1569700000000012	F	F	F
0.6249921938536130	0.1248957086099775	0.2386703446335783	T	T	T
0.6668514072330136	0.2082557129427512	0.3224025304108937	T	T	T
0.6249998296108075	0.2499997876146764	0.0000000000000000	F	F	F
0.6666665443007744	0.3333332169946104	0.0784850000000006	F	F	F
0.7083331247477958	0.2916665023046434	0.1569700000000012	F	F	F
0.6251049058138300	0.2499013922755771	0.2383997948937159	T	T	T
0.6672670608328263	0.3336324540418050	0.3208053901678841	T	T	T
0.6249999638537531	0.3749999316845773	0.0000000000000000	F	F	F
0.6666666785437201	0.4583333610645113	0.0784850000000006	F	F	F
0.7083332589907414	0.4166666463745443	0.1569700000000012	F	F	F
0.6251389689346324	0.3752897449842462	0.2384348168536839	T	T	T
0.6669562556884270	0.4586916298924879	0.3224837905584722	T	T	T
0.6250000980967059	0.5000000757544782	0.0000000000000000	F	F	F
0.6666668127866728	0.5833335051344122	0.0784850000000006	F	F	F
0.7083333932336870	0.5416667904444452	0.1569700000000012	F	F	F
0.6250648661159409	0.5001030378694420	0.2387390537453692	T	T	T
0.6666308068796766	0.5833429744381756	0.3227315992902228	T	T	T
0.6250002323396515	0.6250002198243791	0.0000000000000000	F	F	F
0.6666666967670594	0.7083331486791877	0.0784850000000006	F	F	F
0.7083332772140736	0.6666664339892208	0.1569700000000012	F	F	F
0.6252967772412825	0.6251703598040488	0.2386983449297204	T	T	T
0.6666537896795089	0.7084045756287510	0.3225999709162911	T	T	T
0.6250001163200380	0.7499998633691547	0.0000000000000000	F	F	F
0.6666668310100050	0.8333332927490886	0.0784850000000006	F	F	F
0.7083334114570263	0.7916665780591217	0.1569700000000012	F	F	F
0.6251346315264589	0.7501565258390901	0.2386365125464980	T	T	T
0.6668116048974074	0.8334593575928644	0.3225662375130540	T	T	T
0.6249998170955351	0.8750000074390556	0.0000000000000000	F	F	F
0.6666665317855021	0.9583334368189895	0.0784850000000006	F	F	F
0.7083335456999720	0.9166667221290226	0.1569700000000012	F	F	F
0.6250112129276139	0.8750025114949977	0.2386462531774441	T	T	T
0.6667363265745353	0.9583878349769728	0.3224438894306710	T	T	T
0.7500001204389335	0.0000000000000000	0.0000000000000000	F	F	F
0.7916668351289005	0.0833334293799339	0.0784850000000006	F	F	F
0.8333334155759147	0.0416667146899670	0.1569700000000012	F	F	F
0.7499935798253996	0.0000419776742111	0.2385729269472998	T	T	T
0.7917191529397758	0.0833855993392103	0.3223456655885289	T	T	T
0.7500002546818791	0.1250001440699009	0.0000000000000000	F	F	F
0.7916669693718461	0.2083335734498348	0.0784850000000006	F	F	F
0.8333335498188674	0.1666668587598679	0.1569700000000012	F	F	F
0.7499946995777712	0.1250589547454112	0.2386438135150749	T	T	T
0.7917633126132859	0.2084012767858146	0.3225396693909588	T	T	T
0.7499997051948100	0.2499997876146764	0.0000000000000000	F	F	F
0.7916664198847769	0.3333332169946104	0.0784850000000006	F	F	F
0.8333334337992468	0.2916665023046434	0.1569700000000012	F	F	F
0.7501532233629100	0.2500549792177713	0.2386719082116232	T	T	T
0.7919367484723426	0.3334261049907816	0.3225896962876036	T	T	T
0.7499998394377627	0.3749999316845773	0.0000000000000000	F	F	F
0.7916665541277297	0.4583333610645113	0.0784850000000006	F	F	F
0.8333331345747439	0.4166666463745443	0.1569700000000012	F	F	F
0.7505880514022014	0.3753057786037549	0.2384135951306031	T	T	T
0.7919669042324331	0.4585658359903831	0.3226068533920834	T	T	T

0.7499999736807084	0.5000000757544782	0.0000000000000000	F	F	F
0.7916666883706753	0.5833335051344122	0.0784850000000006	F	F	F
0.8333332688176966	0.5416667904444452	0.1569700000000012	F	F	F
0.7501646659028725	0.5001168607776745	0.2386804482952248	T	T	T
0.7917798244302726	0.5834151521671916	0.3226208676055685	T	T	T
0.7500001079236540	0.6250002198243791	0.0000000000000000	F	F	F
0.7916665723510619	0.7083331486791877	0.0784850000000006	F	F	F
0.8333331527980832	0.6666664339892208	0.1569700000000012	F	F	F
0.7499971307356572	0.6249104857422200	0.2387079497413399	T	T	T
0.7916522157293333	0.7083403845585337	0.3223120819358967	T	T	T
0.7499999919040405	0.7499998633691547	0.0000000000000000	F	F	F
0.7916667065940075	0.8333332927490886	0.0784850000000006	F	F	F
0.8333332870410288	0.7916665780591217	0.1569700000000012	F	F	F
0.7500157452371156	0.7500378002477069	0.2386340335182096	T	T	T
0.7917045073346969	0.8333856987807281	0.3224197694028965	T	T	T
0.7500001261469933	0.8750000074390556	0.0000000000000000	F	F	F
0.7916668408369603	0.9583334368189895	0.0784850000000006	F	F	F
0.8333334212839745	0.9166667221290226	0.1569700000000012	F	F	F
0.7500073176492201	0.8750543082891505	0.2386006087519116	T	T	T
0.7917436875659342	0.9583982539380873	0.3224094545896591	T	T	T
0.874999960229360	0.0000000000000000	0.0000000000000000	F	F	F
0.9166667107129030	0.0833334293799339	0.0784850000000006	F	F	F
0.9583332911599243	0.0416667146899670	0.1569700000000012	F	F	F
0.8750155262793050	0.0000473941815378	0.2385744254945479	T	T	T
0.9167155127123474	0.0833697067755699	0.3224036848938485	T	T	T
0.8750001302658816	0.1250001440699009	0.0000000000000000	F	F	F
0.9166668449558486	0.2083335734498348	0.0784850000000006	F	F	F
0.9583334254028699	0.1666668587598679	0.1569700000000012	F	F	F
0.8750131804513500	0.1250622864507105	0.2385754935325274	T	T	T
0.9167258234050296	0.2083697769612559	0.3224462497277688	T	T	T
0.8750000142462682	0.2499997876146764	0.0000000000000000	F	F	F
0.9166667289362351	0.3333332169946104	0.0784850000000006	F	F	F
0.9583333093832564	0.2916665023046434	0.1569700000000012	F	F	F
0.8750697280111832	0.2500468979927807	0.2386284211267382	T	T	T
0.9167467980002026	0.3333608285789393	0.3225570719579852	T	T	T
0.8750001484892138	0.3749999316845773	0.0000000000000000	F	F	F
0.9166668631791808	0.4583333610645113	0.0784850000000006	F	F	F
0.9583334436262021	0.4166666463745443	0.1569700000000012	F	F	F
0.8752122677461813	0.3750546421836917	0.2386386019699980	T	T	T
0.9166717801712622	0.4583778553955121	0.3225887203283653	T	T	T
0.8749998492647180	0.5000000757544782	0.0000000000000000	F	F	F
0.9166665639546849	0.5833335051344122	0.0784850000000006	F	F	F
0.9583335778691477	0.5416667904444452	0.1569700000000012	F	F	F
0.8752134939490609	0.5001666443695554	0.2386429598413691	T	T	T
0.9167732754713497	0.5834737910203950	0.3225619439065739	T	T	T
0.8749999835076636	0.6250002198243791	0.0000000000000000	F	F	F
0.9166664479350644	0.7083331486791877	0.0784850000000006	F	F	F
0.9583330283820857	0.6666664339892208	0.1569700000000012	F	F	F
0.8750252356849262	0.6250080524586127	0.2386220516913787	T	T	T
0.9167340939742914	0.7083963080124558	0.3224179395096738	T	T	T
0.8749998674880501	0.7499998633691547	0.0000000000000000	F	F	F
0.9166665821780171	0.8333332927490886	0.0784850000000006	F	F	F
0.9583331626250313	0.7916665780591217	0.1569700000000012	F	F	F
0.8749740664801604	0.7499631539913997	0.2385708411323831	T	T	T
0.9167224577399327	0.8333906583533940	0.3223177048380304	T	T	T
0.8750000017309958	0.8750000074390556	0.0000000000000000	F	F	F
0.9166667164209628	0.9583334368189895	0.0784850000000006	F	F	F
0.9583332968679841	0.9166667221290226	0.1569700000000012	F	F	F
0.8750039918027634	0.8750409888948233	0.2385562300716783	T	T	T
0.9167323321438103	0.9583811899545005	0.3223751147385109	T	T	T
0.4492711382364695	0.5394651107700092	0.4245106749105436	T	T	T
0.3397956356859002	0.4295499620609632	0.4250036663639194	T	T	T
0.3393751200602123	0.5389667690673039	0.4246611673662203	T	T	T
0.6215499437043722	0.2563441615207074	0.4249386351089645	T	T	T
0.5128398459581281	0.2581547507136681	0.4250975064396145	T	T	T
0.6234397051382428	0.3669197413517534	0.4245359914742118	T	T	T
0.4116868113909720	0.4675744629510270	0.4249100802454399	T	T	T
0.4112892300370236	0.5733492682030432	0.4245614740040402	T	T	T
0.3054762982737557	0.4670947789011689	0.4250792941901037	T	T	T
0.5497105122316090	0.2231435263098363	0.4253599818137148	T	T	T
0.6566279308899242	0.3282803447343710	0.4247361373740564	T	T	T
0.5515316983789059	0.3300107279183814	0.4249027716830985	T	T	T
0.4373670006779989	0.4422256178640795	0.4242325382513469	T	T	T
0.3099978826547660	0.3694487850967790	0.4251950189122329	T	T	T
0.2544157599188316	0.4414262127271156	0.4247995127194857	T	T	T
0.3091519452909492	0.5688500709160549	0.4245947147891681	T	T	T
0.4366471071773955	0.6244074272300556	0.4238650203318731	T	T	T
0.5093928598795051	0.5696705036161362	0.4243378480248125	T	T	T

0.5235584659640423	0.1720873919211168	0.4251492408895550	T	T	T
0.4527472842331418	0.2289337035450921	0.4251951173152845	T	T	T
0.5266860010476523	0.3561836035819101	0.4240536018097251	T	T	T
0.6542008520354317	0.4270284710679505	0.4242482052345268	T	T	T
0.7076778447280407	0.3531373635215415	0.4240456179625954	T	T	T
0.6508604701306256	0.2255521873380209	0.4249314665177792	T	T	T

Borazine adsorbed on Au(111), hpc, with 9 H₂ molecules

23.0697829620000014	0.0000000000000000	0.0000000000000000
-11.5348914810000007	19.9790169730000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.0000000000000000

Au B N H
320 3 3 24

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0416667146899670	0.0833334293799339	0.0784850000000006	F	F	F
0.0833332951369883	0.0416667146899670	0.1569700000000012	F	F	F
0.9999942302177672	0.9999724617849010	0.2385942084569199	T	T	T
0.0416444834701767	0.0832707018954374	0.3224201531346439	T	T	T
0.0000001342429456	0.1250001440699009	0.0000000000000000	F	F	F
0.0416668489329126	0.2083335734498348	0.0784850000000006	F	F	F
0.0833334293799339	0.1666668587598679	0.1569700000000012	F	F	F
0.0000326268387682	0.1249982851864430	0.2385918248734053	T	T	T
0.0416510909569179	0.2083067368088353	0.3224241695271849	T	T	T
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0.0833333133603205	0.2916665023046434	0.1569700000000012	F	F	F
0.9999979768646937	0.2499856038650661	0.2385958654265448	T	T	T
0.0416357179242383	0.3333084787886944	0.3224785802952575	T	T	T
0.00000001524662778	0.3749999316845773	0.0000000000000000	F	F	F
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0.0833334476032661	0.4166666463745443	0.1569700000000012	F	F	F
0.9999771524925763	0.3749570962745201	0.2386076549849698	T	T	T
0.0416533548587948	0.4583065439634854	0.3224294371264849	T	T	T
0.9999997248487205	0.5000000757544782	0.0000000000000000	F	F	F
0.0416665679317489	0.5833335051344122	0.0784850000000006	F	F	F
0.0833335818462118	0.5416667904444452	0.1569700000000012	F	F	F
0.9999703164252420	0.4999369171881610	0.2385844326156740	T	T	T
0.0416128720399919	0.5832666882028421	0.3223689208740145	T	T	T
0.999998590916661	0.6250002198243791	0.0000000000000000	F	F	F
0.0416664519121284	0.7083331486791877	0.0784850000000006	F	F	F
0.0833330323591497	0.6666664339892208	0.1569700000000012	F	F	F
0.9999539219449908	0.6249576880772950	0.2385819410663911	T	T	T
0.0416050451720956	0.7082636922354987	0.3223739750143809	T	T	T
0.999997430720526	0.749998633691547	0.0000000000000000	F	F	F
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0.0833331666020953	0.7916665780591217	0.1569700000000012	F	F	F
0.9999603088145934	0.7499854158288942	0.2385878736996161	T	T	T
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0.0833333008450481	0.9166667221290226	0.1569700000000012	F	F	F
0.9999673519292822	0.8749739405414388	0.2386087245544236	T	T	T
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0.2083331707209908	0.0416667146899670	0.1569700000000012	F	F	F
0.1249366624834979	0.9999536123444367	0.2386225835835539	T	T	T
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0.1250023405920763	0.1249784010265858	0.2386594319601923	T	T	T
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0.2083331889443230	0.2916665023046434	0.1569700000000012	F	F	F
0.1250027538079080	0.2499865656634011	0.2386587676364375	T	T	T
0.1665762586689002	0.3332981981558484	0.3225256687637407	T	T	T
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0.208333231872686	0.4166666463745443	0.1569700000000012	F	F	F
0.1249469043430942	0.3749449848161339	0.2386196851022682	T	T	T
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0.1250001622932331	0.5000000757544782	0.0000000000000000	F	F	F
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0.2083334574302214	0.5416667904444452	0.1569700000000012	F	F	F

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0.1250002965361787	0.6250002198243791	0.0000000000000000	F	F	F
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0.2083333414106079	0.6666664339892208	0.1569700000000012	F	F	F
0.1249757411259503	0.6249495408715370	0.2385778885008751	T	T	T
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0.2499168714502738	0.9999252162794009	0.2386485797853139	T	T	T
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0.2498511081494417	0.3749657065152144	0.2386419485797786	T	T	T
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0.333333330142239	0.5416667904444452	0.1569700000000012	F	F	F
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0.2500111822675323	0.7499776596387505	0.2385783502348816	T	T	T
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0.3748358930673474	0.1246695330062923	0.2386560784600076	T	T	T
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0.8333335498188674	0.1666668587598679	0.1569700000000012	F	F	F
0.7499706033174121	0.1249997525105022	0.2385915965601133	T	T	T
0.7916577173961935	0.2083070947224146	0.3224249323937683	T	T	T
0.7499997051948100	0.2499997876146764	0.0000000000000000	F	F	F
0.7916664198847769	0.3333332169946104	0.0784850000000006	F	F	F
0.8333334337992468	0.2916665023046434	0.1569700000000012	F	F	F
0.7499853996142662	0.2499863138087894	0.2386580505721557	T	T	T
0.7917218066731482	0.3332985096885442	0.3225246403795908	T	T	T
0.7499998394377627	0.3749999316845773	0.0000000000000000	F	F	F
0.7916665541277297	0.4583333610645113	0.0784850000000006	F	F	F
0.8333331345747439	0.4166666463745443	0.1569700000000012	F	F	F
0.7501136414167450	0.3749641530520822	0.2386413602975517	T	T	T
0.7915431507270927	0.4582010722074439	0.3225013302611439	T	T	T
0.7499999736807084	0.5000000757544782	0.0000000000000000	F	F	F
0.7916666883706753	0.5833335051344122	0.0784850000000006	F	F	F
0.8333332688176966	0.5416667904444452	0.1569700000000012	F	F	F
0.7502258225813684	0.5000946604520384	0.2386737505557089	T	T	T
0.7915318271464153	0.5832428792010855	0.3225154096495851	T	T	T
0.7500001079236540	0.6250002198243791	0.0000000000000000	F	F	F
0.7916665723510619	0.7083331486791877	0.0784850000000006	F	F	F
0.8333331527980832	0.6666664339892208	0.1569700000000012	F	F	F
0.7500811532413164	0.6250802581325574	0.2386485117223376	T	T	T
0.7916928064783828	0.7083083273508261	0.3225194005448566	T	T	T
0.7499999919040405	0.7499998633691547	0.0000000000000000	F	F	F
0.7916667065940075	0.8333332927490886	0.0784850000000006	F	F	F
0.8333332870410288	0.7916665780591217	0.1569700000000012	F	F	F
0.7499741470719936	0.7499446889668762	0.2386541818520551	T	T	T
0.7916389583068347	0.8332495541433542	0.3224179192275117	T	T	T
0.7500001261469933	0.8750000074390556	0.0000000000000000	F	F	F
0.7916668408369603	0.9583334368189895	0.0784850000000006	F	F	F
0.8333334212839745	0.9166667221290226	0.1569700000000012	F	F	F
0.7499660707096407	0.8749269779608648	0.2385894505952614	T	T	T
0.7916386801462754	0.9582635836367104	0.3223672871857532	T	T	T
0.874999960229360	0.0000000000000000	0.0000000000000000	F	F	F
0.9166667107129030	0.0833334293799339	0.0784850000000006	F	F	F
0.9583332911599243	0.0416667146899670	0.1569700000000012	F	F	F
0.8749954430140224	0.9999669012053437	0.2385843910292722	T	T	T
0.9166496968268557	0.0832853073202679	0.3223692508558135	T	T	T
0.8750001302658816	0.1250001440699009	0.0000000000000000	F	F	F
0.9166668449558486	0.2083335734498348	0.0784850000000006	F	F	F
0.9583334254028699	0.1666668587598679	0.1569700000000012	F	F	F
0.8749982826716517	0.1249920280521514	0.2385853778949522	T	T	T
0.9166543654757493	0.2083052925693252	0.3224078591084090	T	T	T
0.8750000142462682	0.2499997876146764	0.0000000000000000	F	F	F
0.9166667289362351	0.3333332169946104	0.0784850000000006	F	F	F
0.9583333093832564	0.2916665023046434	0.1569700000000012	F	F	F
0.8749890553397877	0.2499854753587438	0.2385966174881837	T	T	T
0.9166736502930153	0.3333073401868595	0.3224788401396815	T	T	T
0.8750001484892138	0.3749999316845773	0.0000000000000000	F	F	F
0.9166668631791808	0.4583333610645113	0.0784850000000006	F	F	F

0.9583334436262021	0.4166666463745443	0.1569700000000012	F	F	F
0.8749960892781360	0.3749446972541485	0.2386205241925328	T	T	T
0.9166039226800025	0.4582700583890683	0.3224576984826664	T	T	T
0.8749998492647180	0.5000000757544782	0.0000000000000000	F	F	F
0.9166665639546849	0.5833335051344122	0.0784850000000006	F	F	F
0.9583335778691477	0.5416667904444452	0.1569700000000012	F	F	F
0.8750029100657186	0.4999406645068462	0.2386448888282766	T	T	T
0.9165197718113552	0.5832215528874835	0.3223730251972791	T	T	T
0.8749999835076636	0.6250002198243791	0.0000000000000000	F	F	F
0.9166664479350644	0.7083331486791877	0.0784850000000006	F	F	F
0.9583330283820857	0.6666664339892208	0.1569700000000012	F	F	F
0.8749913713796974	0.6250202043587818	0.2386465165028659	T	T	T
0.9165862451648362	0.7082423301062355	0.3224668461986188	T	T	T
0.8749998674880501	0.7499998633691547	0.0000000000000000	F	F	F
0.9166665821780171	0.8333332927490886	0.0784850000000006	F	F	F
0.9583331626250313	0.7916665780591217	0.1569700000000012	F	F	F
0.8749817186335743	0.7499976561640089	0.2386193019984981	T	T	T
0.9166491978870305	0.8332669288217748	0.3224746275670795	T	T	T
0.8750000017309958	0.8750000074390556	0.0000000000000000	F	F	F
0.9166667164209628	0.9583334368189895	0.0784850000000006	F	F	F
0.9583332968679841	0.9166667221290226	0.1569700000000012	F	F	F
0.8749816989363348	0.8749586328016683	0.2385947102335156	T	T	T
0.9166448467533339	0.9582622185144237	0.3224004847661802	T	T	T
0.5716587584356244	0.4086172469535312	0.4241554279722849	T	T	T
0.4620837250901053	0.4087602140603047	0.4242265105772831	T	T	T
0.4619341485796450	0.2990265996397628	0.4238533553511000	T	T	T
0.5339750122880138	0.4428291958729677	0.4243581030104645	T	T	T
0.5338324555621179	0.3367041706371747	0.4239600596677501	T	T	T
0.4278338547399596	0.3368377634167416	0.4240277476002480	T	T	T
0.6317259677242532	0.4385714798910569	0.4243733453252159	T	T	T
0.5593070801519822	0.3110914005567999	0.4238497421610201	T	T	T
0.4318745981920398	0.2389582929857517	0.4238718962444564	T	T	T
0.3767441379906203	0.3113501120484065	0.4239647845522651	T	T	T
0.4321068618055675	0.4388394627487077	0.4245079486929409	T	T	T
0.5595563768487420	0.4939110222859481	0.4245503182880319	T	T	T
0.6180822153771982	0.6111594588822625	0.4179383884969931	T	T	T
0.6167468200925217	0.6084434359478107	0.4430120614253956	T	T	T
0.6199588234925237	0.2539921757000119	0.4177932284497246	T	T	T
0.6183113595732712	0.2551084037931016	0.4428643111838491	T	T	T
0.2592638682336573	0.2544228870802644	0.4178233643687935	T	T	T
0.2621827952590328	0.2557297788109338	0.4428873853418386	T	T	T
0.2928753752641063	0.4020269351997191	0.4180803409736860	T	T	T
0.2964403901010572	0.4035910818483168	0.4430754497816838	T	T	T
0.2914089416974506	0.1396832755569772	0.4181209236655218	T	T	T
0.2950829260315558	0.1416117629676397	0.4431095707949091	T	T	T
0.4712576443624289	0.5782638797052918	0.4180243413582165	T	T	T
0.4697678961848356	0.5746972225836782	0.4430189518820618	T	T	T
0.4732312098647004	0.1397098318295335	0.4180790777001792	T	T	T
0.4715607010223574	0.1417834907080397	0.4430625837772368	T	T	T
0.7337559700307302	0.4010572760633167	0.4180022352759399	T	T	T
0.7316378200499509	0.4024304209932854	0.4430012218030757	T	T	T
0.7319777143075241	0.5781577576873939	0.4180123934213189	T	T	T
0.7298271648275928	0.5745434015001981	0.4430033550111311	T	T	T

Borazine dimer adsorbed on Au(111), dimer II, with 10 H₂ molecules

23.0697829620000014	0.0000000000000000	0.0000000000000000
-11.5348914810000007	19.9790169730000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.0000000000000000

Au B N H
320 6 6 32

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0416667146899670	0.0833334293799339	0.0784850000000006	F	F	F
0.0833332951369883	0.0416667146899670	0.1569700000000012	F	F	F
0.0000537259102898	0.0000337061172669	0.2385736472189307	T	T	T
0.0416603928195830	0.0833134677777821	0.3224596141669762	T	T	T
0.0000001342429456	0.1250001440699009	0.0000000000000000	F	F	F
0.0416668489329126	0.2083335734498348	0.0784850000000006	F	F	F
0.0833334293799339	0.1666668587598679	0.1569700000000012	F	F	F
0.0000241927953762	0.1250143488915853	0.2385897815480675	T	T	T
0.0416592827734681	0.2083279096828799	0.3225046551897596	T	T	T
0.0000000182233322	0.2499997876146764	0.0000000000000000	F	F	F
0.0416667329132991	0.3333332169946104	0.0784850000000006	F	F	F
0.0833333133603205	0.2916665023046434	0.1569700000000012	F	F	F
0.0000431010417638	0.2500036662687813	0.2386001216882904	T	T	T
0.0417255064910459	0.3333687595853942	0.3223690432462044	T	T	T
0.0000001524662778	0.3749999316845773	0.0000000000000000	F	F	F

0.0416668671562448	0.4583333610645113	0.0784850000000006	F	F	F
0.0833334476032661	0.4166666463745443	0.1569700000000012	F	F	F
0.0000443099743128	0.3749915184566292	0.2385815096901640	T	T	T
0.0417414133967063	0.4583360542918527	0.3224549776348462	T	T	T
0.9999997248487205	0.5000000757544782	0.0000000000000000	F	F	F
0.0416665679317489	0.5833335051344122	0.0784850000000006	F	F	F
0.0833335818462118	0.5416667904444452	0.1569700000000012	F	F	F
0.0000535902490299	0.4999870019828954	0.2385781160668842	T	T	T
0.0417469714018403	0.5833329880065797	0.3224191260705314	T	T	T
0.9999998590916661	0.6250002198243791	0.0000000000000000	F	F	F
0.0416664519121284	0.7083331486791877	0.0784850000000006	F	F	F
0.0833330323591497	0.6666664339892208	0.1569700000000012	F	F	F
0.0000533426413836	0.6250053021029535	0.2385688185644825	T	T	T
0.0418063497780608	0.7083454844421245	0.3223855419658604	T	T	T
0.9999997430720526	0.7499998633691547	0.0000000000000000	F	F	F
0.0416665861550811	0.8333332927490886	0.0784850000000006	F	F	F
0.0833331666020953	0.7916665780591217	0.1569700000000012	F	F	F
0.0000439306827922	0.7499974803496965	0.2385657976354666	T	T	T
0.0417608779594616	0.8333324820589488	0.3223861764220814	T	T	T
0.0000000057080598	0.8750000074390556	0.0000000000000000	F	F	F
0.0416667203980268	0.9583334368189895	0.0784850000000006	F	F	F
0.0833333008450481	0.9166667221290226	0.1569700000000012	F	F	F
0.0000360190559462	0.8750272433558284	0.2385691272108438	T	T	T
0.0417208871415859	0.9583192415118661	0.3224122269942646	T	T	T
0.1249998755840025	0.0000000000000000	0.0000000000000000	F	F	F
0.1666665902739695	0.0833334293799339	0.0784850000000006	F	F	F
0.2083331707209908	0.0416667146899670	0.1569700000000012	F	F	F
0.1250370095693387	0.0000174717402583	0.2386181776040576	T	T	T
0.1666394943699434	0.0832978469785353	0.3224937742178282	T	T	T
0.125000098269552	0.1250001440699009	0.0000000000000000	F	F	F
0.1666667245169222	0.2083335734498348	0.0784850000000006	F	F	F
0.2083333049639364	0.1666668587598679	0.1569700000000012	F	F	F
0.1249872848184486	0.1249988781746724	0.2386662328106949	T	T	T
0.1665182916038495	0.2082762409334075	0.3226430647757285	T	T	T
0.1249998938073347	0.2499997876146764	0.0000000000000000	F	F	F
0.1666666084973016	0.3333332169946104	0.0784850000000006	F	F	F
0.2083331889443230	0.2916665023046434	0.1569700000000012	F	F	F
0.1249711792932841	0.2499590032241031	0.2386519346619407	T	T	T
0.1666448590505689	0.3332596464632445	0.3225319736609839	T	T	T
0.1250000280502874	0.3749999316845773	0.0000000000000000	F	F	F
0.1666667427402544	0.4583333610645113	0.0784850000000006	F	F	F
0.2083333231872686	0.4166666463745443	0.1569700000000012	F	F	F
0.1250515335563242	0.3749983549532425	0.2386554681862490	T	T	T
0.1667317803221489	0.4583381420046051	0.3225566543557503	T	T	T
0.1250001622932331	0.5000000757544782	0.0000000000000000	F	F	F
0.1666668769832000	0.5833335051344122	0.0784850000000006	F	F	F
0.2083334574302214	0.5416667904444452	0.1569700000000012	F	F	F
0.1250222923753512	0.4999580347143096	0.2386258163091978	T	T	T
0.1667284600963333	0.5832946083863887	0.3224685093084451	T	T	T
0.1250002965361787	0.6250002198243791	0.0000000000000000	F	F	F
0.1666667609635866	0.7083331486791877	0.0784850000000006	F	F	F
0.2083333414106079	0.6666664339892208	0.1569700000000012	F	F	F
0.1250256461670656	0.6249699578499347	0.2385932843216596	T	T	T
0.1668086568558568	0.7083511835502325	0.3223663096095525	T	T	T
0.1249997470491166	0.7499998633691547	0.0000000000000000	F	F	F
0.1666664617390836	0.8333332927490886	0.0784850000000006	F	F	F
0.2083334756535535	0.7916665780591217	0.1569700000000012	F	F	F
0.1250509077813027	0.7500095798411854	0.2385552647157595	T	T	T
0.1668174457950435	0.8333880918244395	0.3223913002774593	T	T	T
0.1249998812920623	0.8750000074390556	0.0000000000000000	F	F	F
0.1666665959820293	0.9583334368189895	0.0784850000000006	F	F	F
0.2083331764290506	0.9166667221290226	0.1569700000000012	F	F	F
0.1250284414384063	0.8750188070861188	0.2385734045469895	T	T	T
0.1667093548401243	0.9582845706224515	0.3224793733550400	T	T	T
0.2500001846354607	0.0000000000000000	0.0000000000000000	F	F	F
0.2916668993254277	0.0833334293799339	0.0784850000000006	F	F	F
0.3333334797724490	0.0416667146899670	0.1569700000000012	F	F	F
0.2499549655667978	0.9999283512305650	0.2386113699175641	T	T	T
0.2914875427868485	0.0831929648431144	0.3225556572228452	T	T	T
0.2499998854109577	0.1250001440699009	0.0000000000000000	F	F	F
0.2916666001009247	0.2083335734498348	0.0784850000000006	F	F	F
0.3333336140153946	0.1666668587598679	0.1569700000000012	F	F	F
0.2499271787267835	0.1249146216647411	0.2387107313486918	T	T	T
0.2913673028382369	0.2082417277529130	0.3225715015519427	T	T	T
0.2499997693913443	0.2499997876146764	0.0000000000000000	F	F	F
0.2916664840813112	0.3333332169946104	0.0784850000000006	F	F	F
0.3333330645283255	0.2916665023046434	0.1569700000000012	F	F	F
0.2497211809626771	0.2497794017590265	0.2386330012433708	T	T	T

0.2914092573034348	0.3329884012674882	0.3225703883284903	T	T	T
0.2499999036342899	0.3749999316845773	0.0000000000000000	F	F	F
0.2916666183242569	0.4583333610645113	0.0784850000000006	F	F	F
0.33333331987712782	0.4166666463745443	0.1569700000000012	F	F	F
0.2498479279816614	0.3748742147260059	0.2387171982772860	T	T	T
0.2915142081634615	0.4581523475658494	0.3224377756233763	T	T	T
0.2500000378772356	0.5000000757544782	0.0000000000000000	F	F	F
0.2916667525672025	0.5833335051344122	0.0784850000000006	F	F	F
0.3333333301422239	0.5416667904444452	0.1569700000000012	F	F	F
0.2499166485427648	0.4999934561783893	0.2386758822234151	T	T	T
0.2916424983255976	0.5832947663726394	0.3225575927771299	T	T	T
0.2500001721201883	0.6250002198243791	0.0000000000000000	F	F	F
0.2916666365475891	0.7083331486791877	0.0784850000000006	F	F	F
0.3333332169946104	0.6666664339892208	0.1569700000000012	F	F	F
0.2499632537757901	0.6250147999237755	0.2386436021648267	T	T	T
0.2918057880292846	0.7083167823564438	0.3224216714525129	T	T	T
0.2500000561005749	0.7499998633691547	0.0000000000000000	F	F	F
0.2916667707905418	0.8333332927490886	0.0784850000000006	F	F	F
0.3333333512375560	0.7916665780591217	0.1569700000000012	F	F	F
0.2500697555014383	0.7500223324711105	0.2386003198203032	T	T	T
0.2918398358800405	0.8334243167159047	0.3223103169081480	T	T	T
0.2500001903435205	0.8750000074390556	0.0000000000000000	F	F	F
0.2916669050334875	0.9583334368189895	0.0784850000000006	F	F	F
0.3333334854805088	0.9166667221290226	0.1569700000000012	F	F	F
0.2500520882763219	0.8750350150891272	0.2386178182299284	T	T	T
0.2918025045353179	0.9584693016928262	0.3224889247102914	T	T	T
0.3750000602194632	0.0000000000000000	0.0000000000000000	F	F	F
0.4166667749094302	0.0833334293799339	0.0784850000000006	F	F	F
0.4583333553564515	0.0416667146899670	0.1569700000000012	F	F	F
0.3749958188420949	0.9998619878157392	0.2386867620696790	T	T	T
0.4167054389791185	0.0833429981639519	0.3226200891592658	T	T	T
0.3750001944624159	0.1250001440699009	0.0000000000000000	F	F	F
0.4166669091523829	0.2083335734498348	0.0784850000000006	F	F	F
0.4583334895993971	0.1666668587598679	0.1569700000000012	F	F	F
0.3748276324093565	0.1246235042288826	0.2385427553863062	T	T	T
0.4161829785891512	0.2080437427587666	0.3212348267680657	T	T	T
0.3750000784427954	0.2499997876146764	0.0000000000000000	F	F	F
0.4166667931327623	0.3333332169946104	0.0784850000000006	F	F	F
0.4583333735797837	0.2916665023046434	0.1569700000000012	F	F	F
0.3747074316736331	0.2498348019738290	0.2384869228772683	T	T	T
0.4164908303279060	0.3331509189276436	0.3221977877501157	T	T	T
0.3749997792182995	0.3749999316845773	0.0000000000000000	F	F	F
0.4166664939082665	0.4583333610645113	0.0784850000000006	F	F	F
0.4583335078227293	0.4166666463745443	0.1569700000000012	F	F	F
0.3745613716289756	0.3745809537904126	0.2383681884459332	T	T	T
0.4164747488556736	0.4577520328949286	0.3207928899390536	T	T	T
0.3749999134612452	0.5000000757544782	0.0000000000000000	F	F	F
0.4166666281512121	0.5833335051344122	0.0784850000000006	F	F	F
0.4583332085982335	0.5416667904444452	0.1569700000000012	F	F	F
0.3748119113488544	0.5000174712496086	0.2385039471457722	T	T	T
0.4165509707954384	0.5834780871724923	0.3214811255939780	T	T	T
0.3750000477041908	0.6250002198243791	0.0000000000000000	F	F	F
0.4166665121315987	0.7083331486791877	0.0784850000000006	F	F	F
0.4583330925786129	0.6666664339892208	0.1569700000000012	F	F	F
0.3748506855284417	0.6252214638299324	0.2385397963642453	T	T	T
0.4167023577269330	0.7083857191317517	0.3225974441834371	T	T	T
0.3749999316845773	0.7499998633691547	0.0000000000000000	F	F	F
0.4166666463745443	0.8333332927490886	0.0784850000000006	F	F	F
0.4583332268215656	0.7916665780591217	0.1569700000000012	F	F	F
0.3750734261307122	0.7501174207830830	0.2386456819861152	T	T	T
0.4167733593222854	0.8333860372304679	0.3225679962825770	T	T	T
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0.4166667806174900	0.9583334368189895	0.0784850000000006	F	F	F
0.4583333610645113	0.9166667221290226	0.1569700000000012	F	F	F
0.3751331727659361	0.8750454278177487	0.2386363326802338	T	T	T
0.4168163270405514	0.9584718256957057	0.3224831135504435	T	T	T
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0.5000817365104198	0.9999629507279274	0.2386435903454424	T	T	T
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0.4998634477824988	0.3751036581031177	0.2383807879058949	T	T	T
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0.5001640446128854	0.5000736552267653	0.2383829190080163	T	T	T
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0.5000363657461655	0.7500791915778003	0.2387006161481062	T	T	T
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