

3.8.7 Cyclic hydrocarbons

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3.8.7.1 List of symbols and abbreviations

Geometry, Coverage:

$\sigma(d), \sigma(v)$	orientation with molecular $\sigma(d/v)$ mirror plane parallel to surface mirror plane (see Fig. 1)
hcp site	3-fold coordinated hollow site with a substrate atom in the 2 nd layer underneath.
fcc site	3-fold coordinated hollow site with a substrate atom in the 3 rd layer underneath.
bridge	2-fold coordinated adsorption site.
pedestal site	see Fig. 4.
θ_r	relative coverage (fraction of saturation coverage)
θ	absolute coverage (adsorbed molecules per substrate surface atom)
ML	“monolayer”, unit for absolute coverage. Note: following a common practice, in some cases the word “monolayer” is also used to describe the saturated chemisorbed layer. “ML”, however, always refers to the absolute coverage of molecules, i.e. the ratio of adsorbed molecules to substrate surface atoms.
E_{des}	activation energy for desorption
E_{act}	activation energy for dissociation (dehydrogenation)
E_{diff}	activation energy for diffusion
E_{trans}	translational energy of gas particles
T_{max}	desorption temperature (rate maximum)

Experimental techniques

2PPE	2 Photon Photoemission
$\Delta\Phi$	Work Function Change
AES	Auger Electron Spectroscopy
ARPES	Angle Resolved Photoelectron Spectroscopy
ARUPS	Angle Resolved UV Photoelectron Spectroscopy
DLEED	Diffuse Low Energy Electron Diffraction
(E)ELS	Electron Energy Loss Spectroscopy
ESDIAD	Electron Stimulated Desorption Ion Angular Distribution
FTMS	Fourier Transform Mass Spectroscopy
HAS	Helium Atom Scattering
HREELS	High Resolution Electron Energy Loss Spectroscopy
IETS	In-Elastic Tunnelling Spectroscopy
IPES	Inverse Photoemission Spectroscopy
LEED(-IV)	Low Energy Electron Diffraction (Intensity vs. Voltage dependence)
LITD	Laser Induced Thermal Desorption
MAES	Metastable Atom Electron Spectroscopy
MIES	Metastable Impact Electron Spectroscopy
NEELFS	Near Edge Electron Energy Loss Fine Structure
NEXAFS	Near Edge X-ray Absorption Fine Structure (= XANES)
PED	Photoelectron Diffraction
PhD	Photoelectron Diffraction
RAIRS	Reflection Absorption Infrared Spectroscopy
Raman	Raman Spectroscopy
SRUPS	Spin Resolved UV Photoelectron Spectroscopy

SHG	Second Harmonic Generation
STM	Scanning Tunnelling Microscopy
STS	Scanning Tunnelling Spectroscopy
TPD	Temperature Programmed Desorption
UPS	UV Photoelectron Spectroscopy
XANES	X-ray Absorption Near Edge Spectroscopy (= NEXAFS)
XPD	X-ray Photoelectron Diffraction
XPS	X-ray Photoelectron Spectroscopy

Theoretical techniques

ADC(3)	Algebraic Diagrammatic Construction Green's function method
CI	Configuration Interaction
PM3	Parameterized Method 3 (semi empirical)
DFT (GGA)	Density Functional Theory (General Gradient Approximation) (ab initio)
EHT	Extended Hückel Theory (semi-empirical)
HF	Hartree Fock calculation (ab initio)
LCGTO-DFT	Linear Combination of Gauss-Type Orbitals– DFT (ab initio)
MO calc.	Molecular Orbital calculations (semi-empirical)
MINDO	Modified Intermediate Neglect of Differential Overlap (semi empirical)

3.8.7.2 Benzene (C₆H₆)

Among the cyclic hydrocarbon molecules adsorbed on surfaces, benzene is by far the most intensely studied system. Most surface science techniques have been applied in order to elucidate the geometry and the bond/electronic structure of benzene adsorbed on single crystal surfaces. Due to its high symmetry in the gas phase (D_{6h}), vibrational spectroscopies (HREELS, RAIRS) and photo-electric spectroscopies (ARUPS, NEXAFS) can also be used to retrieve information about the orientation and the symmetry of the adsorption complex besides the actual spectroscopic information. The vast majority of studies concentrate on transition metal surfaces of particular catalytic importance. Recently, there is also growing interest in the adsorption on silicon surfaces.

The present article is restricted to the adsorption and coadsorption with atoms / small molecules on low-index (i.e. non-stepped) single crystal surfaces and flat well-defined thin films. The adsorption of benzene on stepped surfaces (Pt, Ir) has been studied to some extent [e.g. 73Gla, 74Bar] because of their potential importance in catalytic processes involving small metal particles. These results are not included in the tables because they are dominated by step effects and do, therefore, not represent low index surface properties.

The available information is provided in Tables 1a-1c: After listing typical gas phase or multilayer values for comparison, the adsorbate systems are divided into metals and semiconductors / insulators are listed alphabetically starting with pure benzene layers and then listing coadsorption systems for each substrate.

Table 1.a “**Temperature Dependence and Adsorption Geometry**” compiles the desorption temperatures from temperature programmed desorption spectroscopy (TPD) and the information about long range order (LEED patterns) and local adsorption geometries, bond length, molecular orientation, etc.. The adsorption geometry is characterized by spectroscopic methods (see above), local probes (STM), crystallographic diffraction methods (LEED-IV, PhD), and semi-empirical or ab initio theoretical calculations. Especially for the latter two techniques, benzene provides a particular challenge, since these structures are among the most complex surface structures solved with those methods so far.

TPD: Molecular multilayer desorption is observed around 150 K. For the chemisorbed layer a wide range of desorption temperatures has been reported (150 K - 570 K). Hydrogen desorption indicates decomposition of benzene leaving a layer of carbon behind on the surface. Typically, the onset of hydrogen desorption is somewhat above the onset of molecular desorption; the lowest onset is 250 K, reported for Pt(111). As a typical example, TPD spectra of benzene on Ni(111) are shown in Fig. 1.

Adsorption Geometry: On metals the surface bond is formed through the interaction between metal d-states and the molecular π -electrons. Therefore, on unreconstructed close-packed surfaces (fcc 111, 100, hcp 0001) intact molecules usually adsorb with the ring parallel to the surface, whereas on more corrugated surfaces (e.g. fcc 110) also tilted geometries are reported with the ring parallel to one of the facets. There is a great variety of adsorption sites (bridge, hollow) and orientations observed, not following any apparent rule. The key geometrical parameters listed in the table are adsorption site, orientation of the molecule (for a description of the nomenclature, see Fig. 2), C-C bond lengths (usually larger than the gas phase value of 1.40 Å) and the substrate-carbon bond lengths (typically around 2.0 Å). On most metal surfaces benzene does not order very easily and in some cases (e.g. Rh(111)) it was argued that all long range ordered structures observed are actually induced by coadsorption with CO from residual gas. In general, pure ordered overlayers tend to be observed at low temperatures near saturation coverage, with the exception of Ru(0001), where ordered phases are observed for various coverages - as an example the corresponding LEED patterns are shown in Fig. 3. Coadsorption with O, NO, CO helps to induce long range order at higher temperatures and lower coverage.

For insulator surfaces very weak surface bonds are reported with little information about the adsorption geometry available.

On silicon surfaces the situation is different, since benzene is able to form covalent bonds with the surface Si atoms, completely changing the intra-molecular bonding. The main body of structural studies has focussed on Si(100)-(2×1), applying spectroscopic and theoretical techniques. There, a 1,4-cyclohexadiene-like adsorption structure seems to emerge as the most stable adsorption configuration [98Bir, 95Jeo] (see also Fig. 4).

Table 1.b **“Electronic structure”** lists the binding energies of the occupied molecular orbitals and excitation energies for transitions into unoccupied levels. The spatial distribution of the molecular orbitals is shown in Fig. 5. Most data were collected using angle resolved photoelectron spectroscopy (ARUPS). Due to the bond formation through molecular π -electrons on metal surfaces, these orbitals ($1e_{1g}$, $1a_{2u}$) show the largest differential shifts (“bonding” shifts) upon adsorption. The magnitude of the differential shift is also a measure for the surface bond strength (small on group Ib metals, large on group VIII metals).

The spectroscopies of occupied and unoccupied molecular levels (ARUPS, EELS, NEXAFS) allow a characterization of the symmetry of the molecule/adsorption complex. As examples, ARUPS spectra of a dilute benzene layer on Ni(110) and NEXAFS spectra of benzene on Au(111), Rh(111), and Pt(111) are shown in Fig. 6 and Fig. 7, respectively. Detailed descriptions of the application of symmetry selection rules in order to retrieve geometry information and discussions of the electronic structure of adsorbed benzene can be found in several recent reviews [92Sto, 94Ste, 95Fre, 96Ste, 97Dow].

The excitation energies for molecular vibrations are listed in Table 1.c **“Vibrational properties”**. The two main techniques used here are HREELS and RAIRS. The frequencies for adsorption on metal surfaces are very similar to the corresponding values of the molecule in the gas phase, indicating essentially undistorted molecules.

On Si surfaces larger differences are observed due to changes in the bond order of the C-C bonds. No assignment is made to individual frequencies. Instead, the molecular vibrations for each adsorption system are grouped into four main energy ranges (400 - 1000 cm^{-1} , 1000 - 1200 cm^{-1} , 1200 - 1600 cm^{-1} , ~3000 cm^{-1}) with typical modes for each range listed at the top of the table. One band observed for crystalline layers around 1850 cm^{-1} [96Jak] is listed separately. Two additional columns list the frequencies of molecule-surface vibrations. The frustrated vertical translations (C-M, C-S) can be measured by HREELS (Benzene-Metal typically 250 - 400 cm^{-1} , Benzene-Si, up to 600 cm^{-1}), the energies of the lateral modes (frustrated translations and rotations) are usually not obtained by the above mentioned methods. In some cases such data are, however, available from other techniques (HAS, IETS). A detailed discussion of the assignment of vibrational frequencies from adsorbed benzene can be found in the recent review by Sheppard and De la Cruz [98She]; as a typical example a HREELS spectrum of benzene on (2×1) Si(100) together with the calculated normal frequencies of a $\text{C}_6\text{H}_6\text{Si}_{13}\text{H}_{12}$ cluster is shown in Fig. 8.

3.8.7.3 Cyclohexane (c-C₆H₁₂)

The adsorption of cyclohexane has been studied in some detail on low index and stepped metal surfaces of Cu, Ni, Mo, Ru, Pd, Ag, W, Ir and Pt – the key results of these studies are summarized in Table 2. It contains information on the rate maxima in temperature programmed desorption (T_{max}), characteristic vibrational frequencies (soft modes), ordered adsorbate structures, dehydrogenation upon heating as well as the orientation, symmetry and conformation on the surface, along with the corresponding references. The different metals are listed according to their position in the periodic table of elements. For semiconductor or oxide surfaces to the best of our knowledge no detailed studies are available.

The majority of studies focus on the nature of the chemical interaction between cyclohexane, in particular the C-H bonds, and the metal surface. From vibrational spectroscopies (HREELS and RAIRS) the signature of the interaction is a softening (red shift) of one C-H mode from $\sim 2900\text{ cm}^{-1}$ for the free molecule or in the condensed phase to lower wave numbers by up to 400 cm^{-1} . A comparable mode softening has also been observed for a number of different saturated hydrocarbons on metal surfaces – for a detailed discussion of the vibrational spectra see the reviews by Sheppard [88She, 98She].

There is general agreement that the origin of the softened C-H mode is due to H-atoms perturbed by their proximity to the metal surface in a hydrogen bond-like, C-H \cdots M bonding environment, often also termed as agostic (hydrogen-bond-like) bond. However, its relation to the desorption temperature and bond strength as well as the extent of dehydrogenation is subject of ongoing discussion:

For Cu(111), Cu(100), Cu(110), Cu₃Pt(111), Ni(111), Ni(100) and Ni(110) surfaces the observed mode softening is relatively small ($2690 - 2775\text{ cm}^{-1}$) and no dehydrogenation is observed upon heating a monolayer of cyclohexane. The desorption temperatures for these systems range from 178 to 206 K. As examples TPD and RAIRS spectra for Cu(111), Cu(100), Cu(110), Cu₃Pt, Ni(111) are shown in Fig. 9. (Note that in some cases studies of the same system by different authors yield significant differences in the desorption temperatures, which cannot be attributed only to differences in the heating rate). A special case is cyclohexane adsorption on one single layer of K on Ni(111), where the interaction to the substrate is so weak, that three-dimensional growth occurs and cyclohexane desorbs from the condensed phase at 135-140 K, even at nominal submonolayer coverages.

For Mo(110), Ru(0001), Pd(111), Pd(110), Pt(111), Pt(100)-(5 \times 20) a significantly stronger softening of the C-H mode is observed to values between 2550 and 2635 cm^{-1} . For these systems significant dehydrogenation of cyclohexane directly or via stable intermediates to benzene occurs upon heating. In addition, molecular desorption of cyclohexane at temperatures between 182 and 236 K occurs.

However, there are several systems that do not fall into these two categories, indicating that there is no general direct correlation between the magnitude of the mode-softening, the desorption temperature and the reactivity towards dehydrogenation. A very clear example is Mo(110) where a significant difference of nearly 100 cm^{-1} in the vibrational frequency of the soft mode is seen for the clean and the C-modified surface, whereas the desorption temperature remains essentially unchanged. Also for Cu(111) and Cu₃Pt(111) a shift of 21 K is seen in the desorption temperature, while the vibrational frequency of the softened mode is identical. At first sight, there seems to be a general trend that dehydrogenation is observed if the soft mode has a wave number smaller than 2650 cm^{-1} . However, there is again an example, which does not fit in that trend: for the non-reconstructed Pt(100)-(1 \times 1) surface no mode softening, but complete dehydrogenation occurs. Also, a strong isotope effect for dehydrogenation is observed for Pt(111) and Mo(110).

Summarizing these studies, one has to conclude that no general trends and correlations can be derived at the moment, suggesting that the details of the C-H \cdots metal interaction strongly depend on the substrate electronic structure and that there are several factors that contribute to the bonding interaction. Attractive as well as repulsive contributions to the mode-softening and the bonding interaction are discussed. Furthermore, the role of the geometric matching between three of the H-Atoms and specific adsorption sites on the surfaces has been considered [84Hof, 95Zae, 98Tep, 89Rav2, 85Kan, 88She, 98She].

There are only a few studies on the electronic structure of cyclohexane monolayers by UPS or ARUPS. In all studies, no differential shifts, i.e. bonding shifts, of particular molecular orbitals are observed, indicating only minor changes in the electronic structure due to a weak chemical interaction involving a C-H \cdots metal bond.

Concerning the geometric structure, for four surfaces the formation of ordered cyclohexane layers has been observed, namely a $(\sqrt{21} \times \sqrt{21})R10.9^\circ$ structure for Pt(111), $(\sqrt{7} \times \sqrt{7})R19.1^\circ$ structures for Cu(111) and Ni(111) and a (9×9) structure for Ag(111). For none of the surfaces a detailed structural analysis has been performed, which partly may be due to the high sensitivity of cyclohexane to beam damage and the large unit cells.

The conformation of the molecule, its orientation with respect to the surface plane, and the symmetry of the adsorption complex have been investigated using vibrational spectroscopies (HREELS and RAIRS) or ARUPS in combination with symmetry selection rules. In most cases it is concluded that the molecule is adsorbed in the chair form with the molecular plane parallel or slightly inclined to the surface. The symmetry of the adsorption complex differs for the various substrates, from C_{3v} to C_1 .

3.8.7.4 Other saturated cyclic hydrocarbon molecules (cycloalkanes)

Besides cyclohexane, the adsorption of a number of other cycloalkanes has been studied on metal surfaces – an overview is given in Table 3; for each molecule the metals are listed according to their position in the periodic table of elements. The table compiles the rate maxima in temperature programmed desorption (T_{max}), characteristic vibrational frequencies (soft modes), dehydrogenation upon heating and some additional data (column “comments”). For semiconductor or oxide surfaces to the best of our knowledge no detailed studies are available.

One central aspect in these studies is again the nature of the chemical interaction with the substrate, in particular, the formation of C-H...metal bonds, which are reflected in mode softening of a C-H vibration. Studies by TPD show that there is a steady increase of monolayer desorption ranges for the different cycloalkanes, from 123 - 150 K for cyclopropane, 175 K for cyclobutane, 161 - 200 K for cyclopentane, 160 - 236 K for cyclohexane to ~260 K for cyclooctane.

3.8.7.4.1 Cyclopropane (c-C₃H₆)

From a chemical point of view, cyclopropane is interesting, since although saturated, it possesses some “olefinic character”, owing to the strain exerted on the three-membered carbon ring due to the 60° angle between C-C orbitals. Thus cyclopropane lies between a paraffinic and an olefinic hydrocarbon. Cyclopropane adsorption has been studied on Ni(100), Cu(111), Cu(110), Ru(0001), Ir(110) and Ir(111) surfaces. Vibrational studies by HREELS for several of these substrates indicate that, in contrast to cyclohexane (see above) and cyclopentane (see below), no softening of a C-H mode occurs. This is attributed to the fact that the interbond C-C-C angles of 60° for cyclopropane (and 90° for cyclobutane, see below) would not provide convenient geometric requirements for multiple C-H...metal interactions, in contrast to the C_6 ring and also the C_5 ring in cyclohexane and cyclopentane, respectively [98She]. For cyclopropane it has been suggested that surface bonding occurs via a delocalized $\sigma(CC)$ orbital [82Hof]. Upon heating of molecularly adsorbed cyclopropane molecular desorption is observed with rate maxima in the temperature range between 123 and 150 K. For some substrates more or less exclusively molecular desorption occurs, for others significant to nearly complete dehydrogenation occurs upon heating.

3.8.7.4.2 Cyclobutane (c-C₄H₈)

Cyclobutane adsorption has only been studied on Ru(0001). No softening of C-H vibrations has been observed.

3.8.7.4.3 Cyclopentane (c-C₅H₁₀)

Cyclopentane adsorption has been studied for Cu(111), Cu(110), Rh(111), Ru(0001), Ir(111) and Pt(111) surfaces. Quite general, a softening of C-H vibrations is observed, indicating multiple C-H...metal interactions with the substrate; consequently the C₅ ring is assumed to be approximately parallel to the surface. Upon heating of cyclopentane molecularly adsorbed at low temperatures, molecular desorption is observed with rate maxima in the temperature range between 161 and 200 K. For some substrates more or less exclusively molecular desorption occurs, for others significant to nearly complete dehydrogenation is observed upon heating.

3.8.7.4.4 Cyclooctane (c-C₈H₁₆)

Cyclooctane adsorption has only been studied on Ru(0001). Interestingly, no softening of C-H vibrations are observed, indicating that the majority CH₂ groups do not interact with the substrate. Upon heating, molecular desorption of cyclooctane up to temperatures of ~260 K is observed.

3.8.7.5 Non-saturated cyclic hydrocarbon molecules (other than benzene)

The adsorption and dehydrogenation of non-saturated cyclic hydrocarbons has been investigated for various metal surfaces due to the importance of this class of molecules as intermediates in a manifold of surface reactions with great industrial relevance. In contrast to the saturated cycloalkanes, the interaction of the non-saturated cyclic hydrocarbons is significantly stronger, which is attributed to the interaction of the π -electrons with the substrate. A variety of experimental techniques has been applied. Similar to benzene and in contrast to the cycloalkanes there are also a number of studies for group IV semiconductor surfaces with particular emphasis on cycloaddition chemistry. The results are summarized in Table 4, which contains information on various aspects of the adsorbate substrate bonding (column "comments") and the thermal evolution. For each of the included molecules the data for the different metals are listed according to their position in the periodic table of elements, followed by the data for Si and Ge surfaces.

3.8.7.5.1 Cyclopentene (c-C₅H₈)

Measurements have been performed for cyclopentene adsorbed on Mo(110), Rh(111), Ag(111), Ag(112), Ir(111), Pt(111), Si(100), Si(111) and Ge(100). For Ag(111) and Ag(112) reversible adsorption is observed, indicating a very weak interaction with the substrate. For all other metal surfaces decomposition is observed upon heating. Depending on the substrate and the adsorption temperature, c-C₅H₆, c-C₅H₅, and c-C₅H₃ species have been identified as intermediates. On the Si(100)-(2×1) and Ge(100)-(2×1) surfaces cyclopentene forms di- σ Si/Ge-C bonds, which corresponds to a [2+2] cycloaddition reaction with the surface dimers. For these surfaces no decomposition occurs upon heating. For Si(111)-(7×7) molecular desorption of cyclopentene is observed between 300 and 650 K with some dehydrogenation to c-C₆H₅.

3.8.7.5.2 Cyclopentadiene (c-C₅H₆)

The adsorption of cyclopentadiene has been studied on Rh(111), Ir(111), Pt(111) and on Si(111)-(7×7). For Ir(111) and Pt(111) the formation of c-C₅H₅ and c-C₅H₃ intermediates has been proposed upon heating. On Pt(111) a disproportionation reaction to c-C₅H₅ and c-C₅H₈ occurs at 90 K. In contrast to the metal surfaces studied, exclusively molecular desorption of cyclopentadiene is observed for the reconstructed Si(111)-(7×7) surface.

3.8.7.5.3 Cyclohexene (c-C₆H₁₀)

Cyclohexene adsorption has been investigated for Ni(111), Cu(100), Ru(0001), W(100), Pt(111), Pt(100)-(1×1), Pt(100)-(5×20), Si(100)-(2×1) and Ge(100)-(2×1). On Cu(100) cyclohexene adsorption is completely reversible. For the Ni and Pt surfaces decomposition to benzene (C₆H₆) occurs upon heating, partly accompanied by cyclohexene desorption; for Ru(0001) the formation of ethylene (C₂H₄) is reported. For Si(100)-(2×1) and Ge(100)-(2×1) a di-σ type interaction with the Si dimer dangling bond, i.e. a [2+2] cycloaddition reaction, is proposed. For Si(100)-(2×1) there is evidence for two stable adsorption states, assigned to boat type and twist boat type geometries (Fig. 10).

3.8.7.5.4 Cyclohexadiene (c-C₆H₈)

The adsorption of 1,3-cyclohexadiene and/or 1,4-cyclohexadiene has been studied on Ni(111), W(100), Pt(111), Pt(100)-(1×1), and Si(100)-(2×1) surfaces. For the metal surfaces decomposition to benzene is reported for both conformations. Interestingly, for Pt(111) a partial rearrangement of 1,3- to 1,4- cyclohexadiene is proposed as intermediate reaction step. Upon adsorption of 1,4-cyclohexadiene on Si(100)-(2×1) the formation of di-σ Si-C bonds is reported with the Si dimer structure maintained after adsorption; for 1,3-cyclohexadiene a mixture of [2+2] and [4+2] cycloaddition products is observed.

3.8.7.5.5 Cyclooctadiene (c-C₈H₁₂) and Cyclooctatetraene (c-C₈H₈)

These two molecules have been studied on Pt(111) and Si(100)-(1×2). For the latter the interaction of 1,5-Cyclooctadiene indicates the formation of a [2+2] cycloaddition product.

3.8.7.6 Ethylene Oxide (C₂H₄O)

Ethylene oxide (EO) adsorption and reaction on single crystal metal surfaces has been subject to numerous investigations due the industrial importance of ethylene epoxidation – in particular the silver-catalyzed epoxidation represents the largest volume of any catalytic oxidation reaction on an industrial scale. Detailed studies have been performed only for the single crystal surfaces of Fe, Ni, Cu, Mo, Rh, Pd, Ag and Pt. The key results of these studies are summarized in Table 5, listed according to the position of the metal in the periodic table of elements. The table compiles data on the rate maxima in temperature programmed desorption (T_{max}), the work function change upon adsorption ($\Delta\Phi$), ordered adsorbate structures, decomposition upon heating, orientation and symmetry of EO on the surface, bonding shifts of molecular orbitals (2b₁, 6a₁) upon adsorption and some other information (column “comments”).

Overall, the interaction between EO and metal surfaces is weak. At low temperatures EO is reported to adsorb on all surfaces in molecular form. Upon heating the saturated monolayer, molecular desorption in the temperature range between 120 and 255 K is reported. For clean IB metals, Ag and Cu, no decomposition occurs upon heating. For group VIII metals for some substrates ring opening and decomposition occurs; however no general trends can be derived, since e.g. EO decomposition is observed for Pt(111), but not for Pt(110). The situation for Ni(110) is controversial, since reversible and non-reversible adsorption have been reported in different studies.

There is general agreement that the molecule bonds to the surface via the O-atom. Upon adsorption, a strong decrease in the work function ($\Delta\Phi$) is observed, ranging from –1.1 to –2.8 eV (as an example see Fig. 11), which is attributed to an alignment of the large permanent dipole moment of the molecule (6.3×10^{-30} Cm in the gas phase) with a component perpendicular to the surface (O end down).

The electronic structure has been mainly investigated by ARUPS. These studies show bonding shifts of up to 0.9 eV to higher binding energies of the topmost molecular levels (2b₁, 6a₁) due to a weak bonding interaction to substrate. One should note here that in the ARUPS studies until 1993 it was proposed that ordering of these two molecular levels was reversed from that in the free molecules upon

adsorption. However, theoretical studies performed later on for Ni(110) [95Ulr] and Pd(110) [96She] indicate that the order remains the same as in the gas phase, which appears reasonable, considering the relatively weak interaction of EO with the different surfaces.

The vibrational structure of adsorbed EO was studied by HREELS. For molecularly adsorbed EO only small changes in the vibrational frequencies are observed, which indicates a weak bond of EO to metal surfaces.

Ordered EO structures have been reported only for the (110) planes of Ni, Cu, Ag and Pt; in each case a $c(2 \times 2)$ structure was observed. One should note that EO is very sensitive to radiation damage by electrons or photons.

Information on the orientation of the molecule has been derived from ARUPS and HREELS data based on symmetry selection rules, and from XPD. For Ag(111) and Ag(110) EO is proposed to be oriented perpendicular to the surface, for the other substrates studied, a tilt of the molecular plane is suggested. The symmetry of the adsorption complex is reduced to C_s or C_1 , from C_{2v} for the free molecule.

For several surfaces coadsorption of EO with K or O was investigated. Depending on the substrate, O coadsorption leads to a weakening or a strengthening of the EO surface bond; K coadsorption leads to a reaction between EO and K for high K precoverages.

3.8.7.7 Pyridine (C_6H_5N)

Besides benzene, pyridine adsorbed on single crystal metal surfaces represents the second model system for the interaction of aromatic compounds with metals. Whereas the benzene-metal bond is dominated by the interaction with the π -system, pyridine has the additional option of bonding to the metal via the lone pair electrons of the N atom. Due to structural interests, most of the studies have been directed towards the adsorption geometry of pyridine [92Net]. Generally, five different adsorption structures of pyridine on metal surfaces have been proposed (Fig. 12): (a) perpendicular adsorption via the nitrogen lone pair electrons, (b) flat adsorption of the aromatic ring via the π -electrons, (c) tilted adsorption via the nitrogen lone pair orbitals and the π -electrons and (d, e) edge on adsorption through the N and C(2) atoms with the molecular plane more or less perpendicular to the surfaces – i.e. formation of α -pyridile by breaking the C-H bond.

In Table 6 the corresponding results are presented as an overview. It compiles the rate maxima in temperature programmed desorption (T_{max}), ordered adsorbate structures, the orientation of pyridine on the surface and the thermal evolution. The data are listed beginning with different metals according to their position in the periodic table of elements, followed by data for Si and ZnO surfaces.

Structural information has been obtained for the different substrates using predominantly spectroscopies (ARUPS, HREELS, RAIRS, NEXAFS, ESDIAD) and only in very few cases true structural methods (PED) were applied; one should note that *no* structural analysis by LEED is available, which is most likely due to the small number of ordered pyridine phases and the large unit cells for these few structures. The investigations by one or more different methods show that in most cases the molecules are oriented with the molecular plane parallel to the surface (π -bonded) at low surface coverage, and they undergo a transition to an inclined or perpendicular phase (N-bonded) at higher coverages. The distinction between a perpendicular molecule and a molecule with a small inclination angle with respect to the surface normal is in many cases difficult due to the error bars of between 5 and 20° of the different studies. This could explain the observation that for the same system perpendicular and inclined geometries are reported in different studies. Also, the adsorption geometry (and the nature of the species - see below) sometimes depends on the substrate temperature.

The coverage driven (and sometimes also temperature driven) reorientation seems to be a quite general phenomenon of pyridine adsorption on metal surfaces. The only clear exceptions are Pd(110) and Pd(111) where a parallel orientation is maintained from low coverages up to saturation, and Cu(110) where an upright orientation is observed already at low coverages. Interestingly, for these two surfaces a well defined azimuthal orientation is reported.

For a number of systems the formation of a more or less upright α -pyridile species has been proposed at room temperature – for some systems, e.g. Pt(111) and Ir(111) the situation is controversial, since in studies by different authors either pyridine or α -pyridile have been proposed, both being oriented more or less upright. One should note that the identification of α -pyridile in electronic and vibrational spectroscopies is difficult and not necessarily unique [92Net], and the evolution of H_2 from the surface in TPD is often the most direct hint for the formation of α -pyridile.

3.8.7.8 List of Tables

Table 1.a: Benzene ($c-C_6H_6$): Temperature dependence and adsorption geometry

Table 1.b: Benzene ($c-C_6H_6$): Electronic structure

Table 1.c: Benzene ($c-C_6H_6$): Vibrational properties

Table 2: Cyclohexane ($c-C_6H_{12}$)

Table 3: Saturated hydrocarbons other than Cyclohexane: Cyclopropane ($c-C_3H_6$), Cyclobutane ($c-C_4H_8$), Cyclopentane ($c-C_5H_{10}$), Cyclooctane ($c-C_8H_{16}$)

Table 4: Non-saturated hydrocarbons other than Benzene: Cyclopentene ($c-C_5H_8$), Cyclopentadiene ($c-C_5H_6$), Cyclohexene ($c-C_6H_{10}$), Cyclohexadiene ($c-C_6H_8$), Cyclooctadiene ($c-C_8H_{12}$), Cyclooctatetraene ($c-C_8H_8$)

Table 5: Ethylene Oxide (C_2H_4O)

Table 6: Pyridine (C_5H_5N)

3.8.7.9 Tables for 3.8.7

Table 1a. Temperature dependence and adsorption geometries of adsorbed benzene

Metal surfaces								
surface	superstructure (coverage, ML) exp. temperature	Desorption temperature	adsorption site / symmetry/ orientation	C-C bond length [Å]	shortest C- substrate bond length [Å]	comment	method	Refs.
gas phase				1.399				95CRC
Ag(111)		mol. des. 144→230 K					TPD	90Zho
Ag(111)			C _{3v} , ring parallel to surface.				ARUPS	90Dud
Ag(111)	cluster		fcc hollow site, ring parallel to surface.	1.40		C-H bent upwards by 2°	MO calc.	84And
Au(111)			ring parallel to surface				NEXAFS	98Wei3
Co(10-10)	p(3×1) (0.33 ML) 300 K		asymm. near hollow site model 1: σ(v) parallel to [0001] ring tilted by 20° model 2: σ(d) parallel to [0001] ring tilted by 25°	1.50 - 1.60 1.39 - 1.49	2.20 2.02	model 1 slightly favoured by LEED-IV, strong ring distortions in model 1.	LEED-IV	01Pus
Co / W(110)	saturation at 200 K and 300 K		C _{3v} , ring parallel to surface				A/SRUPS	95Get

surface	superstructure (coverage, ML) exp. temperature	Desorption temperature	adsorption site / symmetry/ orientation	C-C bond length [Å]	shortest C- substrate bond length [Å]	comment	method	Refs.
Cu(110)	3 L at 80 K		4-fold hollow, ring parallel to surface, C-C parallel to close packed rows.	1.41 - 1.42	2.21	H-flip structure: ring planar, C-H bonds bent upwards by 17.6° / 5.3°	DFT(GGA) NEXAFS	98Pet 98Wei3
Cu(110)	low cov.: 0.01 ML ads. at 300 K, expt. at 4 K		long bridge site			no step decoration	STM	98Doe
Cu(110)	0.24 ML, 140 K		ring tilted with respect to surface by more than 20°				ARUPS, HREELS	96Lom
Cu(111)	(few % of 1 ML) 4 K, 77 K					up to 4 rows of ordered molecules along step edges (distance 5.1 Å)	STM	94Str 95Str 98Wei2
Cu(111)		mol. des. 140→240 K	1 st layer: ring parallel, 2 nd layer: ring tilted				NEXAFS, TPD	94Xi
Cu(111)		mol. des. 140→240 K					TPD	98Vel
Cu/ Ni(111)	sat. chemisorbed layer, 100 K	mol. des. 160→230 K no hydr. des.	ring parallel to surface			no azimuthal ordering	ARUPS TPD	99Kos2
Cu/ Ru(0001)	sat. chemisorbed layer, 100 K	mol. des. 150→340 K no hydr. des.	ring parallel to surface, $\sigma(d)$			azimuthal ordering	ARUPS TPD	00Kos1 99Kos1
Fe / W(110)	saturation at 200 K and 300 K		C _{3v} , ring parallel to surface				A/SRUPS	95Get

surface	superstructure (coverage, ML) exp. temperature	Desorption temperature	adsorption site / symmetry/ orientation	C-C bond length [Å]	shortest C- substrate bond length [Å]	comment	method	Refs.
Ir(110)	adsorption at 313 K	mol. des. ~ 425 K hydr. des. 450→800 K					TPD	78Nie
Ir(111)	p(3×3) (0.11 ML) at 300 K	mol. des. ~ 400 K hydr. des. 370→500 K	C _{3v} , ring parallel to surface				ARUPS, ESDIAD, TPD	85Mac 76Nie
Mo(110)	adsorption at 120 K	mol. des. ~ 350 K hydr. des. 350→600 K					TPD	88Liu
Ni(100)	c(4×4) (0.125)		4-fold hollow σ(d) or σ(v)	1.44 / 1.45	2.02	C-H bonds bent upwards (0.16 Å) substrate buckling (0.21 Å)	DFT (GGA)	01Mit
Ni(100)	adsorption at 100 K	mol. des. ~ 150 K (multilayer) ~ 480 K hydr. des. 340→510 K				coadsorption w. C, O, and CO inhibit dissociation.	AES, TPD	87Bla 87Mye
Ni(110)	c(4×2) (0.25)		asymmetric site near 4-fold hollow, σ(d) mirror plane parallel to [110] (troughs), ring tilted by 5°	1.42 / 1.45	2.09	C-H bonds bent upwards (19°/35°) .	DFT (GGA)	01Mit

surface	superstructure (coverage, ML) exp. temperature	Desorption temperature	adsorption site / symmetry/ orientation	C-C bond length [Å]	shortest C- substrate bond length [Å]	comment	method	Refs.
Ni(110)	0.1 ML annealed to 200 K, expt. at 60-65 K		4-fold hollow, $\sigma(d)$ mirror plane parallel to [110] (troughs), ring parallel	1.45	1.81	molecular plane parallel to surface	PhD	00Kan
Ni(110)	0.01 ML ads. at 300 K, expt. at 4 K		4-fold hollow site			no step decoration	STM	98Doe
Ni(110)	c(2×4) (0.2 ML) 300 K	mol. des. up to 460 K, hydr. des. up to 435 K	atop or short bridge site, ring parallel to surface		2.24		HREELS MO calculations	92Hun
Ni(110)	c(2×4) (0.2 ML)		C_{2v} ring parallel to surface				ARUPS NEXAFS	91Ram
Ni(110)	diff. coverages, adsorption at 100 K	mol. des. 360, 321, 460 K, hydr. des. up to 390 K	C_{2v} in dilute layer C_1 in saturated layer				ARUPS TPD	91Hub2
Ni(111)			bridge, $\sigma(v)$ or fcc, $\sigma(d)$	1.43 / 1.45 1.44 / 1.45	2.05 2.07	C-H bonds bent upwards, substrate buckling (0.18 / 0.22 Å)	DFT (GGA)	01Mit
Ni(111)			bridge, $\sigma(v)$ or hcp hollow, $\sigma(d)$	1.41 / 1.44 1.42 / 1.44	2.02 2.02	adsorption on bridge sites slightly preferred over hcp, C-H bonds bent upwards by 19-28°, substrate buckling (0.21 / 0.25 Å)	DFT (GGA)	01Yam3

surface	superstructure (coverage, ML) exp. temperature	Desorption temperature	adsorption site / symmetry/ orientation	C-C bond length [Å]	shortest C- substrate bond length [Å]	comment	method	Refs.
Ni(111)	($\sqrt{7}\times\sqrt{7}$)R19.1° (0.14 ML), ads. at 245 K expt. at 160 K		hcp hollow site, $\sigma(d)$	1.43 / 1.55	2.02	buckling in top-most Ni layer (0.14 Å)	LEED-IV	96Hel
Ni(111)	($\sqrt{7}\times\sqrt{7}$)R19.1° (0.14 ML), ads. at 200 K expt. at 300 K		hcp hollow site, $\sigma(d)$	1.40 / 1.46	1.91 (vert.)	substrate buckling <0.10 Å	PhD	96Sch
Ni(111)	disordered phase (0.10 ML), ads. at 300 K expt. at 120 K		bridge, $\sigma(v)$	1.40 / 1.44	1.92 (vert.)	substrate buckling <0.08 Å	PhD	96Sch
Ni(111)	diff.coverages up to 0.14 ML, disordered phase and ($\sqrt{7}\times\sqrt{7}$)R19.1°	mol. des. 154, 136, 146 K (multilayer), 270→460 K hydr. des. 380→650 K	$\sigma(v)$ at low coverage, $\sigma(d)$ in saturated layer			reorientation due to lateral interaction	ARUPS TPD, LEED	91Hub1 89Ste 87Mye
Ni(111)	low coverage		fcc hollow site, $\sigma(d)$	1.43 (2 % ex- pansion)	2.2 (vert.)	C-H bonds bent upwards by 8.5°	CI	91Jin
Ni(111)			hcp hollow site, $\sigma(d)$	1.40	2.0	C-H bonds bent upwards by 8°	MO cluster calc.	84And
Ni(111)	($2\sqrt{3}\times 2\sqrt{3}$)R30° (0.08 ML) coadsorbed w. NO (0.10 ML), 140 K		bridge site, C_{2v} , $\sigma(v)$	1.40 / 1.44	2.02	NO on hcp and fcc sites. buckling of ring (0.13 Å) and 1 st Ni layer (0.08 Å)	PhD	01Bao

surface	superstructure (coverage, ML) exp. temperature	Desorption temperature	adsorption site / symmetry/ orientation	C-C bond length [Å]	shortest C- substrate bond length [Å]	comment	method	Refs.
Ni(111)	(2√3×2√3)R30° (0.08 ML) coads. w. NO, CO, O (0.166 ML) 95 K		σ(v)				ARUPS, LEED	91Hub1 91Zeb1
Ni(111)	p(3×3) (0.11 ML) coadsorbed w. NO (0.22 ML) 95 K		σ(d)			reorientation due to lateral interaction	ARUPS, LEED	91Hub1 91Zeb1
Ni(111)	coadsorbed w. NO 4 ordered structures (0.04 - 0.125 ML)	mol. des. 325→440 K hydr. des. 400→500 K					TPD	91Zeb2
Ni/ Cu(111) (adlayer)	(0.14 ML) 80 K	no mol. des. hydr. des 350→450 K	σ(v)			adlayer (Ni/Cu) -to- sublayer (Cu/Ni/Cu) transition between 300 and 600 K	ARUPS TPD	99Kos1
Os(0001)	(√7×√7)R19.1° 200-290 K	hydr. des 290→830 K	σ(d), ring parallel to surface, C _{3v}				ARUPS TPD	89Gra
Pd(110)	c(4×2)		4-fold hollow site, σ(v)-plane rotated by 11° w/r to [001], C ₂	1.42 - 1.44	1.81	C-H bonds bent upwards (17 - 23°), STM simulations	DFT	00Fav
Pd(110)	diff. coverages at 100 K		4-fold hollow site			diffusion above 220 K (barrier 0.57 eV)	STM	96Yos

surface	superstructure (coverage, ML) exp. temperature	Desorption temperature	adsorption site / symmetry/ orientation	C-C bond length [Å]	shortest C- substrate bond length [Å]	comment	method	Refs.
Pd(110)	c(4×2)	mol. des. 410 K hydr. des >390 K	ring tilted by 10- 20° into troughs, C _s				ARUPS TPD	88Net4
Pd(111)	p(3×3) coads. w. CO (0.11 ML benz, 0.22 ML CO)		fcc hollow site, σ(d)	1.40 / 1.46	2.39	2 CO per unit cell on fcc sites	LEED-IV	88Oht1
Pd(111)		mol. des. 350→600 K					TPD	85Wad
Pt(110)- (1×2)	p(4×2) (0.25 ML) anneal to 275 K expt. at 95 K	mol. des. 180→440 K hydr. des 300→700 K	molecular plane tilted by 30° in [001], C-H bonds parallel to [1-10]				ARUPS NEXAFS TPD	98Zeb
Pt(111)	saturated chemisorbed layer	mol. des. 250→500 K hydr. des 250→750 K					TPD	96Lut2
Pt(111)	0.001 ML, 4 K		3 different adsorption sites: hcp, fcc, top σ(d)				STM STM- simulations	94Sau 96Sau 93Wei3
Pt(111)	saturation at 170 K (ca. 0.16 ML)		bridge site, σ(d), C _{2v}	1.45 / 1.63	2.02	butterfly-like ring distortion	DLEED	91Wan
Pt(111)	saturation at room temp.		σ(d), C _{3v} , ring parallel to surface				ARUPS	87Som1 87Som2

surface	superstructure (coverage, ML) exp. temperature	Desorption temperature	adsorption site / symmetry/ orientation	C-C bond length [Å]	shortest C- substrate bond length [Å]	comment	method	Refs.
Pt(111)		mol. des. 370→570 K hydr. des 500→800 K					TPD	85Abo
Pt(111)			hcp hollow site	1.36 / 1.44	2.0	C-H bent upwards, Kekule-type distortion	MO cluster calculation	84And
Pt(111)	c(2√3×4)rect coads. w. CO (0.13 ML benz, 0.25 ML CO) 140 K		bridge site, ring parallel to surface C _{2v}	1.65/ 1.76	2.25	planar ring (within 0.05 Å) 2 benzene and 4 CO (on bridge sites) per unit cell	LEED-IV	87Ogl 87Van 88Som
Re(0001)							LEED, AES, TPD	82Tat
Rh(111)	diff. coverages at 300 K					no ordering even at satura- tion, only molecules imaged at the upper step edges	STM	97Yoo
Rh(111)	(√19×√19)R23° – (0.159 ML) 20 L at 360 K					high coverage LEED structure	LEED	91Neu
Rh(111)	c(2√3×4)rect (0.13 ML) 4 – 5L at 300 K		σ(d), ring par- allel to surface C _{6v} adsorbate symmetry				ARUPS	87Net2
Rh(111)			3-fold hollow site, σ(d), ring par-allel to surface	1.50 / 1.64	2.06	C-H bonds bent upwards	EHT cluster calc.	86Gar
Rh(111)	adsorption at 290 K	mol. des. 395 K hydr. des 450→700 K					TPD	86Koe 84Koe 83Lin

surface	superstructure (coverage, ML) exp. temperature	Desorption temperature	adsorption site / symmetry/ orientation	C-C bond length [Å]	shortest C- substrate bond length [Å]	comment	method	Refs.
Rh(111)	coads w. CO diff coverages at 300 K, p(3×3) (0.11 ML benz, 0.22 ML CO)					ordering induced through CO	STM	97Yoo 88Oht2
Rh(111)	c(2√3×4)rect coads w. CO (0.13 ML benz, 0.13 ML CO)		hcp hollow site, σ(d), ring par- allel to surface	1.33 / 1.81	2.35	1 CO (on hcp sites) per unit cell	LEED-IV	86Van 88Som
Rh(111)	p(3×3) coads w. CO (0.11 ML benz, 0.22 ML CO)		hcp hollow site, σ(d), ring parallel to surface	1.46 / 1.58	2.30	2 CO (on hcp sites) per unit cell	LEED-IV	87Lin 87Van 88Som
Rh(111)	p(3×3) coads w. CO (0.11 ML benz, 0.22 ML CO)	mol. des. 350→450 K hydr. des 450→550 K CO. des 350→500 K	ring parallel to surface C _{6v} symmetry			molecules essentially undistorted	ARUPS TPD	86Ber
Ru(0001)	(√7×√7)R19.1° (0.143 ML) 200 K		hcp site, σ(v), ring parallel to surface	1.39 / 1.47	2.04	ring buckling (0.07 Å), substrate buckling (<0.06 Å) C-H bond bent upwards by 8.9 / 23.5°	LEED-IV	01Hel
Ru(0001)	(√7×√7)R19.1° (0.143 ML) 200 K		hcp site, σ(v), ring parallel to surface	1.42 / 1.43	2.10	ring buckling (0.06 Å), substrate buckling (<0.06 Å) C-H bond bent upwards by 13.9 / 21.5°	DFT	01Hel

surface	superstructure (coverage, ML) exp. temperature	Desorption temperature	adsorption site / symmetry/ orientation	C-C bond length [Å]	shortest C- substrate bond length [Å]	comment	method	Refs.
Ru(0001)	($\sqrt{7}\times\sqrt{7}$)R19.1° (0.143 ML) 200 K		hcp site, $\sigma(v)$, ring par- allel to surface	1.45 / 1.48	2.11	ring buckling (0.08 Å), substrate buckling (<0.05 Å)	LEED-IV	01Bra 95Ste
Ru(0001)	c($2\sqrt{3}\times 4$)rect (0.125 ML) 200 K		hcp site, $\sigma(v)$, ring par- allel to surface	1.41 / 1.43 / 1.53	2.11	ring buckling (0.10 Å), substrate buckling (<0.07 Å)	LEED-IV	01Bra
Ru(0001)	($2\sqrt{3}\times 2\sqrt{3}$)R30° (0.083 ML) 200 K		hcp site, $\sigma(v)$, ring par- allel to surface	1.41 / 1.46	2.11	ring buckling (0.08 Å), substrate buckling (<0.05 Å)	LEED-IV	01Bra
Ru(0001)	saturation at 230 K					out of plane bending of C- H bonds	NEXAFS	98Wei1
Ru(0001)	adsorption at 120 K	mol. des. 164, 142, 152 K (multilayer) 360 K hydr. des 400→720 K					TPD	89Jak 88Jak
Ru(0001)		multilayer des. 160, 130, 145 K					TPD	87Pol
Ru(0001)	($\sqrt{13}\times\sqrt{13}$)R13.9° coads w. CO (0.08 ML benz, 0.30 ML CO) ads. at 120 K	mol. des. 389 K hydr. des 390→700 K CO des. 380→500 K					LEED TPD workfunction	90Jak2

surface	superstructure (coverage, ML) exp. temperature	Desorption temperature	adsorption site / symmetry/ orientation	C-C bond length [Å]	shortest C- substrate bond length [Å]	comment	method	Refs.
Ru(0001)	p(3×3) coads. w. O (C ₆ D ₆ + 2O) (0.11 ML benz, 0.22 ML O) expt. at 90 K		hcp site, σ(v), ring parallel to surface	1.38 / 1.40	2.22	substrate buckling (<0.04 Å) 2 O atoms (on hcp sites) per unit cell	LEED-IV	97Sti
Ru(0001)	p(3×3) coads w. O < 0.22 ML O ads. at 120 K	mol. des. 320→470 K hydr. des 320→700 K				ratio oxygen/benz < 0.74	LEED TPD workfunction	90Jak1
Ru(0001)	p(3×3) coads. w. NO (C ₆ D ₆ + 2NO) (0.11 ML benz, 0.22 ML NO) expt. at 90 K		hcp site, ring rotated by 20° from σ(v), parallel to surface	1.32 / 1.44	2.23	substrate buckling (<0.02) 2 NO (on hcp sites) per unit cell.	LEED-IV	97Sti
W(110)	coads. w. O (0.55 ML O)	mol. des. 145K (multilayer) 165→220 K					TPD	96Nah
W(110)	coads. w. H (1 ML H)	mol. des. 130→170 K					TPD	99Whi
W(110)	coads. with CO (0.7 ML CO)	mol. des. 125→150 K					TPD	99Whi

Semiconductor / insulator surfaces								
surface	superstructure (coverage, ML) exp. temperature	Desorption temperature	adsorption site / symmetry/ orientation	C-C bond length [Å]	shortest C- substrate bond length [Å]	comment	method	Refs.
Al ₂ O ₃ / Mo(110)	adsorption at 90 K	mol. des. 150→190 K				3 desorption states	TPD	96Str
C(0001) (graphite)	($\sqrt{7}\times\sqrt{7}$)R19.1° (0.14 ML) at 135 K						LEED	86Bar
MgO(100) / Mo(100)	adsorption at 90 K	mol. des. 150→210 K				3 desorption states	TPD	96Str
Ge(100)- (2×1)	adsorption at 90 K	mol. des. 160→270 K (chemis.) peaks at 183, 202, 234, 252 K	C _{2v} symm			di-sigma bonded 1,4-cyclo-hexadiene like molecule	ARUPS TPD	01Fin
Ge / Si(100)- (2×1)	adsorption at 90 K	mol. des. 220→460 K (chemis), peaks at 311, 369, 422 K	C _{2v} symm			di-sigma bonded 1,4-cyclo-hexadiene like molecule (as on Ge(100))	TPD	01Fin
Si(100) – (2×1)			single dimer (metastable) and tight bridge (stable)	1.47/1.50 1.47-1.57, 1.35	1.89/1.98 1.87-2.01		DFT, STM simulation	01Hof
Si(100) – (2×1)			tilted bridge	1.49-1.59 1.34-1.36		tetra-sigma bonded (2 double bonds)	DFT	00Sil

surface	superstructure (coverage, ML) exp. temperature	Desorption temperature	adsorption site / symmetry/ orientation	C-C bond length [Å]	shortest C- substrate bond length [Å]	comment	method	Refs.
Si(100) – (2×1)	0.25 ML 30 K, 90 K	mol. des. 150→210 K (physisorbed) 432, 501 K (chemis.)	C _{2v} symm. “butterfly” structure, flat-lying molecule	1.35, 1.51	1.97	di-sigma bonded 1,4-cyclo-hexadiene like molecule	ARUPS HREELS LCGTO-DF	00Sta 98Bir 98Gok
Si(100) – (2×1)	diff. coverages at 300 K		on top of dimer rows			bonding to Si-Si dimer dangling bonds, saturation at 0.25 ML	STM	98Sel
Si(100) – (2×1)	saturation at 300 K		on top of dimer rows (metastable) two different bridging sites (stable)			dimer – bridge conversion activated (0.94 eV), energy difference > 0.14 eV	STM RAIRS	98Lop1 98Lop2 98Bor
Si(100) – (2×1)	100 K		3 ads. sites: -1,4 single dimer (ontop of dimer rows) - tight bridge - twisted bridge	1.47-1.49, 1.35 1.47-1.53, 1.35	1.86-1.89 1.87-1.89		STM MO cluster calc.	98Wol
Si(100) – (2×1)		mol. des. 450→505 K hydr. des. 780 K					TPD	98Kon
Si(100) – (2×1)			pedestal site (bridging)	1.45, 1.51	1.98	one molecule interacts with 2 Si dimers	cluster PM3	95Jeo
Si(100) – (2×1)			pedestal site	1.33, 1.45-1.47	1.83	tilt by 24° w/r to surface	SLAB- MINDO	93Cra

surface	superstructure (coverage, ML) exp. temperature	Desorption temperature	adsorption site / symmetry/ orientation	C-C bond length [Å]	shortest C- substrate bond length [Å]	comment	method	Refs.
Si(100) – (2×1)	adsorption at 90 K and 300 K	mol. des. 145, 153 K (physisorbed) 460, 505 K (chemis.) no hydr. des.	C _{2v} symm. di-sigma bonded, “butterfly”				HREELS TPD	91Tag1
Si(111) – (7×7)	adsorption at 110 K	mol. des. 130→160 K (physisorbed) 342→363 K (chemis.) no hydr. des.				di-sigma bonded 1,4-cyclo-hexadiene like molecule, desorption energy of physis. layer 92, 96 kJ/mol	HREELS TPD	99Cao
Si(111) – (7×7)	adsorption at 90 K	mol. des. 140→160 K (physisorbed) ~320K (chemis.) no hydr. des.					HREELS TPD	91Tag2
Si(111)	adsorption to saturation at 300 K	mol. des. 330→450 K (peak at 350 K)				high temperature mol. des. states due to defect sites	TPD	91Mac
ZnO(1010)	c(2×2) (0.5 ML) c(4×3) (multilayers) ads. at 113 K	mol. des. 200→260 K				oblique position of low symmetry, $E_{des} = 73\text{-}56$ kJ/mol	LEED ARUPS TPD	81Pos

Table 1b. Electronic Structure of adsorbed BenzeneBinding energies given in eV with respect to Fermi level E_F unless indicated otherwise.

Some of the values have been extracted graphically from diagrams in the relevant publications.

Metal surfaces																	
surface	superstructure (coverage, ML) expt. temp.	C1s binding energy (XPS)	unocc. states, NEXAFS resonances	$1e_{2u}$ (π^*)	$1e_{1g}$ (π)	$2e_{2g}$ (σ)	$1a_{2u}$ (π)	$2e_{1u}$ (σ)	$1b_{2u}$ (σ)	$1b_{1u}$ (σ)	$2a_{1g}$ (σ)	$1e_{2g}$ (σ)	$1e_{1u}$ (σ)	$1a_{1g}$ (σ)	comments	method	Refs.
	gas phase			(4.2)	9.2	11.5	12.3	13.9	14.8	15.5	16.9	19.2	22.5	25.9		with resp. to E_{vac}	87Car
(not specified)	multilayer, 120 K		285.2														98Wei1
(Mo(100))	multilayer, 100 K				9.0	11.8	11.8	13.7	13.7	15.1	16.4					MIES with resp. to E_{vac}	98Gun
(Mo(100))	multilayer, 100 K				8.8	11.4	11.4	14.0	14.0		16.4					UPS (HeI) with resp. to E_{vac}	98Gun
(Fe/W(110))	multilayer, 80 K				8.3	10.5	11.1	12.9	13.5	14.2	15.8					ARUPS	95Get
Ag(110)	$\Theta_r = 0.8$, 90 K		285.5 π^* e_{2u} 289.1 π^* b_{2g} 294.1 σ^* (C-C) 301.0 σ^* (C-C)												maximum ring tilt 10 - 15°	NEXAFS	90Liu
Ag(111)	p(3×3) 0.11 ML at 120 K				8.8	11.2		13.2	13.9	14.7	16.0	18.0	21.8	25.1	ring parallel to surface	ARUPS with resp. to E_{vac}	90Dud
Ag(111)	0.4 L 140 K		4.95 ($^3E_{1u} \leftarrow ^1A_{1g}$) 6.35 ($^1B_{1u} \leftarrow ^1A_{1g}$) 7.0 ($^1E_{1u} \leftarrow ^1A_{1g}$)												C_{3v} $\sigma(d)$ symmetry, ring parallel to surface	HREELS	81Avo1
Au(110)	2 ± 1 ML 80 K			e_{2u} 4.8, b_{2g} 8.3 above E_F												IPES	86Fra
Au(111)	120 K		285.1 π^* e_{2u}													NEXAFS	98Wei1
Co/W(110)	saturation at 200 K				4.7	6.1	7.8	8.1	8.7						ring parallel to surface	A/SRUPS	95Get
Co/W(110)	saturation at 300 K				4.5	5.9	7.6	7.9	8.6						ring parallel to surface	A/SRUPS	95Get

surface	superstructure (coverage, ML) expt. temp.	C1s binding energy (XPS)	unocc. states, NEXAFS resonances	1e _{2u} (π^*)	1e _{1g} (π)	2e _{2g} (σ)	1a _{2u} (π)	2e _{1u} (σ)	1b _{2u} (σ)	1b _{1u} (σ)	2a _{1g} (σ)	1e _{2g} (σ)	1e _{1u} (σ)	1a _{1g} (σ)	comments	method	Refs.
Cu(110)	3 L at 80 K	284.9	284.9 π^* e _{2u}	0 - 0.4	4.4	7.1	7.9	9.3			11.7	13.7	17.5		planar ring parallel top surface, H bent upwards	XES, XPS, NEXAFS DFT	00Nil 98Pet 98Wei3 97Nil
Cu(110)	saturation (0.22 ML) at 160 K				4.6	7.1	8.3 – 10.3				11.8				tilt of ring greater than 20°	ARUPS	96Lom
Cu(111)	$\Theta_r = 0.5$, 95 K														electronic states at –0.23 (bon- ding) and +1.0 eV (antibonding)	2PPE	00Mun 98Mun
Cu(111)	$\Theta_r = 0.6$, 95 K			0.3											electronic states at –0.3 (bon- ding benzene - copper) and +3.8 eV (image potential state)	2PPE	99Mun1
Cu(111)	90 K			0 - 0.25											dispersion of the hybridization state, $m^* = 0.9$ m_e	ARPES (Laser)	99Mun2
Cu(111)					5.4	6.4	7.0	8.4	9.2	10.1	11.5	13.6			no azimuthal orientation, ring parallel to surface	ARUPS	00Kos2
Cu(111)	$\Theta_r = 0.1 - 3$, 85 K, 120 K		image states at 3.30 / 3.45 eV above E_F												image states at +3.30, +3.45 eV above E_F , attributed to 1 st and 2 nd layer	2PPE	98Vel
Cu(111)	monolayer, 90 K		284.8 π^* e _{2u} 288.5 π^* b _{2g} 293.5 σ^* C-C 301.5 σ^* C-C												1 st layer parallel to surface	NEXAFS	94Xi
Cu(111)	multilayer, 90 K		285.0 π^* e _{2u} 287.2 σ^* C-H 288.8 π^* b _{2g} 293.3 σ^* C-C 300.3 σ^* C-C												1 st layer parallel, 2 nd layer tilted	NEXAFS	94Xi

surface	superstructure (coverage, ML) expt. temp.	C1s binding energy (XPS)	unocc. states, NEXAFS resonances	1e _{2u} (π^*)	1e _{1g} (π)	2e _{2g} (σ)	1a _{2u} (π)	2e _{1u} (σ)	1b _{2u} (σ)	1b _{1u} (σ)	2a _{1g} (σ)	1e _{2g} (σ)	1e _{1u} (σ)	1a _{1g} (σ)	comments	method	Refs.
Cu(111)	2 \pm 1 ML 110 K			e _{2u} 4.6 above E_F												IPES	86Fra
1 ML Cu/ Ni(111)	0.08 ML, 80 K				4.0	6.1	6.8	8.5	9.0	9.8	11.3	13.4			ring parallel to surface, no azimuthal ordering	ARUPS	99Kos2
1 ML Cu/ Ni(111)	0.13 ML, 80 K				3.9	6.1	6.6	8.5	9.0	9.8	11.3	13.4			ring parallel to surface, no azi- muthal ordering, small tilt at high coverage	ARUPS	99Kos2
1 ML Cu/ 1 ML Ni/ Cu(111) (sublayer)	none (0.10 ML) 80 K				5.4	6.4	7.0	8.4	9.2	10.1	11.5	13.6			no azimuthal orientation, ring parallel to surface, binding energies like Cu(111)	ARUPS	99Kos1
1 ML Cu/ Ru(0001)	0.14 ML, 80 K				5.2	6.5	7.9	8.8	9.4	10.3	11.7	13.8			ring parallel to surface, σ (d) orientation	ARUPS	00Kos1 99Kos1
Fe / W(110)	saturation at 200 K				4.8	6.2	7.8	8.1	8.7	9.9					ring parallel to surface	A/SRUPS	95Get
Fe / W(110)	saturation at 300 K				4.6	6.0	7.6	8.0	8.4						ring parallel to surface	A/SRUPS	95Get
Ir(111)	p(3 \times 3) (0.11 ML) 30 L at 300 K				5	6-7		7.5 - 9.2			11.3				C _{3v} σ (d) symmetry, ring parallel to surface	ARUPS	85Mac
Ir(111)	20 - 30 L at 300 K		7 $\pi^* \leftarrow \pi$ (weak) 4 - 5 $\pi^* \leftarrow d$												4-5 eV is charge transfer loss, ring parallel to surface	ELS	80Net
Mo(110)	chemisorbed layer (multi- layer anneal- ed to 200 K)	284.1	286.7 π^* 293.0 σ^* 299.2 σ^*												ring parallel to surface	XPS, NEXAFS	88Liu 90Liu

surface	superstructure (coverage, ML) expt. temp.	C1s binding energy (XPS)	unocc. states, NEXAFS resonances	1e _{2u} (π^*)	1e _{1g} (π)	2e _{2g} (σ)	1a _{2u} (π)	2e _{1u} (σ)	1b _{2u} (σ)	1b _{1u} (σ)	2a _{1g} (σ)	1e _{2g} (σ)	1e _{1u} (σ)	1a _{1g} (σ)	comments	method	Refs.
Ni(100)	c(4×4) (0.125 ML) 200 K	284.1	285.2 π^* e _{2u}	1.8	5.1	6.3	7.8	8.7	8.7	8.7	11.2	13.5	17.0		parallel to surface	XES, XPS, NEXAFS	98Wei3 97Nil
Ni(100)	c(4×4) (0.125 ML)			1.7	4.4	4.8 5.1	6.7	6.9	7.5	7.9	9.3	11.5	15.0	17.6	hollow site	DFT (GGA)	01Mit
Ni(110)	c(4×2) (0.125 ML)			1.2/ 2.5	4.5	5.1	7.1	6.6	7.6	8.2	9.3	11.6	15.1	17.7	asymm. hollow site	DFT (GGA)	01Mit
Ni(110)															$\pi - \pi^*$ charge transfer satellite at -10 eV	ADC(3)	97Ohn
Ni(110)	0.10 ML (dilute), 95 K				4.5 4.7	5.8 6.4	7.3	7.8 8.1	8.7	9.7	10.9	13.2			C _{2v} symmtry	ARUPS	91Hub2
Ni(110)	c(4×2) (0.14 ML) 95 K				4.3 4.6	5.5 6.1	7.3	7.5 7.9	8.7	9.8	11.3	13.2			C ₁ symmtry, 0.9 eV band dispersion of 3a _{1g}	ARUPS	91Hub2
Ni(110)		284.5														XPS	92Hun
Ni(110)	c(4×2) (0.125 ML) 170-270 K		285.1 π^* e _{2u} 287.9 / 289.3 π^* b _{2g}		4.3 4.6	5.8 6.4	7.6	8.2 8.4	8.6	9.7	10.6 -11.3	13.0 13.6			2a _{1g} band dispersion of 0.75 eV, C _{2v} symmetry, ring parallel to surface ($\pm 20^\circ$)	ARUPS, NEXAFS	91Ram
Ni(110)	coads. w. CO 0.125 ML ben, 0.125 ML CO 95 K				4.2 4.5	5.4 6.0	7.1	7.8 8.0	8.5	9.5	10.8	13.0			C _{2v} symmetry	ARUPS	91Hub2
Ni(111)	disordered (0.06ML) 95K				4.8	5.8 6.4		8.3	8.5		11.1	13.3			$\sigma(v)$ orientation, ring parallel to surface	ARUPS	89Hub
Ni(111)	disordered (0.105 ML) 95 K				4.9	5.9 6.5	7.8	8.2	8.6		11.1	13.3			$\sigma(v)$ orientation, ring parallel to surface	ARUPS	89Hub
Ni(111)	($\sqrt{7} \times \sqrt{7}$)R19.1° (0.143 ML)			2.1 2.3	4.5 4.7	4.9 5.4 5.3	7.0 7.1	7.0 7.3	7.6 7.8	8.1 8.1	9.6 9.7	11.8 11.8	15.1 15.3	17.8 18.0	bridge site fcc hollow site	DFT (GGA)	01Mit

surface	superstructure (coverage, ML) expt. temp.	C1s binding energy (XPS)	unocc. states, NEXAFS resonances	1e _{2u} (π^*)	1e _{1g} (π)	2e _{2g} (σ)	1a _{2u} (π)	2e _{1u} (σ)	1b _{2u} (σ)	1b _{1u} (σ)	2a _{1g} (σ)	1e _{2g} (σ)	1e _{1u} (σ)	1a _{1g} (σ)	comments	method	Refs.
Ni(111)	($\sqrt{7}\times\sqrt{7}$)R19.1° (0.143 ML) 95 K				5.1	6.2 6.8	8.1	8.3	8.7	10.1	11.3	13.3			σ (d) orientation, ring parallel to surface	ARUPS	89Hub
Ni(111)	condensed layer at 120 K		285.2 π^* e _{2u} 289.5 π^* b _{2g} 294 σ^*												values extracted from diagram	NEXAFS	91Ami
Ni(111)	chemisorbed layer				10.5	11.7	12.1	14.2	15.0	15.4	17.0	19.0			w/r to E_{vac}	UPS	74Dem
Ni(111)	coadsorbed w. O, 95 K: ($2\sqrt{3}\times 2\sqrt{3}$)R30° (0.08 ML ben, 0.17 ML O)				5.0	5.8 6.3	7.6	8.1			10.9	13.1			σ (v) orientation, ring parallel to surface	ARUPS	91Hub1 91Hub3
Ni(111)	coadsorbed w. CO, 95 K: ($2\sqrt{3}\times 2\sqrt{3}$)R30° (0.08 ML ben, 0.17 ML CO)		284.0		4.7	5.7 6.4		8.1	8.3		11.0	13.2			σ (v) orientation, ring parallel to surface	ARUPS	98Hel 91Hub3 90Ste 89Hub
Ni(111)	coadsorbed w. NO, 95 K: ($2\sqrt{3}\times 2\sqrt{3}$)R30° (0.08 ML ben, 0.17 ML NO)				4.7	5.7 6.2		8.1			10.9	13.1			σ (v) orientation, ring parallel to surface		91Hub1 91Hub3
Ni(111)	coadsorbed w. NO, 95 K: p(3×3) (0.11 ML ben, 0.22 ML NO)				4.8	5.5 6.1		8.0		9.5	10.8	13.0			σ (d) orientation, ring parallel to surface	ARUPS	91Hub1 91Hub3 90Ste
1 ML Ni/ Cu(111) (adlayer)	0.14 ML 80 K				5.2	6.2 6.7	8.0	8.4	8.8	10.1	11.4	13.4			σ (v) orientation, ring parallel to surface	ARUPS	99Kos1
Os(0001)	($\sqrt{7}\times\sqrt{7}$)R19° (0.14 ML) 15 L at 200K				4.5 - 5.5		6.5 - 6.8	7.8 - 8.7			11.1	13.1			C _{3v} σ (d) symmetry, ring parallel to sur- face C-H derived band	ARUPS	90Gra1 90Gra2 87Net1

surface	superstructure (coverage, ML) expt. temp.	C1s binding energy (XPS)	unocc. states, NEXAFS resonances	1e _{2u} (π^*)	1e _{1g} (π)	2e _{2g} (σ)	1a _{2u} (π)	2e _{1u} (σ)	1b _{2u} (σ)	1b _{1u} (σ)	2a _{1g} (σ)	1e _{2g} (σ)	1e _{1u} (σ)	1a _{1g} (σ)	comments	method	Refs.
Pd(110)	c(2×4) 320 K														antibonding state (1e _{1g} and Pd 4d) near E_F	STM, MO calculations, MAES, UPS	97Yos
Pd(110)	c(2×4) prep. at 300 K, expt. at 80 K				4.5	5.9	6.9	8.0	8.8	9.4	10.9	13.0			molecules tilted by 10 - 20°	ARUPS	88Net4
Pd(111)	saturation at 300 K, multilayer at 140 K														circular dichro- ism of all orbi- tals; highest asymm. in 2a _{1g} and 1e _{1g}	UPS	91Wes
Pd(111)	saturation at 300 K (3 - 5 L)				5.0	6 - 6.5	8.0 - 8.6				11.3	13.4			C _{6v} , ring parallel to surface,	ARUPS, ELS	83Net1
Pt(100)	saturation at 300 K,				4.3		7.5	8.4			10.7				ring parallel to surface, clean surface reconstruction is lifted	ARUPS	82Ric
Pt(100)	saturation at 333 K (0.22 ML)				4.2	6.0	8.2				10.7	13.2			no band assignment made in the orig. publication	UPS	77Fis
Pt(110)	p(4×2) (0.25ML), anneal to 275 K expt at 95 K		285.0 π^* e _{2u} 288.8 π^* b _{2g} 290.2 σ^* C-H 293.4 σ^* C-C 299/ 304 shape resonance		4.3	6.2	8.5			10.0	11.1	13.5			molecules tilted by 27 / 30°	ARUPS, NEXAFS	98Zeb
Pt(111)	saturation at 230 K		284.2 π^* e _{2u} 285.1 π^* e _{2u}													NEXAFS	98Wei1
Pt(111)	saturation at 300 K, expt. at 95 K														negative ion resonance due to b _{2g} (π^*) at 2.1 eV	HREELS	96Dip
Pt(111)	saturation at 300 K				5.0	6.0						13.3					87Som1 87Som2

surface	superstructure (coverage, ML) expt. temp.	C1s binding energy (XPS)	unocc. states, NEXAFS resonances	1e _{2u} (π^*)	1e _{1g} (π)	2e _{2g} (σ)	1a _{2u} (π)	2e _{1u} (σ)	1b _{2u} (σ)	1b _{1u} (σ)	2a _{1g} (σ)	1e _{2g} (σ)	1e _{1u} (σ)	1a _{1g} (σ)	comments	method	Refs.
Pt(111)	saturation at 200 K ("monolayer")	284.4	286.0 π^* e _{2u} 293.7 σ^* e _{1u} 299.9 σ^* e _{2g} +a _{2g}												ring parallel to surface	NEXAFS	85Hor
Pt(111)	multilayer ("solid") at 100 K	284.9	285.0 π^* e _{2u} 288.9 π^* b _{2g} 293.3 σ^* e _{1u} 300.1 σ^* e _{2g} +a _{2g}													NEXAFS	85Hor
Rh(111)	saturation at 230 K		284.8 π^* e _{2u} 285.8 π^* e _{2u}												out of plane bending of C-H bonds	NEXAFS	98Wei1
Rh(111)	($\sqrt{19} \times \sqrt{19}$) R23.4° – 3C ₆ H ₆														2a _{1g} derived band width 0.5eV	ARUPS	91Neu
Rh(111)	c(2 $\sqrt{3} \times 4$)rect (0.13 ML) 4-5 L at 300K				4.9	5.8 - 6.3	7 - 9				11.0	13.1			C _{6v} adsorbate symmetry, σ (d) orientation ring parallel to surface	ARUPS	87Net2 85Neu
Rh(111)	p(3 \times 3) coads. w. CO at 300 K (0.11 ML benz., 0.22 ML CO)				4.9	5.6 - 6.1	7 - 9				11.2	12.9			C _{6v} adsorbate symmetry, ring parallel to surface	ARUPS	86Ber
Ru(0001)	p($\sqrt{7} \times \sqrt{7}$)R19° (0.14 ML), 80 K				5.1	6.1	7.6	8.5	9.0	9.9	11.2	13.4			σ (v) orientation, ring parallel to surface	ARUPS	00Kos1
Ru(0001)	saturation at 230 K		284.5 π^* e _{2u} 286.1 π^* e _{2u}												out of plane bending of C-H bonds	NEXAFS	98Wei1
Ru(0001)	saturated chemisorbed layer (0.16 ML), 90 K				4.9	6.2	7.8	8.3	8.8	10.0	11.2	13.4					89Hei

surface	superstructure (coverage, ML) expt. temp.	C1s binding energy (XPS)	unocc. states, NEXAFS resonances	1e _{2u} (π^*)	1e _{1g} (π)	2e _{2g} (σ)	1a _{2u} (π)	2e _{1u} (σ)	1b _{2u} (σ)	1b _{1u} (σ)	2a _{1g} (σ)	1e _{2g} (σ)	1e _{1u} (σ)	1a _{1g} (σ)	comments	method	Refs.
Ru(0001)	coadsorbed w. CO: ($\sqrt{13}\times\sqrt{13}$)R14° (0.08 ML ben, 0.33 ML CO)				4.7	6.0	7.8	7.9	8.8	9.8	11.2	13.2			shifts in CO 4 σ and 5 σ levels	ARUPS	90Ste 89Hei
Ru(0001)	coadsorbed w. NO: p(3 \times 3) (0.11 ML ben, 0.22 ML NO)				4.7	5.6	7.8	8.0	8.8	10.0	10.9	13.2			shifts in NO 5 σ level, NO on bridge sites	ARUPS	90Ste 89Hei
W(110)		284.3														XPS	96Whi

Semiconductor / insulator surfaces																	
surface	superstructure (coverage, ML) expt. temp.	C1s binding energy (XPS)	unocc. states, NEXAFS resonances	1e _{2u} (π)	1e _{1g} (π)	2e _{2g} (σ)	1a _{2u} (π)	2e _{1u} (σ)	1b _{2u} (σ)	1b _{1u} (σ)	2a _{1g}	1e _{2g}	1e _{1u}	1a _{1g}	comments	method	Refs.
Al ₂ O ₃ (111) / Mo(110)	ca 1 monolayer (0.03-0.04 L) at 90 K		3.94 (³ B _{1u} ← ¹ A _{1g}) 4.84 (¹ B _{2u} ← ¹ A _{1g}) 6.19 (¹ B _{1u} ← ¹ A _{1g}) 6.86 (¹ E _{1u} ← ¹ A _{1g})												vibronic fine structure (110 meV spacing) observed in the multilayer range	HREELS	96Str
MgO(100) / Mo(100)	ca 1 ML (0.03-0.04 L) at 90 K		3.94 (³ B _{1u} ← ¹ A _{1g}) 4.79 (¹ B _{2u} ← ¹ A _{1g}) 6.20 (¹ B _{1u} ← ¹ A _{1g}) 6.84 (¹ E _{1u} ← ¹ A _{1g})												vibronic fine structure (110 meV spacing) observed in the multilayer range	HREELS	96Str
Ge(100)-(2×1)	physisorbed 90 K				3.9	5.8	6.9	8.1	8.8	9.9	11.3	13.4	17.1	20.3		ARUPS	01Fin
Ge(100)-(2×1)	0.4 ML chemisorbed, 90 K			2.3	4.0 8.4	5.7 6.5	8.9	7.9 8.4	8.9	10.2	11.2	12.9 14.1	17.0 17.1	19.9	C _{2v} symmetry, di-sigma bonded 1,4-cyclo-hexadiene-like adsorption	ARUPS	01Fin
Ge / Si(100)-(2×1)	1.0 ML chemisorbed, 90 K			2.3	4.0 8.4	5.7 6.5	8.9	7.9 8.4	8.9	10.2	11.2	12.9 14.1	17.0 17.1	19.9	levels identical to Ge(100), C _{2v} symmetry, di-sigma bonded 1,4-cyclo-hexadiene-like adsorption	ARUPS	01Fin
Si(100)-(2×1)	(2×1) (0.25 ML) 30 K					11.1 11.8	11.8	13.5 14.3	16.6	16.1	16.9	18.3 19.7	22.5	26.1	w/r to E _{vac}	ARUPS DFT cluster calc.	98Gok 98Car
Si(100)-(2×1)	(2×1) (0.25 ML) 30 K			2b _{1u} 2.3	1b _{3g} 4.0	3b _{1g} 5.7 6a _g 6.5	5b _{3u} 7.9	4b _{2u} 1b _{2g} 8.4	1b _{1u} 3b _{2u} 8.9	4b _{3u} 10.2	5a _g 11.2	2b _{1g} 12.9	4a _g 14.1		C _{2v} symmetry,	ARUPS DFT cluster calc.	98Gok

surface	superstructure (coverage, ML) expt. temp.	C1s binding energy (XPS)	unocc. states, NEXAFS resonances	1e _{2u} (π)	1e _{1g} (π)	2e _{2g} (σ)	1a _{2u} (π)	2e _{1u} (σ)	1b _{2u} (σ)	1b _{1u} (σ)	2a _{1g}	1e _{2g}	1e _{1u}	1a _{1g}	comments	method	Refs.
Si(100) – (2×1)	physisorbed layer (1 L at 100K)		285.0 π^* e _{2u} 288.8 π^* b _{2g}													NEXAFS	98Kon
Si(100) – (2×1)	chemisorbed layer (1 L at 100K)		285.0 / 285.9 π^* e _{2u} 287.7 σ^* C-H 289.5 σ^* C-Si 292.2 σ^* C-C 298.6 σ^* C=C												two chemisorption structures, tilt 30 / 45°	NEXAFS	98Kon
Si(100)- (2×1)															HOMO: -1.2eV LUMO: >3.5eV	STM	98Sel
Si(111) – (7×7)													at low temp physisorbed layer with spectrum identical to gas phase, transition to chemisorbed layer at 75-105 K			UPS	00Car
Si(111) – (7×7)	saturation at 300 K			8.2	9.6	11.1 12.2	12.2	13.5 14.2	16.4	15.3	16.4	18.3 19.6	22.5	26.0	probably C _{2v} symmetry, 2 surface bonds	ARUPS (w/r to E _{vac})	98Car
Si(111) – (2×1) cleaved	5 - 100 L at 60 K				6.3	9.0		11.4			13.8	15.8	19.5		physisorbed and chemisorbed species coexist at low temp. and low coverage	UPS/XPS	87Pia
Si(111) – (2×1) cleaved	saturation at 300 K				5.3 6.2	8.1		10.7 12.4			13.8	16.6			ring parallel to surface	UPS/XPS	87Pia
TiO ₂ (100)	5 L - 20 L at 120 K	285.0			3.5 - 3.9	6.1		8.5			10.8				ring parallel to surface	AES, UPS, XPS	98 Raz
ZnO(10-10)	c(2×2) (0.5 ML) 150 K				2	4.1	5.0	6.4	7.3	8.1					energies extracted from spectrum plot	ARUPS	81Pos
ZnO(10-10)	c(4×3) (multilayers) 150 K				2	4.3	5.0	6.6	7.3	7.9	9.8				energies extracted from spectrum plot	ARUPS	81 Pos

Table 1c. Vibrational properties of adsorbed benzene
 Vibrational energies in cm^{-1} , unless indicated otherwise. Main peaks are underlined.
 Values for deuterated benzene are given in brackets where available.
 (δ = in plane deformation mode, γ = out of plane deformation mode, ν = stretch mode)

Metal surfaces											
surface	preparation, super-structure (coverage, ML), expt. temp.	low vibrational modes (frustrated rotations, lateral translations)	C-M	400 – 1000 γ C-C γ C-H δ C-C ν C-H	1000– 1200 δ C-H ν C-C	1200- 1650 ν C-C	1850	3000 (2300) ν C-H	comments	method	Refs.
gas phase				404 (351) 607 (579) 675 (497) 707 (599) 846 (663) 969 (789) 991 (830)	993 (945) 1010 (970) 1035 (812) 1146 (826) 1177 (868)	1309 (1282) 1346 (1055) 1479 (1330) 1595 (1553)		3047 - 3062 (2267-2294)		IR spectr.	88Jak
Ag(110)		4 meV, 19 meV (chemisorbed) 7 meV, 44 meV (weak ads.)							vibrational modes as finger prints for chemical state	STS - IETS	01Pas
Ag(110)	5 L (sub monolayer) 90 K, only C_6D_6			(495) (650) (780)	(945)				C_{2v} symmetry	Raman	84Hal
Ag(111)	5 L (sub monolayer) 90 K, only C_6D_6			(495)	(945)				C_{3v} $\sigma(\text{d})$ symmetry	Raman	84Hal
Ag(111)	0.4 L 140 K			410 675 820	1000 1155	1360 1480 1590		3030	C_{3v} $\sigma(\text{d})$ symmetry, ring parallel to surface	HREELS	81Avo1
Cu(110)	1 st layer (< 1 L), 85 K			685 - 683					flat-lying ring	RAIRS	96Haq

surface	preparation, super-structure (coverage, ML), expt. temp.	low vibrational modes (frustrated rotations, lateral translations)	C-M	400 – 1000 γ C-C γ C-H δ C-C ν C-H	1000– 1200 δ C-H ν C-C	1200- 1650 ν C-C	1850	3000 (2300) ν C-H	comments	method	Refs.
Cu(110)	multilayers (2 L), 85K			677	1037	1479		3042 3066 3084	2 nd layer molecules tilted	RAIRS	96Haq
Cu(110)	0.24 ML, 140 K			685	970	1550		3050	tilt of ring greater than 20°	HREELS	96Lom
Cu(110)	multilayers 140 K			680	990 1150	1460 1550		3050		HREELS	96Lom
Cu(111)	monolayer 1.5 L at 120 K			675 (500)					ring parallel	HREELS	94Xi
Cu(111)	multilayer 25 L at 120 K			410 680 (500) 845 (680)	1000 (960) 1160 (845)			3060 (2300)	ring tilted	HREELS	94Xi
Cu(111)	multilayer at 140 K			685 845	1000 1165	1480 1595		3060		HREELS	88Pat
Ni(100)	c(4×4) 3L at 300 K		360	750 (540) 845 (645) 845 (820)	1120 (820)	1330 (1225) 1430 (1370)		3025 (2260)	ring parallel to surface, frequencies very similar to Ni(111)	HREELS	79Ber 77Ber
Ni(110)	c(2×4) (0.25 ML) 300 K			743 879					ring parallel to surface	HREELS	92Hun
Ni(110)	c(2×4) (0.25 ML) 300 K			700 845	1110	1420		3020		HREELS	81Ber
Ni(111)	(2√3×2√3)R30° 3 L at 300 K		290	745 (540) 845 (645) 845 (820)	1110 (820)	1320 (1225) 1420 (1360)		3020 (2250)	ring parallel to surface, frequencies very similar to Ni(100)	HREELS	79Ber 77Ber
Ni(111)	2.0 L at 280 K		320	720 830	1130	1430		3000	ring parallel to surface	HREELS	78Leh

surface	preparation, super-structure (coverage, ML), expt. temp.	low vibrational modes (frustrated rotations, lateral translations)	C-M	400 – 1000 γ C-C γ C-H δ C-C ν C-H	1000– 1200 δ C-H ν C-C	1200- 1650 ν C-C	1850	3000 (2300) ν C-H	comments	method	Refs.
Os(0001)	saturation at 273 K		450 - 500	790	1050	1355		2900	phenyl and benzynes as precursors for dissociation	HREELS	90Gra
Pd(100)	saturation at 300 K		280 (285) 435 (400)	720 (520) 870 (675)	1115 (830)	1320 (1220) 1425 (1370)		3010 (2240)	ring parallel to surface, C _s adsorption site	HREELS	85Wad
Pd(111)	saturation at 180 K			695 (505)				3050 (2280)	ring parallel to surface, weak surface bond	HREELS	87Gra
Pd(111)	saturation at 300 K		265 (270)	720 (525) 810 (640)	1100 (830)	1410 (1355)		2990 (2230)	ring parallel to surface, C _s adsorption site	HREELS	85Wad
Pt(110)	300 K, diff. coverages		340 (340)	565 830 (665) 910 (800)	1120 (800)	1335 (1220) 1435 (1370)		3025 (2260)	ring parallel to surface	HREELS	87Sur
Pt(111)	chemisorbed layer at 300 K			814-810 829-827 900-891					ring parallel to surface, up to three different adsorption sites	RAIRS	96Haq
Pt(111)	multilayer (2 L) at 90 K			684 820 831	1037	1478			ring tilted in 2 nd layer	RAIRS	96Haq
Pt(111)	chemisorbed layer at 125 K			825		1480		2990	ring parallel to surface	HREELS (specular)	96Lut2
Pt(111)	multilayer at 125 K			685	1030	1480		3050	ring tilted	HREELS	96Lut2
Pt(111)	multilayer at 100 K			684	1032					RAIRS	86Sch

surface	preparation, super-structure (coverage, ML), expt. temp.	low vibrational modes (frustrated rotations, lateral translations)	C-M	400 – 1000 γ C-C γ C-H δ C-C ν C-H	1000– 1200 δ C-H ν C-C	1200- 1650 ν C-C	1850	3000 (2300) ν C-H	comments	method	Refs.
Pt(111)	0.58/0.30 L at 200 K		365 (345)	550 840 (600) 920 (715)	1145 (820)	1405		3005 (2250)		HREELS	85Abo
Pt(111)	sub monolayer at 300 K, saturation at 2 - 3 L		360 (350)	570 830 (610) 920 (700)	1130 (800)	1420 (1350)		3000 (2240)	ring parallel to surface	HREELS	78Leh
Rh(111)	c(2 $\sqrt{3}$ ×3)rect	13.1 meV (frustrated lateral transl.)								HAS	93Wit
Rh(111)	saturation at 290 K		345 (330)	550 (550) 810 (565) 880 (835)	1130 (835)	1320 (1320) 1420 (1365)		2988 (2250)	C _{3v} σ (d) symmetry, ring parallel to surface, decomposition starts above 400 K.	HREELS	86Koe 84Koe 83Koe
Rh(111)	c(2 $\sqrt{3}$ ×4)rect (0.12 ML) coads w. CO	12.9 meV (frustrated lateral transl.)								HAS	93Wit
Rh(111)	p(3×3) (0.11 ML) coads w. CO	12.7 meV (frustrated lateral transl.)								HAS	93Wit
Rh(111)	c(2 $\sqrt{3}$ ×4)rect coads w. CO 300 K								ring parallel to surface	HREELS, LEED, TPD	87Van
Ru(0001)	(2 $\sqrt{3}$ ×2 $\sqrt{3}$)R30° (< 0.07) 115 K		290 (270)	570 750 (540) 860 (830) 860 (685) 960 (910)	1010 (790) 1110 (790) 1110 (830)	1260 (1210) 1320 1410 (1360)		3020 (2160) (2250)	parallel to surface	HREELS, TPD	88Jak

surface	preparation, super-structure (coverage, ML), expt. temp.	low vibrational modes (frustrated rotations, lateral translations)	C-M	400 – 1000 γ C-C γ C-H δ C-C ν C-H	1000– 1200 δ C-H ν C-C	1200- 1650 ν C-C	1850	3000 (2300) ν C-H	comments	method	Refs.
Ru(0001)	multilayer (α_1 , α_2 , α_3) 115 K		240 (250)	430 610 (580) 690 (510) 700 (580) 850 980 (840) 980 (940)	1040 (820) 1170 (820) 1180 (840)	1345 1480 (1335) 1600 (1550)		3045- 3055 (2275-2290)	α_1 -layer essentially parallel, metastable, α_2 - layer strongly til- ted, α_3 -layer bulk-like	HREELS	89Jak
Ru(0001)	multilayer (α_2 : glassy phase) 53 K			<u>687</u> 703 855 974	1010 <u>1036</u> 1147 1175	1311 1348 1400 1470 1478 1540 1586	1754 1825 1969	<u>3032</u> <u>3069</u> <u>3088</u>	α_2 - α_3 phase transition is irreversible, temperature depends on layer thick- ness	RAIRS,	96Jak
Ru(0001)	multilayers (α_2 : crystalline phase) 120 K			<u>689</u> 707 974 978 987	1009 1032 <u>1034</u> <u>1039</u> 1142 1148	1250 1312 1403 1415 1469 1474 1479 1550 1565	1755 1829 1838 1974 1983	3029 3037 3067 3071 3085 3091	α_2 - α_3 phase transition is irreversible, temperature depends on layer thick- ness	RAIRS,	96Jak
Ru(0001)	p(3×3) coadsorbed w. 0.16 - 0.22 ML O (0.11 ML Benz) at 120 K		280 (270)	650 785 (555) 880 (850) 890 975 (825) 975 (900)	975 (760) 1125 (825)	1360 1440 (1385)		3005 (2230)	ν (O-Ru): 510 (505); net charge transfer from oxygen to benzene.	HREELS	90Jak3

surface	preparation, super-structure (coverage, ML), expt. temp.	low vibrational modes (frustrated rotations, lateral translations)	C-M	400 – 1000 γ C-C γ C-H δ C-C ν C-H	1000– 1200 δ C-H ν C-C	1200- 1650 ν C-C	1850	3000 (2300) ν C-H	comments	method	Refs.
Ru(0001)	($\sqrt{13} \times \sqrt{13}$)R14° coadsorbed w. 0.30 ML CO (0.08 ML) formed at 250 K, exp at 120 K		280 (270)	565 (545) 770 (550) 870 880 (840) 940 (920) 1000 (830) 1000 (840)	1000 (740) 1120 (830) 1270	1360 1430 (1365) 1530 (1480)		3030 (2260)	ν (C-O): 1960 (1960) ν (CO-Ru): 450 (465) attractive in- teraction be- tween benz- ene and CO due to indirect charge trans- fer	HREELS	90Jak2

Semiconductor / insulator surfaces											
surface	preparation, super-structure (coverage, ML), expt. temp.	low vibrational modes (frustrated rotations, lateral translations)	C-S	400 – 1000 γ C-C γ C-H δ C-C ν C-H	1000– 1200 δ C-H ν C-C	1200- 1650 ν C-C	1850	3000 (2300) ν C-H	comments	method	Refs.
MgO(100) / Mo(100)	multilayer 0.3 L at 90 K			406 679 841 989	1158	1468 1564		3068		HREELS	96Str
Si(100) – (2×1)	p($\sqrt{8} \times \sqrt{8}$) R45° supercell			900	1100 1230	1520		2880 3010	adsorption in tight bridge site geometry	DFT, Car- Parrinello approach	00Sil
Si(100) – (2×1)	0.25 ML, 90 K		315 538 604	776 876 949	1050 1160 1286 1378	1623		2935 3050		HREELS, LCGTO- DF cluster calculation	00Sta
Si(100) – (2×1)	0.25 ML		528 (493) 593 (552)	774 (650) 873 (885)	1042 (754) 1152 (853)	1648 (1610)		3000 (2216) 3090 (2304)		LCGTO- DF cluster calculation	98Bir

surface	preparation, super-structure (coverage, ML), expt. temp.	low vibrational modes (frustrated rotations, lateral translations)	C-S	400 – 1000 γ C-C γ C-H δ C-C ν C-H	1000– 1200 δ C-H ν C-C	1200- 1650 ν C-C	1850	3000 (2300) ν C-H	comments	method	Refs.
Si(100) – (2×1)	(2×1) (0.25 ML)		615 (550)	790 (660) 910 (860)	1075 (785) 1170 (860)	1635 (1595)		2935 (2190) 3065 (2300)		HREELS	98Bir
Si(100) – (2×1)	physisorbed at 100 K							3030 3036 3067 3086		RAIRS	98Kon
Si(100) – (2×1)	chemisorbed at 300 K							2945 3044	cyclo- hexadiene- like structure	RAIRS	98Kon
Si(100) – (2×1)	chemisorbed annealed to 350 K							2899 3044	cyclo- hexadiene- like structure	RAIRS	98Kon
Si(100) – (2×1)	physisorbed , 2 L at 90 K			425 (365) 695 (525) 860 (685)	1005 (850) 1040 (850) 1180 (850)	1500 (1340) 1610 (1585)		3075 (2300)		HREELS	91Tag1
Si(100) – (2×1)	c(2×4) chemisorbed at 300 K, expt. at 90 K		615 (550)	790 (550) 910 (660)	1075 (785) 1170 (860) 1170 (1080)	1635 (1595)		2935 (2190) 3065 (2300)	di- σ bonded to two adjacent Si atoms (SB)	HREELS	91Tag1
Si(111)- (7×7)	physisorbed , 1.0 L at 110 K			407 678 851 974	1021 1164	1332 1483 1587		3060		HREELS	99Cao
Si(111)- (7×7)	chemisorbed 0.5 L ann to 300 K, expt. at 110 K		540	785 877 951	1068 1157	1299 1582 1635		2920 3025	di- σ bonded to two ad- jacent Si atoms	HREELS	99Cao
Si(111)- (7×7)	physisorbed , 1.5 L at 90 K			420 (365) 695 (520) 865 (670)	1010 (840) 1040 (840)	1355 1490 (1345) 1620 (1580)		3070 (2295)		HREELS	91Tag1 91Tag2
Si(111)- (7×7)	chemisorbed at 300 K, expt. at 90 K		540 (510)	790 (630) 965 (930)	1075 (805) 1190 (930)	1440		2985 (2195) 3050 (2260)	π -bonded, ring parallel to surface	HREELS	91Tag1 91Tag2

surface	preparation, super-structure (coverage, ML), expt. temp.	low vibrational modes (frustrated rotations, lateral translations)	C-S	400 – 1000 γ C-C γ C-H δ C-C ν C-H	1000– 1200 δ C-H ν C-C	1200- 1650 ν C-C	1850	3000 (2300) ν C-H	comments	method	Refs.
Si(111) – (2×1) cleaved	0.5 – 25 L at 85 K			700	1050	1570		3050	C _{3v} symmetry	HREELS	86Pia
Si(111) – (2×1) cleaved	30 - 75 L at 85 K			700	1050 1170	1570		3050	C _s symmetry	HREELS	86Pia
Si(111) – (2×1) cleaved	saturation at 300 K		540 (500)	780 (500)	1060 1250 (1170)	1610 (1540)		3060 (2190)	ring tilted, breakage of C-H bond and formation of C-Si bond.	HREELS	84Pia

Table 2. Cyclohexane (c-C₆H₁₂)

	T_{max} [K]	Heating rate [K/s]	Soft mode [cm ⁻¹]	Structure	Dehydrogenation upon heating	Methods	Conformation, orientation, symmetry	Comments	References
Ni(111)						UPS		Electronic structure: No bonding shifts	74Dem, 76Dem
	>170		2720		No	HREELS	C _s		78Dem, 79Leh
	180-192	2		($\sqrt{7} \times \sqrt{7}$)R19.1°	No	TPD, LEED, ARUPS	C ₁ , Slightly inclined	Rate maximum: Depends on coverage Electronic structure: No bonding shifts Coadsorption of O and K	90Hub, 91Zeb1
			2730	($\sqrt{7} \times \sqrt{7}$)R19.1°		RAIRS, LEED	C _{3v}	Coadsorption of O	95Coo
						RAIRS		C ₆ HD ₁₁	95Rav
					Not up to 340 K	TPD			82Tsa1, 82Tsa2
						Cluster Calc.			84Hof
Ni[5(111) ×(110)]			2620		To benzene above 220 K	HREELS			79Leh
Ni[9(111) ×(111)]					Not up to 340 K	TPD			82Tsa1, 82Tsa2
K/Ni(111)	135-140				No	TPD		$\theta_K=0.34$ ML, Cluster growth	91Zeb1
Ni(100)					Not up to 470 K	TPD			82Tsa1, 82Tsa2
						Cluster Calc.			84Hof
Ni(110)	195 ⁺		2690		No	HREELS		⁺ no TPD spectra shown	89Rav2
	206	2				TPD, ARUPS		Electronic structure No bonding shifts	91Hub3
					Not up to 380 K	TPD			82Tsa1, 82Tsa2
Cu(111)	178	3	2754			TPD, RAIRS			98Tep
	165 ⁺		2775	($\sqrt{7} \times \sqrt{7}$)R19.1°	No	HREELS, RAIRS, LEED, TPD	Parallel, C _{3v}	⁺ no TPD spectra shown	89Rav1 ⁺ , 89Rav2, 86Che, 93Rav
						NEXAFS		Electronic structure	01Woe, 99Wei
Cu(100)	160 ⁺		2790			HREELS		⁺ no TPD spectra shown	89Rav2
	181-184	3	2746		No	TPD, RAIRS		$E_{des} = 46.4$ kJ/mol	98Tep, 96Tep
						He-scattering		Frustrated translation	95Wit
Cu(110)	181	3	2728		No	TPD, RAIRS			98Tep
Cu ₃ Pt(111)	199		2754		No	TPD, RAIRS			98Tep
Mo(110)	195		2570+2610		C ₆ H ₁₂ : 10% dehydrogenation, 90% molecular desorption	RAIRS	Chair, lower than C _{3v} at low coverage	Coverage dependence Coadsorption of S and O	96Wel
	C ₆ D ₁₂ : 205	3	C ₆ H ₁₂ : 2577		C ₆ H ₁₂ : not investigated C ₆ D ₁₂ : no dehydrogenation	TPD, HREELS			98Tep

	T_{max} [K]	Heating rate [K/s]	Soft mode [cm ⁻¹]	Structure	Dehydrogenation upon heating	Methods	Conformation, orientation, symmetry	Comments	References
C/Mo(110)	C ₆ D ₁₂ : 203	3	C ₆ H ₁₂ : 2685		C ₆ H ₁₂ : not investigated C ₆ D ₁₂ : no dehydrogenation	TPD, HREELS		(4×4) interstitial carbide overlayer	98Tep
Ru(0001)	227	20				ESDIAD, TPD, LEED	Chair	E_{des} =59 kJ/mol	78Mad
	200	5-9				TPD		E_{des} =38-45 kJ/mol	86Pol
	200	10	2520-2600	Disordered	Little	HREELS,TPD, LEED, UPS	C _{3v}	Coverage dependence of mode softening	83Hof2, 81Hof
	200	10	2516		To benzene	HREELS, Cluster Calc.		O Coadsorption	84Hof
						LITD		Surface diffusion, E_{diff} =19 kJ/mol	88Mak
Pd(111)			2635			HREELS			86Wad
					To benzene at 300 K	UPS		Electronic structure: No bonding shifts	78Rub
Pd(110)			2630		Yes	HREELS	Chair	also C ₆ D ₁₂	89Rav1, 89Rav2
Ag(111)				(9×9)		LEED			78Fir
W(100)					Decomposition at 300 K	UPS, $\Delta\phi$		Adsorption at 300 K	80Bha
Ir(111)						LEED, AES, TPD		Adsorption at 303 K	76Nie
Pt(111)				$\sqrt{21}\times\sqrt{21}$ R10.9'		LEED			77Fir
					Some dehydrogenation	TPD			82Tsa1
			~2600			RAIRS	C _{3v}		90Che
			~2600		C ₆ H ₁₂ : to intermediate >200K, to benzene at 300K. C ₆ D ₁₂ : no dehydrogenation	HREELS	C _{3v} , Parallel		93Lan, 78Dem
	236	~7	2550		Starting at 195 K To benzene >290 K Reactivity red. by coads. Bi	LEED, TPD, XPS, AES, HREELS		E_{des} =58 kJ/mol Bi Coadsorption	93Dom, 88Cam, 94Cam, 89Rod, 92Bus
	230				To benzene	TPD, XPS, AES, $\Delta\phi$		Cs coadsorption: Stabilization of cyclohexane Reversal of dipole moment	91Dav, 91Ern
	228					TPD, AES, LEED, HREELS		O Coadsorption (SnPt alloy) Reduction adsorption energy Sticking coefficient at 150 K = 1 Radiation damage	94Xu1, 93Xu
	~230	3			Starting at 180 K To benzene >280 K	TPD, LITD+FTMS			92Par, 89Lan, 91Pet
					To benzene	Cluster Calc.			85Kan

	T_{max} [K]	Heating rate [K/s]	Soft mode [cm ⁻¹]	Structure	Dehydrogenation upon heating	Methods	Conformation, orientation, symmetry	Comments	References
Cont'd.						NEXAFS, $X\alpha$ -calculation			86Hit
						Molecular Beam		Sticking coefficient at 100 K = 1	92Jia
Pt[6(111) ×(111)]					To benzene (more than on Pt(111))	TPD, LEED			82Tsa2, 74Bar
Pt(100) -(5×20)	182	1.7	2550		Molecular desorption dominates, some dehydrogenation to benzene	TPD, HREELS, RAIRS	C _{3v} , chair		94Lam2, 97Lam 90Mar
Pt(100) -(1×1)	No molecular desorption		No soft- mode		Complete dehydrogenation: - to C ₆ H ₉ at 220 K - to benzene at 300 K	TPD, HREELS,RAIRS	Lower than C _{3v}		94Lam2, 97Lam 90Mar

Table 3. Saturated hydrocarbons other than cyclohexane: Cyclopropane (c-C₃H₆), Cyclobutane (c-C₄H₈), Cyclopentane (c-C₅H₁₀), Cyclooctane (c-C₈H₁₆)

	T_{max} [K]	Heating rate [K/s]	Soft mode [cm ⁻¹]	Dehydro- genation upon heating	Methods	Comments	References
Cyclopropane (C ₃ H ₆)							
Ni(100)	123	3	No	Minor	HREELS, TPD	$E_{des} \approx 29$ kJ/mol	95Son, 96Son
Cu(111)				No	HF calculation, NEXAFS	Electronic structure	00Woe
	125	3	No		HREELS, TPD	Electron beam induced bond scission $E_{des} \approx 38$ kJ/mol	97Mar2, 97Mar3, 98Mar
Cu(110)	125	3	No	No	HREELS, TPD	Electron beam induced bond scission $E_{des} \approx 38$ kJ / mol	94Mar, 97Mar1, 97Mar2, 97Mar3, 98Mar, 98Roc
Ru(0001)	150	10	No	No	HREELS, ARUPS, LEED, TPD	90 K: Molecular adsorption One C-C bond parallel to surface plane C _s symmetry, interaction via $\sigma(CC)$ orbital	83Fel 82Hof
	145	-			LEED, TPD, ESDIAD	non dissociative, no ordered LEED pattern $E_{des} = 33$ kJ/mol	78Mad
	145	-			LITD	Surface diffusion, $E_{diff} = 8$ kJ / mol	88Mak
					TPD	400-1000 K: Dissociation via C-C cleavage $E_{act} = 39.5$ kJ/mol (no isotope effect)	97Jac
	145	-	No (<20 cm ⁻¹)		TPD, HREELS		84Hof
Ir(110)1×2				Yes	Molecular beam	$E_{trans} < 21$ kJ/mol: molecular adsorption $E_{trans} > 21$ kJ/mol: dissociative adsorption	96Kel
	~135	10-15		Yes	TPD, UPS, LEED, $\Delta\Phi$	100 K: Low coverage: Dissociation upon adsorption 100 K: High coverage: Additional molecular adsorption	82Wit1, 82Wit2, 83Szu, 84Szu
Ir(111)				Minor	TPD, LEED	100 K: molecular adsorption	83Szu, 84Szu
Cyclobutane (C ₄ H ₈)							
Ru(0001)	175	10	No (<40 cm ⁻¹)		TPD, HREELS		84Hof
Cyclopentane (C ₅ H ₁₀)							
Cu(111)	161	3	2812	No	RAIRS		98Tep

	T_{max} [K]	Heating rate [K/s]	Soft mode [cm ⁻¹]	Dehydro- genation upon heating	Methods	Comments	References
Cu(110)	166	3	2732	No	RAIRS		98Tep
Ru(0001)	180	-			LITD	$E_{des} = 43$ kJ/mol Surface diffusion, $E_{diff} = 13.8$ kJ/mol	88Mak
	180	-	2610		TPD, HREELS		83Hof1, 84Hof
					LITD		90Are
Ir(111)				No	TPD, HREELS		93Ave
Pt(111)	200	1	2690	Partly to C ₅ H ₆	TPD, HREELS, $\Delta\Phi$	90 K: molecular adsorption $E_{des} = 60$ kJ/mol	85Ave, 93Ave
			~2700				90Che
Cyclooctane (C ₈ H ₁₆)							
Ru(0001)	~260	-	157 - 270		LEED, TPD, ESDIAD	Coverage dependent desorption temperature	78Mad
	250	10	No (<40 cm ⁻¹)		TPD, HREELS		84Hof

Table 4. Non-saturated hydrocarbons other than benzene – Cyclopentene (c-C₅H₈), Cyclopentadiene (c-C₅H₆), Cyclohexene (c-C₆H₁₀), Cyclohexadiene (c-C₆H₈), Cyclooctadiene (c-C₈H₁₂), Cyclooctatetraene (c-C₈H₈)

	Methods	Thermal evolution	Comments	References
Cyclopentene (c-C ₅ H ₈)				
Mo(110)	HREELS, NEXAFS, TPD, XPS, AES	Decomposition upon heating		96Fru
Rh(111)	ARUPS, TPD, LEED, $\Delta\Phi$	Adsorption at 290 K: Decomposition to C ₅ H ₅ Heating after adsorption at 80 K: Decomposition to C ₅ H ₆	Weakly π -bonded in monolayer at 150 K	88Net3, 88Net2
Ag(111)	ESDIAD, LEED, TPD	No decomposition upon heating		86Alv
Ag(211)	ESDIAD, LEED, TPD	No decomposition upon heating	T_{des} = 175 K, 220 K Double bond oriented along steps	86Alv
Ir(111)	TPD, HREELS	160 K: Decomposition to c-C ₅ H ₆ 400 K :Decomposition to c-C ₅ H ₃		93Ave
Pt(111)	TPD, HREELS, $\Delta\Phi$	<250 K: molecular adsorption ~300 K: formation of c-C ₅ H ₅ , stable up to 480 K	c-C ₅ H ₈ : di- σ bonded c-C ₅ H ₅ : π -bonded	84Ave1, 84Ave2, 93Ave
	TPD	Molecular desorption + decomposition	Bi coadsorption	88Cam
	NEXAFS, X α -calculations		Electronic structure	86Hit
	TPD, AES, XPS	Dehydrogenation to adsorbed c-C ₅ H ₅ or molecular desorption		89Hen
	TPD, XPS, AES, $\Delta\Phi$		Cs coadsorption: Stabilization at low Cs coverage Reversal of dipole moment	91Ern 91Dav
Si(100)-(2 \times 1)	STM, RAIRS, XPS	No	Formation of [2+2] cycloaddition product (i.e. di- σ Si-C bonds)	97Hov, 98Liu, 98Hov1, 98Hov2, 98Ham, 99Ham, 00Lee
	UPS, XPS		Formation of di- σ Si-C bonds	01Yam1, 01Yam2
Si(111)7 \times 7	TPD	Some dehydrogenation to c-C ₅ H ₆	Molecular desorption: T_{des} = 300-650 K	92Mac
Ge(100)-(2 \times 1)	RAIRS, STM, XPS, UPS, TPD	Formation of [2+2] cycloaddition product	T_{des} = 360 K and 410 K	99Ham, 00Lee

	Methods	Thermal evolution	Comments	References
Cyclopentadiene (c-C₅H₆)				
Rh(111)	ARUPS, TPD, LEED, $\Delta\Phi$	Complete decomposition upon heating Formation of cyclopentadienyl (c-C ₅ H ₅)	Weak π -bonded in monolayer	88Net2, 88Net3
Ir(111)	TPD, HREELS	Heating to 350 K: Decomposition to c-C ₅ H ₅ Heating to 450 K: Decomposition to c-C ₅ H ₃	Irreversible adsorption	93Ave
Pt(111)	TPD, HREELS	1,3: Adsorption at 90 K: Disproportionation reaction to c-C ₅ H ₅ and c-C ₅ H ₈		86Ave, 93Ave
Si(111)7×7	TPD		Molecular desorption: $T_{des} = 300\text{-}650\text{ K}$	92Mac
Cyclohexene (c-C₆H₁₀)				
Ni(111)	TPD	Dyhydrogenation to benzene	Also stepped surface	82Tsa2
Cu(100)	RAIRS, TPD	No decomposition upon heating	$T_{des} = 206\text{ K}$, $E_{des} = 52\text{ kJ/mol}$	96Tep
Ru(0001)	TPD	No molecular desorption from monolayer C-H and C-C bond breaking at 150 K – formation of C ₂ H ₄		87Fly
W(100)	UPS, $\Delta\Phi$, TPD	300 K: Decomposition upon adsorption		80Bha
Pt(111)	TPD	Benzene formation above 300 K		88Cam
	LEED		$E_{des} = 75\text{ kJ/mol}$, Bi coadsorption	93Dom, 94Cam
	TPD		Electron beam induced dissociation	93Xu
	TPD	Dissociation for small coverages Molecular desorption at higher coverages: $T_{des} = 239$ and 281 K	Sticking coefficient: unity di- σ bonding	94Xu2
	TPS, XPS, AES	Decomposition upon heating Molecular desorption at $T_{des} = 255$ and 300 K Also observed: benzene desorption: $T_{des} = 350\text{-}500\text{ K}$		89Rod1
	TPD	Dyhydrogenation to benzene	also stepped surface	82Tsa2
Pt(100)1×1	TPD, HREELS	Dehydrogenation to benzene upon heating to 290 K		97Lam
Pt(100)5×20	TPD, HREELS	Dehydrogenation to benzene upon heating to 290 K		97Lam
Si(100)-(2×1)	UPS, STM		Two stable adsorption states, assigned to boat type and twist boat type geometries	01Yos
			Formation of di- σ Si-C bonds	01Yam2
Ge(100)-(2×1)	RAIRS, STM, XPS, UPS, TPD	Formation of [2+2] cycloaddition products; minor decomposition upon heating	$T_{des} = 370$ and 455 K	00Lee

	Methods	Thermal evolution	Comments	References
Cyclohexadiene (c-C ₆ H ₈)				
Ni(111)	TPD	1,3 and 1,4: Dehydrogenation to benzene	also stepped surface	82Tsa2
W(100)	UPS, $\Delta\Phi$	1,3 and 1,4: Decomposition upon adsorption at 300 K		80Bha
Pt(111)	SFG	1,4: Flat adsorption on surface Dehydrogenation to benzene at ~ 300 K 1,3: partial rearrangement to 1,4; Dehydrogenation to benzene		97Su
	TPD, HREELS, TPD	1,3: Dehydrogenation to benzene upon heating: $E_{act} = 58$ kJ/mol 1,4: Dehydrogenation to benzene upon heating $E_{act} = 58$ kJ/mol	Bi coadsorption	92Hug
	TPD	1,3 and 1,4: Dehydrogenation to benzene	also stepped surface	82Tsa2
Pt(100)1×1	TPD	1,3 and 1,4: Dehydrogenation to benzene		97Lam
Si(100)-(2×1)	STM, RAIRS, XPS		1,3: Mixture of [2+2] and [4+2] cycloaddition products	98Hov2
	LEED, UPS		1,4: Formation of di- σ Si-C bonds	00Ham, 01Yam1, 01Yam2
Cyclooctadiene (c-C ₈ H ₁₂)				
Pt(111)	TPD, HREELS			94Hos
Si(100)1×2	STM, RAIRS		1,5: Formation of [2+2] cycloaddition product	98Hov1, 98Hov2, 99Ham
Cyclooctatetraene (c-C ₈ H ₈)				
Pt(111)	NEXAFS		Electronic structure	86Hit
	TPD, HREELS			94Hos

Table 5. Ethylene oxide (C₂H₄O)

	T_{max} [K]	Heating rate [K/s]	$\Delta\Phi$ [eV]	Structure	Decom- position upon heating	Methods	Orientation, Symmetry	2b ₁ , 6a ₁ Bonding Shift [eV]	Comments	Reference
Fe(100)	120-250		-2.2		-	ARUPS, TPD, $\Delta\Phi$	Molecular plane nearly perpendicular	0.7 / 0.45	$E_{des} = 55$ kJ/mol	87Ben1
						Theory (ASED- MO)			Electronic structure	89Sel
Ni(111)	150-250	2-5	-1.6		No (<0.05 ML)	ARUPS, TPD, $\Delta\Phi$, HREELS		0.75 / 0.6	K coadsorption Reaction at high K coverages	87Ben1, 87Ben2, 90Nie1, 90Nie2, 92Nie
						Theory (ASED- MO)			Electronic structure	89Sel
Ni(110)	120-240	2	-2.8	c(2×2)	No	TPD, $\Delta\Phi$, LEED, XPS, ARUPS, NEXAFS	Molecular plane tilted, C ₁	0.9 / 0.5	Radiation damage observed	93Wei1, 93Wei2
					Yes	XPD, XPS, LEED, UPS	Molecular plane tilted, C _s		Radiation damage observed	93Gro, 94Ham
						Cluster Calculations (DFT)			Orbital assignment	95UlB
Cu(110)	150-240		-1.1	c(2×2)	No (<0.03 ML)	ARUPS, TPD, $\Delta\Phi$, LEED	Molecular plane nearly perpendicular	0.5 / 0.6	$E_{des} = 50$ kJ/mol O coadsorption: weakening of bond	86Ben1, 86Ben2, 87Ben1
Mo(110)	140-190				Yes	TPD, XPS				89Ser
Rh(111)	120-210	4			Yes	TPD, HREELS				93Bro
Pd(111)	255	8			Yes	TPD, LEED, HREELS, XPS			$E_{des} \approx 63$ kJ/mol	94Lam
Pd(110)	170-220	4			Yes	HREELS, TPD DFT calculations	Molecular plane tilted, C ₁		$E_{des} = 42 - 51$ kJ/mol Orbital assignment Ring opening above 200 K	96She, 97She
Ag(111)	158	3			No	RAIRS, TPD	Molecular plane perpendicular		$E_{des} = 45$ kJ/mol O coadsorption: $E_{des} = 51$ kJ/mol Also "High" pressure (1 mbar)	01Sta
									$E_{des} \approx 41$ kJ/mol	87Tan

	T_{max} [K]	Heating rate [K/s]	$\Delta\Phi$ [eV]	Structure	Decom- position upon heating	Methods	Orientation, Symmetry	2b ₁ , 6a ₁ Bonding Shift [eV]	Comments	Reference
Cont'd.						TPD			Adsorption between 300 and 500 K	85Gra
Ag(110)						TPD, LEED, HREELS			$E_{des} \approx 38$ kJ/mol O coadsorption: new adsorption states	83Bac
	~170	4.5	-1.44	c(2×2)	No	AES, TPD, AES, LEED, HREELS, ARUPS, $\Delta\Phi$	Molecular plane nearly perpendicular	No shifts	K-coadsorption Reaction at high K coverages	86Kru, 86Ben2, 87Ben1, 91Nie
	175	11			No	XPS, TPD, AES, HREELS			$E_{des} = 42$ kJ/mol Only molecular desorption	86Cam
				c(2×2)		TPD, LEED, XPS, HREELS			$E_{des} = 40$ kJ/mol	92Bar
						Cluster calculation, INDO/S			Electronic structure	88Rod2
Pt(111)	160-190	11			Yes	XPS, TPD, AES, HREELS			$E_{des} = 41$ to > 50 kJ/mol depending on coverage	86Cam
Pt(110)	140-230	5	-2.1	streaky (2×2)	No (< 0.02 ML)	TPD, $\Delta\Phi$, LEED, XPS, ARUPS, NEXAFS	Mol plane tilted, C ₁	0.6 / 0.4	Two coexisting species	93Wei2

Table 6. Pyridine (C_5H_5N)

	T_{max} [K]	Heating rate [K/s]	Structure	Methods	Orientation / thermal evolution	References
Ni(111)				HREELS, XPS, ARUPS	120 K and 170 K: Low coverage: π -bonded, molecular plane parallel to surface. High coverage: N-bonded, molecular plane tilts towards surface normal. Decomposition at 520 K	90Coh
				NEXAFS	Electronic structure 300 K: tilt angle of molecular plane to surface normal: 20°	91Ami
				PED	N atom close to on top position, tilt angle to surface normal: 18° N-Ni bond length: 1.97 Å	94Fri
Ni(110)				HREELS, ARUPS, XPS	100 K: Low coverage: π -bonded, molecular plane parallel to surface High coverage: Molecular plane tilts towards surface normal Decomposition upon heating to 520 K	91Coh
Ni(100)				HREELS	100 K: Low coverage: π -bonded, molecular plane parallel to surface High coverage: molecular plane tilts towards surface normal 300 K: Reaction to α -pyridine, N-bonded, perpendicular, stable up to 490 K	84Din1, 84Din2, 84Avo
				TPD	300 K: Formation of α -pyridine	82Wex
Cu(111)				NEXAFS	Tilted, tilt angle of molecular plane to surface normal: 20°	86Bad1
	Des. <240K			XPS, HREELS	C_2 axis parallel to surface, π -bonded, C_s -symmetry No decomposition upon heating, complete molecular desorption <240 K O coadsorption: Stabilization of pyridine up to 380 K C_2 axis perpendicular to surface	95Dav
				IPES	Electronic structure	86Fra
				EELS	Charge transfer excitations	01Zyl
Cu(110)	Low cov: 360 K	2	(5×3), (4×3)	LEED, TPD, ESDIAD	Low coverage: Perpendicular, mol plane along [001]; $E_{des} = 94$ kJ/mol Saturation: Perpendicular, mol plane twisted by 25° ; $E_{des} = 109$ kJ/mol No decomposition upon heating	01Lee
					Perpendicular, tilt angle of molecular plane to surface normal: 0°	86Bad1
					240 K: N-bonded, perpendicular, molecular plane along [001]	87Con, 87Bri
				ARUPS	300 K: N-bonded, perpendicular, differential shift of lone pair orbital: 0.9 eV	79Ban, 80Nyb
				RAIRS	85 K: N-bonded, C_{2v} , perpendicular at low coverage some tilting with increasing coverage	96Haq

	T_{max} [K]	Heating rate [K/s]	Structure	Methods	Orientation / thermal evolution	References
Cont'd.				PED	Saturation coverage: near on top-site, N-Cu: 2.00 Å tilt angle of molecular plane to surface normal: 20°, twisted by 30° from [001]	99Gie, 00Ter
				ARUPS	Electronic structure	88Dud
Cu(100)				STM	Electron induced dissociation	00Lau
Ru(0001)				HREELS, TPD	< 200 K: low coverage: π -bonded, molecular plane parallel to surface high coverage: N-bonded, inclined 300 K: reaction to α -pyridile different dehydrogenation pathways for π -bonded and N-bonded pyridine	87Bri, 87Jak, 90Jak
Rh(111)			(2 $\sqrt{3}$ × $\sqrt{3}$)rect	LEED, HREELS TPD, SHG	Adsorption at 80 K: α -pyridile formed upon heating to at 310 K further decomposition upon heating at 400 K	88Mat
				ARUPS, TPD, $\Delta\Phi$	300 K: intact pyrdine, change from parallel to inclined species with coverage $\Delta\Phi$ for saturated layer: -1.65 eV	90Net
Pd(111)			Disordered	ARUPS, EELS	300 K: C _s , tilted, π + N-bonding	83Net1, 83Net2
				HREELS	180 K, all coverages: π -bonded, molecular plane parallel to surface 310 K, all coverages: N-bonded	87Gra
				HREELS	150 K, all coverages: π -bonded, molecular plane parallel to surface	86Wad
Pd(110)			c(4×2)	ARUPS, LEED, $\Delta\Phi$	π -bonded, molecular plane parallel to surface, also at saturation coverage N-atom along [001] azimuth	88Net1
Ag(111)				NEXAFS	Tilted, tilt angle to surface normal changes from 45 to 20° with coverage	86Bad1, 86Bad2
				EELS	Change from π -bonded to N-bonded with coverage Vibrational overtones	80Dem, 81Dem, 82Dem, 81Avo1, 81Avo2, 83Dem
				NEELFS	Change from small to large tilt angle with coverage	90Tyl
			($\sqrt{3}$ × $\sqrt{3}$)R30°	LEED, ARUPS	Perpendicular, N-bonded	86Dud
				UPS, Raman	Electronic structure	80San
				IPES, UPS	Electronic structure	85Ott
Ag(110)				SHG, $\Delta\Phi$	Change from flat to upright with coverage Sticking coefficient at 110 K close to unity	88Hes
				UPS, TPD, AES	Electronic structure	80Kel
Ag(100)				NEELFS	Change from small to large tilt angle with coverage	90Tyl
Ir(111)			(2 $\sqrt{3}$ ×2 $\sqrt{3}$)R30°	ARUPS, ESDIAD	300 K, saturation coverage: C _s , N-bonded, inclined by 20°	85Mac
					300 K, saturation coverage: reaction to α -pyridile (from data in 85Mac)	87Con

	T_{max} [K]	Heating rate [K/s]	Structure	Methods	Orientation / thermal evolution	References
Pt(111)				RAIRS	85 K: Tilted geometry, rotation about C_2 axis with coverage 140 K, low coverage: π -bonded, molecular plane parallel to surface 140 K, high coverage: tilting towards surface normal 300 K: α -pyridile, upright, for all coverages	96Haq
				NEXAFS, $X\alpha$ -calculations	300 K: Perpendicular	85Hor, 83Joh
				TPD, NEXAFS	240 K: Tilted geometry: 38° to surface normal 300 K: α -pyrdile: Perpendicular ($16\pm 10^\circ$)	85Joh
				ARUPS	300 K: reaction to α -pyridile	87Bri, 87Con
				HREELS, Raman	Adsorbed from solution 300 K: Inclined: 15 - 19° to surface normal	90Kah
				HREELS, TPD	120 K – high cov: N + π -bonded, tilted 300 K: reaction to α -pyridile, perpendicularly oriented	86Gra
			Diffuse (2 \times 2)	LEED, $\Delta\Phi$	300 K: $\Delta\Phi = -2.7$ eV	73Gla, 82Gar
Pt(110)				HREELS	Adsorption at 300 K: no dissociation Change from π -bonded to N-bonded with increasing coverage	83Ric, 87Sur
Pt(100)			Diffuse (1 \times 1)	LEED, $\Delta\Phi$	300 K: $\Delta\Phi = -2.4$ eV	73Gla
Au(111)				DFT calculation	Vibrational frequencies	01Tad
Au(110)				IPES	Electronic structure	Fra86
Si(111)7 \times 7				STM	Adsorption across dimer row	00Yag, 00Shi
Si(111)2 \times 1				ARUPS, HREELS	Electronic structure 45 K and 85 K: physisorbed state 300 K: chemisorbed state	83Pia, 85Pia, 86Pia, 90Pia
ZnO(0001)				Cluster Calc. (INDO/S)	Electronic structure, charge transfer	88Rod
				TPD, XPS, NEXAFS	O-terminated surface: $T_{des} = 225$ K, $E_{ad} = 57$ kJ/mol, tilt angle: 24° to SN Zn-terminated surface: $T_{des} = 365$ K, $E_{ad} = 112$ kJ/mol, tilt angle: 19° to SN	00Hov
ZnO(10 $\bar{1}$ 0)				NEXAFS	295 K: upright with ring plane along [0001], N-bonded	93Wal
ZnO(1 $\bar{1}$ 00)				UPS	300 K: N + π -bonded	78Lut

3.8.7.10 Figures for 3.8.7

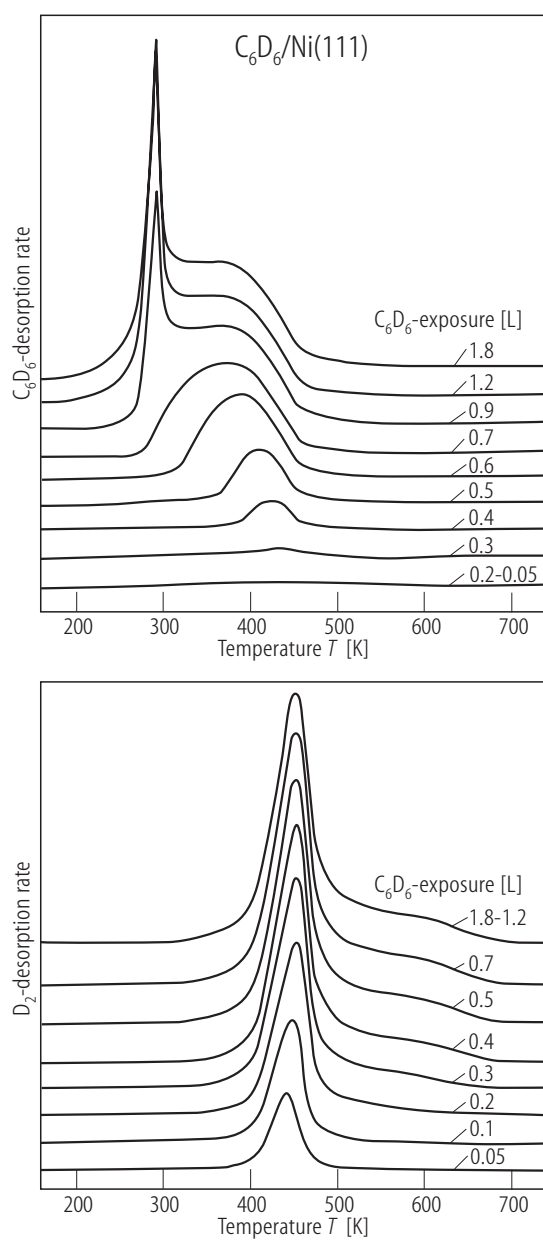


Fig. 1. Temperature programmed desorption spectra of D_2 (lower Fig; $m/e = 4$) and C_6D_6 (upper Fig.; $m/e = 84$) after different exposures of deuterated benzene onto Ni(111) at a surface temperature of 200 K. Heating rate was 5 K/s; [89Ste].

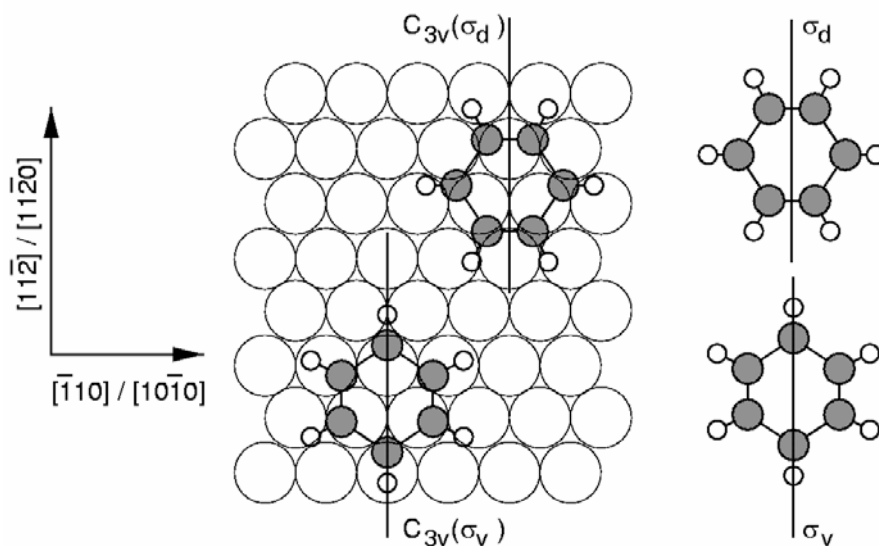


Fig. 2. Schematic drawing of the $\sigma(d)$ and $\sigma(v)$ orientations of benzene adsorbed parallel on a close packed hexagonal surface (fcc 111 or hcp 0001) which lead to the highest possible C_{3v} symmetry of the adsorption complex. Note that either one of the $\sigma(d)$ or $\sigma(v)$ mirror planes is parallel to the mirror plane of the substrate (along $[11\bar{2}] / [11\bar{2}0]$). The adsorption site is chosen arbitrarily; [99Kos1].

Fig. 3: see next page

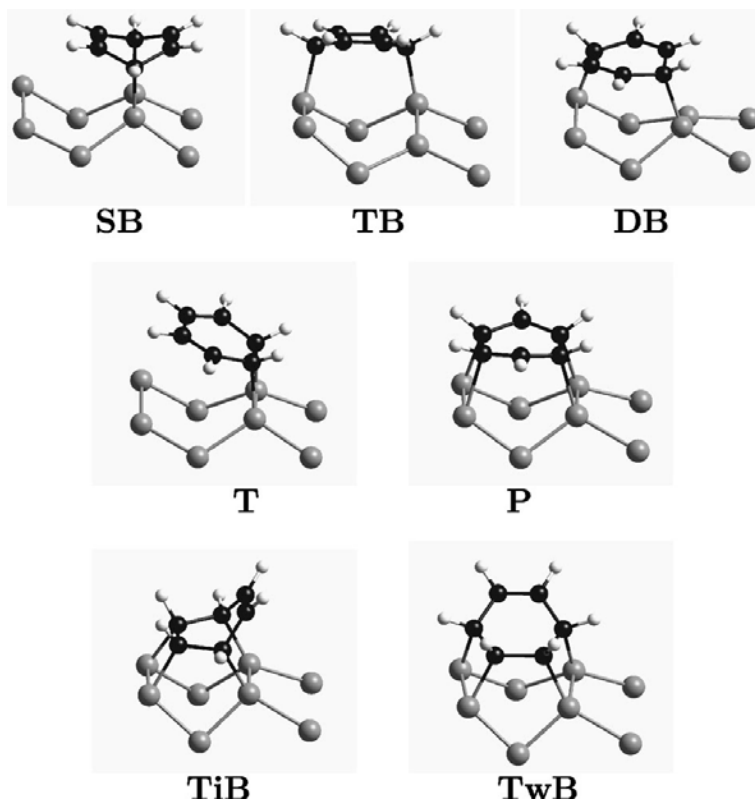
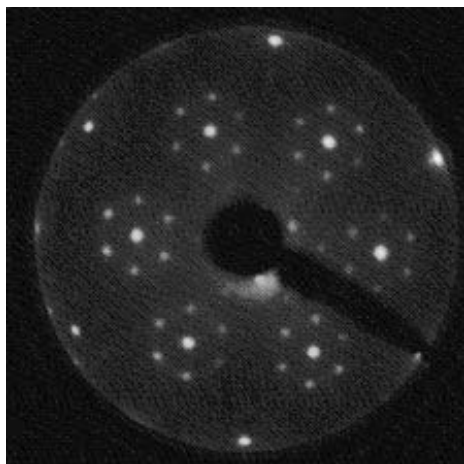


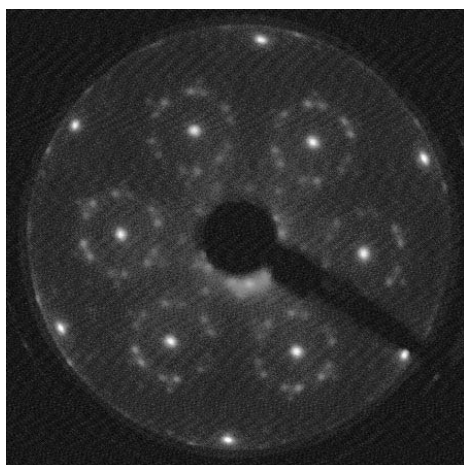
Fig. 4. Stable adsorption geometries for benzene on Si(100)-(1×2):

SB = standard butterfly
(1,4-cyclohexadiene-like, ontop of dimer row)
TB = tilted-bridge butterfly,
DB = diagonal-bridge butterfly,
T = tilted,
P = pedestal,
TiB = tight bridge,
TwB = twisted bridge. Only four Si atoms of the first layer (dimers) and four of the second layer are shown; [00Sil].

Ⓐ $p(2\sqrt{3} \times 2\sqrt{3})R30^\circ$



Ⓑ $c(2\sqrt{3} \times 4)rect$



Ⓒ $p(\sqrt{7} \times \sqrt{7})R19^\circ$

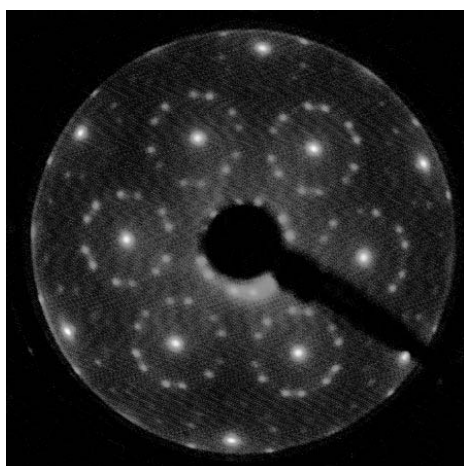


Fig. 3. LEED patterns (200 eV) for the three commensurate adsorption structures of benzene adsorbed on Ru(0001): $p(2\sqrt{3} \times 2\sqrt{3})R30^\circ$, $c(2\sqrt{3} \times 4)rect$, and $p(\sqrt{7} \times \sqrt{7})R19^\circ$; [01Bra].

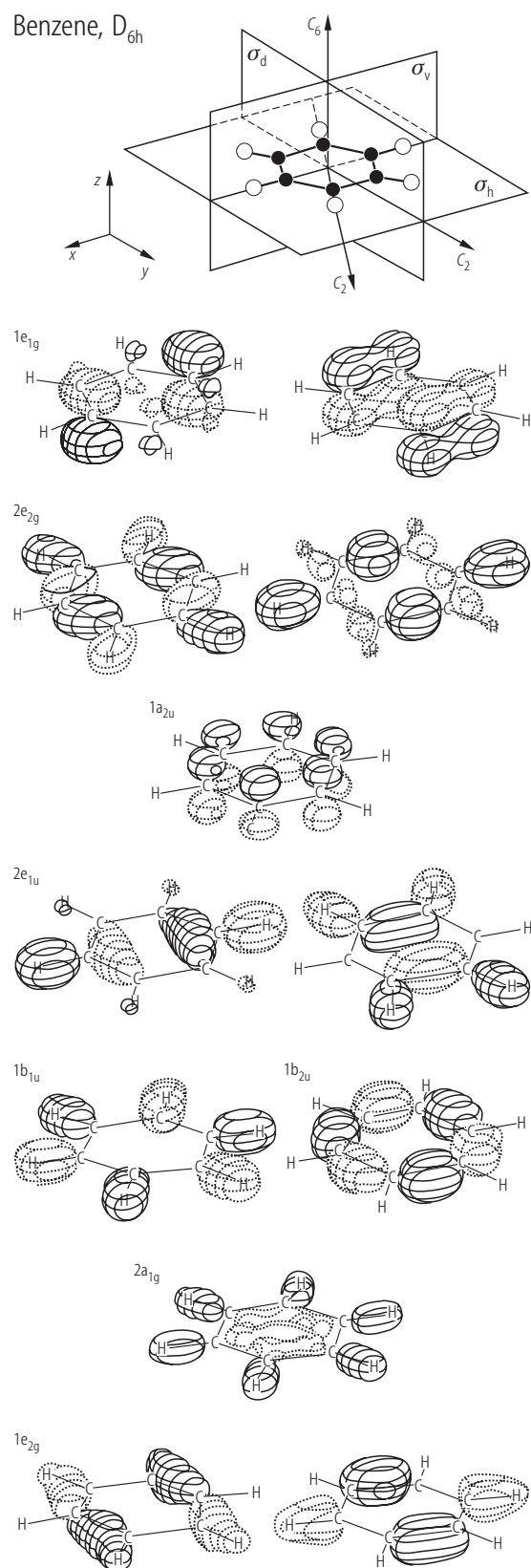
Benzene, D_{6h} 

Fig. 5. Top: schematic drawing of benzene with its symmetry elements in the gas phase. Only one out of three equivalent C_2 rotation axes and $\sigma(d)$ / $\sigma(v)$ mirror planes are indicated. Bottom: occupied molecular orbitals after Jørgensen and Salem [73Jor]; [96Ste].

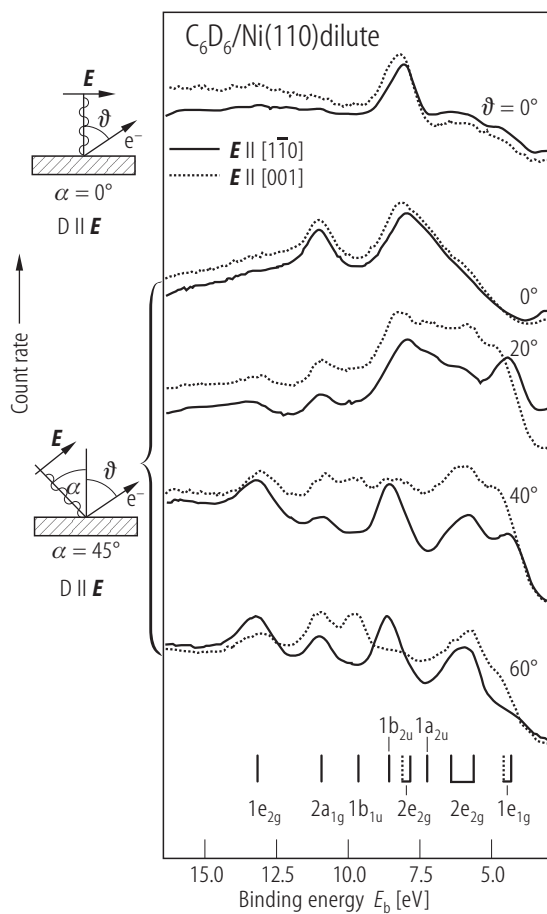


Fig. 6. Angle-resolved UPS spectra of a dilute layer (~ 0.1 ML) of deuterated benzene on Ni(110) at various experimental geometries, using a photon energy of 30 eV. Orbital positions and assignment are indicated in form of a bar diagram. D indicates the plane of electron detection, E the orientation of the electrical field vector. From the pronounced polarization and emission angle dependencies the orientation of the molecule is determined as C_{2v} ; [94Ste].

Fig. 7: see next page

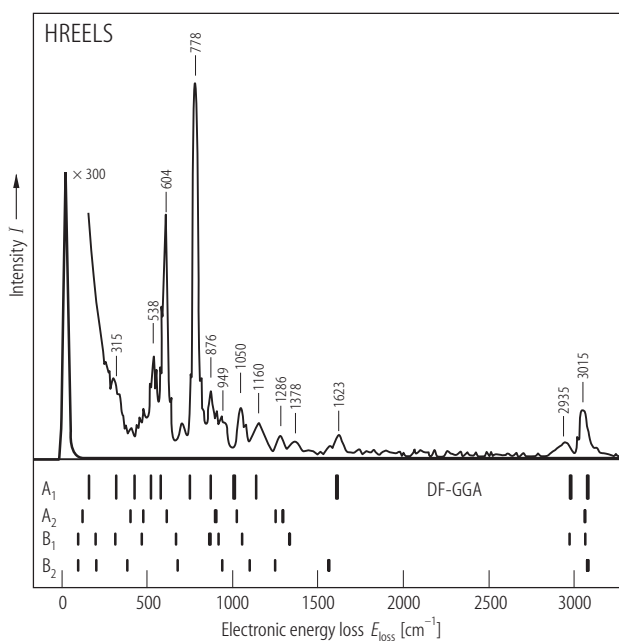


Fig. 8. HREELS spectrum of benzene on (2 \times 1) Si(100) together with the calculated normal frequencies of a $C_6H_6Si_{13}H_{12}$ cluster. The calculated frequencies are indicated by vertical bars, separated according to the four irreducible representations of the symmetry group C_{2v} ; [00Sta].

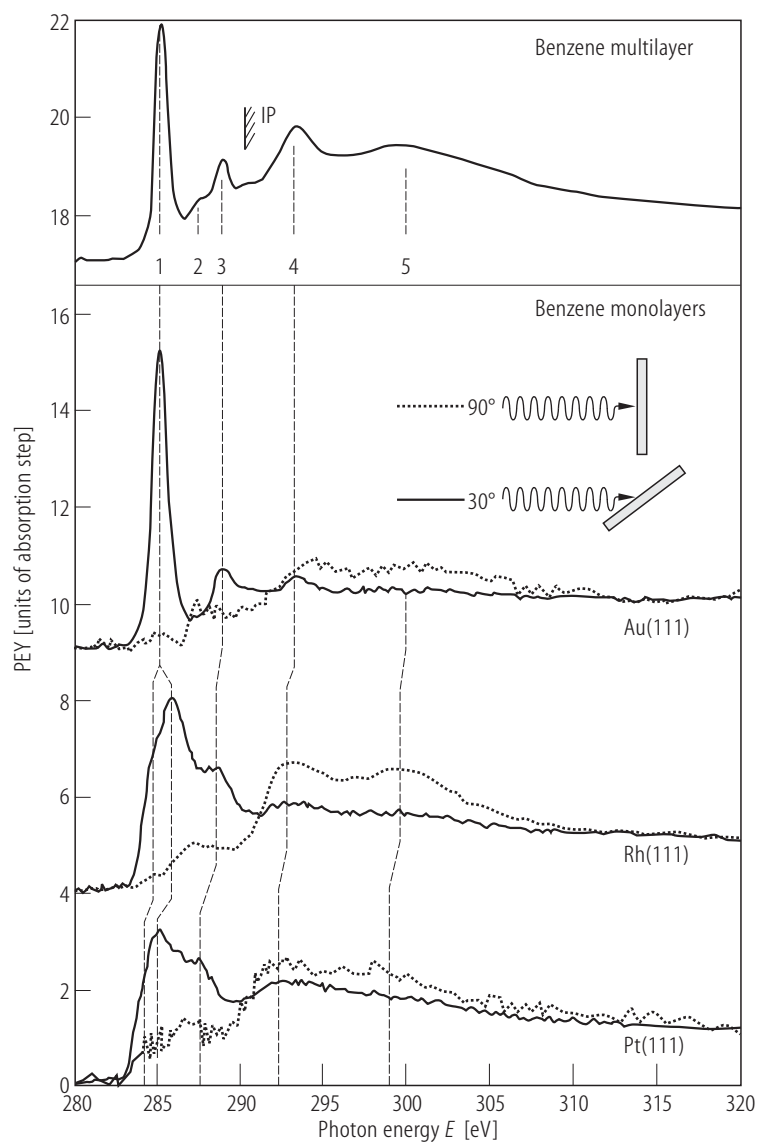


Fig. 7. NEXAFS spectrum of a benzene multilayer at 120 K (top) and polarization dependence of NEXAFS spectra for benzene monolayers adsorbed on Au(111), Rh(111), and Pt(111). The disappearance of the π -resonance at around 285 eV for normal incidence spectra (dotted) indicates flat-lying molecules on all three surfaces (PEY = partial electron yield); [98Wei1].

Fig. 9.: see next page

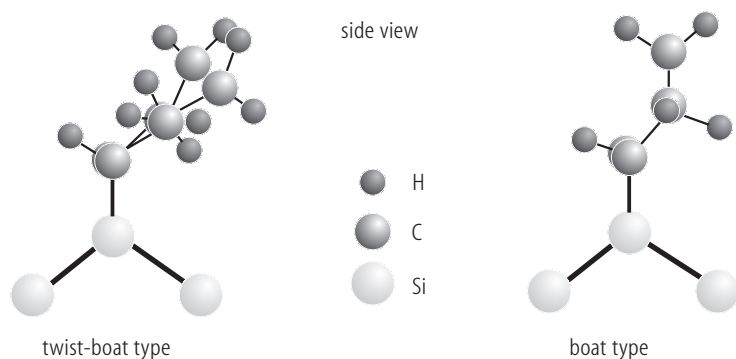


Fig. 10. Models of adsorbed cyclohexene on Si(100)(2x1); [01Yos].

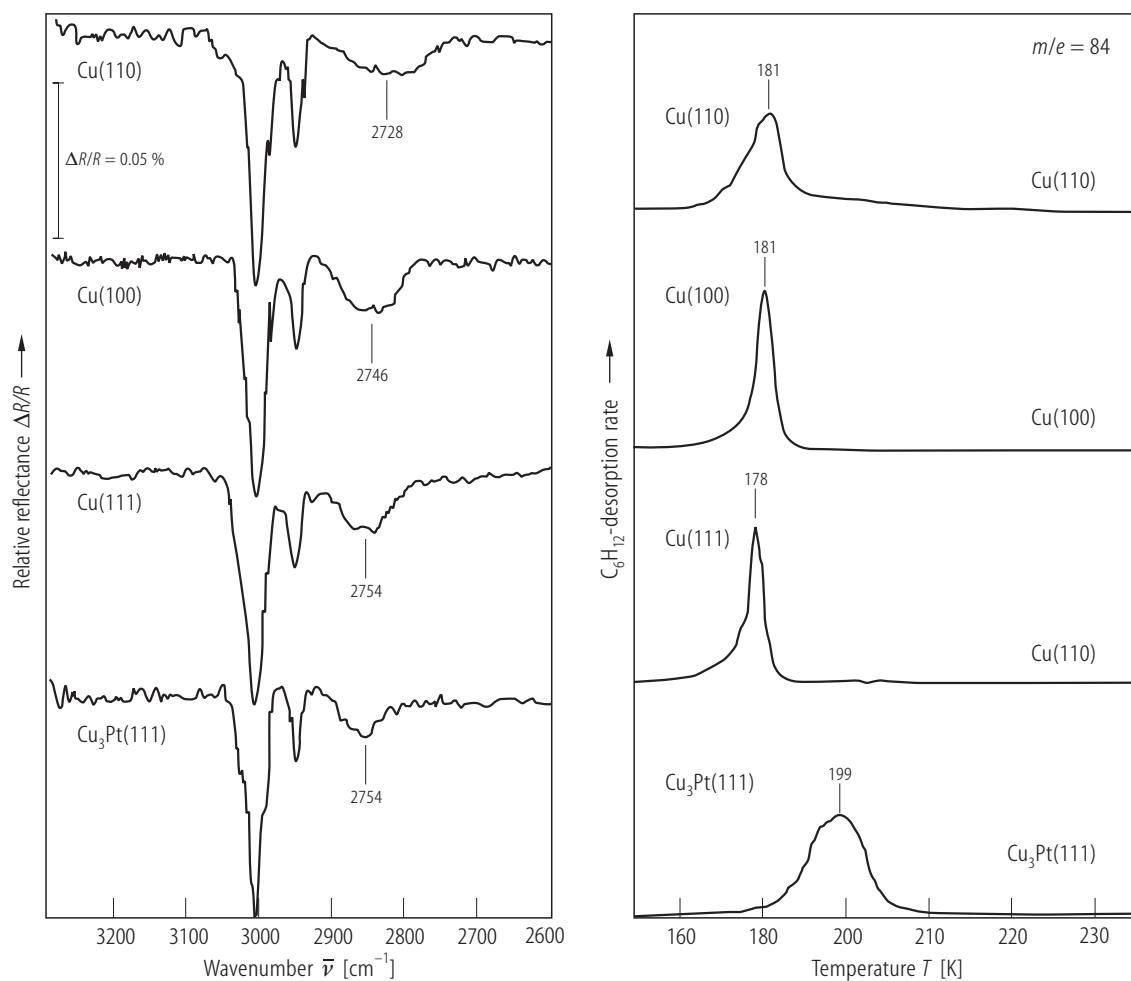


Fig. 9. Comparison of RAIRS (left) and TPD (right) studies of submonolayer coverages of cyclohexane on Cu(110), Cu(100), Cu(111) and $\text{Cu}_3\text{Pt}(111)$ surfaces. The desorption temperature of cyclohexane is independent of the surface coverage up to a monolayer saturation on all surfaces. The wave numbers of the softened modes are denoted; [98Tep].

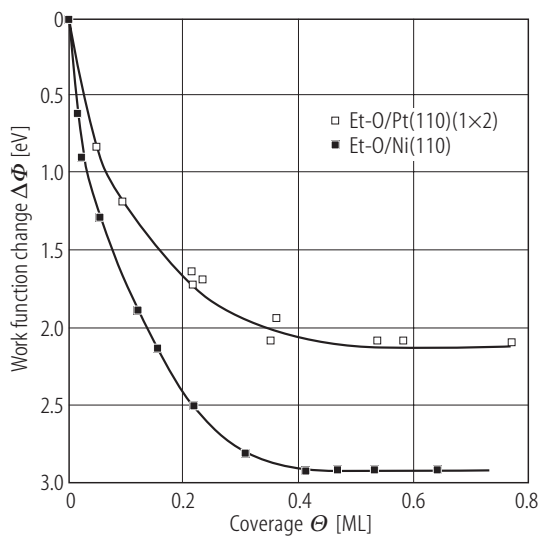


Fig. 11. Change in work function as a function of coverage for ethylene oxide (Et-O) on Pt(110) (1x2) and Ni(110); adsorption temperature: 100 K.; [93Wei2].

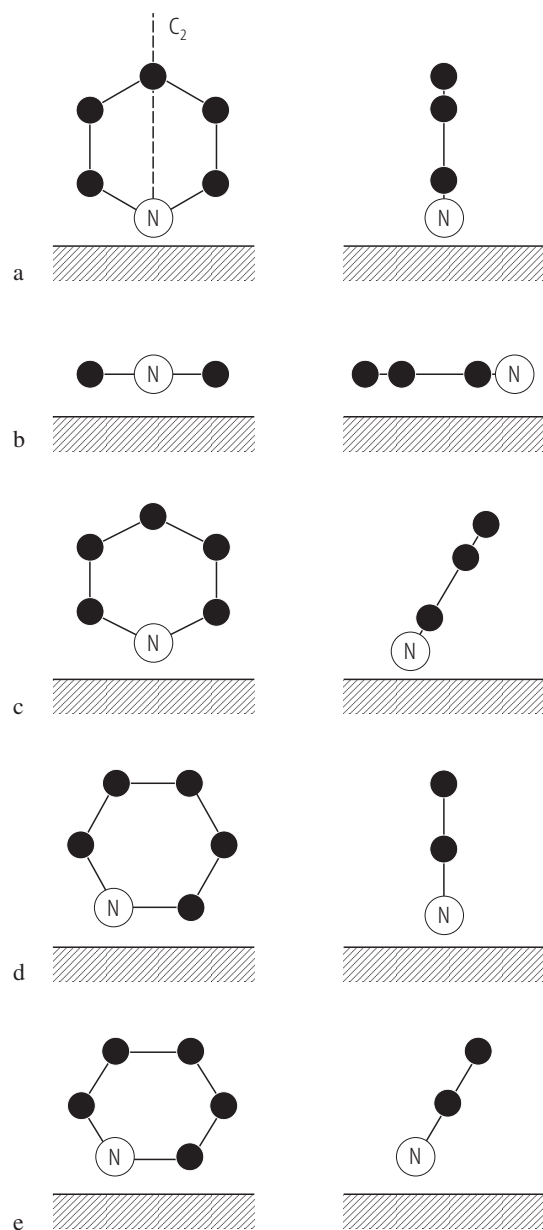


Fig. 12. (a) perpendicular adsorption via the nitrogen lone pair electrons, (b) flat adsorption of the aromatic ring via the π -electrons, (c) tilted adsorption via the nitrogen lone pair orbitals and the π -electrons, and (d,e) edge on adsorption through the N and C(2) atoms with the molecular plane more or less perpendicular to the surfaces - i.e. formation of α -pyridile by breaking the C-H bond; [99Gie].

3.8.7.11 References for 3.8.7

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