

**Supporting Information** for the Manuscript:

**Adsorption Geometry and Self-Assembling of Chiral Modifier (R)-(+)-1-(1-naphthylethylamine) on Pt(111)**

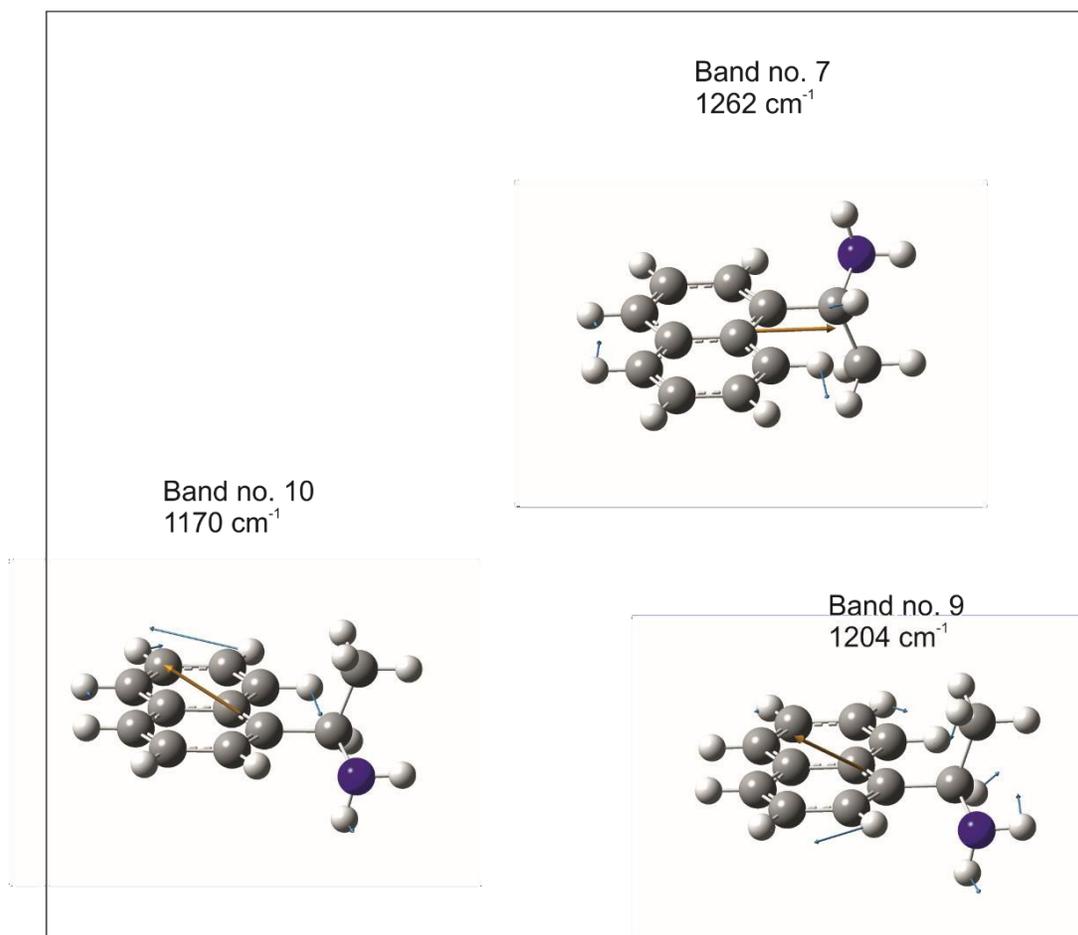
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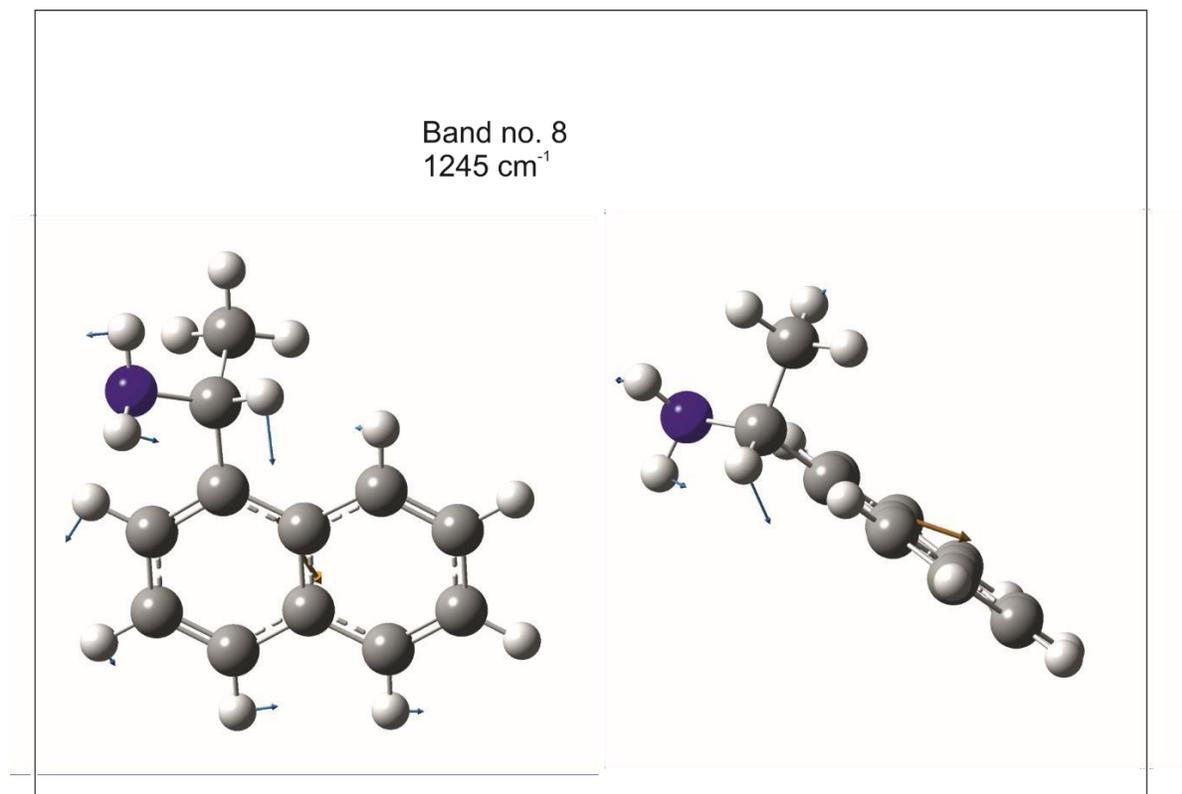
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**1. Graphical representation of the selected vibrational modes.**



**Figure S1:** Visualization of selected vibrational modes of R-NEA, with labels 7,9 and 10 corresponding to the same labels in Figure 1 and Table 1. The experimental IR bands observed in the multilayers of R-NEA are indicated. The displacement vectors and the resulting dynamic

dipole moment for each mode are indicated in blue and orange, respectively. The origin of the dynamic dipole moment is placed arbitrary in the R-NEA center of mass.

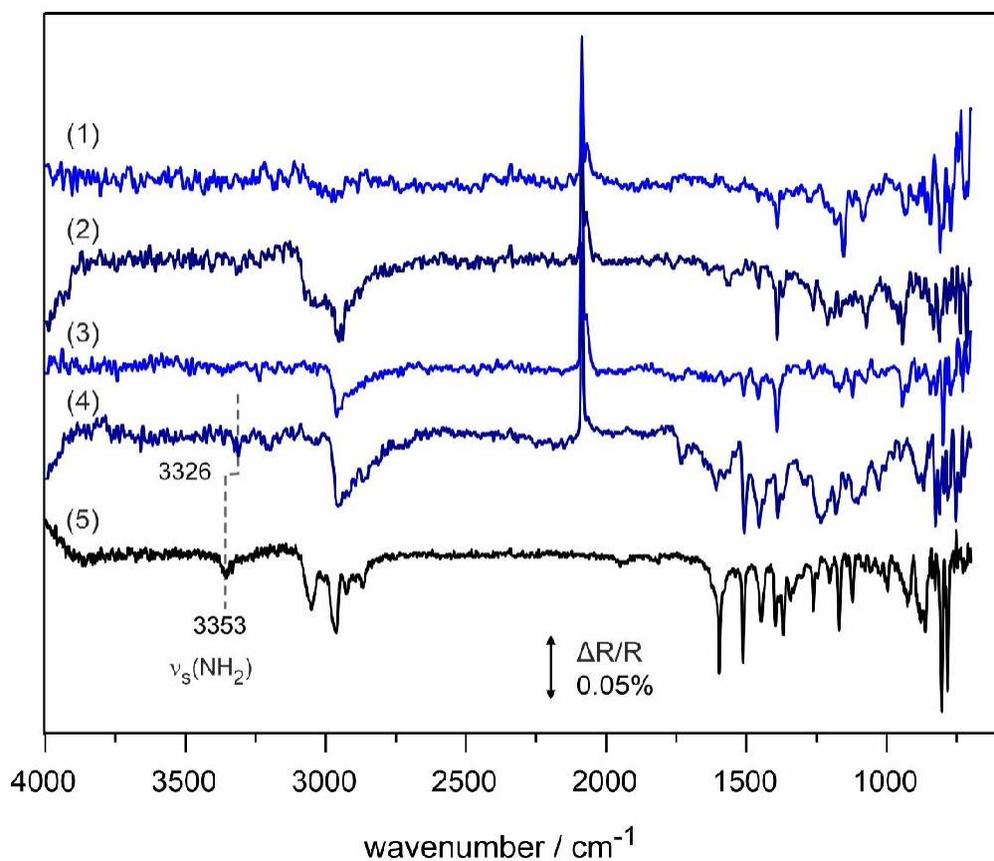


**Figure S2:** Visualization of band (8) corresponding to the same label in Figure 1 and Table 1. The experimental IR band observed in the multilayer of R-NEA is indicated. The displacement vectors and the resulting dynamic dipole moment for each mode are indicated in blue and orange, respectively. The origin of the dynamic dipole moment is placed arbitrary in the R-NEA center of mass. For better representation of the corresponding vibrational mode, it is presented at two different perspectives.

The experimentally observed band at 1245  $\text{cm}^{-1}$ , can be also assigned to band (8), which corresponds mainly to aromatic breathing and amine deformation. The dynamic dipole moment of this band lies slightly out of plane of the naphthyl ring and oriented along its short axis (with a small offset from the axis).

## 2. Full range of the spectrum (5) from Figure 3 of the main manuscript.

The full range IR spectra of R-NEA adsorbed on Pt(111) at 160 K. The region around  $3000\text{ cm}^{-1}$  corresponds to the C-H stretching vibrations of the naphthyl ring and the ethyl-group. The stretching (C-N) vibrational band is also situated in this range, overlapping with the stretching C-H vibrations. The band at  $3353\text{ cm}^{-1}$  (spectrum 5) is related to the N-H symmetric stretching vibration of the amine group. Probably, a very small band at similar frequency ( $3326\text{ cm}^{-1}$ ) exists in the spectrum (4). Note that the sensitivity of the MCT detector employed in this study is rather low in the frequency range above  $3000\text{ cm}^{-1}$ . The calculated frequencies for the symmetric and asymmetric  $\nu(\text{N-H})$  vibrational bands are  $3376$  and  $3451\text{ cm}^{-1}$ , correspondingly (calculated in this study). The positive peak at around  $2100\text{ cm}^{-1}$  arises from the replacement of a small amount of CO molecules, which were adsorbed from background prior to R-NEA exposure.



**Figure S3.** Full range IR spectra of R-NEA on Pt(111) recorded at 160 K after exposure for (1) 1, (2) 1.5, (3) 2, (4) 5 and (5) 10 minutes. The data correspond to the spectra (1) - (5) in the Figure 3 of the main manuscript.

The vibration related to the  $\nu_s(\text{N-H})$  symmetric stretching vibration of the amine group appears as at a notable intensity only in the very last spectrum ( $3353\text{ cm}^{-1}$ ), corresponding to roughly a monolayer coverage of R-NEA. In the spectrum (4), this vibrational band is hardly seen and is shifted to  $3326\text{ cm}^{-1}$ . It should be noted that the baseline in this spectrum is rather noisy and it cannot be excluded that the peak at  $3326\text{ cm}^{-1}$  is not real and arises just as a part of a noisy baseline. Clearly, the  $\nu_s(\text{N-H})$  vibrational band is quite pronounced only at the monolayer coverage, at which the molecules are strongly inclined both along the short and the long axes of the naphthyl ring (see the main text of the manuscript). At lower coverages, this band might be not seen or have a significantly lower intensity due two major reasons – the low coverage and/or the metal surface selections rule. Based on the available dataset, we cannot discriminate between these reasons due to low sensitivity of the MCT detector in this frequency range. The antisymmetric N-H stretching vibration was not observed even at the highest coverage.