Supporting information for: Adsorption behavior of organic molecules: a study of benzotriazole on Cu(111) with spectroscopic and theoretical methods

Chiara Gattinoni[1], Panayiotis Tsaousis[2], Chanan Euaruksakul[2,3], Rachel Price[2], David A. Duncan[3], Tod Pascal[4], David Prendergast[4], Georg Held[2,3], and Angelos Michaelides[1]

[1]Thomas Young Centre, London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, Gower Street, WC1E 6BT, UK
[2]Department of Chemistry, University of Reading, Reading RG6 6AD, UK
[3]Diamond Light Source Harwell Science and Innovation Campus, Didcot OX11 0QX, UK
[4]Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA
E-mail: g.held@reading.ac.uk, angelos.michaelides@ucl.ac.uk

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S1 Formation energy of the adsorbed systems

The complete set of candidate structures considered for this work is shown in Fig. S1. In order to

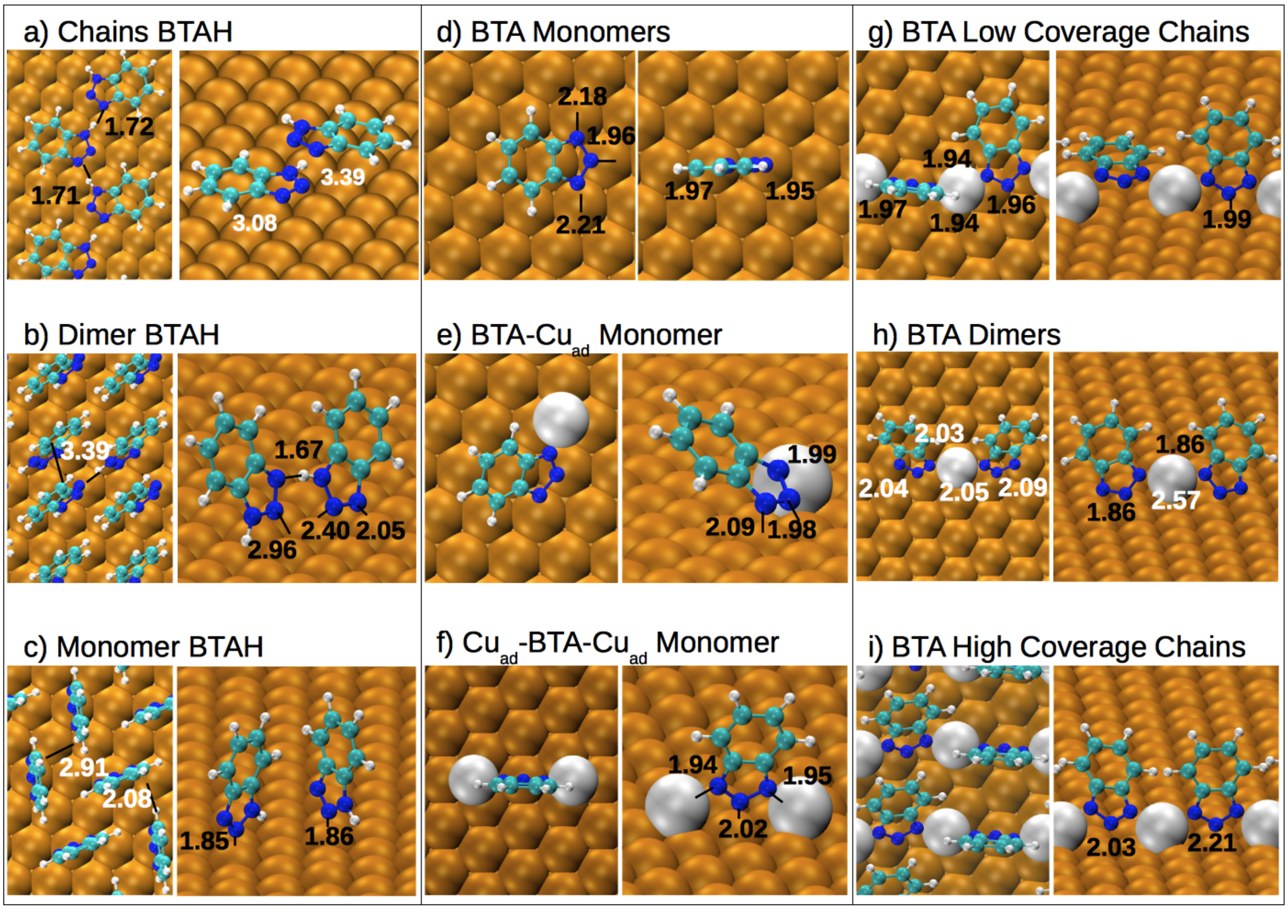

Figure S1: Summary of the benzotriazole structures considered in this work. Cu atoms are copper colored, N blue, C cyan H white. Cu adatoms are in gray. Relevant bond lengths between benzotriazole molecules and the substrate are also shown.

"rank" them in terms of stability, the cost of dissociation into BTA and H and of the formation of copper adatoms needs to be taken into account. We thus use the definition of adsorption energy given in the main manuscript which considers these energy costs:

$$\mathrm{E}^{\alpha}_{\mathrm{ads}} = \mathrm{E}_{\mathrm{system}} - N_{\mathrm{BTAH}}\mathrm{E}_{\mathrm{BTAH}} - \mathrm{E}_{\mathrm{slab}} - \alpha\Delta\mathrm{N}_{\mathrm{Cu}}g_{\mathrm{Cu}}, \tag{S1}$$

where $\mathrm{E}_{\mathrm{system}}$ is the total energy of $\mathrm{N}_{\mathrm{BTAH}}$ adsorbed benzotriazole molecules, dissociated or not, on Cu(111). For the deprotonated case, BTA and H are co-adsorbed on the surface. $\mathrm{E}_{\mathrm{BTAH}}$ is the total energy of BTAH in the gas phase. $\Delta\mathrm{N}_{\mathrm{Cu}}$ is the number of copper adatoms, g_{Cu} their formation energy and $\mathrm{E}_{\mathrm{slab}}$ the total energy of the Cu(111) slab. Considering that some adatoms might already be present on the surface, a prefactor α, ranging from 0 to 1 has been added to $\Delta\mathrm{N}_{\mathrm{Cu}}$, where 0 signifies that all adatoms are already available on the surface and 1 that all adatoms are extracted from the bulk. The experimental reality is likely to lie in between these endpoint values. The adsorption energies are reported in Table S1 for all structures in Fig. S1. They show that structures formed by intact BTAH are less favorable than many dissociated structures, although the energy barrier which could be an obstacle to dissociation is not included here.

Structure	$E_{\text{ads}}^{\alpha=0}$	P($\alpha = 0$)	$E_{\text{ads}}^{\alpha=1}$	P($\alpha = 1$)
50% Coverage				
BTAH Chains (a)	-1.46	0.0	-1.46	0.0
BTA Monomers (d)	-2.42	0.0	-0.69	0.0
BTA-Cu_{ad} Monomer (e)	-2.42	0.0	-0.69	0.0
Cu_{ad}-BTA-Cu_{ad} Monomer (f)	-2.42	97.7	-0.69	0.0
BTA Chains (g)	-2.31	2.2	-1.45	0.3
BTA Dimers (h)	-2.02	0.0	-1.59	99.6
100% Coverage				
BTAH Dimer (b)	-1.24	0.0	-1.24	0.0
BTAH Monomer (c)	-1.24	0.0	-1.24	0.0
BTA Dimers (h)	-2.02	100.0	-1.42	1.7
BTA Chains (i)	-2.36	1.7	-1.15	98.3

Table S1: Formation energies for the structures considered in this study and shown in Fig. 2. The energies, in eV, are calculated using Eq. S1. The Boltzman probability P at 300 K is also reported.

In order to establish which are the most prevalent dissociated structures at room temperature the Boltzman probability is obtained for $\alpha = 0, 1$. The results are shown in Table S1. The Cu_{ad}-BTA-Cu_{ad} monomer (simply referred to as Monomer subsequently and in the main manuscript), chain and dimer structures are the only ones which are competitive at this temperature.

For these three structures, the probability for α varying between 0 and 1 is shown in Fig. S2. It shows that three regimes are to be expected for low coverage of BTA (top graph, Fig. S2): one where the dominant structures are the monomers stabilized by two Cu_{ad}s (Fig. S1f), one where the low coverage chains of Fig. S1g are favorable and a third where dimers chains are observed (Fig. S1h). Similarly, for high coverage two regimes are possible (bottom graph, Fig. S2): for values of α up to ~ 0.8 closely packed chains (Fig. S1i) are expected to be the dominant feature, while for higher values dimers are predicted.

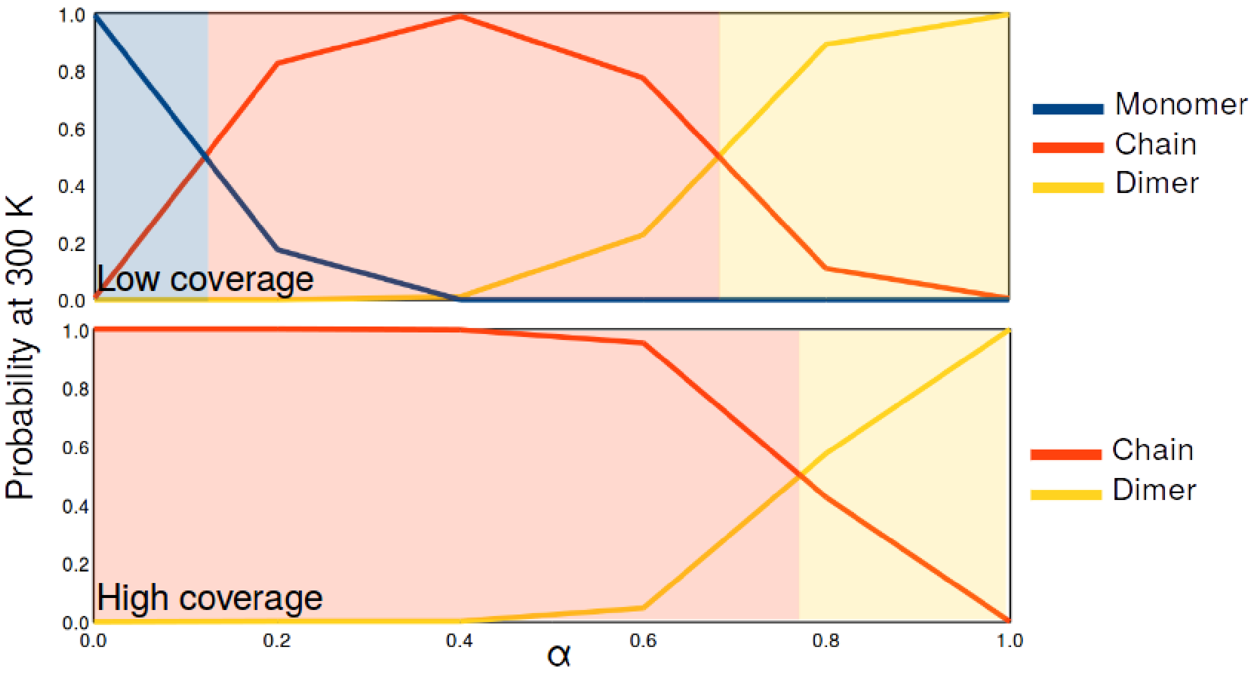

Figure S2: Boltzmann probability at 300 K as a function of the factor α in Eq. S1, representing the number of adatoms which are extracted from the bulk. The following structures are considered: at low coverage (top) the monomer (Fig. 2a), chain (Fig. 2b) and dimer (Fig. 2c, at high coverage (bottom) the chain (Fig. 2d) and dimer (Fig. 2c).

S2 NEXAFS C K-edge spectra

The π^* resonance leads to two strong peaks in all the model C K-edge spectra, as shown in Fig. S3. Most structures give the highest intensity for almost normal incidence ($\theta = 87°$), reflecting the upright position of the molecules with respect to the surface. An exception are the low coverage chains of BTA (Fig. S3b) and of BTAH (Fig. S3e), where some or all of the molecules are lying flat on the Cu(111). The σ^* resonance is instead characterized by a broad feature with one main peak, and multiple smaller peaks. Conversely to the π^* feature, it has the highest intensity for grazing incident angles for all structures except the low coverage chains.

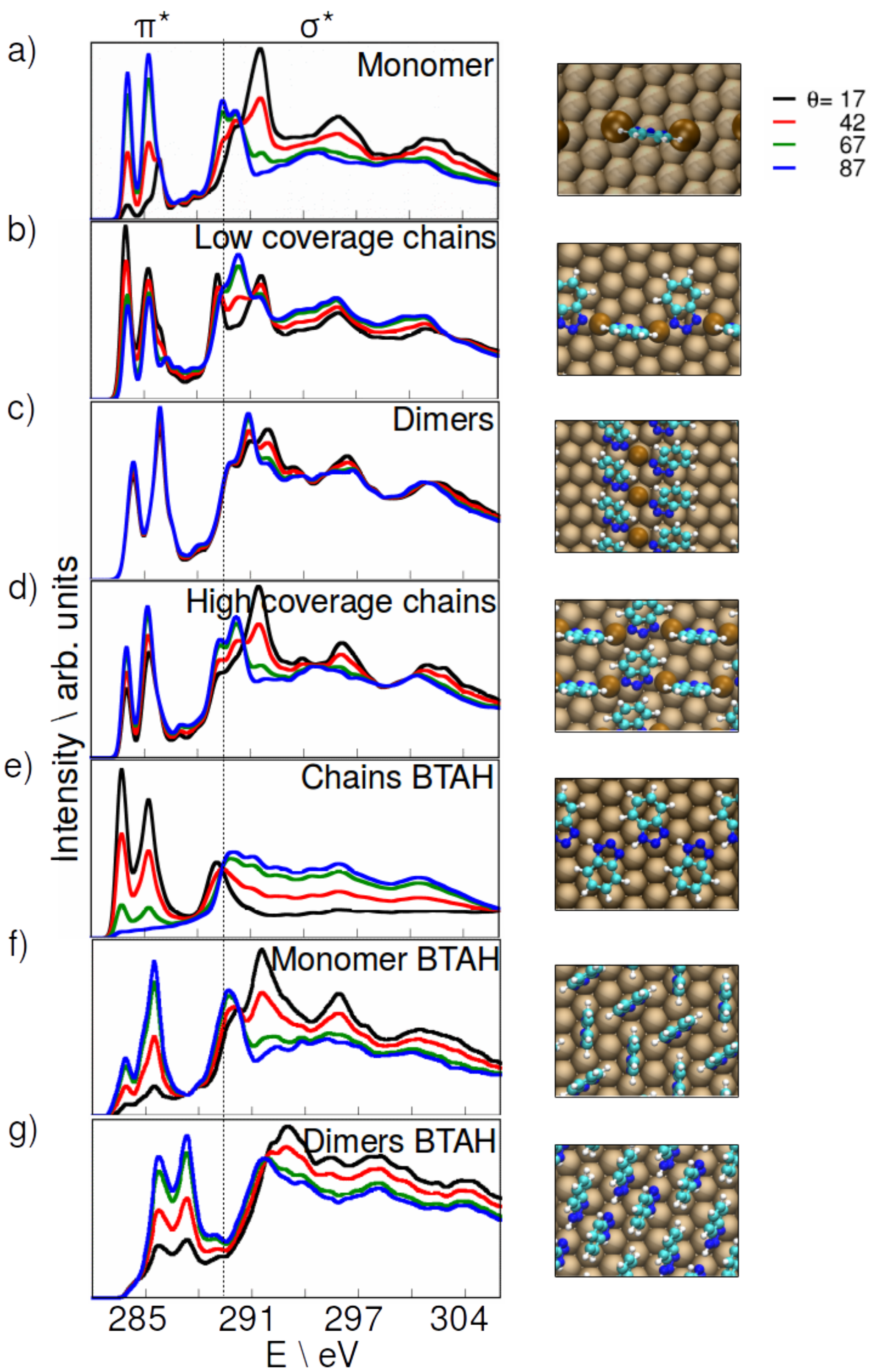

Figure S3: Simulated C K-edge NEXAFS spectra for the structures considered in this work, shown on the right. a) low coverage BTA monomer stabilized by two Cu_{ad}; b) low coverage BTA chains ($\frac{1}{10}$ ML); c) high coverage BTA chains ($\frac{1}{5}$ ML). d) BTA Dimers ($\frac{1}{7}$ ML for low coverage, $\frac{1}{4}$ ML for high coverage). e) low coverage BTAH ($\frac{1}{16}$ ML) f) high coverage BTAH dimers ($\frac{1}{4}$ ML) g) high coverage BTAH monomers ($\frac{1}{4}$ ML) The dark brown atoms shown on top of the Cu(111) surface (depicted in light brown) are copper adatoms. The NEXAFS spectra have been calculated for $\theta = 17, 42, 67, 87°$, where θ is the angle between the polarization and the normal to the surface.

S3 Mixed Dimer-Chain NEXAFS

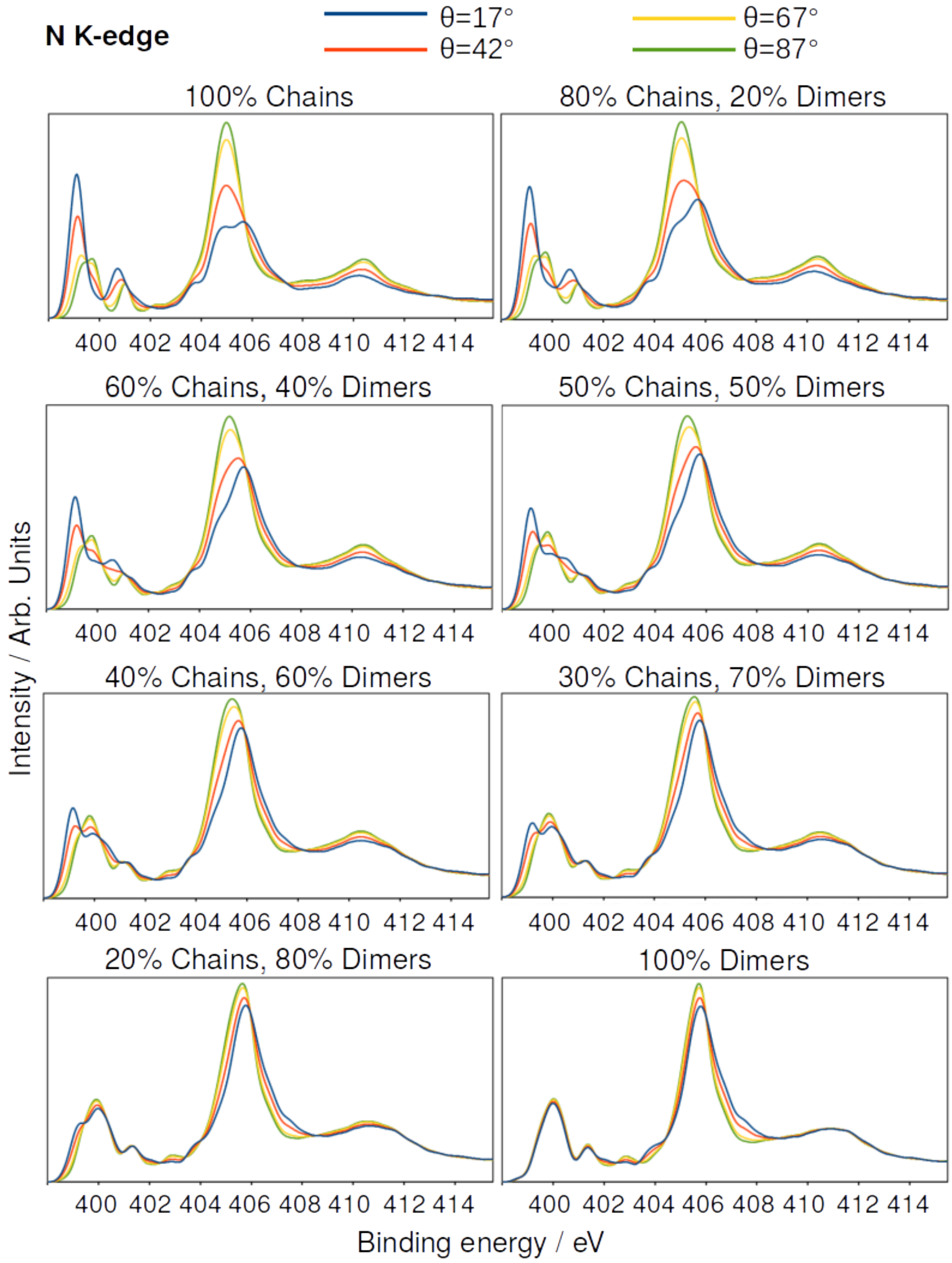

Figure S4: N K-edge calculated spectra corresponding to mixed low coverage chains (Fig. 2b) and dimer (Fig. 2c) structures.

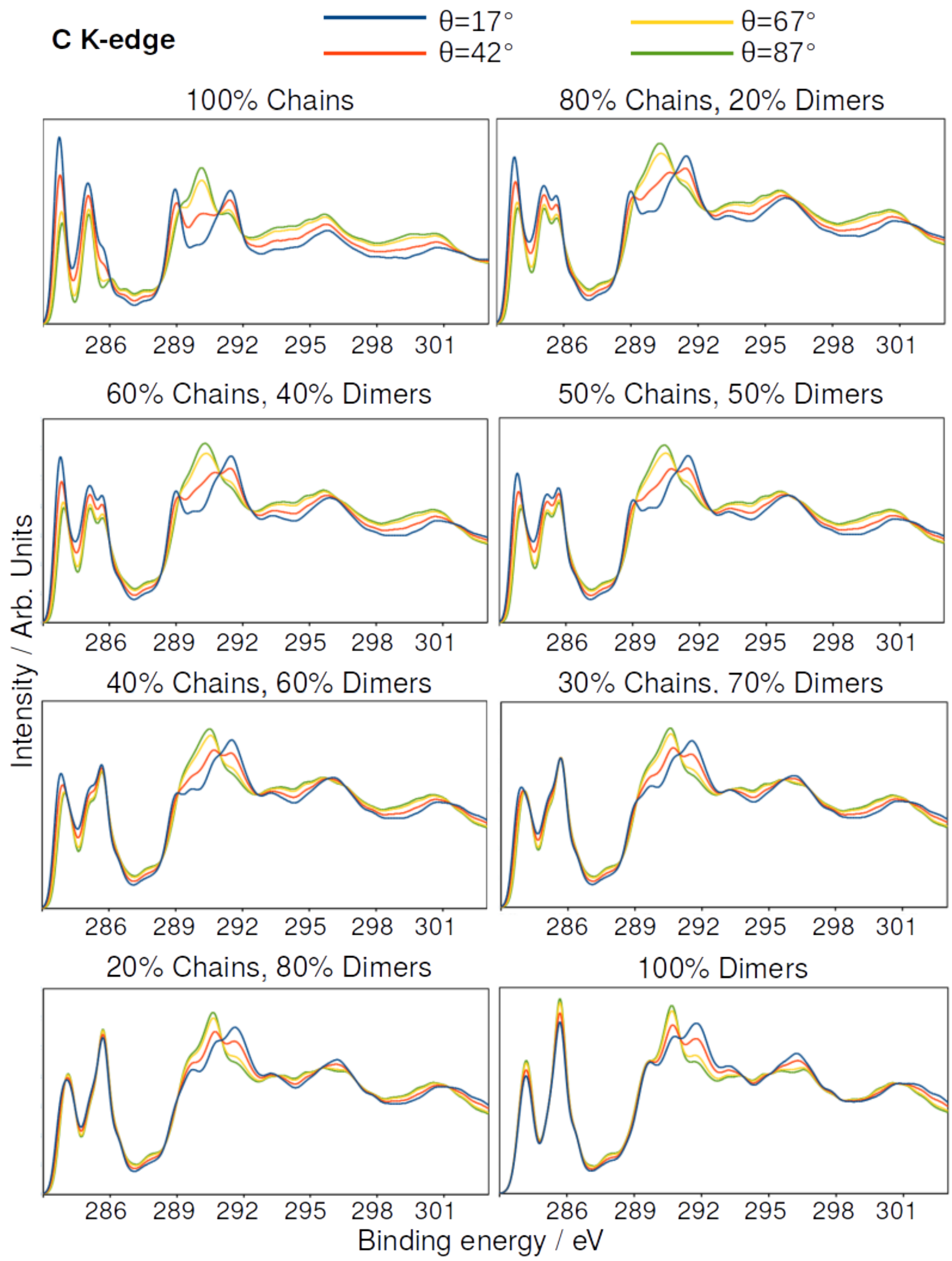

Figure S5: C K-edge calculated spectra corresponding to mixed low coverage chains (Fig. 2b) and dimer (Fig. 2c) structures.

S4 Mixed Dimer-Chain XPS

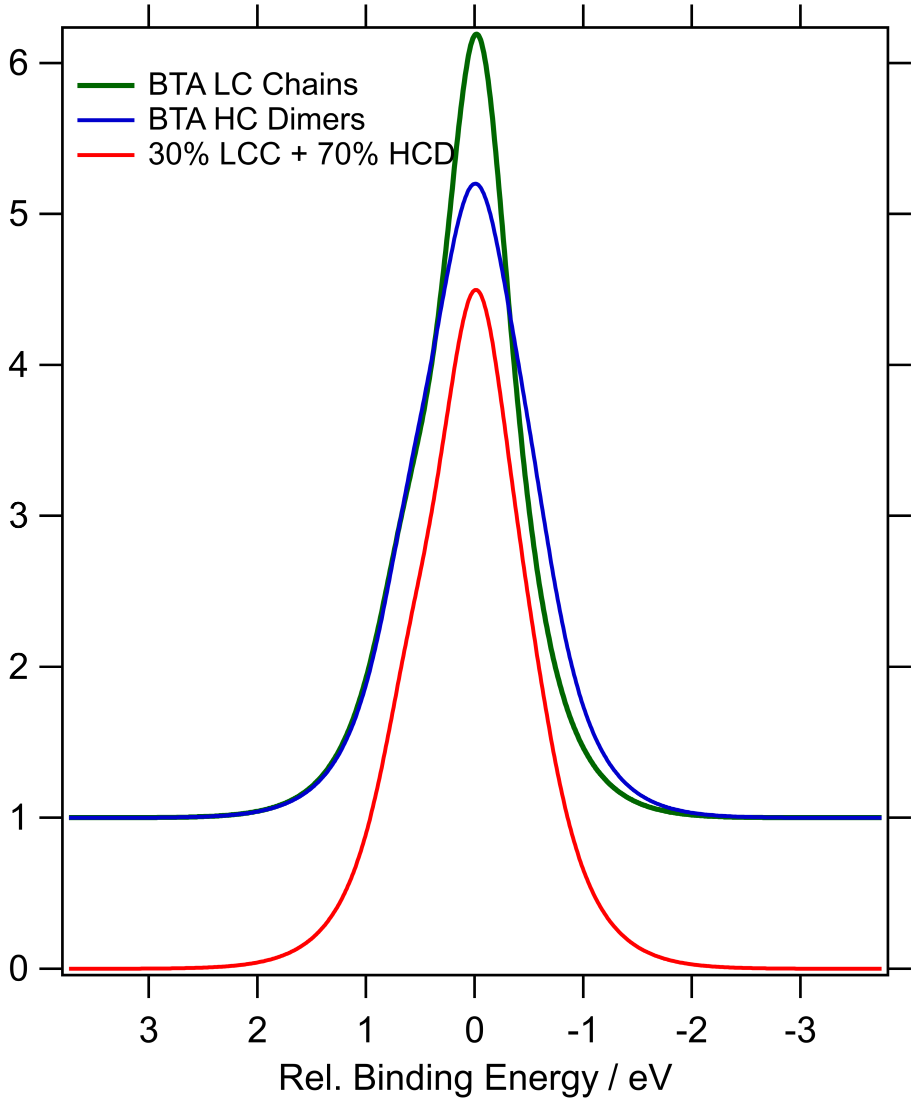

Figure S6: Calculated XPS spectra for the deprotonated low coverage chains (green), high coverage dimers (blue) and a 30% chains-70% dimers mixture (red).

S5 NIXSW

The normal incidence X-ray standing wave (NIXSW) technique exploits the standing wavefield resulting from the coherent interference of incident and reflected beams at the Bragg condition. As the incident photon energy is scanned over the Darwin reflectivity curve the variation in the wavelength of the incident and reflected light results in a comparable variation in the wavelength of the standing wavefield. This results in the antinodes of the standing wavefield moving from half way between the scattering planes to lying on the scattering planes. Thus, as the standing wavefield will extend beyond the surface of the crystal in which it was generated, any adsorbate that lies above the surface will experience a variation in the amplitude of the standing wavefield as a function of the photon energy. This variation in amplitude will result in a modulation of the photoemission intensity that is indicative of the average position of the adsorbate between the projected scattering planes (coherent position) and the fraction of atoms that occupy that position (coherent fraction). If the scattering plane coincides with the surface plane, then the coherent position will be equivalent to the height of the adsorbate above the surface of the crystal, assuming that relaxation of the atoms in the outermost substrate layers can be neglected.

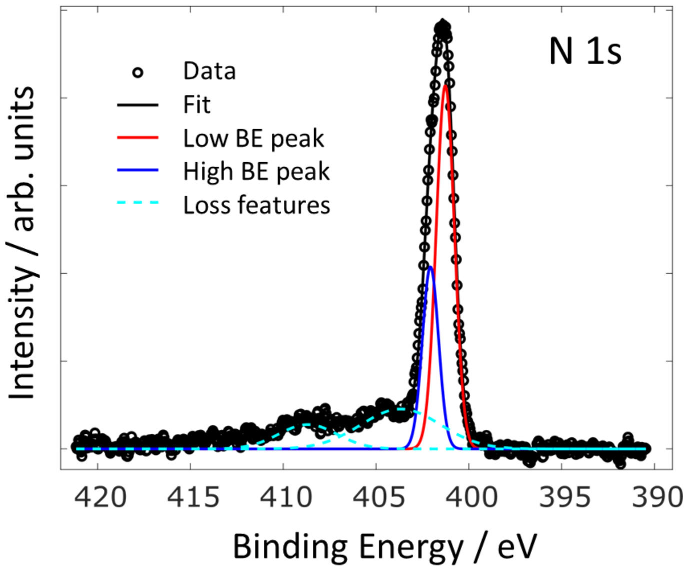

Figure S7: Example of peak fitting of the NIXSW data.

The measurements were performed at beam line I09 at Diamond Light Source in the same end-station that was used for XPS and NEXAFS. The intensity and width of the (111) Bragg reflection of Cu ($\approx$ 2970 eV at 300 K) was acquired from a fluorescent screen mounted onto the port through which the incident photons entered. This Darwin reflectivity curve had a full width half maximum of 0.82 eV. It is as a measure of the energy broadening due to imperfections in the monochromator (Si(111) double-crystal) and the mosaicity of the single crystal substrate (about 0.7° in this case) and was incorporated in the data analyisis through convolution with a Gaussian of the same width. The relative X-ray absorption of the N atoms was monitored through the integrated intensity of the N 1s photoemission peaks. Photoemission spectra were acquired using a VG Scienta EW4000 HAXPES hemispherical electron analyser with an angular acceptance range of $\pm$30°, which was orientated such that there was an angle of 90° between the incident photon beam and the centre of the analyser in the plane of the photon polarisation. The N 1s photoemission spectra were acquired in fixed energy mode with a pass energy of 500 eV. A calibration curve was generated by dividing a fixed energy mode scan by a swept energy mode scan with the same step size and comparable acquisition time acquired over an area of the XP spectrum that was comparably flat. This calibration curve was used to normalise the N 1s photoemission spectra, which were then fitted with a linear background and four Gaussian peaks corresponding to the two chemically distinct N species in the adsorbed molecule and two satellite features at higher binding energy (see Fig. S7). Note that the binding energy axis in Figure S7 is not calibrated. Therefore the energies differ from those stated in the main text.

Non-dipolar effects, due to the angular dependence of the photoemission, were modelled using theoretically calculated values, specifically with a backward-forward asymmetry parameter, Q, of 0.115 (assuming $\Theta = 18°$ as defined in Ref. **?**) and fitted to the energy dependence of the two peak intensities.

The N 1s NIXSW measurements were repeated five times on different spots on the sample and the absorption profiles fitted separately to produce average values for the coherent fraction and coherent position, and the associated random uncertainty (standard error at 2σ). Figure 8 of the main article shows average absorption profiles and fits.

S6 Summary of benzotriazole structures

In the following, .xyz files of the most relevant adsorbed benzotriazole structures, shown in Fig. S1 are shown.

S6.1 Chains BTAH

```
156
btah_chains
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S6.2 Dimer BTAH

```
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N 1.2274009599999993 0.610290035 2.551595374999998
N 2.80580292 1.231394145 1.1859189850000007
N 1.7207658000000001 0.4646936350000004 1.304043704999998
N -2.0434986100000003 -2.4879775449999997 2.097699145
N -0.8727499700000005 -1.021181895 3.1630067949999976
N -1.0245311800000003 -1.619417905 2.001999725000001
Cu -0.4133453 3.312859265 -7.026516255000001
Cu 2.13363055 3.312859265 -7.026516255000001
Cu -4.23380908 -3.3043780949999997 -7.026516255000001
Cu -1.6868332300000004 -3.3043780949999997 -7.026516255000001
Cu -2.96032115 -1.098632305 -7.026516255000001
Cu -0.4133453 -1.098632305 -7.026516255000001
Cu -1.6868332300000004 1.107113475 -7.026516255000001
Cu 0.86014262 1.107113475 -7.026516255000001
Cu 0.8640320199999993 4.038887295 -4.982134695000001
Cu 3.41182378 4.040854525 -4.9803564850000015
Cu -2.95955157 -2.563749595 -4.982473165
Cu -0.4097714800000003 -2.564018625 -4.984856515000001
Cu -1.6796641 -0.3517714150000002 -4.972471805000001
Cu 0.8625094499999997 -0.35191520499999984 -4.959319725
Cu -0.4078406600000002 1.8411327350000002 -4.963963385000001
Cu 2.13918146 1.8426684949999996 -4.970495245
Cu -0.3991866800000001 -4.039070815 -2.947873155
Cu -2.95675552 -4.040854525 -2.951838005000001
Cu 0.8577671099999997 -1.827609365 -2.9198915850000002
```

Cu -1.6817239300000004 -1.823472585 -2.938011105000001
Cu 2.1542985499999996 0.386999525 -2.8815477650000005
Cu -0.41931114 0.38356032500000015 -2.855326625
Cu 3.4156744199999998 2.5726848250000005 -2.891357375
Cu 0.8742689999999995 2.569107155 -2.8991961050000015
Cu -0.37184153000000064 3.357872715 -0.8678332950000005
Cu 2.1394650999999993 3.3644948350000004 -0.8724796350000013
Cu -4.213768420000001 -3.3077127849999997 -0.8557098250000017
Cu -1.6730423200000004 -3.3259634250000003 -0.930574674999999
Cu -2.9575163300000002 -1.136063055 -0.9035299350000017
Cu -0.4237183200000003 -1.1346941449999999 -0.8563728049999995
Cu -1.6320359500000001 1.1702228450000003 -0.750362814999999
Cu 0.8648925999999997 1.1094244949999996 -0.8393849750000015

S6.3 Monomer BTAH

```
60
btah_monomer
H 4.950434515 0.30874271500000017 6.672025655000002
H 5.827283875 0.07606950499999998 9.601416935
H 4.749143555000001 -0.02091534500000014 11.845582525000001
H 2.2815320750000003 0.03270134499999999 12.096632255
H 0.7843408649999999 0.185683225 10.089676305000001
H -1.083366905 -1.315517045 6.741717725000001
H -0.40877341499999975 -1.7868750150000001 9.698600115000001
H -0.8630962049999997 -0.6902792149999999 11.888992215000002
H -2.172157805 1.413806005 12.034103675
H -3.093383605 2.503539725 9.974367664999999
C 3.890363365 0.177925675 8.593143435000002
C 4.740887735 0.09178188500000006 9.703363405000001
C 4.122925424999999 0.040837794999999844 10.949684605000002
C 2.7148186250000004 0.0735618950000001 11.092274845000002
C 1.872017435 0.1551566750000002 9.989549365000002
C 2.478210764999999 0.206300315 8.722218855000001
C -1.5064700850000001 -0.240266235 8.611713635000001
C -0.9838724650000001 -0.860993355 9.754040185000001
C -1.2484842350000003 -0.2366699849999998 10.969804135
C -1.9973674149999998 0.9618741449999999 11.052391295
C -2.511746505 1.5796747449999997 9.918149265
C -2.259545895 0.960287745 8.681573365000002
N 4.093719064999999 0.26567153500000007 7.2518539749999995
N 1.914815775 0.3103712249999999 7.469679984999999
N 2.9013852350000002 0.3428760350000002 6.601058994999999
N -1.4968516149999997 -0.538299095 7.284237924999999
N -2.658955545 1.3144811349999999 7.4127520350000005
N -2.187139565 0.40556668500000015 6.587433964999999
Cu 5.360619525 0.3964602749999999 -1.5966322549999994
Cu -2.280308025 0.3964602749999999 -1.5966322549999994
Cu 0.26666782499999986 0.3964602749999999 -1.5966322549999994
Cu 2.8136436750000007 0.3964602749999999 -1.5966322549999994
Cu 4.087131595 -1.809285515 -1.5966322549999994
Cu -3.553795955 -1.809285515 -1.5966322549999994
Cu -1.006820105 -1.809285515 -1.5966322549999994
Cu 1.5401557449999999 -1.809285515 -1.5966322549999994
Cu -3.551021905 1.123144705 0.45706114500000083
Cu -1.0059132350000004 1.1287660650000002 0.4604257750000009
Cu 1.5414259350000004 1.119712255 0.45769574500000054
Cu 4.091033755000001 1.1253489449999998 0.4577058550000004
Cu -4.825958175 -1.083510215 0.4864288950000013
Cu -2.273448565 -1.076840885 0.4582390350000001
Cu 0.2668174150000002 -1.082532325 0.48749730499999977
Cu 2.8153471750000003 -1.075409745 0.4602119250000012
Cu 5.389052455000001 1.8419000850000002 2.472684685000001
Cu -2.251931575 1.8265871749999998 2.522988455
Cu 0.2915026550000004 1.8371812449999996 2.474909875
```

```
Cu 2.8444722449999995 1.8192018649999997 2.510976095
Cu 4.091852015 -0.35655376500000013 2.5222557850000005
Cu -3.499605635 -0.3487289250000001 2.5104923250000013
Cu -0.9976716550000004 -0.3534441049999999 2.5241136550000007
Cu 1.5870574250000002 -0.34794816500000003 2.5245088449999997
Cu 5.404760925000001 0.37382348499999996 4.494488705000002
Cu -2.246104095 0.3820883949999998 4.7350771850000015
Cu 0.29586393499999986 0.3782829350000001 4.5293774450000015
Cu 2.8362922349999993 0.359179825 4.743376605000002
Cu 4.1084569449999995 -1.836201695 4.5271784749999995
Cu -3.505961985 -1.8337215649999998 4.506253355000002
Cu -0.9719005850000002 -1.848535045 4.501350935000001
Cu 1.5767833949999996 -1.849744375 4.503506695000002
```

S6.4 BTA Tilted Monomer

```
77
bta_tilted
H 2.0956630050000005 0.14723824000000008 9.276402145
H 1.9615307350000002 -2.2521757299999994 9.980310925
H -0.18615413499999978 -3.4750056799999998 9.971972225
H -2.313609275 -2.3635358999999996 9.258227145000001
C -0.04604656500000015 0.22156205000000018 8.850505395
C 1.145723115000001 -0.3945838899999994 9.278008915
C 1.0565327149999995 -1.7229967699999995 9.669177455000002
C -0.17740967499999982 -2.4256731499999997 9.664208495000002
C -1.362800955 -1.8233043199999996 9.267229025
C -1.281601545 -0.4825665099999994 8.844797045000002
N -0.2649206450000001 1.4556746400000007 8.282119685
N -2.2273477449999994 0.33687308000000016 8.272503155
N -1.585289425 1.49332331 7.982065575000002
Cu 3.183719815 -2.3357977099999996 0.0196890750000005
Cu -4.457207735 -2.3357977099999996 0.0196890750000005
Cu -1.910231885 -2.3357977099999996 0.0196890750000005
Cu 0.636743965 -2.3357977099999996 0.0196890750000005
Cu 4.457207735000001 -0.13005191999999965 0.0196890750000005
Cu -3.183719815 -0.13005191999999965 0.0196890750000005
Cu -0.636743965 -0.13005191999999965 0.0196890750000005
Cu 1.910231885 -0.13005191999999965 0.0196890750000005
Cu 5.730695655 2.0756938700000003 0.0196890750000005
Cu -1.910231885 2.0756938700000003 0.0196890750000005
Cu 0.636743965 2.0756938700000003 0.0196890750000005
Cu 3.183719815 2.0756938700000003 0.0196890750000005
Cu 7.004183585 4.281439650000001 0.0196890750000005
Cu -0.636743965 4.281439650000001 0.0196890750000005
Cu 1.910231885 4.281439650000001 0.0196890750000005
Cu 4.457207735000001 4.281439650000001 0.0196890750000005
Cu 4.470460865 -1.5907178899999996 2.0856256350000013
Cu -3.190060505 -1.6010454699999994 2.080344365
Cu -0.6431167750000002 -1.5997288399999996 2.0679441450000002
Cu 1.9190005150000005 -1.5984916099999995 2.057575805000001
Cu 5.731850235 0.6074130500000008 2.0910168250000005
Cu -1.9115828549999998 0.6093032000000003 2.0778509850000013
Cu 0.635394045 0.6138496900000003 2.0744920550000003
Cu 3.1739846650000008 0.61453033 2.088061855000001
Cu 7.000652955 2.80736964 2.0761770449999997
Cu -0.6348767749999995 2.81404779 2.075114505
Cu 1.9066126749999999 2.8099288300000005 2.0928413050000003
Cu 4.455691935000001 2.8123798100000004 2.0793525650000007
Cu 3.1894434149999995 -3.8098939499999993 2.068014175
Cu -4.454992004999999 -3.8167923999999998 2.0873125750000003
Cu -1.9125342549999997 -3.80647471 2.0771357350000006
Cu 0.6389542349999999 -3.8047531399999994 2.072559095000001
Cu 3.199592655 -0.8591295199999998 4.126353845000001
Cu -4.432058505 -0.8449800999999995 4.196530585
```

Cu -1.9381456149999998 -0.8606655499999998 4.134335925
Cu 0.6634086550000005 -0.8748629399999994 4.085226425
Cu 4.446690825000001 1.3436923900000002 4.138097395000001
Cu -3.1803441649999997 1.3337171700000008 4.178244235000001
Cu -0.6408180850000003 1.3594444400000008 4.156524345000001
Cu 1.8804249849999994 1.3516130800000008 4.189160215000001
Cu 5.730872075000001 3.5477085100000005 4.131729425
Cu -1.9104663950000003 3.54767013 4.134703145000001
Cu 0.6288772649999999 3.52109918 4.189726355000001
Cu 3.179050815 3.5461018600000003 4.145136885000001
Cu 1.9262373050000008 -3.0651888199999995 4.111767875
Cu -5.720915785 -3.0621000499999997 4.124530795
Cu -3.1896447749999997 -3.0789836399999997 4.138377205000001
Cu -0.6360629449999999 -3.0704774399999994 4.1257466350000005
Cu 3.1960048949999997 -2.32815609 6.186409825
Cu -4.449546495 -2.3347452599999996 6.208499954999999
Cu -1.9109871050000002 -2.3696297399999997 6.173311615000001
Cu 0.6550155950000001 -2.3591450399999996 6.166414935000001
Cu 4.454586075 -0.12144949999999977 6.208229845
Cu -3.1869329549999996 -0.13760564999999936 6.383435875000002
Cu -0.5780958350000001 -0.22135369999999988 6.035444655000001
Cu 1.9398744850000007 -0.15668031999999954 6.177370535
Cu 5.678186515 2.09770256 6.177877345000001
Cu -1.962892825 2.1848458100000006 6.185130695
Cu 0.6398234550000002 2.0681525700000005 6.393118795000001
Cu 3.173027385000001 2.0758992000000003 6.213386855000001
Cu 6.980067835 4.324415120000001 6.171543945000002
Cu -0.6310612149999999 4.33579771 6.1807769650000015
Cu 1.9081831650000005 4.279251290000001 6.210923335000002
Cu 4.4467850349999996 4.2813506100000005 6.196191975

S6.5 BTA Upright Monomer

```
77
bta_up
H 0.53480112 -0.6219406800000002 10.534120755000002
H -0.6461118500000005 1.30449341 11.614953185
H -1.6561598799999997 3.1090401099999996 10.262835475000001
H -1.5391015799999996 3.0863958999999994 7.765687775000002
C 0.15310621999999974 0.15982459999999943 8.536835654999999
C 0.08623664000000009 0.17918858999999987 9.941677045
C -0.5697330699999998 1.2499566 10.525972265000002
C -1.1499022600000002 2.28787553 9.748923365000001
C -1.09292489 2.2874652299999996 8.364762405000002
C -0.42920552 1.2029338099999993 7.7647309149999995
N 0.7234003600000003 -0.7554085200000005 7.687638715
N -0.19185323000000043 0.8862509699999999 6.461854205
N 0.5011919000000002 -0.2969307300000006 6.476608805
Cu 0.8141891299999999 3.6314022799999996 -1.6149531849999992
Cu 3.3611649800000007 3.6314022799999996 -1.6149531849999992
Cu 5.90814083 3.6314022799999996 -1.6149531849999992
Cu -1.73278672 3.6314022799999996 -1.6149531849999992
Cu -3.00627464 -2.98583508 -1.6149531849999992
Cu -0.45929879000000007 -2.98583508 -1.6149531849999992
Cu 2.087677050000001 -2.98583508 -1.6149531849999992
Cu -5.55325049 -2.98583508 -1.6149531849999992
Cu -1.73278672 -0.7800893000000002 -1.6149531849999992
Cu 0.8141891299999999 -0.7800893000000002 -1.6149531849999992
Cu 3.3611649800000007 -0.7800893000000002 -1.6149531849999992
Cu -4.27976257 -0.7800893000000002 -1.6149531849999992
Cu -0.45929879000000007 1.4256564899999997 -1.6149531849999992
Cu 2.087677050000001 1.4256564899999997 -1.6149531849999992
Cu 4.6346529 1.4256564899999997 -1.6149531849999992
Cu -3.00627464 1.4256564899999997 -1.6149531849999992
Cu 2.0890543100000007 4.36526158 0.4380360250000006
Cu 4.6361021 4.36859772 0.4383540350000015
Cu 7.18581087 4.36831031 0.43903173500000037
Cu -0.4573437 4.35571126 0.4420564150000015
Cu -1.7285545300000003 -2.2502231900000003 0.4403773450000017
Cu 0.8147587199999995 -2.2524377500000003 0.4368605150000011
Cu 3.3539806600000004 -2.2449276900000004 0.442361365
Cu -4.28008545 -2.2524480900000006 0.43912539500000136
Cu -0.4577584100000003 -0.04614048000000004 0.4389656250000016
Cu 2.081618099999999 -0.04535121000000064 0.44413929500000116
Cu 4.634832820000001 -0.04368802000000027 0.4383721350000016
Cu -3.00422774 -0.04359418000000037 0.4392149250000017
Cu 0.8149622699999997 2.1546946599999997 0.44382491500000043
Cu 3.36428 2.1596469099999993 0.43649084500000157
Cu 5.91328915 2.15961731 0.4374200650000013
Cu -1.7317847000000004 2.15966626 0.4350122550000002
Cu -4.2800891 -3.72216314 2.4766484150000014
Cu -1.7338270500000004 -3.7218613300000003 2.477911135000001
```

Cu 0.8173921999999996 -3.7177716800000002 2.484696015000001
Cu -6.82251296 -3.7202000400000004 2.4725531750000016
Cu -3.0017939800000004 -1.5135371100000001 2.4777830650000006
Cu -0.4408944699999999 -1.5074994400000001 2.5036698150000003
Cu 2.0723404800000003 -1.5060618000000003 2.5152472150000005
Cu 4.634438309999999 -1.5174762800000003 2.4774964750000006
Cu -1.7148422300000004 0.7002694799999993 2.5002830950000003
Cu 0.7987797299999997 0.67719212 2.5340040450000014
Cu 3.358935 0.6866627099999993 2.4808666950000013
Cu 5.90920177 0.6888444899999993 2.477294285000001
Cu -0.45722454000000035 2.8742522699999995 2.513718755000001
Cu 2.0818875500000003 2.8928638699999993 2.480156495000001
Cu 4.63581259 2.8956199599999994 2.482653815000001
Cu 7.18518524 2.8948073699999997 2.481660315000001
Cu 0.8291993599999996 3.66220047 4.524930265
Cu 3.3615341699999997 3.63065427 4.536044375000001
Cu 5.90373064 3.6259868299999996 4.536927465
Cu -1.7467147599999997 3.6582902500000003 4.526110505
Cu -3.0026262800000003 -2.9838039200000006 4.5346263350000005
Cu -0.46576964000000043 -3.0189094900000004 4.522230185
Cu 2.109173039999999 -3.01963836 4.5315275050000015
Cu -5.54502015 -2.9838959600000003 4.532399735
Cu -1.7567914900000003 -0.7951008200000005 4.501871745000001
Cu 0.8662872199999994 -0.8617720800000002 4.629702775
Cu 3.3983145699999993 -0.7840362100000005 4.5259934850000025
Cu -4.27386528 -0.7789418000000006 4.533839325000001
Cu -0.4988220100000005 1.4994876599999998 4.630439385000001
Cu 2.11881641 1.4427725199999992 4.507472385000002
Cu 4.635789119999999 1.4247572599999998 4.536535715000001
Cu -3.0368065900000003 1.4354246099999992 4.520204655000002

S6.6 BTA Monomer with Cu_{ad} (Monomer in Fig. 2)

```
95
BTA_monomer
 H       10.402468        4.694794       21.562189
 H        0.576906        4.330880       23.684986
 H        3.020133        3.965180       23.668383
 H        4.317309        3.963699       21.525036
 C        1.115836        4.543141       20.364332
 C       11.484462        4.539071       21.560640
 C        1.100703        4.333453       22.727425
 C        2.505352        4.126817       22.718502
 C        3.236361        4.126509       21.541403
 C        2.518099        4.346291       20.356138
 N        0.728797        4.726511       19.065275
 N        2.928501        4.425018       19.054720
 N        1.835324        4.647211       18.309387
 Cu       3.600026        0.696933       10.000000
 Cu       3.892106        3.227106       10.000000
 Cu       5.937261        1.709071       10.000000
 Cu       7.982415        0.191036       10.000000
 Cu       4.184186        5.757279       10.000000
 Cu       6.229341        4.239244       10.000000
 Cu       8.274494        2.721209       10.000000
 Cu      10.319649        1.203174       10.000000
 Cu       2.430792        9.805839       10.000000
 Cu       4.476266        8.287452       10.000000
 Cu       6.521420        6.769417       10.000000
 Cu       8.566574        5.251382       10.000000
 Cu      10.611729        3.733347       10.000000
 Cu       1.554872        2.215312       10.000000
 Cu       6.813500        9.299590       10.000000
 Cu       8.858654        7.781555       10.000000
 Cu      10.903809        6.263520       10.000000
 Cu       1.846952        4.745485       10.000000
 Cu      11.195889        8.793693       10.000000
 Cu       2.139031        7.275658       10.000000
 Cu       3.008330        2.048001       12.052279
 Cu       5.061274        0.519932       12.045124
 Cu       3.298385        4.575266       12.047230
 Cu       5.354789        3.052708       12.047903
 Cu       7.393831        1.539570       12.065049
 Cu       9.434667        0.019858       12.068913
 Cu       3.592059        7.099981       12.059305
 Cu       5.645077        5.589171       12.050694
 Cu       7.677083        4.071155       12.051794
 Cu       9.725182        2.546909       12.049234
 Cu       0.675362        1.027658       12.049479
 Cu       3.892622        9.631330       12.054708
 Cu       5.939390        8.115766       12.051826
 Cu       7.972275        6.597275       12.053975
```

Cu	10.025850	5.080929	12.055606
Cu	0.965636	3.561774	12.043180
Cu	8.270713	9.126703	12.067698
Cu	10.314432	7.615408	12.053720
Cu	1.260094	6.094659	12.049610
Cu	1.551762	8.623296	12.054906
Cu	4.482100	1.850854	14.078484
Cu	4.767678	4.398652	14.076949
Cu	6.806419	2.890331	14.137409
Cu	8.850267	1.370025	14.130782
Cu	5.064834	6.935155	14.097240
Cu	7.101656	5.405970	14.141994
Cu	9.125262	3.898562	14.090849
Cu	11.189103	2.364285	14.084737
Cu	2.144959	0.849479	14.101576
Cu	5.360622	9.452930	14.105672
Cu	7.395426	7.929886	14.134331
Cu	9.424168	6.420700	14.095634
Cu	11.500486	4.903996	14.115226
Cu	2.410923	3.402025	14.120162
Cu	6.518936	0.354716	14.126870
Cu	9.726890	8.948562	14.131857
Cu	11.775429	7.440094	14.097569
Cu	2.706331	5.899304	14.136481
Cu	12.072135	9.963243	14.113356
Cu	3.020549	8.445519	14.108336
Cu	3.896773	3.156761	16.067429
Cu	4.205019	5.779767	16.113340
Cu	6.218896	4.232221	16.235298
Cu	8.260921	2.719004	16.209332
Cu	4.475550	8.281652	16.165716
Cu	6.515750	6.757134	16.211988
Cu	8.560013	5.237303	16.232248
Cu	10.582991	3.661320	16.078657
Cu	1.539172	2.165004	16.129620
Cu	3.598528	0.669283	16.157940
Cu	6.807581	9.287631	16.179319
Cu	8.844735	7.765474	16.205477
Cu	10.884047	6.304663	16.104918
Cu	1.835381	4.730059	16.289558
Cu	5.929997	1.698195	16.203367
Cu	7.968784	0.182374	16.185644
Cu	11.185079	8.793268	16.174749
Cu	2.130286	7.291378	16.143738
Cu	10.305541	1.174742	16.172663
Cu	2.426265	9.789945	16.173819
Cu	10.209273	5.002751	18.014431
Cu	4.572762	4.337397	18.020336

S6.7 BTA Low Coverage Chains

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108
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H -0.9416164900000004 -1.0532989699999997 11.80718851
H 0.35659039000000003 -1.0705605999999999 9.66083111
H 5.4389220300000005 3.13631835 7.386668149999998
H 3.81034221 5.03097702 7.563775069999998
H 1.37203577 4.618861990000001 7.681133710000001
H 0.44480655999999996 2.2931359799999997 7.617464739999999
C -2.84823358 -0.5001636199999995 8.49855105
C -3.58058525 -0.4872387199999997 9.697209959999999
C -2.86046202 -0.6902678599999996 10.86423056
C -1.45591368 -0.8995334899999996 10.855243339999998
C -0.7252895800000001 -0.9141125599999995 9.67809891
C -1.44760211 -0.7121669099999997 8.490429629999998
C 3.8314027500000005 1.6519163900000002 7.388726379999998
C 4.36075932 2.95419536 7.432885849999998
C 3.4465027700000004 3.999077830000001 7.536246200000001
C 2.0490629599999997 3.76256562 7.604873049999998
C 1.5225763599999995 2.4756259600000003 7.56870486
C 2.44044744 1.4167785400000001 7.451929189999998
N -3.23526317 -0.3316538299999996 7.194411159999998
N -1.0420313200000004 -0.6669721500000003 7.183142119999999
N -2.13248873 -0.4400131499999995 6.4419544
N 4.4297328799999995 0.4222035799999997 7.230149659999999
N 2.261086389999999 0.054718000000000266 7.327542640000001
N 3.4684145100000006 -0.5155088699999997 7.198812709999999
Cu -0.36491726000000035 -4.3340439 -1.8234911300000007
Cu -0.07283750000000033 -1.8038708999999997 -1.8234911300000007
Cu 1.9723167100000003 -3.32190589 -1.8234911300000007
Cu 4.017470919999999 -4.83994088 -1.8234911300000007
Cu 0.2192422599999997 0.7263020899999999 -1.8234911300000007
Cu 2.2643964699999994 -0.7917328999999995 -1.8234911300000007
Cu 4.309550679999999 -2.30976789 -1.8234911300000007
Cu -4.74730611 -3.82780287 -1.8234911300000007
Cu -1.5341519000000003 4.77486214 -1.8234911300000007
Cu 0.5113220199999997 3.2564750900000003 -1.8234911300000007
Cu 2.5564762299999995 1.7384401 -1.8234911300000007
Cu 4.601630439999999 0.22040510999999974 -1.8234911300000007
Cu -4.45522635 -1.2976298800000001 -1.8234911300000007
Cu -2.41007214 -2.81566487 -1.8234911300000007
Cu 2.8485559800000004 4.2686130900000006 -1.8234911300000007
Cu 4.893710199999999 2.75057811 -1.8234911300000007
Cu -4.16314659 1.2325431199999999 -1.8234911300000007
Cu -2.11799238 -0.28549186999999954 -1.8234911300000007
Cu -3.87106683 3.7627161099999995 -1.8234911300000007
Cu -1.82591262 2.24468112 -1.8234911300000007
Cu -0.9550665700000005 -2.98180735 0.23487347000000014
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Cu 3.4298401 -3.49326715 0.23868691999999925
Cu -5.6279729000000005 -5.0105262999999995 0.2392478099999984
Cu -0.3766924300000003 2.0683919499999996 0.23634526999999927
Cu 1.6795399299999998 0.55547301 0.23223418999999978
Cu 3.7208729399999996 -0.9622041000000001 0.23079554999999985
Cu -5.33685389 -2.48185713 0.23337876999999985
Cu -3.28856107 -3.99931576 0.23198842999999947
Cu -0.07307712999999971 4.602042239999999 0.23385509999999954
Cu 1.9712084899999995 3.0848027600000005 0.23278165999999878
Cu 4.01080372 1.5677977500000004 0.2346644599999994
Cu -5.03943854 0.04975459000000004 0.24296024999999943
Cu -2.99903882 -1.4686077499999999 0.23033409999999854
Cu 4.3054841800000005 4.09831376 0.23943781000000008
Cu -4.75201806 2.58293751 0.23380051000000002
Cu -2.70839404 1.06213785 0.23366049999999916
Cu -2.4138982 3.5925230799999994 0.23509483999999858
Cu 0.5079245199999995 -3.16673985 2.2781833999999996
Cu 0.7970346599999996 -0.6357604700000001 2.27300801
Cu 2.8482578600000004 -2.14891256 2.3037065499999994
Cu 4.89011824 -3.66503743 2.2991960099999993
Cu 1.0848316599999999 1.8986688200000001 2.2754924799999987
Cu 3.1399325099999995 0.37189970000000017 2.300973189999999
Cu 5.17687802 -1.1383388599999997 2.287026429999999
Cu -3.87742785 -2.65722674 2.2852065999999986
Cu -1.82480771 -4.17785541 2.2830686
Cu 1.3896332300000003 4.424754419999999 2.2921641699999995
Cu 3.4309826900000004 2.91109305 2.3023536899999986
Cu 5.4721290499999995 1.3958676500000005 2.2837876999999995
Cu -3.5650495600000003 -0.12996963999999966 2.31546176
Cu -1.5470578699999997 -1.6324358700000001 2.3122874399999986
Cu 2.5504772300000003 -4.67371126 2.3048079
Cu 5.76494396 3.92396205 2.29996987
Cu -3.29298004 2.4056102900000003 2.287527259999999
Cu -1.26339821 0.8695649599999999 2.317566359999999
Cu -2.99618995 4.9360794299999995 2.292228999999999
Cu -0.9512589299999998 3.4160703100000003 2.2865884199999993
Cu -0.06633597999999985 -1.8476040399999998 4.32070526
Cu 0.23082378999999964 0.7241187800000004 4.317812189999998
Cu 2.25112384 -0.8083011099999995 4.362702599999999
Cu 4.2996494300000005 -2.3203347 4.375879959999999
Cu 0.5027664300000003 3.2486365100000008 4.346118779999998
Cu 2.5410356400000005 1.7333175800000005 4.323454699999999
Cu 4.609386239999999 0.21257211999999992 4.35293665
Cu -4.48044312 -1.3362754 4.33036791
Cu -2.42721873 -2.864849 4.3214093899999995
Cu -0.3742991600000005 -4.35035475 4.3427913700000005
Cu 2.838470019999999 4.26799606 4.365130309999998
Cu 4.8817723 2.7487939600000004 4.365100559999998

Cu -4.17832542 1.2504329299999997 4.3341205800000004
Cu -2.12763873 -0.2998265499999997 4.453851480000001
Cu 1.9598257099999996 -3.32890186 4.3801525099999985
Cu 4.00762383 -4.84212825 4.353575790000001
Cu -3.88057713 3.7599743300000004 4.352565849999998
Cu -1.8331967100000002 2.26023787 4.332012379999998
Cu -4.76104666 -3.84729949 4.3607095099999995
Cu -1.5419739000000003 4.76064929 4.356541669999999
Cu -4.96629401 0.016889810000000338 6.39271287
Cu 0.7279768300000002 -0.6886769699999995 6.343419189999999

S6.8 BTA Dimers

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75
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H 7.235348279999999 -1.45540124 7.80123508
H 0.6713648799999996 1.7636602199999998 10.13151275
H -0.6211852499999999 -0.9243762800000002 11.40723322
H -2.73771626 0.0037200399999997025 10.53344712
H -3.6578291700000003 -0.7296913900000002 8.312614680000001
C 3.9295208199999996 -0.6342705000000002 8.38873524
C 4.053321209999999 0.2461578900000001 9.476970839999998
C 5.33885625 0.49064788000000004 9.938273959999998
C 6.477284030000001 -0.11152472000000024 9.34093208
C 6.364915320000001 -0.99203686 8.275531899999999
C 5.06462225 -1.25579537 7.812256889999999
C -0.7951194400000006 1.75119939 8.51317772
C -0.26382861999999996 2.1772572799999996 9.743166059999998
C -0.99404424 -1.28365265 10.44344803
C -2.21243443 -0.7533346700000001 9.94374284
C -2.7333050200000004 -1.14933185 8.721038909999999
C -2.0034831200000003 -2.1147486300000002 8.00676763
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Cu -7.63832703 -2.20142615 -1.4072332200000002
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Cu 3.8230642900000005 0.004319639999999847 -1.4072332200000002
Cu 6.3700401399999995 0.004319639999999847 -1.4072332200000002
Cu -6.35863605 -1.4745622600000001 0.6341236400000003
Cu -3.80253358 -1.47354064 0.642812339999999
Cu -1.27296004 -1.47664045 0.653968299999999
Cu 1.2676245600000007 -1.4742125600000002 0.6477217
Cu 3.824950179999999 -1.47343573 0.6394484699999996
Cu 6.37439688 -1.47824785 0.6321357299999999
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Cu 0.008905089999999838 0.7389363799999997 0.6627409399999991
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Cu -7.616256040000001 -0.77229046 2.67750616
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Cu -0.006356819999999708 -0.7364473600000001 2.71973343
Cu 2.55565602 -0.7676131500000001 2.69302261
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Cu 6.36623484 1.4447869500000001 2.71865472
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Cu 2.5322263099999995 2.1564787400000003 4.872100519999998
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Cu -3.88588144 -0.00796177000000009 4.72145499
Cu -1.2300245500000004 -0.04736098000000011 4.809776049999998
Cu 1.31068373 -0.03617815999999996 4.744726989999998
Cu 3.8634157 -0.034492280000000264 4.644334840000001
Cu 6.42805215 -0.062431899999999985 4.716305
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S6.9 BTA High Coverage Chains

```
68
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H 5.02184956 -0.52919049 8.694100815
H 3.8340390000000006 0.71872194 10.521415055
H 1.4190865400000003 0.4181864700000002 10.907653875
H 0.035693239999999626 -1.08154026 9.453245775000001
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C -4.15127635 1.83637638 9.594538124999998
C -3.51480278 1.6376663899999997 10.810679145
C -2.10159342 1.5479395399999998 10.909804164999999
C -1.2838690000000001 1.64197698 9.793444795000001
C -1.9201302199999999 1.8259146399999997 8.555455775
C 3.179318179999999 -1.53634257 8.091750575
C 3.9513195999999997 -0.66359821 8.878746094999999
C 3.2832422999999995 0.022208909999999804 9.881052814999999
C 1.88972023 -0.14439301999999987 10.095572804999998
C 1.11525694 -0.9824353800000001 9.305609304999999
C 1.7840516500000003 -1.6857109700000001 8.287819285
N -3.6245946 2.13675634 7.137027084999998
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Cu -0.4539315000000004 -1.77640698 -1.8958545450000006
Cu 2.1952227099999995 1.7597580300000004 -1.8958545450000006
Cu 4.240376919999999 0.2417230400000001 -1.8958545450000006
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Cu 3.92845668 -2.28230396 -1.8958545450000006
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Cu -0.7074120700000002 2.0967952199999997 0.1902358349999993
Cu 1.3247781500000002 0.5887785500000002 0.18703373499999998
Cu -1.02931728 -0.42505959000000004 0.18626447499999976
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Cu 3.6566704100000003 1.5996447600000003 0.1641297349999995
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Cu 3.349838760000001 -0.9235880999999999 0.17196737499999948
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Cu -3.04591939 1.0922006400000002 0.16310952499999942
Cu -3.34803666 -1.44039724 0.15979779499999935
Cu 0.7895489700000002 1.9290510000000003 2.2839396049999987
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Cu 5.1375864 1.4332000800000002 2.1888171649999997
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Cu -1.88589012 -1.63374181 2.272821875
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Cu -0.3924188099999997 -1.7559680100000001 4.301717805000001
Cu 2.2521270500000004 1.77685518 4.563469875000001
Cu 4.2984737200000005 0.2591465799999999 4.302864944999998
Cu 1.9188560399999997 -0.72550585 4.285434874999998
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Cu -2.45568327 -0.27390033999999996 4.2690970749999995
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