Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information to:

Metalation and coordination reactions of 2H-meso-trans-di(p-cyanophenyl)porphyrin on Ag(111) with coadsorbed cobalt atoms

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Closer Inspection of molecular arrangement of 2HtransDCNPP on Ag(111)

To further elucidate the molecular order in particular the peculiar orientational arrangement of the 2HtransDCNPP molecules on Ag(111) we did measurements of the relevant molecular axes as documented in Fig. SI1 and Table SI1. The values clearly show alternating behavior (…larger value-smaller value-larger value-smaller value….) along the horizontal and vertical directions as expected from the proposed model (c.f. Fig. 1 in main manuscript). However in a few cases (indicated with red background in Table SI1) the ratio of the axes was either wrong or not clear (ratio of 1). This triggered a closer inspection of the STM image and the correspondingly measured values. Since the slow scanning direction of the depicted micrograph was the vertical direction one might expect distortions in that direction due to thermal drift. Indeed we found by averaging the blue values separated by the directions in Table SI1 (8 times each molecular orientation) that the average of the "green" values was 1.52 nm while the corresponding value for the "red" direction amounts to 1.85 nm. This finding indicates a compression (probably due to thermal drift) in the vertical direction with a factor or 1.12. We therefore calculated the corrected values (column C Table SI1) and found that indeed with the comprehensible correction all values are in perfect agreement with the proposed molecular orientations of the 2HtransDCNPP molecules.

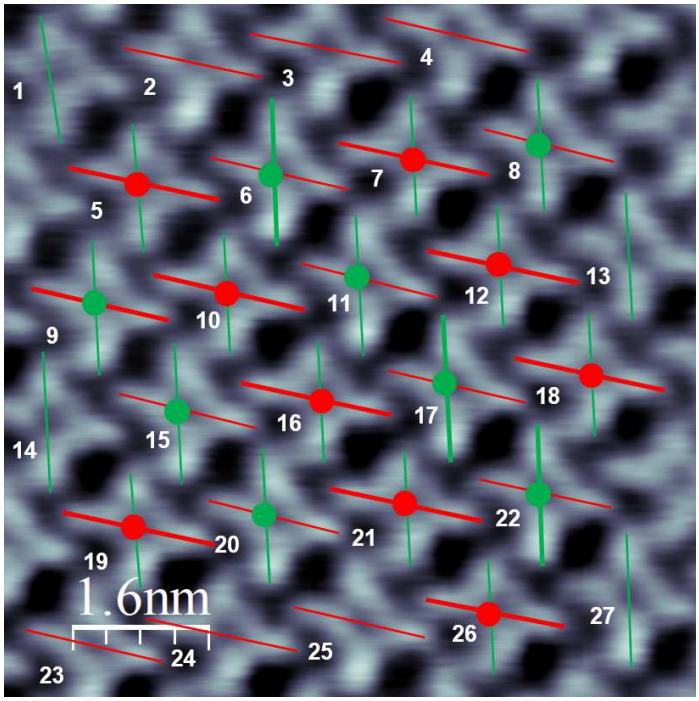

Figure SI1 *Constant current STM images of the self-assembled 2HtransDCNPP on Ag(111) as shown in Fig. 1 b in the original paper. The characteristic molecular axes were measured as indicated by the red (close to horizontal direction) and green (close to vertical direction) lines. The corresponding values are documented in Table SI 1. The individual 2HtransDCNPP are labelled with white numbers left of the molecules. Thicker lines within one molecule indicate which axis is longer for the actual molecule (if both are thin the length is equal). The green and red dots indicate which axis of the corresponding molecule is longer after correcting (drift correction) the vertical length as indicated in text. Tunneling parameters: U = -0.1 V, I = 27 pA.*

A	B	C	D	E	F	G	H
#	Green [nm]	Corr. Green [nm]	Red [nm]	g/r	Longer Axis	Corr g/r	Corr. LA
1	1.5	1.68	-	-	-	-	-
2	-		1.65	-	-	-	-
3	-		1.8	-	-	-	-
4	-		1.73	-	-	-	-
5	1.5	1.68	1.8	0.83	R	0.93	R
6	1.73	1.94	1.65	1.05	G	1.18	G
7	1.43	1.6	1.8	0.79	R	0.89	R
8	1.58	1.77	1.58	1	-	1.12	G
9	1.58	1.77	1.65	0.96	R	1.07	G
10	1.43	1.6	1.8	0.79	R	0.89	R
11	1.65	1.85	1.65	1	-	1.12	G
12	1.43	1.6	1.8	0.79	R	0.89	R
13	1.5	1.68	-	-	-	-	-
14	1.65	1.85	-	-	-	-	-
15	1.65	1.85	1.65	1		1.12	G
16	1.43	1.6	1.8	0.79	R	0.89	R
17	1.73	1.94	1.65	1.04	G	1.18	G
18	1.43	1.6	1.8	0.79	R	0.89	R
19	1.35	1.51	1.8	0.75	R	0.83	R
20	1.58	1.77	1.58	1	-	1.12	G
21	1.35	1.51	1.8	0.75	R	0.84	R
22	1.65	1.85	1.58	1.04	G	1.17	G
23	-		1.65	-	-	-	-
24	-		1.8	-	-	-	-
25	1.5	1.68	-	-	-	-	-
26	1.35	1.51	1.65	0.82	R	0.92	R
27	1.58	1.77	-	-	-	-	-

Table SI1 *Measured and processed values from Figure SI1. The following values are documented in the corresponding columns:* ***A*** *molecular labels;* ***B*** *measured values in nanometer along green lines as indicated in Fig. SI1;* ***C*** *drift corrected (see text) values from A;* ***D*** *correspondingly measured values for red lines;* ***E*** *ratio of axes within one molecule (length of green direction divided by red direction);* ***F*** *colour of longer axes (G:= green, R:= red);* ***G*** *ratio of axes with corrected values from column C analoge to column E;* ***H F*** *colour of longer axes with corrected values from C. The yellow and orange blocks indicate molecules within one "horizontal line". The red background indicate deviations from the proposed molecular order.*