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## Single-molecule conductance of dibenzopentalenes: antiaromaticity and quantum interference<sup>†</sup>

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The effects of antiaromaticity and destructive quantum interference (DQI) are investigated on the charge transport through dibenzo-[*a*,*e*]pentalene (DBP). 5,10-Connectivity gives high single-molecule conductance whereas 2,7 gives low conductance due to DQI. Comparison of the 5,10-DBP with phenyl and anthracene analogues yields the trend  $G_{\text{DBP}} \approx G_{\text{Anth}} > G_{\text{Ph}}$ , despite the aromatic anthracene having a larger HOMO-LUMO gap than 5,10-DBP. This is explained by unfavourable level alignment for 5,10-DBP.

The concept of aromaticity has captivated chemists for many years. It is characterised by the additional stability and lower reactivity of planar, cyclic hydrocarbons possessing 4n + 2 delocalised  $\pi$ -electrons (where *n* is any integer except zero) over olefinic analogues, as codified by Hückel.<sup>1</sup> Aromatic compounds display large anisotropic diamagnetic susceptibilities due to their ability to sustain ring currents under applied magnetic fields. Benzene is the archetypal aromatic molecule

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with six  $\pi$  electrons. Breslow extended the concept by describing cyclic, planar compounds with  $4n \pi$  electrons as antiaromatic,<sup>2</sup> which are chemically less stable than their olefinic counterparts and which sustain paratropic ring currents.

One of the simplest compounds considered antiaromatic is cyclobutadiene (1 in Fig. 1), which contains two double bonds connected *via* two single bonds in a cyclic structure having four  $\pi$  electrons (n = 1).<sup>3</sup> This compound is highly unstable under ambient conditions, where the use of bulky substituents is essential to make (relatively) air stable examples.<sup>4</sup> Pentalene, n = 2, (3 in Fig. 1) is also antiaromatic<sup>5</sup> and again highly unstable, only isolable employing bulky substituents.<sup>6</sup> Both cyclobutadiene and pentalene can be stabilised through annulation yielding biphenylene (2) and dibenzo[a,e]pentalene (DBP, 4), shown in Fig. 1. The presence of the outer rings diminishes, however, the antiaromatic character of the inner rings.<sup>7</sup>

Antiaromatic compounds are predicted to give higher conductance in molecular junctions compared to corresponding aromatic or non-aromatic conjugated compounds. Breslow suggested that the relative conductance can be predicted based on the ease to which the  $\pi$ -system is perturbed due to a shift of electron density between anchor groups.<sup>8</sup> Aromatic molecules are predicted to be less conductive as they will resist this charge redistribution (which disrupts aromatic bonding). Conversely, antiaromatic compounds favour a redistribution which disrupts cyclic conjugation, leading to higher conductance. Furthermore, antiaromatic molecules tend to have smaller HOMO–LUMO gaps compared to aromatic and non-aromatic molecules.<sup>9</sup> When connected to (gold) electrodes, the frontier



Fig. 1 Chemical structures of cyclobutadiene (1), biphenylene (2), pentalene (3) and dibenzo[a,e]pentalene (4).

molecular orbitals of antiaromatic molecules might be expected to lie closer to the Fermi level, also contributing to higher conductance. Both hypotheses consider, fundamentally, isolated molecules. It is unclear, therefore, if this will translate to molecular junctions, where the alignment of the moleculebased orbitals with the electrode Fermi level is critical.<sup>10</sup> Despite such fundamental interest in the behaviour of antiaromatic compounds, there are only a handful of examples of single molecule transport studies. Moreover, there are even fewer theoretical electron-transport calculations to substantiate these claims.

Of distinct relevance is the effect of modulating the degree of aromaticity within a particular structure. There are, however, conflicting reports in the literature. Chen et al. concluded that the conductance of a family of amine-terminated wires was highest for the least aromatic compound.<sup>11</sup> The 2,5-disubstituted thiophene (most aromatic) was the least conductive, followed by the respective furan and finally the cyclopentadiene (least aromatic). Gantenbein et al. found a similar dependence studying pyridyl-terminated compounds with tricyclic cores,12 but the least aromatic fluorene-containing compound did not have the highest conductance. Yang et al. studied a family of 2,5-disubstituted 5-membered heterocycles (similar to Chen et al. but with pyridyl anchor groups).<sup>13</sup> They did not find any relation between conductance and aromaticity. The authors also found no relation when measuring the analogous 2,4-disubstituted compounds, which were instead dominated by DQI effects. Miguel et al. studied a series of oligo(phenyleneethynylene)-type (OPE) compounds<sup>14</sup> (terminated with -SMe) in which the central ring was either phenyl (most aromatic), pyridyl or pyrimidyl (least aromatic). No difference in the conductance could be identified.

Regarding single molecule conductance measurements on antiaromatic compounds, there are few precedents. Fujii *et al.* compared an antiaromatic norcorrole nickel complex with an aromatic nickel-porphyrin analogue. They found the former to be approximately one order of magnitude more conductive than the latter.<sup>15</sup> Gantenbein *et al.* on the other hand investigated a group of OPE-based compounds containing a biphenylene core.<sup>16</sup> They could not, however, find a correlation between the presence of an antiaromatic core and a higher conductance. These studies may suggest that a certain degree of change in aromaticity/antiaromaticity is required to influence the conductance significantly. The question is how much?



Fig. 2 DBP derivatives **5** and **6**, anthracene derivative **7** and compound **8**<sup>14</sup> investigated in this study. **5** and **7** have almost the same number of  $\pi$  bonds in total and thus will constitute the best test of the role of antiaromaticity towards electron transport.

Here, we report the synthesis, single-molecule conductance and electronic transport calculations of two new compounds, **5** and **6**, containing an antiaromatic DBP core with methyl sulphide (SMe)-terminated phenylacetylene anchor groups in either the 5,10- or the 2,7-positions respectively (Fig. 2). In order to ascertain the role of antiaromaticity precisely, we have also investigated aromatic analogues of **5**, anthracene **7** and phenyl **8** (Fig. 2). Compounds **5**, **7** and **8** have the same number of  $\pi$  bonds connecting the anchor groups *via* the shortest pathway and practically identical S–S distance (Table 1).

SMe anchor groups were chosen for **5**, **6** and **7** to facilitate the synthetic route and avoid known issues with thiol anchor groups when used on gold.<sup>17</sup> The mesityl substituents in the respective 2,7- or 5,10-positions of the DBP core were attached to increase the solubility of **5** and **6**. **5**, **6** and **7** were synthesized according to previously described procedures.<sup>18–22</sup> Full details are shown in the ESI† along with X-ray crystal structures and NICS calculations.

To form molecular junctions, we used the statistical breakjunction method<sup>23</sup> as described previously with a home-built scanning tunnelling microscope (STM).<sup>24–26</sup> For details of sample preparation and methodology, see Section 9 in the ESI.†

Table 1	Single molecule conductance and length data from STM-BJ experiments and theory plus UV-vis spectroscopy and electrochemical data								
Molecule	Measured low-bias conductance $(\log(G/G_0))^a$	Theoretical conductance $(\log(G/G_0))$	Mean length (95th percentile $(L_{95}))^b$	Theoretical Au–Au distance (nm)	Theoretical S–S distance (nm)	$E_{ m g} \left( { m UV} / { m vis}  ight)^c \ ({ m eV})$	$E_{\rm HOMO}$ (E-chem) <sup>d</sup> (eV)	$E_{\text{LUMO}}$ (E-chem) <sup>d</sup> (eV)	E <sub>gap</sub> (E-chem) (eV)
5	-4.3(0.9)	-3.66	1.58 (2.04)	2.29	2.03	1.73	-5.45	-3.46	1.99
6	-6.2(0.8)	-5.19	1.87 (2.84)	2.84	2.58	2.06	-5.51	-3.15	2.36
7	-4.4(0.9)	-3.74	1.37 (1.94)	2.28	2.02	2.48	-5.31	-3.02	2.29
8	-4.6(0.8)	-3.87	1.43 (1.97)	2.28	2.02	—		—	—

<sup>*a*</sup> Values in parentheses are the FWHM of the peak. <sup>*b*</sup> Values have 0.4 nm added to account for the gold snap-back. <sup>*c*</sup> Optical gap from the onsets of the longest wavelength absorption band. <sup>*d*</sup> Obtained from the onsets of the first reduction/oxidation peaks, assuming an ionization energy of 4.8 eV for ferrocene.<sup>30</sup>

The main results from the BJ experiments are summarised in Table 1. The 5,10-isomer 5 is clearly more conductive than the 2,7-isomer 6, which is not surprising given that 6 is 0.55 nm longer. The fact that 6 is about 0.01 times as conductive is surprising, however, given the typical conductance decay ( $\beta$ -value) through  $\pi$ -systems (usually between 1–4 nm<sup>-1</sup>).<sup>27</sup> Using the relation  $G_{2,7}/G_{5,10} = e^{(-\beta(L_{5,10}-L_{2,7}))}$  the relative conductance of 6 would be between 0.5 and 0.1 times that of 5 if it behaved just as a longer molecule. As even the lower estimate is a factor ten larger than observed, we conclude that this attenuation arises *via* another mechanism. Considering the conjugation paths through the backbones, it is clear that the anchor groups in 5 are directly conjugated whereas in 6 they are not. This suggests that DQI may play a role as for a *meta*-anchored phenyl ring.<sup>28,29</sup>

Next, we compare the results of 5 with purely aromatic 7 (anthracene) and 8 (phenyl). The difference in S–S distance across compounds is within 0.1 Å, and thus negligible. Fig. 3a shows the 1D histograms for each where 8 has the lowest conductance peak situated at  $\log(G/G_0) = -4.6$ . 7 gives the next highest peak centred at  $\log(G/G_0) = -4.4$  followed by 5 at  $\log(G/G_0) = -4.3$ . Both 5 and 7 are thus notably more conductive than 8. There is significant overlap in the histograms of 5 and 7, but there is, nonetheless, a small shift to higher values for 5. We also studied the conductance *versus* voltage (*G*–*V*) behaviour of 5–8, but we found little difference in their response (see ESI,† Section 9.3 for details).

To shed light on how changing the central unit affects the conductance, we performed theoretical calculations based on a combination of density functional theory (DFT) and Green's function techniques<sup>31</sup> as described in Section 10 in the ESI.<sup>†</sup> The HOMO-LUMO gap was corrected by the DFT+ $\Sigma$  technique.<sup>32,33</sup> We built metal-molecule-metal junctions incorporating 5–8, in which the terminal S atoms are bound to the



**Fig. 3** (a) 1D conductance histograms for **5**, **6**, **7** and **8**.  $N_{\text{junc}} = 1074$  (9%) (**5**), 831 (28%) (**6**), 925 (21%) (**7**), 1210 (57%) (**8**). (b–e)  $\log(G/G_0) - z$  2D histograms generated from all plateau-containing traces for 1–4 respectively. Note, the length scale is uncalibrated. The tip–sample bias was 0.2 V.



Fig. 4 Transmission as a function of energy for the junctions incorporating compounds **5–8** as show in Fig. 2.

undercoordinated last gold atoms of pyramidal electrodes in a top orientation on each side (Fig. 4a).<sup>17,34</sup> In Fig. 4b, we show the zero-bias transmission curves for **5–8** (we also studied the junction formed by replacing the DBP in 5 with pentalene (**5c**), see Section 10.2 in the ESI†). The electronic transport generally takes place through the tail of the HOMO, although in the case of **5** the Fermi level falls almost in the middle of the HOMO–LUMO gap. The conductance for each is given in Table 1. The theoretical values match the trend found experimentally whereby  $G_6 \ll G_8 < G_7 < G_5$ . The theoretical conductance differences between each are very similar to those found experimentally. Between **7** and **8**, the theoretical and experimental conductance differences  $(\log(G/G_0) = 0.13 \text{ and } 0.2 \text{ respectively})$  agree well with previous experimental results on thiol analogues.<sup>35</sup>

Firstly, the most striking difference between the shape of the transmission curves of 5 and 6 is the presence of a strong dip within the HOMO-LUMO gap of 6, which is a clear signature of DQI.<sup>36–38</sup> This fits the "curly-arrow" depiction of conjugation as previously mentioned. Turning to the relation between 5, 7 and 8, the alignment of the frontier molecular orbitals clearly affects the final relative theoretical conductance. We find that the effect of switching the phenyl ring of 8 with an anthracene (7) reduces the HOMO-LUMO gap, shifting both frontier molecular orbitals closer to the Fermi level  $(E_F)$ , which results in a slightly higher conductance, as observed previously.<sup>39</sup> Substituting with the DBP unit of 5 reduces the HOMO-LUMO gap further, resulting in the LUMO-derived peak sitting significantly closer to E<sub>F</sub>. Narrowing of the HOMO-LUMO gap in antiaromatic systems is well known and discussed elsewhere,<sup>40</sup> and in the ESI.<sup>†</sup> The HOMO-peak conversely sits further down in energy compared to that of 7. This behaviour is reflected in the electrochemical oxidation and reduction values (Table 1). It is worth noting that the conductance trend and the shape of the transmission curves can be well reproduced using a simple tight-binding model (see ESI,† Section 10.3).

We now turn to the question of how much the antiaromatic nature of 5 contributes to the conductance. Both theory and experiment show that 5 is more conductive than 8, in agreement with the initial hypothesis. 5, however, has greater overall  $\pi$  conjugation, which likely contributes to the conductance

increase. Comparing 5 with 7, which have similar sized  $\pi$ systems, we detect a very small difference, both experimentally and in the theoretical transmission at the Fermi level, with 5 being slightly more conductive than 7. This is also the case for the absolute transmission minima within the HOMO-LUMO gap. Higher conductance ratios are obtained, however, at higher energy as a consequence of the lower LUMO energy of 5. A similar picture is found comparing (theoretically) 8 with 5c (ESI,<sup>†</sup> Section 10.2). Our results suggest, therefore, that in order to take full advantage of the antiaromatic nature of dibenzo[a,e] pentalene in a molecule junction configuration, chemical or electric field gating, or the use of appropriate anchor groups which promote alignment of the LUMO with the Fermi level, are needed. We envisage most small antiaromatic compounds will require a degree of gating. We anticipate LUMO-aligning anchor groups to help for non-alternant compounds while HOMO-aligning groups may be required in other systems. Exploitation of this will be pursued in later work. We also note our work suggests that as the antiaromatic core grows, the effect on conductance becomes more pronounced. For comparable cores, biphenylene is slightly less conductive than fluorene, DBP is slightly more conductive than anthracene and norcorrole is significantly more conductive than porphyrin. This insight will be useful in predicting the behaviour of other systems, but more work is needed to build a complete picture.

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### Conflicts of interest

There are no conflicts to declare.

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