Journal Name

ARTICLE TYPE

Cite this: DOI: 10.1039/xxxxxxxxxx

The influence of heteroatoms on the aromatic character and the current pathways of B_2N_2-dibenzo[a,e]pentalenes†

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Received Date
Accepted Date

DOI: 10.1039/xxxxxxxxxx

www.rsc.org/journalname

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Current profile plots

Molecule (1)

Current profile plots and integrated domains in the plots (in nA/T). The origin on the abscissa lies at the beginning of the integration plane, which lies at the centre of a ring unless otherwise noted.

Table 1 Plane **a** with origin at the centre of ring A and passing through atom C1.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-0.13	9.87	5.43
Diatropic domains		
0.97	9.87	13.08
Paratropic domains		
-0.13	9.87	-7.74
-0.03	2.07	-4.60
2.07	2.67	-2.12
2.67	3.67	-1.03

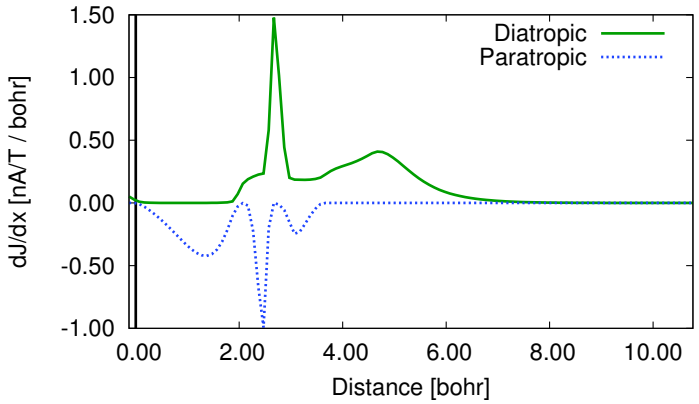


Table 2 Plane **b** with origin at the centre of ring A and passing through the midpoint of the bond between atoms C1 and C2.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-0.03	9.87	6.10
Diatropic domains		
1.07	9.87	12.40
Paratropic domains		
-0.03	2.27	-6.34

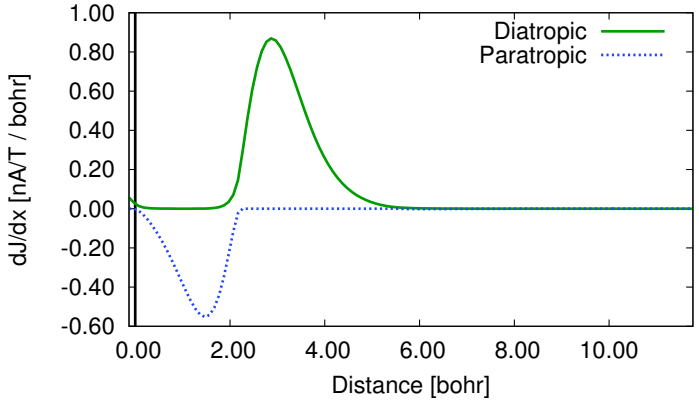


Table 3 Plane **c** with origin at the centre of ring B and passing through the midpoint of the bond between atoms C4 and C7.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-0.07	10.38	-7.23
Diatropic domains		
1.88	5.38	6.48
Paratropic domains		
-0.22	3.78	-13.78

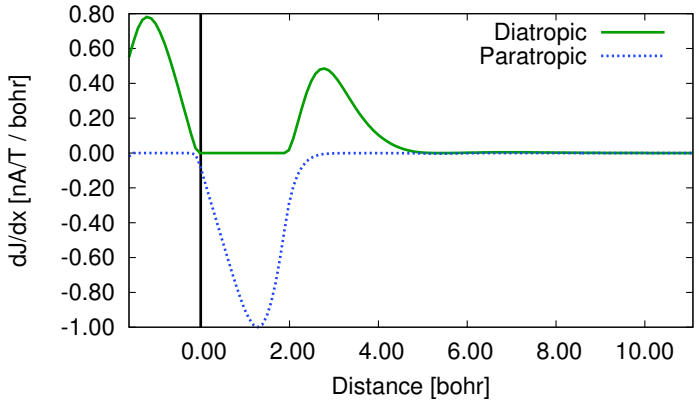


Table 4 Plane **d** along the C7 – C8 bond, with origin at the midpoint of the bond.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-0.01	9.83	3.59
Diatropic domains		
-0.01	9.83	9.25
-0.01	1.33	3.54
1.37	1.71	0.70
1.97	5.19	4.91
Paratropic domains		
0.01	7.83	-5.66

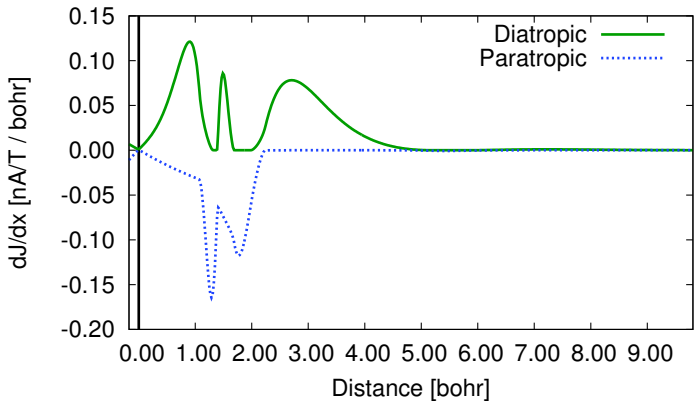


Table 5 Plane **e** with origin at the centre of ring B and passing through atom C9.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-0.01	10.73	-7.31
Diatropic domains		
1.47	10.73	7.96
1.47	2.15	0.53
2.27	2.63	0.70
3.03	10.73	6.71
Paratropic domains		
-0.01	10.73	-15.27

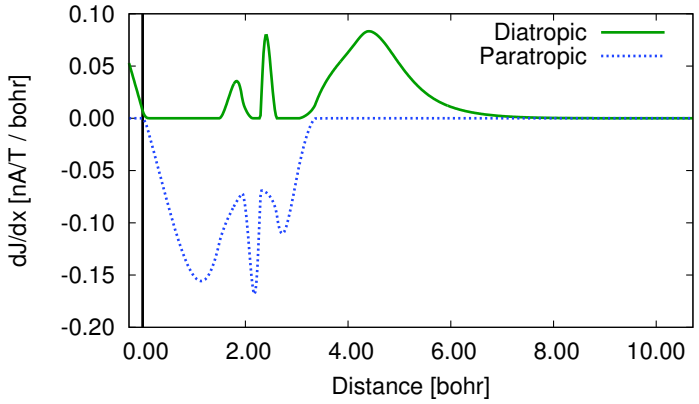


Table 6 Plane **f** with origin at the centre of ring B and passing through the midpoint of the bond between atoms C5 and C9.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.12	11.82	-7.18
Diatropic domains		
1.86	11.82	5.52
Paratropic domains		
0.00	7.82	-12.75

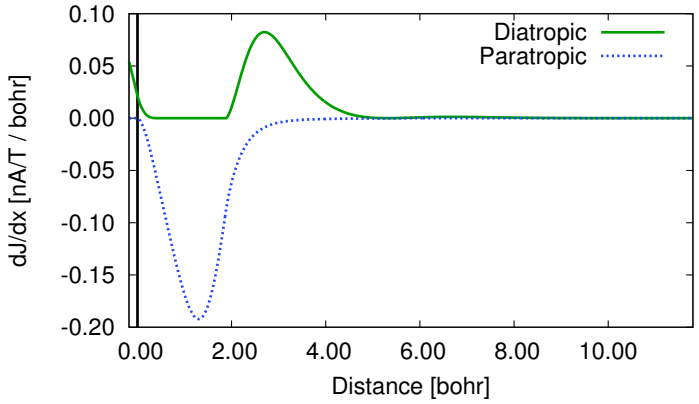


Table 7 Plane **g** along the C4 – C5 bond, with origin at the midpoint of the bond.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.00	9.46	7.27
Diatropic domains		
0.00	9.46	10.24
1.66	5.06	4.69
Paratropic domains		
0.61	5.51	-2.97

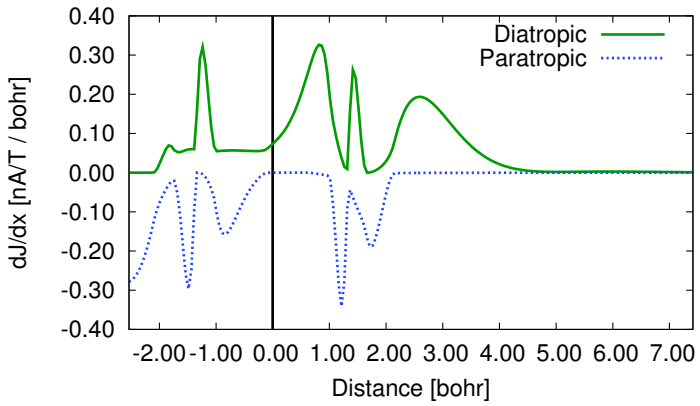


Table 8 Plane **h** with origin at the centre of ring B and ending at the centre of ring A. The point 0 on the abscissa corresponds to the centre of the fusion bond.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-1.90	2.30	-12.85
Diatropic domains		
-0.10	2.80	4.78
Paratropic domains		
-2.20	2.30	-17.74

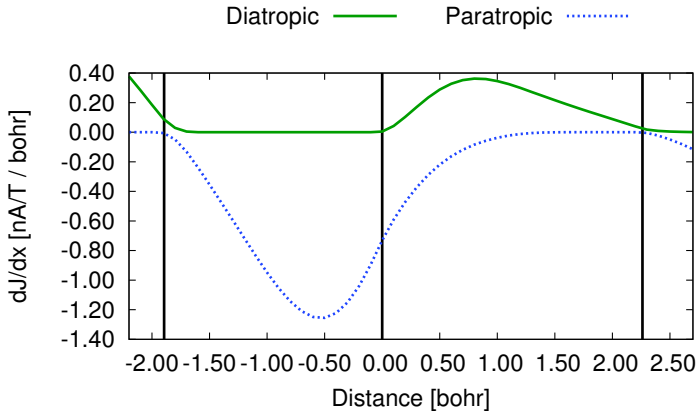


Table 9 Plane **i** with origin at the centre of ring B and ending at the centre of ring C. The point 0 on the abscissa corresponds to the centre of the fusion bond.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-1.98	1.98	-0.01
Diatropic domains		
0.00	2.36	11.11
Paratropic domains		
-2.32	0.00	-11.12

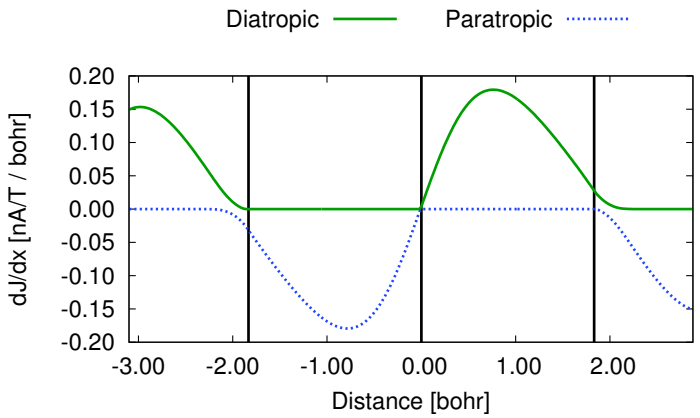
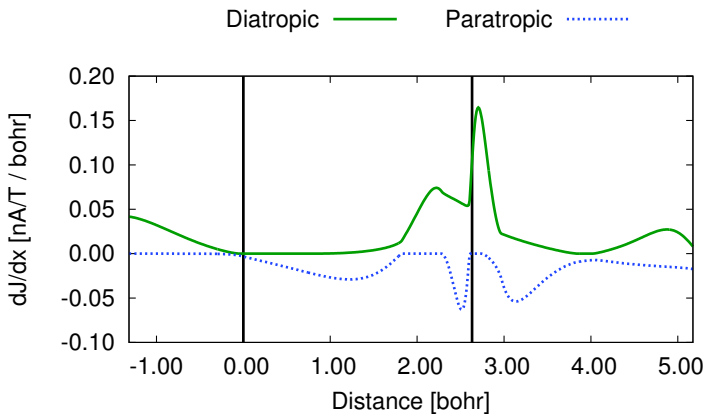


Table 10 Plane **j** with origin at the centre of ring A and passing through atom C5.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Paratropic domains		
-0.32	1.83	-3.37
2.28	2.61	-1.06



Molecule (2)

Table 11 Plane **a** with origin at the centre of ring A and passing through atom C1.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.08	11.62	10.03
Diatropic domains		
0.08	11.62	16.47
Paratropic domains		
0.08	11.62	-6.44
0.08	1.94	-3.55
2.20	2.64	-1.98
2.82	5.62	-0.90

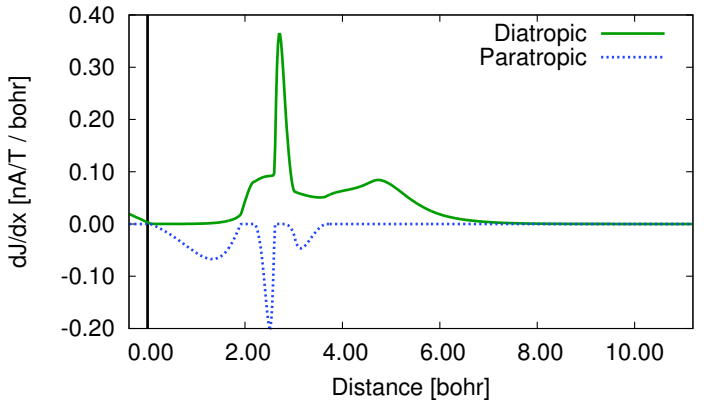


Table 12 Plane **b** with origin at the centre of ring A and passing through the midpoint of the bond between atoms C1 and C2.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.05	11.77	10.16
Diatropic domains		
0.05	11.77	15.45
Paratropic domains		
0.05	11.77	-5.28

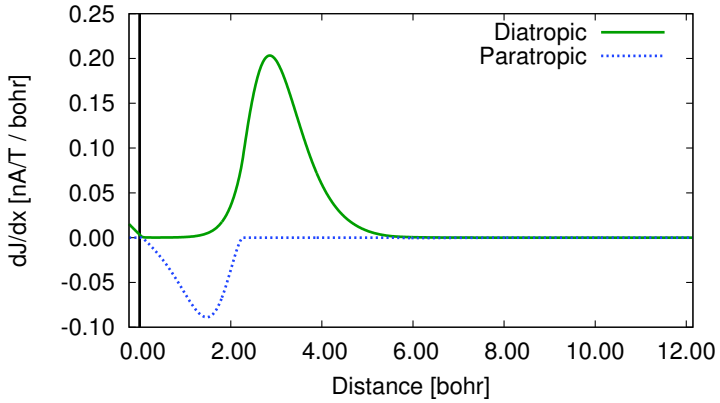


Table 13 Plane **c** with origin at the centre of ring B and passing through the midpoint of the bond between atoms C4 and N2.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.08	11.66	2.58
Diatropic domains		
0.08	11.66	9.41
Paratropic domains		
0.08	11.66	-6.82

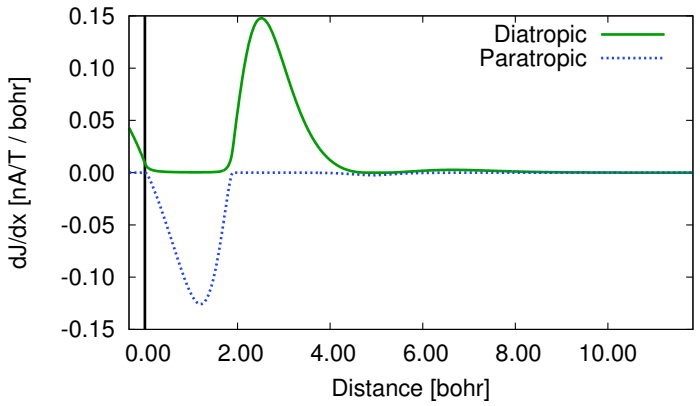


Table 14 Plane **d** along the N1 – N2 bond, with origin at the midpoint of the bond. The domains that are overlapping with each other are marked with an asterisk.

x_1 [bohr]	x_2 [bohr]	current [nA/T]	
Net current			
-0.01	11.53	12.31	
Diatropic domains			
-0.01	11.53	17.35	
-0.03	1.33	5.04	7.38*
1.33	1.55	0.53	1.07*
1.55	9.53	6.65	9.01*
Paratropic domains			
-0.03	9.53	-5.04	
1.03	1.37	-2.12*	
1.37	2.13	-2.55*	

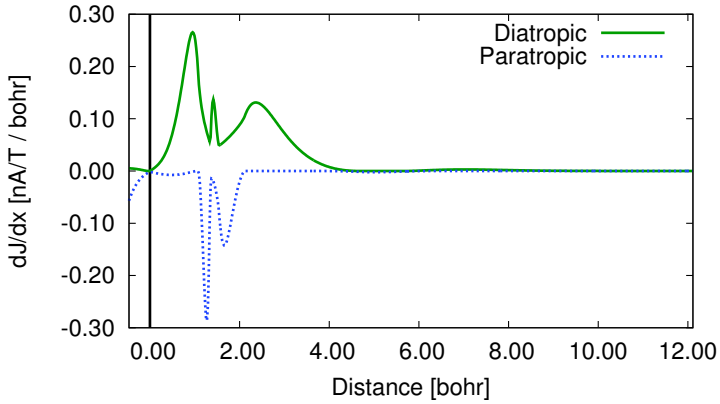


Table 15 Plane **e** with origin at the centre of ring B and passing through atom B1.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-0.10	9.66	2.60
Diatropic domains		
1.36	9.66	8.99
Paratropic domains		
-0.34	9.66	-6.42
-0.34	1.58	-3.00
1.92	2.40	-1.39
2.46	5.66	-2.03

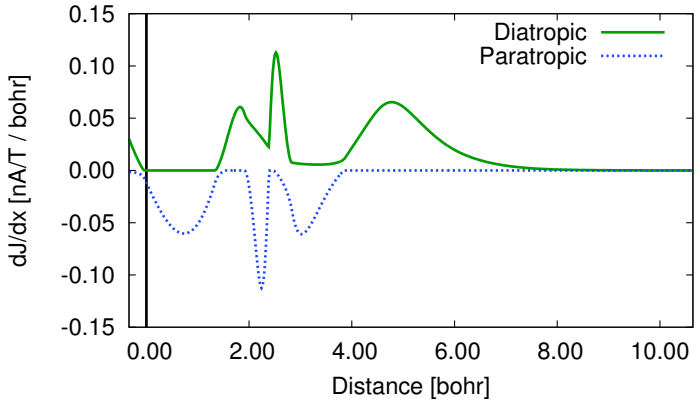


Table 16 Plane **f** with origin at the centre of ring B and passing through the midpoint of the bond between atoms C5 and B1.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-0.07	11.67	2.54
Diatropic domains		
1.61	11.67	8.78
Paratropic domains		
-0.33	5.67	-6.27

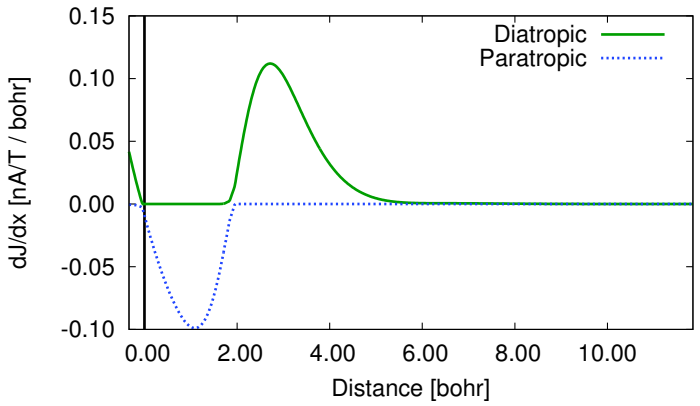


Table 17 Plane **g** along the C4 – C5 bond, with origin at the midpoint of the bond.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.00	11.18	14.09
Diatropic domains		
0.00	11.18	15.48
Paratropic domains		
0.00	11.18	-1.39
1.00	1.36	-0.86
1.42	2.06	-0.43

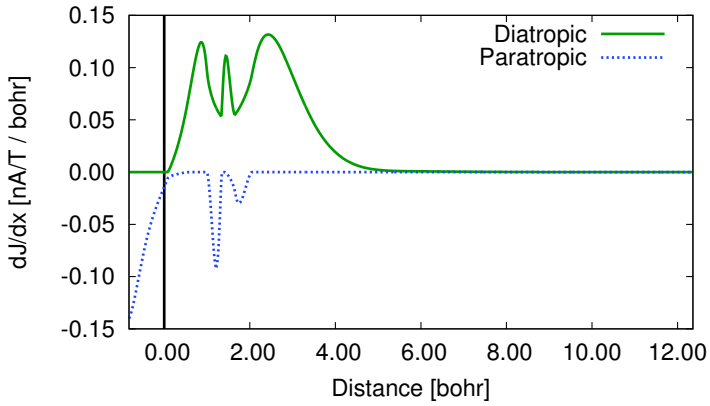


Table 18 Plane **h** with origin at the centre of ring B and ending at the centre of ring A. The point 0 on the abscissa corresponds to the centre of the fusion bond.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-1.88	2.32	-7.68
Diatropic domains		
0.22	2.70	5.42
Paratropic domains		
-1.96	1.88	-13.20

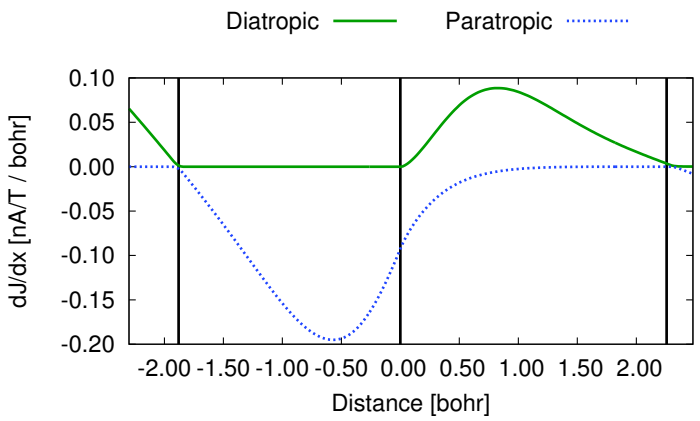


Table 19 Plane **i** with origin at the centre of ring B and ending at the centre of ring C. The point 0 on the abscissa corresponds to the centre of the fusion bond.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-1.82	1.80	0.00
Diatropic domains		
0.00	1.84	10.04
Paratropic domains		
-1.82	1.80	-10.05

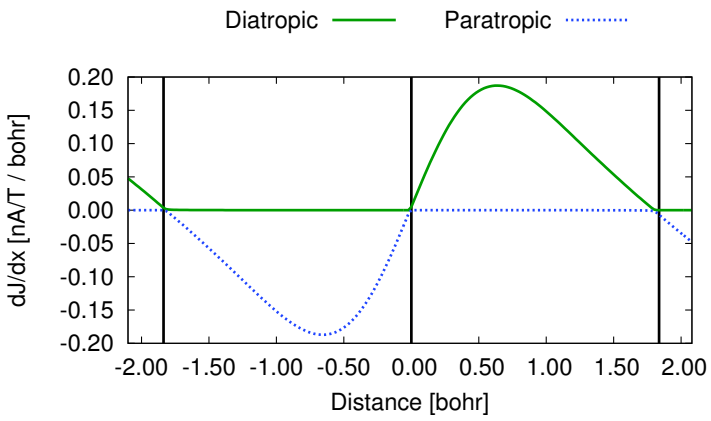


Table 20 Plane **j** with origin at the centre of ring A and passing through atom C4.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Paratropic domains		
-0.19	2.57	-4.15
-0.19	1.79	-2.88
2.23	2.57	-1.27

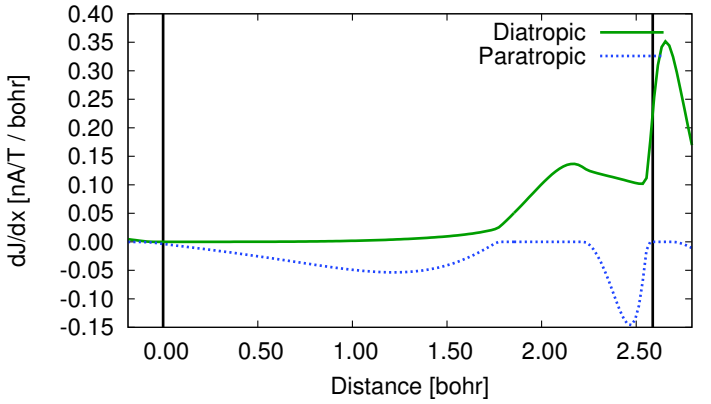
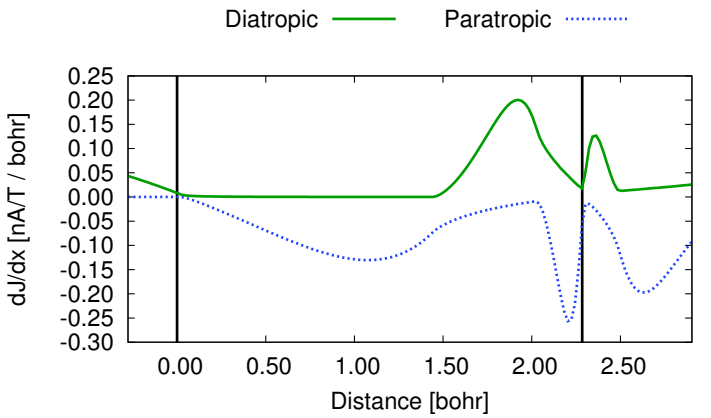


Table 21 Plane **k** with origin at the centre of ring C and passing through atom N2. The domains which are overlapping with each other are marked with an asterisk.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Paratropic domains		
0.04	2.42	-8.93
0.04	2.02	-6.85*
2.02	2.30	-1.89*



Molecule (3)

Table 22 Plane **a** with origin at the centre of ring **A** and passing through atom C1.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.04	11.82	8.81
Diatropic domains		
0.04	11.82	15.44
Paratropic domains		
0.04	11.82	-6.62
0.04	1.96	-3.72
2.20	2.64	-1.93
2.64	3.70	-0.98

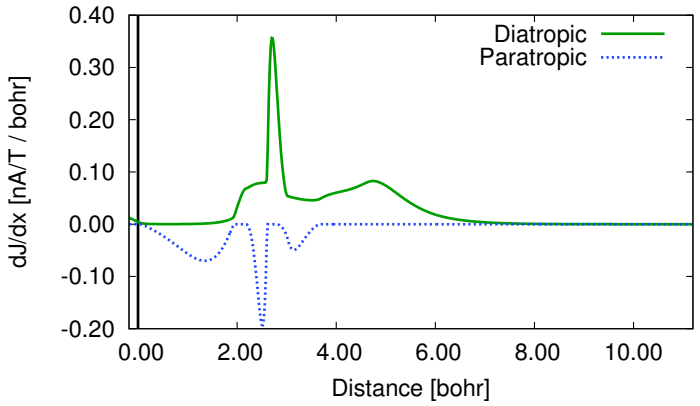


Table 23 Plane **b** with origin at the centre of ring **A** and passing through the midpoint of the bond between atoms C1 and C2.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.10	11.68	8.85
Diatropic domains		
0.66	11.68	14.40
Paratropic domains		
0.04	2.30	-5.52

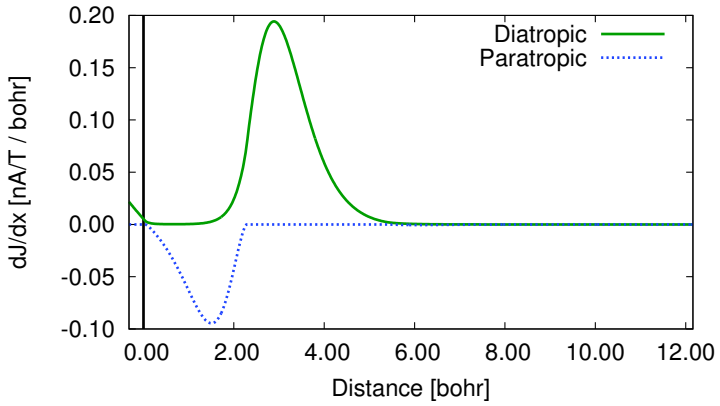


Table 24 Plane **c** with origin at the centre of ring **B** and passing through the midpoint of the bond between atoms C4 and B2.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-0.01	9.81	-3.94
Diatropic domains		
2.07	9.81	5.48
Paratropic domains		
-0.05	3.63	-9.39

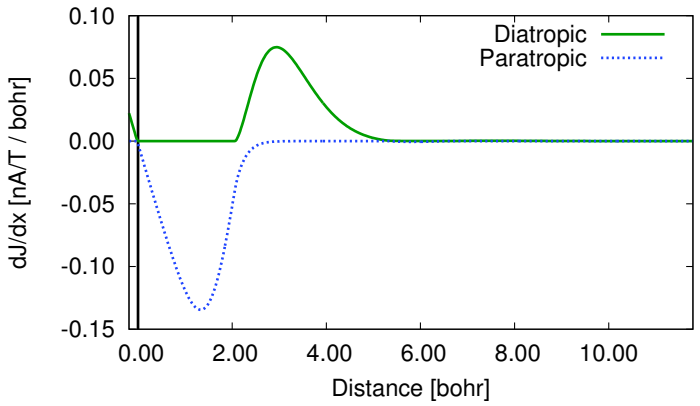


Table 25 Plane **d** along the N1 – B2 bond, with origin at the midpoint of the bond.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.00	9.76	6.29
Diatropic domains		
0.60	9.76	13.07
0.60	1.36	0.94
1.36	9.76	12.14
Paratropic domains		
0.00	9.76	-6.78

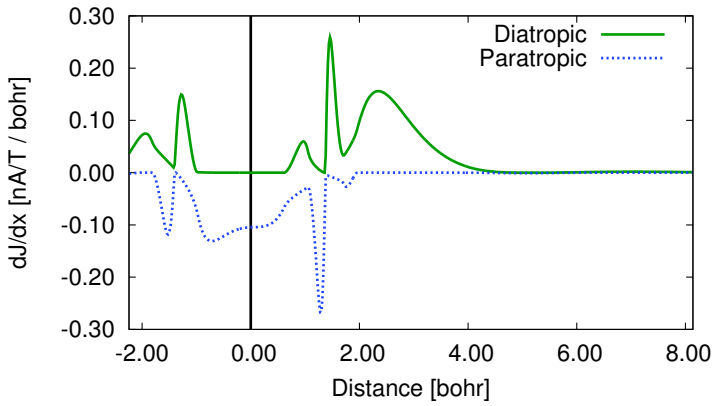


Table 26 Plane **e** with origin at the centre of ring **B** and passing through atom B1.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-0.14	7.70	-3.94
Diatropic domains		
1.20	7.70	7.63
1.20	2.18	0.76
2.24	2.72	1.85
3.58	7.70	5.03
Paratropic domains		
-0.14	7.70	-11.57

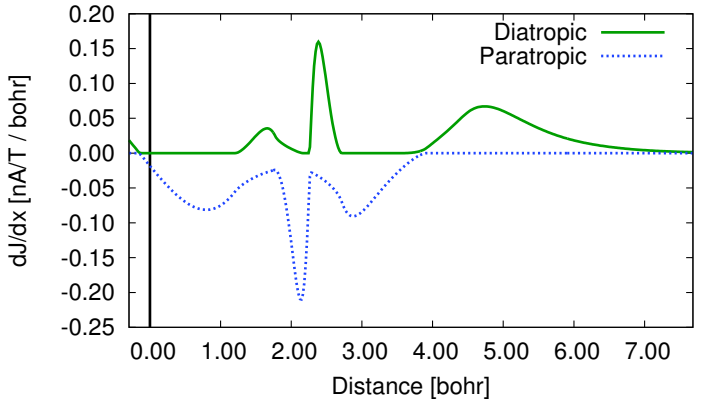


Table 27 Plane **f** with origin at the centre of ring **B** and passing through the midpoint of the bond between atoms B1 and C5.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-0.01	9.87	-3.94
Diatropic domains		
1.95	9.87	5.79
Paratropic domains		
-0.01	9.87	-9.73

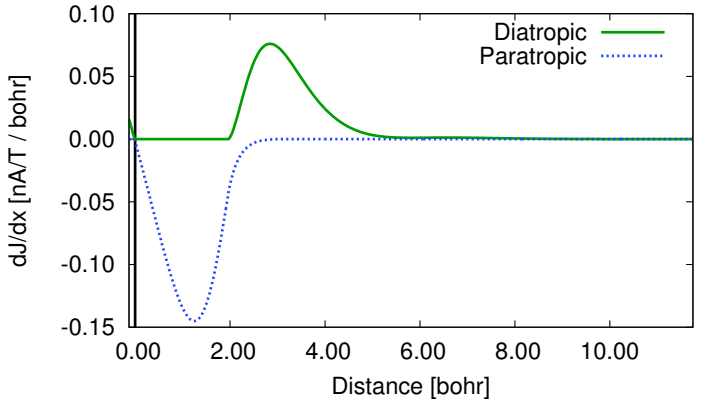


Table 28 Plane **g** along the C4 – C5 bond, with origin at the midpoint of the bond.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-0.01	8.51	10.86
Diatropic domains		
-0.01	8.51	11.95
Paratropic domains		
-0.01	8.51	-1.09

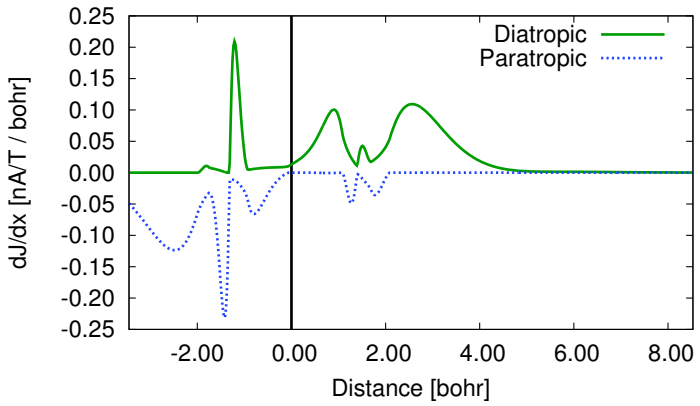


Table 29 Plane **h** with origin at the centre of ring **A** and ending at the centre of ring **B**. The point 0 on the abscissa corresponds to the centre of the fusion bond.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-2.20	2.38	-12.84
Diatropic domains		
0.00	2.60	5.51
Paratropic domains		
-2.20	2.38	-18.48

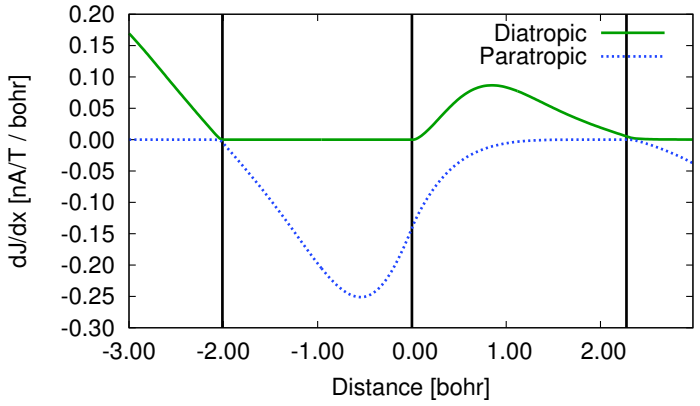


Table 30 Plane **i** with origin at the centre of ring **B** and ending at the centre of ring **C**.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-1.92	1.92	-6.56
Diatropic domains		
-0.02	2.30	4.98
Paratropic domains		
-1.92	1.92	-11.52

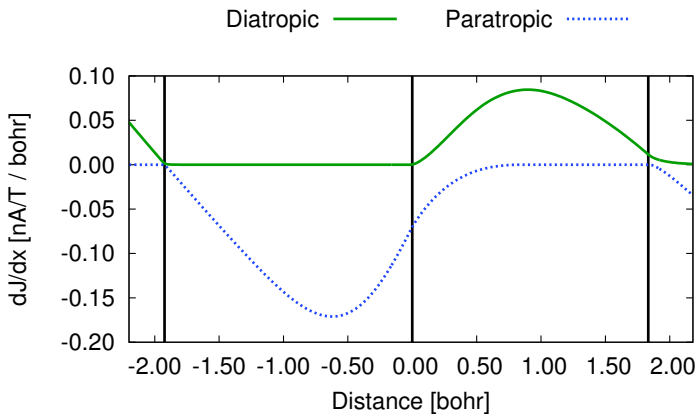


Table 31 Plane **j** with origin at the centre of ring **C** and ending at the centre of ring **D**.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-2.28	1.76	7.88
Diatropic domains		
-2.30	1.76	12.21
Paratropic domains		
-2.30	-0.04	-4.31

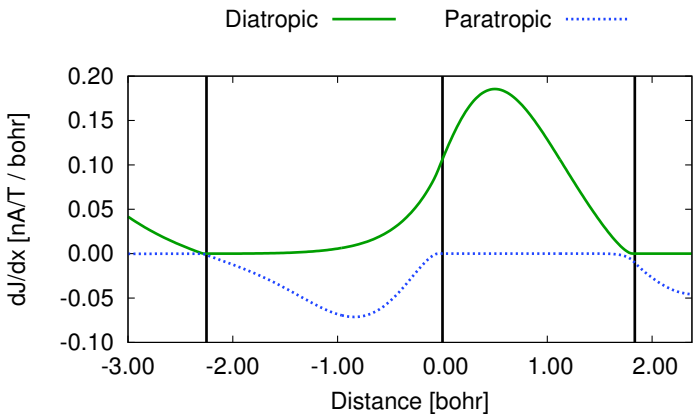


Table 32 Plane **k** with origin at the centre of ring **C** and passing through atom N1.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Paratropic domains		
-0.10	2.34	-9.86
-0.10	1.92	-7.95
1.92	2.30	-1.91

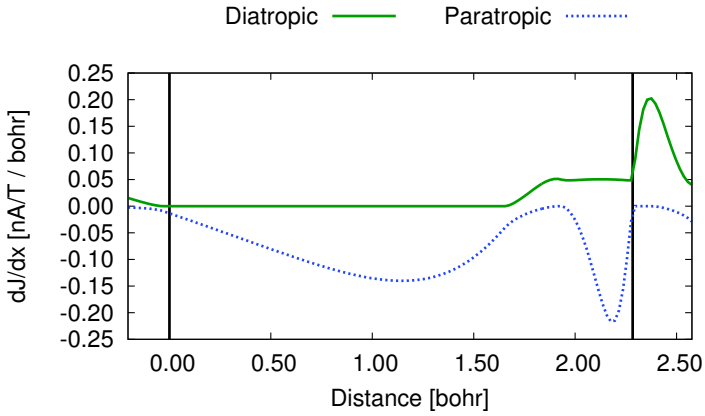


Table 33 Plane **l** with origin at the centre of ring **C** and passing through atom N1.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Paratropic domains		
-0.08	2.32	-3.49
-0.08	1.12	-1.82
1.88	2.32	-1.67

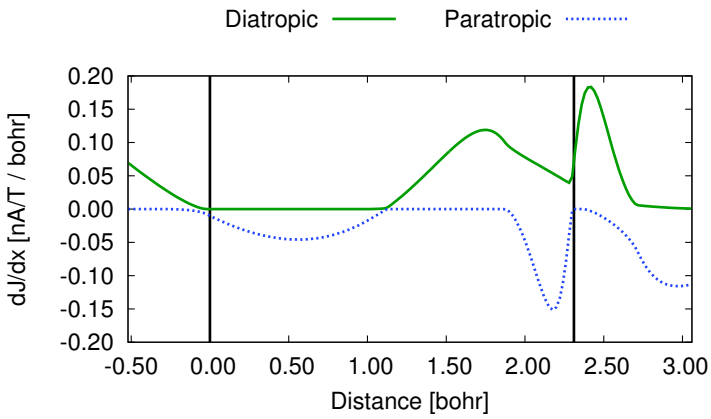


Table 34 Plane **m** with origin at the centre of ring **C** and passing through atom N2.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.04	10.72	2.33
Diatropic domains		
1.62	2.16	0.61*
1.62	2.58	3.18*
2.16	2.58	2.58*
Paratropic domains		
0.02	2.28	-10.18
0.02	1.94	-7.96*
1.94	2.28	-2.25*

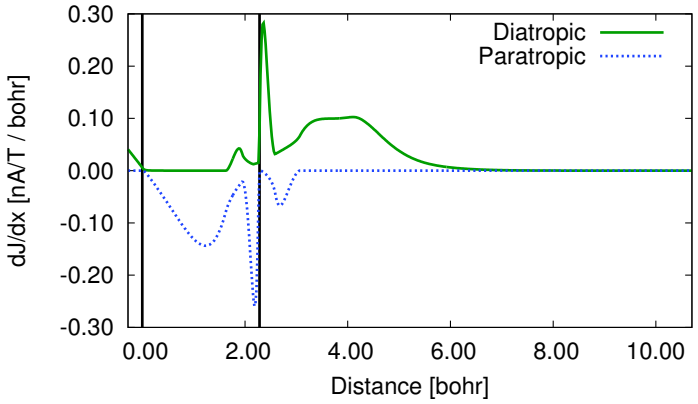


Table 35 Plane **n** with origin at the centre of ring **C** and passing through atom C8.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Paratropic domains		
0.03	2.29	-8.05
0.03	1.89	-4.82
1.89	2.29	-3.25

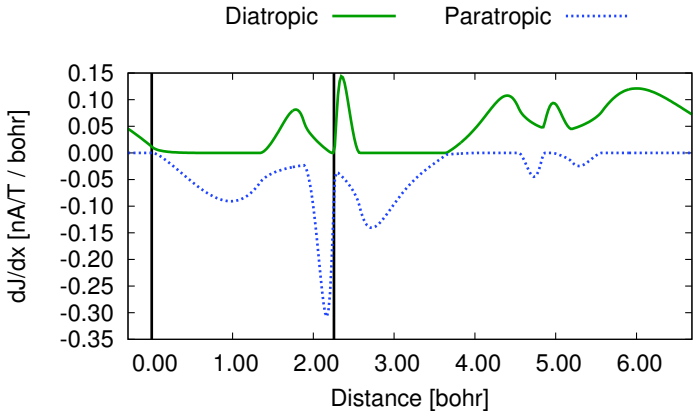


Table 36 Plane **o** with origin at the centre of ring **D** and passing through atom C8.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Paratropic domains		
-0.03	2.59	-3.46
-0.19	1.75	-2.40
2.27	2.59	-1.06

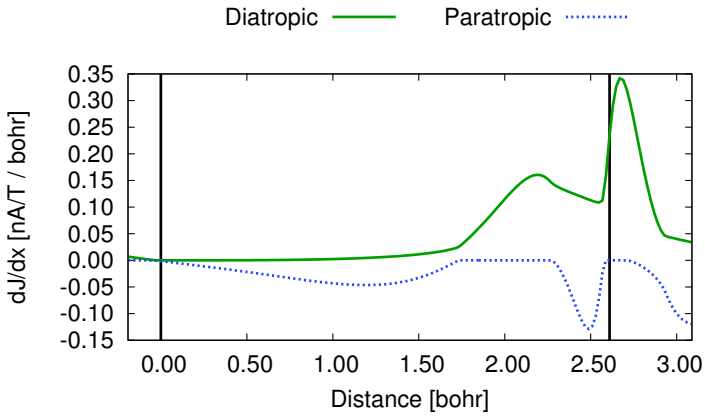


Table 37 Plane **p** along the N1 – B2 bond, with origin at the midpoint of the bond.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.00	11.03	5.35
Diatropic domains		
0.00	11.03	8.96
1.37	1.79	0.78
2.07	6.11	2.41
Paratropic domains		
0.23	2.87	-3.59

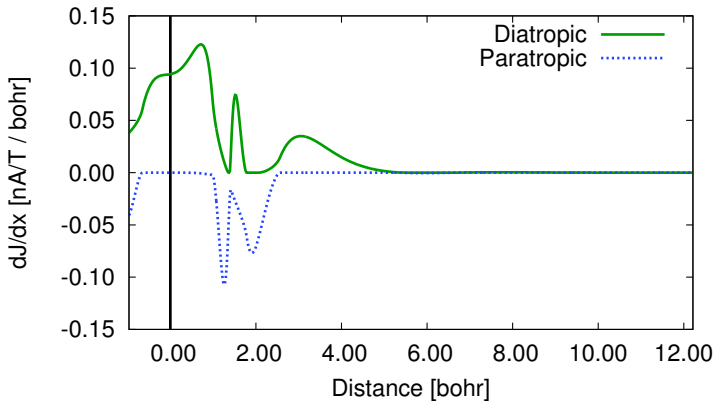


Table 38 Plane **q** along the C7 – C8 bond, with origin at the midpoint of the bond.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.00	12.45	13.29
Diatropic domains		
-0.17	8.73	16.09
Paratropic domains		
0.99	2.21	-2.68
0.99	1.37	-1.64
1.43	2.21	-1.04

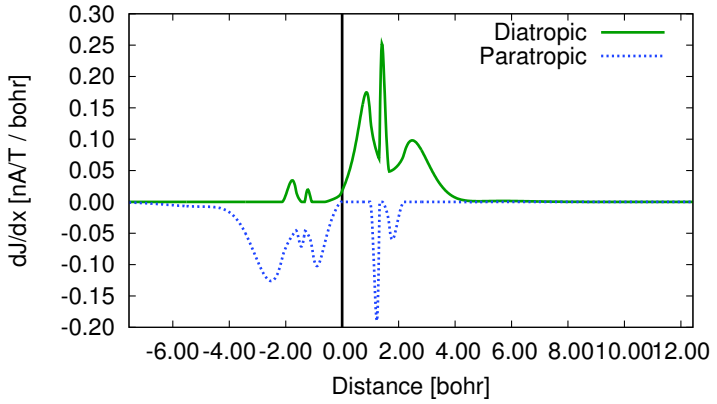


Table 39 Plane **r** with origin at the centre of ring **D** and passing through atom C10.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.01	11.81	10.38
Diatropic domains		
0.01	11.81	16.87
Paratropic domains		
-0.07	3.65	-6.48
-0.07	1.91	-3.56
2.17	2.61	-2.07
2.83	3.65	-0.86

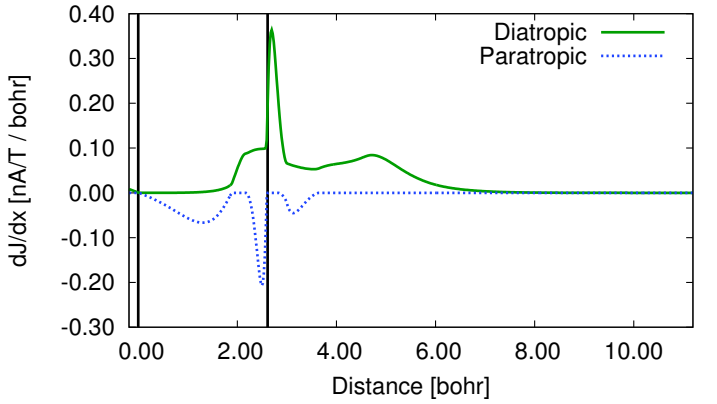


Table 40 Plane **s** with origin at the centre of ring **D** and passing through the midpoint of the bond between atoms C10 and C11.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.00	11.76	10.49
Diatropic domains		
0.16	11.76	15.82
Paratropic domains		
0.02	2.28	-5.31

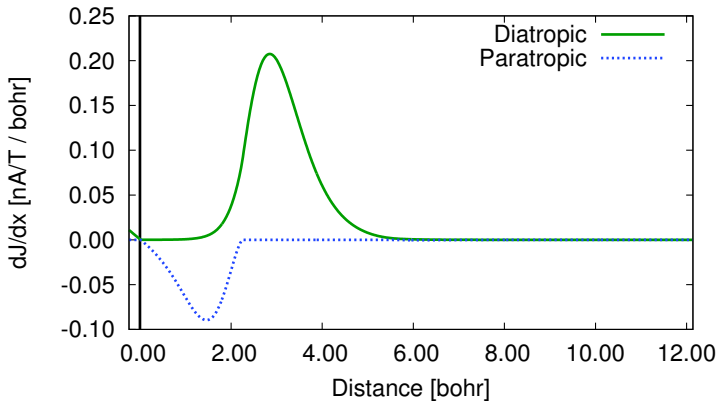
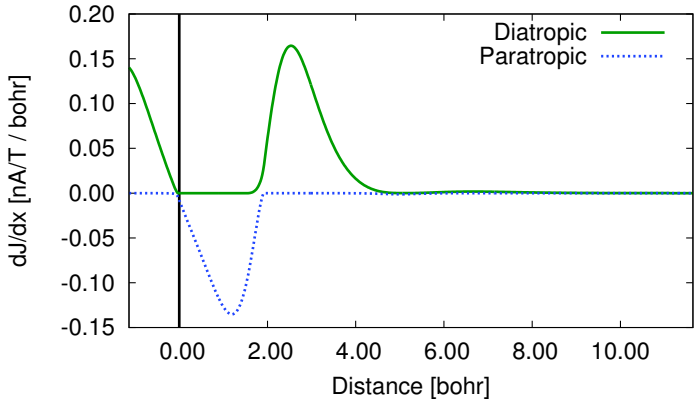


Table 41 Plane **t** with origin at the centre of ring **C** and passing through the midpoint of the bond between atoms C7 and N1.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-0.06	10.86	2.69
Diatropic domains		
1.56	10.86	10.51
Paratropic domains		
-0.14	1.86	-7.74



Molecule (4)

Table 42 Plane **a** with origin at the centre of ring A and passing through atom C1.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-0.01	12.61	8.57
Diatropic domains		
0.69	12.61	22.82
Paratropic domains		
-0.01	12.61	-14.26
0.01	1.97	-4.02
2.17	2.61	-9.01
2.99	3.67	-1.24

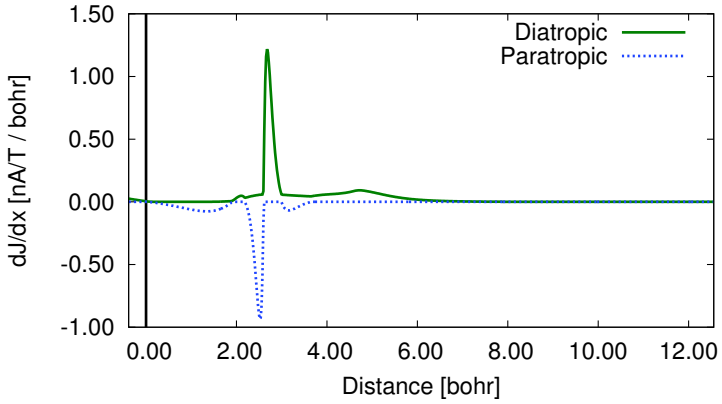


Table 43 Plane **b** with origin at the centre of ring A and passing through the midpoint of the bond between atoms C1 and C2.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.14	12.78	7.13
Diatropic domains		
0.92	12.78	13.23
Paratropic domains		
0.04	12.78	-6.12
0.04	2.30	-6.09

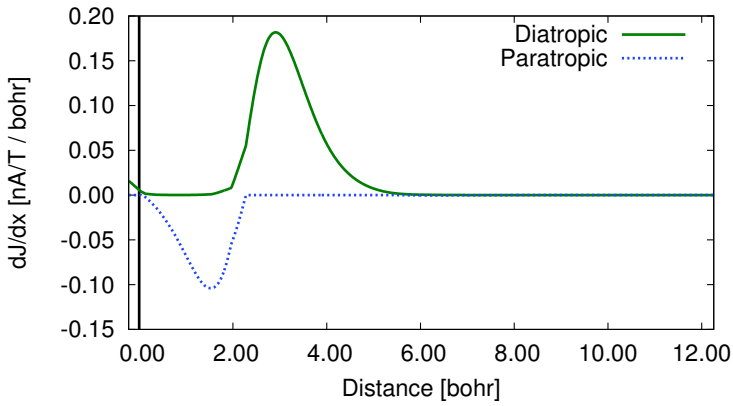


Table 44 Plane **c** with origin at the centre of ring B and passing through the midpoint of the bond between atoms C4 and B2.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-0.30	12.00	-5.41
Diatropic domains		
2.10	7.16	6.43
Paratropic domains		
-1.00	3.40	-11.95

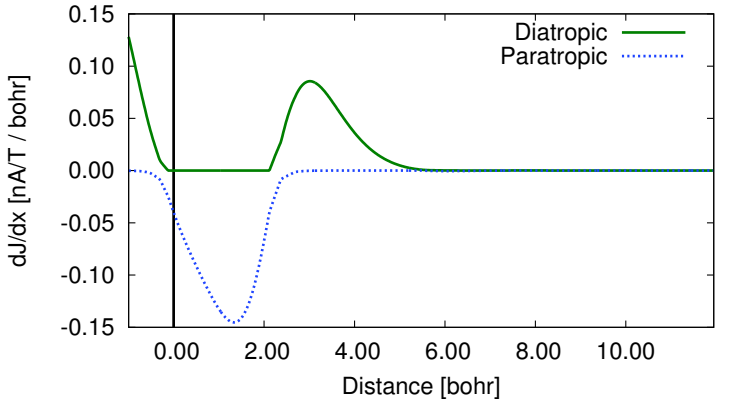


Table 45 Plane **d** along the B1 – B2 bond, with origin at the midpoint of the bond.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.00	10.00	1.63
Diatropic domains		
0.00	10.00	12.77
0.00	1.58	2.60
1.58	2.02	7.78
2.02	5.80	2.62
Paratropic domains		
0.00	10.00	-11.14

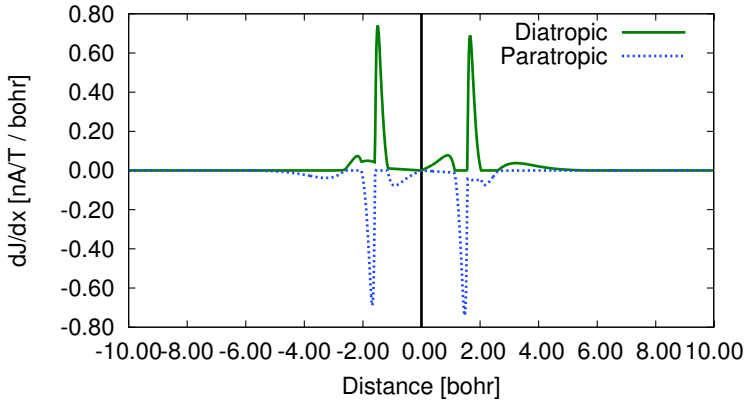


Table 46 Plane **e** with origin at the centre of ring B and passing through atom B1. The domains that are overlapping with each other are marked with an asterisk.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.25	12.85	-4.77
Diatropic domains		
1.67	12.85	19.79
1.67	2.33	0.97
2.33	2.71	10.11
2.71	12.85	8.71
Paratropic domains		
0.07	11.85	-24.69
0.07	2.01	-10.18
2.01	2.63	-12.66*
0.07	2.63	-22.74*
2.63	3.63	-1.97*

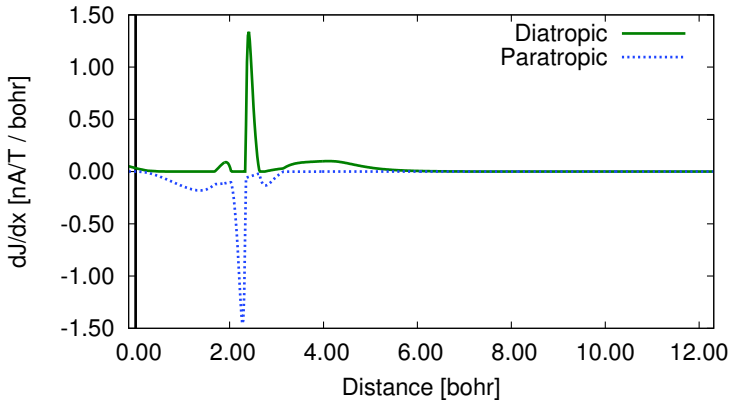


Table 47 Plane **f** with origin at the centre of ring B and passing through the midpoint of the bond between atoms C5 and B1.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.28	11.86	-5.31
Diatropic domains		
1.88	4.62	5.35
Paratropic domains		
0.04	4.12	-11.04

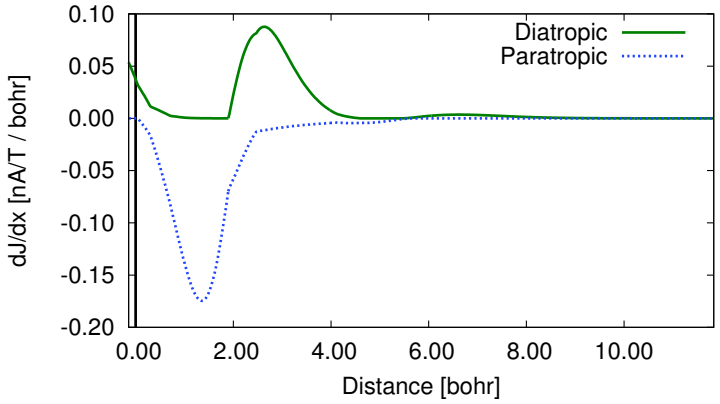


Table 48 Plane **g** along the C4 – C5 bond, with origin at the midpoint of the bond. The domains that are overlapping with each other are marked with an asterisk.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.00	10.00	8.43
0.48	10.00	9.13
Diatropic domains		
0.18	0.98	1.46
1.20	1.78	10.30*
1.78	6.12	8.78*
Paratropic domains		
0.48	10.00	-11.20

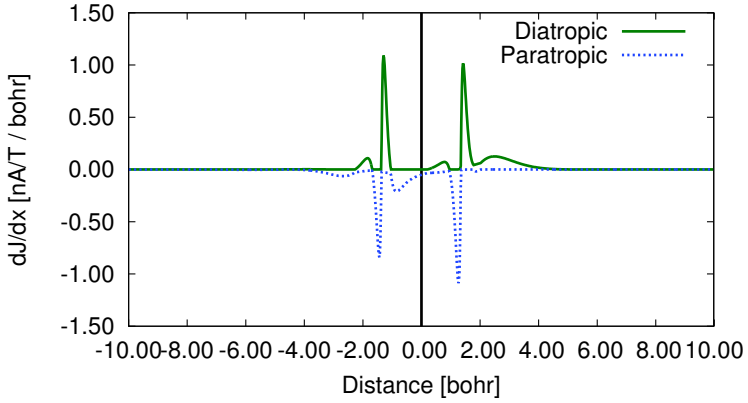


Table 49 Plane **h** with origin at the centre of ring B and ending at the centre of ring A.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-1.90	2.42	-11.99
Diatropic domains		
0.00	2.50	5.01
Paratropic domains		
-1.96	2.32	-16.99

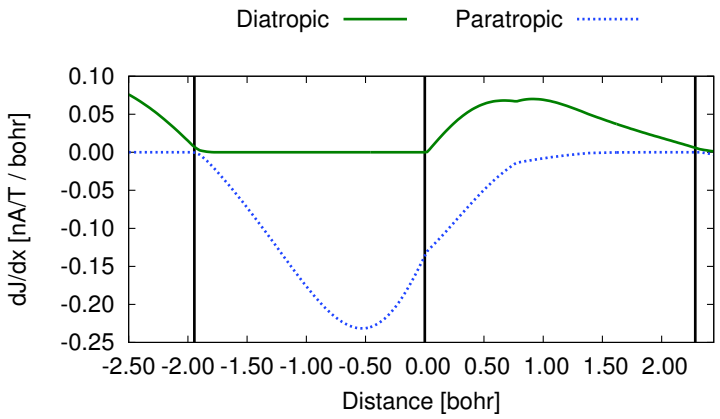


Table 50 Plane **i** with origin at the centre of ring B and ending at the centre of ring C. The point 0 on the abscissa corresponds to the centre of the fusion bond.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-2.08	2.08	0.00
Diatropic domains		
-2.50	0.02	7.33
Paratropic domains		
0.00	2.08	-7.26

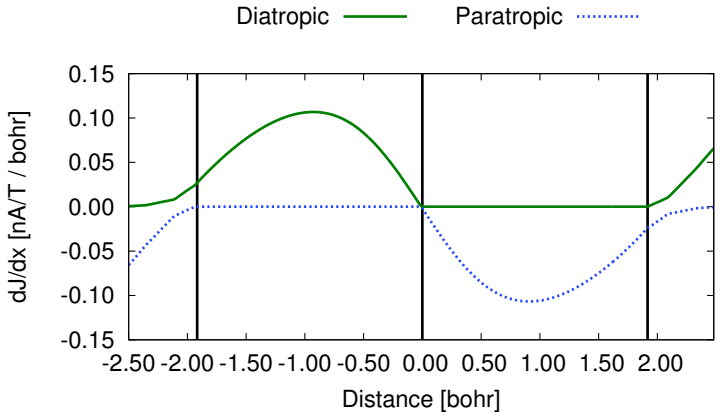
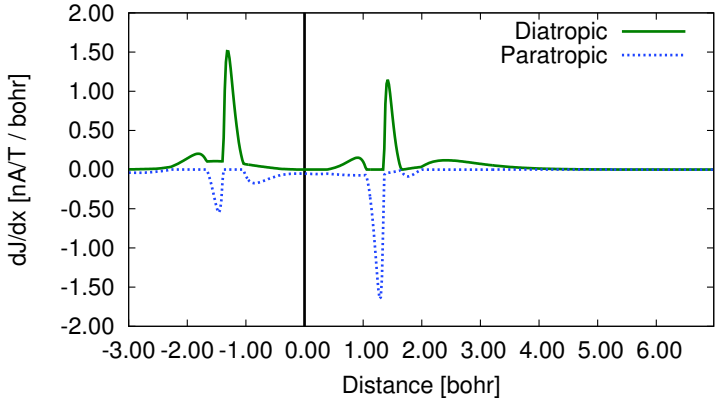


Table 51 Plane **j** along the C5 – N1 bond, with origin at the midpoint of the bond.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.00	7.00	0.71
Diatropic domains		
-1.06	1.06	4.08
1.36	1.66	8.65
1.68	7.00	7.40
Paratropic domains		
-1.04	-0.12	-4.80



Clarification on the meaning of paratropic and diatropic components in the current profile

Sometimes in the current profile plots it appears that currents which are expected to be paratropic appear as the diatropic contribution to the currents flowing across the integration plane. This is not a computational error but a matter of definition. In Fig. 1 the induced current densities along integration plane **a** in molecule (**1**) are illustrated. The line integral convolution (LIC) representation also shows the direction of the vector field at different grid points. The current flow on one side of ring A appears to be flowing in opposite directions on the two sides of the vortex of the ring current.

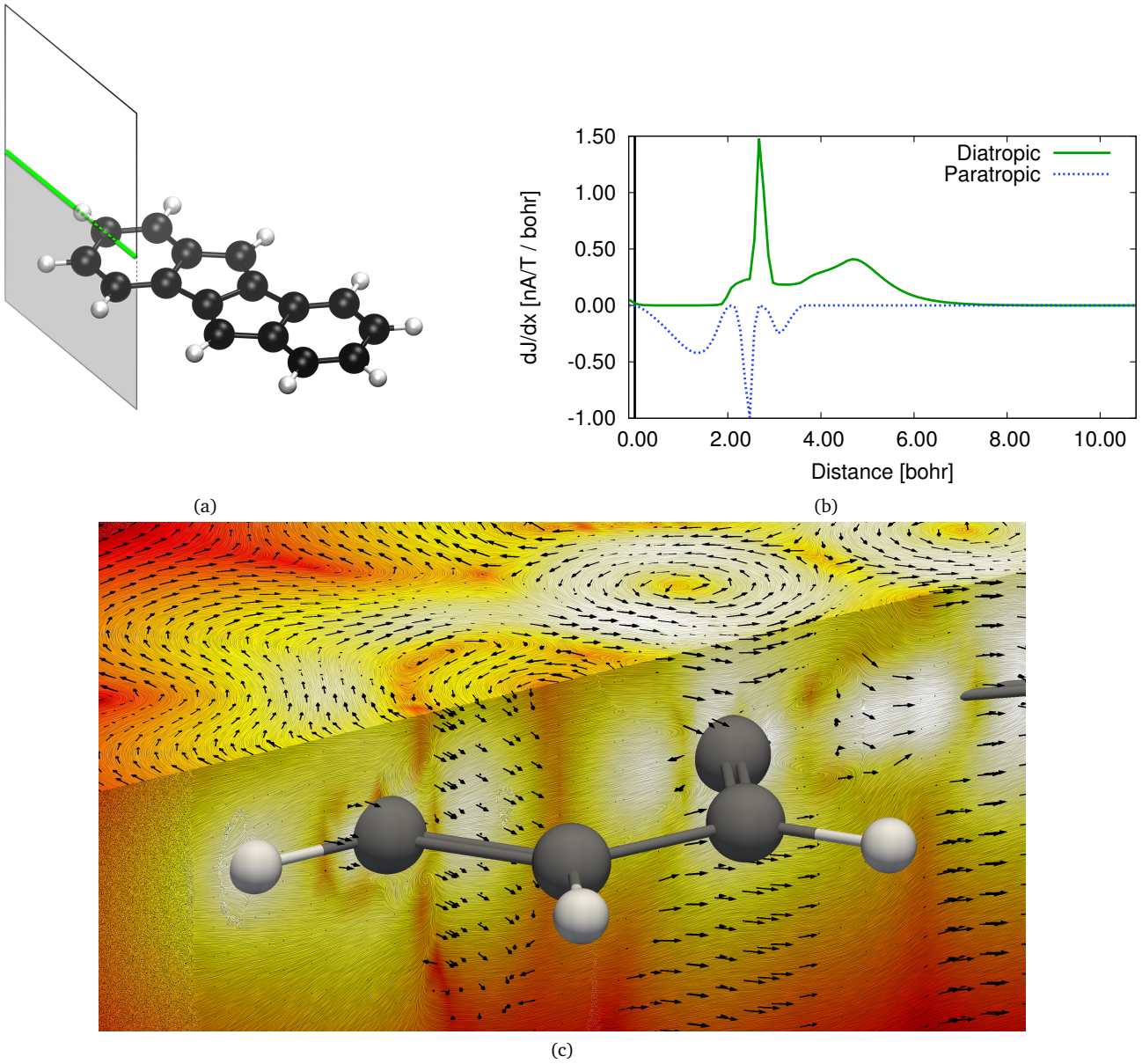


Fig. 1 (a) LIC representation of the current density in molecule (**1**). A horizontal clipping plane has been defined 1.5 bohr above the molecular plane and a vertical clipping plane perpendicular to the molecular plane passed through atom C1. (b) Current profile for the integration along plane **b**

Molecular coordinates

The molecular structures are optimized at the B3LYP/def2-TZVP level of theory. The coordinates are listed in Å.

Molecule (1)

index	element	x	y	z
1	C	-4.3482341129	0.5034908647	0.0000000000
2	C	-4.1229715822	-0.8664652598	0.0000000000
3	C	-3.2764494511	1.4052191353	0.0000000000
4	C	-1.9853738681	0.9081899260	0.0000000000
5	C	-1.7548316259	-0.4971113107	0.0000000000
6	C	-2.8184588970	-1.3785130825	0.0000000000
7	C	-0.3030474641	-0.6692379338	0.0000000000
8	C	0.2937920181	0.6718555141	0.0000000000
9	C	-0.6863346898	1.6043264172	0.0000000000
10	C	1.7454887247	0.4999169191	0.0000000000
11	C	1.9762820420	-0.9053173863	0.0000000000
12	C	0.6772326933	-1.6015991696	0.0000000000
13	C	2.8087887408	1.3816931891	0.0000000000
14	C	4.1134269770	0.8700627856	0.0000000000
15	C	4.3390480701	-0.4998308070	0.0000000000
16	C	3.2675545309	-1.4019111127	0.0000000000
17	H	-5.3636447904	0.8799448369	0.0000000000
18	H	-4.9641214970	-1.5484629559	0.0000000000
19	H	-3.4615795310	2.4729958862	0.0000000000
20	H	-2.6551217912	-2.4495861198	0.0000000000
21	H	2.6450386007	2.4526965706	0.0000000000
22	H	4.9543748758	1.5523063631	0.0000000000
23	H	5.3545777543	-0.8759509364	0.0000000000
24	H	3.4531468279	-2.4695989378	0.0000000000
25	H	0.5661946076	-2.6775277870	0.0000000000
26	H	-0.5750931918	2.6802454502	0.0000000000

Molecule (2)

index	element	x	y	z
1	C	3.9867602103	1.0438644878	0.0000000000
2	C	4.3393761681	-0.3097646570	0.0000000000
3	C	3.3558884099	-1.2897446511	0.0000000000
4	C	2.6570662923	1.4455359883	0.0000000000
5	C	1.6862434626	0.4507367131	0.0000000000
6	C	2.0078489644	-0.9242955061	0.0000000000
7	C	-2.0078489644	0.9242955061	0.0000000000
8	C	-1.6862434626	-0.4507367131	0.0000000000
9	C	-3.3558884099	1.2897446511	0.0000000000
10	C	-4.3393761681	0.3097646570	0.0000000000
11	C	-3.9867602103	-1.0438644878	0.0000000000
12	C	-2.6570662923	-1.4455359883	0.0000000000
13	H	-3.6341968478	2.3370878757	0.0000000000
14	H	-5.3854682144	0.5888522828	0.0000000000
15	H	-4.7653651342	-1.7969681847	0.0000000000
16	H	-2.3891822187	-2.4939771693	0.0000000000
17	H	3.6341968478	-2.3370878757	0.0000000000
18	H	5.3854682144	-0.5888522828	0.0000000000
19	H	4.7653651342	1.7969681847	0.0000000000
20	H	2.3891822187	2.4939771693	0.0000000000
21	N	0.3036582727	0.6365768403	0.0000000000
22	B	-0.6631262707	1.6793553778	0.0000000000
23	H	-0.3786700213	2.8294799372	0.0000000000
24	N	-0.3036582727	-0.6365768403	0.0000000000
25	B	0.6631262707	-1.6793553778	0.0000000000
26	H	0.3786700213	-2.8294799372	0.0000000000

Molecule (3)

index	element	x	y	z
1	C	4.0687118758	1.0134834411	0.0000000000
2	C	4.3722512382	-0.3453635139	0.0000000000
3	C	3.3607763051	-1.3081759090	0.0000000000
4	C	2.7438995069	1.4532881075	0.0000000000
5	C	1.7349880089	0.5046107380	0.0000000000
6	C	2.0467288325	-0.8737622235	0.0000000000
7	C	-2.0528567271	0.8253520693	0.0000000000
8	C	-1.7945781634	-0.5773143588	0.0000000000
9	C	-3.3641090188	1.2797917244	0.0000000000
10	C	-4.4210893441	0.3631555855	0.0000000000
11	C	-4.1652998037	-1.0011338746	0.0000000000
12	C	-2.8487250620	-1.4764284210	0.0000000000
13	H	-3.5768203442	2.3433345874	0.0000000000
14	H	-5.4448631621	0.7179162429	0.0000000000
15	H	-4.9909235694	-1.7028466719	0.0000000000
16	H	-2.6702511263	-2.5463051482	0.0000000000
17	H	3.6013515669	-2.3645979836	0.0000000000
18	H	5.4071398038	-0.6634085120	0.0000000000
19	H	4.8705518234	1.7408535722	0.0000000000
20	H	2.5078578787	2.5097865398	0.0000000000
21	N	0.8484660495	-1.6149112299	0.0000000000
22	N	0.3431380228	0.6345727855	0.0000000000
23	B	-0.6879222941	1.6188399181	0.0000000000
24	B	-0.2392982950	-0.7079672071	0.0000000000
25	H	0.8660305393	-2.6197361561	0.0000000000
26	H	-0.5151545417	2.7969658982	0.0000000000

Molecule (4)

index	element	x	y	z
1	C	4.22345694	1.01556241	-0.002646849
2	C	4.434542986	-0.35644142	-0.005823534
3	C	3.3612966	-1.252618388	-0.00328609
4	C	2.917597236	1.512352301	0.002877238
5	C	1.822125971	0.656301666	0.005399553
6	C	2.070324649	-0.752809979	0.002488948
7	C	-2.070332211	0.752806199	0.003469087
8	C	-1.822131677	-0.656309474	0.0062461
9	C	-3.361290028	1.252617095	-0.002645737
10	C	-4.434533288	0.356436436	-0.005897503
11	C	-4.223446919	-1.015566167	-0.002831458
12	C	-2.917587353	-1.512357003	0.003231488
13	H	-3.542923902	2.321429748	-0.00532458
14	H	-5.446109705	0.744854043	-0.010955362
15	H	-5.067046252	-1.694192425	-0.005367413
16	H	-2.755812858	-2.584500123	0.005374417
17	H	3.54296708	-2.321424317	-0.005864082
18	H	5.446133021	-0.744829131	-0.010311815
19	H	5.067052689	1.694193458	-0.004701076
20	H	2.755859129	2.584499377	0.005105451
21	B	0.27222774	0.788268442	0.009334955
22	N	-0.894531563	1.576944105	0.005864138
23	H	-1.033702155	2.57725084	0.00134754
24	B	-0.272216852	-0.788257831	0.009375566
25	N	0.894489475	-1.576951151	0.004957343
26	H	1.033591248	-2.577258711	0.000583676

Nuclear shielding constants

Isotropic nuclear shielding constants calculated at the B3LYP/def2-TZVP level of theory.

Molecule (1)

index	element	shielding constant
1	C	50.37
2	C	51.03
3	C	55.77
4	C	24.18
5	C	39.43
6	C	56.57
7	C	24.91
9	C	49.04
17	H	24.99
18	H	25.00
19	H	25.07
20	H	24.86
25	H	25.52

Molecule (2)

index	element	shielding constant
1	C	45.90
2	C	55.69
3	C	44.13
4	C	67.79
5	C	26.49
6	C	43.78
13	H	23.86
14	H	24.56
15	H	24.21
16	H	24.13
21	N	22.53
22	B	72.27
23	H	25.84

Molecule (3)

index	element	shielding constant
1	C	57.45
2	C	56.30
3	C	68.32
4	C	65.42
5	C	40.48
6	C	32.43
7	C	20.54
8	C	34.79
9	C	43.83
10	C	47.66
11	C	47.11
12	C	49.31
13	H	24.10
14	H	24.41
15	H	24.42
16	H	24.33
17	H	24.88
18	H	24.72
19	H	24.73
20	H	24.37
21	N	136.06
22	N	63.18
23	B	56.73
24	B	63.62
25	H	26.09
26	H	25.56

Molecule (4)

index	element	shielding constant
1	C	58.04
2	C	43.83
3	C	66.04
4	C	43.09
5	C	49.71
6	C	-2.35
17	H	25.26
18	H	24.63
19	H	25.05
20	H	24.59
21	B	47.62
25	N	113.30
26	H	26.39

NMR shifts

NMR shifts δ_0 (in ppm) calculated for two of the studied molecules at the B3LYP/def2-TZVP level of theory. They are compared to experimental NMR shifts δ_{exp} obtained for the derivatives where the hydrogen atoms H5 and H6 at the heteroatoms are substituted with mesityl groups. The NMR shifts were calculated at the same level of theory and compared to the non-substituted molecules and the experimental data obtained by Wang *et al.* (*J. Am. Chem. Soc.*, 2015, **137**, 7668 – 7671). The labels of the hydrogen atoms are presented in our article.

Molecule (2) with mesityl substituents at the boron atoms

Atom	δ_0	δ_{Mes}	$\delta_0 - \delta_1$	δ_{exp}	$\delta_0 - \delta_{exp}$
H6	8.07	7.86	-0.21	7.55	0.31
H3	7.80	7.29	-0.51	7.26	0.03
H2	7.72	7.48	-0.24	7.055	0.42
H1	7.37	7.08	-0.30	6.81	0.27

Molecule (3) with mesityl substituents at the nitrogen atoms

Atom	δ_0	δ_{Mes}	$\delta_0 - \delta_1$	δ_{exp}	$\delta_0 - \delta_{exp}$
H6	7.83	7.66	-0.17	7.34	0.32
H3	7.60	7.29	-0.30	7.075	0.22
H12	7.56	7.09	-0.46	6.71	0.38
H1	7.52	7.48	-0.04	7.215	0.26
H2	7.51	7.38	-0.13	7.215	0.16
H11	7.20	7.10	-0.10	6.86	0.24
H10	7.21	7.13	-0.08	6.79	0.34
H9	7.05	6.59	-0.46	6.43	0.16