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

Supporting Information
Molecular graphs and molecular conduction - the d-omni-conductors

Patrick W Fowler, Barry T. Pickup, Martha Borg, and Irene Sciriha

1 Conduction behaviour of devices based on general graphs: two-letter codes (2LA)

Table 1 (ESI) Distribution over allowed classes for two-letter codes of general graphs on $n \leq 10$ vertices

Case	η	Vertex count									
		1	2	3	4	5	6	7	8	9	10
CC	0			1	1	3	7	35	483	9572	771377
CI	0		1								
CX	0								31	406	46839
XC	0						4	39	388	16341	795546
XI	0				1		7		129		15356
XX	0				1	5	34	268	4693	114744	6231077
CC	1							3	13	560	12551
XC	1	1			1	1	8	46	591	10663	499908
XX	1			1		7	34	291	3090	80431	2300210
IC	>1						1	2	3	7	24
IX	>1				1	1	1	5	17	100	914
XC	>1				1	3	8	49	370	5564	134397
XX	>1						22	101	1823	22178	908372
Total count		1	1	2	6	20	126	839	11631	260566	11716571

2 Conduction behaviour of devices based on general bipartite graphs: three-letter codes (TLA)

Table 2 (ESI) Distribution over allowed classes for three-letter codes of bipartite graphs on $n \leq 10$ vertices

Case	η	Vertex count									
		1	2	3	4	5	6	7	8	9	10
CII	0						1		3		16
CXI	0		1								
XII	0				1		4		32		597
ICX	1			1							
IXX	1					1		5		40	
XXC	1	1									
XXX	1					2		17		823	
ICC	>1				1				1		2
IIC	>1						1	1	2	2	3
IIX	>1				1	1	1	3	7	19	73
IXC	>1					1	1	2	5	15	47
IXX	>1						5	11	56	198	1204
XIX	>1						2	2	17	29	249
XXX	>1						2	3	59	144	841
Total count		1	1	1	3	5	17	44	182	730	4032

3 Conduction behaviour of devices based on general graphs: three-letter d-omni codes (TLA)

Table 3 (ESI) Distribution over allowed classes for three-letter codes of graphs on $n \leq 10$ vertices

Case	η	Vertex count									
		1	2	3	4	5	6	7	8	9	10
CCC	0					2	6	34	482	9571	771376
CCX	0								31	406	46839
CII	0						1		3		16
CXC	0			1	1	1	1	12	19	2141	50904
CXI	0		1								
CXX	0							4	28	966	51389
XCC	0						1	13	55	2874	78503
XCX	0				1	2	5	16	101	1766	88254
XIC	0						1	1	2	5	8
XII	0				1		5		38		700
XIX	0					1	1	8	15	94	190
XXC	0						2	14	313	11322	666132
XXI	0						1		88		14640
XXX	0					2	28	240	4549	111918	6091244
CCC	1							3	13	560	12551
ICX	1			1							
IXX	1				1		14		514		
XCC	1				1	1	3	6	20	115	1178
XCX	1					1	1	2	6	30	184
XXC	1	1					5	40	571	10548	498730
XXX	1					6	19	289	2570	80401	2300026
ICC	>1				1	1	1	1	2	1	3
IIC	>1						1	2	3	7	24
IIX	>1				1	1	1	5	17	100	914
IXC	>1					1	2	6	27	142	1076
IXX	>1						9	29	281	2211	51805
XCC	>1						1	1	4	7	37
XCX	>1							1	1	3	7
XIC	>1					1	3	6	30	142	980
XIX	>1						4	18	112	864	10789
XXC	>1						1	35	307	5272	132301
XXX	>1						9	53	1429	19100	845771
Total count		1	1	2	6	20	126	839	11631	260566	11716571

4 Expanded d-omni codes

We define the *long code* for a molecular graph as a string of $(D + 1)$ letters drawn from the alphabet {C, I, X}, where each letter refers to the conduction behaviour of devices with a fixed value of graph distance d, drawn from the range $d = 0$, 1, ..., D, where D is the diameter of the graph. Notice that the entries in the long code are ordered strictly by increasing d, with alternating even and odd devices starting from *ipso* ($d = 0$). The TLA has *ipso* at the final position, for consistency with previous usage.Some long codes are obvious, determined entirely by a three-letter acronym that contains no X in the first two positions. Table 4 (ESI, below) analyses long codes for the graph families defined in Fig.1.

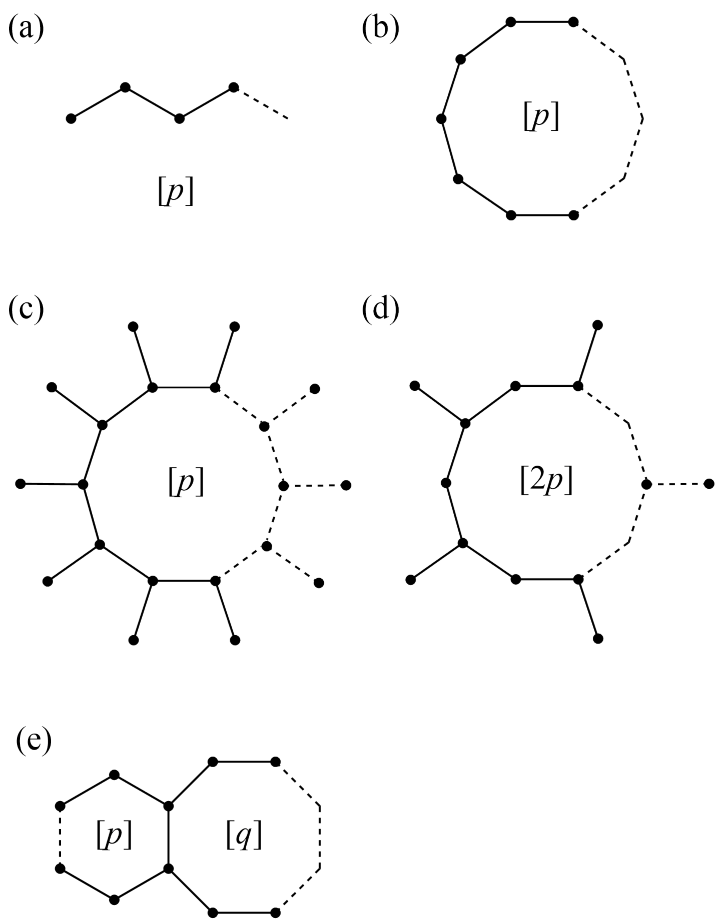

Fig. 1 (ESI) Families of graphs with interesting long codes describing their conduction behaviour: (a) paths, (b) cycles, (c) radialenes, (d) semiradialenes, (e) bi-cycles. The parameters $[p]$ and $[q]$ in (a) to (e) may take both odd and even values.

Table 4 (ESI) Long codes for Fermi-level conduction of the chemical families of molecular graphs defined in Fig. 1(ESI)

Family		Short code	Long code		Notes
Paths, P_n	n even	XII	(IX)^{a}IC	$a = (n-2)/2$	CXI for $n = 2$
	n odd	IXX	(XI)^{a}C	$a = (n-1)/2$	ICX for $n = 3$
Cycles, C_n	$n = 4N+2$	CII	(IC)^a	$a = (n-2)/2$	
	$n = 4N$	ICC	(CI)^{a}C	$a = n/4$	
	n odd	CCC	(C)^a	$a = (n+1)/2$	CXC for $n = 3$
Radialenes, R_n	$n = 2N$	XII	IXIX(I)^a	$a = \lfloor N/2 \rfloor - 1$	IXIC for $N = 3$
Semiradialenes, $n = 3p$	$2p = 4N+2$	XII	(XI)^a	$a = (N+2)/2$	XIIIC for $n = 4$
	$2p = 4N$	XII	(XI)^a	$a = (N+4)/2$	
Bi-cycles, p, q	$p = 4N+2$, $q = 4N'+2$	CII	(IC)^a	$a = N + N' + 1$	
	$p = 4N$, $q = 4N'$, $p \geq q$	XII	(IX)^a(IC)^b	$a = N$, $b = N'$	
	$p = 4N+2$, q odd	CCC	(C)^a	$a = (p+q-1)/2$ $= (n+1)/2$	
	$p = 4N$, q odd	XXX	(X)^a	$a = (p+q-1)/2$ $= (n+1)/2$	
	p, q odd, $p+q = 4N+2$	XXC	C(X)^{a}C	$a = (p+q-4)/2$ $= 2N-1$	XCC for $p = q = 3$
	p, q odd, $p+q = 4N$	XXX	(X)^{a}C	$a = (p+q-2)/2$ $= 2N-1$	