The chemical roots of the matching polynomial

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[a]CNRS ; LCC (Laboratoire de Chimie de Coordination) ; 205, route de Narbonne, F-31077 Toulouse, France. Fax: (+33)5 61 55 30 03. E-mail: chauvin@lcc-toulouse.fr. [b]Université de Toulouse ; UPS, INPT ; LCC ; F-31077 Toulouse, France. †*Department of Chemistry, University of Sheffield, Sheffield S3 7HF, U.K.,* *and* ‡*Laboratoire de Chimie et Physique Quantiques IRSAMC, UMR 5626 CNRS, 118 route de Narbonne, 31062, Toulouse cedex 09, France.*

Supplementary Information

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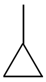
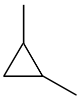
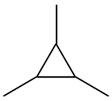
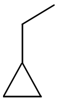
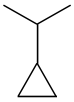
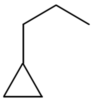
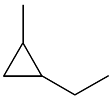
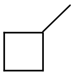
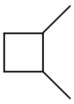
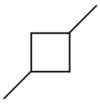
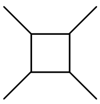
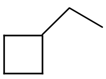
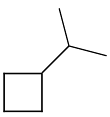
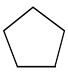
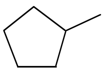
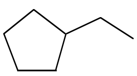
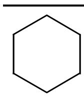
	$P^0(x)$	$P^1(x)$	$P^{ac}(x)$	TRE*
	x^3-3x-2	x^3-3x+2	x^3-3x	–0.464
	x^4-4x^2-2x+1	x^4-4x^2+2x+1	x^4-4x^2+1	–0.063
	$x^5-5x^3-2x^2+3x$	$x^5-5x^3+2x^2+3x$	x^5-5x^3+3x	0.023
	$x^6-6x^4-2x^3+6x^2-1$	$x^6-6x^4+2x^3+6x^2-1$	$x^6-6x^4+6x^2-1$	0.009
	$x^5-5x^3-2x^2+4x+2$	$x^5-5x^3+2x^2+4x-2$	x^5-5x^3+4x	–0.111
	$x^6-6x^4-2x^3+7x^2+4x$	$x^6-6x^4+2x^3+7x^2-4x$	$x^6-6x^4+7x^2$	0.471
	$x^6-6x^4-2x^3+8x^2+4x-1$	$x^6-6x^4+2x^3+8x^2-4x-1$	$x^6-6x^4+8x^2-1$	0.103
	$x^6-6x^4-2x^3+7x^2+2x-1$	$x^6-6x^4+2x^3+7x^2-2x-1$	$x^6-6x^4+7x^2-1$	0.045
	x^4-4x^2	x^4-4x^2+4	x^4-4x^2+2	–1.226
	x^5-5x^3+2x	x^5-5x^3+6x	x^5-5x^3+4x	–0.404
	$x^6-6x^4+5x^2-1$	$x^6-6x^4+9x^2-1$	$x^6-6x^4+7x^2-1$	–0.163
	$x^6-6x^4+5x^2$	$x^6-6x^4+9x^2$	$x^6-6x^4+7x^2$	–0.248
	$x^8-8x^6+14x^4-8x^2+1$	$x^8-8x^6+18x^4-8x^2+1$	$x^8-8x^6+16x^4-8x^2+1$	–0.072
	$x^6-6x^4+6x^2$	$x^6-6x^4+10x^2-4$	$x^6-6x^4+8x^2-2$	–1.060
	$x^7-7x^5+10x^3$	$x^7-7x^5+14x^3-8x$	$x^7-7x^5+12x^3-4x$	–1.124
	x^5-5x^3+5x-2	x^5-5x^3+5x+2	x^5-5x^3+5x	–0.301
	$x^6-6x^4+8x^2-2x-1$	$x^6-6x^4+8x^2+2x-1$	$x^6-6x^4+8x^2-1$	0.020
	$x^7-7x^5+13x^3-2x^2-6x+2$	$x^7-7x^5+13x^3+2x^2-6x-2$	$x^7-7x^5+13x^3-6x$	–0.150
	$x^6-6x^4+9x^2-4$	$x^6-6x^4+9x^2$	$x^6-6x^4+9x^2-2$	0.273

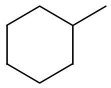
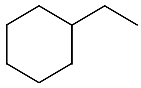
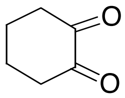
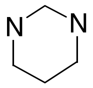
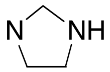
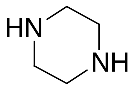
	$x^7-7x^5+13x^3-7x$	$x^7-7x^5+13x^3-3x$	$x^7-7x^5+13x^3-5x$	0.155
	$x^8-8x^6+19x^4-16x^2+4$	$x^8-8x^6+19x^4-12x^2$	$x^8-8x^6+19x^4-14x^3+2$	0.249
	$x^8-0.44x^7-7.912x^6+3.071x^5+17.511x^4-5.685x^3-12.327x^2+3.054x+0.767$	$x^8-0.44x^7-7.912x^6+3.071x^5+17.511x^4-5.685x^3-8.327x^2+1.293x+0.961$	$x^8-0.44x^7-7.912x^6+3.071x^5+17.511x^4-5.685x^3-10.327x^2+2.174x+0.864$	0.053
	$x^6-0.76x^5-3.816x^4+2.265x^3+3.372x-1.117x-0.96$	$x^6-0.76x^5-3.816x^4+2.265x^3+3.372x-1.117x$	$x^6-0.76x^5-3.815x^4+2.267x^3+3.370x-1.118x-0.48$	0.193
	$x^5-1.88x^4-3.03x^3+3.966x^2-1.92x-1.837$	$x^5-1.88x^4-3.03x^3+3.966x^2+1.92x-0,249$	$x^5-1.88x^4-3.03x^3+3.964x^2-1.92x-1.043$	0.196
	$x^6-3x^5-2.99x^4+10.86x^3+2.364x^2-7.86x-0.374$	$x^6-3x^5-2.99x^4+10.86x^3+2.364x^2-7.86x+2.25$	$x^6-3x^5-2.99x^4+10.86x^3+2.364x^2-7.86x-0.938$	–0.132

Table S1. Characteristic and acyclic polynomials of some Hückel and Möbius unicycles with ring size 3-6. The *o*-benzoquinone,[1] 1,4-dihydropyrazine,[2] 1,3-pyrimidine and imidazole graphs are here weighted by the Hess-Schaad parameters: $h_{O\bullet} = 0.22$, $k_{C\text{-}O\bullet} = 0.99$,[3] $h_{N\bullet} = 0.38$, $k_{C\text{-}N\bullet} = 0.70$,[4] $h_{N:} = 1.50$, $k_{C\text{-}N:} = 0.90$.[5] * TRE values for the neutral ground state (in β units).

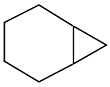
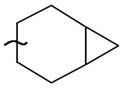
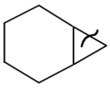
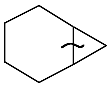
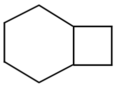
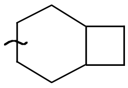
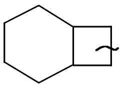
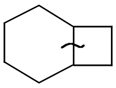
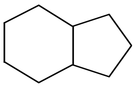
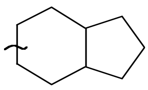
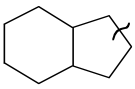
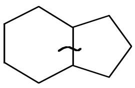
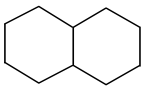
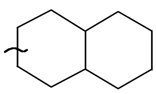
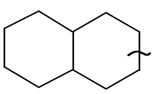
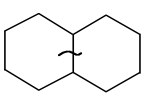
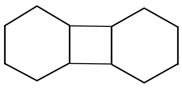
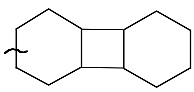
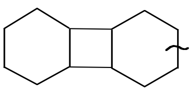
[1] J. Aihara, *J. Am. Chem. Soc.,* 1976, **98**, 2750-2758.

[2] J. Aihara, H. Ichikawa, *Bull. Chem. Soc. Jpn.,* 1988, **61**, 223-228.

[3] B. A. Hess, Jr, L. J. Schaad, C. W. Holyoke, Jr. *Tetrahedron,* 1972, **28**, 5299.

[4] B. A. Hess, Jr, L. J. Schaad, C. W. Holyoke, Jr. *Tetrahedron,* 1975, **31**, 295.

[5] B. A. Hess, Jr, L. J. Schaad, C. W. Holyoke, Jr. *Tetrahedron,* 1972, **28**, 3657.

	Hückel and Möbius characteristic polynomials	Acyclic polynomial
	$P^0(x)=x^7-8x^5-2x^4+17x^3+6x^2-10x-4$	$P^{ac}(x)=x^7-8x^5+17x^3-8x$
	$P^1(x)=x^7-8x^5-2x^4+17x^3+6x^2-6x$	
	$P^2(x)=x^7-8x^5+2x^4+17x^3-6x^2-10x+4$	
	$P^3(x)=x^7-8x^5+2x^4+17x^3-6x^2-6x$	
	$P^0(x)=x^8-9x^6+22x^4-16x^2+1$	$P^{ac}(x)=x^8-9x^6+24x^4-20x^2+3$
	$P^1(x)=x^8-9x^6+22x^4-12x^2+1$	
	$P^2(x)=x^8-9x^6+26x^4-28x^2+9$	
	$P^3(x)=x^8-9x^6+26x^4-24x^2+1$	
	$P^0(x)=x^9-10x^7+32x^5-2x^4-39x^3+6x^2+15x-4$	$P^{ac}(x)=x^9-10x^7+32x^5-37x^3+11x$
	$P^1(x)=x^9-10x^7+32x^5-2x^4-35x^3+6x^2+7x$	
	$P^2(x)=x^9-10x^7+32x^5+2x^4-39x^3-6x^2+15x+4$	
	$P^3(x)=x^9-10x^7+32x^5+2x^4-35x^3-6x^2+7x$	
	$P^0(x)=x^{10}-11x^8+41x^6-65x^4+43x^2-9$	$P^{ac}(x)=x^{10}-11x^8+41x^6-61x^4+31x^2-3$
	$P^1(x)=x^{10}-11x^8+41x^6-61x^4+31x^2-1$	
	$P^2(x)=x^{10}-11x^8+41x^6-61x^4+31x^2-1$	
	$P^3(x)=x^{10}-11x^8+41x^6-57x^4+19x^2-1$	
	$P^0(x)=x^{12}-14x^{10}+69x^8-154x^6+162x^4-72x^2+9$	$P^{ac}(x)=x^{12}-14x^{10}+71x^8-162x^6+164x^4-60x^2+5$
	$P^1(x)=x^{12}-14x^{10}+69x^8-150x^6+142x^4-48x^2+1$	
	$P^2(x)=x^{12}-14x^{10}+69x^8-150x^6+142x^4-48x^2+1$	

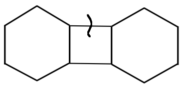
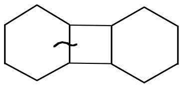
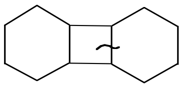
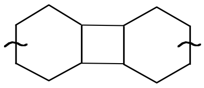
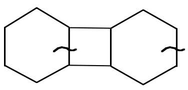
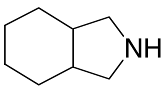
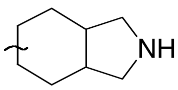
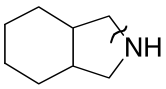
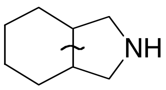
	$P^3(x)=x^{12}-14x^{10}+73x^8-178x^6+214x^4-120x^2+25$	
	$P^4(x)=x^{12}-14x^{10}+73x^8-174x^6+186x^4-72x^2+1$	
	$P^5(x)=x^{12}-14x^{10}+73x^8-174x^6+186x^4-72x^2+1$	
	$P^6(x)=x^{12}-14x^{10}+69x^8-146x^6+122x^4-24x^2+1$	
	$P^7(x)=x^{12}-14x^{10}+73x^8-170x^6+158x^4-24x^2+1$	
	$P^0(x)=x^9-1.5x^8-9.62x^7+12x^6+29.34x^5-28.619x^4-34.059x^3+24.360x^2+12.339x-4.74$	$P^{ac}(x)=x^9-1.5x^8-9.62x^7+12x^6+29.34x^5-27x^4-32.06x^3+16.5x^2+9.10x-1.5$
	$P^1(x)=x^9-1.5x^8-9.62x^7+12x^6+29.34x^5-28.618x^4-30.059x^3+18.359x^2+5.859x-1.5$	
	$P^2(x)=x^9-1.5x^8-9.62x^7+12x^6+29.341x^5-25.379x^4-34.061x^3+14.639x^2+12.34x+1.74$	
	$P^3(x)=x^9-1.50x^8-9.62x^6+12x^6+29.338x^5-25.381x^4-30.057x^3+8.640x^2+5.859x-1.5$	

Table S2. Characteristic and acyclic polynomials of some Hückel and Möbius polycyclic systems. Each Möbius circuit is marked by a tilde: the edge where it is located is weighted by a factor –1, while all other edges are non-weighted. The isoindole graph is weighted by the Hess-Schaad Hückel parameters: $h_{N:}$ = 1.50, $k_{C\text{-}N:}$ = 0.90.[4]