Characteristic and Counting Polynomials on Modeling Nonane Isomers Properties

LORENTZ JÄNTSCHI[1], SORANA-DANIELA BOLBOACĂ[2], CRISTINA MARIA FURDUI[3]

[1] "Iuliu Hațieganu" University of Medicine and Pharmacy
13 Emil Isac Street, 400023 Cluj-Napoca, Romania
http://sorana.cademicdirect.ro
sorana@j.academicdirect.ro

[2] Technical University of Cluj-Napoca,
15 Constantin Daicoviciu Street, 400020 Cluj-Napoca, Romania
http://lori.academicdirect.org
lori@j.academicdirect.org

[3] Wake Forest University Health Sciences,
Medical Center Bvd, Winston-Salem, 27157 NC, USA
http://www1.wfubmc.edu/MolMed_Section/Faculty/CristinaFurdui.htm
cfurdui@wfubmc.edu

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The major goal of this study was to investigate the broad application of graph polynomials to the analysis of Henry's law constants of nonane isomers.

In this context, Henry's law constants of nonane isomers were modeled using characteristic and counting polynomials and the characteristic and counting polynomials on the distance matrix, on the maximal fragments matrix, on the complement of maximal fragments matrix, and on the Szeged matrix were calculated for each compound.

One of included nonane isomers, 4-methyloctane, was identified as an outlier and was withdrawn from further analysis. This report describes the performance and characteristics of top five significant models. The results show that Henry's law constants of nonane isomers can be modeled by applying characteristic and counting polynomials.

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Lorentz JÄNTSCHI, Sorana D. BOLBOACĂ & Cristina M. FURDUI

“Iuliu Hatieganu” University of Medicine and Pharmacy Cluj-Napoca, Romania
&
Technical University of Cluj-Napoca, Romania
&
Wake Forest University Health Sciences, Winston-Salem, USA

Outlines

- Introduction
- Material
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Background

- Characteristic polynomial = one associates a polynomial to any square matrix [Trinajstić, 1983].

$$\varphi(G,X) = \det[XI - A(G)]$$

where A(G) is the adjacency matrix of a pertinently constructed skeleton graph and I is the identity matrix

- Encodes several properties of a matrix, the most important being the matrix eigenvalues, its determinant and its trace [Trinajstić, 1988].

Application of characteristic polynomials

- ***Mathematics***:
  - Correlations of Characteristic Polynomials: Riemann-Hilbert Approach [Strahov and Fyodorov, 2003]
  - Spectral problems for polynomial matrices [Kublanovskaya, 2005]
- ***Computer science***:
  - Algorithms for computing the characteristic polynomial in a domain [Abdeljaoued and Malaschonok, 2001]
  - Stability of discrete-time systems [Lastman and Sinha, 1999]
  - Complexity of computing determinants [Kaltofen and Villard, 2005]

Application of characteristic polynomials

- ***Engineering:***
  - Characteristic polynomial assignment in F-M model II of 2-D systems [Tang and Kang, 2005]
- ***Chemistry:***
  - Characteristic polynomial and topology of molecule [Balaban and Harary, 1971]
  - Cluj weighted adjacency matrices [Kunz, 1998]
  - Properties and relationships of conjugated polyenes having a reciprocal eigenvalue spectrum - Dendralene and radialene hydrocarbons [Dias, 2004]

Application of characteristic polynomials

- ***Physics:***
  - Characteristic polynomials of random matrices at edge singularities [Brézin and Hikami, 2000]
  - D-decomposition theory [Gryazinam 2004]
- ***Management:***
  - Condition of applying the fourth order of characteristic equation to the dynamic stability of wing-in-ground effect vehicles [Zhang et al., 2000]

Counting polynomials & chemical graph theory

- Counting polynomial:

$$\sum_{k\geq 0} a_k X^k, \text{ where } a_k = |\{M_{i,j} \mid M_{i,j} = k\}|$$

a_k being the polynomial-count and i, j = 1, …, n

- Methods for counting polynomials [Diudea et al., 2002]:
  - Distance matrix
  - Szeged matrix
  - Cluj matrix

Research Aim

- To analyze the Henry's law constants of nonane isomers
  - by using characteristic and counting polynomials
- Can characteristic and counting polynomials be used to characterize the relationship between structure and chemical properties for this class of compounds?

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Alkanes isomers

- Acyclic saturated hydrocarbon structures that normally have a linear configuration:

$$C_nH_{2n+2}$$

- The number of isomers increases with the number of carbon atoms:
  - 1 to 10 carbons
  - Isomers: 1, 1, 1, 2, 3, 5, 9, 18, 35, and 75
- Nonane isomers with the general chemical structure C_9H_{20}

Henry’s law constant

- The values of Henry’s law constants were taken from a previously reported research [Yaws and Yang, 1992]

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Counting and Characteristic Polynomial

- Counting polynomials [Jantschi and Bolboaca, unpublished]:
  - the distance matrix (CDi)
  - the maximal fragments matrix (CMx)
  - the complement of the maximal fragments matrix (CcM)
  - Szeged matrix (CSz)

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Characteristic and counting polynomials - generic formulas

- Characteristic polynomial:

$$P(X)_{ChP} = X^7 \cdot (X^2 - 8) + X \cdot Q(X)_{ChP}$$

- Counting polynomial on the distance matrix:

$$P(X)_{CDi} = 2 \cdot X^2 \cdot Q(X)_{CDi} + 16 \cdot X + 9$$

Characteristic and counting polynomials - generic formulas

- Counting polynomial on the maximal fragments matrix:

$$P(X)_{CMx} = 16\cdot X^8 + X\cdot Q(X)_{CMx} + 2\cdot X + 9$$

- Counting polynomial on the complement of the maximal fragments matrix:

$$P(X)_{CcM} = 2\cdot X^8 + X\cdot Q(X)_{CcM} + 16\cdot X + 9$$

Characteristic and counting polynomials - generic formulas

- Counting polynomial on the Szeged matrix:

$$P(X)_{CSz} = 2 \cdot X^{8} + X \cdot Q(X)_{CSz} + 4 \cdot X + 9$$

- Remark:
- The characteristic polynomial can be easily factorized while the counting polynomials are not.

Similarities in counting polynomials

- All formulas contain the "$a_1 \cdot X+9$", where a_1 varies from 2 to 16, but is always an even number;
- The generic formula for counting polynomials on the maximal fragments matrix, on the complement of maximal fragments matrix, and on Szeged matrix, respectively is:

$$P(X) = a_0X^8 + XQ(X) + a_1X + 9$$

- where a_0 and a_1 are even integers with values from 2 to 16;
- The term Q(X) could be factorized in a limited number of cases

Characteristic polynomial - monovariate model

- $\hat{Y}_{ChP\text{-}mono} = 19.54 + 0.17 \cdot P(1.65\ldots)$

- $r^2 = 0.2968$ – 35 compounds
- $r^2 = 0.2968$ – 34 compounds (4-methyloctane)
  - compound 4-methyloctane was considered an outliner and was excluded from further analysis.

Multivariate models

- Characteristic polynomial

$$\hat{Y}_{ChP} = 1765.89 + 0.18\cdot P(24/9) - 0.11\cdot P(26/9) - 3.44\cdot 10^{-5}\cdot P(65/9)$$

- Counting polynomial on the distance matrix:

$$\hat{Y}_{CDi} = 106.16 + 4.89\cdot P(-3/9) - 6.54\cdot P(3/9) - 5.55\cdot 10^{-8}\cdot P(79/9)$$

- Counting polynomial on the maximal fragments matrix:

$$\hat{Y}_{CMx} = 29.65 - 5.90\cdot 10^{-6}\cdot P(-79/9) + 1.15\cdot 10^{-5}\cdot P(-73/9) - 1.19\cdot 10^{-3}\cdot P(-27/9)$$

Multivariate models

- Counting polynomial on the complement of the maximal fragments matrix:

$$\hat{Y}_{CcM} = -1275.16 + 3.37 \cdot P(13/9) + 3.72 \cdot 10^{-5} \cdot P(74/9) - 2.52 \cdot 10^{-5} \cdot P(77/9)$$

- Counting polynomial on the Szeged matrix

$$\hat{Y}_{CSz} = 25.05 - 1.98 \cdot 10^{-5} \cdot P(67/9) + 2.62 \cdot 10^{-5} \cdot P(73/9) - 1.07 \cdot 10^{-5} \cdot P(77/9)$$

Multivariate models assessment

Model	Parameter					
	r	$95\%CI_r$	r^2	StdError	F	n
$\hat{Y}_{ChP}$	0.9338	[0.8704-0.9666]	0.8720	0.6468	68†	34
$\hat{Y}_{CDi}$	0.9246	[0.8530-0.9619]	0.8548	0.6888	59†	34
$\hat{Y}_{CMx}$	0.8520	[0.7217-0.9239]	0.7259	0.9464	68†	34
$\hat{Y}_{CcM}$	0.8269	[0.6783-0.9104]	0.6838	1.0164	22†	34
$\hat{Y}_{CSz}$	0.8363	[0.6944-0.9155]	0.6993	0.9912	23†	34

r = correlation coefficient; $95\%CI_r$ = 95% confidence intervals for correlation coefficient; r^2 = squared correlation coefficient; StdError = standard error; F = Fisher parameter; n = sample size; † $p < 0.0001$

Results of correlated correlation analysis

	$\hat{Y}_{ChP}$	$\hat{Y}_{CDi}$	$\hat{Y}_{CMx}$	$\hat{Y}_{CSz}$
$\hat{Y}_{ChP}$	1			
$\hat{Y}_{CDi}$	0.3012	1		
$\hat{Y}_{CMx}$	0.0036	0.0144	1	
$\hat{Y}_{CcM}$	0.0015	0.0083	0.2442	1
$\hat{Y}_{CSz}$	0.0056	0.0185	0.3816	0.5684

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Conclusion

- The Henry's law constant of the nonane isomers can be modeled using characteristic and counting polynomials.
- The characteristic and counting polynomials approaches provided good models, opening a new venue for the characterization of chemical compounds.

Further research

- Characterization of other properties and/or other chemical compounds
- Testing the robustness of the identified models
- []

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No.	$k_H(\cdot 10^5)$ [M/atm]	$Q(X)_{ChP}$
a_01	1.0	$(2X-1)(2X+1)(5X^2-3)$
a_02	1.5	$17X^4-12X^2+2$
a_03	1.5	$18X^4-16X^2+5$
a_04	1.6	$3X^2(5X^2-2)$
a_05	1.6	$8X^2(2X^2-1)$
a_06	1.7	$21X^4-20X^2+5$
a_07	1.7	$X^2(17X^2-10)$
a_08	1.7	$17X^4-11X^2+2$
a_09	1.7	$18X^4-14X^2+3$
a_10	1.7	$2X^2(8X^2-3)$
a_11	1.8	$19X^4-15X^2+3$
a_12	1.8	$2(3X^2-1)^2$
a_13	1.8	$19X^4-16X^2+4$
a_14	1.8	$X^2(17X^2-10)$
a_15	1.8	$6X^2(3X^2-2)$
a_16	1.9	$19X^4-14X^2+2$
a_17	1.9	$2(3X^2-1)^2$
a_18	1.9	$6X^2(3X^2-2)$
a_19	1.9	$20X^4-18X^2+5$
a_20	1.9	$2(2X^2-1)(5X^2-2)$
a_21	1.9	$X^2(17X^2-9)$
a_22	1.9	$X^2(17X^2-6)$
a_23	1.9	$X^2(17X^2-8)$
a_24	1.9	$19X^4-15X^2+2$
a_25	1.9	$15X^4$
a_26	2.0	$20X^4-17X^2+4$
a_27	2.0	$19X^4-13X^2+2$
a_28	2.0	$19X^4-14X^2+3$
a_29	2.0	$2X^2(9X^2-5)$
a_30	2.1	$2(10X^4-8X^2+1)$
a_31	2.1	$2X^2(9X^2-5)$
a_32	2.1	$X^2(19X^2-13)$
a_33	2.1	$X^2(19X^2-12)$
a_34	2.1	$X^1(17X^2-7)$
a_35	2.1	$19X^4-14X^2+2$

No.	$k_H(\cdot 10^5)$ [M/atm]	$Q(X)_{CDi}$
a_01	1.0	$X^5+2X^4+4X^3+6X^2+7X+8$
a_02	1.5	$5X^2+12X+11$
a_03	1.5	$2(3X^2+6X+5)$
a_04	1.6	$3X^2+12X+13)$
a_05	1.6	$4(X^2+3X+3)$
a_06	1.7	$X^6+2X^5+3X^4+4X^3+5X^2+6X+7$
a_07	1.7	$2X^3+5X^2+10X+11$
a_08	1.7	$X^3+5X^2+11X+11$
a_09	1.7	$2(X^3+3X^2+5X+5)$
a_10	1.7	$2(3X^2+5X+6)$
a_11	1.8	$(X^2+3)(X^2+3X+3)$
a_12	1.8	$2(X^3+3X^2+5X+5)$
a_13	1.8	$2X^3+7X^2+10X+9$
a_14	1.8	$7X^2+10+11$
a_15	1.8	$2(4X^2+5X+5)$
a_16	1.9	$2X^4+4X^3+5X^2+8X+9$
a_17	1.9	$X^4+4X^3+5X^2+8X+10$
a_18	1.9	$X^4+2X^3+7X^2+8X+10$
a_19	1.9	$2(X^4+2X^3+3X^2+4X+4)$
a_20	1.9	$X^4+4X^3+7X^2+8X+8$
a_21	1.9	$3X^3+5X^2+9X+11$
a_22	1.9	$6X^3+5X^2+6X+11$
a_23	1.9	$2X^3+7X^2+8X+11$
a_24	1.9	$3X^3+7X^2+9X+9$
a_25	1.9	$9X^2+6X+13$
a_26	2.0	$X^5+3X^4+4X^3+5X^2+7X+8$
a_27	2.0	$2X^4+5X^3+5X^2+7X+9$
a_28	2.0	$X^4+4X^3+6X^2+8X+9$
a_29	2.0	$2(2X^3+3X^2+4X+5)$
a_30	2.1	$2X^5+3X^4+4X^3+5X^2+6X+8$
a_31	2.1	$3X^4+4X^3+5X^2+6X+10$
a_32	2.1	$2X^4+3X^3+7X^2+7X+9$
a_33	2.1	$4X^4+4X^3+5X^2+6X+9$
a_34	2.1	$3X^3+7X^2+7X+11$
a_35	2.1	$4X^3+7X^2+8X+9$

No.	$k_H(\cdot 10^5)$ [M/atm]	$Q(X)_{CSz}$
a_01	1.0	$X^7+6X^6+13X^5+9X^4+9X^3+16X^2+9X+3$
a_02	1.5	$3X^7+10X^6+9X^5+14X^2+20X+10$
a_03	1.5	$2(X^7+10X^6+20X+2)$
a_04	1.6	$4X^7+5X^6+13X^4+16X^3+10X+18$
a_05	1.6	$2(2X^7+9X^5+14X^2+8)$
a_06	1.7	$2X(X^2+X+1)(3X^3+2X^2+2X+4)$
a_07	1.7	$3X^7+3X^6+19X^5+23X^2+6X+12$
a_08	1.7	$(X+1)(3X^6+6X^5-6X^4+19X^3-6X^2+6X+11)$
a_09	1.7	$2X^7+13X^6+10X^5+11X^2+24X+6$
a_10	1.7	$4X^7+7X^5+10X^4+15X^3+13X^2+17$
a_11	1.8	$(X+1)(2X^6+5X^5+3X^4+7X^3+4X^2+6X+6)$
a_12	1.8	$3X^7+4X^6+7X^5+11X^4+13X^3+11X^2+7X+10$
a_13	1.8	$2X^7+12X^6+11X^4+13X^3+23X+5$
a_14	1.8	$3X^7+8X^6+10X^4+15X^3+18X+12$
a_15	1.8	$3X^7+4X^6+14X^5+26X^2+9X+10$
a_16	1.9	$2X^7+3X^6+13X^5+10X^4+9X^3+18X^2+4X+7$
a_17	1.9	$2X^7+8X^6+7X^5+10X^4+9X^3+10X^2+12X+8$
a_18	1.9	$2(X^7+3X^6+9X^5+10X^2+6X+4)$
a_19	1.9	$X^7+11X^6+6X^5+10X^4+9X^3+9X^2+18X+2$
a_20	1.9	$X^7+10X^6+16X^5+20X^2+17X+2$
a_21	1.9	$3X^7+3X^6+9X^5+10X^4+12X^3+11X^2+5X+13$
a_22	1.9	$3X^7+5X^5+18X^4+20X^3+6X^2+14$
a_23	1.9	$3X^7+5X^6+5X^5+13X^4+10X^3+10X^2+8X+12$
a_24	1.9	$2X^7+7X^6+16X^5+22X^2+13X+6$
a_25	1.9	$2(2X^7+7X^4+14X^3+10)$
a_26	2.0	$(X+1)(X^6+6X^5-X^4+17X^3+7X+3)$
a_27	2.0	$(X+1)(2X^6+2X^5+3X^4+13X^3+7X^2-X+7)$
a_28	2.0	$2(X^7+4X^6+8X^4+11X^3+6X+3)$
a_29	2.0	$3X^7+12X^5+12X^4+11X^3+17X^2+11$
a_30	2.1	$X^7+3X^6+10X^5+15X^4+17X^3+12X^2+4X+4$
a_31	2.1	$2X^7+3X^6+5X^5+17X^4+17X^3+8X^2+4X+10$
a_32	2.1	$2X^7+3X^6+12X^5+10X^4+10X^3+17X^2+5X+7$
a_33	2.1	$2(X^7+5X^5+7X^4+10X^3+6X^2+4)$
a_34	2.1	$(X+1)(3X^6+X^5-X^4+17X^3+7X^2-7X+13)$
a_35	2.1	$2X^7+8X^6+5X^5+12X^4+11X^3+8X^2+14X+6$

No.	$k_H(\cdot 10^5)$ [M/atm]	$Q(X)_{CMx}$
a_01	1.0	$8X^7+14X^6+12X^5+5X^4+4X^3+6X^2+4X+1$
a_02	1.5	$24X^7+14X^6+6X^5+3X^2+4X+3$
a_03	1.5	$2(8X^7+14X^6+4X+1)$
a_04	1.6	$32X^7+7X^6+5X^4+4X^3+2X+4$
a_05	1.6	$2(16X^7+6X^5+3X^2+2)$
a_06	1.7	$2X(7X^5+6X^4+5X^3+4X^2+3X+2)$
a_07	1.7	$24X^7+7X^6+12X^5+6X^2+2X+3$
a_08	1.7	$24X^7+14X^6+5X^4+4X^3+4X+3$
a_09	1.7	$16X^7+21X^6+6X^5+3X^2+6X+2$
a_10	1.7	$32X^7+6X^5+5X^4+4X^3+3X^2+4$
a_11	1.8	$16X^7+14X^6+6X^5+5X^4+4X^3+3X^2+4X+2$
a_12	1.8	$24X^7+7X^6+6X^5+5X^4+4X^3+3X^2+2X+3$
a_13	1.8	$16X^7+21X^6+5X^4+4X^3+6X+2$
a_14	1.8	$24X^7+14X^6+5X^4+4X^3+4X+3$
a_15	1.8	$24X^7+7X^6+12X^5+6X^2+2X+3$
a_16	1.9	$16X^7+7X^6+12X^5+5X^4+4X^3+6X^2+2X+2$
a_17	1.9	$16X^7+14X^6+6X^5+5X^4+4X^3+3X^2+4X+2$
a_18	1.9	$2(8X^7+7X^6+6X^5+3X^2+2X+1)$
a_19	1.9	$8X^7+21X^6+6X^5+5X^4+4X^3+3X^2+6X+1$
a_20	1.9	$8X^7+21X^6+12X^5+6X^2+6X+1$
a_21	1.9	$24X^7+7X^6+6X^5+5X^4+4X^3+3X^2+2X+3$
a_22	1.9	$24X^7+6X^5+10X^4+8X^3+3X^2+3$
a_23	1.9	$24X^7+7X^6+6X^5+5X^4+4X^3+3X^2+2X+3$
a_24	1.9	$2(8X^7+7X^6+6X^5+3X^2+2X+1)$
a_25	1.9	$2(16X^7+5X^4+4X^3+2)$
a_26	2.0	$8X^7+14X^6+6X^5+10X^4+8X^3+3X^2+4X+1$
a_27	2.0	$16X^7+7X^6+6X^5+10X^4+8X^3+3X^2+2X+2$
a_28	2.0	$2(8X^7+7X^6+5X^4+4X^3+2X+1)$
a_29	2.0	$24X^7+12X^5+5X^4+4X^3+6X^2+3$
a_30	2.1	$8X^7+7X^6+12X^5+10X^4+8X^3+6X^2+2X+1$
a_31	2.1	$16X^7+7X^6+6X^5+10X^4+8X^3+3X^2+2X+2$
a_32	2.1	$16X^7+7X^6+12X^5+5X^4+4X^3+6X^2+2X+2$
a_33	2.1	$2(X^2-X+1)(8X^5+8X^4+6X^3+3X^2+X+1)$
a_34	2.1	$24X^7+7X^6+10X^4+8X^3+2X+3$
a_35	2.1	$16X^7+14X^6+6X^5+5X^4+4X^3+3X^2+4X+2$

No.	$k_H(\cdot 10^5)$ [M/atm]	$Q(X)_{CcM}$
a_01	1.0	$X^7+4X^6+6X^5+4X^4+5X^3+12X^2+14X+8$
a_02	1.5	$3X^7+4X^6+3X^5+6X^2+14X+24$
a_03	1.5	$2(X^7+4X^6+14X+8)$
a_04	1.6	$4X^7+2X^6+4X^4+5X^3+7X+32$
a_05	1.6	$2(2X^7+3X^5+6X^2+16)$
a_06	1.7	$2X(2X^5+3X^4+4X^3+5X^2+6X+7)$
a_07	1.7	$3X^7+2X^6+6X^5+12X^2+7X+24$
a_08	1.7	$3X^7+4X^6+4X^4+5X^3+14X+24$
a_09	1.7	$2X^7+6X^6+3X^5+6X^2+21X+16$
a_10	1.7	$4X^7+3X^5+4X^4+5X^3+6X^2+32$
a_11	1.8	$2X^7+4X^6+3X^5+4X^4+5X^3+6X^2+14X+16$
a_12	1.8	$3X^7+2X^6+3X^5+4X^4+5X^3+6X^2+7X+24$
a_13	1.8	$2X^7+6X^6+4X^4+5X^3+21X+16$
a_14	1.8	$3X^7+4X^6+4X^4+5X^3+14X+24$
a_15	1.8	$3X^7+2X^6+6X^5+12X^2+7X+24$
a_16	1.9	$2X^7+2X^6+6X^5+4X^4+5X^3+12X^2+7X+16$
a_17	1.9	$2X^7+4X^6+3X^5+4X^4+5X^3+6X^2+14X+16$
a_18	1.9	$2(X^7+2X^6+3X^5+6X^2+7X+8)$
a_19	1.9	$X^7+6X^6+3X^5+4X^4+5X^3+6X^2+21X+8$
a_20	1.9	$X^7+6X^6+6X^5+12X^2+21X+8$
a_21	1.9	$3X^7+2X^6+3X^5+4X^4+5X^3+6X^2+7X+24$
a_22	1.9	$3X^7+3X^5+8X^4+10X^3+6X^2+24$
a_23	1.9	$3X^7+2X^6+3X^5+4X^4+5X^3+6X^2+7X+24$
a_24	1.9	$2\cdot(X^7+2\cdot X^6+3\cdot X^5+6\cdot X^2+7\cdot X+8)$
a_25	1.9	$2(2X^7+4X^4+5X^3+16)$
a_26	2.0	$X^7+4X^6+3X^5+8X^4+10X^3+6X^2+14X+8$
a_27	2.0	$2X^7+2X^6+3X^5+8X^4+10X^3+6X^2+7X+16$
a_28	2.0	$2(X^7+2X^6+4X^4+5X^3+7X+8)$
a_29	2.0	$3X^7+6X^5+4X^4+5X^3+12X^2+24$
a_30	2.1	$X^7+2X^6+6X^5+8X^4+10X^3+12X^2+7X+8$
a_31	2.1	$2X^7+2X^6+3X^5+8X^4+10X^3+6X^2+7X+16$
a_32	2.1	$2X^7+2X^6+6X^5+4X^4+5X^3+12X^2+7X+16$
a_33	2.1	$2(X^2-X+1)(X^5+X^4+3X^3+6X^2+8X+8)$
a_34	2.1	$3X^7+2X^6+8X^4+10X^3+7X+24$
a_35	2.1	$2X^7+4X^6+3X^5+4X^4+5X^3+6X^2+14X+16$