MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **63** (2010) 737-750

ISSN 0340 - 6253

Some Graphs Are More Strongly-Isospectral than Others*

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(Received March 25, 2009)

Abstract

Let A be the adjacency matrix of a graph G, let D be its distance matrix and let V be the diagonal matrix with elements that indicate the valence of corresponding vertices. We explore possibility of discriminating the degree of similarity between isospectral graphs (having the same eigenvalues of the adjacency matrix A) by examining their spectral properties with respect to additional graph matrices: $A - V$ matrix, which is essentially the Laplace matrix multiplied by -1; $AA^T - V$ matrix, which is obtained from AA^T where elements on the main diagonal are replaced by zeros; natural distance matrix ${}^{N}DD$, constructed from distances between columns of the adjacency matrix viewed as vectors in N-dimensional space; terminal matrix, which is really the distance matrix between the vertices of degree 1, also called terminal vertices. We found that matrices of form $A^m - V$, the elements of which count non-returning walk of length m in a graph, discriminate some isospectral mates, but not others. We refer to pair of graphs which agree in eigenvalues of several matrices as strongly-isospectral, or S-isospectral graphs, as opposed to those less strongly similar. Hence, in other words, some graphs are more S-isospectral than other.

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* On the occasion of 65 anniversary this paper is dedicated to outstanding promoter of Mathematical Chemistry, Professor Paul G. Mezey, the Editor of the Journal of Mathematical Chemistry, for his numerous contributions to Mathematical Chemistry.

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1. Introduction

The eigenvalues of the adjacency matrix, the graph spectrum, are one of most elementary graph invariants. Already in 1943 U. Sinogowitz, who perished in WW II, has found that there are trees that have all eigenvalues equal, hence graph spectra are not unique to a graph [1]. Graphs that have all eigenvalues equal are often referred in chemical literature as *isospectral* and in mathematical literature as *co-spectral*. There was a considerable interest in *isospectral* (or co-spectral) *graphs* in mathematical [2] and chemical circles [3]. In chemistry the eigenvalues of the adjacency matrix represent molecular orbital energies of π -electrons of conjugated polycyclic hydrocarbons [4]. According to one of the early theoretical model of π-electron structure of mid 1930s of E. Hückel, known today as the Hückel Molecular Orbital Theory (HMO), monocyclic conjugated hydrocarbons having $4n+2$ π-electrons are aromatic, while those having 4n π-electrons are anti-aromatic. From mathematical point of view the energies of π -electron molecular orbitals are equivalent to the graph spectral theory.

The Hückel $4n+2$ Rule on aromaticity has been considered one of the early triumphs of Quantum Chemistry even though it has not been widely recognized that it is a consequence of molecular connectivity (Graph Theory) and not Quantum Chemistry. Many attempts have been made over the past 20-30 years to generalize the Hückel $4n+2$ Rule on aromaticity to polycyclic conjugated hydrocarbons but all these attempts failed. Finally in 1976 the notion of conjugated circuits was introduced [5] and it was shown that polycyclic conjugated hydrocarbons having only $4n+2$ conjugated circuits are aromatic and those having only $4n$ conjugated circuits are anti-aromatic [6, 7]. It is interesting to mention that while HMO model dominated theoretical chemistry, which was for at least some 20 years, nothing was known about isospectral graphs (and molecules). It was only in 1973, when HMO was already fading out as a viable chemical model of π-electrons in conjugated systems, that Živković [8] by browsing pages of widely available "Dictionary of π-Electron Calculations" [9], found a pair of simple benzene derivatives: 1,4-divynylbenzene and 2-phenylbutadiene (molecular skeleton of which are illustrated in Figure 1) which are isospectral. Typically molecular orbitals and π-orbital energies of each molecule occupied a single page, and the two isospectral substituted benzenoid compounds having the same HMO eigenvalues were separated by few pages!

Finally we should add that Hückel MO Theory is not dead [10, 11] and even less dead is the "Conjugated Circuits Theory," which as Klein and collaborators have shown [12-20], can be cast in rigorous Quantum Theory formalism.

Although isospectrality is today of no much interest in chemistry, in view that HMO is no longer adequate theoretical model for spectra of conjugated polycyclic hydrocarbons, it is nevertheless of interest to understand structural reasons why isospectrality occurs for some pairs of compounds and not for others. It turned out that the reason that structurally closely related 1,4-divynylbenzene and 2-phenylbutadiene (illustrated in Figure 1) are isospectral because they posses special sites, two critical vertices, which when erased produce subgraphs having the same characteristic polynomial. Therefore, when the two sites are substituted by the same molecular fragment, they will always produce pairs of isospectral graphs [21-23]. However, there are graphs which are isospectral and which do not have such special vertices, which could be classified as "*sporadic.*" Such pairs of graphs are isospectral accidentally, or for yet unknown structural reasons. On the other hand, one can refer to isospectrality of 1,4-divynylbenzene and 2-phenylbutadiene as "*structural*" or "*regular*", because the isospectrality of such graph, as mentioned above, can be traced to definite structural elements.

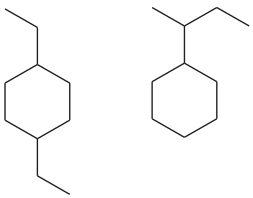


Figure 1: Isospectral pair of graphs found by Živković.

In this contribution, we are interested in characterization of the degree of hidden structural similarity or "*intensity*" of isospectral graphs. Clearly any pair of non-isospectral graphs can already be differentiated by their spectra, while though graph spectra cannot differentiate between isospectral graphs, we believe that in general isospectral graphs can be differentiated by having at least one invariant different – the problem of interest for graph isomorphism testing [24, 25] is that nobody knows in advance which invariants are this to be. Hence, in such cases, one needs to continue with examination of additional graph invariants, an approach which need not to be efficient. For some graphs such discriminatory properties

may be found in few steps but in some cases a pair of graphs may resist differentiation and require considerable effort in finding a set of invariants in which they differ.

Hosoya and coworkers seems to be the first to search for graphs that are isospectral (having the same set of eigenvalues of the adjacency matrix *A*) and have the same set of eigenvalues of graph distance matrix *D* [26]. If in addition such graphs have also identical *Z*-counting polynomial, matching polynomial, the Wiener number [27] and the Hosoya topological index *Z* [28], Hosoya, Nagashima and Hyugaji referred to such graphs colloquially as "*twin graphs*" [26]. Three pairs of such graphs are illustrated at the top in Figure 2. Non-isomorphic graphs may have many common invariants, as is the case with the twin graphs, but, as already mentioned, they should have at least one non-common invariant. For instance, as Hosoya indicated, his twin nonahedra shown at the top of Figure 2, have different connectivity index 3.9285 and 3.9317. In comparison the other two pairs of twin graphs of Figure 2 have the same connectivity indices ${}^1\chi$, which may hint that there are various degrees of structural "isospectrality" in the sense that some isospectral graphs have many common invariants while other may have few. The connectivity index ${}^1\chi$ [29], also often referred to as Randić index, (see, for example, the structure-property-activity software CODESSA [30]) is defined as a bond additive quantity in which bond (*m, n*), where *m, n* are the degrees of vertices forming bond, contribute $\frac{1}{\sqrt{m\,n}}$ to the molecular connectivity index.

Here we will investigate possibility to differentiate among twin graphs based on considering isospectrality of additional graph matrices. We will refer to isospectral graphs having the same eigenvalues of the distance matrix for "historical" reasons as twin graphs, regardless whether they have the same matching polynomial, Wiener number and Hosoya *Z* topological index. Twin graphs (according to our "simplified" definition just stated above) which are found to have the same eigenvalues with respect to any additional (not trivially related) matrix will be referred to as *strongly-isospectral graphs* or *S-isospectral graphs*. Observe the distinction between isospectral graphs and *S*-isospectral graphs, the former have the same eigenvalues of adjacency matrix, the latter have same eigenvalues with respect to *S*-number of matrices. Thus the "twin" graphs are 2-isospectral, the second matrix showing the same spectra being the graph distance matrix. In view that two pairs of graphs having the same *S*-isospectrality may involve different sets of matrices the letter *S* in *S*-isospectrality also stand for a set of matrices *S* to which isospectrality relates. Hence, for 2-isospectral twin graphs $S = \{A, D\}$, where again, *A* and *D* stand for the adjacency and the graph distance

matrix. For example, for important applications of spectral properties of line distance matrices, see [41].

2. Graph Matrices beyond Adjacency and Distance Matrix

There are numerous matrices associated with graph that one can consider as supplementary tool to be used for discrimination of graphs. Recently Janežič *et al*. [32] listed in their monograph on matrices of interest in chemistry several dozen-graph matrices. First matrix suggested specifically for the use in differentiating among isospectral graphs was matrix of Johnson and Newman [33], in which triples (x, 0, 1) in the adjacency matrix were replaced by (λ, 1, x); incidentally, this matrix was not mentioned in the monograph of Janežič *et al.* on graph matrices.

As before, let A be the adjacency matrix of a graph G, let D be its distance matrix and let V be the diagonal matrix having as entries on the diagonal the valences of corresponding vertices of G (sometimes called the *degree matrix* of G). We decided to consider the following matrices:

(i) Matrix AA^T, that can be interpreted as the scalar product of columns of the adjacency matrix A, when viewed as vectors;

(ii) Natural distance matrix ${}^N DD$, where

$$ {}^N DD_{i,j} = \sqrt{\sum_{k=1}^{N} (A_{i,k} - A_{k,j})^2}, $$

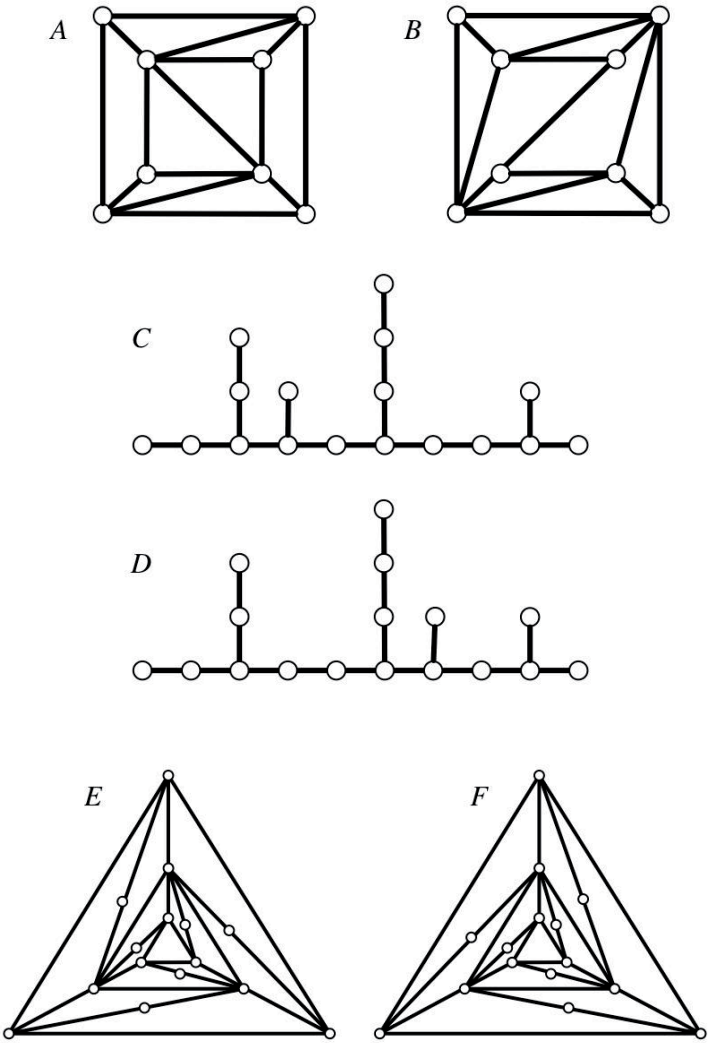
which can be interpreted as the Euclidean distance matrix in N-dimensional space between columns of the adjacency matrix viewed as vectors [34];

(iii) Laplace matrix $L = V - A$, which can be viewed as a proper discretization of the familiar Laplacian differentian operator; It is known, that if G is a regular graph, then the spectra of the Laplacian matrix is determined by the eigenvalues of the adjacency matrix of G [41];

(iv) Matrix $AA^T - V$, which in other words, is the AA^T matrix in which the diagonal entries are set to zero [35];

(v) Terminal matrix T, which is defined as the sub-matrix of D spanned on rows and columns that belong to terminal vertices of G [37, 38];

and Johnson-Newman polynomial $p_{JN}(x,\lambda)$ [33].



(E, F) Fischer twin graphs.

We initiate this project by considering the twin graphs of Figure 2 for which we will construct eigenvalues of above listed matrices in order to see if these graphs will be discriminated by the selected additional matrices. We have designated the three pairs of graphs of Figure 2: (A, B), (C, D) and (E, F), as H_1 and H_2, M_1 and M_2 and F_1 and F_2, respectively, where H, M and F stand for Hosoya *et al.* [26], McKay [35] and Fisher [39], who have introduced those graphs. Graphs H_1 and H_2 are Schlegel projections of eight vertices polyhedra which have the same eigenvalues for A and D matrix. Graphs M_1 and M_2 are the smallest pair of trees (acyclic graphs) which have the same eigenvalues for A and D matrices, while F_1 and F_2 are isospectral graphs of Fisher, which Hosoya *et al.* [26] found to have also the same distance eigenvalues.

3.1 AA^T matrix

Because the adjacency matrix A is symmetric, the matrix AA^T is equivalent to A^2, and therefore its entries count the number of walks of length two between the corresponding column and row vertices. The diagonal entries, which correspond to self-returning walks of length two are the same as vertex valences. Because matrix A is positive semi-definite, all eigenvalues of A^2 are non-negative and, when observing trees M_1 and M_2 all eigenvalues appear at least twice. It is well-known that the eigenvalues of A^2 could be obtained by squaring the eigenvalues of adjacency matrix A and thus, two graphs with the same spectrum will also have the same spectra of corresponding AA^T matrices.

In Table 1 we have listed the eigenvalues of the AA^T matrices for the six graphs considered. The exponent indicates the multiplicities of eigenvalues of corresponding AA^T.

Graph	Eigenvalues
H_1	15.0555; 5.79312; 4.39026; 1.83785; 1.55357; 0.597787; 0.544113; 0.227777
H_2	
M_1	4.9225^2; 3.90925^2; 3.00000^2; 1.75659^2; 1.15567^2; 1.00000^2; 0.255986^2; 0.00000^3
M_2	the same
F_1	^{2}
F_2	

Table 1: The spectra of AA^T matrices.

As is to be expected the eigenvalues of the AA^T matrix do not discriminate the isospectral mates. In the case of Hosoya twin graphs all eigenvalues of AA^T are different, while in the cases of Fisher's and McKay's graphs, some of eigenvalues are degenerate. It is interesting that despite that the twin graphs have apparent symmetry all the eigenvalues are different, while the McKay's trees, which have no apparent symmetry show degenerate eigenvalues.

3.2 Natural distance matrix ^{N}DD

One could expect that ^{N}DD matrix, also referred to as natural distance matrix, will have better chance to discriminate between isospectral graphs in view that its matrix elements in general are not integers, but real numbers. As one can see below, the calculation of eigenvalues for the three pairs of isospectral graphs confirmed our expectations:

Graph	Eigenvalues
H_1	
H_2	14.3999; -3.93886; -3.12959; -1.88845; -1.84319; -1.33998; -1.23001; -1.02986
M_1	^{2}; -1.17814; -1.06686; -0.914618; -0.680228; 0.000000
M_2	^{2}; -1.16858; -1.05313; -0.852104; -0.732321; 0.000000
F_1	
F_2	

Table 2: The spectra of ^{N}DD matrices.

As we see, all twin graphs are discriminated by eigenvalues of the ^{N}DD matrix. Observe that in the case of Fisher's graphs the spectra differ only in the eigenvalues of multiplicity 2. All eigenvalues of Hosoya twin graphs are again different, and this is almost true also for McKay's acyclic twins, except for a single eigenvalue $\sqrt{2}$ of multiplicity 2. Thus for the three sets of twin graphs show identical "behavior," they remain non-differentiated by the AA^T matrix and they are fully discriminated by the natural distance matrix ^{N}DD.

3.3 Negative Laplace matrix $A - V$

It is of interest to continue to explore eigenvalues of different graph matrices to see if isospectral graphs may show different "behavior" with respect to different matrices. We have calculated the characteristic polynomials for the six graphs for the case of the Johnson and Newman matrix (listed in the Appendix), which also as AA^T could not differentiate among isospectral mates, which justifies the statement of Hosoya and coworkers [26] that this "also shows that our twin graphs are strongly similar to each other". This being the case, it is of interest to see if all twin graphs are equally "strongly similar," or perhaps, some are more "strongly similar" than others? We therefore decided to search for a graph matrix that would differentiate some twin graphs, but not others, in analogy with a search for graph invariants (topological indices) that are different for similar graphs.

We decided to examine the eigenvalues of the well-known Laplace matrix $L = V - A$, which can be viewed as a proper discretization of the familiar Laplacian operator, see [41]. Of course, the eigenvalues of negative Laplace matrix $-L$ are essentially the eigenvalues of the Laplace matrix L, multiplied by -1.

Graph	Eigenvalues
H_1	
H_2	
M_1	-0.665458; -0.391223; -0.381966; -0.139194; -0.0651425; 0.00000
M_2	
F_1	
F_2	

Table 3: The spectra of A-V matrices.

As we see, (negative) Laplace matrix A-V can discriminate between the two Hosoya twins, but not between other two isospectral pairs. Thus, using the vocabulary of Hosoya *et al*., one may say, based on the above results, McKay twins M_1 and M_2 are more "strongly similar" than Hosoya twins H_1 and H_2, or in other words that some isospectral graphs (M_1 and M_2) are more isospectral!

3.4 $AA^T - V$ matrix

We decided to test in this respect the recently introduced "next nearest neighbors" matrix [40], the elements of which count the number of neighbors two bonds away. Formally, this matrix can be obtained as $AA^T - V$, where again V is diagonal matrix, the elements of which are given by the valence of vertices. One can view this matrix as the first "higher order adjacency matrix," ${}^2A$, matrix of order 2, while the matrix of the first order being the standard adjacency matrix A. Using this matrix on the six twin graphs gives for their eigenvalues:

Graph	Eigenvalues
H_1	
H_2	
M_1	-0.414214; -0.397982; 0.365175; 0.00000
M_2	^{2}
F_1	12.5279; 5.82805^2; -4.63247; -4.54128^2; -2.23607^2; -2.2099^2; -1.89541; -1.86615^2; -0.210721^2;
F_2	

Table 4: The spectra of AA^T-V matrices.

As we see, matrix $AA^T - V$ can discriminate between all pairs of twins. Thus, using the vocabulary of Hosoya *et al*., one may say, based on the above results, that the McKay twins M_1 and M_2, and the Fisher twins F_1 and F_2 are equally "strongly similar"!

3.5 Terminal matrix T

The terminal matrix is well-defined only for trees (acyclic graphs) and is the distance matrix involving only distances between terminal vertices – the vertices of degree one. The only pair of acyclic twin graphs reported by Hosoya *et al.* are McKay twin trees. The following table shows that the terminal matrix T discriminates between McKay twin graphs.

Graph	
M_1	
M_2	

Table 5: The spectra of terminal matrices of McKay twin trees.

Acknowledgments

Research was supported in part by grants P1-0294, P1-017, J1-6062 and L1-7230 by Slovenian Research Agency (ARRS). Milan Randić thanks the National Institute of Chemistry, Ljubljana for warm hospitality.

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Appendix

Fischer

$p_{JN}(x,\lambda) = -512+4992\,x-19296\,x^2+37256\,x^3-35928\,x^4+11184\,x^5+9476\,x^6-11754\,x^7+6792\,x^8-2820\,x^9+348\,x^{10}+450\,x^{11}-224\,x^{12}+12\,x^{13}+12\,x^{14}-2\,x^{15}+(-2112+25824\,x-118980\,x^2+268848\,x^3-316824\,x^4+179856\,x^5-21531\,x^6-30492\,x^7+26130\,x^8-16848\,x^9+6879\,x^{10}-528\,x^{11}-582\,x^{12}+180\,x^{13}-15\,x^{14})\,\lambda+(-576+33408\,x-241776\,x^2+700128\,x^3-994260\,x^4+721368\,x^5-258780\,x^6+45876\,x^7-864\,x^8-15300\,x^9+13212\,x^{10}-4140\,x^{11}+444\,x^{12})\,\lambda^2+(9100-43536\,x-78888\,x^2+712080\,x^3-1398825\,x^4+1211844\,x^5-538440\,x^6+176436\,x^7-75795\,x^8+21400\,x^9+918\,x^{10}-1464\,x^{11}+165\,x^{12})\,\lambda^3+(13800-149376\,x+383580\,x^2-80970\,x^3-762300\,x^4+910644\,x^5-409164\,x^6+120780\,x^7-61140\,x^8+23880\,x^9-3444\,x^{10}+60\,x^{11})\,\lambda^4+(-3312-107040\,x+555399\,x^2-777876\,x^3+169764\,x^4+226548\,x^5-77784\,x^6-13332\,x^7-3834\,x^8+5124\,x^9-684\,x^{10})\,\lambda^5+(-23308+53172\,x+217068\,x^2-621684\,x^3+372204\,x^4-39396\,x^5+26628\,x^6-31356\,x^7+6720\,x^8-88\,x^9)\,\lambda^6+(-18219+117036\,x-109896\,x^2-164388\,x^3+140040\,x^4-5028\,x^5+780\,x^6-6516\,x^7+1146\,x^8)\,\lambda^7+(-156+54768\,x-131040\,x^2+15810\,x^3+14700\,x^4+12240\,x^5-4908\,x^6-24\,x^7)\,\lambda^8+(6394-3156\,x-44115\,x^2+11940\,x^3+1830\,x^4+2856\,x^5-774\,x^6)\,\lambda^9+(2724-10992\,x-5184\,x^2-120\,x^3+1524\,x^4+36\,x^5)\,\lambda^{10}+(-177-3540\,x-234\,x^2-372\,x^3+228\,x^4)\,\lambda^{11}+(-376-372\,x-156\,x^2-6\,x^3)\,\lambda^{12}+(-78-27\,x^2)\,\lambda^{13}+\lambda^{15}$

Hosoya

$p_{JN}(x,\lambda) = 1-8\,x-4\,x^2+74\,x^3-62\,x^4-108\,x^5+157\,x^6-66\,x^7+9\,x^8+(-4-32\,x+168\,x^2-72\,x^3-300\,x^4+208\,x^5-4\,x^6-12\,x^7)\,\lambda+(-28+138\,x-54\,x^2-156\,x^3-223\,x^4+218\,x^5-35\,x^6)\,\lambda^2+(16+60\,x-128\,x^2-256\,x^3+56\,x^4+28\,x^5)\,\lambda^3+(34-88\,x-65\,x^2-132\,x^3+41\,x^4)\,\lambda^4+(-8-40\,x-52\,x^2-12\,x^3)\,\lambda^5+(-13-15\,x^2)\,\lambda^6+\lambda^8$

McKay

$p_{JN}(x,\lambda) = 20\,x-546\,x^2+4992\,x^3-22042\,x^4+52576\,x^5-66360\,x^6+29624\,x^7+30996\,x^8-56444\,x^9+39078\,x^{10}-14556\,x^{11}+2892\,x^{12}-248\,x^{13}+2\,x^{14}+(20-796\,x+7442\,x^2-24308\,x^3+3187\,x^4+167768\,x^5-438452\,x^6+503640\,x^7-266136\,x^8+13652\,x^9+57946\,x^{10}-29724\,x^{11}+5828\,x^{12}-296\,x^{13}-26\,x^{14})\,\lambda+(-250+1948\,x+11182\,x^2-137104\,x^3+437200\,x^4-497624\,x^5-150808\,x^6+870864\,x^7-816618\,x^8+320576\,x^9-30102\,x^{10}-14520\,x^{11}+3258\,x^{12}+152\,x^{13}-58\,x^{14})\,\lambda^2+(-502+15800\,x-93408\,x^2+90824\,x^3+593786\,x^4-1752912\,x^5+1643460\,x^6-240624\,x^7-559374\,x^8+372080\,x^9-79826\,x^{10}+872\,x^{11}+814\,x^{12}+200\,x^{13}-30\,x^{14})\,\lambda^3+(2352-156\,x-184154\,x^2+818488\,x^3-897130\,x^4-916296\,x^5+2319324\,x^6-1445400\,x^7+194982\,x^8+113580\,x^9-34044\,x^{10}-812\,x^{11}+706\,x^{12})\,\lambda^4+(5537-74380\,x+132410\,x^2+716780\,x^3-2311383\,x^4+1561416\,x^5+590604\,x^6-994200\,x^7+322770\,x^8-12020\,x^9-4780\,x^{10}-1036\,x^{11}+214\,x^{12})\,\lambda^5+(-2474-77372\,x+555254\,x^2-622992\,x^3-1284084\,x^4+2064384\,x^5-702492\,x^6-143424\,x^7+93852\,x^8-2320\,x^9-2092\,x^{10})\,\lambda^6+(-14628+62528\,x+348888\,x^2-1341696\,x^3+438576\,x^4+754992\,x^5-485628\,x^6+52800\,x^7+7956\,x^8+1680\,x^9-500\,x^{10})\,\lambda^7+(-8276+149280\,x-213240\,x^2-739596\,x^3+729162\,x^4-30384\,x^5-92766\,x^6+8784\,x^7+2556\,x^8)\,\lambda^8+(9583+64832\,x-386568\,x^2-57432\,x^3+271725\,x^4-67464\,x^5-4230\,x^6-1168\,x^7+552\,x^8)\,\lambda^9+(13120-41100\,x-200212\,x^2+89160\,x^3+32306\,x^4-8496\,x^5-1466\,x^6)\,\lambda^{10}+(3124-54920\,x-41930\,x^2+32000\,x^3-192\,x^4+360\,x^5-322\,x^6)\,\lambda^{11}+(-3434-24120\,x-766\,x^2+3180\,x^3+388\,x^4)\,\lambda^{12}+(-2895-4968\,x+662\,x^2-40\,x^3+101\,x^4)\,\lambda^{13}+(-918-404\,x-38\,x^2)\,\lambda^{14}+(-120-16\,x^2)\,\lambda^{15}+\lambda^{17}$