CROATICA CHEMICA ACTA CCACAA **73** (4) 957–967 (2000)

ISSN-0011-1643
CCA-2694 *Note*

Note on the Resistance Distances in the Dodecahedron#

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Received January 26, 2000; revised May 2, 2000; accepted May 3, 2000

Resistance distances in the regular dodecahedron are computed. This report together with our previous paper (see Ref. 2) completes the study of resistance distances in Platonic solids (the tetrahedron, the cube, the octahedron, the icosahedron and the dodecahedron). The sum over the resistance distances between all pairs of vertices in a graph is a graph invariant. It is used to order Platonic solids according to the complexity of their Schlegel graphs.

Key words: dodecahedron, Platonic solids, resistance distance, Schlegel graph.

INTRODUCTION

Recently, we computed resistance distances[1] in regular graphs.[2] Two classes of regular graphs have been considered: cycles and complete graphs. We considered Schlegel diagrams[3] of four Platonic solids: the tetrahedron, the cube, the octahedron and the icosahedron. These solids are often used to model the shapes of molecules. While our paper was reviewed, one of the reviewers asked why we did not also discuss the resistance distances in the fifth Platonic solid, that is, the dodecahedron? Several colleagues also asked

Reported in part at the 14th Dubrovnik International Course & Conference on the Interfaces between Mathematics, Chemistry and Computer Sciences & The 5th Croatian Meeting on Fullerenes, Dubrovnik, June 21–26, 1999.

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a similar question after our paper was published. The reason was that the complexity involved in the computation of the resistance distances in dodecahedron is quite high. However, finally we succeeded to compute the resistance distances in the dodecahedron. This is reported here. It should be noted that in the present report we would use the same notation and definitions as in our previous paper.[2]

The regular dodecahedron is a convex polyhedron with 12 faces that are all regular pentagons.[4] It has 20 vertices and 30 edges. It is depicted in Figure 1.

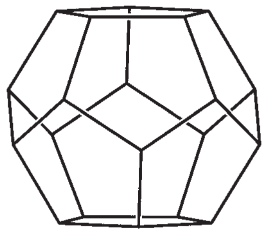

Figure 1. The dodecahedron.

The dodecahedron can be used, for example, to model the carbon skeleton of dodecahedrane, $C_{20}H_{20}$ and the smallest-fullerene (C_{20}). Both these molecules are shown in Figure 2.

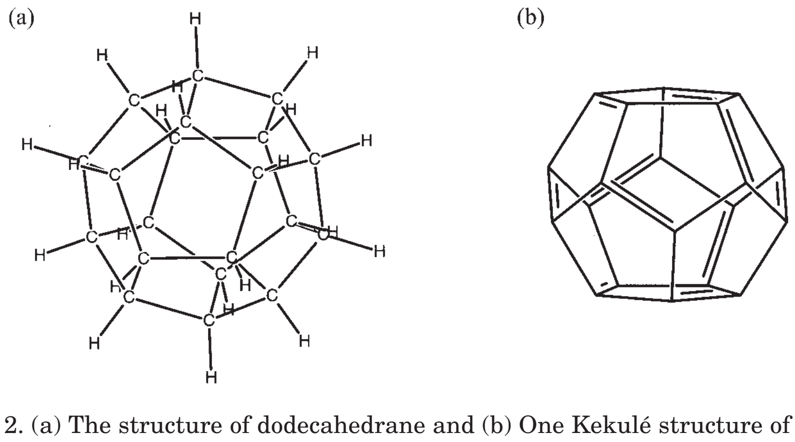

Figure 2. (a) The structure of dodecahedrane and (b) One Kekulé structure of C_{20}-fullerene.

Dodecahedrane was prepared years ago.[5] This molecule has many interesting properties reflecting its high symmetry and spheroidicity. For example, dodecahedrane with one amino group attached to one carbon atom passes readily through membrane of a cell and tends to destroy a virus inside it. C_{20}-fullerene has not yet been prepared. Theoretical studies indicate that this smallest member the fullerene family would undergo Jahn-Teller distortion to a symmetry group somewhat lower than I_h.[6]

RESISTANCE DISTANCES IN DODECAHEDRON

The labeled Schlegel diagram (Schlegel graph) of the dodecahedron is shown in Figure 3.

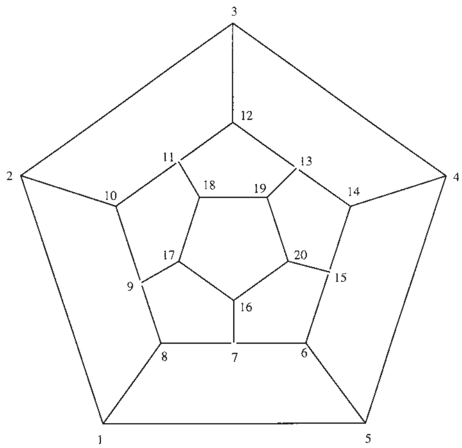

Figure 3. The Schlegel diagram of the dodecahedron.

The number of graph distances equal to one is equal to the number of edges (30), the number of distances equal to two is sixty, the number of distances equal to three is also sixty, while the number of distances equal to four is thirty, and finally the number of distances equal to five is ten. The total number of distances is 190. The usual graph distance matrix for the Schlegel diagram of the dodecahedron is given in Figure 4.

Making use of Kirchoff's rules we derived the algebraic equations for resistance distances: Equations containing three terms were obtained by using Kirchoff's first rule, while equations containing five terms were obtained by using Kirchoff's second rule.

The resistance distance was obtained by using the following approach: It was assumed as before[2] that the total current entering and leaving the set at specified points is equal to one (see Figures 5–9).

0	1	2	2	1	2	2	1	2	2	3	3	4	3	3	3	3	4	5	4
1	0	1	2	2	3	3	2	2	1	2	2	3	3	4	4	3	3	4	5
2	1	0	1	2	3	4	3	3	2	2	1	2	2	3	5	4	3	3	4
2	2	1	0	1	2	3	3	4	3	3	2	2	1	2	4	5	4	3	3
1	2	2	1	0	1	2	2	3	3	4	3	3	2	2	3	4	5	4	3
2	3	3	2	1	0	1	2	3	4	5	4	3	2	1	2	3	4	3	2
2	3	4	3	2	1	0	1	2	3	4	5	4	3	2	1	2	3	3	2
1	2	3	3	2	2	1	0	1	2	3	4	5	4	3	2	2	3	4	3
2	2	3	4	3	3	2	1	0	1	2	3	4	5	4	2	1	2	3	3
2	1	2	3	3	4	3	2	1	0	1	2	3	4	5	3	2	2	3	4
3	2	2	3	4	5	4	3	2	1	0	1	2	3	4	3	2	1	2	3
3	2	1	2	3	4	5	4	3	2	1	0	1	2	3	4	3	2	2	3
4	3	2	2	3	3	4	5	4	3	2	1	0	1	2	3	3	2	1	2
3	3	2	1	2	2	3	4	5	4	3	2	1	0	1	3	4	3	2	2
3	4	3	2	2	1	2	3	4	5	4	3	2	1	0	2	3	3	2	1
3	4	5	4	3	2	1	2	2	3	3	4	3	3	2	0	1	2	2	1
3	3	4	5	4	3	2	2	1	2	2	3	3	4	3	1	0	1	2	2
4	3	3	4	5	4	3	3	2	2	1	2	2	3	3	2	1	0	1	2
5	4	3	3	4	3	3	4	3	3	2	2	1	2	2	2	2	1	0	1
4	5	4	3	3	2	2	3	3	4	3	3	2	2	1	1	2	2	1	0

Figure 4. The distance matrix of the Schlegel diagram of the dodecahedron.

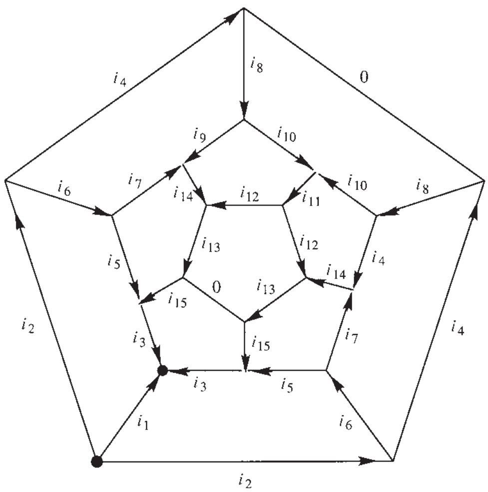

Figure 5. Black dots indicate the adjacent pair of vertices between which the resistance distance has to be determined.

Since $V = IR$ (I = current, R = resistance, V = potential), the potential between the two vertices under consideration (say vertices 1 and 2) is equal to the sum of potential differences $\Sigma\ (1 \times i_k)$ at edges k, lying on the path connecting these two vertices:

$$V = \sum_k (1 \times i_k) = \sum_k i_k \tag{1}$$

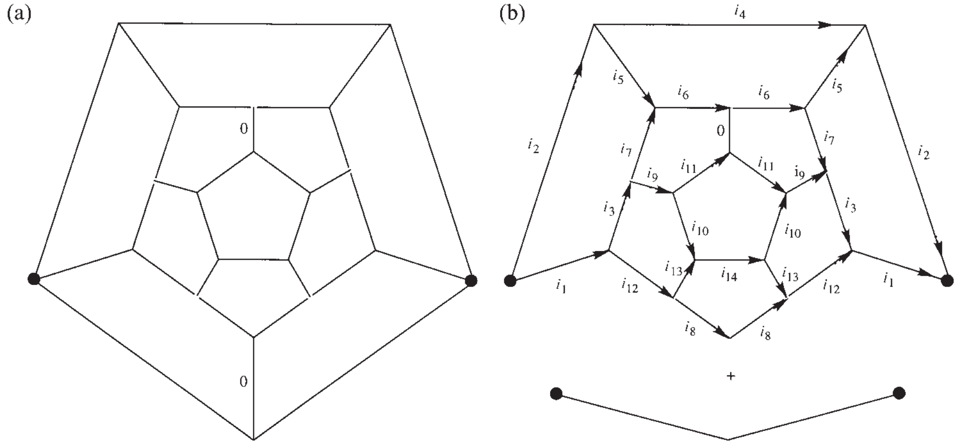

Figure 6. Black dots indicate non-adjacent vertices, separated by two edges, between which the resistance distance has to be determined. The decomposed network (b) was obtained from (a) by removing one edge through which no 'current' is flowing.

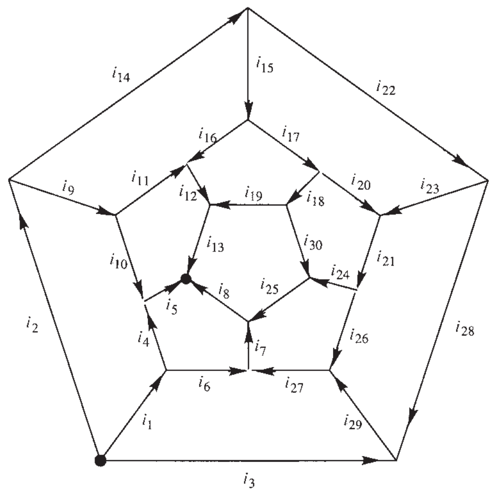

Figure 7. Black dots indicate non-adjacent vertices, separated by three edges, between which the resistance distance has to be determined.

where i_k denotes the 'current' flowing through edge k. The summation in equation (1) goes over all edges lying on path connecting vertices 1 and 2. Consideration of different paths must yield an identical result, but the shortest path was always considered. Using this equation and taking into account that the total current is equal to one ($I = 1$), we obtain the resistance between points 1 and 2, $R_{1,2}$:

$$R_{1,2} = \sum_{k} i_k \ . \tag{2}$$

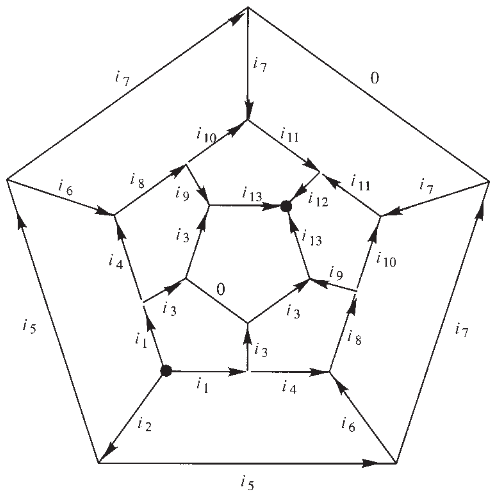

Figure 8. Black dots indicate non-adjacent vertices, separated by four edges, between which the resistance distance has to be determined.

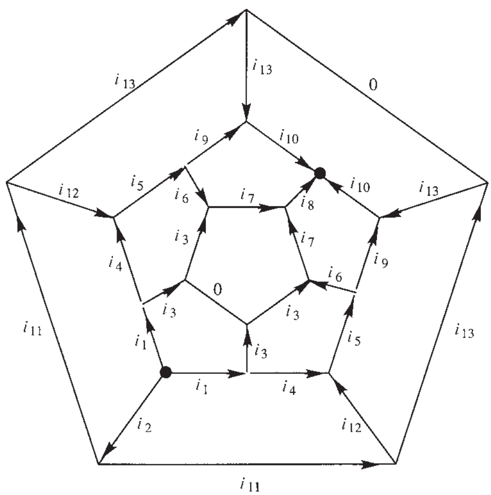

Figure 9. Black dots indicate non-adjacent vertices, separated by five edges, between which the resistance distance has to be determined.

Table I contains the equations and results derived for cases $d_{1,2} = 1$ and $d_{1,2} = 2$, where $d_{1,2}$ is the distance between vertices 1 and 2. Symmetries were used to reduce the number of unknown »currents«; these being shown explicitly only for the cases $d_{1,2} = 1$ and $d_{1,2} = 2$. In order to consider case

TABLE I

Computation of resistance distances between vertices 1 and 2

Distance d and resistance distance R	Equations and symmetry equations	Solutions
$d_{1,2} = 1$ (Figure 5)	$1 = i_1 + 2i_2$	$i_1 = 38/60$
$R_1 = 1 \times i_1/1 = 19/30$	$i_2 = i_4 + i_6$	$i_2 = 11/60$
	$i_6 = i_5 + i_7$	$i_3 = 11/60$
	$i_3 = i_5 + i_{15}$	$i_4 = 3/60$
	$i_{14} = i_7 + i_9$	$i_5 = 8/60$
	$i_{13} = i_{12} + i_{14}$	$i_6 = 8/60$
	$i_8 = i_9 + i_{10}$	$i_7 = 0$
	$i_1 = i_2 + i_3 + i_5 + i_6$	$i_8 = 3/60$
	$i_4 + i_8 + i_9 = i_6 + i_7$	$i_9 = 2/60$
	$i_5 = i_7 + i_{13} + i_{14} + i_{15}$	$i_{10} = 1/60$
	$i_{10} + i_{11} + i_{12} = i_9 + i_{14}$	$i_{11} = 2/60$
	$i_3 = i_2$	$i_{12} = 1/60$
	$i_8 = i_4$	$i_{13} = 3/60$
	$i_{15} = i_{13}$	$i_{14} = 2/60$
	$i_{12} = i_{10}$	$i_{15} = 3/60$
$d_{1,2} = 2$ (Figures 6a and 6b)	$1 = i_1 + i_2$	$i_1 = 14/33$
$R'_2 = 1 \times (2i_2 + i_4)/1 = 54/33$	$i_1 = i_3 + i_{12}$	$i_2 = 19/33$
$R''_2 = 2$	$i_2 = i_4 + i_5$	$i_3 = 6/33$
$1/R_2 = (1/R'_2) + (1/R''_2) = 60/54$	$i_3 = i_7 + i_9$	$i_4 = 16/33$
$R_2 = 54/60 = 9/10$	$i_6 = i_5 + i_7$	$i_5 = 3/33$
	$i_9 = i_{10} + i_{11}$	$i_6 = 5/33$
	$i_{14} = i_{10} + i_{13}$	$i_7 = 2/33$
	$i_{12} = i_8 + i_{13}$	$i_8 = 5/33$
	$i_2 + i_5 = i_1 + i_3 + i_7$	$i_9 = 4/33$
	$i_4 = 2i_5 + 2i_6$	$i_{10} = 1/33$
	$2i_6 + 2i_7 = 2i_9 + 2i_{11}$	$i_{11} = 3/33$
	$i_{12} + i_{13} = i_3 + i_9 + i_{10}$	$i_{12} = 8/33$
	$2i_{11} = 2i_{10} + i_{14}$	$i_{13} = 3/33$
	$2i_8 = 2i_{13} + i_{14}$	$i_{14} = 4/33$

$d_{1,2} = 2$, the symmetries were used to show which currents are zero, and based on this result, Figure 6a could be simplified (see Figure 6b). Note that R_2 was obtained by combining the two subresistances R'_2 and R''_2.

TABLE II

Computing the resistance distances for distances 3, 4 and 5 between vertices 1 and 2

Distance d and resistance distance R	Solutions
$d_{1,2} = 3$ (Figure 7)	$i_1 = 24/60$
$R_3 = 1 \times (i_1 + i_4 + i_5)/1 = 16/15$	$i_2 = 29/60$
	$i_3 = 17/60$
	$i_4 = 16/60$
	$i_5 = 24/60$
	$i_6 = 8/60$
	$i_7 = 13/60$
	$i_8 = 19/60$
	$i_9 = 13/60$
	$i_{10} = 8/60$
	$i_{11} = 5/60$
	$i_{12} = 10/60$
	$i_{13} = 17/60$
	$i_{14} = 6/60$
	$i_{15} = 7/60$
	$i_{16} = 5/60$
	$i_{17} = 2/60$
	$i_{18} = 6/60$
	$i_{19} = 7/60$
	$i_{20} = -4/60$
	$i_{21} = 2/60$
	$i_{22} = -1/60$
	$i_{23} = 6/60$
	$i_{24} = 7/60$
	$i_{25} = 6/60$
	$i_{26} = -5/60$
	$i_{27} = 5/60$
	$i_{28} = -7/60$
	$i_{29} = 10/60$
	$i_{30} = -1/60$

TABLE II (continued)

Distance d and resistance distance R	Solutions
$d_{1,2} = 4$ (Figure 8)	$i_1 = 21/60$
$R_4 = 1 \times (i_1 + 2i_3 + i_{13})/1 = 17/15$	$i_2 = 18/60$
	$i_3 = 13/60$
	$i_4 = 8/60$
	$i_5 = 9/60$
	$i_6 = 2/60$
	$i_7 = 7/60$
	$i_8 = 10/60$
	$i_9 = 8/60$
	$i_{10} = 2/60$
	$i_{11} = 9/60$
	$i_{12} = 18/60$
	$i_{13} = 21/60$
$d_{1,2} = 5$ (Figure 9)	$i_1 = 2/6$
$R_5 = 1 \times (i_1 + 2i_3 + i_7 + i_8)/1 = 7/6$	$i_2 = 2/6$
	$i_3 = 1/6$
	$i_4 = 1/6$
	$i_5 = 1/6$
	$i_6 = 0$
	$i_7 = 1/6$
	$i_8 = 2/6$
	$i_9 = 1/6$
	$i_{10} = 2/6$
	$i_{11} = 1/6$
	$i_{12} = 0$
	$i_{13} = 1/6$

For the rest of cases, given in Table II, the equations are not written out in detail in order to save space, but the results can be checked by using Figures 7–9. A minus sign for a solution indicates that the direction of the partial current is opposite to what was assumed. The number of unknowns was the greatest (30) in the case $d_{1,2} = 3$.

The total resistance (R_T) of the dodecahedron is equal to:

$$R_T = 30\ R_1 + 60\ R_2 + 60\ R_3 + 30\ R_4 + 10\ R_5 \quad (3)$$

or

$$R_T = 30\ (19/30) + 60\ (9/10) + 60\ (16/15) + 30\ (17/15) + 10\ (7/6) = 182.67. \quad (4)$$

CONCLUSIONS

If we now compare the resistances in all five Platonic solids – tetrahedron (T), cube (C), octahedron (O), icosahedron (I) and dodecahedron (D): R(T) = 3, R(C) = 19.3, R(O) = 6.5, R(I) = 32.3 and R(D) = 182.7, they order these solids according to complexity of their Schlegel graphs as T < O < C < I < D. Some other structural characteristics order the Platonic solids in the following ways: (*i*) The number of vertices gives T < O < C < I < D; (*ii*) The number of edges T < O = C < I = D; (*iii*) The number of faces T < C < O < D < I; (*iv*) The number of spanning trees[7] T < O = C < I = D; (*v*) The Bertz complexity index[8] T < C < O < D < I; (*vi*) The Randić vertex-connectivity index[9] T < O < C < I < D; (*vii*) The Estrada first-order edge-connectivity index[10] T < O = C < I = D; (*viii*) The Estrada second-order edge-connectivity index[10] T < O < C < D < I and (*ix*) The Hosoya Z-index[11] T < O < C < I < D. All ten criteria listed here predict the tetrahedron to be the least complex structure. However, in the case of pairs: the cube and the octahedron, and the icosahedron and the dodecahedron, which are dual to each other, different criteria give different ordering. But, judging by the difficulty we had in computing the resistance distances, the order T < O < C < I < D (supported by four criteria) seems to reflect best their complexity.

Acknowledgements. – SN and NT were supported by Grant No. 980605 rewarded by the Ministry of Science and Technology of Croatia. We thank reviewers for helpful comments.

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SAŽETAK

Bilješka o otpornim udaljenostima u dodekaedru

István Lukovits, Sonja Nikolić i Nenad Trinajstić

Izračunane su otporne udaljenosti u dodekaedru. Ova bilješka s prethodnim člankom (vidi Ref. 2) zaokružuje proučavanje otpornih udaljenosti kod Platonskih krutina (tetraedar, kocka, oktaedar, ikozaedar i dodekaedar). Zbroj otpornih udaljenosti između svih parova vrhova u grafu jest invarijanta grafa. Upotrebljena je za redanje Platonskih krutina prema kompleksnosti pripadnih Schlegelovih grafova.