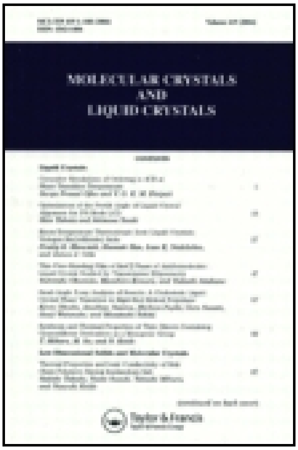

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Visualizing Supramolecular Macrocyclic Formations

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Visualizing Supramolecular Macrocyclic Formations

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A convenient protocol to analyze complicated network structures arising due to noncovalent interactions in the solid state is demonstrated using the remarkably complex and extensively H-bonded crystal structure of the 1:3 cocrystal of *cis,cis*-1,3,5-cyclohexanetricarboxylic acid and urea. The visualization of the H-bond network in terms of macrocyclic formations and their systematic enumeration allows a simple analysis of the complex intermolecular interaction pathways which play a fundamental role in molecular materials design.

Keywords: Supramolecular assemblies; Cocrystal; H-bonding; Graph sets

INTRODUCTION

Hydrogen bonding is one of the most pervasive of all intermolecular interactions that steer the solid state assembly of molecular materials. Such interactions lead to the formation of a wide variety of packing patterns.[1] The specific connectivities and orientations of molecules resulting from the H-bond interactions are known to control material properties such as cooperative magnetism[2] and nonlinear optical effects.[3] The connectivity pattern of supramolecular assemblies resulting from noncovalent interactions such as H-bonding is often the key to the understanding of their physicochemical properties. The visualization and analysis of H-bond networks in crystals is an integral part of structure-property correlations in the solid state and the insight gained from such explorations forms a significant input for advanced materials design. Graph theoretical and related methods are used to systematize the study of H-bond networks in solids; graph set analysis[4] is widely used to classify H-bonded structural motifs and derive

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empirical principles of molecular packing. Graph approach has also been used to analyze the energetics of H-bonded molecular clusters.[5] Though the delineation of H-bond networks is generally a straightforward exercise and is often carried out by visual inspection, it can get complicated when the number of different types of H-bonds in the asymmetric unit of the crystal is large and the symmetry of the connectivity is low. The power of graph concepts has not been exploited to develop a formal approach to this problem. We demonstrate in this paper, a systematic protocol to enumerate and visualize complex structural motifs in supramolecular architectures, using as an example, the highly unsymmetric and extensively H-bonded network structure of the cocrystal formed from two simple molecules, urea and *cis,cis*-1,3,5-cyclohexanetricarboxylic acid (CHTCA).

Crystal structure of urea is a classic case of an extensively H-bonded network generated from a simple structural unit. Each urea molecule is involved in eight H-bonds, accommodation of which leads to a noncentrosymmetric crystal structure.[6] CHTCA with its nonplanar structure and H-bonding arms appeared to be a suitable partner to create complex networks with urea. Interestingly, a search of the Cambridge Crystallographic Database[7] revealed only two crystal structures involving CHTCA;[8] one hit was obtained for its trimethyl ester[9] and nine for the 1,3,5-trimethyl derivative, the Kemp's acid. We have found that CHTCA forms a 1:3 cocrystal with urea. Single crystal x-ray analysis reveals an interesting channel structure arising out of a complex network architecture which can be visualized as a collection of supramolecular macrocyclic formations. It is found to be ideally suited to illustrate the utility of a systematic procedure we have developed for the enumeration and perception of cyclic structural motifs in supramolecular assemblies.

EXPERIMENTAL

CHTCA and urea were mixed in 1:3 ratio in water. Crystals with the morphology of square plates grew over a period of several days. Infra red spectrum of the crystals showed the presence of urea and CHTCA suggesting the formation of a cocrystal. The x-ray diffraction data was collected on an Enraf-Nonius MACH3 diffractometer. Data was reduced using Xtal3.4;[10] Lorentz and polarization corrections were included. Non-hydrogen atoms were found using the direct method analysis in SHELX-97[11] and after several cycles of refinement the positions of the hydrogen atoms were calculated and added to the refinement process. Details of data collection, solution and refinement, anisotropic thermal parameters and full lists of bond lengths and angles are deposited as Supplementary Information.

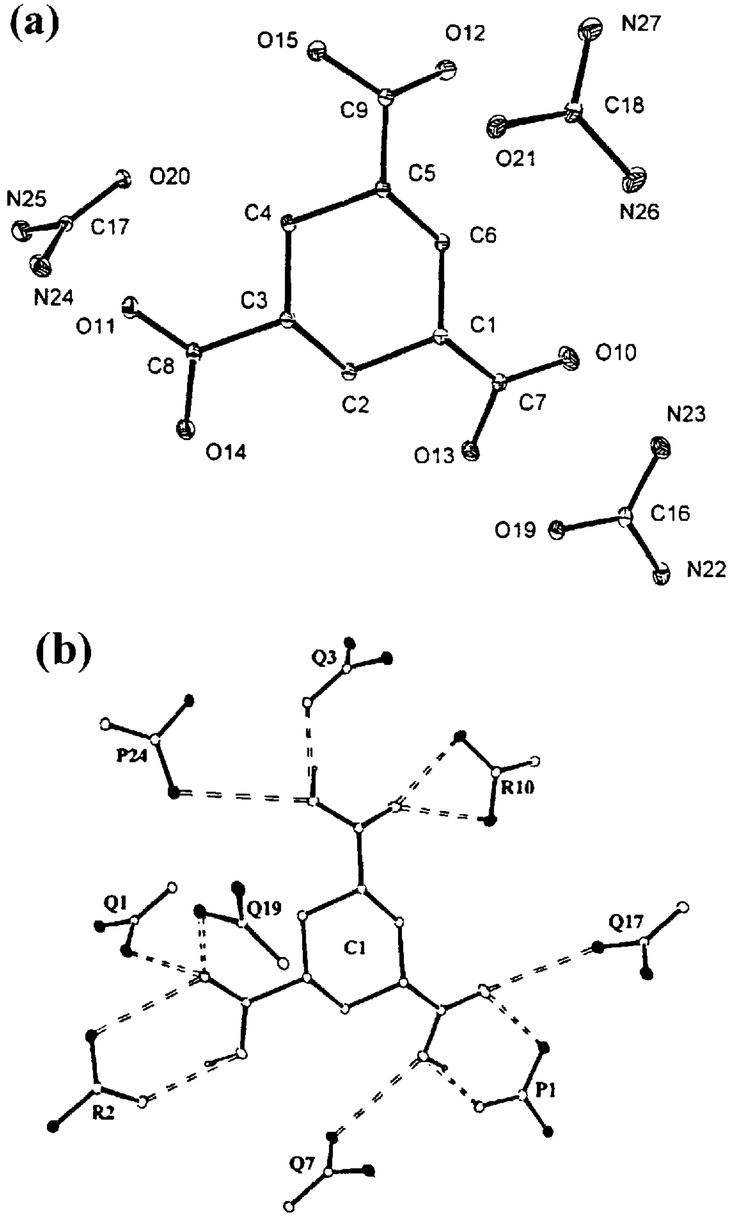

FIGURE 1 (a) Molecular structure of CHTCA-urea from single crystal x-ray analysis. 10% thermal ellipsoids of non hydrogen atoms alone are shown. (b) H-bonds involving the CHTCA molecule in CHTCA-Urea. H-bonds are shown as broken lines; all H atoms except those on the carboxylic acid groups are omitted for clarity; N atoms are shown as filled circles

TABLE I Crystallographic data for CHTCA-Urea

Empirical formula	$C_{12}H_{24}N_6O_9$
Crystal system	Monoclinic
Space group	$P2_1/n$
a (Å)	12.232(10)
b (Å)	12.2555(10)
c (Å)	13.080(9)
β (°)	107.05 (8)
V (Å^3)	1875(2)
Z	4
ρ (gm cm^{-3})	1.404
μ (cm^{-1})	1.20
Number of unique reflections	4291
Number of reflections with $I \geq 2\sigma_I$	2666
Number of parameters	244
Goodness-of-fit	1.060
R (for data with $I \geq 2\sigma_I$)	0.0455
wR^2 (for data with $I \geq 2\sigma_I$)	0.1017

COMPUTATIONAL

A graph is a finite nonempty set, V of vertices together with a prescribed set, E of pairs of vertices or edges.[12] A simple path of length N in a graph is a sequence of N edges and N+1 vertices, each vertex (except the first and the last) being incident with the preceding and with the succeeding edge, no vertex or edge occurring more than once. A ring or a cycle is a closed path where the initial and terminal vertices coincide. Fundamental cycles of a graph having "n" vertices and "m" edges is a set, not necessarily unique, of "n-m+1" (cyclomatic or Frère-jacque number[13]) cycles, combinations of which generate all possible cycles in the graph. A number of algorithms are available in the literature to enumerate the fundamental cycles in a graph.[13]

A directed graph is one in which a direction or orientation is associated with each edge in the graph. The H-bonded cluster of molecules is conveniently described using a directed graph with molecules represented by the vertices and the H-bonds by the edges.[5] The orientation of the edges represent the direction of H-bond donation. Two-way H-bonds formed with each molecule in the pair acting as a H-bond donor as well as an acceptor, are represented by loops. Double H-bonds with one molecule making two H-bond donations to the other are repre-

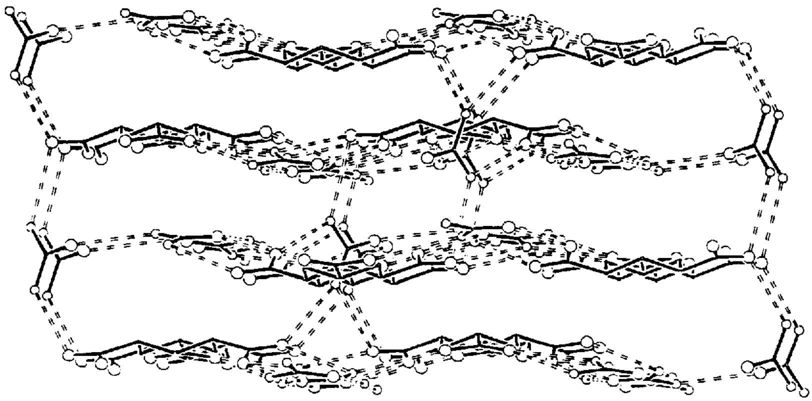

FIGURE 2 View of the CHTCA-urea crystal packing along the *b* axis. C (○), N (○) and O (O) atoms are indicated; H-bonds are shown as broken lines

sented by double edges. A directed cycle preserves the orientation in the sequence of edges *i.e.* starting at any vertex and following the direction of the edges one can traverse the other vertices in the cycle and return to the origin. The algorithm we have developed to generate all possible directed cycles in a directed graph having loops and double edges works as follows. The information regarding the connectivity of vertices is read in as the adjacency or connectivity matrix; double edges are treated as single edges. Then the full set of permutations of the loop edges are generated. For example when there are 10 loop edges, 2^{10} possible orientations of these edges lead to as many directed graphs. In each graph thus created, adjacency matrix multiplication is used to enumerate the directed paths and cycles. Explicit tracking of the vertices passed *en route* allows removal of paths which cross an intermediate vertex already traversed and termination of a cycle when the starting vertex is reached. The Fortran codes developed for creating the permutations and enumerating the directed cycles are provided in the Supplementary Information.

RESULTS AND DISCUSSION

The 1:3 cocrystal formed between CHTCA and urea is found to belong to the $P2_1/n$ space group. The crystallographic data are presented in Table I. There is one CHTCA and three urea molecules in the asymmetric unit (Fig. 1a). The significant bond lengths and angles are collected in Table II. Fifteen inequivalent H-bonds are observed in this crystal ! The geometric details are provided in Table III; the D···A distances lie in the range 2.508 – 3.256 Å and the D-H···A angles in the range 134 – 176°. The CHTCA molecule donates three H-bonds and accepts nine (Fig. 1b) and three H-bonds occur between urea molecules. We denote CHTCA and the inequivalent urea by C and P, Q, R respectively. The symmetry operations generating the relevant molecules are represented by numeric labels: these operations are listed in Table IV. The H-bond network in CHTCA-urea leads to the interesting and complex channel structure shown in Fig. 2.

TABLE II (a) Bond lengths and (b) angles in CHTCA-Urea

(a)

Bond	*Length (Å)*
O(10)-C(7)	1.203(2)
O(11)-C(8)	1.216(2)
O(12)-C(9)	1.197(2)
O(13)-C(7)	1.298(2)
O(14)-C(8)	1.297(2)
O(15)-C(9)	1.308(2)
O(19)-C(16)	1.253(2)
O(20)-C(17)	1.248(2)
O(21)-C(18)	1.249(2)
N(22)-C(16)	1.324(3)
N(23)-C(16)	1.331(3)
N(24)-C(17)	1.323(3)
N(25)-C(17)	1.323(3)
N(26)-C(18)	1.327(3)
N(27)-C(18)	1.320(3)
C(1)-C(7)	1.509(3)
C(1)-C(2)	1.522(3)
C(1)-C(6)	1.522(3)
C(2)-C(3)	1.529(3)
C(3)-C(8)	1.512(3)
C(3)-C(4)	1.522(3)
C(4)-C(5)	1.529(3)
C(5)-C(9)	1.503(3)
C(5)-C(6)	1.526(3)

(b)	
Bond-bond	*Angle (°)*
C(7)-C(1)-C(2)	113.94(17)
C(7)-C(1)-C(6)	109.68(15)
C(2)-C(1)-C(6)	111.85(15)
C(1)-C(2)-C(3)	110.99(16)
C(8)-C(3)-C(4)	110.10(15)
C(8)-C(3)-C(2)	113.39(16)
C(4)-C(3)-C(2)	112.15(15)
C(3)-C(4)-C(5)	111.61(15)
C(9)-C(5)-C(6)	110.19(15)
C(9)-C(5)-C(4)	113.03(16)
C(6)-C(5)-C(4)	112.53(16)
C(1)-C(6)-C(5)	111.94(15)
O(10)-C(7)-O(13)	121.80(18)
O(10)-C(7)-C(1)	123.00(19)
O(13)-C(7)-C(1)	115.19(16)
O(11)-C(8)-O(14)	122.90(17)
O(11)-C(8)-C(3)	122.08(17)
O(14)-C(8)-C(3)	115.02(16)
O(12)-C(9)-O(15)	121.05(19)
O(12)-C(9)-C(5)	123.77(18)
O(15)-C(9)-C(5)	115.18(16)
O(19)-C(16)-N(22)	119.49(19)
O(19)-C(16)-N(23)	121.11(19)
N(22)-C(16)-N(23)	119.39(19)
O(20)-C(17)-N(24)	120.5(2)
O(20)-C(17)-N(25)	121.9(2)
N(24)-C(17)-N(25)	117.6(2)
O(21)-C(18)-N(27)	121.32(18)
O(21)-C(18)-N(26)	120.5(2)
N(27)-C(18)-N(26)	118.19(19)

The extensive H-bonding in CHTCA-urea makes the visualization of the 3-dimensional network structure very difficult. We have chosen to analyze the pattern as follows. First we consider the asymmetric unit consisting of C1, P1, Q1 and R1. The molecules to which this unit donates H-bonds (C6, C7, C8, C9, C10, C11, P4, Q3, Q5, R2 and R4) are determined from the crystal packing information and added as the first shell. In a similar way, a second shell of H-bond acceptors are added leading to a cluster of 42 molecules. The directed graph rep-

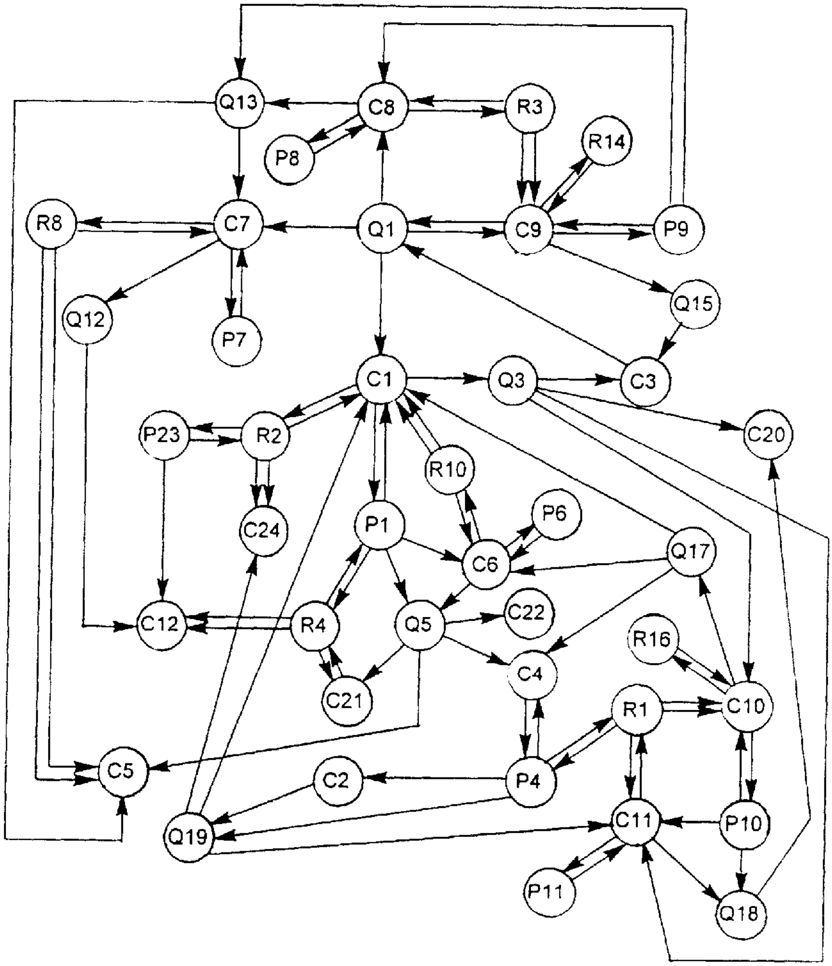

FIGURE 3 The directed graph representation of the CHTCA-urea H-bond network. The letters C, P, Q and R represent CHTCA and the three urea molecules and the numeric labels denote the relevant symmetry operation listed in Table IV. The arrows signify the H-bonds, emanating from the H-bond donor and ending at the acceptor

resentation of this complex H-bonded cluster is shown in Fig. 3. There are 66 H-bond interactions present – 19 are two-way bonds represented by loops and 6 are double H-bonds represented by the double edges. The graph reveals the presence of a large number of *supramolecular macrocyclic formations* enumeration of which is accomplished using the graph theoretical algorithms discussed above. We have carried out this analysis in two ways.

TABLE III The H-bonds involving the asymmetric unit of CHTCA-urea cocrystal. D and A represent the H-bond donor and acceptor atoms, $d_{H...A}$ the H...A distance and $\theta_{D\text{-}H...A}$ the D-H...A angle. See Fig. 1a for the atom labels

D-H	$d_{H...A}$ (Å)	$\theta_{D\text{-}H...A}$ (°)	*A*	*Symmetry operation on A*
O13-H13	1.708	164.56	O19	[x, y, z]
O14-H14	1.759	167.88	O21	[-x+5/2, y-1/2, -z+1/2]
015-H15	1.735	171.95	O20	[-x+3, -y+1, -z+1]
N22-H22A	2.076	160.46	O21	[-x+2, -y, -z+1]
N22-H22B	2.071	157.09	O20	[-x+5/2, y-1/2, -z+3/2]
N23-H23A	2.222	153.28	O10	[x, y, x]
N23-H23B	2.443	157.92	O15	[x-1/2, -y+1/2, z+1/2]
N24-H24A	2.295	157.91	O11	[x, y, z]
N24-H24B	2.162	165.21	O13	[-x+3, -y, -z+1]
N25-H25A	2.175	176.08	O11	[x+1/2, -y+1/2, z+1/2]
N25-H25B	2.378	134.02	O10	[x+1, y, z]
N26-H26A	2.230	159.98	O19	[-x+2, -y, -z+1]
N26-H26B	2.312	145.26	O12	[-x+2, -y+1, -z+1]
N27-H27A	2.137	159.99	O11	[-x+5/2, y+1/2, -z+1/2]
N27-H27B	2.112	153.92	O12	[-x+2, -y+1, -z+1]

First we considered the undirected version of the graph in Fig. 3 and counted one set of fundamental cycles. Since the undirected version is much less complicated than the directed one, this enumeration is easily carried out by inspection. The physical implication of the set of fundamental cycles in the present case is that it represents the collection of basic H-bonded macrocyclic formations in the cluster. The number of cycles of various sizes in the set is presented in Table V. Next we enumerated the directed cycles in the cluster which represent ring structures with H-bonds directed in the same sense. The addition of shells of H-bond acceptors in the generation of the cluster in Fig. 3 facilitates this count. A close examination of the directed graph shows that there are several vertices which cannot participate in a directed cycle; they are C5, C12, C20, C22, C24, P6, P7, P8, P11, R14 and R16. Removal of these vertices exposes some more such vertices and successive prunings lead to the removal of C7, P23, Q12, Q13, Q18, R2 and R8. The final pruned graph has 24 vertices, 10 loops and 29 simple edges with multiple edges being treated as simple edges. Each orientation of every loop was considered explicitly and the directed graphs arising from the 2^{10} permutations of the loop edges were generated and their directed cycles enumerated. The graph with maximum cycle formation was determined by estimating the

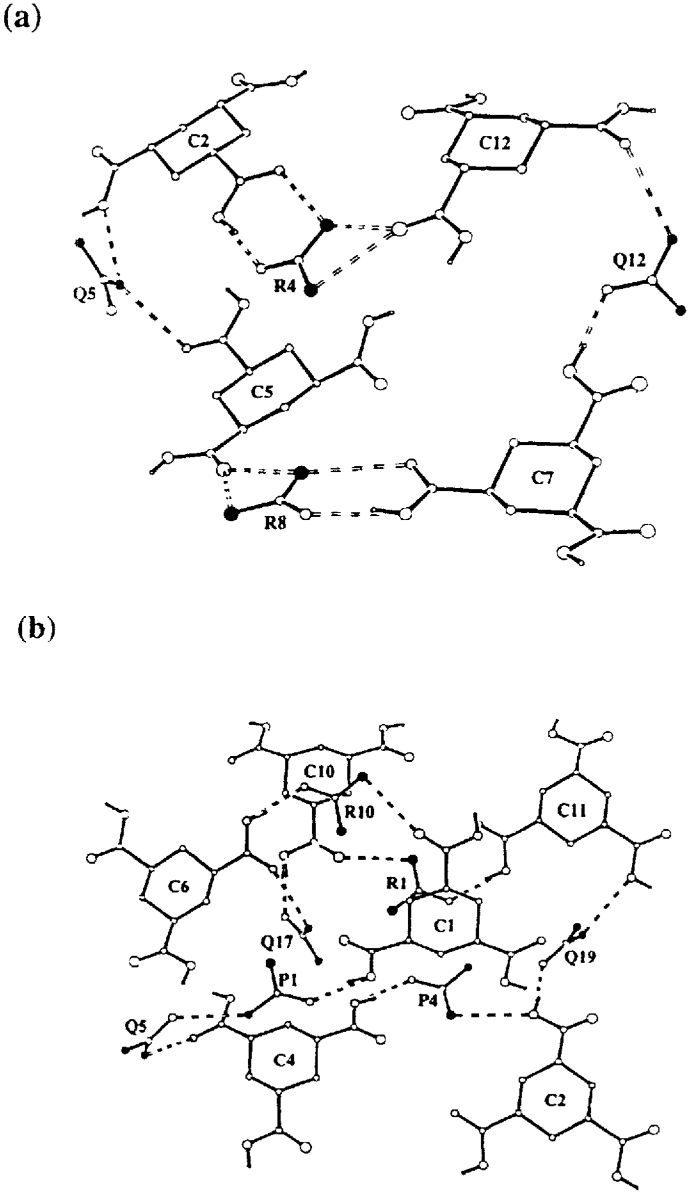

FIGURE 4 (a) An undirected fundamental H-bonded 8-cycle and (b) a directed H-bonded 13-cycle (showing only one H-bond where multiple ones exist) in the CHTCA-urea crystal. H-bonds are shown as broken lines; all H atoms except those on the carboxylic acid groups are omitted for clarity; N atoms are shown as filled circles weighted (by the cycle size) sum of cycles in each graph. The weighted cycle sum is found to be a convenient measure of the complexity of such networks. The number of directed cycles in the graph with the maximum cycle formation is listed in Table V.

TABLE IV List of symmetry operations used in generating two shells of H-bonded molecules around the asymmetric unit (the prime represents the inverse of an operation)

Number	*Symmetry operation*
1	[x, y, z]
2 ≡ 11′	[-x+5/2, y-1/2, -z+1/2]
3	[-x+3, -y+1, -z+1]
4	[-x+2, -y, -z+1]
5	[-x+5/2, y-1/2, -z+3/2]
6	[x-1/2, -y+1/2, z+1/2]
7 ≡ 7′	[-x+3, -y, -z+1]
8	[x+1/2, -y+1/2, z+1/2]
9	[x+1, y, z]
10 ≡ 10′	[-x+2, -y+1,-z+1]
11	[-x+5/2, y+1/2, -z+1/2]
12	[x, y-1, z]
13	[-x+7/2, y-1/2, -z+3/2]
14	[-x+7/2, y-1/2, -z+1/2]
15	[-x+4, -y+1, -z+1]
16	[x-1/2, -y+3/2, z+1/2]
17 ≡ 9′	[x-1, y, z]
18	[x-1/2, -y+3/2, z-1/2]
19 ≡ 8′	[x-1/2, -y+1/2, z-1/2]
20	[x, y+1, z]
21	[x-1/2, -y-1/2, z+1/2]
22	[-x+3/2, y-1/2, -z+3/2]
23	[x+1/2, -y-1/2, z-1/2]
24 ≡ 6′	[x+1/2, -y+1/2, z-1/2]

This analysis allows further, the selection and visualization of cycles in the H-bond network. Our computer program provides a listing of the vertices that constitute the directed cycles. These are used to locate the molecules in the crystal that form the macrocyclic structures. Selected macrocyclic motifs extracted from the CHTCA-urea structure are shown in Fig. 4. Fig. 4a shows an 8-cycle, one of the fundamental cycles in the cluster. The graph set notation[1,4] for this cycle is $R_{12}^{10}(42)$. Being one of the fundamental cycles there are no cross connections between the molecules forming this cycle. One of the largest directed macrocycles in the cluster $(R_{15}^{13}(58))$ is shown in Fig. 4b. These cyclic structures amply illustrate the complexity of the lattice structure in CHTCA-urea. Just as ring perception algorithms based on graph theoretical principles are useful in computer-aided organic synthetic schemes,[13a] the methodology presented in this paper for the visualization of supramolecular fragments in extended lattices should prove useful in the design and construction of molecular crystal architectures.[14]

TABLE V One set of undirected fundamental cycles and directed cycles of different sizes in the H-bond cluster graph in Fig. 3

Cycle size	*No. of undirected fundamental cycles*[a]	*No. of directed cycles*[b]
3	4	0
4	15	7
5	2	2
6	2	4
7	1	5
8	1	5
9	0	4
10	0	5
11	0	3
12	0	3
13	0	1

a. The total number is equal to the cyclomatic number.
b. The weighted cycle sum (see text for definition) is 305.

CONCLUSION

The CHTCA-urea complex provides an interesting case study of a complex H-bond network leading to potentially useful channel structures. The highly unsymmetric architecture allowed us to demonstrate the protocol we have developed for a systematic visualization of complex networks. The methodology developed here should prove to be of general utility in analyzing intermolecular interaction pathways which have strong implications in materials chemistry and biology.

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SUPPLEMENTARY INFORMATION AVAILABLE

Listing of crystallographic data, computational details (??? pages).

X-ray structure determination

X-ray diffraction data were collected on an Enraf-Nonius MACH3 diffractometer. MoK_{α} radiation with a graphite crystal monochromator in the incident beam was used. Data was reduced using Xtal3.4 (Eds., Hall, S.R; King, G.S.D.; Stewart, J.M. *Xtal 3.4*, University of Western Australia, 1995); Lorentz and polarization corrections were included. All non-hydrogen atoms were found using the direct method analysis in SHELX-97 (Sheldrick, G.M. *SHELX-97*; University of Göttingen, 1997) and after several cycles of refinement the positions of the hydrogen atoms were calculated and added to the refinement process. The detailed data are provided in Tables I–VI below.

Molecular structure of the 1:3 CHTCA-Urea cocrystal from single crystal x-ray analysis

10% thermal ellipsoids are shown

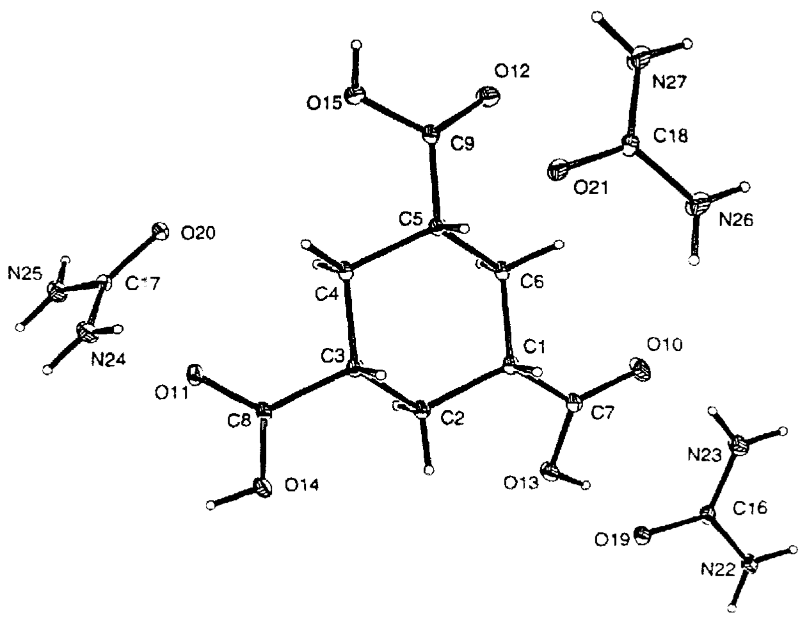

TABLE I Crystal data and structure refinement for CHTCA-Urea

Compound name	*cis,cis-1,3,5-cyclohexane- tricarboxylic acid – urea (1:3)*
Empirical formula	$C_{12}H_{24}N_6O_9$
Formula weight	396.37
Temperature (K)	293(2) K
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	$P2_1/n$
a (Å)	12.232(10)
b (Å)	12.2555(10)
c (Å)	13.080(9)
α (°)	90
β (°)	107.05(8)
γ (°)	90
V (Å^3)	1875(2)
Z	4
ρ (gm cm^{-3})	1.404
μ (cm^{-1})	1.20
F(000)	840
Crystal size	0.64 × 0.40 × 0.36 mm
Number of unique reflections	4291
Number of reflections with $I > 2\sigma_I$	2666
Number of parameters	244
Goodness-of-fit	1.060
R (for data with $I > 2\sigma_I$)	0.0455
wR^2 (for data with $I > 2\sigma_I$)	0.1017
R (for all data)	0.0825
wR^2 (for all data)	0.1251

TABLE II Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for CHTCA-Urea. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor

	x	*y*	*z*	U_{eq}
O(10)	10537(2)	1257(1)	6119(2)	83(1)
O(11)	14241(1)	1461(1)	2712(1)	55(1)
O(12)	11970(2)	4883(1)	5136(2)	85(1)
O(13)	11613(1)	−104(1)	5922(1)	64(1)

	x	y	z	U_{eq}
O(14)	13928(1)	−45(1)	3509(1)	63(1)
O(15)	13013(2)	4911(1)	4039(1)	67(1)
O(19)	11098(1)	−1195(1)	7336(1)	55(1)
O(20)	16483(1)	3130(1)	5346(2)	67(1)
O(21)	9539(1)	3981(1)	2138(1)	53(1)
N(22)	10162(2)	−1750(2)	8467(1)	57(1)
N(23)	10104(2)	47(2)	7969(2)	69(1)
N(24)	16699(2)	1831(2)	4224(2)	66(1)
N(25)	18175(2)	2274(2)	5667(2)	66(1)
N(26)	8482(2)	3548(2)	3214(2)	77(1)
N(27)	9141(2)	5277(2)	3183(2)	74(1)
C(1)	11508(2)	1426(2)	4787(2)	41(1)
C(2)	12480(2)	872(2)	4480(2)	43(1)
C(3)	12766(2)	1487(2)	3574(2)	39(1)
C(4)	13038(2)	2683(2)	3847(2)	42(1)
C(5)	12084(2)	3242(2)	4190(2)	42(1)
C(6)	11768(2)	2622(2)	5074(2)	43(1)
C(7)	11175(2)	860(2)	5675(2)	46(1)
C(8)	13719(2)	965(2)	3226(2)	40(1)
C(9)	12347(2)	4413(2)	4511(2)	47(1)
C(16)	10474(2)	−967(2)	7914(2)	47(1)
C(17)	17100(2)	2429(2)	5096(2)	50(1)
C(18)	9074(2)	4263(2)	2828(2)	49(1)

TABLE III Bond lengths (Å) and angles (°) for CHTCA-Urea

Bond	*Bond length*
O(10)-C(7)	1.203(2)
O(11)-C(8)	1.216(2)
O(12)-C(9)	1.197(2)
O(13)-C(7)	1.298(2)
O(14)-C(8)	1.297(2)
O(15)-C(9)	1.308(2)
O(19)-C(16)	1.253(2)
O(20)-C(17)	1.248(2)
O(21)-C(18)	1.249(2)

N(22)-C(16)	1.324(3)
N(23)-C(16)	1.331(3)
N(24)-C(17)	1.323(3)
N(25)-C(17)	1.323(3)
N(26)-C(18)	1.327(3)
N(27)-C(18)	1.320(3)
C(1)-C(7)	1.509(3)
C(1)-C(2)	1.522(3)
C(1)-C(6)	1.522(3)
C(2)-C(3)	1.529(3)
C(3)-C(8)	1.512(3)
C(3)-C(4)	1.522(3)
C(4)-C(5)	1.529(3)
C(5)-C(9)	1.503(3)
C(5)-C(6)	1.526(3)
Bond-bond	*Angle*
C(7)-C(1)-C(2)	113.94(17)
C(7)-C(1)-C(6)	109.68(15)
C(2)-C(1)-C(6)	111.85(15)
C(1)-C(2)-C(3)	110.99(16)
C(8)-C(3)-C(4)	110.10(15)
C(8)-C(3)-C(2)	113.39(16)
C(4)-C(3)-C(2)	112.15(15)
C(3)-C(4)-C(5)	111.61(15)
C(9)-C(5)-C(6)	110.19(15)
C(9)-C(5)-C(4)	113.03(16)
C(6)-C(5)-C(4)	112.53(16)
C(1)-C(6)-C(5)	111.94(15)
O(10)-C(7)-O(13)	121.80(18)
O(10)-C(7)-C(1)	123.00(19)
O(13)-C(7)-C(1)	115.19(16)
O(11)-C(8)-O(14)	122.90(17)
O(11)-C(8)-C(3)	122.08(17)
O(14)-C(8)-C(3)	115.02(16)
O(12)-C(9)-O(15)	121.05(19)
O(12)-C(9)-C(5)	123.77(18)
O(15)-C(9)-C(5)	115.18(16)

O(19)-C(16)-N(22)	119.49(19)
O(19)-C(16)-N(23)	121.11(19)
N(22)-C(16)-N(23)	119.39(19)
O(20)-C(17)-N(24)	120.5(2)
O(20)-C(17)-N(25)	121.9(2)
N(24)-C(17)-N(25)	117.6(2)
O(21)-C(18))-N(27)	121.32(18)
O(21)-C(18)-N(26)	120.5(2)
N(27)-C(18)-N(26)	118.19(19)

TABLE IV Anisotropic displacement parameters ($Å^2 \times 10^3$) for CHTCA-Urea. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(10)	108(1)	68(1)	110(1)	28(1)	87(1)	35(1)
O(11)	63(1)	49(1)	68(1)	9(1)	44(1)	9(1)
O(12)	132(2)	44(1)	121(2)	−17(1)	102(1)	−11(1)
O(13)	88(1)	45(1)	83(1)	13(1)	64(1)	13(1)
O(14)	83(1)	45(1)	86(1)	12(1)	61(1)	18(1)
O(15)	98(1)	39(1)	91(1)	−11(1)	70(1)	−10(1)
O(19)	64(1)	48(1)	66(1)	6(1)	42(1)	4(1)
O(20)	70(1)	41(1)	112(1)	−16(1)	62(1)	−3(1)
O(21)	66(1)	50(1)	58(1)	−3(1)	39(1)	−10(1)
N(22)	63(1)	61(1)	59(1)	10(1)	38(1)	7(1)
N(23)	90(2)	57(1)	80(1)	3(1)	55(1)	12(1)
N(24)	62(1)	60(1)	77(1)	−18(1)	24(1)	9(1)
N(25)	63(1)	62(1)	75(1)	−20(1)	26(1)	2(1)
N(26)	110(2)	54(1)	98(2)	−5(1)	81(1)	17(1)
N(27)	104(2)	53(1)	95(2)	−14(1)	76(1)	−18(1)
C(1)	42(1)	40(1)	47(1)	−1(1)	23(1)	0(1)
C(2)	49(1)	38(1)	50(1)	0(1)	28(1)	2(1)
C(3)	41(1)	40(1)	40(1)	−2(1)	19(1)	2(1)
C(4)	50(1)	39(1)	45(1)	−2(1)	28(1)	0(1)
C(5)	48(1)	37(1)	46(1)	−1(1)	23(1)	3(1)
C(6)	47(1)	40(1)	50(1)	−3(1)	29(1)	0(1)
C(7)	47(1)	41(1)	59(1)	−2(1)	30(1)	1(1)
C(8)	48(1)	39(1)	40(1)	−2(1)	22(1)	2(1)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(9)	58(1)	39(1)	55(1)	4(1)	34(1)	6(1)
C(16)	49(1)	52(1)	46(1)	−2(1)	22(1)	−2(1)
C(17)	58(1)	35(1)	72(1)	−4(1)	43(1)	−4(1)
C(18)	52(1)	50(1)	54(1)	4(1)	31(1)	−2(1)

TABLE V Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for CHTCA-Urea

	x	y	z	U_{eq}
H(13)	11399	−355	6413	95
H(14)	14458	−268	3300	95
H(15)	13121	5541	4257	101
H(22A)	10387	−2410	8428	68
H(22B)	9733	−1600	8866	68
H(23A)	10293	559	7603	83
H(23B)	9677	191	8369	83
H(24A)	16009	1923	3825	79
H(24B)	17128	1349	4057	79
H(25A)	18469	2661	6229	79
H(25B)	18581	1785	5477	79
H(26A)	8417	2885	2989	92
H(26B)	8164	3747	3689	92
H(27A)	9510	5758	2938	89
H(27B)	8815	5455	3659	89
H(1)	10837	1408	4154	49
H(2A)	12262	129	4255	51
H(2B)	13152	843	5098	51
H(3)	12080	1468	2957	47
H(4A)	13140	3055	3227	50
H(4B)	13748	2736	4421	50
H(5)	11404	3244	3565	50
H(6A)	12395	2669	5729	51
H(6B)	11103	2960	5202	51

TABLE VI The H-bonds in and around the asymmetric unit of CHTCA-urea cocrystal. D and A represent the H-bond donor and acceptor atoms, $d_{H...A}$ the H...A distance and $\theta_{D-H...A}$ the D-H...A angle

D-H	$d_{H...A}$ (Å)	$\theta_{D-H...A}$ (°)	*A*	*Symmetry operation on A*
O13-H13	1.708	164.56	O19	[x, y, z]
O14-H14	1.759	167.88	O21	[-x+5/2, y-1/2, -z+1/2]
O15-H15	1.735	171.95	O20	[-x+3, -y+1, -z+1]
N22-H22A	2.076	160.46	O21	[-x+2, -y, -z+1]
N22-H22B	2.071	157.09	O20	[-x+5/2, y-1/2, -z+3/2]
N23-H23A	2.222	153.28	O10	[x, y, x]
N23-H23B	2.443	157.92	O15	[x-1/2, -y+1/2, z+1/2]
N24-H24A	2.295	157.91	O11	[x, y, z]
N24-H24B	2.162	165.21	O13	[-x+3, -y, -z+1]
N25-H25A	2.175	176.08	O11	[x+1/2, -y+1/2, z+1/2]
N25-H25B	2.378	134.02	O10	[x+1, y, z]
N26-H26A	2.230	159.98	O19	[-x+2, -y, -z+1]
N26-H26B	2.312	145.26	O12	[-x+2, -y+1, -z+1]
N27-H27A	2.137	159.99	O11	[-x+5/2, y+1/2, -z+1/2]
N27-H27B	2.112	153.92	O12	[-x+2, -y+1, -z+1]

TABLE VII List of symmetry transformations used in generating the H-bond shells around the asymmetric unit (the prime represents the inverse of an operation)

Number	*Symmetry operation*
1	[x, y, z]
2 ≡ 11'	[-x+5/2, y-1/2, -z+1/2]
3	[-x+3, -y+1, -z+1]
4	[-x+2, -y, -z+1]
5	[-x+5/2, y-1/2, -z+3/2]
6	[x-1/2, -y+1/2, z+1/2]
7 ≡ 7'	[-x+3, -y, -z+1]
8	[x+1/2, -y+1/2, z+1/2]
9	[x+1, y, z]
10 ≡ 10'	[-x+2, -y+1, -z+1]
11	[-x+5/2, y+1/2, -z+1/2]
12	[x, y-1, z]
13	[-x+7/2, y-1/2, -z+3/2]
14	[-x+7/2, y-1/2, -z+1/2]

Number	*Symmetry operation*
15	[-x+4, -y+1, -z+1]
16	[x-1/2, -y+3/2, z+1/2]
17 ≡ 9′	[x-1, y, z]
18	[x-1/2, -y+3/2, z-1/2]
19 ≡ 8′	[x-1/2, -y+1/2, z-1/2]
20	[x, y+1, z]
21	[x-1/2, -y-1/2, z+1/2]
22	[-x+3/2, y-1/2, -z+3/2]
23	[x+1/2, -y-1/2, z-1/2]
24 ≡ 6′	[x+1/2, -y+1/2, z-1/2]

Enumeration of fundamental cycles

A number of algorithms are available in the literature to enumerate fundamental cycles or chemically relevant Smallest Set of Smallest Rings (SSSR) of graphs. Some relevant references are the following.

1. E.J. Corey and G.A. Petersson, *J. Am. Chem. Soc.*, 1972, **94**, 460
2. B. Schmidt and J. Fleischhauer, *J. Chem. Inf. Comp. Sci.*, 1978, **18**, 204
3. J. Gasteiger and C. Jochum, *J. Chem. Inf. Comp. Sci.*, 1979, **19**, 43
4. B.L. Roos-Kozel and W.L. Jorgensen, *J. Chem. Inf. Comp. Sci.*, 1981, **21**, 101
5. L. Matsyka, *J. Comp. Chem.*, 1988, **9**, 455

In the case of the undirected version of the graph in Fig. 3, we have enumerated one set of fundamental cycles by inspection. The graph has 42 vertices and 66 edges. Hence there are 25 fundamental cycles. One set that is easily observed from the graph is the following.

3-cycles [4]
(C8-P9-Q13), (P1-Q5-C6), (C2-P4-Q19), (P10-C11-Q18)
4-cycles [15]
(Q1-C7-Q13-C8), (Q1-C8-R3-C9), (R3-C8-P9-C9), (C5-R8-C7-Q13), (C1-Q1-C3-Q3), (Q1-C3-Q15-C9), (C1-P1-C6-R10), (C1-R10-C6-Q17), (P1-R4-C21-Q5), (C4-Q5-C6-Q17), (R1-P4-Q19-C11), (R1-C10-P10-C11), (C1-R2-C24-Q19), (C1-Q3-C10-Q17), (Q3-C10-P10-C11)
5-cycles [2]
(R1-P4-C4-Q17-C10), (Q3-C10-P10-Q18-P20)
6-cycle [2]
(C1-P1-R4-C12-P23-R2), (C1-P1-Q5-C4-P4-Q19)

7-cycle [1]
(C1-Q1-C7-Q12-C12-P23-R2)
8-cycle [1]
(R4-C12-Q12-C7-R8-C5-Q5-C21) – Cycle shown in **Fig. 4a**

Algorithm and FORTRAN programme for the generation of the loop edge permutations and enumeration of directed cycles

1. The number of vertices, loop edges and normal edges is read in. Adjacency matrix is generated.
2. Permutations of the 10 loop edges are considered in five "DO LOOPS".
3. In each case, the adjacency matrix is modified correspondingly and the subroutine "CYCLED" is called to enumerate the directed cycles.
4. CYCLED enumerates the directed cycles by adjacency matrix multiplication carried out together with explicit tracking of the vertices passed *en route*. The FORTRAN code, called PERMHC used for this is given below.
5. The calculation was carried out on a Pentium III (450 MHz, 128 MB RAM) machine. The enumeration for the 1024 graphs takes approximately 1 min. 20 sec. of CPU time.

For the graph in Fig. 3 of the manuscript, the graph is initially pruned to get rid of vertices which do not contribute to any directed cycle. These vertices are: C5, C7, C12, C20, C22, C24, P6, P7, P8, P11, P23, Q12, Q13, Q18, R2, R8, R14 and R16. The pruned graph has 24 vertices, 10 loop edges and 29 simple edges.

```
C      PERMHC.FOR (T.P.Radhakrishnan, Feb. 14, 2000)
C PERMUTES LOOP EDGES AND ENUMERATES THE NUMBER OF DIRECTED
C CYCLES IN EACH DIGRAPH
C
C        WEIGHTED CYCLE SUM = SIGMA(CYCLE SIZE * NO. OF CYCLES)
C
C This version is specifically for a graph with 24 vertices and
C 10 loops in it - relevant to the CHTA-Urea complex - in the
C pruned state
C It picks also the digraphs having maximum iwsum value
C
C N = NO. VERTICES; NLOOP = NO. OF LOOPED EDGES;  NSTR = NO. OF
C DIRECTED UNLOOPED EDGES
C
        implicit real*8 (a-h,o-z)
      DIMENSION NS(40),NE(40),NS1(40),NE1(40),NCYCL(25),NC(1024,25)
      DIMENSION IWSUM(1024),IR(1024,10),IM(1024)
      OPEN(5,FILE='PERMHC.DAT',STATUS='OLD')
      OPEN(6,FILE='PERMHC.OUT',STATUS='UNKNOWN')
      READ (5,*) N,NLOOP,NSTR
      READ (5,*) (NS(I),NE(I),I=1,NLOOP)
```

```
      READ (5,*) (NS(I),NE(I),I=NLOOP+1,NLOOP+NSTR)
      M=NLOOP+NSTR
      DO 5 I=1,NLOOP
      NS1(I)=NS(I)
      NE1(I)=NE(I)
5     CONTINUE
      DO 6 I=1,1024
      DO 6 J=1,NLOOP
      IR(I,J)=0
6     CONTINUE
C
      NG=1
      CALL CYCLED(N,M,NS,NE,NCYCL)
      ISUM=0
      DO 8 K=1,N
      ISUM=K*NCYCL(K)+ISUM
      NC(NG,K)=NCYCL(K)
8     CONTINUE
      IWSUM(NG)=ISUM
      FLAG=0
      WRITE (6,200)
     $NG,(NC(NG,K),K=3,14),IWSUM(NG),(IR(NG,K),K=1,NLOOP)
      WRITE (*,200)
     $NG,(NC(NG,K),K=3,14),IWSUM(NG),(IR(NG,K),K=1,NLOOP)
9     DO 10 I1=1,NLOOP
      NG=NG+1
      K=0
      DO 12 I=1,NLOOP
          IF (FLAG.EQ.0.AND.I.NE.I1) GO TO 12
          IF (FLAG.EQ.1.AND.I.EQ.I1) GO TO 12
                K=K+1
                IR(NG,K)=I
             NS(I)=NE1(I)
             NE(I)=NS1(I)
12    CONTINUE
      CALL CYCLED(N,M,NS,NE,NCYCL)
      ISUM=0
      DO 13 K=1,N
      ISUM=K*NCYCL(K)+ISUM
      NC(NG,K)=NCYCL(K)
13    CONTINUE
      IWSUM(NG)=ISUM
      WRITE (6,200)
     $NG,(NC(NG,K),K=3,14),IWSUM(NG),(IR(NG,K),K=1,NLOOP)
      WRITE (*,200)
     $NG,(NC(NG,K),K=3,14),IWSUM(NG),(IR(NG,K),K=1,NLOOP)
      DO 14 I=1,NLOOP
          IF (FLAG.EQ.0.AND.I.NE.I1) GO TO 14
          IF (FLAG.EQ.1.AND.I.EQ.I1) GO TO 14
```

```
              NS(I)=NS1(I)
              NE(I)=NE1(I)
14    CONTINUE
10    CONTINUE
C
      DO 20 I1=1,NLOOP-1
      DO 20 I2=I1+1,NLOOP
      NG=NG+1
      K=0
      DO 22 I=1,NLOOP
          IF (FLAG.EQ.0.AND.(I.NE.I1.AND.I.NE.I2)) GO TO 22
          IF (FLAG.EQ.1.AND.(I.EQ.I1.OR.I.EQ.I2)) GO TO 22
                 K=K+1
                 IR(NG,K)=I
              NS(I)=NE1(I)
              NE(I)=NS1(I)
22    CONTINUE
      CALL CYCLED(N,M,NS,NE,NCYCL)
      ISUM=0
      DO 23 K=1,N
      ISUM=K*NCYCL(K)+ISUM
      NC(NG,K)=NCYCL(K)
23    CONTINUE
      IWSUM(NG)=ISUM
      WRITE (6,200)
     $NG,(NC(NG,K),K=3,14),IWSUM(NG),(IR(NG,K),K=1,NLOOP)
      WRITE (*,200)
     $NG,(NC(NG,K),K=3,14),IWSUM(NG),(IR(NG,K),K=1,NLOOP)
      DO 24 I=1,NLOOP
          IF (FLAG.EQ.0.AND.(I.NE.I1.AND.I.NE.I2)) GO TO 24
          IF (FLAG.EQ.1.AND.(I.EQ.I1.OR.I.EQ.I2)) GO TO 24
              NS(I)=NS1(I)
              NE(I)=NE1(I)
24    CONTINUE
20    CONTINUE
C
      DO 30 I1=1,NLOOP-2
      DO 30 I2=I1+1,NLOOP-1
      DO 30 I3=I2+1,NLOOP
      NG=NG+1
      K=0
      DO 32 I=1,NLOOP
          IF (FLAG.EQ.0.AND.(I.NE.I1.AND.I.NE.I2.AND.I.NE.I3)) GO TO
32
          IF (FLAG.EQ.1.AND.(I.EQ.I1.OR.I.EQ.I2.OR.I.EQ.I3)) GO TO 32
                 K=K+1
                 IR(NG,K)=I
              NS(I)=NE1(I)
              NE(I)=NS1(I)
```

```
32      CONTINUE
        CALL CYCLED(N,M,NS,NE,NCYCL)
        ISUM=0
        DO 33 K=1,N
        ISUM=K*NCYCL(K)+ISUM
        NC(NG,K)=NCYCL(K)
33      CONTINUE
        IWSUM(NG)=ISUM
        WRITE (6,200)
       $NG,(NC(NG,K),K=3,14),IWSUM(NG),(IR(NG,K),K=1,NLOOP)
        WRITE (*,200)
       $NG,(NC(NG,K),K=3,14),IWSUM(NG),(IR(NG,K),K=1,NLOOP)
        DO 34 I=1,NLOOP
            IF (FLAG.EQ.0.AND.(I.NE.I1.AND.I.NE.I2.AND.I.NE.I3)) GO TO
34
            IF (FLAG.EQ.1.AND.(I.EQ.I1.OR.I.EQ.I2.OR.I.EQ.I3)) GO TO 34
                NS(I)=NS1(I)
                NE(I)=NE1(I)
34      CONTINUE
30      CONTINUE
C
        DO 40 I1=1,NLOOP-3
        DO 40 I2=I1+1,NLOOP-2
        DO 40 I3=I2+1,NLOOP-1
        DO 40 I4=I3+1,NLOOP
        NG=NG+1
        K=0
        DO 42 I=1,NLOOP
            IF (FLAG.EQ.0.AND.(I.NE.I1.AND.I.NE.I2.AND.I.NE.I3.
       $AND.I.NE.I4)) GO TO 42
            IF (FLAG.EQ.1.AND.(I.EQ.I1.OR.I.EQ.I2.OR.I.EQ.I3.
       $OR.I.EQ.I4)) GO TO 42
                    K=K+1
                    IR(NG,K)=I
                NS(I)=NE1(I)
                NE(I)=NS1(I)
42      CONTINUE
        CALL CYCLED(N,M,NS,NE,NCYCL)
        ISUM=0
        DO 43 K=1,N
        ISUM=K*NCYCL(K)+ISUM
        NC(NG,K)=NCYCL(K)
43      CONTINUE
        IWSUM(NG)=ISUM
         WRITE (6,200)
       $NG,(NC(NG,K),K=3,14),IWSUM(NG),(IR(NG,K),K=1,NLOOP)
        WRITE (*,200)
       $NG,(NC(NG,K),K=3,14),IWSUM(NG),(IR(NG,K),K=1,NLOOP)
        DO 44 I=1,NLOOP
```

```
          IF (FLAG.EQ.0.AND.(I.NE.I1.AND.I.NE.I2.AND.I.NE.I3.
     $AND.I.NE.I4)) GO TO 44
          IF (FLAG.EQ.1.AND.(I.EQ.I1.OR.I.EQ.I2.OR.I.EQ.I3.
     $OR.I.EQ.I4)) GO TO 44
              NS(I)=NS1(I)
              NE(I)=NE1(I)
44     CONTINUE
40     CONTINUE
       IF (FLAG.EQ.1) GO TO 100
C
       DO 50 I1=1,NLOOP-4
       DO 50 I2=I1+1,NLOOP-3
       DO 50 I3=I2+1,NLOOP-2
       DO 50 I4=I3+1,NLOOP-1
       DO 50 I5=I4+1,NLOOP
       NG=NG+1
       K=0
       DO 52 I=1,NLOOP
          IF (FLAG.EQ.0.AND.(I.NE.I1.AND.I.NE.I2.AND.I.NE.I3.
     $AND.I.NE.I4.AND.I.NE.I5)) GO TO 52
          IF (FLAG.EQ.1.AND.(I.EQ.I1.OR.I.EQ.I2.OR.I.EQ.I3.
     $OR.I.EQ.I4.OR.I.EQ.I5)) GO TO 52
                  K=K+1
                  IR(NG,K)=I
              NS(I)=NE1(I)
              NE(I)=NS1(I)
52     CONTINUE
       CALL CYCLED(N,M,NS,NE,NCYCL)
       ISUM=0
       DO 53 K=1,N
       ISUM=K*NCYCL(K)+ISUM
       NC(NG,K)=NCYCL(K)
53     CONTINUE
       IWSUM(NG)=ISUM
        WRITE (6,200)
     $NG,(NC(NG,K),K=3,14),IWSUM(NG),(IR(NG,K),K=1,NLOOP)
        WRITE (*,200)
     $NG,(NC(NG,K),K=3,14),IWSUM(NG),(IR(NG,K),K=1,NLOOP)
       DO 54 I=1,NLOOP
          IF (FLAG.EQ.0.AND.(I.NE.I1.AND.I.NE.I2.AND.I.NE.I3.
     $AND.I.NE.I4.AND.I.NE.I5)) GO TO 54
          IF (FLAG.EQ.1.AND.(I.EQ.I1.OR.I.EQ.I2.OR.I.EQ.I3.
     $OR.I.EQ.I4.OR.I.EQ.I5)) GO TO 54
              NS(I)=NS1(I)
              NE(I)=NE1(I)
54     CONTINUE
50     CONTINUE
       FLAG = 1
       GO TO 9
```

```
100   NG=NG+1
      K=0
      DO 92 I=1,NLOOP
                  K=K+1
                  IR(NG,K)=I
              NS(I)=NE1(I)
              NE(I)=NS1(I)
92    CONTINUE
      CALL CYCLED(N,M,NS,NE,NCYCL)
      ISUM=0
      DO 93 K=1,N
      ISUM=K*NCYCL(K)+ISUM
      NC(NG,K)=NCYCL(K)
93    CONTINUE
      IWSUM(NG)=ISUM
       WRITE (6,200)
     $NG,(NC(NG,K),K=3,14),IWSUM(NG),(IR(NG,K),K=1,NLOOP)
       WRITE (*,200)
     $NG,(NC(NG,K),K=3,14),IWSUM(NG),(IR(NG,K),K=1,NLOOP)
      DO 94 I=1,NLOOP
              NS(I)=NS1(I)
              NE(I)=NE1(I)
94    CONTINUE
      IMAX=1
      NG1=0
      DO 101 I=1,NG
      IF (IWSUM(I).LT.IMAX) GO TO 103
      IF (IWSUM(I).GT.IMAX) GO TO 104
      NG1=NG1+1
      IM(NG1)=I
      GO TO 103
104   NG1=1
      IMAX=IWSUM(I)
      IM(NG1)=I
103   DO 102 J=15,35
      IF (NC(I,J).EQ.0) GO TO 101
      WRITE (6,201) NG
102   CONTINUE
101   CONTINUE
200   FORMAT (I6,12(I2),I6,10I3)
201   FORMAT (38H CYCLE GREATER THAN 14 FOUND FOR GRAPH,I5)
      WRITE (6,202) IMAX,(IM(I),I=1,NG1)
202   FORMAT (' LARGEST IWSUM =',I5,/'   FOR DIGRAPHS,',5I10)
      STOP
      END
C
      SUBROUTINE CYCLED(N,M,NS,NE,ICYCLE)
C
C     THIS PROGRAM ENUMERATES THE NUMBER OF CYCLES IN A DIRECTED GRAPH
```

```
C      (PATHS ARE ALSO CALCULATED, BUT NOT WRITTEN)
C
C    N=NO. OF VERTICES, M=NO. OF EDGES, NS(I) : START OF Ith EDGE,
C        NE(I) : END OF Ith EDGE
C
C      IP1(I,J,J1,J2), IP2(I,J,J1,J2) :: I,J = START AND END OF PATH;
C      J1 = NO. OF THE IJ PATH (THERE MAY BE SEVERAL);  J2 = VERTEX
C        ALONG THE IJ PATH
C      IPC(L,I,J1,J2)   :: L = PATH LENGTH, I = CYCLE ROOT
C
C      DIMENSIONED FOR 25 VERTICES AND 40 EDGES
C
       DIMENSION NS(40),NE(40),IA(25,25,25),IP1(25,25,500,25)
       DIMENSION IP2(25,25,500,25),IPC(25,25,500,25)
       DIMENSION IC(25,25),ICYCLE(25),IJMAX(25,25)
C
       DO 100 I=1,N
       DO 100 J=1,N
       DO 101 K=1,M
       IF (NS(K).EQ.I.AND.NE(K).EQ.J) GO TO 110
101    CONTINUE
       IA(1,I,J)=0
       GO TO 100
110    IA(1,I,J)=1
100    CONTINUE
C
       DO 152 I=1,N
       DO 152 J=1,N
       IA(2,I,J)=0
       IF (I.EQ.J) GO TO 152
       IJ=0
       DO 151 K=1,N
       IF (IA(1,I,K).EQ.0.OR.IA(1,K,J).EQ.0) GO TO 151
       IA(2,I,J)=IA(2,I,J)+IA(1,I,K)*IA(1,K,J)
       IJ=IJ+1
       IP2(I,J,IJ,1)=K
151    CONTINUE
152    CONTINUE
       DO 200 L=3,N
       do 800 i=1,n
       do 800 j=1,n
       ipath=ia(l-1,i,j)
       do 800 j1=1,ipath
       do 800 j2=1,l-2
       ip1(i,j,j1,j2)=ip2(i,j,j1,j2)
800    continue
       DO 202 I=1,N
       DO 202 J=1,N
       IA(L,I,J)=0
```

```
      IJ=0
      DO 201 K=1,N
      IF (IA(L-1,I,K).EQ.0.OR.IA(1,K,J).EQ.0) GO TO 201
       IPATH=IA(L-1,I,K)
      DO 207 J1=1,IPATH
      DO 203 J2=1,L-2
      IF (J1.EQ.IPATH.AND.J.EQ.IP1(I,K,J1,J2)) GO TO 201
      IF (J.EQ.IP1(I,K,J1,J2)) GO TO 207
203   CONTINUE
      IJ=IJ+1
      IP2(I,J,IJ,L-1)=K
      DO 205 J2=1,L-2
      IP2(I,J,IJ,J2)=IP1(I,K,J1,J2)
205   CONTINUE
209      IA(L,I,J)=IA(L,I,J)+1
207   CONTINUE
201   CONTINUE
       IF (I.NE.J) GO TO 202
      IJMAX(L,I)=IJ
      do 801 j1=1,ij
      do 801 j2=1,l-1
      ipc(l,i,j1,j2)=ip2(i,j,j1,j2)
801   continue
202   CONTINUE
      SUM=0
       DO 206 I=1,N
      IC(L,I)=IA(L,I,I)
      IA(L,I,I)=0
      IF (IC(L,I).EQ.0) GO TO 206
       SUM=IC(L,I)+SUM
206   CONTINUE
      ICYCLE(L)=SUM/L
200   CONTINUE
       RETURN
      END
```

Fortran program to enumerate the directed cycles and list the vertices

Fortran program to enumerate the directed cycles and list the vertices

```
C       CYCLE.FOR  (T.P.Radhakrishnan/ Feb. 15, 2000)
C  THIS PROGRAM ENUMERATES THE NUMBER OF CYCLES IN A DIRECTED GRAPH
C  (PATHS ARE ALSO CALCULATED, BUT NOT WRITTEN)
C WRITES OUT THE VERTICES IN THE (IJMAX)CYCLES OF THE LARGEST SIZE
C      ROOTED AT EACH VERTEX.
C   MAY BE MODIFIED TO WRITE OUT THE VERTICES IN EVERY CYCLE
C      N=NO. OF VERTICES, M=NO. OF EDGES, NS(I) : START OF Ith EDGE,
```

```
C         NE(I)  : END OF Ith EDGE
C       IP1(I,J,J1,J2), IP2(I,J,J1,J2) :: I,J = START AND END OF PATH;
C       J1 = NO. OF THE IJ PATH (THERE MAY BE SEVERAL);  J2 = VERTEX
C         ALONG THE IJ PATH
C       IPC(L,I J1,J2)   :: L = PATH LENGTH, I = CYCLE ROOT
C
C       DIMENSIONED FOR 25 VERTICES AND 40 EDGES
C
        DIMENSION NS(40),NE(40),IA(25,25,25),IP1(25,25,500,25)
        DIMENSION IP2(25,25,500,25),IPC(25,25,500,25)
        DIMENSION IC(25,25),ICYCLE(25),IJMAX(25,25)
C
        OPEN(5,FILE='CYCLE.DAT',STATUS='OLD')
        OPEN(6,FILE='CYCLE.OUT',STATUS='UNKNOWN')
        READ (5,*) N,M
        READ (5,*) (NS(I),NE(I),I=1,M)
        DO 100 I=1,N
        DO 100 J=1,N
        DO 101 K=1,M
        IF (NS(K).EQ.I.AND.NE(K).EQ.J) GO TO 110
101     CONTINUE
        IA(1,I,J)=0
        GO TO 100
110     IA(1,I,J)=1
100     CONTINUE
C
        DO 152 I=1,N
        DO 152 J=1,N
        IA(2,I,J)=0
        IF (I.EQ.J) GO TO 152
        IJ=0
        DO 151 K=1,N
        IF (IA(1,I,K).EQ.0.OR.IA(1,K,J).EQ.0) GO TO 151
        IA(2,I,J)=IA(2,I,J)+IA(1,I,K)*IA(1,K,J)
        IJ=IJ+1
        IP2(I,J,IJ,1)=K
151     CONTINUE
152     CONTINUE
C
        DO 200 L=3,N
        WRITE (6,400) L
        do 800 i=1,n
        do 800 j=1,n
        ipath=ia(l-1,i,j)
        do 800 j1=1,ipath
        do 800 j2=1,l-2
        ip1(i,j,j1,j2)=ip2(i,j,j1,j2)
800     continue
        DO 202 I=1,N
```

```
      DO 202 J=1,N
      IA(L,I,J)=0
      IJ=0
      DO 201 K=1,N
      IF (IA(L-1,I,K).EQ.0.OR.IA(1,K,J).EQ.0) GO TO 201
       IPATH=IA(L-1,I,K)
      DO 207 J1=1,IPATH
      DO 203 J2=1,L-2
      IF (J1.EQ.IPATH.AND.J.EQ.IP1(I,K,J1,J2)) GO TO 201
      IF (J.EQ.IP1(I,K,J1,J2)) GO TO 207
203   CONTINUE
      IJ=IJ+1
      IP2(I,J,IJ,L-1)=K
C
      DO 205 J2=1,L-2
      IP2(I,J,IJ,J2)=IP1(I,K,J1,J2)
C        WRITE (7,700) L,I,J,IJ,J2,IP(L,I,J,IJ,J2)
205   CONTINUE
c        WRITE (7,700) L,I,J,IJ,L-1,IP(L,I,J,IJ,L-1)
209      IA(L,I,J)=IA(L,I,J)+1
207   CONTINUE
201   CONTINUE
          write (*,402) l,i,j,ia(l,i,j)
          WRITE (6,401) I,J,IA(L,I,J)
      IF (I.NE.J) GO TO 202
      IJMAX(L,I)=IJ
      do 801 j1=1,ij
      do 801 j2=1,l-1
      ipc(l,i,j1,j2)=ip2(i,j,j1,j2)
801   continue
202   CONTINUE
      SUM=0
      write (*,500) l
      WRITE (6,500) L
      DO 206 I=1,N
      IC(L,I)=IA(L,I,I)
      IA(L,I,I)=0
      IF (IC(L,I).EQ.0) GO TO 206
```

```
      write (*,510) i
      WRITE (6,510) I
      SUM=IC(L,I)+SUM
206   CONTINUE
      ICYCLE(L)=SUM/L
200   CONTINUE
400   FORMAT (I4,7H -PATHS,/18H VERTICES   NUMBER)
401   FORMAT (2I4,3X,I5)
402   format (i3,'-PATH',2i4,3x,i5)
500   FORMAT (12H VERTICES IN,I3,11H -CYCLE ARE)
510   FORMAT (2X,I3)
      WRITE (6,515)
      WRITE (6,520) (L,ICYCLE(L),L=3,N)
515   FORMAT (//15H SIZE    CYCLES)
520   FORMAT (2X,I3,5X,I5)
      DO 600 L=3,N
      IF (ICYCLE(L).EQ.0) GO TO 600
      LMAX=L
600   CONTINUE
601   WRITE (6,603) LMAX
      L1=LMAX-1
      DO 602 I=1,N
      IF (IC(LMAX,I).EQ.0) GO TO 602
      IJM=IJMAX(LMAX,I)
      WRITE (6,604) I,IJM
      WRITE (6,606)
      DO 607 J1=1,IJM
      WRITE (6,605) (IPC(LMAX,I,J1,J2),J2=1,L1)
607   continue
602   CONTINUE
603   FORMAT (///' CYCLE SIZE =',I3)
604   FORMAT (/' VERTEX =',I3,/' NO. OF CYCLES =',I6)
605   FORMAT (8X,35I3)
606   FORMAT ('         VERTICES EN ROUTE')
700     format (6i5)
      STOP
      END
```

TABLE VIII The 2^{10} permutation of the 10 loop edges in the directed graph (Figure 3) after pruning and the number of directed cycles of variou sizes in each digraph

No.	Permutations										Number of Cycles of size												Cycle
											3	4	5	6	7	8	9	10	11	12	13	14	Sum
1	0	0	0	0	0	0	0	0	0	0	0	5	0	2	0	0	0	0	0	0	0	0	32
2	1	0	0	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
3	2	0	0	0	0	0	0	0	0	0	0	5	0	2	0	0	0	0	0	0	0	0	32
4	3	0	0	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
5	4	0	0	0	0	0	0	0	0	0	0	5	0	2	0	0	0	0	0	0	0	0	32
6	5	0	0	0	0	0	0	0	0	0	0	5	1	3	4	3	2	2	0	0	0	0	133
7	6	0	0	0	0	0	0	0	0	0	0	5	0	2	0	0	0	0	0	0	0	0	32
8	7	0	0	0	0	0	0	0	0	0	0	6	0	3	0	1	0	0	0	0	0	0	50
9	8	0	0	0	0	0	0	0	0	0	0	5	0	2	0	0	0	0	0	0	0	0	32
10	9	0	0	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
11	10	0	0	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
12	1	2	0	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
13	1	3	0	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
14	1	4	0	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
15	1	5	0	0	0	0	0	0	0	0	0	4	1	2	2	1	1	1	0	0	0	0	74
16	1	6	0	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
17	1	7	0	0	0	0	0	0	0	0	0	5	0	3	0	1	0	0	0	0	0	0	46
18	1	8	0	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
19	1	9	0	0	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
20	1	10	0	0	0	0	0	0	0	0	0	3	0	2	0	0	0	0	0	0	0	0	24
21	2	3	0	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
22	2	4	0	0	0	0	0	0	0	0	0	6	1	2	0	0	0	0	0	0	0	0	41
23	2	5	0	0	0	0	0	0	0	0	0	5	1	3	4	3	2	2	0	0	0	0	133
24	2	6	0	0	0	0	0	0	0	0	0	5	0	2	0	0	0	0	0	0	0	0	32
25	2	7	0	0	0	0	0	0	0	0	0	6	0	3	0	1	0	0	0	0	0	0	50
26	2	8	0	0	0	0	0	0	0	0	0	5	0	2	0	0	0	0	0	0	0	0	32
27	2	9	0	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
28	2	10	0	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
29	3	4	0	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
30	3	5	0	0	0	0	0	0	0	0	0	4	1	2	4	3	2	1	0	0	0	0	113
31	3	6	0	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
32	3	7	0	0	0	0	0	0	0	0	0	5	0	2	0	0	0	0	0	0	0	0	32
33	3	8	0	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
34	3	9	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
35	3	10	0	0	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
36	4	5	0	0	0	0	0	0	0	0	0	5	1	3	4	3	2	2	0	0	0	0	133
37	4	6	0	0	0	0	0	0	0	0	0	5	0	2	0	0	0	0	0	0	0	0	32
38	4	7	0	0	0	0	0	0	0	0	0	6	0	3	0	1	0	0	0	0	0	0	50
39	4	8	0	0	0	0	0	0	0	0	0	5	0	2	0	0	0	0	0	0	0	0	32
40	4	9	0	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
41	4	10	0	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
42	5	6	0	0	0	0	0	0	0	0	0	5	0	3	3	2	1	1	0	0	0	0	94
43	5	7	0	0	0	0	0	0	0	0	0	6	1	4	5	5	4	5	3	3	1	0	296

44	5	8	0	0	0	0	0	0	0	0	0	5	1	3	4	3	2	2	0	0	0	0	133
45	5	9	0	0	0	0	0	0	0	0	0	4	1	2	4	3	2	2	0	0	0	0	123
46	5	10	0	0	0	0	0	0	0	0	0	4	1	3	4	3	2	2	0	0	0	0	129
47	6	7	0	0	0	0	0	0	0	0	0	7	1	4	1	2	1	0	0	0	0	0	89
48	6	8	0	0	0	0	0	0	0	0	0	5	0	2	0	0	0	0	0	0	0	0	32
49	6	9	0	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
50	6	10	0	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
51	7	8	0	0	0	0	0	0	0	0	0	5	0	3	0	1	0	0	0	0	0	0	46
52	7	9	0	0	0	0	0	0	0	0	0	5	0	2	0	1	0	0	0	0	0	0	40
53	7	10	0	0	0	0	0	0	0	0	0	5	0	3	0	1	0	0	0	0	0	0	46
54	8	9	0	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
55	8	10	0	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
56	9	10	0	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
57	1	2	3	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
58	1	2	4	0	0	0	0	0	0	0	0	5	1	2	0	0	1	0	0	0	0	0	46
59	1	2	5	0	0	0	0	0	0	0	0	4	1	2	2	1	1	1	0	0	0	0	74
60	1	2	6	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
61	1	2	7	0	0	0	0	0	0	0	0	5	0	3	0	1	0	0	0	0	0	0	46
62	1	2	8	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
63	1	2	9	0	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
64	1	2	10	0	0	0	0	0	0	0	0	3	0	2	0	0	0	0	0	0	0	0	24
65	1	3	4	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
66	1	3	5	0	0	0	0	0	0	0	0	4	1	1	2	1	1	1	0	0	0	0	68
67	1	3	6	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
68	1	3	7	0	0	0	0	0	0	0	0	5	0	2	0	0	0	0	0	0	0	0	32
69	1	3	8	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
70	1	3	9	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
71	1	3	10	0	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
72	1	4	5	0	0	0	0	0	0	0	0	4	1	2	2	1	1	1	0	0	0	0	74
73	1	4	6	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
74	1	4	7	0	0	0	0	0	0	0	0	5	0	3	0	1	0	0	0	0	0	0	46
75	1	4	8	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
76	1	4	9	0	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
77	1	4	10	0	0	0	0	0	0	0	0	3	0	2	0	0	0	0	0	0	0	0	24
78	1	5	6	0	0	0	0	0	0	0	0	4	0	2	1	1	1	1	0	0	0	0	62
79	1	5	7	0	0	0	0	0	0	0	0	5	1	3	3	3	3	3	1	1	0	0	168
80	1	5	8	0	0	0	0	0	0	0	0	4	1	2	2	1	1	1	0	0	0	0	74
81	1	5	9	0	0	0	0	0	0	0	0	3	1	1	2	1	1	1	0	0	0	0	64
82	1	5	10	0	0	0	0	0	0	0	0	3	1	2	2	1	1	1	0	0	0	0	70
83	1	6	7	0	0	0	0	0	0	0	0	6	1	4	1	2	1	0	0	0	0	0	85
84	1	6	8	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
85	1	6	9	0	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
86	1	6	10	0	0	0	0	0	0	0	0	3	0	2	0	0	0	0	0	0	0	0	24
87	1	7	8	0	0	0	0	0	0	0	0	4	0	3	0	1	0	0	0	0	0	0	42
88	1	7	9	0	0	0	0	0	0	0	0	4	0	2	0	1	0	0	0	0	0	0	36
89	1	7	10	0	0	0	0	0	0	0	0	4	0	3	0	1	0	0	0	0	0	0	42
90	1	8	9	0	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
91	1	8	10	0	0	0	0	0	0	0	0	3	0	2	0	0	0	0	0	0	0	0	24
92	1	9	10	0	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18

93	2	3	4	0	0	0	0	0	0	0	0	5	1	1	0	0	0	0	0	0	0	0	31
94	2	3	5	0	0	0	0	0	0	0	0	4	1	2	4	3	2	1	0	0	0	0	113
95	2	3	6	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
96	2	3	7	0	0	0	0	0	0	0	0	5	0	2	0	0	0	0	0	0	0	0	32
97	2	3	8	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
98	2	3	9	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
99	2	3	10	0	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
100	2	4	5	0	0	0	0	0	0	0	0	6	2	3	4	3	2	2	0	0	0	0	142
101	2	4	6	0	0	0	0	0	0	0	0	6	1	2	0	0	0	0	0	0	0	0	41
102	2	4	7	0	0	0	0	0	0	0	0	7	1	3	0	1	0	0	0	0	0	0	59
103	2	4	8	0	0	0	0	0	0	0	0	6	1	2	0	0	0	0	0	0	0	0	41
104	2	4	9	0	0	0	0	0	0	0	0	5	1	1	0	0	0	0	0	0	0	0	31
105	2	4	10	0	0	0	0	0	0	0	0	5	1	2	0	0	0	0	0	0	0	0	37
106	2	5	6	0	0	0	0	0	0	0	0	5	0	3	3	2	1	1	0	0	0	0	94
107	2	5	7	0	0	0	0	0	0	0	0	6	1	4	5	5	4	5	3	3	1	0	296
108	2	5	8	0	0	0	0	0	0	0	0	5	1	3	4	3	2	2	0	0	0	0	133
109	2	5	9	0	0	0	0	0	0	0	0	4	1	2	4	3	2	2	0	0	0	0	123
110	2	5	10	0	0	0	0	0	0	0	0	4	1	3	4	3	2	2	0	0	0	0	129
111	2	6	7	0	0	0	0	0	0	0	0	7	1	4	1	2	1	0	0	0	0	0	89
112	2	6	8	0	0	0	0	0	0	0	0	5	0	2	0	0	0	0	0	0	0	0	32
113	2	6	9	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
114	2	6	10	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
115	2	7	8	0	0	0	0	0	0	0	0	5	0	3	0	1	0	0	0	0	0	0	46
116	2	7	9	0	0	0	0	0	0	0	0	5	0	2	0	1	0	0	0	0	0	0	40
117	2	7	10	0	0	0	0	0	0	0	0	5	0	3	0	1	0	0	0	0	0	0	46
118	2	8	9	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
119	2	8	10	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
120	2	9	10	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
121	3	4	5	0	0	0	0	0	0	0	0	4	1	2	4	3	2	1	0	0	0	0	113
122	3	4	6	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
123	3	4	7	0	0	0	0	0	0	0	0	5	0	2	0	0	0	0	0	0	0	0	32
124	3	4	8	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
125	3	4	9	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
126	3	4	10	0	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
127	3	5	6	0	0	0	0	0	0	0	0	4	0	2	3	2	1	1	0	0	0	0	84
128	3	5	7	0	0	0	0	0	0	0	0	5	1	3	5	4	4	4	3	2	0	0	243
129	3	5	8	0	0	0	0	0	0	0	0	4	1	2	4	3	2	1	0	0	0	0	113
130	3	5	9	0	0	0	0	0	0	0	0	3	1	1	4	3	2	1	0	0	0	0	103
131	3	5	10	0	0	0	0	0	0	0	0	3	1	2	4	3	2	1	0	0	0	0	109
132	3	6	7	0	0	0	0	0	0	0	0	6	1	3	1	1	1	0	0	0	0	0	71
133	3	6	8	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
134	3	6	9	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
135	3	6	10	0	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
136	3	7	8	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
137	3	7	9	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
138	3	7	10	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
139	3	8	9	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
140	3	8	10	0	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
141	3	9	10	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12

142	4	5	6	0	0	0	0	0	0	0	0	5	0	3	3	2	1	1	0	0	0	0	94
143	4	5	7	0	0	0	0	0	0	0	0	6	1	4	5	5	4	5	3	3	1	0	296
144	4	5	8	0	0	0	0	0	0	0	0	5	1	3	4	3	2	2	0	0	0	0	133
145	4	5	9	0	0	0	0	0	0	0	0	4	1	2	4	3	2	2	0	0	0	0	123
146	4	5	10	0	0	0	0	0	0	0	0	4	1	3	4	3	2	2	0	0	0	0	129
147	4	6	7	0	0	0	0	0	0	0	0	7	1	4	1	2	1	0	0	0	0	0	89
148	4	6	8	0	0	0	0	0	0	0	0	5	0	2	0	0	0	0	0	0	0	0	32
149	4	6	9	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
150	4	6	10	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
151	4	7	8	0	0	0	0	0	0	0	0	5	0	3	0	1	0	0	0	0	0	0	46
152	4	7	9	0	0	0	0	0	0	0	0	5	0	2	0	1	0	0	0	0	0	0	40
153	4	7	10	0	0	0	0	0	0	0	0	5	0	3	0	1	0	0	0	0	0	0	46
154	4	8	9	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
155	4	8	10	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
156	4	9	10	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
157	5	6	7	0	0	0	0	0	0	0	0	7	1	5	5	5	4	4	3	3	1	0	296
158	5	6	8	0	0	0	0	0	0	0	0	5	0	3	3	2	1	1	0	0	0	0	94
159	5	6	9	0	0	0	0	0	0	0	0	4	0	2	3	2	1	1	0	0	0	0	84
160	5	6	10	0	0	0	0	0	0	0	0	4	0	3	3	2	1	1	0	0	0	0	90
161	5	7	8	0	0	0	0	0	0	0	0	5	1	4	5	5	4	5	3	3	1	0	292
162	5	7	9	0	0	0	0	0	0	0	0	5	1	3	5	5	4	5	3	3	1	0	286
163	5	7	10	0	0	0	0	0	0	0	0	5	1	4	5	5	4	5	3	3	1	0	292
164	5	8	9	0	0	0	0	0	0	0	0	4	1	2	4	3	2	2	0	0	0	0	123
165	5	8	10	0	0	0	0	0	0	0	0	4	1	3	4	3	2	2	0	0	0	0	129
166	5	9	10	0	0	0	0	0	0	0	0	4	1	2	4	3	2	2	0	0	0	0	123
167	6	7	8	0	0	0	0	0	0	0	0	6	1	4	1	1	0	0	0	0	0	0	68
168	6	7	9	0	0	0	0	0	0	0	0	6	1	3	1	2	1	0	0	0	0	0	79
169	6	7	10	0	0	0	0	0	0	0	0	6	1	4	1	2	1	0	0	0	0	0	85
170	6	8	9	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
171	6	8	10	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
172	6	9	10	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
173	7	8	9	0	0	0	0	0	0	0	0	4	0	2	0	1	0	0	0	0	0	0	36
174	7	8	10	0	0	0	0	0	0	0	0	4	0	3	0	1	0	0	0	0	0	0	42
175	7	9	10	0	0	0	0	0	0	0	0	5	0	2	0	1	0	0	0	0	0	0	40
176	8	9	10	0	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
177	1	2	3	4	0	0	0	0	0	0	0	5	1	1	0	0	1	0	0	0	0	0	40
178	1	2	3	5	0	0	0	0	0	0	0	4	1	1	2	1	1	1	0	0	0	0	68
179	1	2	3	6	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
180	1	2	3	7	0	0	0	0	0	0	0	5	0	2	0	0	0	0	0	0	0	0	32
181	1	2	3	8	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
182	1	2	3	9	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
183	1	2	3	10	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
184	1	2	4	5	0	0	0	0	0	0	0	5	2	2	2	1	2	1	0	0	0	0	92
185	1	2	4	6	0	0	0	0	0	0	0	5	1	2	0	0	1	0	0	0	0	0	46
186	1	2	4	7	0	0	0	0	0	0	0	6	1	3	0	1	1	0	1	0	0	0	75
187	1	2	4	8	0	0	0	0	0	0	0	5	1	2	0	0	1	0	0	0	0	0	46
188	1	2	4	9	0	0	0	0	0	0	0	4	1	1	0	0	1	0	0	0	0	0	36
189	1	2	4	10	0	0	0	0	0	0	0	4	1	2	0	0	1	0	0	0	0	0	42
190	1	2	5	6	0	0	0	0	0	0	0	4	0	2	1	1	1	1	0	0	0	0	62

191	1	2	5	7	0	0	0	0	0	0	0	5	1	3	3	3	3	3	1	1	0	0	168
192	1	2	5	8	0	0	0	0	0	0	0	4	1	2	2	1	1	1	0	0	0	0	74
193	1	2	5	9	0	0	0	0	0	0	0	3	1	1	2	1	1	1	0	0	0	0	64
194	1	2	5	10	0	0	0	0	0	0	0	3	1	2	2	1	1	1	0	0	0	0	70
195	1	2	6	7	0	0	0	0	0	0	0	6	1	4	1	2	1	0	0	0	0	0	85
196	1	2	6	8	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
197	1	2	6	9	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
198	1	2	6	10	0	0	0	0	0	0	0	3	0	2	0	0	0	0	0	0	0	0	24
199	1	2	7	8	0	0	0	0	0	0	0	4	0	3	0	1	0	0	0	0	0	0	42
200	1	2	7	9	0	0	0	0	0	0	0	4	0	2	0	1	0	0	0	0	0	0	36
201	1	2	7	10	0	0	0	0	0	0	0	4	0	3	0	1	0	0	0	0	0	0	42
202	1	2	8	9	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
203	1	2	8	10	0	0	0	0	0	0	0	3	0	2	0	0	0	0	0	0	0	0	24
204	1	2	9	10	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
205	1	3	4	5	0	0	0	0	0	0	0	4	1	1	2	1	1	1	0	0	0	0	68
206	1	3	4	6	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
207	1	3	4	7	0	0	0	0	0	0	0	5	0	2	0	0	0	0	0	0	0	0	32
208	1	3	4	8	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
209	1	3	4	9	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
210	1	3	4	10	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
211	1	3	5	6	0	0	0	0	0	0	0	4	0	1	1	1	1	1	0	0	0	0	56
212	1	3	5	7	0	0	0	0	0	0	0	5	1	2	3	2	3	3	1	1	0	0	154
213	1	3	5	8	0	0	0	0	0	0	0	4	1	1	2	1	1	1	0	0	0	0	68
214	1	3	5	9	0	0	0	0	0	0	0	3	1	0	2	1	1	1	0	0	0	0	58
215	1	3	5	10	0	0	0	0	0	0	0	3	1	1	2	1	1	1	0	0	0	0	64
216	1	3	6	7	0	0	0	0	0	0	0	6	1	3	1	1	1	0	0	0	0	0	71
217	1	3	6	8	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
218	1	3	6	9	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
219	1	3	6	10	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
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221	1	3	7	9	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
222	1	3	7	10	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
223	1	3	8	9	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
224	1	3	8	10	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
225	1	3	9	10	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
226	1	4	5	6	0	0	0	0	0	0	0	4	0	2	1	1	1	1	0	0	0	0	62
227	1	4	5	7	0	0	0	0	0	0	0	5	1	3	3	3	3	3	1	1	0	0	168
228	1	4	5	8	0	0	0	0	0	0	0	4	1	2	2	1	1	1	0	0	0	0	74
229	1	4	5	9	0	0	0	0	0	0	0	3	1	1	2	1	1	1	0	0	0	0	64
230	1	4	5	10	0	0	0	0	0	0	0	3	1	2	2	1	1	1	0	0	0	0	70
231	1	4	6	7	0	0	0	0	0	0	0	6	1	4	1	2	1	0	0	0	0	0	85
232	1	4	6	8	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
233	1	4	6	9	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
234	1	4	6	10	0	0	0	0	0	0	0	3	0	2	0	0	0	0	0	0	0	0	24
235	1	4	7	8	0	0	0	0	0	0	0	4	0	3	0	1	0	0	0	0	0	0	42
236	1	4	7	9	0	0	0	0	0	0	0	4	0	2	0	1	0	0	0	0	0	0	36
237	1	4	7	10	0	0	0	0	0	0	0	4	0	3	0	1	0	0	0	0	0	0	42
238	1	4	8	9	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
239	1	4	8	10	0	0	0	0	0	0	0	3	0	2	0	0	0	0	0	0	0	0	24

240	1	4	9	10	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
241	1	5	6	7	0	0	0	0	0	0	0	6	1	4	3	4	4	3	1	1	0	0	195
242	1	5	6	8	0	0	0	0	0	0	0	4	0	2	1	1	1	1	0	0	0	0	62
243	1	5	6	9	0	0	0	0	0	0	0	3	0	1	1	1	1	1	0	0	0	0	52
244	1	5	6	10	0	0	0	0	0	0	0	3	0	2	1	1	1	1	0	0	0	0	58
245	1	5	7	8	0	0	0	0	0	0	0	4	1	3	3	3	3	3	1	1	0	0	164
246	1	5	7	9	0	0	0	0	0	0	0	4	1	2	3	3	3	3	1	1	0	0	158
247	1	5	7	10	0	0	0	0	0	0	0	4	1	3	3	3	3	3	1	1	0	0	164
248	1	5	8	9	0	0	0	0	0	0	0	3	1	1	2	1	1	1	0	0	0	0	64
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250	1	5	9	10	0	0	0	0	0	0	0	3	1	1	2	1	1	1	0	0	0	0	64
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253	1	6	7	10	0	0	0	0	0	0	0	5	1	4	1	2	1	0	0	0	0	0	81
254	1	6	8	9	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
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261	2	3	4	5	0	0	0	0	0	0	0	5	2	2	4	3	2	1	0	0	0	0	122
262	2	3	4	6	0	0	0	0	0	0	0	5	1	1	0	0	0	0	0	0	0	0	31
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267	2	3	5	6	0	0	0	0	0	0	0	4	0	2	3	2	1	1	0	0	0	0	84
268	2	3	5	7	0	0	0	0	0	0	0	5	1	3	5	4	4	4	3	2	0	0	243
269	2	3	5	8	0	0	0	0	0	0	0	4	1	2	4	3	2	1	0	0	0	0	113
270	2	3	5	9	0	0	0	0	0	0	0	3	1	1	4	3	2	1	0	0	0	0	103
271	2	3	5	10	0	0	0	0	0	0	0	3	1	2	4	3	2	1	0	0	0	0	109
272	2	3	6	7	0	0	0	0	0	0	0	6	1	3	1	1	1	0	0	0	0	0	71
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285	2	4	5	9	0	0	0	0	0	0	0	5	2	2	4	3	2	2	0	0	0	0	132
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289	2	4	6	9	0	0	0	0	0	0	0	5	1	1	0	0	0	0	0	0	0	0	31
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291	2	4	7	8	0	0	0	0	0	0	0	6	1	3	0	1	0	0	0	0	0	0	55
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296	2	4	9	10	0	0	0	0	0	0	0	5	1	1	0	0	0	0	0	0	0	0	31
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299	2	5	6	9	0	0	0	0	0	0	0	4	0	2	3	2	1	1	0	0	0	0	84
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301	2	5	7	8	0	0	0	0	0	0	0	5	1	4	5	5	4	5	3	3	1	0	292
302	2	5	7	9	0	0	0	0	0	0	0	5	1	3	5	5	4	5	3	3	1	0	286
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304	2	5	8	9	0	0	0	0	0	0	0	4	1	2	4	3	2	2	0	0	0	0	123
305	2	5	8	10	0	0	0	0	0	0	0	4	1	3	4	3	2	2	0	0	0	0	129
306	2	5	9	10	0	0	0	0	0	0	0	4	1	2	4	3	2	2	0	0	0	0	123
307	2	6	7	8	0	0	0	0	0	0	0	6	1	4	1	1	0	0	0	0	0	0	68
308	2	6	7	9	0	0	0	0	0	0	0	6	1	3	1	2	1	0	0	0	0	0	79
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310	2	6	8	9	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
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316	2	8	9	10	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
317	3	4	5	6	0	0	0	0	0	0	0	4	0	2	3	2	1	1	0	0	0	0	84
318	3	4	5	7	0	0	0	0	0	0	0	5	1	3	5	4	4	4	3	2	0	0	243
319	3	4	5	8	0	0	0	0	0	0	0	4	1	2	4	3	2	1	0	0	0	0	113
320	3	4	5	9	0	0	0	0	0	0	0	3	1	1	4	3	2	1	0	0	0	0	103
321	3	4	5	10	0	0	0	0	0	0	0	3	1	2	4	3	2	1	0	0	0	0	109
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323	3	4	6	8	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
324	3	4	6	9	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
325	3	4	6	10	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
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333	3	5	6	8	0	0	0	0	0	0	0	4	0	2	3	2	1	1	0	0	0	0	84
334	3	5	6	9	0	0	0	0	0	0	0	3	0	1	3	2	1	1	0	0	0	0	74
335	3	5	6	10	0	0	0	0	0	0	0	3	0	2	3	2	1	1	0	0	0	0	80
336	3	5	7	8	0	0	0	0	0	0	0	4	1	3	5	4	4	4	3	2	0	0	239
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338	3	5	7	10	0	0	0	0	0	0	0	4	1	3	5	4	4	4	3	2	0	0	239
339	3	5	8	9	0	0	0	0	0	0	0	3	1	1	4	3	2	1	0	0	0	0	103
340	3	5	8	10	0	0	0	0	0	0	0	3	1	2	4	3	2	1	0	0	0	0	109
341	3	5	9	10	0	0	0	0	0	0	0	3	1	1	4	3	2	1	0	0	0	0	103
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343	3	6	7	9	0	0	0	0	0	0	0	5	1	2	1	1	1	0	0	0	0	0	61
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345	3	6	8	9	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
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353	4	5	6	8	0	0	0	0	0	0	0	5	0	3	3	2	1	1	0	0	0	0	94
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356	4	5	7	8	0	0	0	0	0	0	0	5	1	4	5	5	4	5	3	3	1	0	292
357	4	5	7	9	0	0	0	0	0	0	0	5	1	3	5	5	4	5	3	3	1	0	286
358	4	5	7	10	0	0	0	0	0	0	0	5	1	4	5	5	4	5	3	3	1	0	292
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363	4	6	7	9	0	0	0	0	0	0	0	6	1	3	1	2	1	0	0	0	0	0	79
364	4	6	7	10	0	0	0	0	0	0	0	6	1	4	1	2	1	0	0	0	0	0	85
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371	4	8	9	10	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
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373	5	6	7	9	0	0	0	0	0	0	0	6	1	4	5	5	4	4	3	3	1	0	286
374	5	6	7	10	0	0	0	0	0	0	0	6	1	5	5	5	4	4	3	3	1	0	292
375	5	6	8	9	0	0	0	0	0	0	0	4	0	2	3	2	1	1	0	0	0	0	84
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377	5	6	9	10	0	0	0	0	0	0	0	4	0	2	3	2	1	1	0	0	0	0	84
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379	5	7	8	10	0	0	0	0	0	0	0	4	1	4	5	5	4	5	3	3	1	0	288
380	5	7	9	10	0	0	0	0	0	0	0	5	1	3	5	5	4	5	3	3	1	0	286
381	5	8	9	10	0	0	0	0	0	0	0	4	1	2	4	3	2	2	0	0	0	0	123
382	6	7	8	9	0	0	0	0	0	0	0	5	1	3	1	1	0	0	0	0	0	0	58
383	6	7	8	10	0	0	0	0	0	0	0	5	1	4	1	1	0	0	0	0	0	0	64
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385	6	8	9	10	0	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
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402	1	2	3	7	8	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
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404	1	2	3	7	10	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	28
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406	1	2	3	8	10	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
407	1	2	3	9	10	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
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413	1	2	4	6	7	0	0	0	0	0	0	7	2	4	1	2	2	0	1	0	0	0	114
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415	1	2	4	6	9	0	0	0	0	0	0	4	1	1	0	0	1	0	0	0	0	0	36
416	1	2	4	6	10	0	0	0	0	0	0	4	1	2	0	0	1	0	0	0	0	0	42
417	1	2	4	7	8	0	0	0	0	0	0	5	1	3	0	1	1	0	1	0	0	0	71
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420	1	2	4	8	9	0	0	0	0	0	0	4	1	1	0	0	1	0	0	0	0	0	36
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426	1	2	5	6	10	0	0	0	0	0	0	3	0	2	1	1	1	1	0	0	0	0	58
427	1	2	5	7	8	0	0	0	0	0	0	4	1	3	3	3	3	3	1	1	0	0	164
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446	1	3	4	5	9	0	0	0	0	0	0	3	1	0	2	1	1	1	0	0	0	0	58
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466	1	3	5	8	10	0	0	0	0	0	0	3	1	1	2	1	1	1	0	0	0	0	64
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483	1	4	5	7	9	0	0	0	0	0	0	4	1	2	3	3	3	3	1	1	0	0	158
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501	1	5	6	8	9	0	0	0	0	0	0	3	0	1	1	1	1	1	0	0	0	0	52
502	1	5	6	8	10	0	0	0	0	0	0	3	0	2	1	1	1	1	0	0	0	0	58
503	1	5	6	9	10	0	0	0	0	0	0	3	0	1	1	1	1	1	0	0	0	0	52
504	1	5	7	8	9	0	0	0	0	0	0	3	1	2	3	3	3	3	1	1	0	0	154
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506	1	5	7	9	10	0	0	0	0	0	0	4	1	2	3	3	3	3	1	1	0	0	158
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532	2	3	5	7	8	0	0	0	0	0	0	4	1	3	5	4	4	4	3	2	0	0	239
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563	2	4	6	9	10	0	0	0	0	0	0	5	1	1	0	0	0	0	0	0	0	0	31
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567	2	4	8	9	10	0	0	0	0	0	0	5	1	1	0	0	0	0	0	0	0	0	31
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569	2	5	6	7	9	0	0	0	0	0	0	6	1	4	5	5	4	4	3	3	1	0	286
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577	2	5	8	9	10	0	0	0	0	0	0	4	1	2	4	3	2	2	0	0	0	0	123
578	2	6	7	8	9	0	0	0	0	0	0	5	1	3	1	1	0	0	0	0	0	0	58
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581	2	6	8	9	10	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
582	2	7	8	9	10	0	0	0	0	0	0	4	0	2	0	1	0	0	0	0	0	0	36

583	3	4	5	6	7	0	0	0	0	0	0	6	1	4	5	4	4	4	3	2	0	0	253
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615	3	6	7	9	10	0	0	0	0	0	0	5	1	2	1	1	1	0	0	0	0	0	61
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619	4	5	6	7	9	0	0	0	0	0	0	6	1	4	5	5	4	4	3	3	1	0	286
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621	4	5	6	8	9	0	0	0	0	0	0	4	0	2	3	2	1	1	0	0	0	0	84
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623	4	5	6	9	10	0	0	0	0	0	0	4	0	2	3	2	1	1	0	0	0	0	84
624	4	5	7	8	9	0	0	0	0	0	0	4	1	3	5	5	4	5	3	3	1	0	282
625	4	5	7	8	10	0	0	0	0	0	0	4	1	4	5	5	4	5	3	3	1	0	288
626	4	5	7	9	10	0	0	0	0	0	0	5	1	3	5	5	4	5	3	3	1	0	286
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628	4	6	7	8	9	0	0	0	0	0	0	5	1	3	1	1	0	0	0	0	0	0	58
629	4	6	7	8	10	0	0	0	0	0	0	5	1	4	1	1	0	0	0	0	0	0	64
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631	4	6	8	9	10	0	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22

632	4	7	8	9	10	0	0	0	0	0	0	4	0	2	0	1	0	0	0	0	0	0	36
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635	5	6	7	9	10	0	0	0	0	0	0	6	1	4	5	5	4	4	3	3	1	0	286
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642	1	2	3	5	6	7	8	9	10	0	0	4	1	2	3	2	3	3	1	1	0	0	150
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644	1	2	3	4	5	7	8	9	10	0	0	4	2	1	3	2	4	3	2	1	0	0	169
645	1	2	3	4	5	6	8	9	10	0	0	4	1	0	1	1	2	1	0	0	0	0	64
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649	3	4	5	6	7	8	9	10	0	0	0	4	1	3	5	3	3	4	3	2	0	0	222
650	2	4	5	6	7	8	9	10	0	0	0	6	2	4	5	4	3	4	3	3	1	0	274
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653	2	3	4	5	7	8	9	10	0	0	0	4	2	2	5	4	4	4	3	2	0	0	238
654	2	3	4	5	6	8	9	10	0	0	0	4	1	1	3	2	1	1	0	0	0	0	83
655	2	3	4	5	6	7	9	10	0	0	0	6	2	3	5	4	4	4	3	2	0	0	252
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663	1	3	4	5	6	7	9	10	0	0	0	5	1	2	3	3	4	3	1	1	0	0	171
664	1	3	4	5	6	7	8	10	0	0	0	4	1	3	3	2	3	3	1	1	0	0	156
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669	1	2	4	5	6	8	9	10	0	0	0	4	1	1	1	1	2	1	0	0	0	0	70
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676	1	2	3	5	6	7	9	10	0	0	0	5	1	2	3	3	4	3	1	1	0	0	171
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678	1	2	3	5	6	7	8	9	0	0	0	4	1	2	3	2	3	3	1	1	0	0	150
679	1	2	3	4	7	8	9	10	0	0	0	4	1	1	0	0	1	0	1	0	0	0	47
680	1	2	3	4	6	8	9	10	0	0	0	4	1	0	0	0	1	0	0	0	0	0	30

681	1	2	3	4	6	7	9	10	0	0	0	6	2	2	1	1	2	0	1	0	0	0	90
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694	4	5	6	7	8	9	10	0	0	0	0	5	1	4	5	4	3	4	3	3	1	0	265
695	3	5	6	7	8	9	10	0	0	0	0	4	1	3	5	3	3	4	3	2	0	0	222
696	3	4	6	7	8	9	10	0	0	0	0	4	1	2	1	0	0	0	0	0	0	0	40
697	3	4	5	7	8	9	10	0	0	0	0	3	1	2	5	4	4	4	3	2	0	0	229
698	3	4	5	6	8	9	10	0	0	0	0	3	0	1	3	2	1	1	0	0	0	0	74
699	3	4	5	6	7	9	10	0	0	0	0	5	1	3	5	4	4	4	3	2	0	0	243
700	3	4	5	6	7	8	10	0	0	0	0	4	1	4	5	3	3	4	3	2	0	0	228
701	3	4	5	6	7	8	9	0	0	0	0	4	1	3	5	3	3	4	3	2	0	0	222
702	2	5	6	7	8	9	10	0	0	0	0	5	1	4	5	4	3	4	3	3	1	0	265
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704	2	4	5	7	8	9	10	0	0	0	0	5	2	3	5	5	4	5	3	3	1	0	291
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706	2	4	5	6	7	9	10	0	0	0	0	7	2	4	5	5	4	4	3	3	1	0	295
707	2	4	5	6	7	8	10	0	0	0	0	6	2	5	5	4	3	4	3	3	1	0	280
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711	2	3	5	6	8	9	10	0	0	0	0	3	0	1	3	2	1	1	0	0	0	0	74
712	2	3	5	6	7	9	10	0	0	0	0	5	1	3	5	4	4	4	3	2	0	0	243
713	2	3	5	6	7	8	10	0	0	0	0	4	1	4	5	3	3	4	3	2	0	0	228
714	2	3	5	6	7	8	9	0	0	0	0	4	1	3	5	3	3	4	3	2	0	0	222
715	2	3	4	7	8	9	10	0	0	0	0	4	1	1	0	0	0	0	0	0	0	0	27
716	2	3	4	6	8	9	10	0	0	0	0	4	1	0	0	0	0	0	0	0	0	0	21
717	2	3	4	6	7	9	10	0	0	0	0	6	2	2	1	1	1	0	0	0	0	0	70
718	2	3	4	6	7	8	10	0	0	0	0	5	2	3	1	0	0	0	0	0	0	0	55
719	2	3	4	6	7	8	9	0	0	0	0	5	2	2	1	0	0	0	0	0	0	0	49
720	2	3	4	5	8	9	10	0	0	0	0	4	2	1	4	3	2	1	0	0	0	0	112
721	2	3	4	5	7	9	10	0	0	0	0	5	2	2	5	4	4	4	3	2	0	0	242
722	2	3	4	5	7	8	10	0	0	0	0	4	2	3	5	4	4	4	3	2	0	0	244
723	2	3	4	5	7	8	9	0	0	0	0	4	2	2	5	4	4	4	3	2	0	0	238
724	2	3	4	5	6	9	10	0	0	0	0	4	1	1	3	2	1	1	0	0	0	0	83
725	2	3	4	5	6	8	10	0	0	0	0	4	1	2	3	2	1	1	0	0	0	0	89
726	2	3	4	5	6	8	9	0	0	0	0	4	1	1	3	2	1	1	0	0	0	0	83
727	2	3	4	5	6	7	10	0	0	0	0	6	2	4	5	4	4	4	3	2	0	0	258
728	2	3	4	5	6	7	9	0	0	0	0	6	2	3	5	4	4	4	3	2	0	0	252
729	2	3	4	5	6	7	8	0	0	0	0	6	2	4	5	3	3	4	3	2	0	0	241

730	1	5	6	7	8	9	10	0	0	0	0	4	1	3	3	3	3	3	1	1	0	0	164
731	1	4	6	7	8	9	10	0	0	0	0	4	1	3	1	1	0	0	0	0	0	0	54
732	1	4	5	7	8	9	10	0	0	0	0	3	1	2	3	3	3	3	1	1	0	0	154
733	1	4	5	6	8	9	10	0	0	0	0	3	0	1	1	1	1	1	0	0	0	0	52
734	1	4	5	6	7	9	10	0	0	0	0	5	1	3	3	4	4	3	1	1	0	0	185
735	1	4	5	6	7	8	10	0	0	0	0	4	1	4	3	3	3	3	1	1	0	0	170
736	1	4	5	6	7	8	9	0	0	0	0	4	1	3	3	3	3	3	1	1	0	0	164
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738	1	3	5	7	8	9	10	0	0	0	0	3	1	1	3	2	3	3	1	1	0	0	140
739	1	3	5	6	8	9	10	0	0	0	0	3	0	0	1	1	1	1	0	0	0	0	46
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741	1	3	5	6	7	8	10	0	0	0	0	4	1	3	3	2	3	3	1	1	0	0	156
742	1	3	5	6	7	8	9	0	0	0	0	4	1	2	3	2	3	3	1	1	0	0	150
743	1	3	4	7	8	9	10	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
744	1	3	4	6	8	9	10	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
745	1	3	4	6	7	9	10	0	0	0	0	5	1	2	1	1	1	0	0	0	0	0	61
746	1	3	4	6	7	8	10	0	0	0	0	4	1	3	1	0	0	0	0	0	0	0	46
747	1	3	4	6	7	8	9	0	0	0	0	4	1	2	1	0	0	0	0	0	0	0	40
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749	1	3	4	5	7	9	10	0	0	0	0	4	1	1	3	2	3	3	1	1	0	0	144
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764	1	2	4	7	8	9	10	0	0	0	0	4	1	2	0	1	1	0	1	0	0	0	61
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777	1	2	4	5	6	7	9	0	0	0	0	6	2	3	3	4	5	3	2	1	0	0	214
778	1	2	4	5	6	7	8	0	0	0	0	6	2	4	3	3	4	3	2	1	0	0	203

779	1	2	3	7	8	9	10	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
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781	1	2	3	6	7	9	10	0	0	0	0	5	1	2	1	1	1	0	0	0	0	0	61
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815	4	6	7	8	9	10	0	0	0	0	0	5	1	3	1	1	0	0	0	0	0	0	58
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821	3	6	7	8	9	10	0	0	0	0	0	4	1	2	1	0	0	0	0	0	0	0	40
822	3	5	7	8	9	10	0	0	0	0	0	3	1	2	5	4	4	4	3	2	0	0	229
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828	3	4	6	8	9	10	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
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831	3	4	6	7	8	9	0	0	0	0	0	4	1	2	1	0	0	0	0	0	0	0	40
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843	2	5	7	8	9	10	0	0	0	0	0	4	1	3	5	5	4	5	3	3	1	0	282
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847	2	5	6	7	8	9	0	0	0	0	0	5	1	4	5	4	3	4	3	3	1	0	265
848	2	4	7	8	9	10	0	0	0	0	0	5	1	2	0	1	0	0	0	0	0	0	45
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871	2	3	5	7	8	9	0	0	0	0	0	3	1	2	5	4	4	4	3	2	0	0	229
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875	2	3	5	6	7	10	0	0	0	0	0	5	1	4	5	4	4	4	3	2	0	0	249
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895	2	3	4	5	6	9	0	0	0	0	0	4	1	1	3	2	1	1	0	0	0	0	83
896	2	3	4	5	6	8	0	0	0	0	0	5	1	2	3	2	1	1	0	0	0	0	93
897	2	3	4	5	6	7	0	0	0	0	0	7	2	4	5	4	4	4	3	2	0	0	262
898	1	6	7	8	9	10	0	0	0	0	0	4	1	3	1	1	0	0	0	0	0	0	54
899	1	5	7	8	9	10	0	0	0	0	0	3	1	2	3	3	3	3	1	1	0	0	154
900	1	5	6	8	9	10	0	0	0	0	0	3	0	1	1	1	1	1	0	0	0	0	52
901	1	5	6	7	9	10	0	0	0	0	0	5	1	3	3	4	4	3	1	1	0	0	185
902	1	5	6	7	8	10	0	0	0	0	0	4	1	4	3	3	3	3	1	1	0	0	170
903	1	5	6	7	8	9	0	0	0	0	0	4	1	3	3	3	3	3	1	1	0	0	164
904	1	4	7	8	9	10	0	0	0	0	0	3	0	2	0	1	0	0	0	0	0	0	32
905	1	4	6	8	9	10	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
906	1	4	6	7	9	10	0	0	0	0	0	5	1	3	1	2	1	0	0	0	0	0	75
907	1	4	6	7	8	10	0	0	0	0	0	4	1	4	1	1	0	0	0	0	0	0	60
908	1	4	6	7	8	9	0	0	0	0	0	4	1	3	1	1	0	0	0	0	0	0	54
909	1	4	5	8	9	10	0	0	0	0	0	3	1	1	2	1	1	1	0	0	0	0	64
910	1	4	5	7	9	10	0	0	0	0	0	4	1	2	3	3	3	3	1	1	0	0	158
911	1	4	5	7	8	10	0	0	0	0	0	3	1	3	3	3	3	3	1	1	0	0	160
912	1	4	5	7	8	9	0	0	0	0	0	3	1	2	3	3	3	3	1	1	0	0	154
913	1	4	5	6	9	10	0	0	0	0	0	3	0	1	1	1	1	1	0	0	0	0	52
914	1	4	5	6	8	10	0	0	0	0	0	3	0	2	1	1	1	1	0	0	0	0	58
915	1	4	5	6	8	9	0	0	0	0	0	3	0	1	1	1	1	1	0	0	0	0	52
916	1	4	5	6	7	10	0	0	0	0	0	5	1	4	3	4	4	3	1	1	0	0	191
917	1	4	5	6	7	9	0	0	0	0	0	5	1	3	3	4	4	3	1	1	0	0	185
918	1	4	5	6	7	8	0	0	0	0	0	5	1	4	3	3	3	3	1	1	0	0	174
919	1	3	7	8	9	10	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
920	1	3	6	8	9	10	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
921	1	3	6	7	9	10	0	0	0	0	0	5	1	2	1	1	1	0	0	0	0	0	61
922	1	3	6	7	8	10	0	0	0	0	0	4	1	3	1	0	0	0	0	0	0	0	46
923	1	3	6	7	8	9	0	0	0	0	0	4	1	2	1	0	0	0	0	0	0	0	40
924	1	3	5	8	9	10	0	0	0	0	0	3	1	0	2	1	1	1	0	0	0	0	58
925	1	3	5	7	9	10	0	0	0	0	0	4	1	1	3	2	3	3	1	1	0	0	144

975	1	2	4	6	8	9	0	0	0	0	0	4	1	1	0	0	1	0	0	0	0	0	36
976	1	2	4	6	7	10	0	0	0	0	0	6	2	4	1	2	2	0	1	0	0	0	110
977	1	2	4	6	7	9	0	0	0	0	0	6	2	3	1	2	2	0	1	0	0	0	104
978	1	2	4	6	7	8	0	0	0	0	0	6	2	4	1	1	1	0	1	0	0	0	93
979	1	2	4	5	9	10	0	0	0	0	0	4	2	1	2	1	2	1	0	0	0	0	82
980	1	2	4	5	8	10	0	0	0	0	0	4	2	2	2	1	2	1	0	0	0	0	88
981	1	2	4	5	8	9	0	0	0	0	0	4	2	1	2	1	2	1	0	0	0	0	82
982	1	2	4	5	7	10	0	0	0	0	0	5	2	3	3	3	4	3	2	1	0	0	193
983	1	2	4	5	7	9	0	0	0	0	0	5	2	2	3	3	4	3	2	1	0	0	187
984	1	2	4	5	7	8	0	0	0	0	0	5	2	3	3	3	4	3	2	1	0	0	193
985	1	2	4	5	6	10	0	0	0	0	0	4	1	2	1	1	2	1	0	0	0	0	76
986	1	2	4	5	6	9	0	0	0	0	0	4	1	1	1	1	2	1	0	0	0	0	70
987	1	2	4	5	6	8	0	0	0	0	0	5	1	2	1	1	2	1	0	0	0	0	80
988	1	2	4	5	6	7	0	0	0	0	0	7	2	4	3	4	5	3	2	1	0	0	224
989	1	2	3	8	9	10	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
990	1	2	3	7	9	10	0	0	0	0	0	4	0	1	0	0	0	0	0	0	0	0	22
991	1	2	3	7	8	10	0	0	0	0	0	3	0	2	0	0	0	0	0	0	0	0	24
992	1	2	3	7	8	9	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
993	1	2	3	6	9	10	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
994	1	2	3	6	8	10	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	0	18
995	1	2	3	6	8	9	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	12
996	1	2	3	6	7	10	0	0	0	0	0	5	1	3	1	1	1	0	0	0	0	0	67
997	1	2	3	6	7	9	0	0	0	0	0	5	1	2	1	1	1	0	0	0	0	0	61
998	1	2	3	6	7	8	0	0	0	0	0	5	1	3	1	0	0	0	0	0	0	0	50
999	1	2	3	5	9	10	0	0	0	0	0	3	1	0	2	1	1	1	0	0	0	0	58
1000	1	2	3	5	8	10	0	0	0	0	0	3	1	1	2	1	1	1	0	0	0	0	64
1001	1	2	3	5	8	9	0	0	0	0	0	3	1	0	2	1	1	1	0	0	0	0	58
1002	1	2	3	5	7	10	0	0	0	0	0	4	1	2	3	2	3	3	1	1	0	0	150
1003	1	2	3	5	7	9	0	0	0	0	0	4	1	1	3	2	3	3	1	1	0	0	144
1004	1	2	3	5	7	8	0	0	0	0	0	4	1	2	3	2	3	3	1	1	0	0	150
1005	1	2	3	5	6	10	0	0	0	0	0	3	0	1	1	1	1	1	0	0	0	0	52
1006	1	2	3	5	6	9	0	0	0	0	0	3	0	0	1	1	1	1	0	0	0	0	46
1007	1	2	3	5	6	8	0	0	0	0	0	4	0	1	1	1	1	1	0	0	0	0	56
1008	1	2	3	5	6	7	0	0	0	0	0	6	1	3	3	3	4	3	1	1	0	0	181
1009	1	2	3	4	9	10	0	0	0	0	0	4	1	0	0	0	1	0	0	0	0	0	30
1010	1	2	3	4	8	10	0	0	0	0	0	4	1	1	0	0	1	0	0	0	0	0	36
1011	1	2	3	4	8	9	0	0	0	0	0	4	1	0	0	0	1	0	0	0	0	0	30
1012	1	2	3	4	7	10	0	0	0	0	0	5	1	2	0	0	1	0	1	0	0	0	57
1013	1	2	3	4	7	9	0	0	0	0	0	5	1	1	0	0	1	0	1	0	0	0	51
1014	1	2	3	4	7	8	0	0	0	0	0	5	1	2	0	0	1	0	1	0	0	0	57
1015	1	2	3	4	6	10	0	0	0	0	0	4	1	1	0	0	1	0	0	0	0	0	36
1016	1	2	3	4	6	9	0	0	0	0	0	4	1	0	0	0	1	0	0	0	0	0	30
1017	1	2	3	4	6	8	0	0	0	0	0	5	1	1	0	0	1	0	0	0	0	0	40
1018	1	2	3	4	6	7	0	0	0	0	0	7	2	3	1	1	2	0	1	0	0	0	100
1019	1	2	3	4	5	10	0	0	0	0	0	4	2	1	2	1	2	1	0	0	0	0	82
1020	1	2	3	4	5	9	0	0	0	0	0	4	2	0	2	1	2	1	0	0	0	0	76
1021	1	2	3	4	5	8	0	0	0	0	0	5	2	1	2	1	2	1	0	0	0	0	86
1022	1	2	3	4	5	7	0	0	0	0	0	6	2	2	3	2	4	3	2	1	0	0	183
1023	1	2	3	4	5	6	0	0	0	0	0	5	1	1	1	1	2	1	0	0	0	0	74
1024	1	2	3	4	5	6	7	8	9	10	0	5	2	2	3	2	4	3	2	1	0	0	179

LARGEST IWSUM : 305
FOR DIGRAPHS : 283, 548

Vertices in the directed 13-cycle (permutation 283 above)

(C1-P1-Q5-C4-P4-C2-Q19-C11-R1-C10-Q17-C6-R10)

This cycle is shown in **Fig. 4b**