match no. 23 pp. 201-207 1988

THERE ARE EXACTLY NINETY-EIGHT CONCEALED NON-KEKULÉAN BENZENOIDS WITH TWELVE HEXAGONS. APPENDIX: BENZENOIDS WITH HEXAGONAL SYMMETRY AND FOURTY-NINE HEXAGONS*

HE WENCHEN,[a] HE WENJIE[b]

[a]*Hebei Chemical Engineering Institute,* [b]*Hebei Academy of Sciences. Shijiazhuang, The People's Republic of China*

B. N. CYVIN, S. J. CYVIN, J. BRUNVOLL

Division of Physical Chemistry, The University of Trondheim, N-7034 Trondheim-NTH, Norway

(Received: January 1988)

The existing 98 systems of concealed non-Kekuléan benzenoids with h=12 are displayed (h = number of hexagons). Also the 42 concealed non-Kekuléans with hexagonal symmetry and h=49 were depicted. They are shown in the appendix.

The search for concealed non-Kekuléan (Δ=0, K=0) benzenoid systems through the years 1974-1986 is described in Part IV of this article series [1]. It was demonstrated that there are 8 concealed non-Kekuléans with h=11, where h is the number of hexagons. In the present work we have extended the search to h=12 benzenoid systems and found that there are exactly 99 concealed non-Kekuléans among them.

Description of the forms

Figure 1 shows the set of 58 systems generated by adding one hexagon to one of the 8 concealed non-Kekuléans with h=11 [1] so that the two parts share exactly one edge. Here we will say by definition that such two parts are fused (in a strict sense). Consequently the 58 systems (Fig. 1) possess a hexagon with five edges belonging to the perimeter, which is equivalent to a vertex of degree one in the dualist graph. They are attributed to the class F according to He and He [2, 3].

---

*Part VI of the series "Enumeration and Classification of Benzenoid Hydrocarbons".

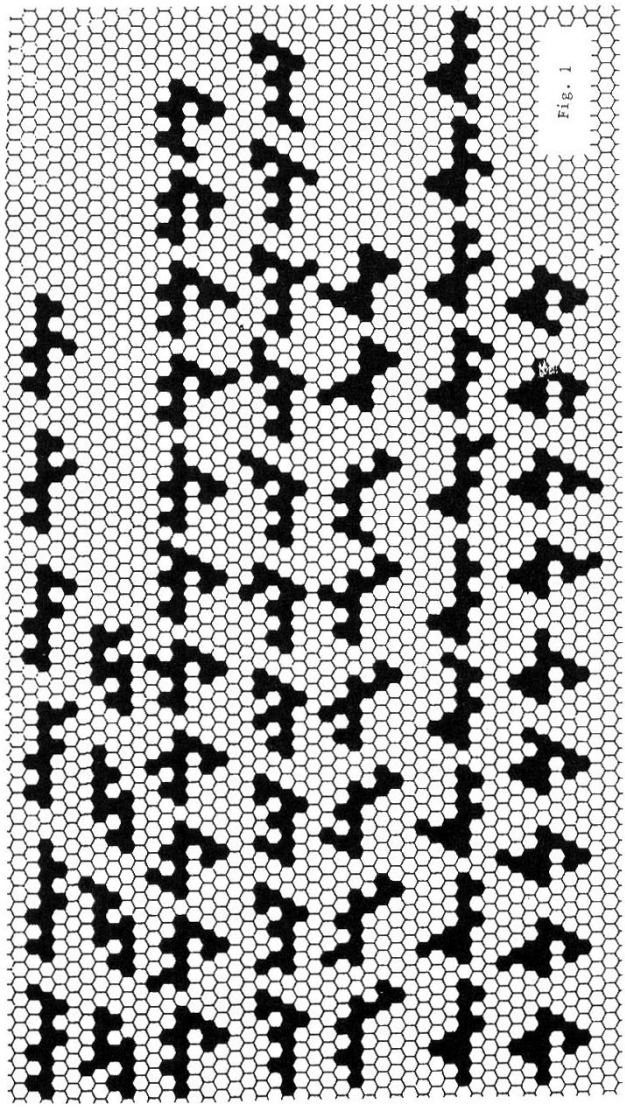


Fig. 1

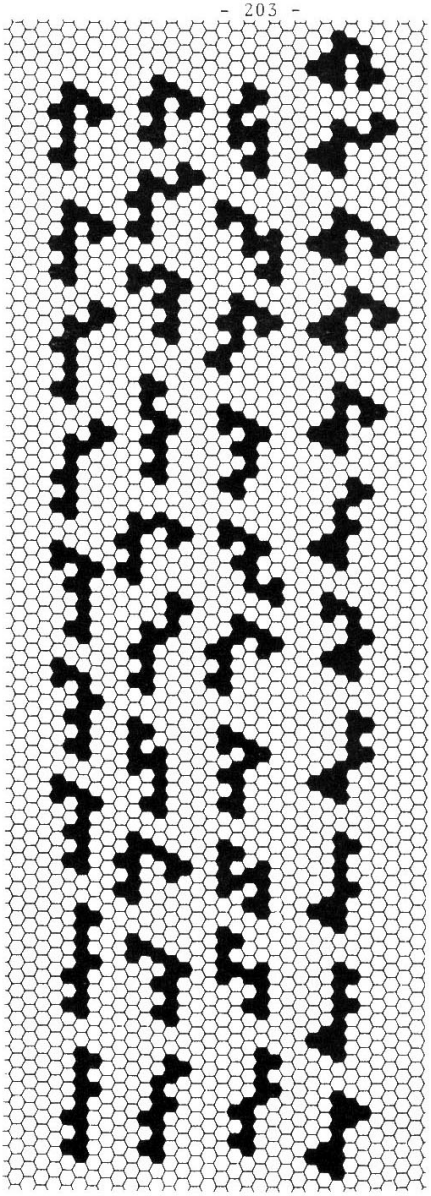
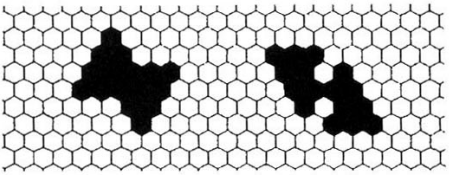


Fig. 2

In the second set of 40 systems, displayed in Fig. 2, the benzenoids have no hexagon with five free edges (on the perimeter); they belong to the class *D* [2, 3].

The 8 concealed non-Kekuléans with h=11 [1] were described by means of two types of triangular conformations, viz. phenalene (3 hexagons) and triangulene (6 hexagons). These sub-units are of course recognized also in the 58 systems of Fig. 1. But also the 41 systems of Fig. 2 may be described in terms of the same sub-units: (a) two triangulenes, (b) one triangulene and two phenalenes or (c) four phenalenes. In all cases we have systems where these units are simply fused. But also two phenalenes in cases (c) or one triangulene with one phenalene in cases (b) may merge together to form a perylene sub-unit. In those cases a linking hexagon is recognized, characterized by either 2+2 or 3+1 free edges in two disconnected paths (i.e. linear or angular annelation, respectively).

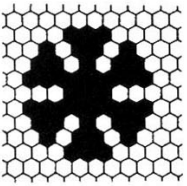
The described occurrence of only the two smallest triangular conformations is not a general feature of concealed non-Kekuléans. Below we show two examples with h=16. The left-hand system [4] is completely pericondensed in the sense that it can not be divided into fused sub-units. In the right-hand system [5] two identical sub-units of eight hexagons each are fused.



APPENDIX

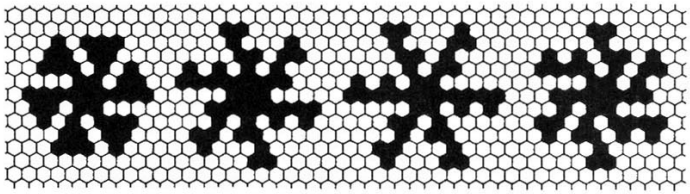
Benzenoids with hexagonal symmetry ("Snowflakes")

The first concealed non-Kekuléan snowflake was found by Hosoya [6], who depicted the below system of D_{6h} symmetry.



(1986)

Hosoya [6] conjectured that it is the smallest system (h=43) of that kind. Brunvoll et al. [7] confirmed by computer generations that no concealed non-Kekulēan snowflake exists for $h < 43$. At the same time they identified four additional systems (symmetry C_{6h}) for h=43:



(1986)

The analysis of snowflakes was carried on to a higher h value, viz. h=49. It was found that there are exactly 42 concealed non-Kekulēan snowflakes with h=49; all of them posses the C_{6h} symmetry. Figure 3 shows the 19 systems of class F, where one hexagon is fused to one of the five systems with h=43 (see above). In Fig. 4 the 23 systems of class D are depicted;

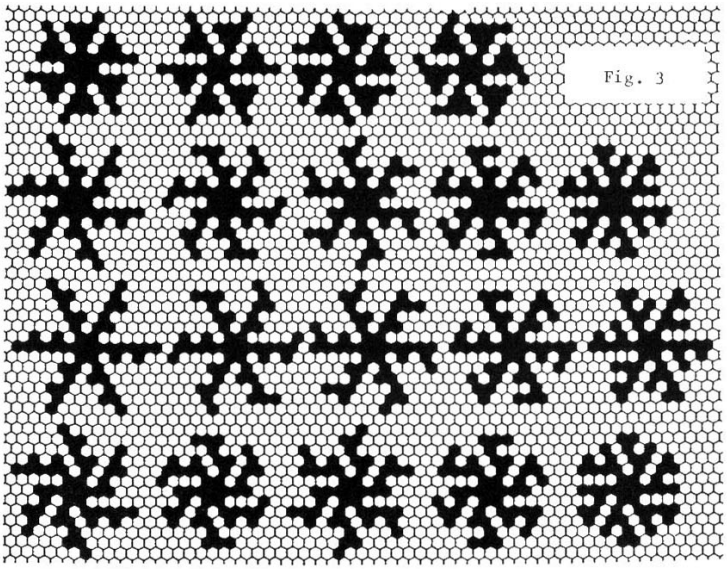


Fig. 3

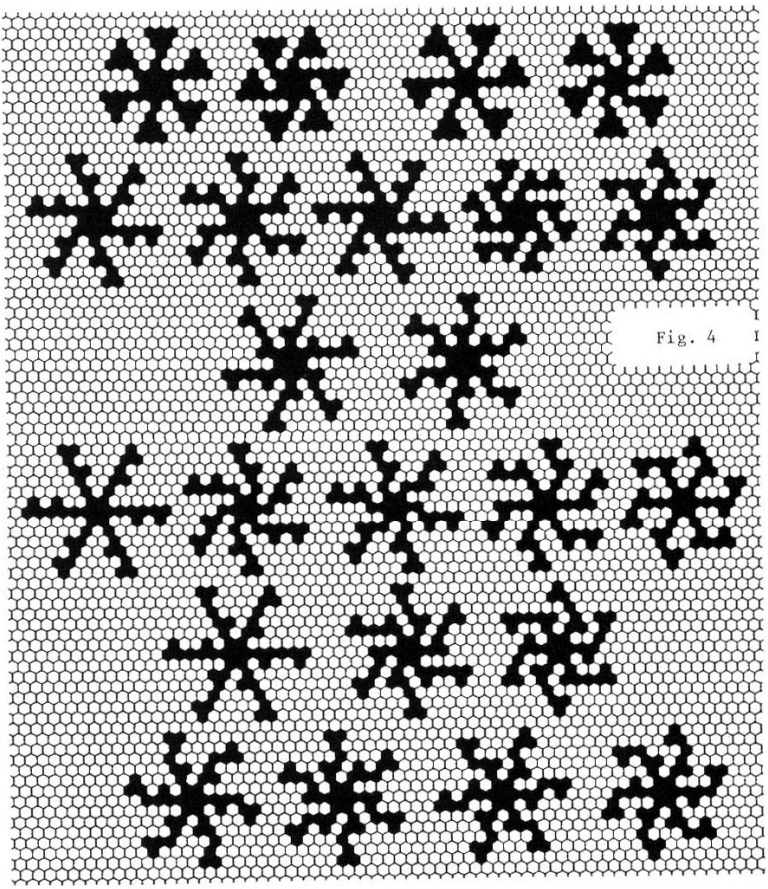


Fig. 4

they have no hexagon with five free edges.

In a way there are no surprises in the depicted forms (Figs. 3 and 4) when the systems with lower symmetries for h = 11 and 12 are known. In all arms of the snowflakes the elements from these systems are recognized.

Acknowledgement: Financial support to BNC from the Norwegian Research Council for Science and the Humanities is gratefully acknowledged.

REFERENCES

[1] J. Brunvoll, S.J. Cyvin, B.N. Cyvin, I. Gutman, W. He and W. He, Match 22, 105 (1987).

[2] W. He and W. He, Theor. Chim. Acta 68, 301 (1985).

[3] W. He and W. He, Tetrahedron 42, 5291 (1986).

[4] S.J. Cyvin, B.N. Cyvin and I. Gutman, Z. Naturforsch. 40a, 1253 (1985).

[5] S.J. Cyvin and I. Gutman, J. Mol. Struct. (Theochem) 150, 157 (1987).

[6] H. Hosoya, Comp. & Maths. with Appls. 12B, 271 (1986).

[7] J. Brunvoll, B.N. Cyvin and S.J. Cyvin, RUN·NYTT, Informasjonsorgan for RUNIT, Regnesentret ved Universitetet i Trondheim 13(4), 20 (1986); J. Brunvoll, B.N. Cyvin and S.J. Cyvin, J. Chem. Inf. Comput. Sci. 27, 171 (1987).