

# Mobility of ‘*N*-loops’: bodies cyclically connected by intersecting revolute hinges

BY S. D. GUEST<sup>1,\*</sup> AND P. W. FOWLER<sup>2</sup>

<sup>1</sup>*Department of Engineering, University of Cambridge, Trumpington Street, Cambridge CB2 1PZ, UK*

<sup>2</sup>*Department of Chemistry, University of Sheffield, Sheffield S3 7HF, UK*

The mobilities of many objects from toys and molecular models to large-scale deployable structures can be understood in terms of *N*-loops: sets of *N* bodies, cyclically connected by pairs of intersecting revolute hinges. A symmetry-extended version of the Grübler criterion for counting kinematic degrees of freedom is used to explain and rationalize the observed mobilities of *N*-loops with small *N*. Compared with simple counting, the symmetry-based approach gives improved detection and visualization of mechanisms and states of self-stress. It can also give a better account of the differing mobilities of conformers occupying different regions of the phase space, such as the rigid chair and flexible boat forms of cyclohexane.

**Keywords:** symmetry; mobility; mechanisms

## 1. Introduction

Mobility counting and rigidity theory provide concepts that are used and re-used in contexts from conformational analysis of small molecules (Dunitz & Waser 1972), mechanics of protein structures (Jacobs *et al.* 2001), modelling of pH-dependent expansion of nano-scale viral particles (Kovács *et al.* 2004), through robotics (Porta *et al.* 2009), to the generation of designs for deployable engineering structures (Chen *et al.* 2005). Many systems at these different length scales can be described as cycles of bodies linked by intersecting revolute hinges. The present paper is concerned with the mobility of such cycles, and in particular with the kinematic insights that can be gained by exploiting symmetry.

We define an *N*-loop as consisting of *N* rigid bodies, linked in a cycle by joints, such that each joint is a revolute hinge allowing torsional freedom about a line, and such that the two hinge lines for each body intersect. All distances between neighbouring intersections and all angles of intersection are allowed, and indeed much of our treatment will be applicable to this general situation. However, in applications, the configurations of interest are usually *regular N*( $\theta$ )-loops, in which all distances between neighbouring intersections are equal, and all intersection angles are equal to some angle  $\theta$  (which is taken to be greater than or equal to  $\pi/2$ ).

\*Author for correspondence (sdg@eng.cam.ac.uk).

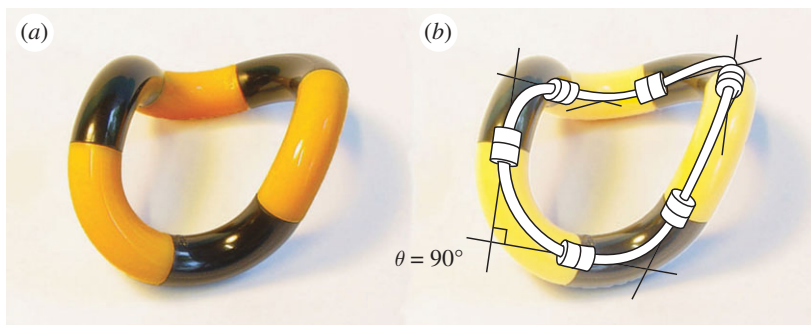


Figure 1. (a) Tangle model of the six-loop in the twist-boat conformation; (b) line drawing showing bodies, hinges and intersecting hinge lines. The angle of intersection is  $\theta = 90^\circ$ .

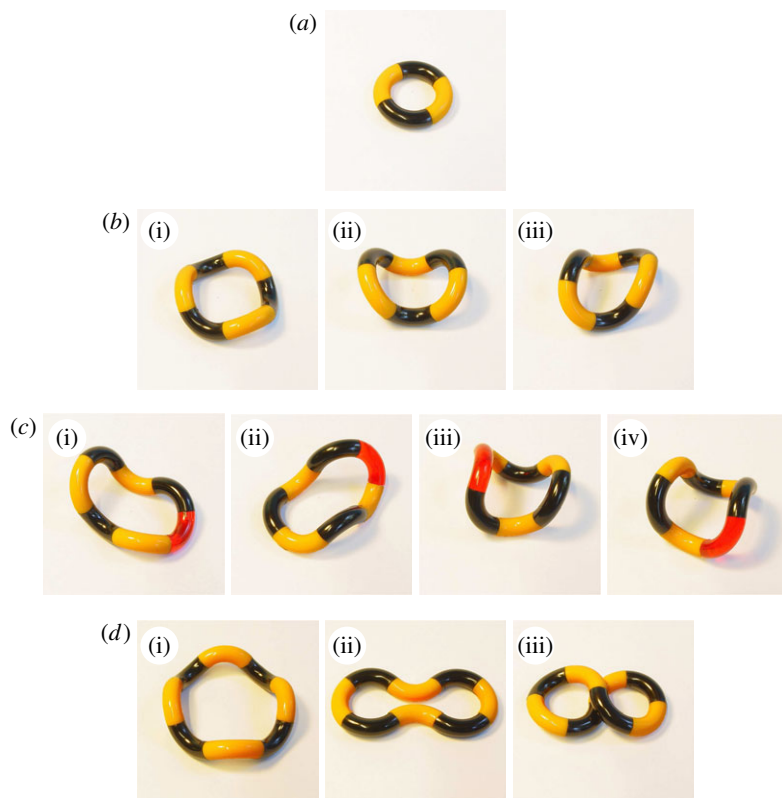


Figure 2. Conformations of Tangle models of  $N$ -loops, with  $N = 4, 6, 7, 8$ . Here  $\theta = 90^\circ$  for all links.

The ‘Tangle’ toy (<http://www.tanglecreations.com>) provides a simple means of building tangible realizations of  $N$ -loops with  $\theta = 90^\circ$  that allow exploration of their mobility properties. Figure 1 shows one conformation of a six-loop constructed from Tangle pieces, together with an analysis in terms of the bodies, hinges and hinge lines of the  $N$ -loop description.

The interesting properties of Tangles have been used as the basis for educational workshops in mathematics (Freudenthal 2003). Constructing and handling Tangle models (figure 2) leads to a number of immediate observations.

- $N = 4$ . As  $\theta = 90^\circ$ , a four-loop can be constructed in a planar conformation (figure 2a), but the physical model allows small out-of-plane deformations without the apparent distortion of the components.
- $N = 5$ . It proves to be impossible to assemble a regular five-loop with  $\theta = 90^\circ$ . It is easy to show by a geometrical argument (Freudenthal 2003) that it is not possible to close a chain of five  $90^\circ$  ‘elbows’ and simultaneously align the hinges.
- $N = 6$ . There are two ways in which a six-loop can be constructed from Tangle pieces. One leads to a rigid conformation (figure 2b(i)). The other leads to a family of non-rigid conformations lying on a one-parameter pathway. The two high-symmetry conformations are shown in figure 2b(ii)(iii). To convert from the rigid to a non-rigid conformation of the Tangle model requires dismantling and re-assembling. The three illustrated models are  $\theta = 90^\circ$  equivalents of the three well-known conformations of cyclohexane (see below).
- $N = 7$ . There are also two ways in which a seven-loop can be constructed from Tangle pieces, but now both lead to one-parameter families of non-rigid conformations, and passage from one family to the other is possible only by dismantling and re-assembling. Figure 2c(i)(ii) shows high-symmetry points on the path connecting ‘chair’-like conformations, while figure 2c(iii)(iv) shows high-symmetry points on the path connecting ‘boat’-like conformations. The four illustrated models again have their equivalents in molecular conformations (of cycloheptane) (Graveron-Demilly 1977; Crippen 1992).
- $N = 8$ . Figure 2d shows three conformations of a Tangle model of an eight-loop. All are interconvertible, in what is clearly a multi-parameter family. Porta *et al.* (2007) showed that, for cyclooctane (an eight-loop with  $\theta$  equal to the tetrahedral angle,  $\theta_T = \cos^{-1}(-1/3) \approx 109^\circ 28'$ ), all conformations form a single interconnected family.
- $N > 8$ . Some examples of loops with larger  $N$  are discussed in Freudenthal (2003).

The ‘Dreiding’ models (Dreiding 1959), used in chemistry to study conformations and flexibility of cycloalkenes and related molecules, are also the physical realizations of  $N$ -loops. The atom components linked by peg-and-socket joints are rigid bodies linked by torsional revolute hinges; these bodies are free to rotate around the linking bond. For a given hybridization of the carbon atom, the angle of intersection of the hinges is fixed, i.e.  $\theta = \theta_T$  for  $\text{sp}^3$  (where a saturated carbon centre participates in four single bonds),  $\theta = 2\pi/3$  for  $\text{sp}^2$  (where an unsaturated carbon centre participates in bonds to three neighbours). Figure 3 illustrates the use of Dreiding models for the well-studied case of the cyclohexane ring (Eliel 1962), where the models are six-loops with  $\theta = \theta_T$ . The figure shows the three conformations identified in chemical nomenclature as chair, boat and ‘twist’-boat. The chair model, representing the low-energy molecular conformer, is rigid, whereas the boat and twist-boat models can be interconverted by rotation

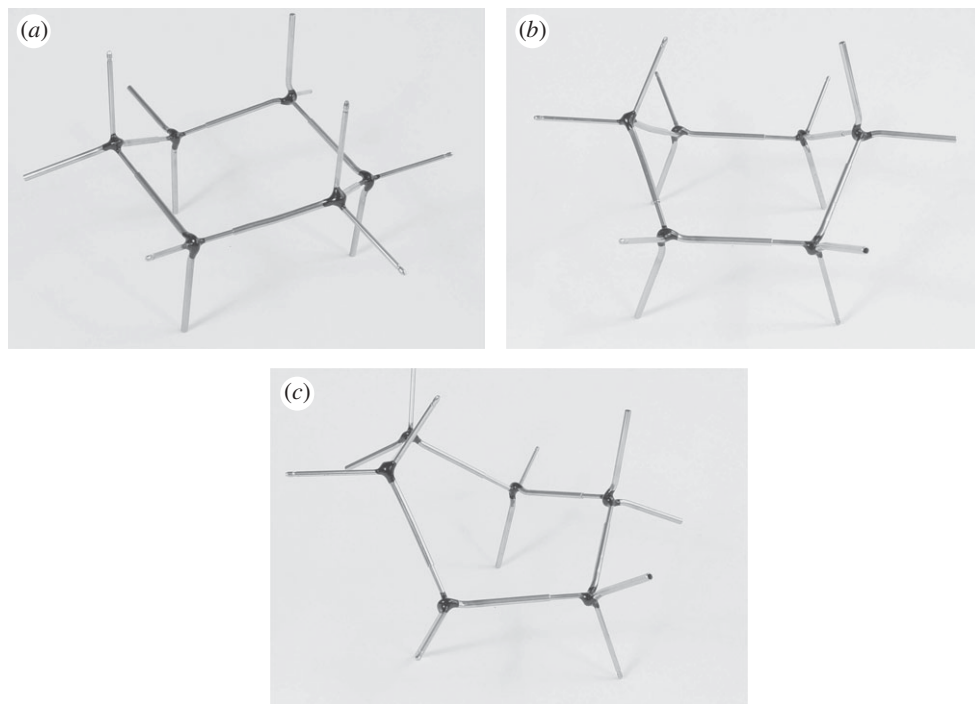


Figure 3. Dreiding models of the cyclohexane ring in: (a) chair; (b) boat; and (c) twist-boat conformations.

of hinges, following a one-parameter continuous path (e.g. Baker (1986), and the complete map of the conformation space given in a recent computational study (Porta *et al.* 2007)). Unlike the stiffer Tangle model, the chair Dreiding model can be ‘snapped through’ to the boat form by the deformation of the components.

Even simpler models of  $N$ -loops are possible. Goldberg (1978) gave a net from which a paper model of Bricard’s (1897) flexible octahedron can be made, and, as we show in figure 4, this generates a corresponding non-regular six-loop.

The concept of mobility is central to the analysis of the kinematic properties of all these models. The mobility criterion associated with the classic work of Kutzbach and Grübler (Hunt 1978) is usually interpreted as a counting rule that quantifies the kinematic degrees of freedom of a system, and, in favourable cases, reveals the existence of mechanisms (freedoms) or states of self-stress (overconstraints). However, counting alone cannot distinguish, for example, between the rigid chair and non-rigid boat forms of the six-loop. A key difference between the chair and the boat forms is their point-group symmetry, and it turns out that symmetry considerations explain the difference in mobility. In the present paper, we cast the general symmetry-extended mobility criterion (Guest & Fowler 2005) in a form suitable for the analysis of the kinematics of the  $N$ -loop, and use this to examine generically symmetric configurations for different values of  $N$ , strengthening the counting results, and rationalizing the observed mobility in many cases.

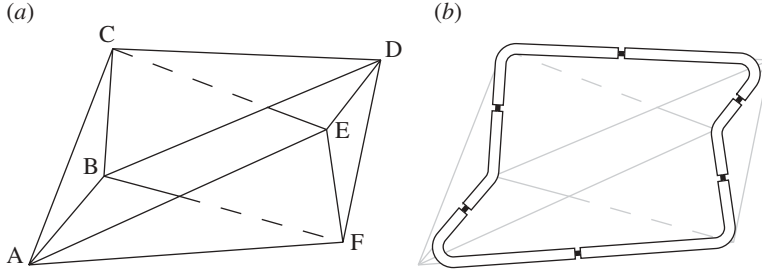


Figure 4. Flexibility of the Bricard octahedron. (a) Flattened form (after Goldberg 1978) in which the intersecting faces BDF and ACE have been removed, thus allowing the rest of the structure to flex. (b) An equivalent planar non-regular six-loop.

## 2. Preliminary counting analysis

As a simple generic counting relationship for calculating the degrees of freedom of a mechanical linkage, the mobility criterion is a familiar concept in mechanism theory. In Hunt's (1978) formulation, as extended by the present authors (Guest & Fowler 2005), a mechanical linkage consisting of  $n$  bodies connected by  $g$  joints, where joint  $i$  permits  $f_i$  relative freedoms, has relative mobility

$$m - s = 6(n - 1) - 6g + \sum_{i=1}^g f_i, \quad (2.1)$$

where  $m - s$  is the difference between the mobility, or the number of mechanisms,  $m$ , and the number of independent states of self-stress,  $s$ . This equation counts the degrees of freedom by taking the difference between the *relative body freedoms*, of which there are  $6(n - 1)$ , and the constraints imposed by the joints, of which there are  $\sum_{i=1}^g (6 - f_i)$ .

For a loop of  $N$  components, the numbers of bodies and joints are equal,  $n = g = N$ , and each revolute hinge allows a single relative freedom,  $f_i = 1$  for all  $i$ . Therefore,

$$m - s = 6(N - 1) - 6N + N = N - 6, \quad (2.2)$$

and the  $N$ -loop is guaranteed to have  $m > 0$  mechanisms for all  $N > 6$ . For  $N = 4$ , the  $N$ -loop has at least two states of self-stress, and for  $N = 5$  it has at least one. For  $N = 6$ , the loop has equal numbers of mechanisms and states of self-stress,  $m - s = 0$ . For  $N > 6$ , each mechanism beyond the minimum count of  $N - 6$  necessarily implies a corresponding extra state of self-stress.

Clearly, from the observations described in the introduction, this simple counting exercise has not captured all aspects of the mobility of an  $N$ -loop. For example, the four-loop has in fact infinitesimal mobility,  $m = 1$ . The six-loop has two forms, both with  $m - s = 0$ , but one is rigid ( $m = s = 0$ ) and the other has finite mobility ( $m = s = 1$ ). To gain further insight, we need a symmetry-extended mobility criterion for  $N$ -loops that compares not only total numbers, but also symmetries, of the mechanisms and the states of self-stress.

### 3. A symmetry-extended mobility analysis

The extended mobility criterion (Guest & Fowler 2005) relates the *representations* of the mechanisms and states of self-stress to those of various features of the structure. A representation  $\Gamma(\text{object})$  describes the symmetry of a set of objects (which may be joints, bars, vectors or other local structural or dynamical motifs) in the relevant point group of the structure.  $\Gamma(\text{object})$  collects the *characters*  $\chi(S)$  of sets of objects, i.e. for each symmetry operation  $S$ ,  $\chi(S)$  is the trace of the matrix that relates the set before and after the application of  $S$ . For further details, see Bishop (1973).

In the language of representations, the extended mobility criterion for a collection of bodies can be written (Guest & Fowler 2005)

$$\Gamma(m) - \Gamma(s) = \Gamma(\text{relative body freedoms}) - \Gamma(\text{hinge constraints}), \quad (3.1)$$

where  $\Gamma(m)$  and  $\Gamma(s)$  are, respectively, the representations of the mobility and the states of self-stress. The relative body freedoms are the freedoms of all the bodies of the mechanical linkage, in the absence of connections, and taken relative to one body considered as a reference. The *hinge constraints* are those constraints imposed by hypothetical rigid joints, minus the actual freedoms at the joints. A rigid joint removes six freedoms, i.e. three relative rotations and three relative translations. In the present case, all joints are revolute hinges, each of which restores one relative rotational freedom about the line of the hinge joining a pair of bodies.

An alternative way of formulating the extended mobility criterion is to consider the relative mobility of the structure where all joints are fixed and rigid-body motions are prevented, which we will call  $\Gamma_{\text{fix}}$ . To obtain  $\Gamma(m) - \Gamma(s)$ , we then restore the various hinge freedoms spanning  $\Gamma(\text{hinge freedoms}) \equiv \Gamma_f$ , and write

$$\Gamma(m) - \Gamma(s) = \Gamma_{\text{fix}} + \Gamma_f. \quad (3.2)$$

For a structure with all joints fixed, there can be no mechanisms,  $\Gamma(m) = 0$ , and it is apparent that  $\Gamma_{\text{fix}}$  is the negative of the representation of the states of self-stress of a completely rigid structure that has the same topology as the original linkage.

In describing the mobility of a general mechanical linkage, it is useful to define the linkage topology through what is often loosely called the contact *polyhedron*  $C$ , a graph embedded in three-dimensional space that has ‘vertices’ at bodies, and ‘edges’ through joints. The point group of this embedded graph is  $G(C)$ . (In fact, in the case of the  $N$ -loop,  $C$  reduces to a (non-planar) contact polygon, as each body is joined to exactly two others.) In terms of the properties of  $C$ , the symmetry-extended mobility rule of the general mechanical linkage is (Guest & Fowler 2005)

$$\Gamma(m) - \Gamma(s) = (\Gamma_\sigma(v, C) - \Gamma_{\parallel}(e, C) - \Gamma_0) \times (\Gamma_T + \Gamma_R) + \Gamma_f, \quad (3.3)$$

where  $\Gamma_\sigma(v, C)$  is the *permutation representation* of the vertices of  $C$  (a permutation representation of a set has character  $\chi(S)$  equal to the number of elements of the set left in place by the operation  $S$ ), and where  $\Gamma_{\parallel}(e, C)$  is the representation of a set of vectors along the edges of  $C$ .  $\Gamma_0$  is the totally symmetric representation, with  $\chi_0(S) = 1$  for all  $S$ , and  $\Gamma_T$  and  $\Gamma_R$  are the

representations of rigid-body translations and rotations, respectively.  $\Gamma_0$ ,  $\Gamma_T$  and  $\Gamma_R$  can be read off from standard point-group theory tables (e.g. Atkins *et al.* 1970; Altmann & Herzog 1994).

Substituting the formulation (3.2) in (3.3), we see that, for the general  $N$ -loop,  $\Gamma_{\text{fix}}$  is the six-dimensional representation

$$\Gamma_{\text{fix}} = (\Gamma_\sigma(v, C) - \Gamma_{\parallel}(e, C) - \Gamma_0) \times (\Gamma_T + \Gamma_R). \quad (3.4)$$

This expression can be simplified, as we will see below.

The other term in this approach to the calculation of mobility,  $\Gamma_f$ , which describes the set of hinge freedoms, is also associated with a structural representation of the contact polyhedron. The freedom of a revolute hinge, the axis of which is parallel to an edge of the contact polyhedron, is described in group-theoretical terms by Guest & Fowler (2005). Such a freedom has the nature of a local pseudo-scalar: if an operation  $S$  leaves a particular hinge unshifted, then the contribution to the overall character for the set of hinges is  $+1$  for proper, and  $-1$  for improper operations  $S$ . Therefore,  $\Gamma_f$  for the set of revolute hinges in an  $N$ -loop is

$$\Gamma_f = \Gamma_\sigma(e, C) \times \Gamma_\epsilon, \quad (3.5)$$

where  $\Gamma_\sigma(e, C)$  is the permutation representation of the edges of  $C$ , and  $\Gamma_\epsilon$  is the representation of a central pseudo-scalar, having character  $\chi(S) = +1$  for proper, and  $-1$  for improper  $S$ .

Substituting equation (3.5) into (3.3) gives a specific form of the mobility criterion applicable to an  $N$ -loop, the loop equation

$$\Gamma(m) - \Gamma(s) = (\Gamma_\sigma(v, C) - \Gamma_{\parallel}(e, C) - \Gamma_0) \times (\Gamma_T + \Gamma_R) + \Gamma_\sigma(e, C) \times \Gamma_\epsilon. \quad (3.6)$$

This equation too can be greatly simplified by taking into account the properties of the different representations associated with  $C$ , as we will see below. It is convenient to split the discussion of  $\Gamma_{\text{fix}}$  (§3a) and  $\Gamma_f$  (§3b) before producing unified expressions for the mobility of the  $N$ -loop (§3c).

### (a) States of self-stress in a ring structure

The highest point-group symmetry  $G(C)$  achievable by an  $N(\theta)$ -loop is  $D_{Nh}$  (for the planar structure that exists when  $\theta = 2\pi/N$ ). Any other conformation belongs to a subgroup of  $D_{Nh}$ , and results obtained in the higher group can be specialized to particular conformations using descent in symmetry or inspection of characters.

We use the standard  $D_{Nh}$  setting with the  $z$ -direction along the principal rotational axis. It is useful to present the odd  $N = 2p + 1$  and even  $N = 2p$  (both with  $p > 0$ ) cases separately before writing the fully general formula.

#### (i) $N$ odd

For odd cycles, the edge and vertex representations are equal

$$(N \text{ odd}): \quad \Gamma_\sigma(e, C) = \Gamma_\sigma(v, C), \quad (3.7)$$

and, independently of the parity of  $N$ , the representation of a set of vectors along the edges of the cycle is

$$\Gamma_{\parallel}(e, C) = \Gamma(R_z) \times \Gamma_\sigma(e, C), \quad (3.8)$$

where  $\Gamma(R_z)$  is the representation of the rotation about the principal axis.

The form of equation (3.4) conceals a high degree of cancellation, which can be removed by considering an angular-momentum type expansion of the two vertex-related terms. In general, the odd cycle has contributions to  $\Gamma_\sigma(v, C)$  from complete sets with axial angular momentum components 0 to  $p = (N - 1)/2$ ,

$$(N \text{ odd}): \quad \Gamma_\sigma(v, C) = \Gamma_\sigma(e, C) = \Gamma_0 + \sum_{L=1}^p \Gamma_L = A'_1 + \sum_{L=1}^p E'_L, \quad (3.9)$$

where  $\Gamma_0$  is the symmetry of the nodeless in-phase combination of all vertices and the notation  $\Gamma_L$  stands for the representation of the two independent combinations of vertices (or edges) with  $L$  angular nodal planes (corresponding to the set of two degenerate functions with components  $\pm L$  of angular momentum about the principal axis).

As the vector representation  $\Gamma_\parallel(e, C)$  arises by the multiplication of  $\Gamma_\sigma(e, C)$  with the one-dimensional representation  $\Gamma(R_z) = A'_2$ , the summation term is left unchanged, and  $\Gamma_\parallel(e, C)$  and  $\Gamma_\sigma(v, C)$  differ in only one term

$$(N \text{ odd}): \quad \Gamma_\parallel(e, C) - \Gamma_\sigma(v, C) = \Gamma(R_z) - \Gamma_0 = A'_2 - A'_1. \quad (3.10)$$

Thus, for the odd- $N$  loop, equation (3.4) becomes

$$(N \text{ odd}): \quad \Gamma_{\text{fix}} = -\Gamma(R_z) \times (\Gamma_T + \Gamma_R) = -A'_1 - E'_1 - A''_1 - E''_1. \quad (3.11)$$

(ii)  $N$  even

For even cycles, edge and vertex representations are in general different. An even cycle is a *bipartite* graph, one in which vertices can be partitioned into two sets, such that no two members of a set are adjacent. Vertices of the cycle belong alternately to these ‘starred’ and ‘unstarred’ sets. The vertex representation for even  $N$ , as before, can be written as an expansion in angular momentum, but now also includes a final, non-degenerate, fully antisymmetric combination that has a change of sign between each adjacent pair of vertices. The symmetry of this special combination is the *alternating representation*,  $\Gamma_\star$ , which has character  $\chi_\star(S) = +1$  for operations that preserve, and  $\chi_\star(S) = -1$  for operations that swap, the starred and unstarred sets.

For even cycles, the difference between the vertex and the edge permutation representations can be calculated from  $\Gamma_\star$ , as  $\Gamma_\sigma(v, C)$  includes  $\Gamma_\star$ , but the edge representation includes  $\Gamma_\star \times \Gamma(R_z)$ , where  $\Gamma_\star$  and  $\Gamma_\star \times \Gamma(R_z)$  form the two halves of the  $L = p$  angular-momentum pair. The vertex and edge representations, for  $D_{ph}$  with  $p$  finite, are therefore

$$(N \text{ even}): \quad \Gamma_\sigma(v, C) = A_{1g} + \Gamma_\star + \sum_{L=1}^{p-1} E_{Lg/u} \quad (3.12)$$

and

$$(N \text{ even}): \quad \Gamma_\sigma(e, C) = \Gamma_\sigma(v, C) - \Gamma_\star + \Gamma_\star \times \Gamma(R_z), \quad (3.13)$$

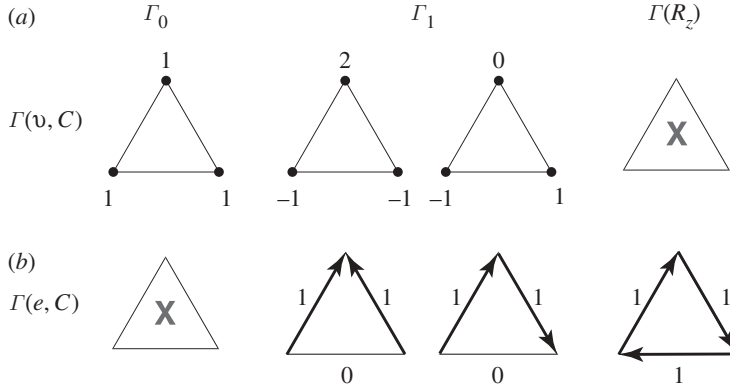


Figure 5. Correspondence between vertex- and edge-vector representations for cycles. Weights in the (a) vertex combinations correspond to net flows into vertices in the (b) edge-vector combinations. Only one combination of each type is unmatchable (X).

and the edge-vector representation (3.8) is

$$(N \text{ even}): \quad \Gamma_{\parallel}(e, C) = A_{2g} + \Gamma_{\star} + \sum_{L=1}^{p-1} E_{Lg/u}. \quad (3.14)$$

In equations (3.12) and (3.14), the notation means that  $E_{Lg/u}$  has  $g$  symmetry for even  $L$  and  $u$  symmetry for odd  $L$ .

Thus, for the even- $N$  loop, equation (3.4) becomes

$$(N \text{ even}): \quad \Gamma_{\text{fix}} = -\Gamma(R_z) \times (\Gamma_T + \Gamma_R) = -A_{1g} - E_{1g} - A_{2u} - E_{1u}. \quad (3.15)$$

### (iii) General formulation

Although the end results (3.11) and (3.15) appear superficially different because of the different notation for representations of  $D_{Nh}$  with odd and even  $N$ , they carry the same information, which is topological in character. The generic form for  $\Gamma_{\text{fix}}$  arises from the fact that, for any cycle,  $\Gamma_{\parallel}(e, C)$  differs from  $\Gamma_{\sigma}(v, C)$  only by substitution of  $\Gamma(R_z)$  for  $\Gamma_0$ . A cyclic array of arrows cannot be totally symmetric in  $D_{Nh}$  but it can achieve the symmetry of a rotation when all  $N$  arrows point in the same sense; a cyclic array of vertices can have a totally symmetric set of weights, but cannot have weights corresponding to rotation (figure 5). Both odd- $N$  and even- $N$  cases are therefore represented by the general formula

$$\Gamma_{\text{fix}} = -\Gamma(R_z) \times (\Gamma_T + \Gamma_R) = -\Gamma_0 - \Gamma_{\epsilon} - \Gamma(x, y) - \Gamma(R_x, R_y), \quad (3.16)$$

which can be easily specialized for any particular group. This can be done either by following the fate of the irreducible representations under descent in symmetry, or by using the characters  $\chi(S)$  for the individual operations.  $\Gamma_{\text{fix}}$  has character zero under all improper operations (as it is proportional to  $(\Gamma_T + \Gamma_R)$ ) and under proper operations it has  $\chi_{\text{fix}}(E) = -6$ ,  $\chi_{\text{fix}}(C_n) = -2 - 4 \cos \phi$ ,  $\chi_{\text{fix}}(C'_2) = -2$ .

The r.h.s. of equation (3.16) is the (negative of the) generic symmetry description of the set of states of self-stress arising from the linking together of  $N$  bodies in a cycle. This is a direct consequence of the toroidal topology of the linked

bodies, and other rigid toroidal assemblies also have the same set of states of self-stress. The same symmetry has been derived for the states of self-stress of toroidal deltahedra using symmetry-extended Maxwell analysis (Fowler & Guest 2002), and occurs as a contribution to the mobility equation for the toroidal rotating rings of tetrahedra (Fowler & Guest 2005). The deltahedra are rigid and so have no term  $\Gamma(m)$ ; compared with the  $N$ -loops, the rotating rings have a different mode of linkage and a different partial cancellation of  $\Gamma(m)$  and  $\Gamma(s)$ . However, in all three cases, equation (3.16) appears as the symmetry description of the states of self-stress imposed by the closure of a chain of bodies into a rigid torus.

(b) *Hinge freedoms for the  $N$ -loop*

An angular-momentum type expansion is also useful for the representation of the hinge freedoms,  $\Gamma_f = \Gamma_\epsilon \times \Gamma_\sigma(e, C)$ . In  $D_{(2p+1)h}$ , multiplication by  $\Gamma_\epsilon = A_1''$  interconverts  $E_L'$  and  $E_L''$ , and, from equation (3.9),

$$(N = 2p + 1): \quad \Gamma_f = \Gamma_\epsilon + \sum_{L=1}^p \Gamma_L \times \Gamma_\epsilon = A_1'' + \sum_{L=1}^p E_L''. \quad (3.17)$$

In  $D_{2ph}$ , multiplication by  $\Gamma_\epsilon = A_{1u}$  interconverts  $E_{Lg}$  and  $E_{Lu}$ , and, from equation (3.13),

$$(N = 2p): \quad \Gamma_f = \Gamma_\epsilon + \Gamma_\star \times \Gamma(z) + \sum_{L=1}^{p-1} \Gamma_L \times \Gamma_\epsilon = A_{1u} + \Gamma_\star \times \Gamma(z) + \sum_{L=1}^{p-1} E_{Lu/g}, \quad (3.18)$$

where the reversal of  $g/u$  subscripts in equation (3.18) means that odd  $L$  values now imply  $g$ , even  $L$  values imply  $u$ .

The general expression subsuming odd and even cases is therefore

$$\Gamma_f = \Gamma_\epsilon + [\Gamma_\star \times \Gamma(z)] + \sum_{L=1}^{\lfloor (N-1)/2 \rfloor} \Gamma_L \times \Gamma_\epsilon, \quad (3.19)$$

where the term in square brackets is understood to be omitted for odd  $N$ . This expression is easily specialized for any particular group:  $\Gamma_f$  has characters  $\chi_f(E) = N = -\chi_f(\sigma_h)$ ,  $\chi_f(C_n) = \chi_f(S_n) = \chi_f(i) = 0$ ,  $\chi_f(\sigma_v) = e_v$ ,  $\chi_f(C_2') = e_2$ , where  $e_v$  and  $e_2$  are the numbers of edges on the  $\sigma_v$  and  $C_2'$  symmetry elements, respectively.

(c) *Mobility of the  $N$ -loop*

Substitution of equations (3.11), (3.17) and (3.15), (3.18) into the mobility criterion (3.6) leads to explicit expressions for the mobility of the  $N$ -loop

$$(N = 2p + 1): \quad \Gamma(m) - \Gamma(s) = -A_1' - E_1' + \sum_{L=2}^p E_L'', \quad (3.20)$$

$$(N = 2p): \quad \Gamma(m) - \Gamma(s) = A_{2u} \times \Gamma_\star - A_{1g} - E_{1u} + \sum_{L=2}^{p-1} E_{Lu/g} \quad (3.21)$$

and

$$(\text{all } N): \quad \Gamma(m) - \Gamma(s) = [\Gamma_\star \times \Gamma(z)] - \Gamma_0 - \Gamma(x, y) + \sum_{L=2}^{\lfloor (N-1)/2 \rfloor} \Gamma_L \times \Gamma_\epsilon, \quad (3.22)$$

where  $\Gamma(x, y)$  is the representation of the two translations in the plane perpendicular to the principal axis.

In equations such as (3.22) and (3.19),  $\Gamma_\star$  (defined only when  $N$  is even) depends on both the size of the  $N$ -loop and its setting within the point group. If we agree to fix the even- $N$ -cycle in  $D_{Nh}$  so that  $C_2''$  and  $\sigma_d$  symmetry elements each pass through vertices of the cycle, then  $\Gamma_\star$  has  $\chi_\star(C_2'') = \chi_\star(\sigma_d) = -1$ ,  $\chi_\star(C_2') = \chi_\star(\sigma_d) = +1$ , and is  $\Gamma_\star = B_{2g}$  for  $N = 4m$  and  $\Gamma_\star = B_{2u}$  for  $N = 4m + 2$ . The term appearing in  $\Gamma_f$  and  $\Gamma(m) - \Gamma(s)$  is then  $\Gamma_\star \times \Gamma(z) = B_{1u}$  for  $N = 4m$  and  $\Gamma_\star \times \Gamma(z) = B_{1g}$  for  $N = 4m + 2$ .

Equation (3.22) is the generic symmetry description of the mobility arising from the linking together of  $N$  bodies in a cycle where the links are revolute hinges whose axes intersect. In many applications, the  $N$ -loop will be regular, i.e. it will be characterized by a single nearest-neighbour distance, and a constant intersection angle. However, equation (3.22) applies more generally, both for a regular object adopting a less symmetrical conformation and for an object with a more general distribution of distances and angles, when specialized to the appropriate point group.

#### 4. Examples

In this section, we will look at some general classes of conformations of  $N$ -loops, and examine the behaviour of small cases.

##### (a) Planar conformations of $N$ -loops

If the intersection angle  $\theta$  is  $\pi - 2\pi/N$ , then a unique planar conformation is possible for a regular  $N$ -loop. We can use the present approach to derive a general formula for the mechanisms and states of self-stress in such conformations.

The group of the regular polygon is  $D_{Nh}$ . In the groups of this type there is no cancellation between the positive and the negative terms of the r.h.s. of equation (3.22), i.e. the non-degenerate representations  $\Gamma_\star \times \Gamma(z)$ ,  $\Gamma_0$  are not equal, and the degenerate  $\Gamma(x, y)$  is not repeated by any of the terms under the summation sign. Hence, we can be sure that the negative terms are included in the symmetry of the states of self-stress and the positive terms in the symmetry of the mechanisms

$$\Gamma(s) \supset \Gamma_0 + \Gamma(x, y) \quad (4.1)$$

$$\text{and} \quad \Gamma(m) \supset [\Gamma_\star \times \Gamma(z)] + \sum_{L=2}^{\lfloor (N-1)/2 \rfloor} \Gamma_L \times \Gamma_\epsilon. \quad (4.2)$$

We can strengthen these inequality results by the following argument which fixes  $\Gamma(s)$ . Consider building up the cycle by introducing the  $N$  joints between the bodies one by one in a cyclic order. When  $N - 1$  joints have been introduced, we

have a chain of  $N$  bodies connected by  $N - 1$  revolute hinges, each of which lies in the plane, and so far there are no states of self-stress. States of self-stress arise from possible misfits when connecting the final joint. No in-plane misalignment can be corrected by the rotation of an in-plane hinge, but any out-of-plane misalignment can be corrected by appropriate hinge rotation. Thus,  $s = 3$ . Inequalities (4.1) and (4.2) become equalities, applicable for any  $N$ ,

$$\Gamma(s) = \Gamma_0 + \Gamma(x, y) \quad (4.3)$$

$$\text{and} \quad \Gamma(m) = [\Gamma_\star \times \Gamma(z)] + \sum_{L=2}^{\lfloor (N-1)/2 \rfloor} \Gamma_L \times \Gamma_\epsilon. \quad (4.4)$$

Note that the term containing  $\Gamma_\star$  is defined only for  $N$  even, and the summation over  $L$  is non-empty only for  $N \geq 5$ .

- $N = 3$ . The three-loop can exist only in a planar confirmation, and hence is generically rigid. Evaluation of  $\Gamma(s)$  and  $\Gamma(m)$  in  $D_{3h}$  leads straightforwardly in  $\Gamma(s) = A'_1 + E'$  and  $\Gamma(m) = 0$ .
- $N = 4$ . In  $D_{4h}$  symmetry, with the convention that  $C_2''$  and  $\sigma_d$  pass through a pair of vertices in the contact polyhedron, we have for the four-loop  $\Gamma(m) - \Gamma(s) = B_{1u} - A_{1g} - E_u$ , and hence  $\Gamma(s) = A_{1g} + E_u$  and  $\Gamma(m) = B_{1u}$ . There is therefore an infinitesimal mechanism which may be blocked by the totally symmetric state of self-stress (Kangwai & Guest 1999), and hence may not extend to a finite path.
- $N \geq 5$ . The five-loop ( $D_{5h}$ ) has  $\Gamma(s) = A'_1 + E'_1$  and  $\Gamma(m) = E''_2$ . The six-loop ( $D_{6h}$ ) has  $\Gamma(s) = A_{1g} + E_{1u}$  and  $\Gamma(m) = B_{1g} + E_{2u}$ . The series continues with  $s = 3$  and  $m = N - 3$ , and the general forms of  $\Gamma(s)$  and  $\Gamma(m)$  in  $D_{Nh}$  are deducible from equations (3.21) and (3.20).

### (b) Crown conformations of $N$ -loops

For even values of  $N$ , and intersection angles  $\theta$  smaller than  $\pi - 2\pi/N$ , ‘crown’ conformations of  $D_{(N/2)d}$  symmetry, in which the bodies lie alternately above and below the median plane, are possible. In  $D_{(N/2)d}$ ,  $\Gamma_\star$  is equal to  $\Gamma(z)$  ( $B_2$  when  $N/2$  is even,  $A_{2u}$  when  $N/2$  is odd), and the product  $\Gamma(z) \times \Gamma_\star$  is equal to  $\Gamma_0$ . Degenerate representations in these groups obey

$$\Gamma_L \times \Gamma_\epsilon = \Gamma_{N/2-L}, \quad (4.5)$$

and therefore the summation of  $\Gamma_L \times \Gamma_\epsilon$  from  $L = 2$  to  $L = \lfloor (N - 1)/2 \rfloor$  contains  $\Gamma(x, y)$  for  $N \geq 6$ . Thus, both terms describing the states of self-stress in equation (3.22) are cancelled out, leaving the following expressions for the mechanisms in the two distinct cases of even  $N$ :

$$(N = 4p + 2 \geq 6): \quad \Gamma(m) \supset \sum_{i=2}^{(N-2)/4} (E_{ig} + E_{iu}) \quad (4.6)$$

and

$$(N = 4p > 6): \quad \Gamma(m) \supset \sum_{i=2}^{(N-4)/2} E_i. \quad (4.7)$$

- $N = 4$ . In the  $D_{2d}$  crown conformation of the four-loop,  $\Gamma(m) - \Gamma(s) = -\Gamma(x, y)$ , indicating that  $\Gamma(s)$  contains  $\Gamma(x, y) = E$ . The loop is generically rigid, and hence  $s = 2$  and  $\Gamma(s) = E$ .
- $N = 6$ . In the  $D_{3d}$  crown conformation of the six-loop,  $\Gamma(m) - \Gamma(s) = 0$ . This conformation is generically rigid with  $m = s = 0$ . The chair form of cyclohexane is a specific instance with  $\theta = \theta_T$ .
- $N = 8$ . In the  $D_{4d}$  crown conformation of the eight-loop,  $\Gamma(m) - \Gamma(s) = E_2$ . There is a degenerate pair of mechanisms, related by a rotation of  $\pi/4$  about the principal axis. Each follows one of the pair of two-noded  $(xy, x^2 - y^2)$  harmonics. In each mechanism, one pair of bodies moves simultaneously outward, and another inward.

Mobilities for each crown conformation could also have been found by taking the mobility for the flat conformation, and making a descent in symmetry within the point-group chain  $D_{Nh} \rightarrow D_{(N/2)d}$ .

### (c) Special cases

Manipulation of models, as described in the introduction, reveals a number of conformations that do not fit into the previous classes.

- $N = 6$ . For  $\theta = \pi/2$ , the smallest special case occurs for  $N = 6$ , and is an analogue of the well-known boat form of cyclohexane. Unlike the chair, this is a flexible conformation. Generically, it retains only a  $C_2$  axis through the ring centre, but can attain the higher symmetries  $C_{2v}$  and  $D_{2d}$  at special points along the path of the mechanism (figure 2b(ii)(iii)). In the generic  $C_2$  conformation,  $\Gamma(m) = \Gamma(s) = A - B$ . At the  $D_{2h}$  conformation ( $C_2(y)$  passing through two hinges),  $\Gamma(m) = \Gamma(s) = B_1 - B_3$ . At the  $C_{2v}$  conformation ( $\sigma(y)$  passing through two hinges),  $\Gamma(m) = \Gamma(s) = A_2 - B_2$ . Hence, there is a mechanism preserving a  $C_2$  axis, and, in the absence of an equisymmetric state of self-stress, this mechanism must extend to a finite one-dimensional path.
- $N = 7$ . The mobility count for generic conformations of the seven-loop implies the existence of at least one mechanism. Manipulation of the models with  $\theta = \pi/2$  reveals two independent sets of non-interconverting conformations, analogues of the boat and chair of cycloheptane. Both are observed to be flexible, but generally with only the trivial symmetry  $C_1$ . The maximum point groups, reached at special conformations, are  $C_s$  (boat and chair) and  $C_2$  (twist-boat and twist-chair). For all conformations,  $\Gamma(m) - \Gamma(s)$  is a single irreducible representation. In the three accessible groups  $C_s$ ,  $C_2$  and  $C_1$ , this representation is, respectively,  $A''$ ,  $B$  and  $A$ . This indicates at least one mechanism that acts to lower the symmetry at the high-symmetry points.

## 5. Conclusions

We have given a general description of the mobility of the  $N$ -loop. Given any particular geometric configuration of an  $N$ -loop, we can predict its mechanisms and states of self-stress in greater detail than would be possible by counting

arguments alone, and in favourable cases can give a complete symmetry description of the mechanisms and states of self-stress. To complete the picture, it would be interesting to determine for given  $N$  the ranges of  $\theta$  for which conformations are realizable, and any induced partitioning of conformation space. For each realizable conformation, the symmetry machinery of the present approach can be applied. Techniques exist for numerical determination of realizability, and tracking of mechanisms in conformation space (Porta *et al.* 2007). Their application could give further insight into fields as diverse as chemical conformation analysis, and rigidity theory of engineering structures.

We note that it would be possible to extend the concept of  $N$ -loops to polycyclic and three-dimensional cage topologies by allowing more than two hinged contacts per body. Such cases are equally amenable to a symmetry treatment of the type that we have described here. However, full polyhedra tend to be highly overconstrained.

S.D.G. acknowledges the support of the Leverhulme Trust, and thanks Prof. C. R. Calladine for a timely Christmas present and Mark Schenk for the help with the translation from the Dutch. P.W.F. is grateful for a Royal Society/Wolfson Research Merit Award.

## References

- Altmann, S. L. & Herzig, P. 1994 *Point-group theory tables*. Oxford, UK: Clarendon Press.
- Atkins, P. W., Child, M. S. & Phillips, C. S. G. 1970 *Tables for group theory*. Oxford, UK: Oxford University Press.
- Baker, J. E. 1986 Limiting positions of a bricard linkage and their possible relevance to the cyclohexane molecule. *Mech. Mach. Theory*, **21**, 253–260. (doi:10.1016/0094-114X(86)90101-1)
- Bishop, D. M. 1973 *Group theory and chemistry*. Oxford, UK: Clarendon Press.
- Bricard, R. 1897 Mémoire sur la théorie de l'octaèdre articulé. *J. Math. Pures Appl., Liouville*, **3**, 113–148.
- Chen, Y., You, Z. & Tarnai, T. 2005 Three-fold symmetric bricard linkages for deployable structures. *Int. J. Solid Struct.*, **42**, 2287–2301. (doi:10.1016/j.ijsolstr.2004.09.014)
- Crippen, G. M. 1992 Exploring the conformation space of cycloalkenes by linearized embedding. *J. Comput. Chem.*, **13**, 351–361. (doi:10.1002/jcc.540130308)
- Dreiding, A. S. 1959 Einfache molekularmodelle. *Helvet. Chim. Acta*, **42**, 1339–1344. (doi:10.1002/hlca.19590420433)
- Dunitz, J. & Waser, J. 1972 Geometric constraints in six- and eight-membered rings. *J. Amer. Chem. Soc.*, **94**, 5645–5650. (doi:10.1021/ja00771a018)
- Eliel, E. L. 1962 *Stereochemistry of carbon compounds*. New York, NY: McGraw-Hill Book Company Inc.
- Fowler, P. W. & Guest, S. D. 2002 Symmetry and states of self stress in triangulated toroidal frames. *Int. J. Solid Struct.*, **39**, 4385–4393. (doi:10.1016/S0020-7683(02)00350-5)
- Fowler, P. W. & Guest, S. D. 2005 A symmetry analysis of mechanisms in rotating rings of tetrahedra. *Proc. R. Soc. A*, **461**, 1829–1846. (doi:10.1098/rspa.2004.1439)
- Freudenthal. 2003 B-dag 2003. For information about Freudenthal Instituut's Wiskunde B-Dag see <http://www.fi.uu.nl/wisbdag>; for results from tangle investigation see [http://www.fi.uu.nl/wisbdag/2003/voorblad\\_2003.doc](http://www.fi.uu.nl/wisbdag/2003/voorblad_2003.doc).
- Goldberg, M. 1978 Unstable polyhedral structures. *Math. Mag.*, **51**, 165–170.
- Graveron-Demilly, D. 1977 Conformation maps of some saturated six and seven membered rings. *J. Chem. Phys.*, **66**, 2874–2877. (Graveron-Demilly, D. 1978 Erratum: conformational maps of some saturated six and seven membered rings. *J. Chem. Phys.*, **68**, 785.) (doi:10.1063/1.434346)
- Guest, S. D. & Fowler, P. W. 2005 A symmetry-extended mobility rule. *Mech. Mach. Theory*, **40**, 1002–1014. (doi:10.1016/j.mechmachtheory.2004.12.017)

- Hunt, K. H. 1978 *Kinematic geometry of mechanisms*. Oxford, UK: Clarendon Press.
- Jacobs, D., Rader, A., Kuhn, L. & Thorpe, M. 2001 Protein flexibility predictions using graph theory. *Prot. Struct. Funct. Genet.* **44**, 150–165. (doi:10.1002/prot.1081)
- Kangwai, R. D. & Guest, S. D. 1999 Detection of finite mechanisms in symmetric structures. *Int. J. Solid Struct.* **36**, 5507–5527. (doi:10.1016/S0020-7683(98)00234-0)
- Kovács, F., Tarnai, T., Guest, S. D. & Fowler, P. W. 2004 Double-link expandedhedra: a mechanical model for expansion of a virus. *Proc. R. Soc. Lond. A* **460**, 3191–3202. (doi:10.1098/rspa.2004.1344)
- Porta, J., Ros, L., Thomas, F., Corcho, F., Cantó, J. & Pérez, J. 2007 Complete maps of molecular-loop conformational spaces. *J. Comput. Chem.* **28**, 2170–2189. (doi:10.1002/jcc.20733)
- Porta, J., Ros, L. & Thomas, F. 2009 A linear relaxation technique for the position analysis of multiloop linkages. *IEEE Trans. Robot.* **25**, 225–239. (doi:10.1109/TRO.2008.2012337)