ONLINE SUPPLEMENT 2

The effect of internal angles that deviate from ideal is small

[Please place Supplement 2 Figure S1 here.]

The curvature at a vertex in a discrete surface is given by the "angle deficit", 360° minus the sum of the three internal angles at the vertex. Thus, the angle deficits of ideal 666, 566, 556, and 555 vertices are 0°, 12°, 24°, and 36°, respectively. [The total angle deficit in a fullerene cage, like that in any convex polyhedron, is 720° (4π), the solid angle of a sphere (S1, S2).]

Here, following the Key diagram in the upper right of Supplement 2 Figure S1, we describe the three dihedral angles I, II, and III and their fall from their ideal values at a vertex due to internal angles A, B, and C that are 1° less than ideal. For example, the three dihedral angles about the three edges emerging from an ideal 666 vertex are 180°. If one of the internal angles is 119°, giving an angle deficit of 1° at the vertex, all three dihedral angles fall to almost the identical value, ~168.5°. (See 666 vertex in Supplement 2 Table S1.) If instead, all three internal angles are 119.67°, giving the same angle deficit of 1°, all three dihedral angles fall to virtually the same value, 168.5°. This example illustrates a general principle: Angle deficit is the key parameter in determining the three dihedral angles at a vertex, nearly independent of how that angle deficit is distributed among the three internal angles at that vertex.

[Please place Supplement 2 Table S1 here.]

We compare the effect on dihedral angle of reducing one internal angle by 1° at different types of vertex. [We already showed that even in the most distorted cages, internal angles vary little from the ideal angles (10).] Although there are just four combinations of faces about a three-connected vertex (666, 566, 556, and 555), there are eight permutations of faces, as shown in Supplement 2 Figure S1. Following the organization of that figure, Supplement 2 Table S1 shows eight sets of data. This table shows that a 1° reduction in one internal angle causes a reduction of ~11.5° in the dihedral angles about a vertical edge for the 666 vertex, 1.2°-1.9° for the three permutations of a 566 vertex, 0.7°-1.4° for the three permutations of a 556 vertex, and 0.5°-1.2° for the 555 vertex.

Thus, imperfect angles may cause a major change in the magnitude of the *D* about a green DAD edge, which involves a 666 vertex, but are likely to cause only a minor change about a red or a blue DAD edge. Indeed, the magnitude of the green *D*'s in Table 1 and Supplement 1 Table S1 is typically ~28° instead of the ideal 41.8°, whereas the magnitudes of the red and blue *D*'s typically approach their ideal values 18.4° and 14.6° closely.

Nonzero sum of internal and external rotations around a whole Ring

Imperfect angles, arranged in just the right way, can cause violation of equations 9 and 10, the rules that the internal and external rotations around a whole Ring sum to zero. However, as described here, the magnitude of the violation is small.

[Please place Supplement 2 Figure S2 here.]

In Supplement 2 Figure S2A, each of the surround pentagons in a hex-Ring 661 has a 107° internal angle in the same relative position. This imperfect angle is responsible for a *D* about each central edge of 0.48° (Supplement 2 Fig. S2B), with the vectors all pointing in the same (clockwise) direction. Thus, $\sum D = 2.88°$, not zero.

Normally, extension of equation 1 over the whole central face would yield

$$\sum_{whole} D = \sum_{whole} I - \sum_{whole} E \quad \text{(S1)}$$

and equations 9 and 10 mean that the $\sum D$ around the whole central face equals zero. Conversely, the nonzero $\sum D$ in Supplement 2 Figure 2A would cause a nonzero $\sum E$ with $\sum I = 0$ (with potentially a planar central face), a nonzero $\sum I$ with $\sum E = 0$ (with potentially planar surround faces), or a combination of nonzero $\sum I$ and $\sum$E. Thus, equations 9 and 10 can be violated. However, the magnitude of the violation is small.

LITERATURE CITED

S1. Sutton, D. 2002. Platonic and Archimedean solids. Walker and Co., New York.
S2. Grünbaum, B. 2003. Convex Polytopes, 2nd Edition. Springer-Verlag, New York.

SUPPLEMENT 2 TABLE S1

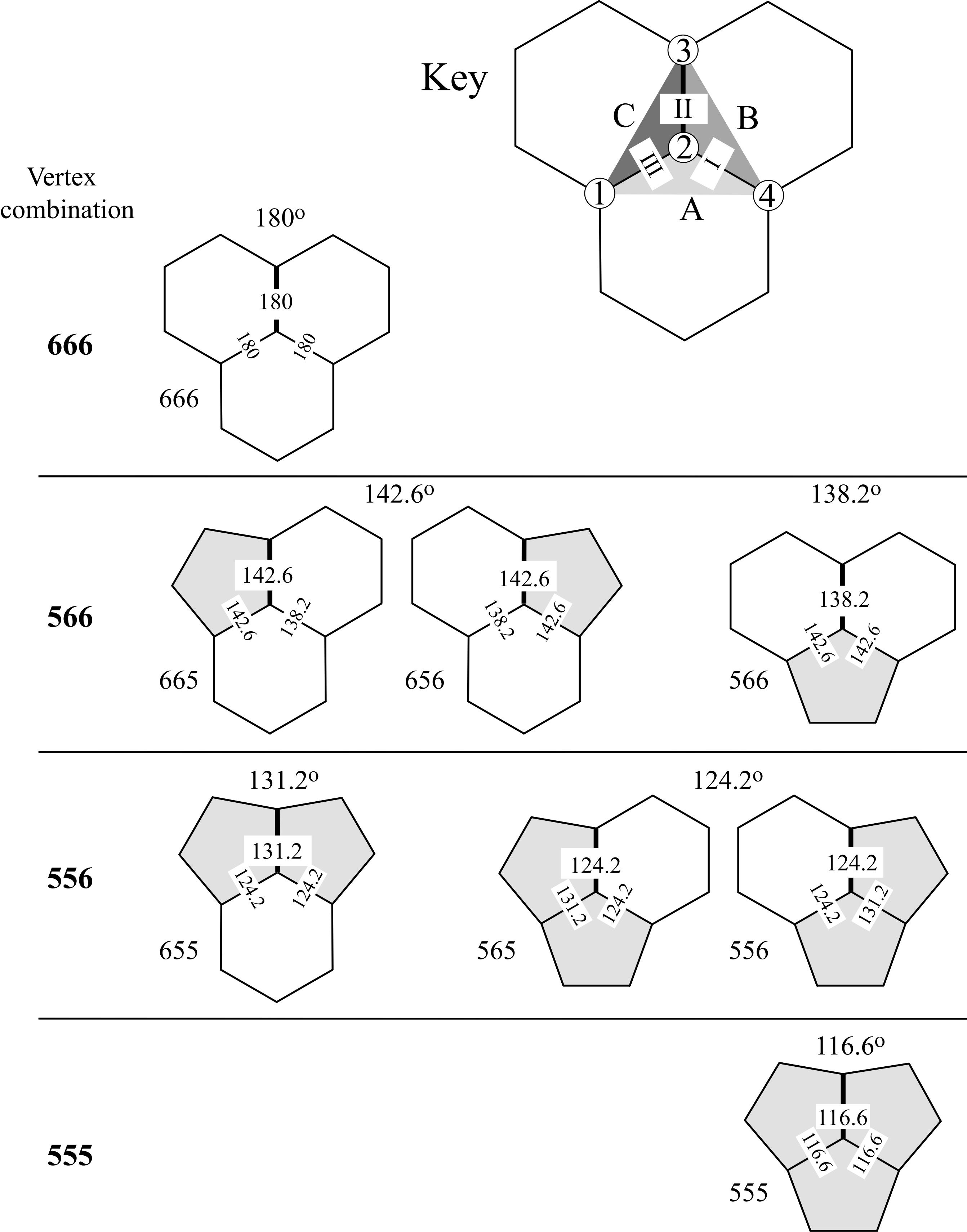
Vertex Combin-ations	Vertex Permut-ations	Internal angles A	Internal angles B	Internal angles C	Dihedral angles I	Dihedral angles II	Dihedral angles III	Fall in dihedral angles I	Fall in dihedral angles II	Fall in dihedral angles III
666	666	120	120	120	180.00	180.00	180.00	0.00	00.00	0.00
		119	120	120	168.56	168.45	168.56	11.44	11.55	11.44
		120	119	120	168.56	168.56	168.45	11.44	11.44	11.55
		119.67	119.67	119.67	168.53	168.53	168.53	11.47	11.47	11.47
566	665	120	120	108	138.19	142.62	142.62	0.00	0.00	0.00
		119	120	108	136.72	140.91	141.37	1.47	1.71	1.25
		120	119	108	136.72	141.37	140.91	1.47	1.25	1.71
	656	120	108	120	142.62	142.62	138.19	0.00	0.00	0.00
		119	108	120	141.37	140.91	136.72	1.25	1.71	1.47
		120	107	120	141.28	141.28	136.32	1.34	1.34	1.87
	566	108	120	120	142.62	138.19	142.62	0.00	0.00	0.00
		107	120	120	141.28	136.32	141.28	1.34	1.87	1.34
		108	119	120	141.37	136.72	140.91	1.25	1.47	1.71
556	655	120	108	108	124.25	131.17	124.25	0.00	0.00	0.00
		119	108	108	123.48	129.91	123.48	0.77	1.27	0.77
		120	107	108	123.34	130.47	122.86	0.91	0.70	1.39
	565	108	120	108	124.25	124.25	131.17	0.00	0.00	0.00
		107	120	108	123.34	122.86	130.47	0.91	1.39	0.70
		108	119	108	123.48	123.48	129.91	0.77	0.77	1.27
	556	108	108	120	131.17	124.25	124.25	0.00	0.00	0.00
		107	108	120	130.47	122.86	123.34	0.70	1.39	0.91
		108	107	120	130.47	123.34	122.86	0.70	0.91	1.39
555	555	108	108	108	116.57	116.57	116.57	0.00	0.00	0.00
		107	108	108	116.05	115.39	116.05	0.52	1.17	0.52
		108	107	108	116.05	116.05	115.39	0.52	0.52	1.17

Supplement 2 Table S1. Reduction in dihedral angles from their ideal values due to reduction in internal angles from their ideal values
Internal angles A, B, and C and dihedral angles I, II, and III follow the "Key" diagram in Supplement 2 Figure S1. The shaded entries in the A, B, and C columns are the ones that are changed by 1°, and the shaded entries in the two "II" columns are the resulting dihedral angle about the lower end of the vertical (thick) edge in Supplement 2 Figure 1 and the change in that dihedral angle II from its ideal value.

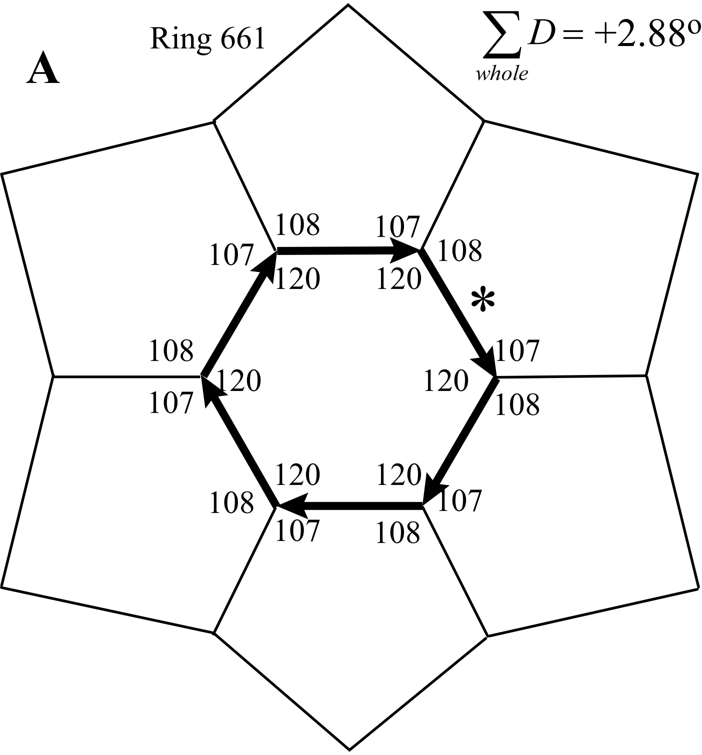
SUPPLEMENT 2 FIGURE LEGENDS

Supplement 2 Figure 1. Four combinations and eight permutations of three types of face about a vertex.
Key. With ideal internal angles A, B, and C of 120° in hexagons and 108° in pentagons, the diagram shows ideal dihedral angles I, II, and III about the three edges at a vertex. Given points 1, 2, 3, and 4 in this configuration, clicking those points in order with Spartan's dihedral angle function produces the angle between the 123 and the 324 planes, that is, the dihedral angle about their common (thick, vertical) edge 23 at the end of that edge near vertex 2.
Diagrams. For the eight permutations of the four combinations of vertex (666, 566, 556, and 666), there are six ideal dihedral angles about the lower end of thick, vertical edge 23 near vertex 2: These are 180°, 142.6°, 138.2°, 131.2°, 124.2°, and 116.6°.

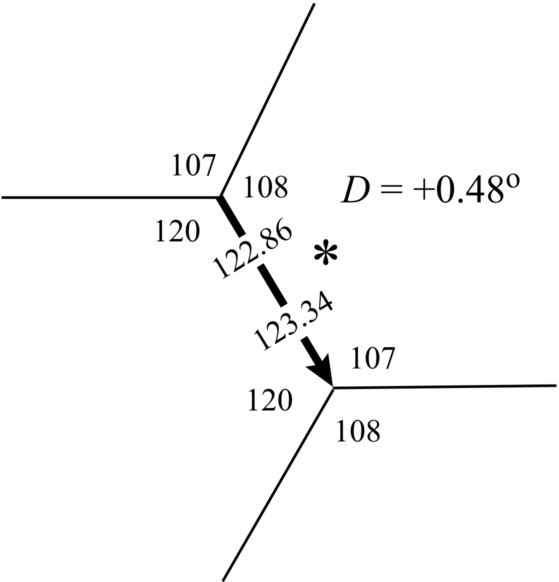
Supplement 2 Figure 2. A systematic arrangement of non-ideal internal angles can produce a nonzero ∑*D* around a whole Ring.
A. Each of the surround pentagons in this imperfect Ring 661 has a 107° internal angle in the corresponding site. The edges have DAD, the vectors all point in the same (clockwise; positive) direction, and the six *D*'s add to produce a nonzero ∑*D* = +2.88° about the edges of the central face. The edge with the asterisk is diagrammed in part **B**.
B. The *D* of the edge marked by the asterisk (and indeed that of all of the central edges) in **A** is +0.48°.


Key
3
C
II
B
2
III
I
1
4
A
Vertex combination
180°
180
180
180
666
666
142.6°
142.6
142.6
138.2
665
142.6
138.2
142.6
656
138.2°
138.2
142.6
142.6
566
566
131.2°
131.2
124.2
124.2
655
124.2°
124.2
131.2
124.2
565
124.2
124.2
131.2
556
556
116.6°
116.6
116.6
116.6
555
555

A


Ring 661
$\sum_{whole} D = +2.88^o$
108
107
107
108
120
120
*
108
107
120
120
107
108
120
120
108
107
107
108

B


107
108
$D = +0.48^o$
120
122.86
*
123.34
107
120
108