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Supporting information for article:

Isogonal weavings on the sphere: knots, links, polycatenanes

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A note on the symmetry of embeddings of knots and links

As materials scientists we think of symmetry as a rigid-body symmetry. Applied to knots, we mean the symmetry of a model of the knot or, more to the point, of a molecular assembly with that underlying topology. An abstract knot is a topology, not a rigid body and, as shown here, can have embeddings in symmetries that are not related as group-subgroup. Fig. S1 shows three depictions of the figure-8 knot 4_1 (Flapan, 1987, 2015). The piecewise linear representations have, we think, the highest possible symmetry (both groups of order 4). The symmetry $\bar{4}$ is generally preferred as it has lower transitivity and the knot is demonstrably achiral. Also shown in the figure are depictions of the Borromean rings. The most common illustrations are chiral, such as the piecewise linear drawing shown on the left. However, a different symmetry of higher order (but *not* a supergroup!) is also commonly used. As shown in that symmetry, embeddings with transitivity 1 2 and 2 1 are both possible, so even the transitivity is not unique for a given symmetry.

Another problem of concern is that of possible symmetries of isogonal embeddings knots and links. We consider this in three parts:

1. Chiral structures. We have systematically explored all the chiral groups in this paper. For axial symmetries the groups n (n an integer) obviously cannot support an isogonal knot as all n points are coplanar. For the groups $n2$ (n odd), $n22$ (n even), the cubic groups 23 and 432 , and the icosahedral group 235 we have systematically explored all space.
2. Achiral groups without mirrors. These are the groups \bar{n} (n odd or a multiple of 4). From experimentation we believe that no *isogonal* knots are possible although there are corner 2-transitive structures in each symmetry (cf. knot 4_1 cited above).
3. Groups with mirrors. There are knots with mirror symmetry: the square knot, composite of two 3_1 [torus knots (3,2)] in RCSR as **kok**, has an embedding with symmetry $2/m$ (C_{2h}). However, we are concerned here with knots and links with isogonal embeddings. We offer the speculation that these cannot contain mirror planes in their symmetries. Excepting of course the Borromean rings and the "Borromean twins".

On the catenanes of Hu *et al.*

In the main text we mentioned the interesting work of Hu *et al.* (2009) enumerating certain classes of cubic and icosahedral polycatenane structures. These were derived by replacing faces of regular polyhedra with polygons with entwined edges. We show the two simplest examples here and illustrate that they are corner

(vertex) 2-transitive in a piecewise linear embedding (Fig. S2). The link **rly**, derived from the tetrahedron, has symmetry 23 (*T*) and crossing number 12 and might be confused with the regular link **rka** (symmetry 432), described in the text, which also has crossing number 12. We note that Sawada *et al.* (2019) made polycatenanes based on both structures and proved mathematically that they were distinct links.

References

- Flapan, E. (1987). *Pacific J. Math.* **129**, 57-66.
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 Hu, G., Zhai, X.-D., Lu, D. & Qiu, W.-Y. (2009). *J. Math. Chem.* **46**, 592-603.
 Sawada, T., Saito, A., Tamiya, K., Shimokawa, K., Hisada, Y. & Fujita, M. (2019). *Nature Commun.* **10**, 921.

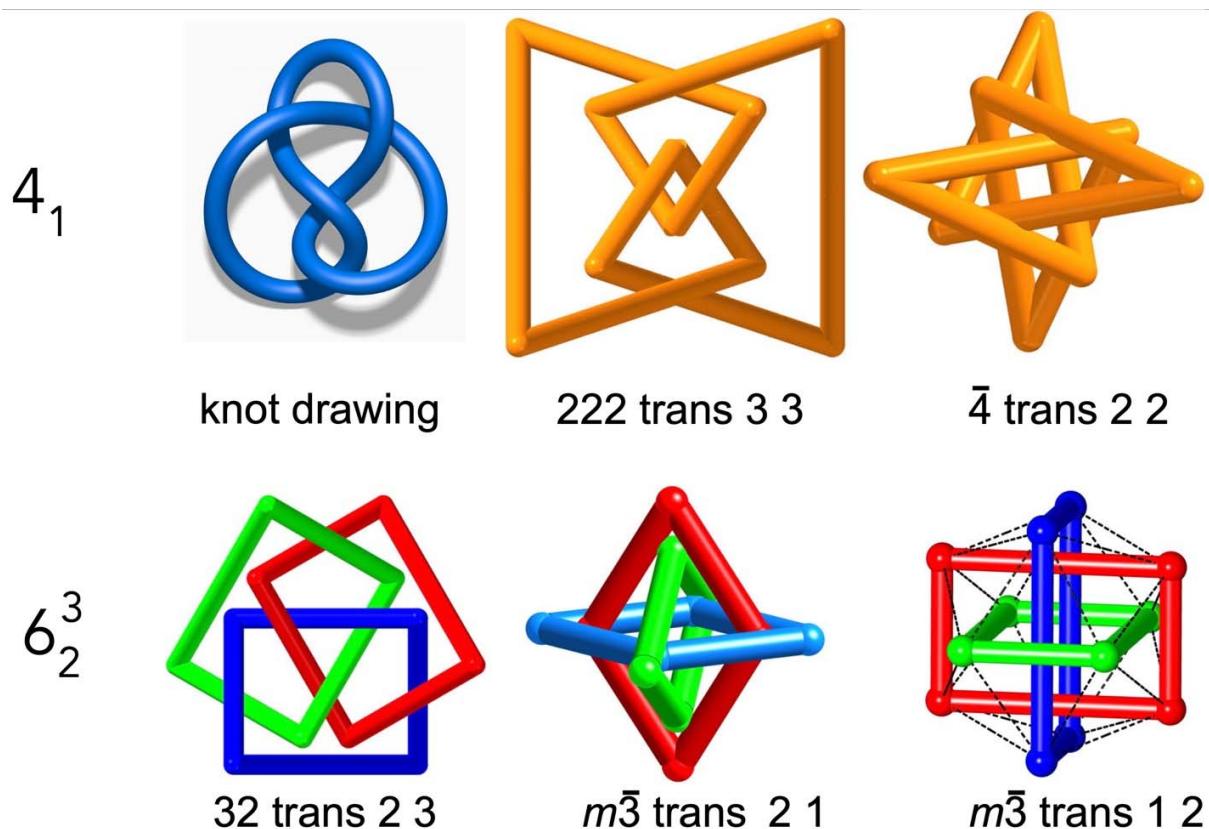


Figure S1. Embeddings of the figure-8 knot (top) and the Borromean rings (bottom). *Trans* refers to transitivity. Broken lines at bottom right outline an icosahedron. The drawing at top left comes from http://commons.wikimedia.org/wiki/File:Blue_Figure-Eight_Knot.png.

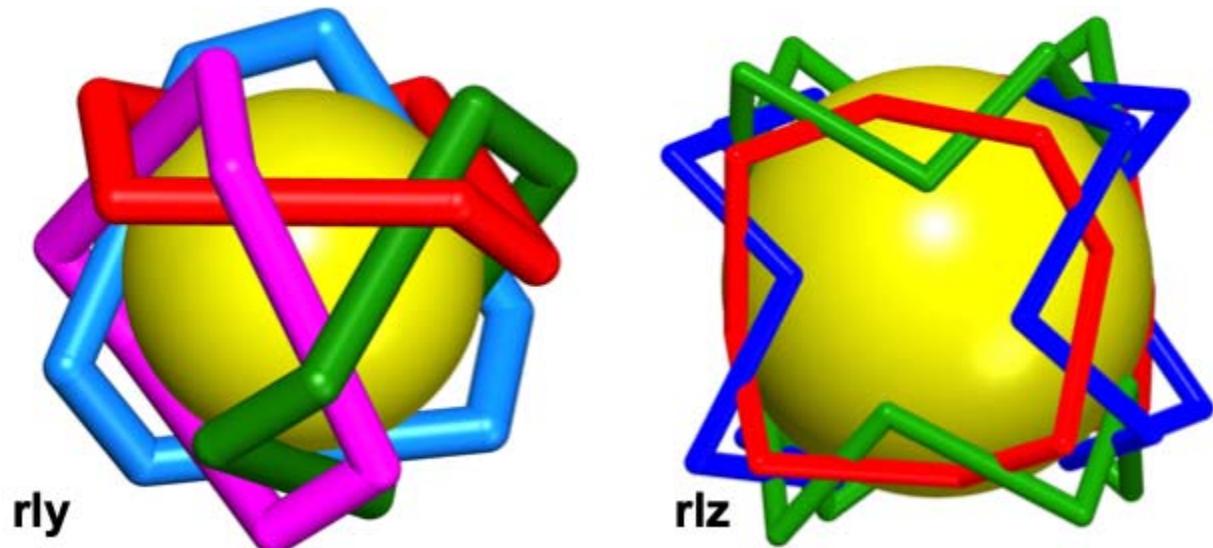


Figure S2. Piecewise linear embeddings of the simplest of the catenane structures of Hu *et al.* (2009). Both have transitivity 2 2.

TableS1. Supporting data for torus knots (p,q) with $p = 11\text{--}13$. Cartesian coordinates are for a 2-fold axis along the x direction, and for longer stick length = 1.0.

symbol	girth	x	y	z	stick 2	angle ($^{\circ}$)
(11,2)	0.1514	0.5155	-0.4314	-0.2528	0.5329	44.84
(11,3)	0.1428	0.4358	-0.4124	-0.2828	0.5778	63.72
(11,4)	0.1197	0.3438	-0.3993	-0.3010	0.6698	66.70
(11,5)	0.0964	0.2653	-0.3887	-0.3145	0.7534	62.33
(11,6)	0.0754	0.2011	0.3800	0.3249	0.8237	54.61
(11,7)	0.0568	0.1479	0.3730	0.3330	0.8825	45.10
(11,8)	0.0403	0.1030	0.3673	0.3392	0.9305	34.52
(11,9)	0.0254	0.0641	0.3628	0.3440	0.9672	23.29
(11,10)	0.0118	0.0296	0.3595	0.3475	0.9911	11.71
(12,5)	0.0977	0.2970	-0.3913	-0.3112	0.7248	64.48
(12,7)	0.0620	0.1779	0.3756	0.3300	0.8515	50.63
(12,11)	0.0099	0.0270	0.3585	0.3485	0.9925	10.71
(13,2)	0.1371	0.5702	-0.4355	-0.2456	0.5473	38.65
(13,3)	0.1341	0.4968	-0.4168	-0.2762	0.5536	59.20
(13,4)	0.1167	0.4061	-0.4041	-0.2945	0.6250	66.34
(13,5)	0.0981	0.3267	-0.3938	-0.3081	0.6998	65.78
(13,6)	0.0809	0.2608	-0.3853	-0.3187	0.7660	61.39
(13,7)	0.0656	0.2059	0.3782	0.3271	0.8234	54.90
(13,8)	0.0518	0.1596	0.3723	0.3338	0.8730	47.11
(13,9)	0.0395	0.1198	0.3673	0.3392	0.9153	38.47
(13,10)	0.0283	0.0848	0.3633	0.3435	0.9501	29.25
(13,11)	0.0180	0.0534	0.3602	0.3468	0.9766	19.67
(13,12)	0.0084	0.0249	0.3578	0.3493	0.9937	9.87

Table S2. Data for torus knots (p,q) for $p \leq 10$ and links (p,q) $p \leq 12$ (marked *). Cartesian coordinates are for a 2-fold axis along the x direction, and longer stick length equal to 1.0.

symbol	girth	x	y	z	stick 2	angle (°)
(3,2)	0.1748	0.1354	0.4363	0.2442	0.8297	50.19
(4,2)*	0.2051	0.4225	0.2175	0.2673	0.6892	65.50
(4,3)	0.0977	0.0955	0.4017	0.2978	0.9214	35.08
(5,2)	0.2057	0.2800	-0.4197	-0.2718	0.6083	68.34
(5,3)	0.1351	0.1691	0.4002	0.2997	0.8265	52.77
(5,4)	0.0606	0.0718	0.3836	0.3207	0.9531	27.04
(6,2)*	0.1981	0.3318	-0.4203	-0.2708	0.5632	66.07
(6,3)	0.1492	0.2289	0.4011	0.2986	0.7525	61.71
(6;4)*	0.0915	0.1326	0.3857	0.3181	0.8852	43.49
(6,5)	0.0412	0.0576	0.3741	0.3317	0.9685	22.10
(7,2)	0.1882	0.3767	-0.4221	-0.2679	0.5395	61.89
(7,3)	0.1535	0.2799	-0.4029	-0.2961	0.6964	65.85
(7,4)	0.1072	0.1847	0.3884	0.3149	0.8251	53.67
(7,5)	0.0657	0.1088	0.3770	0.3285	0.9173	37.01
(7,6)	0.0299	0.0483	0.3685	0.3379	0.9773	18.73
(8,2)*	0.1781	0.4164	-0.4244	-0.2643	0.5287	57.23
(8,3)	0.1532	0.3248	-0.4052	-0.2929	0.6537	67.20
(8,4)*	0.1152	0.2306	0.3912	0.3114	0.7750	59.96
(8,5)	0.0800	0.1539	0.3800	0.3250	0.8680	47.20
(8,6)*	0.0494	0.0924	0.3714	0.3348	0.9373	32.24
(8,7)	0.0227	0.0417	0.3649	0.3418	0.9829	16.27
(9,2)	0.1685	0.4523	-0.4268	-0.2604	0.5259	52.70
(9,3)*	0.1506	0.3651	-0.4076	-0.2896	0.6213	66.89
(9,4)	0.1188	0.2717	-0.3939	-0.3079	0.7334	63.72
(9,5)	0.0886	0.1944	0.3830	0.3214	0.8243	54.23
(9,6)*	0.0619	0.1320	0.3743	0.3315	0.8961	42.07
(9,7)	0.0385	0.0804	0.3675	0.3390	0.9507	28.57
(9,8)	0.0178	0.0366	0.3625	0.3444	0.9866	14.39
(10,2)*	0.1596	0.4852	-0.4292	-0.2566	0.5279	48.56

(10,3)	0.1469	0.4019	-0.4100	-0.2862	0.5965	65.60
(10,4)*	0.1200	0.3092	-0.3967	-0.3044	0.6988	65.79
(10,5)	0.0936	0.2313	0.3859	0.3179	0.7864	59.06
(10,6)*	0.0701	0.1679	0.3772	0.3282	0.8580	49.29
(10,7)	0.0493	0.1156	0.3703	0.3360	0.9159	37.93
(10,8)*	0.0309	0.0713	0.3648	0.3419	0.9602	25.66
(10,9)	0.0144	0.0327	0.3608	0.3462	0.9892	12.91
(12,2)*	0.1439	0.5438	-0.4335	-0.2491	0.5396	41.56
(12,3)*	0.1384	0.4673	-0.4146	-0.2795	0.5639	61.54
(12,4)*	0.1184	0.3759	-0.4017	-0.2977	0.6455	66.80
(12,6)*	0.0788	0.2319	0.3827	0.3217	0.7932	58.53
(12,8)*	0.0470	0.1323	0.3698	0.3365	0.9010	41.53
(12,9)*	0.0335	0.0930	0.3651	0.3416	0.9415	31.67
(12,10)*	0.0212	0.0582	0.3613	0.3456	0.9725	21.33

Table S3. Additional maximum-girth data for the edge-2-transitive structures. Not all of these have been examined yet, and some structures may be degenerate. One edge has a length of 1.0; the length of the second edge, which is ≤ 1 , is listed in the table.

group 23; x,y,z to -x,-y,z and to -x,y,z

#	Girth	x	y	z	length	angle(°)
1	0.25	0	-0.5	0.250000	0.50000	90
2	0.081246	0.424300	-0.264518	-0.164906	0.91044	37.7246

group $m\bar{3}$; x,y,z to -x,y,z and to x,y,z

#	Girth	x	y	z	length	angle(°)
1	0.200000	0.300000	-0.500000	0.100000	0.60000	90.0000

group 432; x,y,z to y, x, -z and z,-y,x

#	Girth	x	y	z	length	angle(°)
1	0.217258	0.540213	0.059313	0.366561	0.27273	111.7011
2	0.094797	0.141403	0.478867	0.344805	0.83865	50.6180
3	0.094349	0.127129	-0.429333	0.308505	0.89616	56.9456

4	0.074669	0.008686	-0.344811	0.433036	0.91418	59.6955
5	0.074242	0.040287	0.283839	-0.469405	0.91751	57.5261
6	0.073859	0.022157	0.308426	-0.457193	0.91655	58.5895
7	0.055212	0.073635	0.440801	-0.260114	0.73502	59.3437
8	0.051415	0.175539	0.358960	-0.316696	0.68445	58.9360
9	0.045540	0.538834	-0.160260	-0.075060	0.92545	36.3470
10	0.044506	0.239142	0.149399	-0.435662	0.88052	45.0832
11	0.032713	0.244186	-0.105655	-0.434518	0.98282	23.5178
12	0.032154	0.191527	-0.491693	0.063165	0.97444	40.2841
13	0.022903	0.287212	-0.158704	-0.383330	0.99270	15.9208
14	0.022657	0.200434	-0.121887	-0.445033	0.94482	24.2971
15	0.022514	0.274678	-0.099120	-0.418396	0.98978	22.6975
16	0.017960	0.218324	-0.270014	-0.361612	0.98198	10.2378
17	0.017926	0.221492	-0.270721	-0.358975	0.98338	9.8237
18	0.015275	0.141079	-0.440801	-0.192671	0.90866	23.1009
19	0.014156	0.349539	-0.299650	-0.198184	0.97937	10.8890
20	0.012022	0.260494	-0.224298	-0.363989	0.99055	10.2222
21	0.011049	0.073474	-0.403382	-0.344336	0.96387	25.2640
22	0.010362	0.312891	-0.355307	-0.163573	0.97929	14.2695
23	0.009874	0.307244	0.197980	-0.342070	0.70137	47.7143

group 432; x,y,z to z, -y, x and to -z,-y,-x

#	Girth	x	y	z	length	angle(°)
1	0.125674	0.112384	0.222678	-0.520727	0.72927	74.2182
2	0.036876	0.104600	-0.440801	0.229150	0.89903	30.1725
3	0.021789	0.206322	0.366272	-0.275019	0.73896	43.4325
4	0.008864	0.047046	0.411620	-0.354375	0.93093	43.2803

group 235; x,y,z to -x,-y,z and -x,y,-z

#	Girth	x	y	z	length	angle(°)
1	0.062814	0.200577	0.458005	0.395192	0.88636	79.5396
2	0.055426	0.269926	0.420880	0.365454	0.90866	71.2927

3	0.053033	0.296694	0.402458	0.262063	0.79172	63.5932
4	0.051142	0.320200	0.250969	0.384021	0.81367	59.7331
5	0.049878	0.151864	0.426501	0.476379	0.90546	84.1524
6	0.044039	0.383649	0.320645	0.216001	0.88055	48.0400
7	0.043423	0.221877	0.319824	0.448074	0.77850	75.3482
8	0.039241	0.293618	0.365467	0.404708	0.93761	68.4204
9	0.038216	0.384391	0.281540	0.319755	0.95293	51.6680
10	0.038120	0.383079	0.190687	0.321326	0.85583	46.6950
11*	0.038110	0.430259	0.210253	0.254711	0.95777	39.3630
12*	0.038102	0.432138	0.206507	0.251510	0.95789	38.7568
13	0.038100	0.432761	0.205245	0.250436	0.95793	38.5535
14	0.033505	0.370139	0.336151	0.302645	0.95624	55.0339
15	0.032990	0.189333	0.232078	0.462767	0.59902	76.1506
16	0.030484	0.320645	0.149513	0.383649	0.70758	54.4643
17	0.029941	0.199940	0.458284	0.188838	0.55004	73.0993
18	0.028030	0.160399	0.473574	0.211827	0.53141	78.8337
19	0.027859	0.384121	0.134472	0.320080	0.81396	43.5234
20	0.025458	0.332269	0.189229	0.373627	0.76475	54.7280
21	0.021511	0.448472	0.221073	0.155482	0.94932	32.0638
22	0.020327	0.441995	0.233754	0.208869	0.97772	36.9422
23	0.019438	0.451446	0.214935	0.123099	0.93586	29.4147
24	0.017879	0.364714	0.241597	0.342029	0.87495	52.5472
25	0.016945	0.473447	0.130731	0.160772	0.98233	24.1136
26	0.015864	0.450768	0.094297	0.216351	0.92105	28.0624
27	0.015303	0.463443	0.187673	0.164816	0.98376	29.1553
28	0.014835	0.439818	0.237824	0.176660	0.94794	35.2887
29	0.011055	0.451446	0.214935	0.070011	0.91368	26.8457
30	0.010330	0.384021	0.320200	0.050693	0.77471	40.4090
31	0.009232	0.473574	0.069768	0.160399	0.95737	20.4408
32	0.004665	0.320080	0.384121	0.022516	0.64174	50.3138
33	0.003067	0.473574	0.023179	0.160399	0.94828	18.9124
34	0.002760	0.458412	0.017424	0.199645	0.91749	23.6286

35	0.002352	0.486610	0.114940	0.026082	0.97462	13.6333
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group 235, 2-fold axes at 45°

#	Girth	x	y	z	length	angle(°)
1	0.117064	0.290772	0.406758	0.583181	0.58400	109.0507
2	0.064284	0.155462	-0.475218	-0.499138	0.78932	74.4613
3	0.049003	0.383649	0.320645	0.240346	0.48838	59.6324
4	0.045017	0.451446	0.214935	0.285088	0.70256	52.4213
5	0.039505	0.401880	0.297476	0.326058	0.55734	65.6711
6	0.039266	0.217368	0.450279	-0.232613	0.90508	59.7383
7	0.033469	0.262866	-0.425325	-0.175244	0.79465	37.3774
8	0.033345	0.384021	0.320200	-0.163634	0.86999	50.5379
9	0.031167	0.160399	0.473574	-0.235534	0.90840	59.9469
10	0.030739	0.325994	-0.379115	-0.178343	0.88249	30.9503
11	0.029667	0.203355	-0.456779	0.184690	0.97604	40.9640
12	0.029242	0.448517	0.220982	0.412006	0.76373	63.9361
13	0.025813	0.112470	0.487186	-0.268723	0.97049	59.3533
14	0.025496	0.160543	-0.473525	0.194206	0.96300	44.6837
15	0.024997	-0.239295	-0.422691	0.293938	0.97145	59.2774
16	0.024855	0.376205	-0.329347	-0.163242	0.94427	24.2818
17	0.024452	0.461610	0.192135	-0.182422	0.98078	39.8165
18	0.024445	0.413591	0.280967	0.390208	0.63095	69.7441
19	0.023166	0.160399	-0.473574	-0.175071	0.64289	47.0365
20	0.022546	0.451446	0.214935	-0.142779	0.92048	40.8155
21	0.022012	0.424312	-0.206711	-0.220609	0.94397	22.8442
22	0.021368	0.189332	-0.462767	-0.262857	0.68995	50.9342
23	0.021247	0.199645	0.458412	-0.134160	0.73328	59.9097
24	0.021123	0.451669	0.214465	-0.134006	0.91083	40.5744
25	0.021122	0.320080	0.384121	-0.101950	0.72590	55.3984
26	0.021033	0.188703	0.463024	-0.274583	0.97572	59.9834
27	0.021032	0.160399	0.473574	-0.158942	0.77587	59.9395
28	0.020963	0.160492	-0.473542	0.159238	0.91847	43.9452

29	0.020960	-0.190412	-0.462324	0.274605	0.97581	59.9774
30	0.020943	0.107622	-0.488280	0.227218	0.97989	49.1526
31	0.020901	0.401276	0.280685	-0.248352	0.97940	49.1521
32	0.020873	0.415428	0.195604	-0.254182	0.91835	44.0124
33	0.019544	0.408940	0.287694	-0.226383	0.98136	48.7754
34	0.019380	0.249118	-0.433521	0.104733	0.92078	34.6366
35	0.019358	-0.404531	-0.293861	0.228925	0.98135	49.3148
36	0.019306	0.195824	-0.460058	0.148736	0.92910	40.7231
37	0.018610	0.273302	0.418696	-0.269718	0.97901	58.4723
38	0.017693	0.474526	0.157561	-0.146320	0.96131	35.8007
39	0.016407	0.451446	0.214935	0.103903	0.71364	40.5785
40	0.016042	0.384021	0.320200	-0.078722	0.75290	49.5175
41	0.015528	0.132888	-0.482017	0.138621	0.87418	45.7664
42	0.015462	0.215716	-0.451073	-0.270975	0.73562	49.0110
43	0.015447	0.199645	-0.458412	0.097534	0.87568	39.2659
44	0.014859	0.160399	-0.473574	0.112290	0.86174	43.0372
45	0.014647	0.437405	0.242233	-0.210993	0.98713	44.7428
46	0.013756	0.466717	0.179374	0.101389	0.76068	37.1304
47	0.013474	-0.094976	0.490897	-0.179702	0.90563	49.2552
48	0.012345	0.345498	-0.361429	-0.237405	0.92464	33.1650
49	0.012278	0.429139	0.256593	0.575547	0.86465	80.3153
50	0.012062	0.361535	-0.345388	-0.228875	0.94399	30.8138
51	0.011973	0.086343	-0.492488	0.160193	0.87316	49.5654
52	0.011819	0.437030	0.242909	-0.175927	0.94151	44.0302
53	0.011530	0.451446	0.214935	-0.073019	0.84539	39.4367
54	0.011326	0.320080	0.384121	-0.054668	0.65363	55.1532
55	0.009894	0.114452	-0.486725	-0.101334	0.60970	47.2887
56	0.009682	0.384021	-0.320200	-0.047513	0.94935	17.0069
57	0.008828	0.495426	-0.067477	0.164184	0.98862	20.0263
58	0.008297	0.369641	-0.336698	-0.077310	0.93218	20.0866
59	0.007903	-0.302141	-0.027561	0.407024	0.60679	47.6412
60	0.007267	0.402955	-0.296020	-0.062673	0.96441	14.7293

61	0.007248	0.160399	0.473574	-0.054771	0.59573	59.9298
62	0.007170	0.349040	0.358010	-0.244769	0.96794	54.4640
63	0.007121	0.199645	0.458412	-0.044962	0.57917	59.8983
64	0.007051	0.475346	0.155068	-0.059160	0.88219	33.5126
65	0.006865	0.384021	-0.320200	0.033690	0.97134	16.6455
66	0.006842	-0.431841	-0.252019	0.186124	0.94863	45.0329
67	0.005728	0.199645	-0.458412	-0.036166	0.75951	38.3914
68	0.005709	0.456887	-0.195177	-0.079778	0.99366	8.1703
69	0.005170	0.022455	-0.499496	0.261328	0.99453	54.5633
70	0.004676	0.408645	-0.288113	0.053244	0.99278	13.4038
71	0.004639	0.492093	0.088567	-0.066113	0.93385	27.3604
72	0.004537	0.321333	-0.383073	0.022698	0.91828	25.0171
73	0.004385	0.320080	-0.384121	-0.021168	0.89660	25.1632
74	0.004239	0.486602	0.114972	-0.046994	0.90301	29.5012
75	0.004206	0.403059	0.295877	0.036434	0.64899	46.8653
76	0.004041	0.186072	-0.266206	0.381570	0.64958	47.0327
77	0.004017	0.408740	-0.287978	0.045992	0.99018	13.1291
78	0.003966	0.412996	-0.281841	0.060355	0.99742	13.0137
79	0.003893	0.483311	-0.128105	0.038965	0.99452	6.5247
80	0.003422	0.495326	-0.068208	-0.062974	0.99911	12.8727
81	0.003164	0.383649	-0.320645	0.015519	0.96442	16.4355
82	0.003130	0.488961	-0.104485	-0.038025	0.99837	8.5247
83	0.003068	0.495621	-0.066032	-0.058280	0.99682	12.8549
84	0.003048	-0.440313	0.236906	-0.035033	0.99955	7.2642
85	0.002972	0.447383	-0.223267	0.022634	0.99910	5.3546
86	0.002875	0.302935	-0.397782	0.053976	0.92180	27.6758
87	0.002814	0.320080	-0.384121	0.013580	0.91244	25.1061
88	0.002813	0.436457	-0.243453	0.043265	0.99953	8.3189
89	0.002709	0.354434	-0.347847	0.124220	0.99322	23.4763
90	0.002580	0.322310	-0.382252	0.013290	0.91426	24.8267
91	0.002452	0.022651	-0.499487	-0.122873	0.46839	54.5472
92	0.002185	0.446520	-0.224988	0.017376	0.99810	5.3387

93	0.002122	0.356384	-0.350700	0.114315	0.99902	23.0665
94	0.001564	-0.488112	0.108384	0.018343	0.99483	7.4807
95	0.001506	0.309853	0.392417	-0.007332	0.57382	55.7378
96	0.001330	-0.443242	0.231379	0.012658	0.99391	5.9005
97	0.000939	-0.426574	0.260834	0.135552	0.99352	16.3311
98	0.000908	0.457891	-0.200837	-0.006081	0.99892	2.4799
99	0.000848	-0.454651	0.208069	0.005515	0.99819	3.2382
100	0.000518	-0.434188	0.247954	-0.010272	0.99267	7.7026
101	0.000511	-0.435263	0.246060	-0.009005	0.99292	7.4729
102	0.000501	0.487686	-0.110285	-0.005785	0.99318	7.0864
103	0.000449	0.484016	-0.125412	0.004586	0.99495	5.5403
104	0.000416	0.327805	-0.284145	0.248645	0.86763	30.1056

group 235, 2-fold axes at 72°

#	Girth	x	y	z	length	angle(°)
1	0.150338	0.376283	0.329258	0.730695	0.17546	97.0723
2	0.140428	0.435306	0.245986	0.802366	0.14043	139.9330
3	0.073904	0.466521	-0.179884	0.543344	0.81050	46.1663
4	0.035884	-0.270365	-0.420598	-0.185046	0.66973	33.2641
5	0.032407	0.451446	-0.214935	0.205230	0.86319	23.3175
6	0.030020	0.384021	-0.320200	0.147318	0.95216	14.7017
7	0.026368	-0.383649	-0.320645	-0.129328	0.66415	35.6426
8	0.025201	0.060975	-0.496268	-0.472953	0.93415	36.4339
9	0.023417	-0.332553	-0.373374	-0.176325	0.63578	34.8167
10	0.020679	0.160399	0.473574	0.156276	0.77417	28.5312
11	0.019934	0.166534	0.471452	0.227612	0.72432	30.8739
12	0.018213	0.418496	-0.273607	0.492493	0.93569	37.8279
13	0.018140	0.321820	0.382664	-0.092075	0.93078	34.0214
14	0.017556	0.376281	0.329261	-0.114907	0.94747	35.4681
15	0.016728	0.323071	-0.381609	0.088194	0.98906	7.7863
16	0.016667	0.461446	0.192529	-0.115589	0.94798	35.5121
17	0.015361	0.320362	0.383886	-0.131829	0.97517	34.0473

18	0.015253	0.151440	-0.476514	-0.121177	0.97146	11.6382
19	0.015079	0.377985	0.327303	-0.091641	0.92031	35.4906
20	0.014753	0.478436	0.145255	-0.131396	0.97088	34.7269
21	0.014724	0.109293	0.487909	0.157447	0.81003	26.2408
22	0.013611	0.384021	0.320200	-0.066791	0.89068	35.5947
23	0.013571	0.451446	0.214935	0.085944	0.71156	35.7668
24	0.013143	-0.335420	-0.370802	0.114067	0.95270	34.4678
25	0.012274	0.088643	0.492080	0.160132	0.82319	25.3426
26	0.011578	-0.451446	-0.214935	0.073320	0.89704	35.7589
27	0.011406	0.467739	-0.176694	0.085179	0.88468	21.6900
28	0.011264	0.142064	0.479393	-0.094694	0.97702	26.4149
29	0.010752	-0.397718	0.303019	-0.080321	0.95390	13.2879
30	0.010240	0.483681	-0.126698	-0.103567	0.99315	24.5183
31	0.009266	0.320080	0.384121	-0.044727	0.87902	33.9039
32	0.008899	0.479809	-0.140654	-0.081738	0.97918	23.5533
33	0.008895	0.363161	0.343678	-0.139918	0.97795	35.2100
34	0.008858	0.494775	-0.072093	0.154361	0.77803	28.3288
35	0.008857	0.493524	0.080214	-0.139030	0.98798	33.1458
36	0.008844	0.161647	0.473149	-0.071750	0.95203	27.2285
37	0.008824	0.197238	0.459453	-0.062858	0.93370	28.9036
38	0.008790	-0.495186	0.069215	-0.159434	0.77268	28.5665
39	0.008654	0.472574	0.163321	-0.069292	0.89795	35.0196
40	0.008347	0.187175	-0.463644	-0.128031	0.98570	10.3898
41	0.008178	0.279079	0.414867	-0.095488	0.94410	32.5287
42	0.007912	0.160399	0.473574	-0.059792	0.94198	27.1017
43	0.007788	0.199645	0.458412	-0.049176	0.92030	28.9656
44	0.007641	0.451349	0.215137	-0.048590	0.86817	35.7574
45	0.007577	-0.205320	-0.455899	0.046827	0.91629	29.2250
46	0.007457	0.483450	-0.127578	-0.074933	0.97065	24.2000
47	0.007444	0.405344	-0.292739	0.071411	0.95122	13.8148
48	0.006939	0.384021	-0.320200	-0.034053	0.99372	10.9533
49	0.006603	0.486433	-0.115683	0.144109	0.81426	26.1248

50	0.006478	0.187568	-0.463485	-0.100496	0.98591	8.8614
51	0.006407	0.492424	-0.086712	-0.093218	0.97561	26.4329
52	0.006390	0.474724	-0.156963	-0.053022	0.96230	22.3932
53	0.006319	0.089034	-0.492009	-0.082095	0.95181	13.5821
54	0.006125	0.471306	0.166945	-0.146043	0.98537	35.1462
55	0.005418	0.097421	0.490417	-0.064586	0.96388	23.8688
56	0.005317	0.492986	-0.083453	-0.080303	0.96373	26.4953
57	0.005239	0.387282	-0.316248	0.027683	0.97318	11.2107
58	0.005158	0.061689	-0.496180	-0.095708	0.93637	15.5581
59	0.004810	0.402262	-0.296960	-0.056881	0.99844	13.1436
60	0.004733	0.126448	-0.483747	0.044206	0.99881	10.3436
61	0.004571	-0.470450	0.169341	0.052027	0.96515	21.6626
62	0.004369	0.498129	-0.043215	-0.126274	0.99621	28.6690
63	0.004333	0.487489	0.111151	-0.049611	0.88507	33.8205
64	0.004174	0.384021	-0.320200	-0.020485	0.98908	10.8101
65	0.004122	0.203288	-0.456808	-0.025669	0.99403	4.8510
66	0.003840	0.137253	-0.480793	0.033298	0.99659	9.4565
67	0.003775	0.493887	0.077949	-0.060939	0.90454	32.8831
68	0.003772	0.375588	-0.330051	0.025484	0.97842	10.0255
69	0.003766	0.320080	-0.384121	-0.018176	0.99924	4.8960
70	0.003694	0.443462	-0.230958	-0.034709	0.97212	17.6305
71	0.003596	0.439766	-0.237920	-0.042982	0.97856	17.2252
72	0.003526	0.160399	-0.473574	-0.026647	0.98594	7.8083
73	0.003502	0.499441	-0.023627	0.184709	0.72269	30.9128
74	0.003364	0.498522	-0.038411	-0.109326	0.97932	28.7537
75	0.003187	0.121736	-0.484954	0.030823	0.99367	10.4480
76	0.002870	-0.199645	0.458412	-0.018123	0.99918	4.9502
77	0.002825	0.199645	-0.458412	-0.017838	0.99429	4.9470
78	0.002697	0.160399	-0.473574	0.020379	0.99589	7.7208
79	0.002676	0.193898	-0.460873	0.023190	0.99965	5.4424
80	0.002604	0.432011	-0.251727	-0.068997	0.99593	16.5963
81	0.002548	0.164538	-0.472152	0.024941	0.99746	7.4964

82	0.002394	0.061264	-0.496233	0.044725	0.98897	14.4854
83	0.002371	0.451126	-0.215606	-0.015221	0.95652	18.5579
84	0.002360	0.395402	-0.306034	-0.015524	0.98395	11.9462
85	0.002344	0.498277	-0.041475	-0.070582	0.94417	28.3934
86	0.002241	0.168251	-0.470841	0.029890	0.99902	7.3236
87	0.002227	0.293014	-0.405146	0.011060	0.99841	2.5537
88	0.002225	0.034143	-0.498833	0.074089	0.99908	16.5464
89	0.002142	0.330607	-0.375099	-0.025745	0.99969	5.9230
90	0.002112	0.331099	-0.374665	0.014907	0.99277	5.7997
91	0.002099	0.320080	-0.384121	-0.010134	0.99801	4.7910
92	0.002080	0.114185	-0.486787	-0.021353	0.97616	10.8508
93	0.002059	0.311425	-0.391171	0.010007	0.99651	4.0512
94	0.001976	0.199645	0.458412	-0.012478	0.88683	28.8849
95	0.001947	0.151794	-0.476402	0.015437	0.99353	8.2640
96	0.001940	0.160399	0.473574	-0.014662	0.90361	26.9522
97	0.001919	0.137171	-0.480816	0.016650	0.99167	9.2715
98	0.001888	0.344363	-0.362511	-0.031879	0.99967	7.2263
99	0.001775	0.195304	-0.460279	0.014096	0.99819	5.2017
100	0.001683	0.172176	-0.469420	-0.036487	0.98692	7.2034
101	0.001665	-0.344613	0.362273	0.028897	0.99894	7.1935
102	0.001633	0.363609	-0.343203	0.024531	0.98278	8.8662
103	0.001562	0.199645	-0.458412	0.009862	0.99790	4.8447
104	0.001516	0.015358	-0.499764	-0.111949	0.90821	18.6168
105	0.001513	0.499309	-0.026283	-0.071767	0.94125	29.0620
106	0.001264	0.416624	-0.276450	-0.026966	0.98084	14.3305
107	0.001251	0.027239	-0.499258	0.052155	0.98595	16.6527
108	0.001167	0.317866	-0.385955	-0.005642	0.99760	4.5659
109	0.000722	0.346920	-0.360065	-0.016833	0.99584	7.2324

group 235, 2-fold axes at 36°

#	Girth	x	y	z	length	angle(°)
1	0.081064	-0.354613	-0.352490	-0.552936	0.78430	102.8558

2	0.072492	0.247539	0.434424	0.393303	0.67573	81.4981
3	0.069287	0.384021	0.320200	0.340011	0.36881	103.2274
4	0.067381	0.451446	0.214935	0.426720	0.51614	106.0945
5	0.061401	0.320080	0.384121	0.296373	0.41679	87.0932
6	0.059198	0.442187	0.233390	0.600932	0.83749	107.5651
7	0.056673	0.483835	0.126110	0.575720	0.85213	100.1149
8	0.055439	0.320080	0.384121	-0.267593	0.86243	67.1041
9	0.053255	0.383649	0.320645	-0.261199	0.81520	70.9755
10	0.041955	0.454899	0.207526	-0.273347	0.83596	71.2229
11	0.037335	0.488196	-0.108003	0.439406	0.92908	67.8823
12	0.035475	0.451446	-0.214935	0.224660	0.87960	41.1170
13	0.033608	0.158134	0.474335	0.257124	0.68843	59.3679
14	0.027535	0.113180	0.487022	0.284969	0.78016	56.3000
15	0.025710	0.383432	-0.320905	0.127046	0.96003	22.5269
16	0.024560	0.383649	0.320645	-0.120460	0.55356	70.6028
17	0.024320	0.465566	-0.182340	-0.176708	0.95482	39.5385
18	0.023041	-0.406295	0.291418	-0.231481	0.97735	33.6374
19	0.021118	-0.438463	0.240313	-0.278706	0.94833	42.5071
20	0.020995	0.476586	-0.151214	0.180229	0.77144	44.8782
21	0.019895	-0.402116	0.297157	-0.165769	0.94976	27.9680
22	0.019503	0.320080	0.384121	-0.094136	0.56866	65.1656
23	0.018689	0.115814	-0.486402	-0.189319	0.98504	27.2637
24	0.018500	0.146643	0.478012	-0.151200	0.83950	48.5968
25	0.017931	-0.384021	0.320200	-0.087991	0.95108	20.1406
26	0.017254	0.159719	-0.473804	-0.130875	0.99033	19.0314
27	0.016914	0.451446	-0.214935	-0.107117	0.91870	33.2418
28	0.013900	0.199645	0.458412	-0.087765	0.70851	52.4575
29	0.013139	0.451446	0.214935	-0.083206	0.47804	71.0986
30	0.012933	0.132400	-0.482152	-0.115842	0.96871	20.2164
31	0.011848	0.320080	-0.384121	0.057187	0.99221	9.9200
32	0.011088	0.195229	-0.460310	-0.088458	0.99582	12.7554
33	0.010977	0.338492	-0.367999	0.114140	0.99473	16.2416

34	0.010695	0.495207	-0.069063	0.194415	0.65168	54.7720
35	0.010022	0.169474	0.470403	0.151837	0.62387	52.9747
36	0.009498	0.491844	0.089939	-0.133366	0.65253	63.7666
37	0.009472	0.404282	-0.294204	-0.086537	0.96749	23.1339
38	0.009291	0.199645	-0.458412	-0.058665	0.99212	10.0947
39	0.009014	0.101724	-0.489543	0.103134	0.98707	22.0124
40	0.008854	0.109341	-0.487898	-0.094639	0.94832	21.0395
41	0.008837	0.130333	0.482715	-0.080294	0.78172	44.9397
42	0.008808	0.454682	-0.208002	-0.057278	0.87794	32.5268
43	0.007697	0.027498	-0.499243	-0.317922	0.99004	44.6896
44	0.007219	0.446962	-0.224109	-0.056134	0.89271	30.6219
45	0.006838	0.441978	-0.233786	-0.070337	0.90997	29.8527
46	0.006694	0.394902	-0.306679	-0.043371	0.95614	19.9975
47	0.006522	-0.199645	-0.458412	0.041182	0.65974	51.6624
48	0.006240	0.320637	-0.383656	0.030600	0.98996	8.4615
49	0.006126	0.071791	-0.494819	-0.098010	0.91951	24.9526
50	0.005918	0.147856	-0.477639	0.048013	0.98268	14.7626
51	0.005631	0.390852	-0.311825	-0.053568	0.96376	19.6141
52	0.005600	0.175094	0.468340	-0.227961	0.91370	53.6997
53	0.005512	-0.347409	0.359592	-0.138573	0.99688	19.1636
54	0.005332	0.199645	0.458412	0.033666	0.60077	51.6101
55	0.005208	0.320080	-0.384121	-0.025139	0.99426	8.1637
56	0.004874	0.199645	-0.458412	-0.030774	0.98992	8.4815
57	0.004115	0.358263	-0.348780	0.132893	0.98623	19.8353
58	0.003933	0.383649	-0.320645	0.019291	0.95085	17.5981
59	0.003681	0.412105	-0.283143	-0.052377	0.94211	23.3078
60	0.003577	0.205027	-0.456031	0.022127	0.99485	7.5376
61	0.003511	0.320080	-0.384121	-0.016945	0.99295	7.9082
62	0.003316	0.320080	-0.384121	0.016005	0.99014	7.8858
63	0.002875	0.371402	-0.334754	-0.024096	0.96911	15.6662
64	0.002629	0.155253	-0.475286	0.020441	0.97824	13.1432
65	0.002523	0.199645	-0.458412	-0.015932	0.98991	7.9743

66	0.002504	0.160399	-0.473574	-0.018921	0.97492	12.5354
67	0.002432	0.411857	-0.283503	0.033992	0.91732	22.8483
68	0.002398	0.447483	-0.223068	-0.018173	0.87262	30.1394
69	0.002280	0.362362	-0.344519	-0.039157	0.97918	14.6396
70	0.002274	0.199645	-0.458412	0.014360	0.99238	7.9375
71	0.002218	0.199645	0.458412	-0.014005	0.63528	51.4266
72	0.002201	0.160399	0.473574	-0.016634	0.69183	47.1961
73	0.002102	0.133983	-0.481714	-0.018628	0.96175	15.5024
74	0.001958	0.404590	-0.293780	0.018140	0.92891	21.2534
75	0.001843	0.485093	0.121181	-0.019436	0.44962	65.0156
76	0.001197	0.166926	-0.471313	0.014131	0.98171	11.7120
77	0.001000	0.172155	-0.469428	0.021624	0.98507	11.2569
78	0.000894	0.446707	-0.224617	0.007043	0.86468	29.8906
79	0.000529	-0.355508	0.351588	0.064083	0.99124	14.6889
80	0.000459	0.424774	-0.263756	-0.150606	0.99072	29.7623
81	0.000454	0.179542	-0.466653	0.054096	0.99566	11.7316