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EXAMPLE 1, Cyclohexane twistboat, D2  
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INPUT:

1  
Cyclohexane twistboat, D2  
6 0 0 0 2  
1 6 0 0.000000 0.000000 -1.527965  
2 6 0 -0.381467 1.227991 -0.665784  
3 6 0 0.381467 1.227991 0.665784  
4 6 0 0.000000 0.000000 1.527965  
5 6 0 -0.381467 -1.227991 0.665784  
6 6 0 0.381467 -1.227991 -0.665784

EOF

LONG OUTPUT:

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CONFORMATIONAL ANALYSIS OF PUCKERED RINGS  
Analysis of Ring Molecules in terms of Ring Puckering and Ring Deformation

D. Cremer 1988, D. Izotov, E. Kraka, D. Cremer, January 2011

OUTPUT FILES, puckering data: output.dat, B-matrix output: matrices.dat

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\*\*\*\* MOLECULE: \*\*\*\*

6 Membered Ring: Cyclohexane twistboat, D2

Cell coordinates: NO  
Cartesian coordinates: YES  
Substituent coordinates: NO  
Re-ordering of Ring coordinates: NO  
Coordinate input format: G98, G03, G09 format

Initial ring coordinates

1	6	0.000000	0.000000	-1.527965
2	6	-0.381467	1.227991	-0.665784
3	6	0.381467	1.227991	0.665784
4	6	0.000000	0.000000	1.527965
5	6	-0.381467	-1.227991	0.665784
6	6	0.381467	-1.227991	-0.665784

Ring analysis: Coordinates in ring standard orientation  
(Cartesian system, Origin = Geometrical center of the ring  
XY-Plane = Mean Ringplane, Atom 1 in the 9 o clock position)

1	-1.527965	0.000000	0.000000
2	-0.665784	1.227991	0.381467
3	0.665784	1.227991	-0.381467
4	1.527965	0.000000	0.000000
5	0.665784	-1.227991	0.381467
6	-0.665784	-1.227991	-0.381467

A. (N-3) Puckering coordinates

Total puckering amplitude Q = 0.76293

n	q(n)	phi(n)	theta(n)	%
2	0.76293	270.00000	90.00000	100.00
3	0.00000			0.00

Sum of z-coordinates = 0.0000 Sum of z\*z = 0.582068 Sum of q(n)\*q(n) = 0.582068

#### B. (3N-2) Planar deformation coordinates

Radius of reference polygon R = 1.44023  
Total deformation amplitude T = 0.06915

n	A	B	t(n)	tau(n)	%	Omega
1	0.00000	0.00000	0.00000	0.000	0.0	
2	-0.06547	0.00000	0.06547	180.000	89.6	0.00000
3	0.00000	0.00000	0.00000	0.000	0.0	90.00000
4	-0.02227	0.00000	0.02227	180.000	10.4	71.21380

#### Transformed Coordinates With Regard To Least Squares Plane (LSP Calculated By Iteration Method)

1	0.000000	1.527965	0.000000
2	1.227991	0.665784	0.381467
3	1.227991	-0.665784	-0.381467
4	0.000000	-1.527965	0.000000
5	-1.227991	-0.665784	0.381467
6	-1.227991	0.665784	-0.381467

Number of Iterations 3 Convergence Criterium 0.000001

Angle between the normal of the mean plane and that of the Least-Squares Plane = 0.00

(EULER angles defining the orientation of the Least-Squares Plane are: 0.0000 0.0000 0.0000)

#### Bond Angles

Angle 6 1 2 = 112.32  
Angle 1 2 3 = 111.14  
Angle 2 3 4 = 111.14  
Angle 3 4 5 = 112.32  
Angle 4 5 6 = 111.14  
Angle 5 6 1 = 111.14

#### Calculated Dihedral Angles

Dihedral Angle 6 1 2 3 = 30.60  
Dihedral Angle 1 2 3 4 = -63.48  
Dihedral Angle 2 3 4 5 = 30.60  
Dihedral Angle 3 4 5 6 = 30.60  
Dihedral Angle 4 5 6 1 = -63.48  
Dihedral Angle 5 6 1 2 = 30.60

#### Distance Matrix

	1	2	3	4	5	6
1	0.0000					
2	1.5482	0.0000				
3	2.5428	1.5346	0.0000			
4	3.0559	2.5428	1.5482	0.0000		
5	2.5428	2.7937	2.5718	1.5482	0.0000	
6	1.5482	2.5718	2.7937	2.5428	1.5346	0.0000



1	0.000000	0.000000
2	-0.088410	0.153130
3	0.000000	0.000000
4	-0.071053	0.123067
5	-0.038523	0.066724
6	0.000000	0.000000
7	-0.071053	0.123067
8	0.038523	-0.066724
9	0.000000	0.000000
10	0.000000	0.000000
11	0.088410	-0.153130
12	0.000000	0.000000
13	0.071053	-0.123067
14	0.038523	-0.066724
15	0.000000	0.000000
16	0.071053	0.876933
17	0.961477	0.066724
18	0.000000	0.000000

XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX

B. Puckering part

B.I) Puckering part : (N-3) x 3N Partial derivatives (d zeta\_n /d r\_beta)

	x1	y1	z1	x2	y2	z2	x3	y3
q(2)	0.000000	0.000000	0.000000	0.000000	0.000000	-0.500000	0.000000	0.000000
q(3)	0.000000	0.000000	0.408248	0.000000	0.000000	-0.408248	0.000000	0.000000
phi(2)	0.000000	0.000000	0.756750	0.000000	0.000000	-0.378375	0.000000	0.000000
	z3	x4	y4	z4	x5	y5	z5	x6
q(2)	0.500000	0.000000	0.000000	0.000000	0.000000	0.000000	-0.500000	0.000000
q(3)	0.408248	0.000000	0.000000	-0.408248	0.000000	0.000000	0.408248	0.000000
phi(2)	-0.378375	0.000000	0.000000	0.756750	0.000000	0.000000	-0.378375	0.000000
	y6	z6						
q(2)	0.000000	0.500000						
q(3)	0.000000	-0.408248						
phi(2)	0.000000	-0.378375						

B. II) Puckering part : B-matrix elements for N-3 puckering coordinates: (N-3) x 3N partial derivatives (d zeta\_n /d r\_alpha)

	x1	y1	z1	x2	y2	z2	x3	y3
q(2)	0.000000	0.000000	0.000000	0.500000	0.000000	0.000000	-0.500000	0.000000
q(3)	-0.371700	0.000000	0.000000	0.426523	0.000000	0.000000	-0.426523	0.000000
phi(2)	-0.756750	0.000000	0.000000	0.378375	0.000000	0.000000	0.378375	0.000000
	z3	x4	y4	z4	x5	y5	z5	x6
q(2)	0.000000	0.000000	0.000000	0.000000	0.500000	0.000000	0.000000	-0.500000
q(3)	0.000000	0.371700	0.000000	0.000000	-0.426523	0.000000	0.000000	0.426523
phi(2)	0.000000	-0.756750	0.000000	0.000000	0.378375	0.000000	0.000000	0.378375
	y6	z6						
q(2)	0.000000	0.000000						
q(3)	0.000000	0.000000						
phi(2)	0.000000	0.000000						

B. III) Puckering part : Derivatives of B matrix: (d B\_i /d r\_alpha) (N-3) x 3N x 3N

coord = q(2)

	1	2	3	4	5	6	7	8
1	0.476542	0.000000	0.000000	-0.198639	0.000000	0.113960	-0.238271	0.000000
2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
4	-0.198639	0.000000	0.000000	0.150757	-0.101792	0.056980	0.130940	0.101792
5	0.000000	0.000000	0.000000	-0.101792	0.000000	0.000000	-0.101792	0.000000

6	0.113960	0.000000	0.000000	0.056980	0.000000	0.000000	-0.056980	0.000000
7	-0.238271	0.000000	0.000000	0.130940	-0.101792	-0.056980	0.150757	0.101792
8	0.000000	0.000000	0.000000	0.101792	0.000000	0.000000	0.101792	0.000000
9	-0.113960	0.000000	0.000000	-0.056980	0.000000	0.000000	0.056980	0.000000
10	0.397277	0.000000	0.000000	-0.238271	0.000000	-0.113960	-0.198639	0.000000
11	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
12	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
13	-0.238271	0.000000	0.000000	0.067698	0.101792	-0.056980	0.087515	-0.101792
14	0.000000	0.000000	0.000000	-0.101792	0.000000	0.000000	-0.101792	0.000000
15	0.113960	0.000000	0.000000	0.056980	0.000000	0.000000	-0.056980	0.000000
16	-0.198639	0.000000	0.000000	0.087515	0.101792	0.056980	0.067698	-0.101792
17	0.000000	0.000000	0.000000	0.101792	0.000000	0.000000	0.101792	0.000000
18	-0.113960	0.000000	0.000000	-0.056980	0.000000	0.000000	0.056980	0.000000

	9	10	11	12	13	14	15	16
1	-0.113960	0.397277	0.000000	0.000000	-0.238271	0.000000	0.113960	-0.198639
2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
4	-0.056980	-0.238271	0.000000	0.000000	0.067698	-0.101792	0.056980	0.087515
5	0.000000	0.000000	0.000000	0.000000	0.101792	0.000000	0.000000	0.101792
6	0.000000	-0.113960	0.000000	0.000000	-0.056980	0.000000	0.000000	0.056980
7	0.056980	-0.198639	0.000000	0.000000	0.087515	-0.101792	-0.056980	0.067698
8	0.000000	0.000000	0.000000	0.000000	-0.101792	0.000000	0.000000	-0.101792
9	0.000000	0.113960	0.000000	0.000000	0.056980	0.000000	0.000000	-0.056980
10	0.113960	0.476542	0.000000	0.000000	-0.198639	0.000000	-0.113960	-0.238271
11	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
12	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
13	0.056980	-0.198639	0.000000	0.000000	0.150757	0.101792	-0.056980	0.130940
14	0.000000	0.000000	0.000000	0.000000	0.101792	0.000000	0.000000	0.101792
15	0.000000	-0.113960	0.000000	0.000000	-0.056980	0.000000	0.000000	0.056980
16	-0.056980	-0.238271	0.000000	0.000000	0.130940	0.101792	0.056980	0.150757
17	0.000000	0.000000	0.000000	0.000000	-0.101792	0.000000	0.000000	-0.101792
18	0.000000	0.113960	0.000000	0.000000	0.056980	0.000000	0.000000	-0.056980

	17	18
1	0.000000	-0.113960
2	0.000000	0.000000
3	0.000000	0.000000
4	0.101792	-0.056980
5	0.000000	0.000000
6	0.000000	0.000000
7	0.101792	0.056980
8	0.000000	0.000000
9	0.000000	0.000000
10	0.000000	0.113960
11	0.000000	0.000000
12	0.000000	0.000000
13	-0.101792	0.056980
14	0.000000	0.000000
15	0.000000	0.000000
16	-0.101792	-0.056980
17	0.000000	0.000000
18	0.000000	0.000000

coord = q(3)

	1	2	3	4	5	6	7	8
1	0.000000	0.000000	-0.084718	0.000000	0.000000	0.097213	0.000000	0.000000
2	0.000000	0.000000	0.000000	0.075672	0.000000	0.000000	0.075672	0.000000
3	-0.084718	0.000000	0.000000	-0.042359	0.000000	0.000000	0.042359	0.000000
4	0.000000	0.075672	-0.042359	0.000000	-0.086833	0.048607	0.000000	0.086833
5	0.000000	0.000000	0.000000	-0.086833	0.000000	0.000000	-0.086833	0.000000
6	0.097213	0.000000	0.000000	0.048607	0.000000	0.000000	-0.048607	0.000000
7	0.000000	0.075672	0.042359	0.000000	-0.086833	-0.048607	0.000000	0.086833
8	0.000000	0.000000	0.000000	0.086833	0.000000	0.000000	0.086833	0.000000
9	-0.097213	0.000000	0.000000	-0.048607	0.000000	0.000000	0.048607	0.000000
10	0.000000	0.000000	0.084718	0.000000	0.000000	-0.097213	0.000000	0.000000
11	0.000000	0.000000	0.000000	-0.075672	0.000000	0.000000	-0.075672	0.000000
12	0.084718	0.000000	0.000000	0.042359	0.000000	0.000000	-0.042359	0.000000

13	0.000000	-0.075672	0.042359	0.000000	0.086833	-0.048607	0.000000	-0.086833
14	0.000000	0.000000	0.000000	0.086833	0.000000	0.000000	0.086833	0.000000
15	-0.097213	0.000000	0.000000	-0.048607	0.000000	0.000000	0.048607	0.000000
16	0.000000	-0.075672	-0.042359	0.000000	0.086833	0.048607	0.000000	-0.086833
17	0.000000	0.000000	0.000000	-0.086833	0.000000	0.000000	-0.086833	0.000000
18	0.097213	0.000000	0.000000	0.048607	0.000000	0.000000	-0.048607	0.000000
	9	10	11	12	13	14	15	16
1	-0.097213	0.000000	0.000000	0.084718	0.000000	0.000000	-0.097213	0.000000
2	0.000000	0.000000	0.000000	0.000000	-0.075672	0.000000	0.000000	-0.075672
3	0.000000	0.084718	0.000000	0.000000	0.042359	0.000000	0.000000	-0.042359
4	-0.048607	0.000000	-0.075672	0.042359	0.000000	0.086833	-0.048607	0.000000
5	0.000000	0.000000	0.000000	0.000000	0.086833	0.000000	0.000000	0.086833
6	0.000000	-0.097213	0.000000	0.000000	-0.048607	0.000000	0.000000	0.048607
7	0.048607	0.000000	-0.075672	-0.042359	0.000000	0.086833	0.048607	0.000000
8	0.000000	0.000000	0.000000	0.000000	-0.086833	0.000000	0.000000	-0.086833
9	0.000000	0.097213	0.000000	0.000000	0.048607	0.000000	0.000000	-0.048607
10	0.097213	0.000000	0.000000	-0.084718	0.000000	0.000000	0.097213	0.000000
11	0.000000	0.000000	0.000000	0.000000	0.075672	0.000000	0.000000	0.075672
12	0.000000	-0.084718	0.000000	0.000000	-0.042359	0.000000	0.000000	0.042359
13	0.048607	0.000000	0.075672	-0.042359	0.000000	-0.086833	0.048607	0.000000
14	0.000000	0.000000	0.000000	0.000000	-0.086833	0.000000	0.000000	-0.086833
15	0.000000	0.097213	0.000000	0.000000	0.048607	0.000000	0.000000	-0.048607
16	-0.048607	0.000000	0.075672	0.042359	0.000000	-0.086833	-0.048607	0.000000
17	0.000000	0.000000	0.000000	0.000000	0.086833	0.000000	0.000000	0.086833
18	0.000000	-0.097213	0.000000	0.000000	-0.048607	0.000000	0.000000	0.048607
	17	18						
1	0.000000	0.097213						
2	0.000000	0.000000						
3	0.000000	0.000000						
4	-0.086833	0.048607						
5	0.000000	0.000000						
6	0.000000	0.000000						
7	-0.086833	-0.048607						
8	0.000000	0.000000						
9	0.000000	0.000000						
10	0.000000	-0.097213						
11	0.000000	0.000000						
12	0.000000	0.000000						
13	0.086833	-0.048607						
14	0.000000	0.000000						
15	0.000000	0.000000						
16	0.086833	0.048607						
17	0.000000	0.000000						
18	0.000000	0.000000						

coord = phi(2)

	1	2	3	4	5	6	7	8
1	0.000000	0.000000	-0.172479	0.495947	0.000000	0.086239	-0.495947	0.000000
2	0.000000	0.000000	0.000000	0.154063	0.000000	0.000000	0.154063	0.000000
3	-0.172479	0.000000	0.000000	-0.086239	0.000000	0.000000	0.086239	0.000000
4	0.495947	0.154063	-0.086239	-0.495947	-0.077031	0.043120	0.000000	-0.077031
5	0.000000	0.000000	0.000000	-0.077031	0.000000	0.000000	-0.077031	0.000000
6	0.086239	0.000000	0.000000	0.043120	0.000000	0.000000	-0.043120	0.000000
7	-0.495947	0.154063	0.086239	0.000000	-0.077031	-0.043120	0.495947	-0.077031
8	0.000000	0.000000	0.000000	-0.077031	0.000000	0.000000	-0.077031	0.000000
9	0.086239	0.000000	0.000000	0.043120	0.000000	0.000000	-0.043120	0.000000
10	0.000000	0.000000	0.172479	0.495947	0.000000	-0.086239	-0.495947	0.000000
11	0.000000	0.000000	0.000000	0.154063	0.000000	0.000000	0.154063	0.000000
12	-0.172479	0.000000	0.000000	-0.086239	0.000000	0.000000	0.086239	0.000000
13	0.495947	-0.154063	0.086239	-0.495947	0.077031	-0.043120	0.000000	0.077031
14	0.000000	0.000000	0.000000	-0.077031	0.000000	0.000000	-0.077031	0.000000
15	0.086239	0.000000	0.000000	0.043120	0.000000	0.000000	-0.043120	0.000000
16	-0.495947	-0.154063	-0.086239	0.000000	0.077031	0.043120	0.495947	0.077031
17	0.000000	0.000000	0.000000	-0.077031	0.000000	0.000000	-0.077031	0.000000
18	0.086239	0.000000	0.000000	0.043120	0.000000	0.000000	-0.043120	0.000000
	9	10	11	12	13	14	15	16



tau(4)	0.000000	0.000000	7.484336	0.000000	-6.481625	3.742168	0.000000	-6.481625
	y6	z6						
t(1)	0.166667	0.000000						
t(2)	0.000000	0.000000						
t(3)	0.166667	0.000000						
t(4)	0.144338	0.000000						
R	-0.144338	0.000000						
tau(1)	0.000000	0.000000						
tau(2)	2.545864	0.000000						
tau(3)	0.000000	0.000000						
tau(4)	-3.742168	0.000000						

C. II) Deformation part: B-matrix elements for N-3 puckering coordinates: (2N-3) x 3N partial derivatives (d zeta\_n /d r\_alpha)

	x1	y1	z1	x2	y2	z2	x3	y3
t(1)	0.000000	0.166667	0.166667	0.000000	0.166667	0.166667	0.000000	0.166667
t(2)	0.000000	0.000000	-0.166667	0.000000	0.000000	0.166667	0.000000	0.000000
t(3)	0.000000	0.166667	0.166667	0.000000	0.166667	0.166667	0.000000	0.166667
t(4)	0.000000	0.000000	-0.166667	0.000000	-0.144338	-0.083333	0.000000	-0.144338
R	0.000000	0.000000	-0.166667	0.000000	0.144338	-0.083333	0.000000	0.144338
tau(1)	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
tau(2)	0.000000	-2.430142	0.000000	0.000000	2.603725	0.100218	0.000000	-2.603725
tau(3)	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
tau(4)	0.000000	-7.368613	0.000000	0.000000	-3.684307	6.581843	0.000000	3.684307
	z3	x4	y4	z4	x5	y5	z5	x6
t(1)	0.166667	0.000000	0.166667	0.166667	0.000000	0.166667	0.166667	0.000000
t(2)	-0.166667	0.000000	0.000000	0.166667	0.000000	0.000000	-0.166667	0.000000
t(3)	0.166667	0.000000	0.166667	0.166667	0.000000	0.166667	0.166667	0.000000
t(4)	0.083333	0.000000	0.000000	0.166667	0.000000	0.144338	0.083333	0.000000
R	0.083333	0.000000	0.000000	0.166667	0.000000	-0.144338	0.083333	0.000000
tau(1)	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
tau(2)	0.100218	0.000000	2.430142	0.000000	0.000000	-2.603725	-0.100218	0.000000
tau(3)	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
tau(4)	6.581843	0.000000	7.368613	0.000000	0.000000	3.684307	-6.581843	0.000000
	y6	z6						
t(1)	0.166667	0.166667						
t(2)	0.000000	0.166667						
t(3)	0.166667	0.166667						
t(4)	0.144338	-0.083333						
R	-0.144338	-0.083333						
tau(1)	0.000000	0.000000						
tau(2)	2.603725	-0.100218						
tau(3)	0.000000	0.000000						
tau(4)	-3.684307	-6.581843						

C. III) Deformation part: Derivatives of B matrix: (d B\_i /d r\_alpha) (2N-3) x 3N x 3N

coord = t(1)

	1	2	3	4	5	6	7	8
1	-0.075973	0.000000	0.000000	-0.023049	0.000000	0.000000	0.014937	0.000000
2	0.000000	-0.038574	0.019287	0.000000	-0.028931	0.002584	0.000000	-0.009644
3	0.000000	0.019287	0.000000	0.000000	0.009644	0.016703	0.000000	-0.009644
4	-0.023049	0.000000	0.000000	0.029875	0.000000	0.000000	0.067862	0.000000
5	0.000000	-0.028931	0.009644	0.000000	-0.019287	-0.007060	0.000000	0.000000
6	0.000000	0.002584	0.016703	0.000000	-0.007060	0.033406	0.000000	-0.026347
7	0.014937	0.000000	0.000000	0.067862	0.000000	0.000000	0.105848	0.000000
8	0.000000	-0.009644	-0.009644	0.000000	0.000000	-0.026347	0.000000	0.019287
9	0.000000	0.002584	0.016703	0.000000	-0.007060	0.033406	0.000000	-0.026347
10	0.000000	0.000000	0.000000	0.052924	0.000000	0.000000	0.090911	0.000000
11	0.000000	0.000000	-0.019287	0.000000	0.009644	-0.035990	0.000000	0.028931
12	0.000000	0.019287	0.000000	0.000000	0.009644	0.016703	0.000000	-0.009644
13	-0.052924	0.000000	0.000000	0.000000	0.000000	0.000000	0.037987	0.000000
14	0.000000	-0.009644	-0.009644	0.000000	0.000000	-0.026347	0.000000	0.019287



15	0.000000	0.035990	-0.016703	0.000000	0.026347	0.000000	0.000000	0.007060
16	-0.090911	0.000000	0.000000	-0.037987	0.000000	0.000000	0.000000	0.000000
17	0.000000	-0.028931	0.009644	0.000000	-0.019287	-0.007060	0.000000	0.000000
18	0.000000	0.035990	-0.016703	0.000000	0.026347	0.000000	0.000000	0.007060
	9	10	11	12	13	14	15	16
1	0.000000	0.000000	0.000000	0.000000	-0.052924	0.000000	0.000000	-0.090911
2	0.002584	0.000000	0.000000	0.019287	0.000000	-0.009644	0.035990	0.000000
3	0.016703	0.000000	-0.019287	0.000000	0.000000	-0.009644	-0.016703	0.000000
4	0.000000	0.052924	0.000000	0.000000	0.000000	0.000000	0.000000	-0.037987
5	-0.007060	0.000000	0.009644	0.009644	0.000000	0.000000	0.026347	0.000000
6	0.033406	0.000000	-0.035990	0.016703	0.000000	-0.026347	0.000000	0.000000
7	0.000000	0.090911	0.000000	0.000000	0.037987	0.000000	0.000000	0.000000
8	-0.026347	0.000000	0.028931	-0.009644	0.000000	0.019287	0.007060	0.000000
9	0.033406	0.000000	-0.035990	0.016703	0.000000	-0.026347	0.000000	0.000000
10	0.000000	0.075973	0.000000	0.000000	0.023049	0.000000	0.000000	-0.014937
11	-0.035990	0.000000	0.038574	-0.019287	0.000000	0.028931	-0.002584	0.000000
12	0.016703	0.000000	-0.019287	0.000000	0.000000	-0.009644	-0.016703	0.000000
13	0.000000	0.023049	0.000000	0.000000	-0.029875	0.000000	0.000000	-0.067862
14	-0.026347	0.000000	0.028931	-0.009644	0.000000	0.019287	0.007060	0.000000
15	0.000000	0.000000	-0.002584	-0.016703	0.000000	0.007060	-0.033406	0.000000
16	0.000000	-0.014937	0.000000	0.000000	-0.067862	0.000000	0.000000	-0.105848
17	-0.007060	0.000000	0.009644	0.009644	0.000000	0.000000	0.026347	0.000000
18	0.000000	0.000000	-0.002584	-0.016703	0.000000	0.007060	-0.033406	0.000000
	17	18						
1	0.000000	0.000000						
2	-0.028931	0.035990						
3	0.009644	-0.016703						
4	0.000000	0.000000						
5	-0.019287	0.026347						
6	-0.007060	0.000000						
7	0.000000	0.000000						
8	0.000000	0.007060						
9	-0.007060	0.000000						
10	0.000000	0.000000						
11	0.009644	-0.002584						
12	0.009644	-0.016703						
13	0.000000	0.000000						
14	0.000000	0.007060						
15	0.026347	-0.033406						
16	0.000000	0.000000						
17	-0.019287	0.026347						
18	0.026347	-0.033406						

coord = t(2)

	1	2	3	4	5	6	7	8
1	0.072573	0.000000	0.000000	-0.020694	0.000000	0.000000	0.020694	0.000000
2	0.000000	0.424311	0.000000	0.000000	-0.424311	0.000000	0.000000	0.424311
3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
4	-0.020694	0.000000	0.000000	-0.038837	0.000000	0.000000	0.038837	0.000000
5	0.000000	-0.424311	0.000000	0.000000	0.424311	0.000000	0.000000	-0.424311
6	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
7	0.020694	0.000000	0.000000	0.038837	0.000000	0.000000	-0.038837	0.000000
8	0.000000	0.424311	0.000000	0.000000	-0.424311	0.000000	0.000000	0.424311
9	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
10	-0.072573	0.000000	0.000000	0.020694	0.000000	0.000000	-0.020694	0.000000
11	0.000000	-0.424311	0.000000	0.000000	0.424311	0.000000	0.000000	-0.424311
12	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
13	0.020694	0.000000	0.000000	0.038837	0.000000	0.000000	-0.038837	0.000000
14	0.000000	0.424311	0.000000	0.000000	-0.424311	0.000000	0.000000	0.424311
15	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
16	-0.020694	0.000000	0.000000	-0.038837	0.000000	0.000000	0.038837	0.000000
17	0.000000	-0.424311	0.000000	0.000000	0.424311	0.000000	0.000000	-0.424311
18	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
	9	10	11	12	13	14	15	16
1	0.000000	-0.072573	0.000000	0.000000	0.020694	0.000000	0.000000	-0.020694
2	0.000000	0.000000	-0.424311	0.000000	0.000000	0.424311	0.000000	0.000000

3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
4	0.000000	0.020694	0.000000	0.000000	0.038837	0.000000	0.000000	-0.038837
5	0.000000	0.000000	0.424311	0.000000	0.000000	-0.424311	0.000000	0.000000
6	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
7	0.000000	-0.020694	0.000000	0.000000	-0.038837	0.000000	0.000000	0.038837
8	0.000000	0.000000	-0.424311	0.000000	0.000000	0.424311	0.000000	0.000000
9	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
10	0.000000	0.072573	0.000000	0.000000	-0.020694	0.000000	0.000000	0.020694
11	0.000000	0.000000	0.424311	0.000000	0.000000	-0.424311	0.000000	0.000000
12	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
13	0.000000	-0.020694	0.000000	0.000000	-0.038837	0.000000	0.000000	0.038837
14	0.000000	0.000000	-0.424311	0.000000	0.000000	0.424311	0.000000	0.000000
15	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
16	0.000000	0.020694	0.000000	0.000000	0.038837	0.000000	0.000000	-0.038837
17	0.000000	0.000000	0.424311	0.000000	0.000000	-0.424311	0.000000	0.000000
18	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

	17	18
1	0.000000	0.000000
2	-0.424311	0.000000
3	0.000000	0.000000
4	0.000000	0.000000
5	0.424311	0.000000
6	0.000000	0.000000
7	0.000000	0.000000
8	-0.424311	0.000000
9	0.000000	0.000000
10	0.000000	0.000000
11	0.424311	0.000000
12	0.000000	0.000000
13	0.000000	0.000000
14	-0.424311	0.000000
15	0.000000	0.000000
16	0.000000	0.000000
17	0.424311	0.000000
18	0.000000	0.000000

coord = t(3)

	1	2	3	4	5	6	7	8
1	-0.075973	0.000000	0.000000	-0.023049	0.000000	0.000000	0.014937	0.000000
2	0.000000	-0.038574	0.019287	0.000000	-0.028931	0.002584	0.000000	-0.009644
3	0.000000	0.019287	0.000000	0.000000	0.009644	0.016703	0.000000	-0.009644
4	-0.023049	0.000000	0.000000	0.029875	0.000000	0.000000	0.067862	0.000000
5	0.000000	-0.028931	0.009644	0.000000	-0.019287	-0.007060	0.000000	0.000000
6	0.000000	0.002584	0.016703	0.000000	-0.007060	0.033406	0.000000	-0.026347
7	0.014937	0.000000	0.000000	0.067862	0.000000	0.000000	0.105848	0.000000
8	0.000000	-0.009644	-0.009644	0.000000	0.000000	-0.026347	0.000000	0.019287
9	0.000000	0.002584	0.016703	0.000000	-0.007060	0.033406	0.000000	-0.026347
10	0.000000	0.000000	0.000000	0.052924	0.000000	0.000000	0.090911	0.000000
11	0.000000	0.000000	-0.019287	0.000000	0.009644	-0.035990	0.000000	0.028931
12	0.000000	0.019287	0.000000	0.000000	0.009644	0.016703	0.000000	-0.009644
13	-0.052924	0.000000	0.000000	0.000000	0.000000	0.000000	0.037987	0.000000
14	0.000000	-0.009644	-0.009644	0.000000	0.000000	-0.026347	0.000000	0.019287
15	0.000000	0.035990	-0.016703	0.000000	0.026347	0.000000	0.000000	0.007060
16	-0.090911	0.000000	0.000000	-0.037987	0.000000	0.000000	0.000000	0.000000
17	0.000000	-0.028931	0.009644	0.000000	-0.019287	-0.007060	0.000000	0.000000
18	0.000000	0.035990	-0.016703	0.000000	0.026347	0.000000	0.000000	0.007060
	9	10	11	12	13	14	15	16
1	0.000000	0.000000	0.000000	0.000000	-0.052924	0.000000	0.000000	-0.090911
2	0.002584	0.000000	0.000000	0.019287	0.000000	-0.009644	0.035990	0.000000
3	0.016703	0.000000	-0.019287	0.000000	0.000000	-0.009644	-0.016703	0.000000
4	0.000000	0.052924	0.000000	0.000000	0.000000	0.000000	0.000000	-0.037987
5	-0.007060	0.000000	0.009644	0.009644	0.000000	0.000000	0.026347	0.000000
6	0.033406	0.000000	-0.035990	0.016703	0.000000	-0.026347	0.000000	0.000000
7	0.000000	0.090911	0.000000	0.000000	0.037987	0.000000	0.000000	0.000000
8	-0.026347	0.000000	0.028931	-0.009644	0.000000	0.019287	0.007060	0.000000
9	0.033406	0.000000	-0.035990	0.016703	0.000000	-0.026347	0.000000	0.000000

10	0.000000	0.075973	0.000000	0.000000	0.023049	0.000000	0.000000	-0.014937
11	-0.035990	0.000000	0.038574	-0.019287	0.000000	0.028931	-0.002584	0.000000
12	0.016703	0.000000	-0.019287	0.000000	0.000000	-0.009644	-0.016703	0.000000
13	0.000000	0.023049	0.000000	0.000000	-0.029875	0.000000	0.000000	-0.067862
14	-0.026347	0.000000	0.028931	-0.009644	0.000000	0.019287	0.007060	0.000000
15	0.000000	0.000000	-0.002584	-0.016703	0.000000	0.007060	-0.033406	0.000000
16	0.000000	-0.014937	0.000000	0.000000	-0.067862	0.000000	0.000000	-0.105848
17	-0.007060	0.000000	0.009644	0.009644	0.000000	0.000000	0.026347	0.000000
18	0.000000	0.000000	-0.002584	-0.016703	0.000000	0.007060	-0.033406	0.000000

	17	18
1	0.000000	0.000000
2	-0.028931	0.035990
3	0.009644	-0.016703
4	0.000000	0.000000
5	-0.019287	0.026347
6	-0.007060	0.000000
7	0.000000	0.000000
8	0.000000	0.007060
9	-0.007060	0.000000
10	0.000000	0.000000
11	0.009644	-0.002584
12	0.009644	-0.016703
13	0.000000	0.000000
14	0.000000	0.007060
15	0.026347	-0.033406
16	0.000000	0.000000
17	-0.019287	0.026347
18	0.026347	-0.033406

coord = t(4)

	1	2	3	4	5	6	7	8
1	0.037987	0.000000	0.000000	0.018993	0.000000	0.000000	-0.018993	0.000000
2	0.000000	1.247389	0.000000	0.000000	0.623695	-1.080271	0.000000	-0.623695
3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
4	0.018993	0.000000	0.000000	-0.019888	0.000000	0.000000	-0.038882	0.000000
5	0.000000	0.623695	0.000000	0.000000	0.311847	-0.540135	0.000000	-0.311847
6	0.000000	-1.080271	0.000000	0.000000	-0.540135	0.935542	0.000000	0.540135
7	-0.018993	0.000000	0.000000	-0.038882	0.000000	0.000000	-0.019888	0.000000
8	0.000000	-0.623695	0.000000	0.000000	-0.311847	0.540135	0.000000	0.311847
9	0.000000	-1.080271	0.000000	0.000000	-0.540135	0.935542	0.000000	0.540135
10	-0.037987	0.000000	0.000000	-0.018993	0.000000	0.000000	0.018993	0.000000
11	0.000000	-1.247389	0.000000	0.000000	-0.623695	1.080271	0.000000	0.623695
12	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
13	-0.018993	0.000000	0.000000	0.019888	0.000000	0.000000	0.038882	0.000000
14	0.000000	-0.623695	0.000000	0.000000	-0.311847	0.540135	0.000000	0.311847
15	0.000000	1.080271	0.000000	0.000000	0.540135	-0.935542	0.000000	-0.540135
16	0.018993	0.000000	0.000000	0.038882	0.000000	0.000000	0.019888	0.000000
17	0.000000	0.623695	0.000000	0.000000	0.311847	-0.540135	0.000000	-0.311847
18	0.000000	1.080271	0.000000	0.000000	0.540135	-0.935542	0.000000	-0.540135
	9	10	11	12	13	14	15	16
1	0.000000	-0.037987	0.000000	0.000000	-0.018993	0.000000	0.000000	0.018993
2	-1.080271	0.000000	-1.247389	0.000000	0.000000	-0.623695	1.080271	0.000000
3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
4	0.000000	-0.018993	0.000000	0.000000	0.019888	0.000000	0.000000	0.038882
5	-0.540135	0.000000	-0.623695	0.000000	0.000000	-0.311847	0.540135	0.000000
6	0.935542	0.000000	1.080271	0.000000	0.000000	0.540135	-0.935542	0.000000
7	0.000000	0.018993	0.000000	0.000000	0.038882	0.000000	0.000000	0.019888
8	0.540135	0.000000	0.623695	0.000000	0.000000	0.311847	-0.540135	0.000000
9	0.935542	0.000000	1.080271	0.000000	0.000000	0.540135	-0.935542	0.000000
10	0.000000	0.037987	0.000000	0.000000	0.018993	0.000000	0.000000	-0.018993
11	1.080271	0.000000	1.247389	0.000000	0.000000	0.623695	-1.080271	0.000000
12	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
13	0.000000	0.018993	0.000000	0.000000	-0.019888	0.000000	0.000000	-0.038882
14	0.540135	0.000000	0.623695	0.000000	0.000000	0.311847	-0.540135	0.000000
15	-0.935542	0.000000	-1.080271	0.000000	0.000000	-0.540135	0.935542	0.000000
16	0.000000	-0.018993	0.000000	0.000000	-0.038882	0.000000	0.000000	-0.019888

17	-0.540135	0.000000	-0.623695	0.000000	0.000000	-0.311847	0.540135	0.000000
18	-0.935542	0.000000	-1.080271	0.000000	0.000000	-0.540135	0.935542	0.000000
	17	18						
1	0.000000	0.000000						
2	0.623695	1.080271						
3	0.000000	0.000000						
4	0.000000	0.000000						
5	0.311847	0.540135						
6	-0.540135	-0.935542						
7	0.000000	0.000000						
8	-0.311847	-0.540135						
9	-0.540135	-0.935542						
10	0.000000	0.000000						
11	-0.623695	-1.080271						
12	0.000000	0.000000						
13	0.000000	0.000000						
14	-0.311847	-0.540135						
15	0.540135	0.935542						
16	0.000000	0.000000						
17	0.311847	0.540135						
18	0.540135	0.935542						

coord = R

	1	2	3	4	5	6	7	8
1	0.037987	0.000000	0.000000	0.018993	0.000000	0.000000	-0.018993	0.000000
2	0.000000	0.019287	0.000000	0.000000	0.009644	0.016703	0.000000	-0.009644
3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
4	0.018993	0.000000	0.000000	0.038882	0.000000	0.000000	0.019888	0.000000
5	0.000000	0.009644	0.000000	0.000000	0.004822	0.008352	0.000000	-0.004822
6	0.000000	0.016703	0.000000	0.000000	0.008352	0.014465	0.000000	-0.008352
7	-0.018993	0.000000	0.000000	0.019888	0.000000	0.000000	0.038882	0.000000
8	0.000000	-0.009644	0.000000	0.000000	-0.004822	-0.008352	0.000000	0.004822
9	0.000000	0.016703	0.000000	0.000000	0.008352	0.014465	0.000000	-0.008352
10	-0.037987	0.000000	0.000000	-0.018993	0.000000	0.000000	0.018993	0.000000
11	0.000000	-0.019287	0.000000	0.000000	-0.009644	-0.016703	0.000000	0.009644
12	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
13	-0.018993	0.000000	0.000000	-0.038882	0.000000	0.000000	-0.019888	0.000000
14	0.000000	-0.009644	0.000000	0.000000	-0.004822	-0.008352	0.000000	0.004822
15	0.000000	-0.016703	0.000000	0.000000	-0.008352	-0.014465	0.000000	0.008352
16	0.018993	0.000000	0.000000	-0.019888	0.000000	0.000000	-0.038882	0.000000
17	0.000000	0.009644	0.000000	0.000000	0.004822	0.008352	0.000000	-0.004822
18	0.000000	-0.016703	0.000000	0.000000	-0.008352	-0.014465	0.000000	0.008352
	9	10	11	12	13	14	15	16
1	0.000000	-0.037987	0.000000	0.000000	-0.018993	0.000000	0.000000	0.018993
2	0.016703	0.000000	-0.019287	0.000000	0.000000	-0.009644	-0.016703	0.000000
3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
4	0.000000	-0.018993	0.000000	0.000000	-0.038882	0.000000	0.000000	-0.019888
5	0.008352	0.000000	-0.009644	0.000000	0.000000	-0.004822	-0.008352	0.000000
6	0.014465	0.000000	-0.016703	0.000000	0.000000	-0.008352	-0.014465	0.000000
7	0.000000	0.018993	0.000000	0.000000	-0.019888	0.000000	0.000000	-0.038882
8	-0.008352	0.000000	0.009644	0.000000	0.000000	0.004822	0.008352	0.000000
9	0.014465	0.000000	-0.016703	0.000000	0.000000	-0.008352	-0.014465	0.000000
10	0.000000	0.037987	0.000000	0.000000	0.018993	0.000000	0.000000	-0.018993
11	-0.016703	0.000000	0.019287	0.000000	0.000000	0.009644	0.016703	0.000000
12	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
13	0.000000	0.018993	0.000000	0.000000	0.038882	0.000000	0.000000	0.019888
14	-0.008352	0.000000	0.009644	0.000000	0.000000	0.004822	0.008352	0.000000
15	-0.014465	0.000000	0.016703	0.000000	0.000000	0.008352	0.014465	0.000000
16	0.000000	-0.018993	0.000000	0.000000	0.019888	0.000000	0.000000	0.038882
17	0.008352	0.000000	-0.009644	0.000000	0.000000	-0.004822	-0.008352	0.000000
18	-0.014465	0.000000	0.016703	0.000000	0.000000	0.008352	0.014465	0.000000
	17	18						
1	0.000000	0.000000						
2	0.009644	-0.016703						
3	0.000000	0.000000						
4	0.000000	0.000000						



12	0.000000	0.000000
13	0.000000	0.000000
14	0.000000	0.000000
15	0.000000	0.000000
16	0.000000	0.000000
17	0.000000	0.000000
18	0.000000	0.000000

coord = tau(2)

	1	2	3	4	5	6	7	8
1	0.000000	0.000000	0.000000	-0.494739	0.000000	0.000000	-0.494739	0.000000
2	0.000000	0.000000	-6.468031	0.000000	-0.011597	6.488118	0.000000	-0.011597
3	0.000000	-6.468031	0.000000	0.000000	6.488118	0.011597	0.000000	-6.488118
4	-0.494739	0.000000	0.000000	1.060156	0.000000	0.000000	0.000000	0.000000
5	0.000000	-0.011597	6.488118	0.000000	-0.011597	-6.488118	0.000000	0.000000
6	0.000000	6.488118	0.011597	0.000000	-6.488118	0.011597	0.000000	6.468031
7	-0.494739	0.000000	0.000000	0.000000	0.000000	0.000000	-1.060156	0.000000
8	0.000000	-0.011597	-6.488118	0.000000	0.000000	6.468031	0.000000	0.011597
9	0.000000	-6.488118	0.011597	0.000000	6.468031	0.000000	0.000000	-6.488118
10	0.000000	0.000000	0.000000	0.494739	0.000000	0.000000	0.494739	0.000000
11	0.000000	0.000000	6.468031	0.000000	0.011597	-6.488118	0.000000	0.011597
12	0.000000	6.468031	0.000000	0.000000	-6.488118	-0.011597	0.000000	6.488118
13	0.494739	0.000000	0.000000	-1.060156	0.000000	0.000000	0.000000	0.000000
14	0.000000	0.011597	-6.488118	0.000000	0.011597	6.488118	0.000000	0.000000
15	0.000000	-6.488118	-0.011597	0.000000	6.488118	-0.011597	0.000000	-6.468031
16	0.494739	0.000000	0.000000	0.000000	0.000000	0.000000	1.060156	0.000000
17	0.000000	0.011597	6.488118	0.000000	0.000000	-6.468031	0.000000	-0.011597
18	0.000000	6.488118	-0.011597	0.000000	-6.468031	0.000000	0.000000	6.488118
	9	10	11	12	13	14	15	16
1	0.000000	0.000000	0.000000	0.000000	0.494739	0.000000	0.000000	0.494739
2	-6.488118	0.000000	0.000000	6.468031	0.000000	0.011597	-6.488118	0.000000
3	0.011597	0.000000	6.468031	0.000000	0.000000	-6.488118	-0.011597	0.000000
4	0.000000	0.494739	0.000000	0.000000	-1.060156	0.000000	0.000000	0.000000
5	6.468031	0.000000	0.011597	-6.488118	0.000000	0.011597	6.488118	0.000000
6	0.000000	0.000000	-6.488118	-0.011597	0.000000	6.488118	-0.011597	0.000000
7	0.000000	0.494739	0.000000	0.000000	0.000000	0.000000	0.000000	1.060156
8	-6.488118	0.000000	0.011597	6.488118	0.000000	0.000000	-6.468031	0.000000
9	-0.011597	0.000000	6.488118	-0.011597	0.000000	-6.468031	0.000000	0.000000
10	0.000000	0.000000	0.000000	0.000000	-0.494739	0.000000	0.000000	-0.494739
11	6.488118	0.000000	0.000000	-6.468031	0.000000	-0.011597	6.488118	0.000000
12	-0.011597	0.000000	-6.468031	0.000000	0.000000	6.488118	0.011597	0.000000
13	0.000000	-0.494739	0.000000	0.000000	1.060156	0.000000	0.000000	0.000000
14	-6.468031	0.000000	-0.011597	6.488118	0.000000	-0.011597	-6.488118	0.000000
15	0.000000	0.000000	6.488118	0.011597	0.000000	-6.488118	0.011597	0.000000
16	0.000000	-0.494739	0.000000	0.000000	0.000000	0.000000	0.000000	-1.060156
17	6.488118	0.000000	-0.011597	-6.488118	0.000000	0.000000	6.468031	0.000000
18	0.011597	0.000000	-6.488118	0.011597	0.000000	6.468031	0.000000	0.000000
	17	18						
1	0.000000	0.000000						
2	0.011597	6.488118						
3	6.488118	-0.011597						
4	0.000000	0.000000						
5	0.000000	-6.468031						
6	-6.468031	0.000000						
7	0.000000	0.000000						
8	-0.011597	6.488118						
9	6.488118	0.011597						
10	0.000000	0.000000						
11	-0.011597	-6.488118						
12	-6.488118	0.011597						
13	0.000000	0.000000						
14	0.000000	6.468031						
15	6.468031	0.000000						
16	0.000000	0.000000						
17	0.011597	-6.488118						
18	-6.488118	-0.011597						



5	0.000000	-48.522253	-28.000944	0.000000	-48.522253	28.000944	0.000000	0.000000
6	0.000000	-28.000944	48.522253	0.000000	28.000944	48.522253	0.000000	56.001888
7	-1.500136	0.000000	0.000000	0.000000	0.000000	0.000000	1.500136	0.000000
8	0.000000	-48.522253	28.000944	0.000000	0.000000	56.001888	0.000000	48.522253
9	0.000000	28.000944	48.522253	0.000000	56.001888	0.000000	0.000000	28.000944
10	0.000000	0.000000	0.000000	1.500136	0.000000	0.000000	1.500136	0.000000
11	0.000000	0.000000	56.001888	0.000000	48.522253	28.000944	0.000000	48.522253
12	0.000000	56.001888	0.000000	0.000000	28.000944	-48.522253	0.000000	-28.000944
13	1.500136	0.000000	0.000000	1.500136	0.000000	0.000000	0.000000	0.000000
14	0.000000	48.522253	28.000944	0.000000	48.522253	-28.000944	0.000000	0.000000
15	0.000000	28.000944	-48.522253	0.000000	-28.000944	-48.522253	0.000000	-56.001888
16	1.500136	0.000000	0.000000	0.000000	0.000000	0.000000	-1.500136	0.000000
17	0.000000	48.522253	-28.000944	0.000000	0.000000	-56.001888	0.000000	-48.522253
18	0.000000	-28.000944	-48.522253	0.000000	-56.001888	0.000000	0.000000	-28.000944
	9	10	11	12	13	14	15	16
1	0.000000	0.000000	0.000000	0.000000	1.500136	0.000000	0.000000	1.500136
2	28.000944	0.000000	0.000000	56.001888	0.000000	48.522253	28.000944	0.000000
3	48.522253	0.000000	56.001888	0.000000	0.000000	28.000944	-48.522253	0.000000
4	0.000000	1.500136	0.000000	0.000000	1.500136	0.000000	0.000000	0.000000
5	56.001888	0.000000	48.522253	28.000944	0.000000	48.522253	-28.000944	0.000000
6	0.000000	0.000000	28.000944	-48.522253	0.000000	-28.000944	-48.522253	0.000000
7	0.000000	1.500136	0.000000	0.000000	0.000000	0.000000	0.000000	-1.500136
8	28.000944	0.000000	48.522253	-28.000944	0.000000	0.000000	-56.001888	0.000000
9	-48.522253	0.000000	-28.000944	-48.522253	0.000000	-56.001888	0.000000	0.000000
10	0.000000	0.000000	0.000000	0.000000	-1.500136	0.000000	0.000000	-1.500136
11	-28.000944	0.000000	0.000000	-56.001888	0.000000	-48.522253	-28.000944	0.000000
12	-48.522253	0.000000	-56.001888	0.000000	0.000000	-28.000944	48.522253	0.000000
13	0.000000	-1.500136	0.000000	0.000000	-1.500136	0.000000	0.000000	0.000000
14	-56.001888	0.000000	-48.522253	-28.000944	0.000000	-48.522253	28.000944	0.000000
15	0.000000	0.000000	-28.000944	48.522253	0.000000	28.000944	48.522253	0.000000
16	0.000000	-1.500136	0.000000	0.000000	0.000000	0.000000	0.000000	1.500136
17	-28.000944	0.000000	-48.522253	28.000944	0.000000	0.000000	56.001888	0.000000
18	48.522253	0.000000	28.000944	48.522253	0.000000	56.001888	0.000000	0.000000
	17	18						
1	0.000000	0.000000						
2	48.522253	-28.000944						
3	-28.000944	-48.522253						
4	0.000000	0.000000						
5	0.000000	-56.001888						
6	-56.001888	0.000000						
7	0.000000	0.000000						
8	-48.522253	-28.000944						
9	-28.000944	48.522253						
10	0.000000	0.000000						
11	-48.522253	28.000944						
12	28.000944	48.522253						
13	0.000000	0.000000						
14	0.000000	56.001888						
15	56.001888	0.000000						
16	0.000000	0.000000						
17	48.522253	28.000944						
18	28.000944	-48.522253						