



FOUNDATIONS  
ADVANCES

**Volume 80 (2024)**

**Supporting information for article:**

**Periodic Borromean rings, rods and chains**

**Michael O'Keeffe and Michael M. J. Treacy**

# Systre-format data for structures in O'Keeffe & Treacy "Periodic Borromean Rings"

# Structures identified by Figure number and girth.

# Figure 1

# Systre file created by KLiNG v0.420 on Sun May 7 12:35:20 2023

CRYSTAL

NAME 3triangles\_P3\_0.1301277804\_MT

GROUP P3

CELL 20.0000 20.0000 10.0000 90.0000 90.0000 120.0000

NODE 1 2 0.204013 -0.031509 0.222235

EDGE 1 -0.454352 -0.187562 -0.264749

EDGE 1 0.158935 0.445110 -0.586870

NODE 2 2 -0.454352 -0.187562 -0.264749

EDGE 2 0.158935 0.445110 -0.586870

EDGE 2 0.204013 -0.031509 0.222235

NODE 3 2 0.158935 0.445110 -0.586870

EDGE 3 0.204013 -0.031509 0.222235

EDGE 3 -0.454352 -0.187562 -0.264749

END

# \_\_\_\_\_

#

# Figure 6

# Systre file created by KLiNG v0.420 on Fri May 5 21:11:15 2023

CRYSTAL

NAME P622\_BinoBorro2\_0.3568902497\_MG

GROUP P622

CELL 10.0000 10.0000 100.0000 90.0000 90.0000 120.0000

NODE 1 2 -0.426393 0.158733 0.011069

EDGE 1 -0.426393 0.414874 -0.011069

```
EDGE 1  -0.167736  0.128703  -0.008691

NODE 2 2  -0.167736  0.128703  -0.008691
EDGE 2   0.167736  0.296439  0.008691
EDGE 2  -0.426393  0.158733  0.011069
END
```

```
# _____
```

```
# Systre file created by KLiNG v0.422 on Thu Jun 22 10:03:46 2023
```

```
CRYSTAL
```

```
NAME 24r_P622_0.2809226385_MG
```

```
GROUP P622
```

```
CELL 10.0000 10.0000 100.0000 90.0000 90.0000 120.0000
```

```
NODE 1 2  -0.255359  -0.729859  0.006074
```

```
EDGE 1  -0.474500  -0.729859  -0.006074
```

```
EDGE 1  -0.089184  -0.509397  -0.009157
```

```
NODE 2 2  -0.089184  -0.509397  -0.009157
```

```
EDGE 2   0.089184  -0.420214  0.009157
```

```
EDGE 2  -0.255359  -0.729859  0.006074
```

```
END
```

```
# Systre file created by KLiNG v0.425 on Tue Aug 8 07:20:55 2023
```

```
CRYSTAL
```

```
NAME 5BorroCM_C2m_0.1298904519_MG
```

```
GROUP C2/m
```

```
CELL 10.0000 49.9524 100.0000 90.0000 90.0000 90.0000
```

```
NODE 1 2  0.583303  0.000000  0.121642
```

```
EDGE 1  -0.652074  -0.458832  -0.058549
```

```
EDGE 1  -0.652074  0.458832  -0.058549
```

```
NODE 2 2 0.347926 -0.458832 -0.058549
EDGE 2 -1.347926 -0.458832 0.058549
EDGE 2 1.583303 0.000000 0.121642
END
```

```
# Systre file created by KLiNG v0.425 on Tue Aug 8 08:51:43 2023
```

```
CRYSTAL
```

```
NAME hcb-c5_C2m_0.2000000000_MG
```

```
GROUP C2/m
```

```
CELL 10.0000 28.8675 100.0000 90.0000 90.0000 90.0000
```

```
NODE 1 3 0.166667 0.000000 0.058926
EDGE 1 1.833333 0.000000 -0.058926
EDGE 1 -0.666667 0.500000 -0.058926
EDGE 1 -0.666667 -0.500000 -0.058926
END
```

```
# _____
```

```
# Figure 7
```

```
# Systre file created by KLiNG v0.420 on Sat May 6 14:35:44 2023
```

```
CRYSTAL
```

```
NAME BorroNT_P63cm_0.2030756474_MT
```

```
GROUP P63cm
```

```
CELL 100.0000 100.0000 10.0000 90.0000 90.0000 120.0000
```

```
NODE 1 3 0.063541 0.000000 0.250000
EDGE 1 0.118037 0.118037 -0.250000
EDGE 1 0.000000 -0.118037 -0.250000
EDGE 1 0.118037 0.000000 1.250000
```

```
NODE 2 3 0.118037 0.000000 1.250000
EDGE 2 0.063541 0.000000 0.250000
EDGE 2 0.000000 -0.063541 1.750000
```

EDGE 2 0.063541 0.063541 1.750000

END

#

---

# Systre file created by KLiNG v0.420 on Sat May 6 17:36:32 2023

CRYSTAL

NAME BorroNT\_4vtx\_P63cm\_0.1755619976\_MG

GROUP P63cm

CELL 100.0000 100.0000 1.1108 90.0000 90.0000 120.0000

NODE 1 2 0.000000 -0.016853 0.583324

EDGE 1 -0.008212 -0.009621 0.246525

EDGE 1 0.008212 -0.001409 0.246525

NODE 2 2 -0.008212 -0.009621 0.246525

EDGE 2 -0.012432 -0.013840 -0.778486

EDGE 2 0.000000 -0.016853 0.583324

NODE 3 2 -0.012432 -0.013840 -0.778486

EDGE 3 0.000000 -0.009737 -1.060780

EDGE 3 -0.008212 -0.009621 0.246525

NODE 4 2 0.000000 -0.009737 -1.060780

EDGE 4 -0.012432 -0.013840 -0.778486

EDGE 4 0.012432 -0.001409 -0.778486

END

#

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# Figure 12

# Systre file created by KLiNG v0.420 on Sat May 6 21:19:27 2023

CRYSTAL

NAME borroChinas6-per\_0.1485166410\_MG

GROUP Fd-3c:1

CELL 10.0000 10.0000 10.0000 90.0000 90.0000 90.0000

NODE 1 2 -0.001598 0.163937 0.073047

EDGE 1 0.001598 0.163937 -0.073047

EDGE 1 0.001598 -0.163937 0.073047

NODE 2 2 -0.113441 -0.026711 0.074323

EDGE 2 -0.383315 -0.061737 0.022408

EDGE 2 -0.116685 -0.022408 -0.061737

NODE 3 2 -0.383315 0.061737 -0.022408

EDGE 3 -0.386559 -0.074323 -0.026711

EDGE 3 -0.113441 0.026711 -0.074323

END

# \_\_\_\_\_

# Figure 13

# Systre file created by KLiNG v0.422 on Thu Jun 15 12:56:13 2023

CRYSTAL

NAME 3Chains\_Fm-3c\_0.1666666667\_MG

GROUP Fm-3c

CELL 10.0000 10.0000 10.0000 90.0000 90.0000 90.0000

NODE 1 2 0.500000 0.300000 0.100000

EDGE 1 0.500000 0.300000 -0.100000

EDGE 1 0.500000 -0.300000 0.100000

END

# Systre file created by KLiNG v0.401 on Sun Mar 12 20:43:44 2023

CRYSTAL

NAME pCM\_p4212\_0.0785285936\_MG

GROUP P4212

CELL 10.0000 10.0000 100.0000 90.0000 90.0000 90.0000

NODE 1 2 0.827414 0.630169 -0.055817

EDGE 1 0.630169 0.827414 0.055817

EDGE 1 -0.630169 -0.827414 0.055817

END

# Data for structures reported in Table 1. Identified by girth

# Systre file created by KLiNG v0.401 on Thu Mar 16 09:17:15 2023

CRYSTAL

NAME PCM\_P-3\_0.2500000000\_MG

GROUP P-3

CELL 10.0000 10.0000 100.0000 90.0000 90.0000 120.0000

NODE 1 2 0.952381 0.761905 0.030861

EDGE 1 0.190476 0.952381 -0.030861

EDGE 1 0.761905 -0.190476 -0.030861

END

#

---

# Systre file created by KLiNG v0.401 on Thu Mar 16 09:17:16 2023

CRYSTAL

NAME PCM\_P-3\_0.1111111111\_MG

GROUP P-3

CELL 10.0000 10.0000 100.0000 90.0000 90.0000 120.0000

NODE 1 2 1.615385 1.153846 0.050953

EDGE 1 0.461538 1.615385 -0.050953

EDGE 1 1.153846 -0.461538 -0.050953

END

# \_\_\_\_\_

# Systre file created by KLiNG v0.382 on Sat Dec 3 17:17:02 2022

CRYSTAL

NAME P-3\_(5,3)\_0.11111111\_MG

GROUP P-3

CELL 10.0000 10.0000 100.0000 90.0000 90.0000 120.0000

NODE 1 2 2.615385 2.153846 0.050952

EDGE 1 1.461538 2.615385 -0.050952

EDGE 1 2.153846 0.538462 -0.050952

END

# \_\_\_\_\_

# Systre file created by KLiNG v0.401 on Thu Mar 16 09:17:17 2023

CRYSTAL

NAME PCM\_P-3\_0.0909090909\_MG

GROUP P-3

CELL 10.0000 10.0000 100.0000 90.0000 90.0000 120.0000

NODE 1 2 1.543860 1.350877 0.051512

EDGE 1 0.192982 1.543860 -0.051512

EDGE 1 1.350877 -0.192982 -0.051512

END

# \_\_\_\_\_

# Systre file created by KLiNG v0.401 on Thu Mar 16 09:17:18 2023

CRYSTAL

NAME PCM\_P-3\_0.0714285714\_MG

GROUP P-3

CELL 10.0000 10.0000 100.0000 90.0000 90.0000 120.0000

NODE 1 2 1.964912 1.719298 0.065561

EDGE 1 0.245614 1.964912 -0.065561



```
EDGE 1 1.719298 -0.245614 -0.065561
END
#
# Systre file created by KLiNG v0.401 on Thu Mar 16 09:17:19 2023
CRYSTAL
NAME PCM_P-3_0.0625000000_MG
GROUP P-3
CELL 10.0000 10.0000 100.0000 90.0000 90.0000 120.0000

NODE 1 2 2.285714 1.523810 0.071270
EDGE 1 0.761905 2.285714 -0.071270
EDGE 1 1.523810 -0.761905 -0.071270
END
#
# Systre file created by KLiNG v0.401 on Thu Mar 16 09:17:20 2023
CRYSTAL
NAME PCM_P-3_0.0555555556_MG
GROUP P-3
CELL 10.0000 10.0000 100.0000 90.0000 90.0000 120.0000

NODE 1 2 1.846154 1.384615 0.058835
EDGE 1 0.461538 1.846154 -0.058835
EDGE 1 1.384615 -0.461538 -0.058835
END
#
# Systre file created by KLiNG v0.401 on Thu Mar 16 09:17:21 2023
CRYSTAL
NAME PCM_P-3_0.0500000000_MG
GROUP P-3
CELL 10.0000 10.0000 100.0000 90.0000 90.0000 120.0000
NODE 1 2 2.051282 1.538462 0.065372
EDGE 1 0.512821 2.051282 -0.065372
EDGE 1 1.538462 -0.512821 -0.065372
END
```

```
#  
# Systre file created by KLiNG v0.401 on Thu Mar 16 09:17:22 2023  
CRYSTAL  
NAME PCM_P-3_0.0454545455_MG  
GROUP P-3  
CELL 10.0000 10.0000 100.0000 90.0000 90.0000 120.0000  
  
NODE 1 2 2.256410 1.692308 0.071909  
EDGE 1 0.564103 2.256410 -0.071909  
EDGE 1 1.692308 -0.564103 -0.071909  
END
```

```
#  
# Systre file created by KLiNG v0.401 on Thu Mar 16 09:17:23 2023  
CRYSTAL  
NAME PCM_P-3_0.0434782609_MG  
GROUP P-3  
CELL 10.0000 10.0000 100.0000 90.0000 90.0000 120.0000  
  
NODE 1 2 2.279279 2.072072 0.077184  
EDGE 1 0.207207 2.279279 -0.077184  
EDGE 1 2.072072 -0.207207 -0.077184  
END
```

```
#  
#
```

```
# Data for Table 2 structures identified by girth
```

```
#
```

```
# Systre file created by KLiNG v0.420 on Mon May 8 09:49:05 2023  
CRYSTAL  
NAME 3perTriBorro_R-3m_0.1575510127_MG  
GROUP R-3m:H  
CELL 10.0000 10.0000 3.1948 90.0000 90.0000 120.0000  
  
NODE 1 2 0.633854 1.267708 0.707545
```

EDGE 1 0.032813 0.967187 -0.374211

EDGE 1 0.934374 0.967187 -0.374211

END

# \_\_\_\_\_

# Systre file created by KLiNG v0.420 on Mon May 8 09:49:13 2023

CRYSTAL

NAME 3perTriBorro\_R-3m\_0.1205115959\_MG

GROUP R-3m:H

CELL 10.0000 10.0000 2.5871 90.0000 90.0000 120.0000

NODE 1 2 0.640681 1.281362 -0.543648

EDGE 1 0.025986 0.974014 0.876982

EDGE 1 0.948028 0.974014 0.876982

END

# \_\_\_\_\_

# Systre file created by KLiNG v0.420 on Mon May 8 09:15:29 2023

CRYSTAL

NAME 3perTriBorro\_P-31m\_0.0976310729\_MG

GROUP P-31m

CELL 10.0000 10.0000 3.7637 90.0000 90.0000 120.0000

NODE 1 2 1.935423 0.000000 -0.878677

EDGE 1 1.000000 -0.935423 0.878677

EDGE 1 1.935423 0.935423 0.878677

END

# \_\_\_\_\_

# Systre file created by KLiNG v0.421 on Wed May 17 16:23:52 2023

CRYSTAL

NAME 3perTriBorro\_R-3\_0.1250000000\_MG

GROUP R-3:H

CELL 10.0000 10.0000 8.0178 90.0000 90.0000 120.0000

NODE 1 2 -0.047619 -0.476190 0.611111

EDGE 1 1.095238 0.285714 -0.277778

EDGE 1 -0.809524 -0.095238 -0.277778

END

#

---

# Systre file created by KLiNG v0.421 on Wed May 17 16:15:03 2023

CRYSTAL

NAME 3perTriBorro\_R-3\_0.1000000000\_MG

GROUP R-3:H

CELL 10.0000 10.0000 10.9986 90.0000 90.0000 120.0000

NODE 1 2 1.086022 0.236559 -0.166667

EDGE 1 1.516129 1.419355 0.500000

EDGE 1 -0.096774 -0.516129 0.500000

END

#

---

# Systre file created by KLiNG v0.420 on Sat Apr 1 10:15:27 2023

CRYSTAL

NAME 3R\_P213\_0.0500626906\_MG

GROUP P213

CELL 10.0000 10.0000 10.0000 90.0000 90.0000 90.0000

NODE 1 2 0.612517 -0.230071 -0.580162

EDGE 1 -0.230071 -0.580162 0.612517

EDGE 1 -0.580162 0.612517 -0.230071

END

#

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# Systre file created by KLiNG v0.420 on Fri Mar 31 07:44:08 2023

CRYSTAL

NAME 3R\_Pa-3\_0.0451469297\_MG

GROUP Pa-3

CELL 10.0000 10.0000 10.0000 90.0000 90.0000 90.0000

NODE 1 2 0.571213 -0.220684 -0.543444

```
EDGE 1  -0.220684 -0.543444  0.571213
EDGE 1  -0.543444  0.571213 -0.220684
END
```