

**Supplementary Material for: [Gaussian Basis
sets for Crystalline Solids: All-Purpose Basis Set
Libraries Vs System-Specific Optimizations]**

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This document explicitly reports most of the CRYSTAL17 inputs used to obtain the results reported in the paper. The basis set in the inputs are the dcm-XZVP obtained by using the BDIIS optimizer. The shells labelled by an asterisk are those that have been optimized.

1 Diamond - triple ζ

DIAMOND-TZ-PBE

CRYSTAL

0 0 1

227

3.56679

1

6 0. 0. 0.

END

6 11

0 0 6 2. 1.

1.35753496820E+04 2.22458143520E-04

2.03523336800E+03 1.72327382520E-03

4.63225623590E+02 8.92557153140E-03

1.31200195980E+02 3.57279845020E-02

4.28530158910E+01 1.10762599310E-01

1.55841857660E+01 2.42956276260E-01

0 0 2 2. 1.

6.20671385080E+00 4.14402634480E-01

2.57648965270E+00 2.37449686550E-01

0 0 1 0. 1. *

2.72877227664E+00 1.00000000000E+00

0 0 1 0. 1. *

7.08254466129E-01 1.00000000000E+00

0 0 1 0. 1. *

2.75435053993E-01 1.00000000000E+00

```

0 2 4 2. 1.
    3.46972322440E+01  5.33336578050E-03
    7.95826228260E+00  3.58641090920E-02
    2.37808268830E+00  1.42158733290E-01
    8.14332081830E-01  3.42704718450E-01
0 2 1 0. 1. *
    6.18739070583E-01  1.00000000000E+00
0 2 1 0. 1. *
    2.71282775658E-01  1.00000000000E+00
0 3 1 0. 1. *
    2.01143808439E+00  1.00000000000E+00
0 3 1 0. 1. *
    6.26539832528E-01  1.00000000000E+00
0 4 1 0. 1. *
    1.06242225484E+00  1.00000000000E+00
99 0
END
DFT
PBE
END
MAXCYCLE
100
TOLINTEG
8 8 8 12 24
TOLDEE
8
SHRINK
8 8
END

```

2 Diamond - quadruple ζ

DIAMOND-QZ-PBE

CRYSTAL

0 0 1

227

3.56679

1

6 0. 0. 0.

END

6 17

0 0 8 2. 1.

6.70250710290E+04 3.87363085010E-05

1.00399865380E+04 3.01079175750E-04

2.28493169110E+03 1.57879180950E-03

6.47141221300E+02 6.60870871950E-03

2.11094723350E+02 2.33671232500E-02

7.61776438620E+01 7.04207168980E-02

2.96338391630E+01 1.73603449530E-01

1.21877850810E+01 3.22923056480E-01

0 0 2 2. 1.

5.30260062990E+01 7.48974044920E-02

1.52585027760E+01 7.61362209830E-01

0 0 1 0. 1. *

6.20602927512E+00 1.00000000000E+00

0 0 1 0. 1. *

3.32497590179E+00 1.00000000000E+00

0 0 1 0. 1. *

1.09521378286E+00 1.00000000000E+00

0 0 1 0. 1. *

6.30358128105E-01 1.00000000000E+00

0 0 1 0. 1. *

3.43646141101E-01 1.00000000000E+00

```

0 2 5 2. 1.
    1.05125550820E+02  8.46475538440E-04
    2.48844610660E+01  6.62740385340E-03
    7.86372308260E+00  3.01203904190E-02
    2.84070018350E+00  9.99514354760E-02
    1.12271373350E+00  2.38262992820E-01
0 2 1 0. 1. *
    8.74041963051E-01  1.00000000000E+00
0 2 1 0. 1. *
    5.42561494412E-01  1.00000000000E+00
0 2 1 0. 1. *
    1.83247854025E-01  1.00000000000E+00
0 3 1 0. 1. *
    1.96394180988E+00  1.00000000000E+00
0 3 1 0. 1. *
    9.68369087225E-01  1.00000000000E+00
0 3 1 0. 1. *
    5.47772457307E-01  1.00000000000E+00
0 4 1 0. 1. *
    1.51085897443E+00  1.00000000000E+00
0 4 1 0. 1. *
    7.42254560983E-01  1.00000000000E+00
0 5 1 0. 1. *
    1.18250314805E+00  1.00000000000E+00
99 0
END
DFT
PBE
END
MAXCYCLE
100
TOLINTEG
8 8 8 12 24

```

TOLDEE
8
SHRINK
8 8
NOBIPOLA
END

3 Graphene - triple ζ

GRAPHENE-TZ-PBE
SLAB
77
2.47
1
6 -0.33333333333 0.33333333333 0.
END
6 11
0 0 6 2. 1.
1.35753496820E+04 2.22458143520E-04
2.03523336800E+03 1.72327382520E-03
4.63225623590E+02 8.92557153140E-03
1.31200195980E+02 3.57279845020E-02
4.28530158910E+01 1.10762599310E-01
1.55841857660E+01 2.42956276260E-01
0 0 2 2. 1.
6.20671385080E+00 4.14402634480E-01
2.57648965270E+00 2.37449686550E-01
0 0 1 0. 1. *
1.09605489209E+00 1.00000000000E+00
0 0 1 0. 1. *
5.91106934956E-01 1.00000000000E+00

```

0 0 1 0. 1. *
    2.37383807053E-01  1.00000000000E+00
0 2 4 2. 1.
    3.46972322440E+01  5.33336578050E-03
    7.95826228260E+00  3.58641090920E-02
    2.37808268830E+00  1.42158733290E-01
    8.14332081830E-01  3.42704718450E-01
0 2 1 0. 1. *
    3.38693223652E-01  1.00000000000E+00
0 2 1 0. 1. *
    1.59434147140E-01  1.00000000000E+00
0 3 1 0. 1. *
    1.25021363036E+00  1.00000000000E+00
0 3 1 0. 1. *
    7.19402508165E-01  1.00000000000E+00
0 4 1 0. 1. *
    7.06699996366E-01  1.00000000000E+00
99 0
END
DFT
PBE
XLGRID
END
SCFDIR
FMIXING
30
LDREMO
1
MAXCYCLES
100
TOLINTEG
8 8 8 8 16
TOLDEE

```

8
SHRINK
64 64
END

4 Graphene - quadruple ζ

GRAPHENE-QZ-PBE

SLAB

77

2.47

1

6 -0.3333333333 0.3333333333 0.

END

6 17

0 0 8 2. 1.

6.70250710290E+04 3.87363085010E-05

1.00399865380E+04 3.01079175750E-04

2.28493169110E+03 1.57879180950E-03

6.47141221300E+02 6.60870871950E-03

2.11094723350E+02 2.33671232500E-02

7.61776438620E+01 7.04207168980E-02

2.96338391630E+01 1.73603449530E-01

1.21877850810E+01 3.22923056480E-01

0 0 2 2. 1.

5.30260062990E+01 7.48974044920E-02

1.52585027760E+01 7.61362209830E-01

0 0 1 0. 1. *

5.24039574640E+00 1.00000000000E+00

0 0 1 0. 1. *

2.32777405666E+00 1.00000000000E+00

0 0 1 0. 1. *

| | |
|-------------------|-------------------|
| 1.04613233770E+00 | 1.00000000000E+00 |
| 0 0 1 0. 1. * | |
| 5.21832251512E-01 | 1.00000000000E+00 |
| 0 0 1 0. 1. * | |
| 2.00431897163E-01 | 1.00000000000E+00 |
| 0 2 5 2. 1. | |
| 1.05125550820E+02 | 8.46475538440E-04 |
| 2.48844610660E+01 | 6.62740385340E-03 |
| 7.86372308260E+00 | 3.01203904190E-02 |
| 2.84070018350E+00 | 9.99514354760E-02 |
| 1.12271373350E+00 | 2.38262992820E-01 |
| 0 2 1 0. 1. * | |
| 4.50031980659E-01 | 1.00000000000E+00 |
| 0 2 1 0. 1. * | |
| 3.28748485841E-01 | 1.00000000000E+00 |
| 0 2 1 0. 1. * | |
| 1.24896018560E-01 | 1.00000000000E+00 |
| 0 3 1 0. 1. * | |
| 1.91295701725E+00 | 1.00000000000E+00 |
| 0 3 1 0. 1. * | |
| 8.63019243591E-01 | 1.00000000000E+00 |
| 0 3 1 0. 1. * | |
| 4.52624895593E-01 | 1.00000000000E+00 |
| 0 4 1 0. 1. * | |
| 1.41426143665E+00 | 1.00000000000E+00 |
| 0 4 1 0. 1. * | |
| 5.98189433168E-01 | 1.00000000000E+00 |
| 0 5 1 0. 1. * | |
| 9.93072428023E-01 | 1.00000000000E+00 |
| 99 0 | |
| END | |
| DFT | |
| PBE | |

```
XLGRID
END
SCFDIR
FMIXING
30
LDREMO
1
MAXCYCLES
100
TOLINTEG
8 8 8 8 16
TOLDEE
8
SHRINK
64 64
END
```

5 Carbyne - triple ζ

```
C_Chain
POLYMER
1
2.56620186
2
6 9.624791798260E-02 -1.258372661974E-18 -4.072637834921E-09
6 -3.962479179826E-01 -2.785734209432E-16 4.072638114753E-09
END
6 11
0 0 6 2. 1.
1.35753496820E+04 2.22458143520E-04
2.03523336800E+03 1.72327382520E-03
4.63225623590E+02 8.92557153140E-03
```

1.31200195980E+02 3.57279845020E-02
4.28530158910E+01 1.10762599310E-01
1.55841857660E+01 2.42956276260E-01
0 0 2 2. 1.
6.20671385080E+00 4.14402634480E-01
2.57648965270E+00 2.37449686550E-01
0 0 1 0. 1. *
1.13833219587E+00 1.00000000000E+00
0 0 1 0. 1. *
6.55714337901E-01 1.00000000000E+00
0 0 1 0. 1. *
2.32302377804E-01 1.00000000000E+00
0 2 4 2. 1.
3.46972322440E+01 5.33336578050E-03
7.95826228260E+00 3.58641090920E-02
2.37808268830E+00 1.42158733290E-01
8.14332081830E-01 3.42704718450E-01
0 2 1 0. 1. *
2.85725969158E-01 1.00000000000E+00
0 2 1 0. 1. *
9.05806201973E-02 1.00000000000E+00
0 3 1 0. 1. *
1.30952322712E+00 1.00000000000E+00
0 3 1 0. 1. *
6.13241389114E-01 1.00000000000E+00
0 4 1 0. 1. *
1.13300431880E+00 1.00000000000E+00
99 0
END
DFT
PBE
XLGRID
END

```
LDREMO
1
SCFDIR
LEVSHIFT
10 1
FMIXING
30
MAXCYCLES
100
TOLINTEG
8 8 8 8 16
TOLDEE
8
SHRINK
64 64
END
```

6 NaCl - triple ζ

```
NaCl_crystal-TZ-PBE0
CRYSTAL
0 0 0
225
5.6402
2
17 0.0 0.0 0.0
11 0.5 0.5 0.5
END
11 11
0 0 7 2. 1.
2.60411099270E+04 6.18063428110E-04
3.90612685480E+03 4.77486044140E-03
```

| | |
|-------------------|--------------------|
| 8.88974549930E+02 | 2.44716848290E-02 |
| 2.51454979610E+02 | 9.47553949770E-02 |
| 8.16501435120E+01 | 2.68674969200E-01 |
| 2.89041584010E+01 | 4.79254754400E-01 |
| 1.06257829320E+01 | 3.32485914690E-01 |
| 0 0 3 2. 1. | |
| 5.37694101790E+01 | 1.95277318720E-02 |
| 1.63082430250E+01 | 9.26480107940E-02 |
| 2.37303841250E+00 | -3.99386701720E-01 |
| 0 0 2 1. 1. | |
| 9.57307726030E-01 | 1.64285953910E+00 |
| 4.08064609590E-01 | 5.56925969660E-01 |
| 0 0 1 0. 1. * | |
| 3.43569978393E-01 | 9.99992062637E-01 |
| 0 0 1 0. 1. * | |
| 8.28104267544E-02 | 9.99700925116E-01 |
| 0 2 5 6. 1. | |
| 1.38079799890E+02 | 5.79518919290E-03 |
| 3.22327003930E+01 | 4.16208462510E-02 |
| 9.98160753600E+00 | 1.62819168850E-01 |
| 3.48220339280E+00 | 3.60117846470E-01 |
| 1.22991346200E+00 | 4.48589798890E-01 |
| 0 2 1 0. 1. * | |
| 4.02257637589E-01 | 1.00001437874E+00 |
| 0 2 1 0. 1. * | |
| 9.81092534535E-02 | 1.00010780928E+00 |
| 0 3 1 0. 1. * | |
| 2.60738659094E+00 | 1.00000000000E+00 |
| 0 3 1 0. 1. * | |
| 4.03951011422E-01 | 1.00000000000E+00 |
| 0 3 1 0. 1. * | |
| 9.84682729829E-02 | 1.00000000000E+00 |

17 13

0 0 7 2. 1.
 6.95079909450E+04 5.43148974970E-04
 1.04261568800E+04 4.19904639610E-03
 2.37323340610E+03 2.15921416790E-02
 6.71564200710E+02 8.45988500940E-02
 2.18419997900E+02 2.47572497240E-01
 7.75722497140E+01 4.70169302280E-01
 2.88888152770E+01 3.74363707160E-01
 0 0 3 2. 1.
 1.27105271850E+02 2.51821666030E-02
 3.93395829610E+01 1.07861124560E-01
 7.67406799890E+00 -2.74088215740E-01
 0 0 2 2. 1.
 3.87456276300E+00 1.32138750140E+00
 1.83858325730E+00 6.86369553680E-01
 0 0 1 0. 1. *
 5.72362924707E-01 1.00000000308E+00
 0 0 1 0. 1. *
 2.31162823985E-01 9.99999997835E-01
 0 2 5 6. 1.
 6.66504232840E+02 2.36326638360E-03
 1.57642416900E+02 1.88793003740E-02
 5.02625209780E+01 8.72063412730E-02
 1.85360781050E+01 2.52856129700E-01
 7.29405327770E+00 4.35071548200E-01
 0 2 1 5. 1. *
 2.93863280310E+00 1.00000000143E+00
 0 2 1 0. 1. *
 1.19026410565E+00 1.00000000000E+00
 0 2 1 0. 1. *
 4.69704038156E-01 1.00000000000E+00
 0 2 1 0. 1. *
 1.74720163208E-01 1.00000000000E+00

```

0 3 2 0. 1.
    4.61000000000E+00  2.00000000000E-01
    1.01100000000E+00  1.00000000000E+00
0 3 1 0. 1. *
    2.83798017576E-01  1.00000000000E+00
0 4 1 0. 1. *
    6.89848600893E-01  1.00000000000E+00
99 0
END
DFT
PBE0
END
TOLINTEG
8 8 8 8 16
TOLDEE
8
SHRINK
8 8
END

```

7 Na - triple ζ

```

Na_crystal-TZ-PBE0
CRYSTAL
0 0 0
229
4.2906
1
11 0. 0. 0.
END
    11 11
0 0 7 2. 1.

```

| | |
|-------------------|--------------------|
| 2.60411099270E+04 | 6.18063428110E-04 |
| 3.90612685480E+03 | 4.77486044140E-03 |
| 8.88974549930E+02 | 2.44716848290E-02 |
| 2.51454979610E+02 | 9.47553949770E-02 |
| 8.16501435120E+01 | 2.68674969200E-01 |
| 2.89041584010E+01 | 4.79254754400E-01 |
| 1.06257829320E+01 | 3.32485914690E-01 |
| 0 0 3 2. 1. | |
| 5.37694101790E+01 | 1.95277318720E-02 |
| 1.63082430250E+01 | 9.26480107940E-02 |
| 2.37303841250E+00 | -3.99386701720E-01 |
| 0 0 2 1. 1. | |
| 9.57307726030E-01 | 1.64285953910E+00 |
| 4.08064609590E-01 | 5.56925969660E-01 |
| 0 0 1 0. 1. * | |
| 2.12721167582E-01 | 9.99992062637E-01 |
| 0 0 1 0. 1. * | |
| 7.82096876345E-02 | 9.99700925116E-01 |
| 0 2 5 6. 1. | |
| 1.38079799890E+02 | 5.79518919290E-03 |
| 3.22327003930E+01 | 4.16208462510E-02 |
| 9.98160753600E+00 | 1.62819168850E-01 |
| 3.48220339280E+00 | 3.60117846470E-01 |
| 1.22991346200E+00 | 4.48589798890E-01 |
| 0 2 1 0. 1. * | |
| 4.03415531731E-01 | 1.00001437874E+00 |
| 0 2 1 0. 1. * | |
| 8.50539333916E-02 | 1.00010780928E+00 |
| 0 3 1 0. 1. * | |
| 2.60862497919E+00 | 1.00000000000E+00 |
| 0 3 1 0. 1. * | |
| 4.33739110192E-01 | 1.00000000000E+00 |
| 0 3 1 0. 1. * | |


```

1.11542851169E-01 1.00000000000E+00
99 0
END
DFT
PBE0
END
TOLINTEG
8 8 8 8 16
TOLDEE
8
SHRINK
8 8
END

```

8 Cl₂ - triple ζ

```

Cl_crystal-TZ-PBE0
CRYSTAL
0 0 0
64
7.77875 4.34941 9.02754
8
17 0          0.40882      0.89848
17 0          0.09118      0.39848
17 0          0.90882      0.60152
17 0          0.59118      0.10152
17 0.50000    0.90882      0.89848
17 0.50000    0.59118      0.39848
17 0.50000    0.40882      0.60152
17 0.50000    0.09118      0.10152
END
17 13

```

0 0 7 2. 1.
 6.95079909450E+04 5.43148974970E-04
 1.04261568800E+04 4.19904639610E-03
 2.37323340610E+03 2.15921416790E-02
 6.71564200710E+02 8.45988500940E-02
 2.18419997900E+02 2.47572497240E-01
 7.75722497140E+01 4.70169302280E-01
 2.88888152770E+01 3.74363707160E-01
 0 0 3 2. 1.
 1.27105271850E+02 2.51821666030E-02
 3.93395829610E+01 1.07861124560E-01
 7.67406799890E+00 -2.74088215740E-01
 0 0 2 2. 1.
 3.87456276300E+00 1.32138750140E+00
 1.83858325730E+00 6.86369553680E-01
 0 0 1 0. 1.
 5.07498154767E-01 1.00000000308E+00
 0 0 1 0. 1.
 1.83127456586E-01 9.9999997835E-01
 0 2 5 6. 1.
 6.66504232840E+02 2.36326638360E-03
 1.57642416900E+02 1.88793003740E-02
 5.02625209780E+01 8.72063412730E-02
 1.85360781050E+01 2.52856129700E-01
 7.29405327770E+00 4.35071548200E-01
 0 2 1 5. 1.
 2.89826632488E+00 1.00000000143E+00
 0 2 1 0. 1.
 1.10442102086E+00 1.00000000000E+00
 0 2 1 0. 1.
 4.09232170559E-01 1.00000000000E+00
 0 2 1 0. 1.
 1.36452167048E-01 1.00000000000E+00

```

0 3 2 0. 1.
    4.61000000000E+00  2.00000000000E-01
    1.01100000000E+00  1.00000000000E+00
0 3 1 0. 1.
    3.32581229403E-01  1.00000000000E+00
0 4 1 0. 1.
    5.98970631104E-01  1.00000000000E+00
99 0
END
DFT
PBE0
END
TOLDEE
8
TOLINTEG
8 8 8 8 16
SHRINK
8 8
END

```

9 LiH - SVP

```

LiH-SVP-HF
CRYSTAL
0 0 0
225
4.084
2
3 0.0 0.0 0.0
1 0.5 0.5 0.5
END
3 5

```

```

0 0 5 2. 1.
    2.66277855160E+02  6.49201503250E-03
    4.00697834470E+01  4.77478632150E-02
    9.05599443890E+00  2.02687961110E-01
    2.45030090510E+00  4.86065748170E-01
    7.22095718550E-01  4.36269779550E-01
0 0 1 1. 1. *
    9.22176144583E-01  1.00000000000E+00
0 0 1 0. 1. *
    3.26710606911E-01  1.00000000000E+00
0 2 2 0. 1.
    1.45000000000E+00  2.58600000000E-01
    3.00000000000E-01  1.00000000000E+00
0 2 1 0. 1. *
    2.44108651001E-01  1.00000000000E+00
1 3
0 0 3 1. 1.
    1.30107010000E+01  1.96821580000E-02
    1.96225720000E+00  1.37965240000E-01
    4.44537960000E-01  4.78319350000E-01
0 0 1 0. 1. *
    1.12026126213E-01  1.00000000000E+00
0 2 1 0. 1. *
    7.04259338539E-01  1.00000000000E+00
99 0
END
TOLINTEG
8 8 8 15 30
SHRINK
8 8
FMIXING
50
TOLDEE

```

10
END

10 LiH - triple ζ

LiH-TZ-HF

CRYSTAL

0 0 0

225

4.084

2

3 0.0 0.0 0.0

1 0.5 0.5 0.5

END

3 8

0 0 6 2. 1.

6.26926280100E+03 2.05409688260E-04

9.40316124310E+02 1.59165540890E-03

2.14221075280E+02 8.28698297070E-03

6.07598401840E+01 3.38563742490E-02

1.99151520320E+01 1.11032258760E-01

7.31715097970E+00 2.74493833290E-01

0 0 2 1. 1.

2.97246742160E+00 2.37924564110E-01

1.26398523140E+00 3.07654119240E-01

0 0 1 0. 1. *

7.80051836987E-01 1.00000000000E+00

0 0 1 0. 1. *

3.56751423380E-01 1.00000000000E+00

0 0 1 0. 1. *

1.32441081592E-01 1.00000000000E+00

0 2 1 0. 1. *

```

5.32524694781E-01  1.00000000000E+00
0 2 1 0. 1. *
1.24297352468E-01  1.00000000000E+00
0 2 1 0. 1. *
3.32168908872E+00  1.00000000000E+00
1 4
0 0 3 1. 1.
3.40613410000E+01  6.02519780000E-03
5.12357460000E+00  4.50210940000E-02
1.16466260000E+00  2.01897260000E-01
0 0 1 0. 1. *
7.93610197287E-01  1.00000000000E+00
0 0 1 0. 1. *
2.38040797833E-01  1.00000000000E+00
0 2 1 0. 1. *
7.51152930456E-01  1.00000000000E+00
99 0
END
TOLINTEG
10 10 10 15 30
SHRINK
8 8
FMIXING
50
TOLDEE
10
NOBIPOLA
END

```

11 LiH - quadruple ζ

LiH-QZ-HF

CRYSTAL

0 0 0

225

4.084

2

3 0.0 0.0 0.0

1 0.5 0.5 0.5

LATVEC

100000

END

1 10

0 0 4 1. 1.

1.90691690000E+02 7.08151670000E-04

2.86055320000E+01 5.46788270000E-03

6.50959430000E+00 2.79666050000E-02

1.84124550000E+00 1.07645380000E-01

0 0 1 0. 1. *

6.39685855118E-01 1.00000000000E+00

0 0 1 0. 1. *

2.72584652976E-01 1.00000000000E+00

0 0 1 0. 1. *

1.44295727123E-01 1.00000000000E+00

0 2 1 0. 1. *

2.29203807546E+00 1.00000000000E+00

0 2 1 0. 1. *

8.37965510305E-01 1.00000000000E+00

0 2 1 0. 1. *

2.95979305342E-01 1.00000000000E+00

0 3 1 0. 1. *

2.06195543104E+00 1.00000000000E+00

0 3 1 0. 1. *

6.61486854173E-01 1.00000000000E+00

0 4 1 0. 1. *

| | |
|-------------------|-------------------|
| 1.39686108048E+00 | 1.00000000000E+00 |
| 3 13 | |
| 0 0 9 2. 1. | |
| 1.48539770850E+04 | 4.27113888150E-05 |
| 2.22522364770E+03 | 3.32353108000E-04 |
| 5.04887390080E+02 | 1.75184366490E-03 |
| 1.42458475480E+02 | 7.34779958500E-03 |
| 4.63155995800E+01 | 2.58998376830E-02 |
| 1.66553354740E+01 | 7.66706824310E-02 |
| 6.43311861990E+00 | 1.82760757650E-01 |
| 2.60270438580E+00 | 3.26554340380E-01 |
| 1.08972454050E+00 | 3.70004298280E-01 |
| 0 0 2 1. 1. | |
| 4.42365959710E+00 | 1.11209879210E-01 |
| 1.23563949900E+00 | 7.99873358620E-01 |
| 0 0 1 0. 1. * | |
| 1.47258539716E+00 | 1.00000000000E+00 |
| 0 0 1 0. 1. * | |
| 9.61687138188E-01 | 1.00000000000E+00 |
| 0 0 1 0. 1. * | |
| 5.44705804681E-01 | 1.00000000000E+00 |
| 0 0 1 0. 1. * | |
| 2.59775255362E-01 | 1.00000000000E+00 |
| 0 2 3 0. 1. | |
| 3.26051092060E+00 | 8.65047490230E-03 |
| 6.50030431150E-01 | 4.76141237360E-02 |
| 1.69416710730E-01 | 2.10011380000E-01 |
| 0 2 1 0. 1. * | |
| 3.83906409071E-01 | 1.00000000000E+00 |
| 0 2 1 0. 1. * | |
| 1.98706020944E-01 | 1.00000000000E+00 |
| 0 2 1 0. 1. * | |
| 3.72683460316E+00 | 1.00000000000E+00 |


```
0 3 1 0. 1. *
    3.33113752884E-01  1.00000000000E+00
0 3 1 0. 1. *
    3.68482801264E-01  1.00000000000E+00
0 4 1 0. 1. *
    1.75294244744E-01  1.00000000000E+00
99 0
END
TOLINTEG
10 10 10 40 160
SHRINK
12 12
NOBIPOLA
LDREMO
1
FMIXING
96
THREDIIS
2
TOLDEE
10
ILASIZE
20000
END
```