

## Supporting information

### The Origin of Isotope-Induced Helical-Sense Bias in Supramolecular Polymers of Benzene-1,3,5-Tricarboxamides

#### Table of Contents

## Geometries

The geometries are reported as written in the CONTCAR files by the VASP program.

The dimension of the coordinates for the unit cell (lines 3-5) are in angstroms. The positions of the atoms are given in direct coordinates. In order to convert from these direct coordinates to the Cartesian coordinates; multiply the matrix of the unit cell with the position vector of each atom.

All VASP calculations, unless stated otherwise, were performed using the following set of parameters and conditions:

- Perdew-Becke-Ernzerhof (PBE) functional with plane augmented waves (PAW)
- Kpoints: 1x1x1 (gamma point)
- Cutoff: 500eV
- Gaussian smearing with  $\sigma = 0.0002$  eV
- Conjugate-gradient algorithm
- Kosugi algorithm as integer selecting algorithm
- Energetic threshold of  $10^{-5}$  eV for the energetic SC-loop and a threshold of 0.005 eV/A for the ionic loop
- A stepsize of 0.02 Å for the construction of the Hessian matrix (calculation of frequencies) using the finite difference method

## BTA dimer, relaxed geometry using VASP, CONTCAR FILE

Note that the sequence of atoms is: C, H, N, O

BTA dimer

```
1.000000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
30 42 6 6
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Direct

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0.5669521240219123 0.5198310692052709 0.4112310346854136
0.5510597662509976 0.4517369002086742 0.4117580005707003
0.4837051134210709 0.4321091805865847 0.4112360570998616
0.5372534733593429 0.6406917756536957 0.4129726792582772
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0.4604596797750600 0.7957743822555773 0.4029995312644912
0.2760400542683893 0.3781647931957614 0.4484274956653906
0.2636136266729285 0.3178706981860177 0.4030020778935862
0.7175058805375546 0.3669808954390046 0.4484289477963668
0.7759410584313651 0.3863509946014156 0.4030081150268928
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0.3973500279686149 0.6459298328044650 0.5558048317286527

## BTA trimer, relaxed geometry using VASP, CONTCAR FILE

Note that the sequence of atoms is: C, H, N, O

BTA trimer

```
1.000000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.0000000000000000
45 63 9 9
```

Direct

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## BTA tetramer, relaxed geometry using VASP, CONTCAR FILE

Note that the sequence of atoms is: C, H, N, O

BTA Tetramer

```
1.000000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.0000000000000000
60 84 12 12
```

Direct

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0.4841463396978479 0.4315905516566888 0.4387986542989588
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## BTA pentamer, relaxed geometry using VASP, CONTCAR FILE

Note that the sequence of atoms is: C, H, N, O

BTA pentamer

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0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.0000000000000000
75 105 15 15
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Direct

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## BTA hexamer, relaxed geometry using VASP, CONTCAR FILE

Note that the sequence of atoms is: C, H, N, O

BTA hexamer

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0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.0000000000000000
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Direct

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## BTA heptamer, relaxed geometry using VASP, CONTCAR FILE

Note that the sequence of atoms is: C, H, N, O

BTA Heptamer

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Direct

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0.6139177214727611 0.7549374612613395 0.1428982544573381  
0.7078629472234930 0.7153016535984498 0.1862824536341231  
0.6803082441846701 0.7968670677076848 0.1986801840609177  
0.6547252273041371 0.7269769911364694 0.2265991836723995  
0.6986664115336785 0.3147226312393530 0.1833643610550567  
0.6636289351169524 0.2741700837973953 0.1428849806414554  
0.6669143236257190 0.1957688906651945 0.1986969414262414  
0.6191400316190027 0.2528491842676852 0.2266114942782525  
0.5824559499878492 0.2126042914467186 0.1863187252674879  
0.6831598525194058 0.5084965736100823 0.4840247421420895  
0.4010148142313924 0.6543718963853565 0.4840771862899029  
0.4156829933387196 0.3371237858322159 0.4840808003461252  
0.5977310439821831 0.3448594354025155 0.5894934528240757  
0.5854245149843180 0.6621086284589818 0.5894821081068354  
0.3168159063201222 0.4928021550044689 0.5895026636015963  
0.5830311721548829 0.6636033305778229 0.3784774082821333  
0.3166649676362444 0.4901655620168167 0.3784551057869234  
0.6000368543213772 0.3462084247822828 0.3784891900258835  
0.4124463221840926 0.3392968964890706 0.6951768932042088  
0.6829137909888234 0.5046109774142781 0.6951311177317553  
0.4045357219818416 0.6562821073258069 0.6951585371770290  
0.3976604585455431 0.6526600235729206 0.2727048104289717  
0.4190405597964087 0.3347400080055085 0.2726653913446544  
0.6836884951404836 0.5122372229666120 0.2727362085931328  
0.3180571620520561 0.5001208186561089 0.8022354103250039  
0.5909992100880778 0.3423209133299549 0.8021181883335053  
0.5911719478269059 0.6576127455465623 0.8021588545001530  
0.3148990482829020 0.4868605646487687 0.1689597614302073  
0.6039649817619102 0.3464591083217568 0.1689242027212467  
0.5811597720820275 0.6670830022805607 0.1689025811270466  
0.6545662786320448 0.5900595120072722 0.5270542457320841  
0.3447620467780301 0.5888471505106716 0.5271549578078951  
0.5007430114209007 0.3210945553576997 0.5270303572745380  
0.6545628412220361 0.4095923752683491 0.6326620553991554  
0.5008222993659445 0.6789692852479227 0.6325714660651199  
0.3444744768411377 0.4112127316494743 0.6326667511070146  
0.4980690233078462 0.6786717642572493 0.4216107076028375  
0.3460834368818382 0.4090866873861019 0.4216122751940380  
0.6555468037930589 0.4122592330954282 0.4216284787693771  
0.4958389638344915 0.3207272578551896 0.7387310048378365  
0.6573343634519151 0.5864341833747579 0.7385035346700027  
0.3466418520135277 0.5933805856470831 0.7386882329624244  
0.3435939985535623 0.5853018625168730 0.3157402571242464  
0.5043718737349169 0.3215647289609844 0.3157265178944239  
0.6523994422300122 0.5926382865718539 0.3158415534096308  
0.3404372001495541 0.4128628859907261 0.8427886539003913  
0.6554264063736212 0.4052254103587758 0.8426962184866483



0.5045639174422024 0.6818865639742948 0.8428043895086643  
0.3509149872133323 0.4031117185909802 0.2084373751305698  
0.6586862323353200 0.4194924078327872 0.2083288799786813  
0.4907409236776583 0.6778767898865178 0.2084568784826830

## BTA dimer frequencies (semicolon delimited)

R:

3548.255879;3545.502537;3544.896569;3418.065135;3416.883901;3415.588171;3125.667788;3124.3  
83671;3122.741581;3117.851855;3117.553790;3116.398722;3057.531883;3057.057350;3056.834675;  
3056.780298;3056.671971;3056.102185;3054.160874;3053.702124;3052.351741;3049.740950;3048.4  
06822;3047.372206;3034.731087;3034.495529;3033.130127;3026.133606;3024.816171;3023.906569;  
2975.613199;2974.194474;2973.513137;2970.710651;2970.595303;2969.779847;2193.016105;2192.6  
50723;2192.383547;2187.870439;2187.755463;2187.338874;1653.228211;1652.813784;1648.245204;  
1643.276635;1642.611502;1637.641400;1577.950788;1577.696777;1576.582885;1576.418046;1513.6  
21924;1506.989443;1506.781788;1506.218201;1498.729279;1497.572447;1453.700499;1453.489522;  
1452.989422;1450.501835;1450.375767;1450.000508;1444.816890;1444.218211;1444.107468;1441.1  
45061;1440.901598;1440.488451;1414.545592;1414.065189;1413.562557;1413.248572;1367.078625;  
1366.767790;1366.636699;1355.181873;1355.006132;1354.413053;1353.086557;1348.256892;1329.8  
56080;1329.387370;1319.092040;1318.807526;1313.376912;1311.689211;1305.490019;1300.494084;  
1299.200656;1298.744143;1290.730776;1289.708714;1274.919192;1272.449343;1252.061939;1244.5  
02345;1241.331315;1241.114134;1231.321922;1230.134987;1183.376294;1174.900846;1137.557590;  
1137.288317;1130.659378;1130.404444;1121.173464;1117.168746;1111.427910;1110.907820;1107.3  
31821;1107.230165;1106.514689;1106.003540;1104.729745;1104.575496;1104.391906;1104.274798;  
1047.127714;1046.880660;1046.217086;1041.801051;1041.567276;1040.771069;986.454329;986.157  
360;980.044121;979.821687;977.885557;977.824678;930.429189;929.332129;924.156002;918.81878  
6;918.324271;917.889911;905.374044;898.580279;886.042577;885.352434;883.343074;882.994089;  
879.944225;877.737803;845.622298;845.072644;841.942054;841.683167;795.583120;792.558857;75  
9.243796;759.119327;751.586278;751.476985;737.260368;724.552908;722.411634;722.006991;720.4  
39342;720.422586;684.444218;682.138868;666.442382;664.095736;654.096871;653.408613;650.745  
562;650.541125;638.183930;632.398689;632.095019;550.430215;547.837806;547.430405;530.17453  
9;528.364828;528.333814;511.546608;498.763744;498.148845;457.938096;457.720331;452.395496;  
452.229976;403.220942;399.484438;387.129307;387.046216;380.319156;380.079373;331.646372;32  
4.097735;323.060823;321.403146;315.589598;315.320748;286.322639;285.166298;282.164663;281.1  
25108;277.650395;271.446121;247.377206;246.084349;227.160381;224.500762;220.215565;218.372  
310;205.846133;197.063413;178.211506;177.643191;173.261894;172.525757;111.755524;110.87142  
7;107.591036;104.688946;104.407872;101.518266;82.171786;78.182017;77.360524;75.990751;69.48  
3448;68.214687;63.705500;59.961125;58.963024;53.698717;52.889545;51.632844;45.854949;41.773  
667;39.493792;38.374999;37.340676;36.660206;28.996892;25.047571;20.851874;18.394285;8.65923  
1;1.881389

S:

3548.196913;3545.441673;3544.836323;3417.948880;3416.768190;3415.472301;3125.667174;3124.3  
83103;3122.741280;3117.852754;3117.554712;3116.399952;3057.981399;3057.828478;3057.683000;  
3057.117460;3057.069925;3057.025728;3046.743650;3045.433247;3044.410766;3041.433116;3041.3  
59180;3039.709023;2986.873035;2986.315292;2985.951846;2980.555070;2980.384023;2979.813178;  
2975.531134;2974.257397;2973.490884;2970.894991;2970.771634;2969.895318;2237.123750;2236.6  
99250;2235.839954;2223.182919;2222.526841;2221.708845;1654.042492;1653.652678;1648.913949;  
1644.310035;1643.658308;1638.674743;1578.017880;1577.766395;1576.579720;1576.412583;1515.2  
91309;1508.206485;1507.990286;1506.845403;1498.798033;1497.736461;1453.344754;1453.112850;  
1452.481198;1450.678582;1450.488846;1450.145222;1445.345683;1444.795495;1444.769669;1441.1  
85597;1440.867844;1440.428403;1414.457930;1413.923889;1413.420559;1413.068638;1366.688354;  
1366.358435;1366.294993;1354.682177;1354.483886;1353.877247;1353.041559;1348.321261;1315.1  
39486;1313.444132;1313.181867;1310.014746;1308.863387;1307.789707;1303.438055;1299.734667;  
1281.927499;1281.335430;1278.611593;1274.117249;1273.995782;1273.925345;1252.364710;1244.4  
49874;1242.191805;1241.962762;1233.284449;1232.212520;1187.338569;1175.848826;1138.351122;  
1138.268110;1133.310161;1132.910218;1112.834537;1110.819414;1108.059589;1107.484470;1106.0  
39741;1105.700046;1080.971343;1080.809131;1077.589031;1077.291999;1075.006157;1072.258083;  
1055.881812;1055.580774;1052.701972;1052.648073;1042.154307;1040.537324;999.857502;999.768  
079;999.238499;993.787532;991.111463;990.712691;984.248590;982.174699;929.826362;928.76094  
8;923.149470;922.962216;915.941696;915.807573;914.014821;913.698508;912.896171;901.842726;  
860.245929;858.879507;826.513655;825.862714;825.714943;825.169497;780.964285;775.666318;75  
8.553194;758.438034;751.262584;751.171559;737.451080;725.231822;725.127814;724.656903;722.6

60267;721.932897;684.557357;681.447006;675.329106;671.739434;653.557025;652.894914;649.119  
392;648.932719;638.592673;631.314525;631.124359;550.911022;547.673838;547.283841;529.96470  
9;529.914884;528.682069;510.399842;499.868287;499.266213;454.293156;454.080021;448.664004;  
448.598046;401.179006;397.405458;386.645283;386.536747;379.835615;379.592930;328.002990;32  
1.158950;320.161913;317.887928;312.651091;312.328152;287.861221;286.635380;283.650582;282.6  
52953;276.039293;269.994870;248.098304;247.715011;226.473433;223.745542;219.513005;217.728  
057;207.186193;198.790858;177.895059;177.306344;172.958954;172.153070;113.142801;112.22066  
3;108.113567;106.411560;105.779234;101.834195;82.256879;78.369006;77.618546;76.125938;69.58  
7946;68.564142;63.848949;60.253823;59.056315;53.746278;52.795187;51.414868;45.122903;41.340  
835;39.388620;38.094312;37.673101;36.274954;28.503024;24.311500;20.368276;17.691625;8.81327  
2;2.756741

## BTA trimer frequencies

(semicolon delimited)

R:

3550.155755;3548.718097;3548.148778;3393.447124;3392.112282;3391.253842;3385.858950;3384.4  
20419;3383.612560;3128.631225;3128.126835;3125.884213;3125.534824;3124.869003;3123.773854;  
3119.620657;3118.494671;3116.289599;3062.066656;3061.638910;3061.291919;3061.103222;3061.0  
53061;3060.875151;3060.488613;3060.230154;3060.003385;3057.237138;3056.129181;3055.400733;  
3052.794370;3052.146890;3051.066450;3048.458010;3048.062811;3046.368388;3038.801271;3037.7  
97335;3036.572012;3025.212877;3024.759360;3024.431445;3005.214242;3003.096817;3003.037435;  
2979.363897;2978.635756;2978.187850;2977.966415;2977.695875;2976.740326;2976.712598;2976.5  
28063;2975.951683;2203.794236;2203.490139;2203.141355;2201.119562;2200.929112;2200.676459;  
2199.062947;2198.797485;2198.510518;1653.056604;1652.025970;1648.993326;1645.963592;1644.7  
22735;1640.194348;1629.955625;1629.398721;1627.401975;1578.715305;1578.568749;1578.070503;  
1577.823500;1577.214877;1577.091995;1526.648584;1519.278744;1518.811150;1510.121401;1505.3  
27961;1502.844697;1502.259340;1497.596745;1496.370596;1452.238057;1452.184335;1452.144366;  
1451.538696;1451.483590;1450.825487;1450.716634;1449.941320;1449.709579;1443.359321;1443.0  
24181;1442.717506;1441.957137;1441.524579;1441.331667;1439.238203;1438.746550;1438.133655;  
1416.869026;1416.343144;1415.009517;1414.738931;1414.039988;1413.618307;1363.247760;1363.0  
26758;1362.803190;1359.488873;1359.145238;1358.935762;1352.998516;1351.985468;1351.891767;  
1351.276959;1349.083336;1347.469331;1339.949605;1336.265086;1332.906721;1329.375076;1328.4  
13197;1322.306952;1321.927506;1317.693374;1316.520013;1308.254356;1307.132468;1300.216475;  
1296.877347;1296.322128;1289.878546;1289.495799;1279.193369;1278.341809;1277.818175;1273.7  
69079;1266.806108;1257.262071;1256.885884;1253.189696;1252.874864;1246.562349;1243.912876;  
1243.564995;1232.202401;1231.038000;1189.439815;1186.329053;1175.634692;1142.557353;1142.3  
97608;1137.334931;1136.716594;1131.051082;1130.956478;1125.143055;1120.736671;1116.449595;  
1112.363592;1111.590867;1110.629841;1110.580137;1108.890549;1107.668578;1104.855020;1104.2  
50181;1104.180961;1104.098895;1103.617801;1103.560533;1102.605223;1102.275823;1102.051610;  
1052.825602;1052.720612;1052.437803;1047.982721;1047.895149;1047.884467;1042.884656;1042.7  
64320;1042.312476;986.945818;986.687530;985.963723;984.720342;984.412758;982.989181;982.70  
6327;980.917410;980.857470;927.047703;926.446789;924.994511;921.933894;921.422545;920.9225  
47;918.800847;918.308524;917.805341;908.551947;903.504941;899.357596;886.959976;886.313378  
;885.461723;885.217934;882.822056;882.535829;878.079871;875.739743;875.200576;842.792457;8  
42.584612;838.398387;838.150950;833.420137;832.972444;793.297572;788.940967;785.924239;762.  
018052;761.988689;759.957953;759.757765;750.987864;750.877952;747.487158;742.261867;728.39  
6748;722.736012;722.398293;721.122305;720.988803;720.159342;719.974267;692.872753;688.0103  
20;687.466820;672.255862;669.966561;668.674338;663.612632;662.700328;659.433799;650.948580  
;650.389375;648.941304;648.783053;647.746295;646.950379;646.773329;643.359408;642.991182;5  
51.711890;551.488267;547.195527;546.885096;545.680815;538.085226;537.913810;524.246302;522.  
967439;507.719066;500.065724;499.519267;462.472649;462.367570;458.096778;457.995323;451.55  
7343;451.193102;415.596826;410.303617;400.963205;386.829588;386.645921;382.021139;381.7424  
89;378.679658;378.552529;327.443687;324.090588;321.684807;321.187250;319.252383;318.851201  
;316.452332;309.827210;309.243650;287.604184;287.469847;282.013715;281.512197;278.576621;2  
78.291490;274.490169;271.801154;266.017886;246.090167;241.486965;241.211572;221.011381;219.  
879109;216.347019;215.238276;212.533786;210.321488;209.046932;196.967457;193.809953;176.43  
6301;175.970813;173.783002;173.073492;170.228655;169.571597;113.359000;112.757696;108.2166  
85;107.770392;107.299392;103.813496;103.275581;102.707742;101.599112;95.509605;90.092763;8  
9.629790;88.500828;84.808551;84.035400;79.051153;76.114238;74.562243;73.258470;65.747824;64  
.489124;59.170179;58.355545;56.723402;55.683171;55.345199;52.103935;49.650334;45.119260;44.  
079516;43.072194;40.638600;39.607377;36.730181;36.494652;34.363267;33.158552;32.526930;30.3  
92150;29.524052;28.934947;27.075293;26.041442;23.572330;21.736340;19.093099;18.834373;17.24  
8678;15.895386;10.053230;7.207935

S:

3550.101756;3548.660658;3548.093457;3393.332102;3392.035128;3391.136466;3385.760866;3384.3  
44140;3383.507881;3128.632134;3128.127867;3125.885484;3125.534722;3124.868498;3123.773585;  
3119.620725;3118.494816;3116.289731;3063.601888;3063.153041;3062.810984;3062.315784;3062.2  
46072;3062.209941;3061.585268;3061.118482;3059.724010;3049.871672;3049.164075;3049.079609;  
3048.161577;3047.921866;3047.550649;3047.096850;3046.409600;3022.576960;3009.134166;3000.2

75231;3000.122840;2997.501059;2997.307503;2997.028895;2994.602796;2994.064412;2993.908127;  
2979.493241;2978.696588;2978.445607;2978.338076;2977.995429;2977.840248;2976.866538;2976.8  
42946;2975.739544;2236.554518;2236.085226;2234.133226;2222.417154;2222.058738;2221.679345;  
2210.803209;2205.907627;2202.962408;1654.055450;1653.122751;1649.879247;1647.111623;1645.8  
55555;1641.217658;1631.098091;1630.561163;1628.405503;1578.763530;1578.616576;1578.082971;  
1577.831909;1577.200050;1577.118884;1529.488943;1521.644315;1521.220890;1515.842723;1508.8  
78067;1506.946316;1506.828815;1498.631435;1497.608143;1453.346742;1451.802100;1451.596470;  
1451.322321;1450.712163;1450.611687;1449.838562;1449.646265;1443.717025;1443.278753;1442.9  
79206;1442.305112;1441.914388;1441.731243;1439.907581;1439.727615;1430.034295;1421.042978;  
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**BTA tetramer frequencies**  
(semicolon delimited)

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**BTA pentamer frequencies**  
(semicolon delimited)

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(semicolon delimited)

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(semicolon delimited)

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