Table S1. Cartesian coordinates of the LDA-OPT (an optimized structure from the LDA calculation) for the N-spring at the lattice angle β = 99.05 in the monoclinic unit cell. Each of four columns represent the atom type, x, y, z coordinates, atomic index, and atom serial number, respectively. Atom types correspond to C=1, H=2,O=3,N=4, and Ag=5. Atomic index is used only in the DFT program and bears no significance elsewhere. Atom serial number begins from 0, not from 1.

```
# Coordinates for the conformation No.      18 in no3_3dc_100x100_v20.6_t142_lda.out.
# No. of atoms read =  104
# xmin,xmax,xmax-xmin:  -2.625687  24.765513  27.391200
# ymin,ymax,ymax-ymin:   0.113395  20.215176  20.101781
# zmin,zmax,zmax-zmin:   0.045468  13.956325  13.910857
  5  14.548831  19.399896   7.102452 1    0
  3  24.765513   5.449483   3.265272 1    1
  3  13.240218   0.264195   8.471634 1    2
  3  10.901882   2.781541   6.203611 1    3
  3   6.899030  19.296293   6.175482 1    4
  4  19.057584   2.450561   5.678782 1    5
  4  13.996942  15.807518   8.880909 1    6
  4  11.426997   0.578273   6.950307 1    7
  1  17.421963   4.360565   5.405562 1    8
  1  18.157175   6.634847   4.354791 1    9
  1  20.621496   6.958703   3.585082 1   10
  1  22.318173   4.994672   3.916100 1   11
  1  21.469660   2.751174   4.971488 1   12
  1  11.804602  15.329749  10.055075 1   13
  1  11.416951  13.113799  11.376357 1   14
  1  13.329407  11.344934  11.492816 1   15
  1  15.578828  11.858577  10.276350 1   16
  1  15.861829  14.101796   8.967773 1   17
  2  15.483469   4.020593   6.051700 1   18
  2  16.818276   8.190417   4.133294 1   19
  2  21.224205   8.742802   2.754484 1   20
  2  22.744926   1.154095   5.252281 1   21
  2  10.333528  16.779346   9.904816 1   22
  2   9.570208  12.825587  12.270311 1   23
  2  13.103284   9.561424  12.510066 1   24
  2  17.609444  14.543055   7.966406 1   25
  5  -1.617306  16.614189   0.098959 1   26
  5  11.324668  16.612797   2.851419 1   27
  5   1.616066  19.378445   9.919756 1   28
  3  17.401210  10.004132  10.261987 1   29
  3   4.434723   9.991187   6.737852 1   30
```

3 11.803771 5.446175 13.742716 1 31
3 3.069675 15.166166 1.359619 1 32
3 15.981037 15.196206 1.600391 1 33
3 0.431836 0.240537 8.606582 1 34
3 5.518101 12.661641 13.237179 1 35
3 18.522035 12.613862 3.551342 1 36
3 23.841152 2.827301 10.576381 1 37
3 6.222717 16.719337 13.232734 1 38
3 19.160089 16.676706 3.780182 1 39
3 19.922877 19.332410 10.808445 1 40
4 23.096696 12.987701 12.705301 1 41
4 10.118893 12.992861 4.291223 1 42
4 6.112040 2.426250 11.325743 1 43
4 -1.040626 20.215176 1.883785 1 44
4 11.924165 20.213790 1.073333 1 45
4 1.033550 15.789664 8.115221 1 46
4 4.945223 14.862752 13.956325 1 47
4 17.895819 14.842006 2.980089 1 48
4 24.454507 0.597879 10.000800 1 49
1 -1.198174 11.075918 12.434429 1 50
1 11.756823 11.084624 4.546237 1 51
1 4.473888 4.336622 11.565456 1 52
1 24.006817 8.806845 11.366960 1 53
1 11.037906 8.808163 5.605047 1 54
1 5.201132 6.621170 12.599060 1 55
1 21.548672 8.489664 10.575501 1 56
1 8.584340 8.486316 6.408425 1 57
1 7.658175 6.945332 13.388077 1 58
1 19.849220 10.446524 10.913327 1 59
1 6.879932 10.444241 6.083560 1 60
1 9.360457 4.983696 13.084561 1 61
1 20.690776 12.683068 11.985223 1 62
1 7.714910 12.686168 5.019111 1 63
1 8.519057 2.731404 12.044227 1 64
1 4.424796 0.117481 3.060096 1 65
1 17.386685 0.113395 13.929888 1 66
1 -1.155655 15.318748 6.932011 1 67
1 4.819407 2.328677 4.386371 1 68
1 17.776310 2.315542 12.587180 1 69
1 -1.539105 13.115499 5.588992 1 70
1 2.916091 4.108574 4.506804 1 71
1 15.871735 4.095898 12.473282 1 72

```
 1   0.370280  11.342815   5.472818 1   73
 1   0.667052   3.604002   3.284415 1   74
 1  13.631958   3.597593  13.711891 1   75
 1   2.610557  11.844949   6.708058 1   76
 1   0.377897   1.364100   1.973781 1   77
 1  13.340226   1.359323   0.983298 1   78
 1   2.895784  14.082697   8.022867 1   79
 2   0.732403  11.417156  13.093241 1   80
 2  13.684174  11.428787   3.876474 1   81
 2   2.542238   3.990400  10.902071 1   82
 2  -0.586935   7.246223  11.148460 1   83
 2  12.373968   7.243801   5.792759 1   84
 2   3.864573   8.182917  12.782615 1   85
 2  20.958001   6.716526   9.724026 1   86
 2   7.997206   6.705538   7.253814 1   87
 2   8.252494   8.730828   0.169745 1   88
 2  19.407313  14.273132  12.270548 1   89
 2   6.431763  14.279030   4.739330 1   90
 2   9.796509   1.130965  11.776597 1   91
 2   2.621199  19.235651   2.901880 1   92
 2  15.582759  19.231562   0.045468 1   93
 2  -2.625687  16.767760   7.083945 1   94
 2   6.662901   2.606140   5.284423 1   95
 2  19.612092   2.595899  11.662989 1   96
 2  22.553750  12.837596   4.673142 1   97
 2   3.154491   5.889921   5.525621 1   98
 2  16.101398   5.869042  11.439640 1   99
 2   0.146216   9.569356   4.440798 1  100
 2  24.558098   0.937745   0.968190 1  101
 2  11.588877   0.934092   1.986546 1  102
 2   4.646782  14.510877   9.025907 1  103
-----------------------------------------------------------------------
```

Table S2. Cartesian coordinates of the PBE-OPT (an optimized structure from the PBE calculation) for the N-spring at the lattice angle $\beta = 94.05$ in the monoclinic unit cell. See Table caption for Table S1 for for more information.

Coordinates for the conformation No. 10 in no3_3dc_100x100_v20.6_t571.out.
No. of atoms read = 104
xmin,xmax,xmax-xmin: -0.992557 25.266976 26.259533
ymin,ymax,ymax-ymin: 0.100385 20.203919 20.103534
zmin,zmax,zmax-zmin: 0.034715 13.955551 13.920836

5	14.697545	19.346412	7.065589	1	0
3	23.078045	5.488586	3.249402	1	1
3	11.564767	0.236844	8.158007	1	2
3	9.002828	2.808455	6.164523	1	3
3	6.764273	19.283024	6.191511	1	4
4	17.387214	2.390859	5.653700	1	5
4	14.036855	15.797554	8.905483	1	6
4	9.582012	0.572242	6.835600	1	7
1	15.740010	4.297326	5.361050	1	8
1	16.483697	6.572512	4.295027	1	9
1	18.948224	6.920141	3.537507	1	10
1	20.634692	4.957597	3.895144	1	11
1	19.805599	2.695577	4.950342	1	12
1	11.825546	15.335935	10.076048	1	13
1	11.397813	13.110123	11.387429	1	14
1	13.300523	11.320061	11.497298	1	15
1	15.563064	11.826937	10.282408	1	16
1	15.897595	14.080807	8.988392	1	17
2	13.818490	3.926988	5.985324	1	18
2	15.170160	8.096840	4.023619	1	19
2	19.551504	8.696236	2.736971	1	20
2	21.054866	1.106311	5.238470	1	21
2	10.391872	16.792921	9.922270	1	22
2	9.572345	12.816714	12.269531	1	23
2	13.061389	9.555708	12.506851	1	24
2	17.646915	14.528203	8.023626	1	25
5	24.309851	16.645760	0.073275	1	26
5	11.340408	16.620588	2.829824	1	27
5	1.735868	19.366766	9.859560	1	28
3	17.361725	9.947539	10.273665	1	29
3	4.399108	9.945844	6.747357	1	30
3	10.103709	5.486777	13.768697	1	31

3 3.015564 15.152883 1.379162 1 32
3 15.950689 15.175803 1.562465 1 33
3 24.543805 0.246495 8.576958 1 34
3 5.557809 12.702849 13.230519 1 35
3 18.545253 12.619034 3.546324 1 36
3 21.971830 2.815976 10.565990 1 37
3 6.131196 16.828138 13.220334 1 38
3 19.098244 16.734576 3.807312 1 39
3 19.941628 19.266842 10.823489 1 40
4 23.061474 13.039428 12.670412 1 41
4 10.090936 13.037362 4.310868 1 42
4 4.419777 2.392932 11.325762 1 43
4 -0.992557 20.203919 1.889121 1 44
4 11.975748 20.195995 1.041222 1 45
4 1.064227 15.795155 8.072294 1 46
4 4.909468 14.906930 13.955551 1 47
4 17.871652 14.854273 2.977620 1 48
4 22.626740 0.575047 9.996715 1 49
1 24.701229 11.126060 12.387298 1 50
1 11.734456 11.126743 4.592525 1 51
1 2.771528 4.298409 11.612221 1 52
1 23.958375 8.849976 11.320377 1 53
1 10.993737 8.850030 5.658019 1 54
1 3.514349 6.578425 12.671099 1 55
1 21.496687 8.509905 10.553522 1 56
1 8.532823 8.508380 6.427962 1 57
1 5.975642 6.930815 13.437252 1 58
1 19.812022 10.476066 10.908585 1 59
1 6.845223 10.475153 6.084960 1 60
1 7.663385 4.962928 13.097575 1 61
1 20.643126 12.738563 11.960736 1 62
1 7.673138 12.737915 5.026713 1 63
1 6.837195 2.701854 12.035326 1 64
1 2.673967 0.100385 3.051120 1 65
1 15.642584 0.106625 13.924171 1 66
1 24.783873 15.328669 6.902327 1 67
1 3.105774 2.324790 4.361424 1 68
1 16.061018 2.330173 12.609318 1 69
1 24.363697 13.105753 5.585990 1 70
1 1.204071 4.113026 4.478561 1 71
1 14.153735 4.115499 12.496770 1 72
1 0.338516 11.315090 5.483797 1 73

```
 1  24.874420   3.604068   3.259845 1   74
 1  11.903137   3.603429  13.726023 1   75
 1   2.593646  11.822287   6.710197 1   76
 1  24.527755   1.352720   1.968179 1   77
 1  11.562226   1.340852   0.960575 1   78
 1   2.927559  14.080132   7.991573 1   79
 2   0.692660  11.490157  13.020719 1   80
 2  13.652786  11.493522   3.952857 1   81
 2   0.853240   3.929748  10.979458 1   82
 2  25.266976   7.319217  11.052290 1   83
 2  12.302820   7.317760   5.912562 1   84
 2   2.200237   8.104260  12.932364 1   85
 2  20.890738   6.739441   9.752756 1   86
 2   7.928272   6.730589   7.220060 1   87
 2   6.571681   8.716202   0.189600 1   88
 2  19.394231  14.328757  12.247001 1   89
 2   6.421767  14.326826   4.735792 1   90
 2   8.085486   1.109566  11.745758 1   91
 2   2.654007  19.208241   2.899873 1   92
 2  15.627082  19.220502   0.034715 1   93
 2  23.354019  16.788422   7.048907 1   94
 2   4.936833   2.615546   5.238375 1   95
 2  17.882235   2.626368  11.716253 1   96
 2  22.549631  12.815409   4.681246 1   97
 2   1.440455   5.875303   5.492555 1   98
 2  14.386169   5.879214  11.484055 1   99
 2   0.098656   9.552259   4.472506 1  100
 2  22.773076   0.912437   1.003857 1  101
 2   9.799898   0.898279   1.906672 1  102
 2   4.676318  14.528405   8.951474 1  103
```

Table S3. Cartesian coordinates of the PBE-OPT (an optimized structure from the PBE calculation) for the N-spring at the lattice angle $\beta = 99.05$ in the monoclinic unit cell. See Table caption for Table S1 for for more information.

Coordinates for the conformation No. 8 in no3_3dc_100x100_v20.6_t141.out.
No. of atoms read = 104
xmin,xmax,xmax-xmin: -2.620329 24.775563 27.395892
ymin,ymax,ymax-ymin: 0.121955 20.229903 20.107948
zmin,zmax,zmax-zmin: 0.041716 13.959497 13.917781

5	14.552323	19.392935	7.103203	1	0
3	24.775563	5.484078	3.242115	1	1
3	13.245009	0.260742	8.484633	1	2
3	10.897008	2.800493	6.200623	1	3
3	6.886366	19.276519	6.181015	1	4
4	19.054934	2.467231	5.682814	1	5
4	13.990859	15.796852	8.885834	1	6
4	11.422680	0.579456	6.953092	1	7
1	17.409056	4.379255	5.407331	1	8
1	18.140185	6.660835	4.347300	1	9
1	20.617647	6.981581	3.577883	1	10
1	22.318532	5.004965	3.910992	1	11
1	21.475601	2.752561	4.968859	1	12
1	11.789444	15.322867	10.063950	1	13
1	11.395932	13.099902	11.384510	1	14
1	13.320247	11.329544	11.501051	1	15
1	15.572730	11.850077	10.274484	1	16
1	15.869335	14.097077	8.962778	1	17
2	15.493763	4.028613	6.045982	1	18
2	16.812828	8.202406	4.122601	1	19
2	21.225455	8.745285	2.752560	1	20
2	22.720036	1.156446	5.246096	1	21
2	10.339715	16.763393	9.915988	1	22
2	9.571242	12.807528	12.269605	1	23
2	13.101548	9.562466	12.507754	1	24
2	17.602012	14.555798	7.980017	1	25
5	-1.618759	16.621153	0.100444	1	26
5	11.330670	16.626828	2.845766	1	27
5	1.617185	19.358682	9.915225	1	28
3	17.385303	9.970415	10.251641	1	29

3 4.420869 9.959999 6.757288 1 30
3 11.813719 5.480602 13.768309 1 31
3 3.064524 15.168090 1.373029 1 32
3 15.973642 15.189433 1.590203 1 33
3 0.445551 0.243145 8.600856 1 34
3 5.533361 12.646579 13.232861 1 35
3 18.531487 12.597214 3.543115 1 36
3 23.838316 2.843462 10.569376 1 37
3 6.238789 16.735015 13.230152 1 38
3 19.181729 16.695384 3.778936 1 39
3 19.901599 19.311536 10.803703 1 40
4 23.095635 12.970226 12.709053 1 41
4 10.119317 12.980702 4.290513 1 42
4 6.109721 2.435977 11.324698 1 43
4 -1.036441 20.228619 1.886630 1 44
4 11.930565 20.229903 1.070972 1 45
4 1.025920 15.773775 8.111567 1 46
4 4.952370 14.862323 13.959497 1 47
4 17.902847 14.842012 2.978041 1 48
4 24.451798 0.595285 9.998929 1 49
1 -1.186709 11.055770 12.436156 1 50
1 11.767550 11.067708 4.546226 1 51
1 4.463565 4.352567 11.566223 1 52
1 24.020646 8.779100 11.360356 1 53
1 11.052130 8.783783 5.612825 1 54
1 5.187708 6.645941 12.606583 1 55
1 21.548439 8.462445 10.561405 1 56
1 8.586058 8.461774 6.422235 1 57
1 7.657133 6.971801 13.398497 1 58
1 19.846939 10.434336 10.907776 1 59
1 6.878533 10.432657 6.090246 1 60
1 9.360062 4.994096 13.090310 1 61
1 20.682250 12.681638 11.982441 1 62
1 7.707278 12.684899 5.021082 1 63
1 8.527039 2.731517 12.045704 1 64
1 4.438918 0.125897 3.066628 1 65
1 17.402974 0.121955 13.923640 1 66
1 -1.171986 15.309720 6.924863 1 67
1 4.841901 2.343124 4.396398 1 68
1 17.797680 2.329622 12.576350 1 69
1 -1.562250 13.100575 5.580273 1 70
1 2.927310 4.128071 4.516402 1 71

```
 1  15.881976   4.114279  12.462210 1   72
 1   0.358901  11.326945   5.462201 1   73
 1   0.674484   3.615954   3.282471 1   74
 1  13.639759   3.611035  13.713158 1   75
 1   2.603307  11.836047   6.708421 1   76
 1   0.369144   1.372052   1.971395 1   77
 1  13.333922   1.368328   0.983032 1   78
 1   2.903929  14.076063   8.024661 1   79
 2   0.723854  11.404655  13.088016 1   80
 2  13.670158  11.416742   3.870096 1   81
 2   2.558100   4.004245  10.896102 1   82
 2  -0.581972   7.238241  11.139794 1   83
 2  12.378057   7.237390   5.798329 1   84
 2   3.862313   8.194117  12.788863 1   85
 2  20.955174   6.701284   9.718673 1   86
 2   7.996986   6.695373   7.259204 1   87
 2   8.257461   8.741288   0.174114 1   88
 2  19.426728  14.269434  12.265539 1   89
 2   6.449770  14.270272   4.735792 1   90
 2   9.777282   1.137700  11.774077 1   91
 2   2.609320  19.245237   2.913072 1   92
 2  15.573091  19.242415   0.041716 1   93
 2  -2.620329  16.750506   7.081868 1   94
 2   6.664185   2.620387   5.293158 1   95
 2  19.611341   2.603674  11.661776 1   96
 2  22.552122  12.819649   4.671129 1   97
 2   3.156679   5.891779   5.525201 1   98
 2  16.103752   5.870294  11.440160 1   99
 2   0.143641   9.568885   4.443921 1  100
 2  24.564127   0.933596   0.984622 1  101
 2  11.598971   0.933444   1.968688 1  102
 2   4.639124  14.518868   9.008847 1  103
```

Table S4. Cartesian coordinates of the PBE-OPT (an optimized structure from the PBE calculation) for the N-spring at the lattice angle $\beta = 104.05$ in the monoclinic unit cell. See Table caption for Table S1 for for more information.

Coordinates for the conformation No. 8 in no3_3dc_100x100_v20.6_t492.out.
No. of atoms read = 104
xmin,xmax,xmax-xmin: -2.757376 24.642647 27.400023
ymin,ymax,ymax-ymin: 0.108660 20.208543 20.099882
zmin,zmax,zmax-zmin: 0.047326 13.955245 13.907920

5	14.637972	19.397902	7.119345	1	0
3	0.726816	5.445259	3.220826	1	1
3	15.051368	0.280330	8.422008	1	2
3	12.785243	2.978136	6.213810	1	3
3	6.654620	19.506967	6.195967	1	4
4	20.969970	2.410311	5.676164	1	5
4	14.078735	15.835109	8.900341	1	6
4	13.205755	0.722360	6.944571	1	7
1	19.310849	4.314567	5.413976	1	8
1	20.008717	6.585982	4.313858	1	9
1	22.469597	6.885524	3.494818	1	10
1	24.199229	4.940310	3.865151	1	11
1	23.385170	2.693421	4.950703	1	12
1	11.876319	15.347349	10.074984	1	13
1	11.491176	13.108441	11.373989	1	14
1	13.429084	11.352649	11.462682	1	15
1	15.675907	11.879414	10.237796	1	16
1	15.963497	14.136218	8.948953	1	17
2	17.405630	3.975179	6.076830	1	18
2	18.664220	8.116893	4.095883	1	19
2	23.048171	8.610463	2.576971	1	20
2	24.642647	1.103872	5.237287	1	21
2	10.418779	16.786295	9.939132	1	22
2	9.669905	12.806304	12.269127	1	23
2	13.288414	9.582873	12.460058	1	24
2	17.690336	14.601641	7.959283	1	25
5	-1.541545	16.640698	0.067976	1	26
5	11.422737	16.656968	2.889257	1	27
5	1.687821	19.391268	9.865630	1	28
3	17.498488	10.000981	10.225107	1	29
3	4.547612	10.001704	6.787963	1	30
3	13.681342	5.447169	13.801671	1	31
3	3.030602	15.151654	1.398000	1	32

3 15.962374 15.146028 1.582208 1 33
3 2.125595 0.262530 8.565417 1 34
3 5.466612 12.615668 13.226892 1 35
3 18.453813 12.481190 3.547482 1 36
3 -0.230693 3.054114 10.553754 1 37
3 6.172403 16.722428 13.197828 1 38
3 19.206653 16.568231 3.790038 1 39
3 19.636410 19.578002 10.807774 1 40
4 -2.757376 13.052755 12.692422 1 41
4 10.206854 13.071480 4.300258 1 42
4 8.007669 2.403586 11.315720 1 43
4 -0.999491 20.197562 1.866552 1 44
4 11.967220 20.208543 1.087645 1 45
4 1.113253 15.824323 8.097235 1 46
4 4.902302 14.839565 13.955245 1 47
4 17.884900 14.746642 2.977944 1 48
4 0.248273 0.766723 9.983826 1 49
1 -1.103599 11.142520 12.435149 1 50
1 11.867274 11.163372 4.528331 1 51
1 6.347700 4.311779 11.554482 1 52
1 -1.789741 8.864601 11.341878 1 53
1 11.181287 8.873747 5.605456 1 54
1 7.045011 6.590643 12.639261 1 55
1 21.680554 8.551757 10.519803 1 56
1 8.727286 8.559197 6.441699 1 57
1 9.499456 6.885605 13.476574 1 58
1 19.952488 10.500364 10.886522 1 59
1 6.994016 10.508690 6.105529 1 60
1 11.232052 4.938899 13.131281 1 61
1 20.757372 12.752334 11.971756 1 62
1 7.794328 12.768690 5.030204 1 63
1 10.421359 2.688121 12.049644 1 64
1 6.346289 0.108660 3.042503 1 65
1 19.309012 0.118668 13.944038 1 66
1 -1.083207 15.336629 6.910886 1 67
1 6.732042 2.333908 4.361357 1 68
1 19.687550 2.338392 12.616540 1 69
1 -1.458444 13.108072 5.593452 1 70
1 4.789976 4.084452 4.464187 1 71
1 17.746673 4.092572 12.521925 1 72
1 0.480903 11.350772 5.509621 1 73
1 2.546485 3.567401 3.231989 1 74

1	15.509070	3.575518	13.766457	1	75
1	2.717775	11.875364	6.754441	1	76
1	2.255066	1.320225	1.930994	1	77
1	15.219620	1.327068	1.024071	1	78
1	3.002260	14.131799	8.046858	1	79
2	0.801369	11.478952	13.101542	1	80
2	13.765481	11.506620	3.843475	1	81
2	4.446664	3.973760	10.871236	1	82
2	-0.433232	7.344140	11.128665	1	83
2	12.533767	7.345840	5.785026	1	84
2	5.705414	8.130673	12.831052	1	85
2	21.100976	6.825605	9.597003	1	86
2	8.153413	6.825544	7.349682	1	87
2	10.072100	8.608857	0.352087	1	88
2	19.483272	14.327833	12.263708	1	89
2	6.520676	14.348145	4.750626	1	90
2	11.678262	1.095551	11.772606	1	91
2	2.655892	19.235125	2.893671	1	92
2	15.617070	19.242312	0.047326	1	93
2	-2.542096	16.774249	7.046958	1	94
2	8.552648	2.632080	5.253227	1	95
2	21.496503	2.629314	11.701739	1	96
2	22.660978	12.812964	4.672684	1	97
2	4.927452	5.845954	5.473296	1	98
2	17.888619	5.855923	11.517115	1	99
2	0.342118	9.582370	4.506024	1	100
2	0.530730	0.859392	0.941055	1	101
2	13.490722	0.864705	2.006883	1	102
2	4.733432	14.599839	9.027494	1	103

Table S5. Cartesian coordinates of the LDA-OPT (an optimized structure from the LDA calculation) for the Cl-spring at the lattice angle β = 106.7 in the monoclinic unit cell. Atom types correspond to C=1, H=2,O=3,N=4, Ag=5, and Cl=6. See Table caption for Table S1 for more information.

```
# Coordinates for the conformation No.      18 in clo4_3dc_100x100_v20.6_t2058_lda.out.
# No. of atoms read =  108
# xmin,xmax,xmax-xmin:  -3.201508  24.762609  27.964117
# ymin,ymax,ymax-ymin:   0.208132  18.926477  18.718344
# zmin,zmax,zmax-zmin:   0.112455  16.777942  16.665487
  5  -1.973055  15.415165   5.823727 1    0
  3  18.019638   9.269895   0.239728 1    1
  4  -1.675305  18.896057   7.976872 1    2
  4  -2.623169  11.934934   3.751489 1    3
  6   4.984671  14.142466   7.003933 1    4
  3   5.460622  15.701974   9.212438 1    5
  3   3.026982  15.327585   5.461424 1    6
  3   7.272722  13.898471   5.522327 1    7
  3   4.125162  11.662232   7.799569 1    8
  1   2.240068   1.539623   7.751858 1    9
  1   2.264653   3.729926   9.179982 1   10
  1   4.198849   4.155174  10.882109 1   11
  1   6.086224   2.358995  11.073014 1   12
  1   5.962385   0.208132   9.593499 1   13
  1  21.008766  11.703413   2.670032 1   14
  1  20.368632   9.600132   1.245196 1   15
  1  22.153996   7.719089   0.874517 1   16
  1  -1.418382   7.970379   2.018652 1   17
  1  -0.913941  10.090576   3.467519 1   18
  2   0.723711   1.176148   6.391958 1   19
  2   4.211346   5.856607  12.055143 1   20
  2   7.678466   2.577906  12.376539 1   21
  2   1.729341  17.879666   9.681492 1   22
  2  19.656633  13.232967   2.991218 1   23
  2  21.714112   6.069889  16.777942 1   24
  2   0.007770   6.492818   1.753818 1   25
  2   0.889203  10.337544   4.453275 1   26
  5  14.800586  18.603516  14.512609 1   27
  5   1.764973  18.555695   1.307710 1   28
  5  11.115995  15.425188   9.870922 1   29
  3   0.443476   5.565215   8.793727 1   30
  3  13.413678   5.544321   6.896417 1   31
  3   5.078517   9.303376  15.413025 1   32
```

4 14.443182 15.064279 16.511089 1 33
4 1.451227 15.055433 16.253668 1 34
4 11.372912 18.926477 7.739991 1 35
4 21.124836 2.954934 12.390126 1 36
4 8.160040 2.940199 3.340420 1 37
4 10.359530 11.940772 11.908921 1 38
6 13.570799 0.716533 15.557839 1 39
6 0.554580 0.631883 0.112455 1 40
6 17.818628 13.765600 8.245293 1 41
3 7.419444 18.264375 0.710081 1 42
3 20.238810 18.177402 14.969809 1 43
3 18.434313 15.727200 6.420519 1 44
3 9.854211 18.706550 14.035866 1 45
3 -3.201508 18.547508 1.626162 1 46
3 16.090891 14.785767 10.131978 1 47
3 11.280550 0.840943 14.065309 1 48
3 24.179668 0.848597 1.612824 1 49
3 20.111347 12.907258 9.481252 1 50
3 14.316960 3.240066 16.332365 1 51
3 1.385804 3.117284 16.385084 1 52
3 16.625675 11.655370 6.972506 1 53
1 16.244515 13.309989 16.273454 1 54
1 3.259347 13.308560 16.495236 1 55
1 15.275315 1.555223 7.977588 1 56
1 16.184749 11.097758 0.590511 1 57
1 3.264933 11.144810 15.028015 1 58
1 15.235966 3.712417 6.498488 1 59
1 14.206492 10.643641 2.230267 1 60
1 1.372149 10.746204 13.276877 1 61
1 17.110589 4.115655 4.727842 1 62
1 12.331854 12.449569 2.429755 1 63
1 -0.512581 12.543437 13.071944 1 64
1 19.013221 2.338073 4.526958 1 65
1 12.506620 14.638015 1.017048 1 66
1 -0.419150 14.668960 14.589122 1 67
1 18.960651 0.224253 6.061204 1 68
1 23.391988 3.189859 11.298690 1 69
1 10.432352 3.161633 4.425211 1 70
1 8.075666 11.709178 12.970041 1 71
1 24.001278 5.262260 9.816803 1 72
1 11.070274 5.252057 5.869489 1 73
1 7.428062 9.610894 14.398437 1 74

```
 1  22.202516   7.126512   9.414782 1   75
 1   9.293557   7.142146   6.245138 1   76
 1   9.201745   7.719747  14.773605 1   77
 1  19.876065   6.861942  10.566107 1   78
 1   6.961767   6.898664   5.100000 1   79
 1  11.538773   7.965839  13.644206 1   80
 1  19.390287   4.766112  12.056579 1   81
 1   6.452093   4.782454   3.644045 1   82
 1  12.060392  10.094361  12.213191 1   83
 2  17.772136  13.685907  14.934238 1   84
 2   4.740308  13.648079   0.827782 1   85
 2  13.803092   1.204677   9.388001 1   86
 2  14.165598   8.922356   3.370083 1   87
 2   1.395927   9.059798  12.080644 1   88
 2  17.066370   5.790446   3.517356 1   89
 2  10.725719  12.218948   3.711454 1   90
 2  -2.069951  12.340478  11.723829 1   91
 2  20.562935   2.543157   3.171094 1   92
 2  11.037929  16.094853   1.131841 1   93
 2  -1.905742  16.108078  14.492489 1   94
 2  14.739785  17.908946   5.960574 1   95
 2  24.762609   1.684952  11.658162 1   96
 2  11.786259   1.634548   4.087422 1   97
 2   6.720309  13.231713  12.627824 1   98
 2  22.614691   8.774100   8.235729 1   99
 2   9.739523   8.789137   7.411177 1  100
 2   8.757313   6.070214  15.939821 1  101
 2  18.434301   8.318256  10.289572 1  102
 2   5.538880   8.379122   5.368296 1  103
 2  12.958695   6.482669  13.912347 1  104
 2  17.586698   4.514846  13.040493 1  105
 2   4.643420   4.537845   2.668671 1  106
 2  13.879334  10.355573  11.264792 1  107
```

Table S6. Cartesian coordinates of the PBE-OPT (an optimized structure from the PBE calculation) for the Cl-spring at the lattice angle $\beta = 101.7$ in the monoclinic unit cell. See Table captions for Tables S1 and S5 for more information.

```
# Coordinates for the conformation No.      17 in clo4_3dc_100x100_v20.6_t5044.out.
# No. of atoms read =  108
# xmin,xmax,xmax-xmin:  -3.751517  24.888984  28.640501
# ymin,ymax,ymax-ymin:   0.180266  18.887524  18.707257
# zmin,zmax,zmax-zmin:   0.056212  16.884222  16.828010
  5  -1.781733  15.417484   5.800880 1    0
  3  17.993818   9.305156   0.223544 1    1
  4  -1.610192  18.871267   7.936356 1    2
  4  23.313543  12.036638   3.673192 1    3
  6   5.076589  14.099836   6.958697 1    4
  3   5.536023  15.832636   9.075159 1    5
  3   3.569575  15.399245   5.010173 1    6
  3   7.497277  13.291734   5.879457 1    7
  3   3.675913  11.880840   7.857710 1    8
  1   0.503293   1.502544   7.696193 1    9
  1   0.561090   3.702819   9.123399 1   10
  1   2.494631   4.110220  10.842986 1   11
  1   4.407734   2.330471  11.031524 1   12
  1   4.278809   0.180266   9.541511 1   13
  1  21.005213  11.807355   2.636267 1   14
  1  20.355563   9.669804   1.248274 1   15
  1  22.126449   7.757562   0.887361 1   16
  1  -1.412579   8.037209   1.977447 1   17
  1  -0.874665  10.193871   3.370871 1   18
  2  24.888984   1.112388   6.363244 1   19
  2   2.489478   5.772445  12.033094 1   20
  2   5.979717   2.572139  12.325128 1   21
  2   1.795626  17.852153   9.611687 1   22
  2  19.689703  13.349112   2.956616 1   23
  2  21.645719   6.078336  16.884222 1   24
  2  -0.007043   6.572062   1.714370 1   25
  2   0.938437  10.505646   4.278642 1   26
  5  14.570230  18.553068  14.335616 1   27
  5   1.610913  18.541123   1.299757 1   28
  5  11.234358  15.438596   9.833505 1   29
  3  24.658355   5.578532   8.756042 1   30
  3  11.690372   5.551819   6.890989 1   31
  3   5.059508   9.319688  15.419068 1   32
```

4 14.382936 15.101428 16.483295 1 33
4 1.425367 15.103233 16.185515 1 34
4 11.416141 18.887524 7.644789 1 35
4 19.349943 2.834023 12.215400 1 36
4 6.400293 2.821069 3.399749 1 37
4 10.359389 12.062528 11.943804 1 38
6 11.724208 0.741526 15.529899 1 39
6 24.677734 0.737616 0.056212 1 40
6 18.047618 14.112261 8.630209 1 41
3 7.293659 18.239986 0.676489 1 42
3 20.176222 18.259120 14.911052 1 43
3 18.619613 15.896605 6.583304 1 44
3 9.163085 18.379126 13.618215 1 45
3 -3.751517 18.337949 1.907510 1 46
3 16.466526 15.382177 10.535380 1 47
3 9.316478 1.588964 14.445757 1 48
3 22.308069 1.589660 1.212831 1 49
3 20.404799 13.269872 9.817385 1 50
3 13.237952 2.939960 16.307057 1 51
3 0.279953 2.938539 16.346640 1 52
3 16.681620 11.926656 7.602749 1 53
1 16.228639 13.370409 16.246600 1 54
1 3.272085 13.375811 16.432812 1 55
1 13.507985 1.494633 7.897594 1 56
1 16.179465 11.171562 0.603863 1 57
1 3.239108 11.173765 15.009792 1 58
1 13.514210 3.698747 6.474912 1 59
1 14.245626 10.754227 2.323037 1 60
1 1.330069 10.751918 13.265821 1 61
1 15.407763 4.127583 4.715639 1 62
1 12.330679 12.532937 2.507579 1 63
1 -0.578800 12.533731 13.056520 1 64
1 17.338330 2.367955 4.502882 1 65
1 12.451875 14.684147 1.017298 1 66
1 -0.486389 14.679797 14.557966 1 67
1 17.276530 0.226260 6.012727 1 68
1 21.651015 3.063566 11.162205 1 69
1 8.698105 3.049151 4.458587 1 70
1 8.056891 11.832054 12.992100 1 71
1 22.294896 5.206326 9.778182 1 72
1 9.338652 5.195493 5.837761 1 73
1 7.410219 9.682181 14.364635 1 74

```
 1  20.524226   7.120950   9.431408 1   75
 1   7.576673   7.124139   6.157494 1   76
 1   9.175971   7.758533  14.683126 1   77
 1  18.164724   6.837304  10.531078 1   78
 1   5.222607   6.841037   5.047140 1   79
 1  11.535089   8.038649  13.582021 1   80
 1  17.634079   4.680128  11.927150 1   81
 1   4.688828   4.672767   3.670739 1   82
 1  12.071018  10.210963  12.213271 1   83
 2  17.741961  13.756472  14.906684 1   84
 2   4.778510  13.768953   0.704365 1   85
 2  12.007870   1.077993   9.240126 1   86
 2  14.249462   9.087997   3.509000 1   87
 2   1.345655   9.085445  12.079227 1   88
 2  15.368751   5.785281   3.519097 1   89
 2  10.759994  12.289638   3.801483 1   90
 2  -2.129542  12.291982  11.737977 1   91
 2  18.878015   2.619453   3.171990 1   92
 2  10.973103  16.106713   1.089113 1   93
 2  -1.973919  16.093367  14.477213 1   94
 2  14.826143  17.931447   5.934915 1   95
 2  22.970234   1.525566  11.481093 1   96
 2  10.017408   1.509077   4.145797 1   97
 2   6.744319  13.380504  12.691291 1   98
 2  20.996922   8.798657   8.354136 1   99
 2   8.052238   8.811937   7.221490 1  100
 2   8.695459   6.068555  15.735528 1  101
 2  16.755985   8.299755  10.270272 1  102
 2   3.821858   8.314700   5.278921 1  103
 2  12.935204   6.564132  13.817343 1  104
 2  15.828972   4.373030  12.850499 1  105
 2   2.885639   4.363045   2.743815 1  106
 2  13.880221  10.528255  11.298734 1  107

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Table S7. Cartesian coordinates of the PBE-OPT (an optimized structure from the PBE calculation) for the Cl-spring at the lattice angle $\beta = 106.7$ in the monoclinic unit cell. See Table captions for Tables S1 and S5 for more information.

Coordinates for the conformation No. 15 in clo4_3dc_100x100_v20.6_t2057.out.

No. of atoms read = 108
xmin,xmax,xmax-xmin: -3.178614 24.742923 27.921537
ymin,ymax,ymax-ymin: 0.206346 18.928705 18.722359
zmin,zmax,zmax-zmin: 0.104564 16.778836 16.674271

5	-1.967609	15.399558	5.832474	1	0
3	18.007304	9.221324	0.211077	1	1
4	-1.677236	18.895902	7.993481	1	2
4	-2.615259	11.923419	3.745023	1	3
6	4.978115	14.146760	7.006353	1	4
3	5.449110	15.726487	9.243488	1	5
3	3.002654	15.346300	5.445681	1	6
3	7.284574	13.916810	5.486227	1	7
3	4.114478	11.637338	7.820859	1	8
1	2.231051	1.546317	7.744845	1	9
1	2.280374	3.750687	9.166798	1	10
1	4.212659	4.171268	10.892048	1	11
1	6.110450	2.367268	11.092162	1	12
1	5.978472	0.206346	9.610145	1	13
1	21.006221	11.708577	2.650107	1	14
1	20.369854	9.589450	1.231758	1	15
1	22.164178	7.698543	0.861374	1	16
1	-1.397766	7.942004	2.016300	1	17
1	-0.894984	10.070834	3.471425	1	18
2	0.724496	1.176077	6.394170	1	19
2	4.217328	5.858707	12.054215	1	20
2	7.688967	2.594212	12.385640	1	21
2	1.724917	17.881206	9.692444	1	22
2	19.676312	13.234835	2.970268	1	23
2	21.713054	6.068397	16.778836	1	24
2	0.019931	6.477541	1.763841	1	25
2	0.892412	10.322610	4.454209	1	26
5	14.824824	18.630443	14.562194	1	27
5	1.764273	18.577849	1.292453	1	28
5	11.132456	15.408730	9.840274	1	29
3	0.458636	5.616068	8.758732	1	30
3	13.429671	5.594453	6.919027	1	31

3 5.064065 9.253475 15.441349 1 32
4 14.438103 15.064009 16.520539 1 33
4 1.444721 15.049627 16.248231 1 34
4 11.377130 18.928705 7.734935 1 35
4 21.116733 2.964035 12.378927 1 36
4 8.154770 2.952270 3.350363 1 37
4 10.363029 11.932605 11.920508 1 38
6 13.582329 0.708322 15.563068 1 39
6 0.562140 0.625738 0.104564 1 40
6 17.808928 13.767530 8.229651 1 41
3 7.435270 18.239768 0.747470 1 42
3 20.241738 18.147951 14.933549 1 43
3 18.438224 15.761142 6.396152 1 44
3 9.882718 18.688362 14.015246 1 45
3 -3.178614 18.527254 1.641032 1 46
3 16.067548 14.799342 10.144812 1 47
3 11.276209 0.812954 14.026792 1 48
3 24.175467 0.831055 1.650149 1 49
3 20.118251 12.896158 9.498643 1 50
3 14.324578 3.264300 16.355964 1 51
3 1.389995 3.143688 16.359770 1 52
3 16.601175 11.648793 6.905901 1 53
1 16.249901 13.303953 16.263239 1 54
1 3.265490 13.298742 16.506110 1 55
1 15.266209 1.560887 7.989528 1 56
1 16.169734 11.080108 0.577838 1 57
1 3.251483 11.123337 15.040519 1 58
1 15.250385 3.730010 6.511427 1 59
1 14.192559 10.629263 2.237965 1 60
1 1.362301 10.727554 13.267561 1 61
1 17.124281 4.133128 4.721789 1 62
1 12.309005 12.444871 2.450506 1 63
1 -0.534155 12.531329 13.052309 1 64
1 19.035022 2.346580 4.508727 1 65
1 12.489049 14.641466 1.032402 1 66
1 -0.435852 14.666008 14.575180 1 67
1 18.976586 0.223406 6.049977 1 68
1 23.394470 3.185359 11.275086 1 69
1 10.435468 3.156273 4.450066 1 70
1 8.068810 11.712076 12.993276 1 71
1 24.001371 5.274035 9.801109 1 72
1 11.069315 5.260174 5.888078 1 73

```
 1   7.428814   9.594818  14.415159 1   74
 1  22.193201   7.147782   9.402638 1   75
 1   9.284701   7.162258   6.258635 1   76
 1   9.210798   7.692946  14.790361 1   77
 1  19.854119   6.891073  10.564199 1   78
 1   6.942351   6.923194   5.101899 1   79
 1  11.557231   7.937796  13.646908 1   80
 1  19.371105   4.784229  12.058870 1   81
 1   6.433860   4.798579   3.642430 1   82
 1  12.076477  10.077132  12.213768 1   83
 2  17.768894  13.684758  14.935083 1   84
 2   4.739105  13.646519   0.826621 1   85
 2  13.802345   1.202516   9.387392 1   86
 2  14.159208   8.922856   3.368204 1   87
 2   1.394624   9.053166  12.088487 1   88
 2  17.071366   5.793304   3.521796 1   89
 2  10.720687  12.207482   3.725949 1   90
 2  -2.077342  12.324556  11.713867 1   91
 2  20.568473   2.559480   3.161495 1   92
 2  11.041049  16.093962   1.140506 1   93
 2  -1.902124  16.100937  14.479428 1   94
 2  14.735949  17.912042   5.956583 1   95
 2  24.742923   1.681777  11.631736 1   96
 2  11.768395   1.632488   4.115050 1   97
 2   6.734926  13.231337  12.651206 1   98
 2  22.614591   8.778565   8.233453 1   99
 2   9.737957   8.795665   7.411077 1  100
 2   8.758809   6.060581  15.942843 1  101
 2  18.422276   8.337091  10.300044 1  102
 2   5.528950   8.390194   5.355020 1  103
 2  12.967415   6.466886  13.898863 1  104
 2  17.584521   4.526020  13.040162 1  105
 2   4.642644   4.543750   2.669147 1  106
 2  13.880075  10.341876  11.268083 1  107

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Table S8. Cartesian coordinates of the PBE-OPT (an optimized structure from the PBE calculation) for the Cl-spring at the lattice angle $\beta = 111.7$ in the monoclinic unit cell. See Table captions for Tables S1 and S5 for more information.

Coordinates for the conformation No. 12 in clo4_3dc_100x100_v20.6_t4098.out.
No. of atoms read = 108
xmin,xmax,xmax-xmin: -5.639238 22.806073 28.445311
ymin,ymax,ymax-ymin: 0.268645 19.094966 18.826320
zmin,zmax,zmax-zmin: 0.155186 16.797756 16.642570

5	-1.573794	15.162959	6.238223	1	0
3	18.127567	9.520428	0.214164	1	1
4	-1.398394	18.732203	8.203698	1	2
4	-2.334362	12.136703	3.580874	1	3
6	5.051475	13.973398	6.821793	1	4
3	5.457807	15.878896	8.803120	1	5
3	3.652896	15.102167	4.712072	1	6
3	7.515534	13.077739	5.903512	1	7
3	3.613725	11.835364	7.846281	1	8
1	4.248305	1.229628	7.890987	1	9
1	4.124638	3.483650	9.215553	1	10
1	6.040647	4.135994	10.874326	1	11
1	8.091858	2.520206	11.099096	1	12
1	8.109982	0.268645	9.760219	1	13
1	-4.641535	12.021700	2.512890	1	14
1	20.524243	9.902176	1.140416	1	15
1	22.247859	7.942069	0.765894	1	16
1	-1.265732	8.129060	1.814370	1	17
1	-0.670320	10.248414	3.242342	1	18
2	2.800198	0.713728	6.535087	1	19
2	5.921104	5.869893	11.942804	1	20
2	9.679600	2.949010	12.314246	1	21
2	2.082965	18.055176	9.895113	1	22
2	20.011244	13.616531	2.831165	1	23
2	21.671731	6.279268	16.797756	1	24
2	0.104478	6.615042	1.584407	1	25
2	1.137681	10.448688	4.189192	1	26
5	14.459173	18.844907	14.841986	1	27
5	1.505089	18.950552	0.589014	1	28
5	11.369200	15.084991	9.127037	1	29
3	2.220032	5.222909	8.699568	1	30
3	15.123498	5.229159	6.896560	1	31
3	5.271792	9.701095	15.433365	1	32

4 14.265977 15.172822 16.610738 1 33
4 1.246306 15.238708 15.968057 1 34
4 11.554202 18.778596 7.341151 1 35
4 22.806073 2.931378 12.432495 1 36
4 9.877727 3.017985 3.003518 1 37
4 10.564561 11.975656 11.623111 1 38
6 15.331463 0.939551 15.332017 1 39
6 2.362327 0.853087 0.235914 1 40
6 18.009863 14.007626 8.727236 1 41
3 7.302083 18.054128 0.155186 1 42
3 -5.639238 18.039521 15.342133 1 43
3 18.528745 15.731931 6.614354 1 44
3 9.378799 19.094966 13.308926 1 45
3 -3.540261 18.960887 2.191116 1 46
3 16.550082 15.344646 10.674073 1 47
3 12.896250 1.661499 14.210963 1 48
3 -0.083088 1.441153 1.416813 1 49
3 20.411918 13.129536 9.811758 1 50
3 16.504312 3.135167 16.558964 1 51
3 3.485771 3.117528 16.160150 1 52
3 16.563707 11.821764 7.814835 1 53
1 16.188039 13.537018 16.348005 1 54
1 3.215679 13.654569 16.238143 1 55
1 17.191813 1.263578 7.654550 1 56
1 16.241841 11.305235 0.642508 1 57
1 3.338510 11.407826 14.906850 1 58
1 17.052353 3.522499 6.342434 1 59
1 14.292327 10.726550 2.291119 1 60
1 1.414454 10.753873 13.256908 1 61
1 18.952722 4.187131 4.671277 1 62
1 12.268042 12.384138 2.464914 1 63
1 -0.648421 12.362999 13.054866 1 64
1 21.018916 2.586911 4.440418 1 65
1 12.317195 14.598539 1.069472 1 66
1 -0.668687 14.597116 14.421991 1 67
1 21.060583 0.340256 5.790828 1 68
1 -0.823395 2.970546 11.300172 1 69
1 12.148543 3.047654 4.147994 1 70
1 8.283461 11.939553 12.749982 1 71
1 -0.130017 4.979148 9.756826 1 72
1 12.807980 5.010940 5.761298 1 73
1 7.597493 9.941180 14.312989 1 74

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 1  -1.861463   6.913244   9.291799 1   75
 1  11.056321   6.917858   6.249606 1   76
 1   9.333764   8.010300  14.772621 1   77
 1  21.683082   6.804522  10.423987 1   78
 1   8.703126   6.826312   5.108016 1   79
 1  11.687334   8.103971  13.632184 1   80
 1  21.134656   4.798776  12.025860 1   81
 1   8.177774   4.855100   3.457461 1   82
 1  12.239224  10.109784  12.032455 1   83
 2  17.675721  14.011544  15.022356 1   84
 2   4.690413  14.171424   0.488252 1   85
 2  15.734289   0.743422   8.994782 1   86
 2  14.372893   9.008210   3.392016 1   87
 2   1.534469   9.025137  12.182030 1   88
 2  18.808716   5.918085   3.600934 1   89
 2  10.653474  12.009565   3.666672 1   90
 2  -2.240083  11.945329  11.837335 1   91
 2  22.613027   3.039252   3.238850 1   92
 2  10.766105  15.943489   1.141488 1   93
 2  -2.245246  15.910403  14.309995 1   94
 2  15.043903  18.137639   5.658313 1   95
 2   0.437418   1.394427  11.670778 1   96
 2  13.428911   1.493189   3.747455 1   97
 2   7.020698  13.511610  12.361146 1   98
 2  -1.327369   8.480674   8.096358 1   99
 2  11.568654   8.455451   7.486862 1  100
 2   8.810103   6.461314  15.994713 1  101
 2  20.298068   8.286948  10.102218 1  102
 2   7.311356   8.294546   5.469470 1  103
 2  13.069207   6.618466  13.954295 1  104
 2  19.349400   4.661260  13.029611 1  105
 2   6.392915   4.729335   2.451010 1  106
 2  14.018087  10.234852  11.013715 1  107
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