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1 TODO Write up fitting and optimisation

- Used Genetic Algorithm and CMAES.
- Add in quantities to fit to.
- Realised that the prismatic fault was not high enough.

This caused incredibly large dissociation along the prismatic plane for a screw dislocation.

This was unreasonable, and it has been assumed that this can be rectified by a short ranged, very quickly decaying power law added to the pair potential.

Although this means that we need a refitting of the pair potential.

Unfortunately it seems that the accordance with the DFT results of the correct energetic ordering of the phases is lost: omega phase is **not** lower in energy than that of the hcp phase.

1.1 Reasonable starting point is:

```
PARAMETERS b2=60204900.7590034157 m2=-13.7544131202 p2=0.0000000000
fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849
b0=49.7557565400 p0=1.1050685730 b1=-5.097 3416100 p1=0.6991977165
ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000
redd=10.0000000000 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18
VARGS -vb2=60204900.7590034157 -vm2=-13.7544131202 -vp2=0.0000000000
-vfdd=0.2648249504 -vqdds=0.5697753882 -vqddp=0.5648597117 -vqddd=0.8213593849
-vb0=49.7557565400 -vp0=1. 1050685730 -vb1=-5.0973416100 -vp1=0.6991977165
-vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.2217589360 -vr1dd=6.5000000000
-vrcdd=10.0000000000 -vcr3=-1.1418272350 -vrma xhm=10.1000000000
```

Quantity predicted target norm_{pred} norm_{tar} sq diff. weight objective *
100²

```
ahcp : 5.69823736 5.57678969 5.69823736 5.57678969 0.01474954 1000.00000000
147495.36 c/a : 1.57540221 1.58731122 15.29618259 15.41181168 0.01337009
100.00000000 13370.09 aomega : 9.11713244 8.73254342 1.13964156 1.09156793
0.00231107 10.00000000 231.11 comega : 5.50357270 5.32343103 0.68794659
0.66542888 0.00050705 10.00000000 50.70 a4h : 5.68949374 5.56325146 1.02269218
1.00000000 0.00051493 1.00000000 5.15 c4h : 18.46292975 17.75908031 1.03963321
1.00000000 0.00157079 1.00000000 15.71 a6h : 5.68593900 5.54639384 1.02515962
1.00000000 0.00063301 1.00000000 6.33 c6h : 27.74967218 26.77136353 1.03654310
1.00000000 0.00133540 1.00000000 13.35 abcc : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 afcc : 8.03310655 7.88677000 1.14758665
1.12668143 0.00043703 1.00000000 4.37 DE(o,h) : 1.19189500 -0.63343333
0.07945967 -0.04222889 0.01480810 3000.00000000 444243.14 DE(4h,h): 1.83337000
3.17160000 0.00733348 0.01268640 0.00002865 2000.00000000 573.08 DE(6h,h):
2.75695000 3.72005000 0.01102780 0.01488020 0.00001484 2000.00000000 296.82
DE(b,h) : 9.39020500 7.63520000 0.09485056 0.07712323 0.00031426 1.00000000
3.14 DE(f,h) : 4.17199500 4.51880000 0.04214136 0.04564444 0.00001227
2000.00000000 245.43 c11 : 211.10292175 176.10000000 0.92212869 0.76923077
0.02337778 100.00000000 23377.78 c33 : 232.93926611 190.50000000 0.94059869
0.76923077 0.02936697 100.00000000 29366.97 c44 : 55.49057353 50.80000000
0.84025702 0.76923077 0.00504473 100.00000000 5044.73 c12 : 110.56430372
```

86.90000000 0.97870500 0.76923077 0.04387945 100.00000000 43879.45 c_{13}
: 73.53441848 68.30000000 0.82818356 0.76923077 0.00347543 10.00000000
347.54 $M_{\text{freq}0}$: 2.86541811 2.85858719 0.20883117 0.20833333 0.00000025
0.10000000 0.00 $M_{\text{freq}1}$: 2.86541812 2.85858719 0.20883117 0.20833333 0.00000025
0.10000000 0.00 $M_{\text{freq}2}$: 2.86541812 2.85858719 0.20883117 0.20833333 0.00000025
0.10000000 0.00 $M_{\text{freq}3}$: 2.86541813 2.85858719 0.20883117 0.20833333 0.00000025
0.10000000 0.00 $M_{\text{freq}4}$: 6.16074486 5.66706047 0.22648223 0.20833333 0.00032938
0.10000000 0.33 $M_{\text{freq}5}$: 6.16074486 5.66706047 0.22648223 0.20833333 0.00032938
0.10000000 0.33 $H_{\text{freq}0}$: 4.29880135 4.80643423 0.18633015 0.20833333 0.00048414
0.10000000 0.48 $H_{\text{freq}1}$: 4.29880135 5.58010025 0.16049597 0.20833333 0.00228841
0.10000000 2.29 $H_{\text{freq}2}$: 6.76073943 5.65316738 0.24915013 0.20833333 0.00166601
0.10000000 1.67 $H_{\text{freq}3}$: 6.76073943 6.36651842 0.22123354 0.20833333 0.00016642
0.10000000 0.17 $H_{\text{freq}4}$: 8.32761036 6.40050186 0.27105981 0.20833333 0.00393461
0.10000000 3.93 $H_{\text{freq}5}$: 8.32761036 7.64082373 0.22705913 0.20833333 0.00035066
0.10000000 0.35 bandw. G: 4.58784139 5.87085872 1.30243337 1.66666667
0.13266589 15.00000000 19899.88 bandw. K: 5.68718179 4.97424321 1.03938731
0.90909091 0.01697715 15.00000000 2546.57 bandw. M: 6.52257165 7.78109872
1.39709740 1.66666667 0.07266759 15.00000000 10900.14 bandw. L: 5.25996287
6.34433701 1.38179999 1.66666667 0.08114903 15.00000000 12172.35 bandw.
H: 4.39872218 9.70902614 0.41186812 0.90909091 0.24723050 5.00000000 12361.53
DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
0.00 DOSerr_c: 95.30342229 0.00000000 95.30342229 0.00000000 9082.74230017
0.00000000 0.00 E_{prisf}: 119.59113352 220.00000000 119.59113352 220.00000000
10081.94046857 100000.00000000 10081940468565.85

PARAMETERS b2=73362700.7877650857 m2=-13.9508390550 p2=0.0000000000
fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849
b0=49.7557565400 p0=1.1050685730 b1=-5.097 3416100 p1=0.6991977165
ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000
redd=10.0000000000 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18
VARGS -vb2=73362700.7877650857 -vm2=-13.9508390550 -vp2=0.0000000000
-vfdd=0.2648249504 -vqdds=0.5697753882 -vqddp=0.5648597117 -vqddd=0.8213593849
-vb0=49.7557565400 -vp0=1. 1050685730 -vb1=-5.0973416100 -vp1=0.6991977165
-vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.2217589360 -vr1dd=6.5000000000
-vrcdd=10.0000000000 -vcr3=-1.1418272350 -vrma xhm=10.1000000000

Quantity predicted target norm_{pred} norm_{tar} sq diff. weight objective *
100²

a_{hcp} : 5.68326063 5.57678969 5.68326063 5.57678969 0.01133606 1000.00000000
113360.60 c/a : 1.58164523 1.58731122 15.35679851 15.41181168 0.00302645
100.00000000 3026.45 a_{omega} : 9.09093887 8.73254342 1.13636736 1.09156793

0.00200699 10.00000000 200.70 c_{omega} : 5.49075443 5.32343103 0.68634430
 0.66542888 0.00043745 10.00000000 43.75 a_{4h} : 5.67495771 5.56325146 1.02007931
 1.00000000 0.00040318 1.00000000 4.03 c_{4h} : 18.41194892 17.75908031 1.03676252
 1.00000000 0.00135148 1.00000000 13.51 a_{6h} : 5.67118026 5.54639384 1.02249866
 1.00000000 0.00050619 1.00000000 5.06 c_{6h} : 27.67479817 26.77136353 1.03374631
 1.00000000 0.00113881 1.00000000 11.39 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 8.01192626 7.88677000 1.14456089
 1.12668143 0.00031968 1.00000000 3.20 DE(o,h) : 1.09675833 -0.63343333
 0.07311722 -0.04222889 0.01330473 3000.00000000 399141.76 DE(4h,h): 1.84836500
 3.17160000 0.00739346 0.01268640 0.00002802 2000.00000000 560.30 DE(6h,h):
 2.77866667 3.72005000 0.01111467 0.01488020 0.00001418 2000.00000000 283.58
 DE(b,h) : 8.85897500 7.63520000 0.08948460 0.07712323 0.00015280 1.00000000
 1.53 DE(f,h) : 4.20064500 4.51880000 0.04243076 0.04564444 0.00001033
 2000.00000000 206.56 c_{11} : 209.98522208 176.10000000 0.91724642 0.76923077
 0.02190863 100.00000000 21908.63 c_{33} : 232.98310764 190.50000000 0.94077572
 0.76923077 0.02942767 100.00000000 29427.67 c_{44} : 54.68686450 50.80000000
 0.82808699 0.76923077 0.00346405 100.00000000 3464.05 c_{12} : 109.06955946
 86.90000000 0.96547366 0.76923077 0.03851127 100.00000000 38511.27 c_{13}
 : 73.74195452 68.30000000 0.83052094 0.76923077 0.00375649 10.00000000
 375.65 M_{freq0} : 2.85519402 2.85858719 0.20808604 0.20833333 0.00000006
 0.10000000 0.00 M_{freq1} : 2.85519403 2.85858719 0.20808604 0.20833333 0.00000006
 0.10000000 0.00 M_{freq2} : 2.85519403 2.85858719 0.20808604 0.20833333 0.00000006
 0.10000000 0.00 M_{freq3} : 2.85519404 2.85858719 0.20808604 0.20833333 0.00000006
 0.10000000 0.00 M_{freq4} : 6.14081288 5.66706047 0.22574949 0.20833333 0.00030332
 0.10000000 0.30 M_{freq5} : 6.14081288 5.66706047 0.22574949 0.20833333 0.00030332
 0.10000000 0.30 H_{freq0} : 4.24870561 4.80643423 0.18415877 0.20833333 0.00058441
 0.10000000 0.58 H_{freq1} : 4.24870561 5.58010025 0.15862565 0.20833333 0.00247085
 0.10000000 2.47 H_{freq2} : 6.73808691 5.65316738 0.24831533 0.20833333 0.00159856
 0.10000000 1.60 H_{freq3} : 6.73808691 6.36651842 0.22049227 0.20833333 0.00014784
 0.10000000 0.15 H_{freq4} : 8.32193375 6.40050186 0.27087504 0.20833333 0.00391147
 0.10000000 3.91 H_{freq5} : 8.32193375 7.64082373 0.22690436 0.20833333 0.00034488
 0.10000000 0.34 bandw. G: 4.63954304 5.87085872 1.31711085 1.66666667
 0.12218927 15.00000000 18328.39 bandw. K: 5.74840743 4.97424321 1.05057689
 0.90909091 0.02001828 15.00000000 3002.74 bandw. M: 6.57699445 7.78109872
 1.40875444 1.66666667 0.06651871 15.00000000 9977.81 bandw. L: 5.31166452
 6.34433701 1.39538209 1.66666667 0.07359532 15.00000000 11039.30 bandw.
 H: 4.44226042 9.70902614 0.41594476 0.90909091 0.24319312 5.00000000 12159.66
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 98.57124703 0.00000000 98.57124703 0.00000000 9716.29074056
 0.00000000 0.00 E_{prisf}: 119.88060210 220.00000000 119.88060210 220.00000000

10023.89383558 100000.00000000 10023893835581.32
b2=91394018.8920019716 m2=-14.4689417704 p2=0.0000000000 fdd=0.2648249504
qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=49.7557565400
p0=1.1050685730 b1=-5.097 3416100 p1=0.6991977165 ndt=2.0000000000
cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000
cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18 VARGS -vb2=91394018.8920019716
-vm2=-14.4689417704 -vp2=0.0000000000 -vfdd=0.2648249504 -vqdds=0.5697753882
-vqddp=0.5648597117 -vqddd=0.8213593849 -vb0=49.7557565400 -vp0=1.
1050685730 -vb1=-5.0973416100 -vp1=0.6991977165 -vndt=2.0000000000 -
vcr1=-6.0000000000 -vcr2=3.2217589360 -vr1dd=6.5000000000 -vrccd=10.0000000000
-vcr3=-1.1418272350 -vrma xhm=10.1000000000

Quantity predicted target norm_{pred} norm_{tar} sq diff. weight objective *
100²

a_{hcp} : 5.62525983 5.57678969 5.62525983 5.57678969 0.00234935 1000.00000000
23493.55 c/a : 1.60613643 1.58731122 15.59459288 15.41181168 0.03340896
100.00000000 33408.96 a_{omega} : 8.98530887 8.73254342 1.12316361 1.09156793
0.00099829 10.00000000 99.83 c_{omega} : 5.44549052 5.32343103 0.68068632
0.66542888 0.00023279 10.00000000 23.28 a_{4h} : 5.61807095 5.56325146 1.00985386
1.00000000 0.00009710 1.00000000 0.97 c_{4h} : 18.21768083 17.75908031 1.02582344
1.00000000 0.00066685 1.00000000 6.67 a_{6h} : 5.61365761 5.54639384 1.01212748
1.00000000 0.00014708 1.00000000 1.47 c_{6h} : 27.38802263 26.77136353 1.02303428
1.00000000 0.00053058 1.00000000 5.31 a_{bcc} : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.93028587 7.88677000 1.13289798
1.12668143 0.00003865 1.00000000 0.39 DE(o,h) : 0.56552167 -0.63343333
0.03770144 -0.04222889 0.00638886 3000.00000000 191665.75 DE(4h,h): 1.90610750
3.17160000 0.00762443 0.01268640 0.00002562 2000.00000000 512.47 DE(6h,h):
2.86158833 3.72005000 0.01144635 0.01488020 0.00001179 2000.00000000 235.83
DE(b,h) : 7.52522500 7.63520000 0.07601237 0.07712323 0.00000123 1.00000000
0.01 DE(f,h) : 4.31089500 4.51880000 0.04354439 0.04564444 0.00000441
2000.00000000 88.20 c₁₁ : 199.90553801 176.10000000 0.87321687 0.76923077
0.01081311 100.00000000 10813.11 c₃₃ : 226.98933014 190.50000000 0.91657311
0.76923077 0.02170976 100.00000000 21709.76 c₄₄ : 52.69685443 50.80000000
0.79795358 0.76923077 0.00082500 100.00000000 825.00 c₁₂ : 98.48673287
86.90000000 0.87179546 0.76923077 0.01051952 100.00000000 10519.52 c₁₃
: 72.19938307 68.30000000 0.81314769 0.76923077 0.00192870 10.00000000
192.87 M_{freq0}: 2.78990046 2.85858719 0.20332746 0.20833333 0.00002506
0.10000000 0.03 M_{freq1}: 2.78990047 2.85858719 0.20332746 0.20833333 0.00002506
0.10000000 0.03 M_{freq2}: 2.78990047 2.85858719 0.20332746 0.20833333 0.00002506
0.10000000 0.03 M_{freq3}: 2.78990048 2.85858719 0.20332746 0.20833333 0.00002506

0.10000000 0.03 M_{freq4}: 6.00974100 5.66706047 0.22093101 0.20833333 0.00015870
 0.10000000 0.16 M_{freq5}: 6.00974100 5.66706047 0.22093101 0.20833333 0.00015870
 0.10000000 0.16 H_{freq0}: 3.99826489 4.80643423 0.17330350 0.20833333 0.00122709
 0.10000000 1.23 H_{freq1}: 3.99826489 5.58010025 0.14927543 0.20833333 0.00348784
 0.10000000 3.49 H_{freq2}: 6.58970446 5.65316738 0.24284706 0.20833333 0.00119120
 0.10000000 1.19 H_{freq3}: 6.58970446 6.36651842 0.21563671 0.20833333 0.00005334
 0.10000000 0.05 H_{freq4}: 8.23482251 6.40050186 0.26803961 0.20833333 0.00356484
 0.10000000 3.56 H_{freq5}: 8.23482251 7.64082373 0.22452920 0.20833333 0.00026231
 0.10000000 0.26 bandw. G: 4.85043136 5.87085872 1.37697953 1.66666667
 0.08391864 15.00000000 12587.80 bandw. K: 5.99194943 4.97424321 1.09508653
 0.90909091 0.03459437 15.00000000 5189.16 bandw. M: 6.79332504 7.78109872
 1.45509122 1.66666667 0.04476417 15.00000000 6714.63 bandw. L: 5.51847114
 6.34433701 1.44971049 1.66666667 0.04706998 15.00000000 7060.50 bandw.
 H: 4.61097107 9.70902614 0.43174174 0.90909091 0.22786222 5.00000000 11393.11
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 111.68287062 0.00000000 111.68287062 0.00000000 12473.06358905
 0.00000000 0.00 E_{prisf}: 105.39637060 220.00000000 105.39637060 220.00000000
 13133.99187172 100000.00000000 13133991871718.04

PARAMETERS b2=901772799.4098891020 m2=-15.7042290440 p2=0.0000000000
 fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849
 b0=47.9215925588 p0=1.1092837121 b1=-3.99 59790920 p1=0.6574344463
 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000
 rcdd=10.0000000000 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18
 VARGS -vb2=901772799.4098891020 -vm2=-15.7042290440 -vp2=0.0000000000
 -vfdd=0.2648249504 -vqdds=0.5697753882 -vqddp=0.5648597117 -vqddd=0.8213593849
 -vb0=47.9215925588 -vp0=1.1092837121 -vb1=-3.9959790920 -vp1=0.6574344463
 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.2217589360 -vr1dd=6.5000000000
 -vrdd=10.0000000000 -vcr3=-1.1418272350 -vrm axhm=10.1000000000

Quantity predicted target norm_{pred} norm_{tar} sq diff. weight objective *
 100²

a_{hcp} : 5.58632034 5.57678969 5.58632034 5.57678969 0.00009083 1000.00000000
 908.33 c/a : 1.58324912 1.58731122 15.37237127 15.41181168 0.00155555
 100.00000000 1555.55 a_{omega} : 8.94268260 8.73254342 1.11783533 1.09156793
 0.00068998 10.00000000 69.00 c_{omega} : 5.41189311 5.32343103 0.67648664
 0.66542888 0.00012227 10.00000000 12.23 a_{4h} : 5.57986672 5.56325146 1.00298661
 1.00000000 0.00000892 1.00000000 0.09 c_{4h} : 18.08926296 17.75908031 1.01859233
 1.00000000 0.00034567 1.00000000 3.46 a_{6h} : 5.57525690 5.54639384 1.00520393
 1.00000000 0.00002708 1.00000000 0.27 c_{6h} : 27.19488908 26.77136353 1.01582010
 1.00000000 0.00025028 1.00000000 2.50 a_{bcc} : 6.20079768 6.17948863 0.88582824

0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.87598731 7.88677000 1.12514104
 1.12668143 0.00000237 1.00000000 0.02 DE(o,h) : 1.34781000 -0.63343333
 0.08985400 -0.04222889 0.01744589 3000.00000000 523376.69 DE(4h,h): 2.01890750
 3.17160000 0.00807563 0.01268640 0.00002126 2000.00000000 425.18 DE(6h,h):
 3.01372500 3.72005000 0.01205490 0.01488020 0.00000798 2000.00000000 159.65
 DE(b,h) : 7.98701000 7.63520000 0.08067687 0.07712323 0.00001263 1.00000000
 0.13 DE(f,h) : 4.52676000 4.51880000 0.04572485 0.04564444 0.00000001
 2000.00000000 0.13 c₁₁ : 221.16376396 176.10000000 0.96607594 0.76923077
 0.03874802 100.00000000 38748.02 c₃₃ : 262.04112894 190.50000000 1.05811076
 0.76923077 0.08345165 100.00000000 83451.65 c₄₄ : 61.54190626 50.80000000
 0.93188834 0.76923077 0.02645749 100.00000000 26457.49 c₁₂ : 103.69257328
 86.90000000 0.91787708 0.76923077 0.02209572 100.00000000 22095.72 c₁₃
 : 80.66574593 68.30000000 0.90850035 0.76923077 0.01939602 10.00000000
 1939.60 M_{freq0}: 3.01657581 2.85858719 0.21984752 0.20833333 0.00013258
 0.10000000 0.13 M_{freq1}: 3.01657582 2.85858719 0.21984752 0.20833333 0.00013258
 0.10000000 0.13 M_{freq2}: 3.01657582 2.85858719 0.21984752 0.20833333 0.00013258
 0.10000000 0.13 M_{freq3}: 3.01657583 2.85858719 0.21984752 0.20833333 0.00013258
 0.10000000 0.13 M_{freq4}: 6.55202353 5.66706047 0.24086648 0.20833333 0.00105841
 0.10000000 1.06 M_{freq5}: 6.55202353 5.66706047 0.24086648 0.20833333 0.00105841
 0.10000000 1.06 H_{freq0}: 4.22631935 4.80643423 0.18318844 0.20833333 0.00063227
 0.10000000 0.63 H_{freq1}: 4.22631935 5.58010025 0.15778985 0.20833333 0.00255464
 0.10000000 2.55 H_{freq2}: 7.21414462 5.65316738 0.26585924 0.20833333 0.00330923
 0.10000000 3.31 H_{freq3}: 7.21414462 6.36651842 0.23607044 0.20833333 0.00076935
 0.10000000 0.77 H_{freq4}: 8.98961736 6.40050186 0.29260783 0.20833333 0.00710219
 0.10000000 7.10 H_{freq5}: 8.98961736 7.64082373 0.24510930 0.20833333 0.00135247
 0.10000000 1.35 bandw. G: 4.99873347 5.87085872 1.41908073 1.66666667
 0.06129880 15.00000000 9194.82 bandw. K: 6.15929951 4.97424321 1.12567138
 0.90909091 0.04690710 15.00000000 7036.06 bandw. M: 6.94162715 7.78109872
 1.48685668 1.66666667 0.03233163 15.00000000 4849.74 bandw. L: 5.69262407
 6.34433701 1.49546072 1.66666667 0.02931148 15.00000000 4396.72 bandw.
 H: 4.72525894 9.70902614 0.44244293 0.90909091 0.21776034 5.00000000 10888.02
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 93.81903067 0.00000000 93.81903067 0.00000000 8802.01051603
 0.00000000 0.00 E_{prisf}: 121.13361833 220.00000000 121.13361833 220.00000000
 9774.56142366 1.00000000 97745614.24

PARAMETERS b2=999299811.2360876799 m2=-15.0812332826 p2=0.0000000000
 fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849
 b0=47.4028718523 p0=1.1110171622 b1=-4.0276308878 p1=0.6595005412 ndt=2.0000000000
 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000
 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18 VARGS -vb2=999299811.2360876799

-vm2=-15.0812332826 -vp2=0.0000000000 -vfdd=0.2648249504 -vqdds=0.5697753882
-vqddp=0.5648597117 -vqddd=0.8213593849 -vb0=47.4028718523 -vp0=1 .1110171622
-vb1=-4.0276308878 -vp1=0.6595005412 -vndt=2.0000000000 -vcr1=-6.0000000000
-vcr2=3.2217589360 -vr1dd=6.5000000000 -vrdd=10.0000000000 -vcr3=-1.1418272350
-vrm axhm=10.1000000000

b2=652671393.2498187 m2=-15.0812332826 p2=0.0000000000 fdd=0.24600988946160712
qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=41.05771937127483
p0=1.1110171622 b1=-3.698308573780551 p1=0.6595005412 ndt=2.0000000000
cr1=-6.0000000000 cr2=3.22380803 r1dd=6.37 rcdd=9.87 cr3=-1.10526908
rmaxhm=9.88 npar=18

Quantity predicted target norm_{pred} norm_{tar} sq diff. weight objective *
100²

a_{hcp} : 5.70613418 5.57678969 5.70613418 5.57678969 0.01673000 1000.00000000
167299.96 c/a : 1.57212363 1.58731122 15.26434959 15.41181168 0.02174507
100.00000000 21745.07 a_{omega} : 9.16691334 8.73254342 1.14586417 1.09156793
0.00294808 10.00000000 294.81 c_{omega} : 5.50859785 5.32343103 0.68857473
0.66542888 0.00053573 10.00000000 53.57 a_{4h} : 5.69646904 5.56325146 1.02394599
1.00000000 0.00057341 1.00000000 5.73 c_{4h} : 18.49515166 17.75908031 1.04144761
1.00000000 0.00171790 1.00000000 17.18 a_{6h} : 5.69332284 5.54639384 1.02649091
1.00000000 0.00070177 1.00000000 7.02 c_{6h} : 27.79206990 26.77136353 1.03812680
1.00000000 0.00145365 1.00000000 14.54 a_{bcc} : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 8.04427434 7.88677000 1.14918205
1.12668143 0.00050628 1.00000000 5.06 DE(o,h) : 3.32247167 -0.63343333
0.22149811 -0.04222889 0.06955193 3000.00000000 2086557.92 DE(4h,h): 1.86745000
3.17160000 0.00746980 0.01268640 0.00002721 2000.00000000 544.26 DE(6h,h):
2.80055333 3.72005000 0.01120221 0.01488020 0.00001353 2000.00000000 270.55
DE(b,h) : 11.65659500 7.63520000 0.11774338 0.07712323 0.00165000 1.00000000
16.50 DE(f,h) : 4.23754500 4.51880000 0.04280348 0.04564444 0.00000807
2000.00000000 161.42 c₁₁ : 256.25825401 176.10000000 1.11937384 0.76923077
0.12260017 100.00000000 122600.17 c₃₃ : 285.11928542 190.50000000 1.15129936
0.76923077 0.14597640 100.00000000 145976.40 c₄₄ : 69.13492938 50.80000000
1.04686447 0.76923077 0.07708047 100.00000000 77080.47 c₁₂ : 132.18803667
86.90000000 1.17011628 0.76923077 0.16070920 100.00000000 160709.20 c₁₃
: 85.78433896 68.30000000 0.96614865 0.76923077 0.03877665 10.00000000
3877.67 M_{freq0}: 3.29251267 2.85858719 0.23995775 0.20833333 0.00100010
0.10000000 1.00 M_{freq1}: 3.29251269 2.85858719 0.23995775 0.20833333 0.00100010
0.10000000 1.00 M_{freq2}: 3.29251269 2.85858719 0.23995775 0.20833333 0.00100010
0.10000000 1.00 M_{freq3}: 3.29251270 2.85858719 0.23995775 0.20833333 0.00100010
0.10000000 1.00 M_{freq4}: 7.05767677 5.66706047 0.25945538 0.20833333 0.00261346

0.10000000 2.61 M_{freq5} : 7.05767677 5.66706047 0.25945538 0.20833333 0.00261346
 0.10000000 2.61 H_{freq0} : 4.96582422 4.80643423 0.21524204 0.20833333 0.00004773
 0.10000000 0.05 H_{freq1} : 4.96582422 5.58010025 0.18539931 0.20833333 0.00052597
 0.10000000 0.53 H_{freq2} : 7.78709460 5.65316738 0.28697388 0.20833333 0.00618434
 0.10000000 6.18 H_{freq3} : 7.78709460 6.36651842 0.25481924 0.20833333 0.00216094
 0.10000000 2.16 H_{freq4} : 9.46161176 6.40050186 0.30797102 0.20833333 0.00992767
 0.10000000 9.93 H_{freq5} : 9.46161176 7.64082373 0.25797861 0.20833333 0.00246465
 0.10000000 2.46 bandw. G: 4.56062999 5.87085872 1.29470838 1.66666667
 0.13835297 15.00000000 20752.94 bandw. K: 5.65452812 4.97424321 1.03341954
 0.90909091 0.01545761 15.00000000 2318.64 bandw. M: 6.49399969 7.78109872
 1.39097744 1.66666667 0.07600455 15.00000000 11400.68 bandw. L: 5.23275148
 6.34433701 1.37465151 1.66666667 0.08527285 15.00000000 12790.93 bandw.
 H: 4.37695307 9.70902614 0.40982980 0.90909091 0.24926165 5.00000000 12463.08
 DOSerr_h : 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o : 79.18263924 0.00000000 79.18263924 0.00000000 6269.89035742
 0.00000000 0.00 E_{prisf} : 216.93072664 220.00000000 216.93072664 220.00000000
 9.42043896 0.01000000 942.04
 fdd=0.2190266935 qdds=0.5572087651 qddp=0.5381815801 qddd=0.6434459902
 b0=114.9100355472 p0=1.5292737725 b1=-1.5098252002 p1=1.1777650147
 b2=0.0000000000 m2=-12.0000000000 p2=0.0000000000 ndt=2.0000000000
 cr1=-6.0000000000 cr2=3.9979719633 cr3=-0.9045369332 r1dd=5.8500000000
 rcdd=8.3500000000 rmaxhm=8.4335000000 npar=18

a_{hcp} : 5.47876018 5.57678969 5.47876018 5.57678969 0.00960978 1000.00000000
 96097.84 c/a : 1.62991301 1.58731122 15.82544878 15.41181168 0.17109564
 100.00000000 171095.64 a_{omega} : 8.63155804 8.73254342 1.07894475 1.09156793
 0.00015934 10.00000000 15.93 c_{omega} : 5.36018127 5.32343103 0.67002266
 0.66542888 0.00002110 10.00000000 2.11 a_{4h} : 5.47852076 5.56325146 0.98476957
 1.00000000 0.00023197 1.00000000 2.32 c_{4h} : 17.63579650 17.75908031 0.99305798
 1.00000000 0.00004819 1.00000000 0.48 a_{6h} : 5.46932156 5.54639384 0.98610407
 1.00000000 0.00019310 1.00000000 1.93 c_{6h} : 26.56143981 26.77136353 0.99215865
 1.00000000 0.00006149 1.00000000 0.61 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.71193633 7.88677000 1.10170519
 1.12668143 0.00062381 1.00000000 6.24 $\text{DE}(o,h)$: 1.61649333 -0.63343333
 0.10776622 -0.04222889 0.02249853 3000.00000000 674956.00 $\text{DE}(4h,h)$: 0.92534000
 3.17160000 0.00370136 0.01268640 0.00008073 2000.00000000 1614.62 $\text{DE}(6h,h)$:
 2.10467833 3.72005000 0.00841871 0.01488020 0.00004175 2000.00000000 835.02
 $\text{DE}(b,h)$: 9.73094000 7.63520000 0.09829232 0.07712323 0.00044813 1.00000000
 4.48 $\text{DE}(f,h)$: 4.09731000 4.51880000 0.04138697 0.04564444 0.00001813
 2000.00000000 362.52 c_{11} : 168.12165612 176.10000000 0.73438019 0.76923077

0.00121456 100.00000000 1214.56 c_{33} : 179.76089644 190.50000000 0.72586673
 0.76923077 0.00188044 100.00000000 1880.44 c_{44} : 46.67844234 50.80000000
 0.70682075 0.76923077 0.00389501 100.00000000 3895.01 c_{12} : 53.67757565
 86.90000000 0.47514894 0.76923077 0.08648412 100.00000000 86484.12 c_{13}
 : 47.93463367 68.30000000 0.53986523 0.76923077 0.05260855 10.00000000
 5260.86 $M_{\text{freq}0}$: 2.62512088 2.85858719 0.19131835 0.20833333 0.00028951
 0.10000000 0.29 $M_{\text{freq}1}$: 2.62512089 2.85858719 0.19131835 0.20833333 0.00028951
 0.10000000 0.29 $M_{\text{freq}2}$: 2.62512089 2.85858719 0.19131835 0.20833333 0.00028951
 0.10000000 0.29 $M_{\text{freq}3}$: 2.62512090 2.85858719 0.19131835 0.20833333 0.00028951
 0.10000000 0.29 $M_{\text{freq}4}$: 4.51284044 5.66706047 0.16590172 0.20833333 0.00180044
 0.10000000 1.80 $M_{\text{freq}5}$: 4.51284044 5.66706047 0.16590172 0.20833333 0.00180044
 0.10000000 1.80 $H_{\text{freq}0}$: 3.21166322 4.80643423 0.13920850 0.20833333 0.00477824
 0.10000000 4.78 $H_{\text{freq}1}$: 3.21166322 5.58010025 0.11990761 0.20833333 0.00781911
 0.10000000 7.82 $H_{\text{freq}2}$: 3.88331804 5.65316738 0.14310997 0.20833333 0.00425409
 0.10000000 4.25 $H_{\text{freq}3}$: 3.88331804 6.36651842 0.12707488 0.20833333 0.00660294
 0.10000000 6.60 $H_{\text{freq}4}$: 5.53372345 6.40050186 0.18012010 0.20833333 0.00079599
 0.10000000 0.80 $H_{\text{freq}5}$: 5.53372345 7.64082373 0.15088151 0.20833333 0.00330071
 0.10000000 3.30 bandw. G: 5.06404082 5.87085872 1.43762070 1.66666667
 0.05246205 15.00000000 7869.31 bandw. K: 5.84092618 4.97424321 1.06748558
 0.90909091 0.02508887 15.00000000 3763.33 bandw. M: 7.52803274 7.78109872
 1.61246139 1.66666667 0.00293821 15.00000000 440.73 bandw. L: 5.92936322
 6.34433701 1.55765244 1.66666667 0.01188410 15.00000000 1782.62 bandw.
 H: 4.64770646 9.70902614 0.43518141 0.90909091 0.22459021 1.00000000 2245.90
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 2.76808960 0.00000000 2.76808960 0.00000000 7.66232003
 0.00000000 0.00 E_{prisf}: 80.96885878 220.00000000 80.96885878 220.00000000
 19329.65822763 0.00100000 193296.58

PARAMETERS b2=883425978.8605744839 m2=-15.9116989631 p2=0.0000000000
 fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849
 b0=48.9271746890 p0=1.1172295299 b1=-3.80 34356258 p1=0.6525724680
 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000
 rcdd=10.0000000000 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18
 VARGS -vb2=883425978.8605744839 -vm2=-15.9116989631 -vp2=0.0000000000
 -vfdd=0.2648249504 -vqdds=0.5697753882 -vqddp=0.5648597117 -vqddd=0.8213593849
 -vb0=48.9271746890 -vp0=1.1172295299 -vb1=-3.8034356258 -vp1=0.6525724680
 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.2217589360 -vr1dd=6.5000000000
 -vrccd=10.0000000000 -vcr3=-1.1418272350 -vrm axhm=10.1000000000

Quantity predicted target norm_{pred} norm_{tar} sq diff. weight objective *
 100²

a_{hcp} : 5.55915799 5.57678969 5.55915799 5.57678969 0.00031088 1000.00000000
3108.77 c/a : 1.59486281 1.58731122 15.48513296 15.41181168 0.00537601
100.00000000 5376.01 a_{omega} : 8.89176293 8.73254342 1.11147037 1.09156793
0.00039611 10.00000000 39.61 c_{omega} : 5.39115562 5.32343103 0.67389445
0.66542888 0.00007167 10.00000000 7.17 $a_{4\text{h}}$: 5.55256003 5.56325146 0.99807820
1.00000000 0.00000369 1.00000000 0.04 $c_{4\text{h}}$: 17.99793925 17.75908031 1.01344996
1.00000000 0.00018090 1.00000000 1.81 $a_{6\text{h}}$: 5.54765195 5.54639384 1.00022683
1.00000000 0.00000005 1.00000000 0.00 $c_{6\text{h}}$: 27.05991164 26.77136353 1.01077824
1.00000000 0.00011617 1.00000000 1.16 a_{bcc} : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.83651495 7.88677000 1.11950214
1.12668143 0.00005154 1.00000000 0.52 DE(o,h) : 1.00654333 -0.63343333
0.06710289 -0.04222889 0.01195344 3000.00000000 358603.13 DE(4h,h) : 2.04859250
3.17160000 0.00819437 0.01268640 0.00002018 2000.00000000 403.57 DE(6h,h) :
3.05533667 3.72005000 0.01222135 0.01488020 0.00000707 2000.00000000 141.39
 DE(b,h) : 8.01955000 7.63520000 0.08100556 0.07712323 0.00001507 1.00000000
0.15 DE(f,h) : 4.58537000 4.51880000 0.04631687 0.04564444 0.00000045
2000.00000000 9.04 c_{11} : 214.45221283 176.10000000 0.93675889 0.76923077
0.02806567 100.00000000 28065.67 c_{33} : 256.78024884 190.50000000 1.03686755
0.76923077 0.07162945 100.00000000 71629.45 c_{44} : 59.46475943 50.80000000
0.90043549 0.76923077 0.01721468 100.00000000 17214.68 c_{12} : 97.32695765
86.90000000 0.86152923 0.76923077 0.00851901 100.00000000 8519.01 c_{13}
: 79.57600099 68.30000000 0.89622706 0.76923077 0.01612806 10.00000000
1612.81 M_{freq0} : 2.97174880 2.85858719 0.21658053 0.20833333 0.00006802
0.10000000 0.07 M_{freq1} : 2.97174881 2.85858719 0.21658053 0.20833333 0.00006802
0.10000000 0.07 M_{freq2} : 2.97174881 2.85858719 0.21658053 0.20833333 0.00006802
0.10000000 0.07 M_{freq3} : 2.97174882 2.85858719 0.21658053 0.20833333 0.00006802
0.10000000 0.07 M_{freq4} : 6.47507794 5.66706047 0.23803779 0.20833333 0.00088235
0.10000000 0.88 M_{freq5} : 6.47507794 5.66706047 0.23803779 0.20833333 0.00088235
0.10000000 0.88 H_{freq0} : 4.07088683 4.80643423 0.17645127 0.20833333 0.00101647
0.10000000 1.02 H_{freq1} : 4.07088683 5.58010025 0.15198677 0.20833333 0.00317494
0.10000000 3.17 H_{freq2} : 7.12197475 5.65316738 0.26246255 0.20833333 0.00292997
0.10000000 2.93 H_{freq3} : 7.12197475 6.36651842 0.23305434 0.20833333 0.00061113
0.10000000 0.61 H_{freq4} : 8.92842683 6.40050186 0.29061611 0.20833333 0.00677045
0.10000000 6.77 H_{freq5} : 8.92842683 7.64082373 0.24344089 0.20833333 0.00123254
0.10000000 1.23 bandw. G : 5.10621848 5.87085872 1.44959444 1.66666667
0.04712035 15.00000000 7068.05 bandw. K : 6.27902966 4.97424321 1.14755321
0.90909091 0.05686427 15.00000000 8529.64 bandw. M : 7.04639103 7.78109872
1.50929650 1.66666667 0.02476537 15.00000000 3714.81 bandw. L : 5.79466681
6.34433701 1.52226750 1.66666667 0.02085112 15.00000000 3127.67 bandw. H : 4.80961427 9.70902614 0.45034142 0.90909091 0.21045109 5.00000000 10522.55

DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
0.00 DOSerr_o: 98.86547597 0.00000000 98.86547597 0.00000000 9774.38233945
0.00000000 0.00 E_{prsf}: 109.76244599 220.00000000 109.76244599 220.00000000
12152.31831491 0.01000000 1215231.83

PARAMETERS b2=905445972.6509201527 m2=-15.9446815961 p2=0.0000000000
fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849
b0=47.7899139676 p0=1.1088003756 b1=-3.93 45715688 p1=0.6568823915
ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000
rcdd=10.0000000000 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18
VARGS -vb2=905445972.6509201527 -vm2=-15.9446815961 -vp2=0.0000000000
-vfdd=0.2648249504 -vqdds=0.5697753882 -vqddp=0.5648597117 -vqddd=0.8213593849
-vb0=47.7899139676 -vp0=1.1088003756 -vb1=-3.9345715688 -vp1=0.6568823915
-vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.2217589360 -vr1dd=6.5000000000
-vrcdd=10.0000000000 -vcr3=-1.1418272350 -vrmaxhm=10.1000000000

Quantity predicted target norm_{pred} norm_{tar} sq diff. weight objective *
100²

a_{hcp} : 5.57461126 5.57678969 5.57461126 5.57678969 0.00000475 1000.00000000
47.46 c/a : 1.58824164 1.58731122 15.42084557 15.41181168 0.00008161 100.00000000
81.61 a_{omega} : 8.91266648 8.73254342 1.11408331 1.09156793 0.00050694
10.00000000 50.69 c_{omega} : 5.40535546 5.32343103 0.67566943 0.66542888
0.00010487 10.00000000 10.49 a_{4h} : 5.56863112 5.56325146 1.00096700 1.00000000
0.00000094 1.00000000 0.01 c_{4h} : 18.04635261 17.75908031 1.01617608 1.00000000
0.00026167 1.00000000 2.62 a_{6h} : 5.56371838 5.54639384 1.00312357 1.00000000
0.00000976 1.00000000 0.10 c_{6h} : 27.13379120 26.77136353 1.01353789 1.00000000
0.00018327 1.00000000 1.83 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409
0.00000927 1.00000000 0.09 a_{fcc} : 7.85904307 7.88677000 1.12272044 1.12668143
0.00001569 1.00000000 0.16 DE(o,h) : 0.75090833 -0.63343333 0.05006056 -
0.04222889 0.00851734 3000.00000000 255520.25 DE(4h,h): 2.02638500 3.17160000
0.00810554 0.01268640 0.00002098 2000.00000000 419.69 DE(6h,h): 3.02486000
3.72005000 0.01209944 0.01488020 0.00000773 2000.00000000 154.65 DE(b,h)
: 7.76340500 7.63520000 0.07841823 0.07712323 0.00000168 1.00000000 0.02
DE(f,h) : 4.54128500 4.51880000 0.04587157 0.04564444 0.00000005 2000.00000000
1.03 c₁₁ : 209.20671277 176.10000000 0.91384577 0.76923077 0.02091350
100.00000000 20913.50 c₃₃ : 248.51083574 190.50000000 1.00347602 0.76923077
0.05487084 100.00000000 54870.84 c₄₄ : 57.70646584 50.80000000 0.87381081
0.76923077 0.01093698 100.00000000 10936.98 c₁₂ : 96.52645635 86.90000000
0.85444327 0.76923077 0.00726117 100.00000000 7261.17 c₁₃ : 77.57509665
68.30000000 0.87369182 0.76923077 0.01091211 10.00000000 1091.21 M_{freq0}:
2.90595602 2.85858719 0.21178557 0.20833333 0.00001192 0.10000000 0.01

M_{freq1} : 2.90595603 2.85858719 0.21178557 0.20833333 0.00001192 0.10000000
 $0.01 M_{\text{freq2}}$: 2.90595603 2.85858719 0.21178557 0.20833333 0.00001192 0.10000000
 $0.01 M_{\text{freq3}}$: 2.90595604 2.85858719 0.21178557 0.20833333 0.00001192 0.10000000
 $0.01 M_{\text{freq4}}$: 6.32257889 5.66706047 0.23243160 0.20833333 0.00058073 0.10000000
 $0.58 M_{\text{freq5}}$: 6.32257889 5.66706047 0.23243160 0.20833333 0.00058073 0.10000000
 $0.58 H_{\text{freq0}}$: 3.99946914 4.80643423 0.17335569 0.20833333 0.00122344 0.10000000
 $1.22 H_{\text{freq1}}$: 3.99946914 5.58010025 0.14932039 0.20833333 0.00348253 0.10000000
 $3.48 H_{\text{freq2}}$: 6.95348945 5.65316738 0.25625345 0.20833333 0.00229634 0.10000000
 $2.30 H_{\text{freq3}}$: 6.95348945 6.36651842 0.22754095 0.20833333 0.00036893 0.10000000
 $0.37 H_{\text{freq4}}$: 8.72200055 6.40050186 0.28389703 0.20833333 0.00570987 0.10000000
 $5.71 H_{\text{freq5}}$: 8.72200055 7.64082373 0.23781251 0.20833333 0.00086902 0.10000000
0.87 bandw. G: 5.04499284 5.87085872 1.43221321 1.66666667 0.05496842
15.00000000 8245.26 bandw. K: 6.21100117 4.97424321 1.13512035 0.90909091
0.05108931 15.00000000 7663.40 bandw. M: 6.98652596 7.78109872 1.49647374
1.66666667 0.02896563 15.00000000 4344.84 bandw. L: 5.73616230 6.34433701
1.50689828 1.66666667 0.02552594 15.00000000 3828.89 bandw. H: 4.76063375
9.70902614 0.44575520 0.90909091 0.21467998 5.00000000 10734.00 DOSerr_h :
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00
 DOSerr_o : 106.23490802 0.00000000 106.23490802 0.00000000 11285.85568098
0.00000000 0.00 E_{prisf} : 94.24578590 220.00000000 94.24578590 220.00000000
15814.12236427 0.01000000 1581412.24

PARAMETERS $b_2=997988120.0035278797$ $m_2=-15.4004196434$ $p_2=0.0000000000$
 $\text{fdd}=0.2648249504$ $\text{qdds}=0.5697753882$ $\text{qddp}=0.5648597117$ $\text{qddd}=0.8213593849$
 $b_0=53.3178751943$ $p_0=1.1084242896$ $b_1=-4.8102743429$ $p_1=0.6630121162$ $\text{ndt}=2.0000000000$
 $\text{cr}_1=-6.0000000000$ $\text{cr}_2=3.2217589360$ $\text{r}_1\text{dd}=6.5000000000$ $\text{rcdd}=10.0000000000$
 $\text{cr}_3=-1.1418272350$ $\text{rmaxhm}=10.1000000000$ $\text{npar}=18$ VARGS - $\text{vb}_2=997988120.0035278797$
- $\text{vm}_2=-15.4004196434$ - $\text{vp}_2=0.0000000000$ - $\text{vfdd}=0.2648249504$ - $\text{vqdds}=0.5697753882$
- $\text{vqddp}=0.5648597117$ - $\text{vqddd}=0.8213593849$ - $\text{vb}_0=53.3178751943$ - $\text{vp}_0=1.1084242896$
- $\text{vb}_1=-4.8102743429$ - $\text{vp}_1=0.6630121162$ - $\text{vndt}=2.0000000000$ - $\text{vcr}_1=-6.0000000000$
- $\text{vcr}_2=3.2217589360$ - $\text{vr}_1\text{dd}=6.5000000000$ - $\text{vrcdd}=10.0000000000$ - $\text{vcr}_3=-1.1418272350$
- $\text{vrmaxhm}=10.1000000000$

Quantity predicted target $\text{norm}_{\text{pred}}$ norm_{tar} sq diff. weight objective *
 100^2

a_{hcp} : 5.63778583 5.57678969 5.63778583 5.57678969 0.00372053 1000.00000000
37205.29 c/a : 1.60080459 1.58731122 15.54282399 15.41181168 0.01716423
100.00000000 17164.23 a_{omega} : 9.04280677 8.73254342 1.13035085 1.09156793
0.00150411 10.00000000 150.41 c_{omega} : 5.44646765 5.32343103 0.68080846
0.66542888 0.00023653 10.00000000 23.65 a_{4h} : 5.63101774 5.56325146 1.01218106
1.00000000 0.00014838 1.00000000 1.48 c_{4h} : 18.26169876 17.75908031 1.02830205

1.00000000 0.00080101 1.00000000 8.01 a_{6h} : 5.62716702 5.54639384 1.01456319
1.00000000 0.00021209 1.00000000 2.12 c_{6h} : 27.45232488 26.77136353 1.02543618
1.00000000 0.00064700 1.00000000 6.47 a_{bcc} : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.94992578 7.88677000 1.13570368
1.12668143 0.00008140 1.00000000 0.81 DE(o,h) : 2.48206667 -0.63343333
0.16547111 -0.04222889 0.04313929 3000.00000000 1294178.70 DE(4h,h): 2.01600500
3.17160000 0.00806402 0.01268640 0.00002137 2000.00000000 427.33 DE(6h,h):
3.00347000 3.72005000 0.01201388 0.01488020 0.00000822 2000.00000000 164.32
DE(b,h) : 8.86714000 7.63520000 0.08956707 0.07712323 0.00015485 1.00000000
1.55 DE(f,h) : 4.51670000 4.51880000 0.04562323 0.04564444 0.00000000
2000.00000000 0.01 c_{11} : 247.46650824 176.10000000 1.08097020 0.76923077
0.09718147 100.00000000 97181.47 c_{33} : 292.48964963 190.50000000 1.18106057
0.76923077 0.16960378 100.00000000 169603.78 c_{44} : 67.56639226 50.80000000
1.02311315 0.76923077 0.06445626 100.00000000 64456.26 c_{12} : 126.49949516
86.90000000 1.11976184 0.76923077 0.12287203 100.00000000 122872.03 c_{13}
: 86.58455848 68.30000000 0.97516115 0.76923077 0.04240732 10.00000000
4240.73 M_{freq0} : 3.27389129 2.85858719 0.23860062 0.20833333 0.00091611
0.10000000 0.92 M_{freq1} : 3.27389130 2.85858719 0.23860062 0.20833333 0.00091611
0.10000000 0.92 M_{freq2} : 3.27389130 2.85858719 0.23860062 0.20833333 0.00091611
0.10000000 0.92 M_{freq3} : 3.27389132 2.85858719 0.23860063 0.20833333 0.00091611
0.10000000 0.92 M_{freq4} : 7.17344228 5.66706047 0.26371117 0.20833333 0.00306670
0.10000000 3.07 M_{freq5} : 7.17344228 5.66706047 0.26371117 0.20833333 0.00306670
0.10000000 3.07 H_{freq0} : 4.80388952 4.80643423 0.20822303 0.20833333 0.00000001
0.10000000 0.00 H_{freq1} : 4.80388952 5.58010025 0.17935347 0.20833333 0.00083983
0.10000000 0.84 H_{freq2} : 7.98041792 5.65316738 0.29409833 0.20833333 0.00735563
0.10000000 7.36 H_{freq3} : 7.98041792 6.36651842 0.26114541 0.20833333 0.00278912
0.10000000 2.79 H_{freq4} : 9.75868685 6.40050186 0.31764068 0.20833333 0.01194810
0.10000000 11.95 H_{freq5} : 9.75868685 7.64082373 0.26607861 0.20833333 0.00333452
0.10000000 3.33 bandw. G: 4.80417199 5.87085872 1.36384704 1.66666667
0.09169972 15.00000000 13754.96 bandw. K: 5.93888721 4.97424321 1.08538890
0.90909091 0.03108098 15.00000000 4662.15 bandw. M: 6.74570510 7.78109872
1.44489130 1.66666667 0.04918431 15.00000000 7377.65 bandw. L: 5.47221176
6.34433701 1.43755808 1.66666667 0.05249074 15.00000000 7873.61 bandw.
H: 4.57287512 9.70902614 0.42817468 0.90909091 0.23128042 5.00000000 11564.02
DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
0.00 DOSerr_o: 77.64288259 0.00000000 77.64288259 0.00000000 6028.41721726
0.00000000 0.00 E_{prisf}: 222.07696896 220.00000000 222.07696896 220.00000000
4.31380004 0.01000000 431.38
b2=0.0000000000 m2=0.0000000000 p2=0.0000000000 fdd=0.2648249504
qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=59.5259478032

p0=1.1493643262 b1=-4.5351789513 p1=0.6943513856 ndt=2.0000000000 cr1=-
6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-
1.1418272350 rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.62308140 5.57678969 5.62308140 5.57678969 0.00214292 1000.00000000
21429.23 c/a : 1.60706613 1.58731122 15.60361970 15.41181168 0.03679032
100.00000000 36790.32 a_{omega} : 8.95511122 8.73254342 1.11938890 1.09156793
0.00077401 10.00000000 77.40 c_{omega} : 5.44595238 5.32343103 0.68074405
0.66542888 0.00023455 10.00000000 23.46 a_{4h} : 5.61681826 5.56325146 1.00962869
1.00000000 0.00009271 1.00000000 0.93 c_{4h} : 18.20540238 17.75908031 1.02513205
1.00000000 0.00063162 1.00000000 6.32 a_{6h} : 5.61197437 5.54639384 1.01182399
1.00000000 0.00013981 1.00000000 1.40 c_{6h} : 27.37377796 26.77136353 1.02250219
1.00000000 0.00050635 1.00000000 5.06 a_{bcc} : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.92759020 7.88677000 1.13251289
1.12668143 0.00003401 1.00000000 0.34 DE(o,h) : -0.34139500 -0.63343333 -
0.02275967 -0.04222889 0.00037905 3000.00000000 11371.52 DE(4h,h): 1.90152000
3.17160000 0.00760608 0.01268640 0.00002581 2000.00000000 516.19 DE(6h,h):
2.85588500 3.72005000 0.01142354 0.01488020 0.00001195 2000.00000000 238.97
DE(b,h) : 6.94059500 7.63520000 0.07010702 0.07712323 0.00004923 1.00000000
0.49 DE(f,h) : 4.30125500 4.51880000 0.04344702 0.04564444 0.00000483
2000.00000000 96.57 c₁₁ : 184.83130888 176.10000000 0.80737041 0.76923077
0.00145463 100.00000000 1454.63 c₃₃ : 210.64384444 190.50000000 0.85057074
0.76923077 0.00661619 100.00000000 6616.19 c₄₄ : 49.26324195 50.80000000
0.74596066 0.76923077 0.00054150 100.00000000 541.50 c₁₂ : 93.83944584
86.90000000 0.83065810 0.76923077 0.00377332 100.00000000 3773.32 c₁₃
: 67.50316906 68.30000000 0.76025644 0.76923077 0.00008054 10.00000000
8.05 M_{freq0}: 2.62482946 2.85858719 0.19129711 0.20833333 0.00029023 0.10000000
0.29 M_{freq1}: 2.62482947 2.85858719 0.19129711 0.20833333 0.00029023 0.10000000
0.29 M_{freq2}: 2.62482947 2.85858719 0.19129711 0.20833333 0.00029023 0.10000000
0.29 M_{freq3}: 2.62482948 2.85858719 0.19129711 0.20833333 0.00029023 0.10000000
0.29 M_{freq4}: 5.69996224 5.66706047 0.20954287 0.20833333 0.00000146 0.10000000
0.00 M_{freq5}: 5.69996224 5.66706047 0.20954287 0.20833333 0.00000146 0.10000000
0.00 H_{freq0}: 3.74539370 4.80643423 0.16234288 0.20833333 0.00211512 0.10000000
2.12 H_{freq1}: 3.74539370 5.58010025 0.13983447 0.20833333 0.00469209 0.10000000
4.69 H_{freq2}: 6.26248075 5.65316738 0.23078805 0.20833333 0.00050421 0.10000000
0.50 H_{freq3}: 6.26248075 6.36651842 0.20492888 0.20833333 0.00001159 0.10000000
0.01 H_{freq4}: 7.87194364 6.40050186 0.25622807 0.20833333 0.00229391 0.10000000
2.29 H_{freq5}: 7.87194364 7.64082373 0.21463501 0.20833333 0.00003971 0.10000000
0.04 bandw. G: 4.85859478 5.87085872 1.37929702 1.66666667 0.08258131
15.00000000 12387.20 bandw. K: 6.00147342 4.97424321 1.09682713 0.90909091

0.03524489 15.00000000 5286.73 bandw. M: 6.80148846 7.78109872 1.45683977
1.66666667 0.04402732 15.00000000 6604.10 bandw. L: 5.52527398 6.34433701
1.45149760 1.66666667 0.04629772 15.00000000 6944.66 bandw. H: 4.61641335
9.70902614 0.43225132 0.90909091 0.22737599 5.00000000 11368.80 DOSerr_h:
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00
DOSerr_o: 110.29822598 0.00000000 110.29822598 0.00000000 12165.69865409
0.00000000 0.00 E_{prisf}: 70.80322562 220.00000000 70.80322562 220.00000000
22259.67748515 0.00100000 222596.77
b2=529957467.2048873901 m2=-15.8531159425 p2=0.0000000000 fdd=0.2648249504
qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=47.1964963231
p0=1.0523246525 b1=-4.9366489527 p1=0.6329489051 ndt=2.0000000000 cr1=-
6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-
1.1418272350 rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.57188821 5.57678969 5.57188821 5.57678969 0.00002402 1000.00000000
240.24 c/a : 1.58940570 1.58731122 15.43214786 15.41181168 0.00041356
100.00000000 413.56 a_{omega} : 8.90037874 8.73254342 1.11254734 1.09156793
0.00044014 10.00000000 44.01 c_{omega} : 5.40408192 5.32343103 0.67551024
0.66542888 0.00010163 10.00000000 10.16 a_{4h} : 5.57268326 5.56325146 1.00169538
1.00000000 0.00000287 1.00000000 0.03 c_{4h} : 18.01242981 17.75908031 1.01426591
1.00000000 0.00020352 1.00000000 2.04 a_{6h} : 5.56660954 5.54639384 1.00364484
1.00000000 0.00001328 1.00000000 0.13 c_{6h} : 27.10263712 26.77136353 1.01237418
1.00000000 0.00015312 1.00000000 1.53 a_{bcc} : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.86058346 7.88677000 1.12294049
1.12668143 0.00001399 1.00000000 0.14 DE(o,h) : -0.49262667 -0.63343333 -
0.03284178 -0.04222889 0.00008812 3000.00000000 2643.54 DE(4h,h): 2.28232000
3.17160000 0.00912928 0.01268640 0.00001265 2000.00000000 253.06 DE(6h,h):
3.36564500 3.72005000 0.01346258 0.01488020 0.00000201 2000.00000000 40.19
DE(b,h) : 7.56147000 7.63520000 0.07637848 0.07712323 0.00000055 1.00000000
0.01 DE(f,h) : 5.02996000 4.51880000 0.05080768 0.04564444 0.00002666
2000.00000000 533.18 c₁₁ : 199.75935696 176.10000000 0.87257833 0.76923077
0.01068072 100.00000000 10680.72 c₃₃ : 257.57041942 190.50000000 1.04005822
0.76923077 0.07334751 100.00000000 73347.51 c₄₄ : 57.74878709 50.80000000
0.87445165 0.76923077 0.01107143 100.00000000 11071.43 c₁₂ : 99.00485786
86.90000000 0.87638185 0.76923077 0.01148135 100.00000000 11481.35 c₁₃
: 78.58125619 68.30000000 0.88502372 0.76923077 0.01340801 10.00000000
1340.80 M_{freq0}: 2.89853526 2.85858719 0.21124474 0.20833333 0.00000848
0.10000000 0.01 M_{freq1}: 2.89853527 2.85858719 0.21124474 0.20833333 0.00000848
0.10000000 0.01 M_{freq2}: 2.89853527 2.85858719 0.21124474 0.20833333 0.00000848
0.10000000 0.01 M_{freq3}: 2.89853528 2.85858719 0.21124474 0.20833333 0.00000848

0.10000000 0.01 M_{freq4} : 6.67131393 5.66706047 0.24525185 0.20833333 0.00136298
 0.10000000 1.36 M_{freq5} : 6.67131393 5.66706047 0.24525185 0.20833333 0.00136298
 0.10000000 1.36 H_{freq0} : 3.83835538 4.80643423 0.16637227 0.20833333 0.00176073
 0.10000000 1.76 H_{freq1} : 3.83835538 5.58010025 0.14330520 0.20833333 0.00422866
 0.10000000 4.23 H_{freq2} : 7.48779156 5.65316738 0.27594382 0.20833333 0.00457118
 0.10000000 4.57 H_{freq3} : 7.48779156 6.36651842 0.24502506 0.20833333 0.00134628
 0.10000000 1.35 H_{freq4} : 9.36361994 6.40050186 0.30478144 0.20833333 0.00930224
 0.10000000 9.30 H_{freq5} : 9.36361994 7.64082373 0.25530679 0.20833333 0.00220651
 0.10000000 2.21 bandw. G : 5.05587740 5.87085872 1.43530320 1.66666667
 0.05352905 15.00000000 8029.36 bandw. K : 6.22324630 4.97424321 1.13735827
 0.90909091 0.05210599 15.00000000 7815.90 bandw. M : 6.99741052 7.78109872
 1.49880515 1.66666667 0.02817749 15.00000000 4226.62 bandw. L : 5.74704686
 6.34433701 1.50975767 1.66666667 0.02462043 15.00000000 3693.07 bandw. H : 4.77015774 9.70902614 0.44664696 0.90909091 0.21385440 5.00000000 10692.72
 DOSerr_h : 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o : 104.85200112 0.00000000 104.85200112 0.00000000 10993.94213887
 0.00000000 0.00 E_{prisf} : 72.80642405 220.00000000 72.80642405 220.00000000
 21665.94880152 0.00100000 216659.49

$b_2=238992966.9478154778$ $m_2=-15.0156845030$ $p_2=0.0000000000$ $fdd=0.2648249504$
 $qdds=0.5697753882$ $qddp=0.5648597117$ $qddd=0.8213593849$ $b_0=47.0500980357$
 $p_0=1.0556839408$ $b_1=-5.13$ 00359501 $p_1=0.6507410387$ $ndt=2.0000000000$
 $cr_1=-6.0000000000$ $cr_2=3.2217589360$ $r_1dd=6.5000000000$ $rcdd=10.0000000000$
 $cr_3=-1.1418272350$ $r_{\text{maxhm}}=10.1000000000$ $n_{\text{par}}=18$

a_{hcp} : 5.65153719 5.57678969 5.65153719 5.57678969 0.00558719 1000.00000000
 55871.89 c/a : 1.59497837 1.58731122 15.48625502 15.41181168 0.00554181
 100.00000000 5541.81 a_{omega} : 9.03327448 8.73254342 1.12915931 1.09156793
 0.00141311 10.00000000 141.31 c_{omega} : 5.46261177 5.32343103 0.68282647
 0.66542888 0.00030268 10.00000000 30.27 a_{4h} : 5.65046462 5.56325146 1.01567665
 1.00000000 0.00024576 1.00000000 2.46 c_{4h} : 18.28532568 17.75908031 1.02963247
 1.00000000 0.00087808 1.00000000 8.78 a_{6h} : 5.64546730 5.54639384 1.01786268
 1.00000000 0.00031908 1.00000000 3.19 c_{6h} : 27.50655214 26.77136353 1.02746175
 1.00000000 0.00075415 1.00000000 7.54 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.97380174 7.88677000 1.13911453
 1.12668143 0.00015458 1.00000000 1.55 $\text{DE}(o,h)$: -0.27297000 -0.63343333 -
 0.01819800 -0.04222889 0.00057748 3000.00000000 17324.51 $\text{DE}(4h,h)$: 2.06699250
 3.17160000 0.00826797 0.01268640 0.00001952 2000.00000000 390.45 $\text{DE}(6h,h)$:
 3.06958667 3.72005000 0.01227835 0.01488020 0.00000677 2000.00000000 135.39
 $\text{DE}(b,h)$: 7.84221000 7.63520000 0.07921424 0.07712323 0.00000437 1.00000000
 0.04 $\text{DE}(f,h)$: 4.60577000 4.51880000 0.04652293 0.04564444 0.00000077

2000.00000000 15.43 c_{11} : 200.13394216 176.10000000 0.87421457 0.76923077
 0.01102160 100.00000000 11021.60 c_{33} : 238.53684776 190.50000000 0.96320148
 0.76923077 0.03762464 100.00000000 37624.64 c_{44} : 54.80421660 50.80000000
 0.82986397 0.76923077 0.00367639 100.00000000 3676.39 c_{12} : 111.18853892
 86.90000000 0.98423067 0.76923077 0.04622496 100.00000000 46224.96 c_{13}
 : 72.65583597 68.30000000 0.81828850 0.76923077 0.00240666 10.00000000
 240.67 $M_{\text{freq}0}$: 2.84168323 2.85858719 0.20710138 0.20833333 0.00000152
 0.10000000 0.00 $M_{\text{freq}1}$: 2.84168324 2.85858719 0.20710138 0.20833333 0.00000152
 0.10000000 0.00 $M_{\text{freq}2}$: 2.84168324 2.85858719 0.20710138 0.20833333 0.00000152
 0.10000000 0.00 $M_{\text{freq}3}$: 2.84168325 2.85858719 0.20710138 0.20833333 0.00000152
 0.10000000 0.00 $M_{\text{freq}4}$: 6.35692654 5.66706047 0.23369429 0.20833333 0.00064318
 0.10000000 0.64 $M_{\text{freq}5}$: 6.35692654 5.66706047 0.23369429 0.20833333 0.00064318
 0.10000000 0.64 $H_{\text{freq}0}$: 4.05308243 4.80643423 0.17567954 0.20833333 0.00106627
 0.10000000 1.07 $H_{\text{freq}1}$: 4.05308243 5.58010025 0.15132204 0.20833333 0.00325029
 0.10000000 3.25 $H_{\text{freq}2}$: 7.14466972 5.65316738 0.26329892 0.20833333 0.00302122
 0.10000000 3.02 $H_{\text{freq}3}$: 7.14466972 6.36651842 0.23379699 0.20833333 0.00064840
 0.10000000 0.65 $H_{\text{freq}4}$: 8.81982929 6.40050186 0.28708131 0.20833333 0.00620124
 0.10000000 6.20 $H_{\text{freq}5}$: 8.81982929 7.64082373 0.24047989 0.20833333 0.00103340
 0.10000000 1.03 bandw. G: 4.75383090 5.87085872 1.34955581 1.66666667
 0.10055929 15.00000000 15083.89 bandw. K: 5.88038270 4.97424321 1.07469664
 0.90909091 0.02742526 15.00000000 4113.79 bandw. M: 6.69400345 7.78109872
 1.43381710 1.66666667 0.05421892 15.00000000 8132.84 bandw. L: 5.42187068
 6.34433701 1.42433340 1.66666667 0.05872541 15.00000000 8808.81 bandw.
 H: 4.53341860 9.70902614 0.42448023 0.90909091 0.23484751 5.00000000 11742.38
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 106.26772307 0.00000000 106.26772307 0.00000000 11292.82896546
 0.00000000 0.00 E_{prisf}: 105.96058776 220.00000000 105.96058776 220.00000000
 13004.98754412 0.00100000 130049.88
 b2=0.0000000000 m2=0.0000000000 p2=0.0000000000 fdd=0.2648249504
 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=140.6250881140
 p0=1.5000000000 b1=-0.3349120798 p1=0.5103314042 ndt=2.0000000000 cr1=-
 6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-
 1.1418272350 rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.56058759 5.57678969 5.56058759 5.57678969 0.00026251 1000.00000000
 2625.08 c/a : 1.59424873 1.58731122 15.47917067 15.41181168 0.00453723
 100.00000000 4537.23 a_{omega} : 8.85711014 8.73254342 1.10713877 1.09156793
 0.00024245 10.00000000 24.25 c_{omega} : 5.41409627 5.32343103 0.67676203
 0.66542888 0.00012844 10.00000000 12.84 a_{4h} : 5.54693871 5.56325146 0.99706777
 1.00000000 0.00000860 1.00000000 0.09 c_{4h} : 18.02419033 17.75908031 1.01492814

1.00000000 0.00022285 1.00000000 2.23 a_{6h} : 5.54272137 5.54639384 0.99933786
1.00000000 0.00000044 1.00000000 0.00 c_{6h} : 27.08087241 26.77136353 1.01156119
1.00000000 0.00013366 1.00000000 1.34 a_{bcc} : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.83131615 7.88677000 1.11875945
1.12668143 0.00006276 1.00000000 0.63 DE(o,h) : 1.24301500 -0.63343333
0.08286767 -0.04222889 0.01564915 3000.00000000 469474.45 DE(4h,h): 1.72554000
3.17160000 0.00690216 0.01268640 0.00003346 2000.00000000 669.15 DE(6h,h):
2.63205667 3.72005000 0.01052823 0.01488020 0.00001894 2000.00000000 378.79
DE(b,h) : 8.05059500 7.63520000 0.08131914 0.07712323 0.00001761 1.00000000
0.18 DE(f,h) : 3.97823500 4.51880000 0.04018419 0.04564444 0.00002981
2000.00000000 596.29 c_{11} : 192.43892517 176.10000000 0.84060160 0.76923077
0.00509380 100.00000000 5093.80 c_{33} : 204.85827777 190.50000000 0.82720887
0.76923077 0.00336146 100.00000000 3361.46 c_{44} : 50.34135405 50.80000000
0.76228580 0.76923077 0.00004823 100.00000000 48.23 c_{12} : 75.61328960
86.90000000 0.66932185 0.76923077 0.00998179 100.00000000 9981.79 c_{13}
: 68.71389026 68.30000000 0.77389222 0.76923077 0.00002173 10.00000000
2.17 M_{freq0} : 2.67628898 2.85858719 0.19504747 0.20833333 0.00017651 0.10000000
0.18 M_{freq1} : 2.67628899 2.85858719 0.19504747 0.20833333 0.00017651 0.10000000
0.18 M_{freq2} : 2.67628899 2.85858719 0.19504747 0.20833333 0.00017651 0.10000000
0.18 M_{freq3} : 2.67628900 2.85858719 0.19504747 0.20833333 0.00017651 0.10000000
0.18 M_{freq4} : 5.25767874 5.66706047 0.19328358 0.20833333 0.00022650 0.10000000
0.23 M_{freq5} : 5.25767874 5.66706047 0.19328358 0.20833333 0.00022650 0.10000000
0.23 H_{freq0} : 3.63161265 4.80643423 0.15741107 0.20833333 0.00259308 0.10000000
2.59 H_{freq1} : 3.63161265 5.58010025 0.13558645 0.20833333 0.00529211 0.10000000
5.29 H_{freq2} : 5.48887273 5.65316738 0.20227867 0.20833333 0.00003666 0.10000000
0.04 H_{freq3} : 5.48887273 6.36651842 0.17961389 0.20833333 0.00082481 0.10000000
0.82 H_{freq4} : 7.13585316 6.40050186 0.23226867 0.20833333 0.00057290 0.10000000
0.57 H_{freq5} : 7.13585316 7.64082373 0.19456490 0.20833333 0.00018957 0.10000000
0.19 bandw. G: 5.10077620 5.87085872 1.44804944 1.66666667 0.04779349
15.00000000 7169.02 bandw. K: 6.27358738 4.97424321 1.14655858 0.90909091
0.05639090 15.00000000 8458.63 bandw. M: 7.04094875 7.78109872 1.50813079
1.66666667 0.02513362 15.00000000 3770.04 bandw. L: 5.78922453 6.34433701
1.52083780 1.66666667 0.02126606 15.00000000 3189.91 bandw. H: 4.80417199
9.70902614 0.44983184 0.90909091 0.21091889 5.00000000 10545.94 DOSerr_h:
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00
DOSerr_o: 101.31732878 0.00000000 101.31732878 0.00000000 10265.20111043
0.00000000 0.00 E_{prisf} : 51.15374553 220.00000000 51.15374553 220.00000000
28509.05764790 0.00100000 28509.58
b2=0.0000000000 m2=0.0000000000 p2=0.0000000000 fdd=0.2648249504
qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=114.1564941581

p0=1.3883912590 b1=-1.8695661213 p1=0.7021069541 ndt=2.0000000000 cr1=-
6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-
1.1418272350 rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.62641713 5.57678969 5.62641713 5.57678969 0.00246288 1000.00000000
24628.83 c/a : 1.60564282 1.58731122 15.58980022 15.41181168 0.03167992
100.00000000 31679.92 a_{omega} : 8.96538123 8.73254342 1.12067265 1.09156793
0.00084709 10.00000000 84.71 c_{omega} : 5.45575817 5.32343103 0.68196977
0.66542888 0.00027360 10.00000000 27.36 a_{4h} : 5.61278398 5.56325146 1.00890352
1.00000000 0.00007927 1.00000000 0.79 c_{4h} : 18.24121329 17.75908031 1.02714853
1.00000000 0.00073704 1.00000000 7.37 a_{6h} : 5.60912152 5.54639384 1.01130963
1.00000000 0.00012791 1.00000000 1.28 c_{6h} : 27.40562165 26.77136353 1.02369166
1.00000000 0.00056129 1.00000000 5.61 a_{bcc} : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.92527962 7.88677000 1.13218280
1.12668143 0.00003027 1.00000000 0.30 DE(o,h) : 1.26412500 -0.63343333
0.08427500 -0.04222889 0.01600323 3000.00000000 480097.02 DE(4h,h): 1.69892000
3.17160000 0.00679568 0.01268640 0.00003470 2000.00000000 694.01 DE(6h,h):
2.59242333 3.72005000 0.01036969 0.01488020 0.00002034 2000.00000000 406.89
DE(b,h) : 7.56535500 7.63520000 0.07641773 0.07712323 0.00000050 1.00000000
0.00 DE(f,h) : 3.93098500 4.51880000 0.03970692 0.04564444 0.00003525
2000.00000000 705.08 c₁₁ : 195.05516670 176.10000000 0.85202973 0.76923077
0.00685567 100.00000000 6855.67 c₃₃ : 206.27436836 190.50000000 0.83292699
0.76923077 0.00405721 100.00000000 4057.21 c₄₄ : 49.63461769 50.80000000
0.75158416 0.76923077 0.00031140 100.00000000 311.40 c₁₂ : 86.92490619
86.90000000 0.76945124 0.76923077 0.00000005 100.00000000 0.05 c₁₃ : 68.73179082
68.30000000 0.77409383 0.76923077 0.00002365 10.00000000 2.36 M_{freq0}: 2.68061683
2.85858719 0.19536288 0.20833333 0.00016823 0.10000000 0.17 M_{freq1}: 2.68061684
2.85858719 0.19536289 0.20833333 0.00016823 0.10000000 0.17 M_{freq2}: 2.68061684
2.85858719 0.19536289 0.20833333 0.00016823 0.10000000 0.17 M_{freq3}: 2.68061685
2.85858719 0.19536289 0.20833333 0.00016823 0.10000000 0.17 M_{freq4}: 5.45403129
5.66706047 0.20050192 0.20833333 0.00006133 0.10000000 0.06 M_{freq5}: 5.45403129
5.66706047 0.20050192 0.20833333 0.00006133 0.10000000 0.06 H_{freq0}: 3.89335853
4.80643423 0.16875636 0.20833333 0.00156634 0.10000000 1.57 H_{freq1}: 3.89335853
5.58010025 0.14535874 0.20833333 0.00396580 0.10000000 3.97 H_{freq2}: 5.77373518
5.65316738 0.21277656 0.20833333 0.00001974 0.10000000 0.02 H_{freq3}: 5.77373518
6.36651842 0.18893552 0.20833333 0.00037627 0.10000000 0.38 H_{freq4}: 7.33883803
6.40050186 0.23887574 0.20833333 0.00093284 0.10000000 0.93 H_{freq5}: 7.33883803
7.64082373 0.20009945 0.20833333 0.00006780 0.10000000 0.07 bandw. G:
4.84634965 5.87085872 1.37582078 1.66666667 0.08459133 15.00000000 12688.70
bandw. K: 5.98650715 4.97424321 1.09409190 0.90909091 0.03422537 15.00000000

5133.81 bandw. M: 6.78924333 7.78109872 1.45421694 1.66666667 0.04513489
 15.00000000 6770.23 bandw. L: 5.51302886 6.34433701 1.44828079 1.66666667
 0.04769239 15.00000000 7153.86 bandw. H: 4.60552880 9.70902614 0.43123216
 0.90909091 0.22834898 5.00000000 11417.45 DOSerr_h: 0.00000000 0.00000000
 0.00000000 0.00000000 0.00000000 1.00000000 0.00 DOSerr_o: 106.36466941
 0.00000000 106.36466941 0.00000000 11313.44289798 0.00000000 0.00 E_{prisf}:
 92.22065278 220.00000000 92.22065278 220.00000000 16327.56157472 0.00100000
 163275.62
 b2=100000000.000000000 m2=-17.000000000 p2=0.000000000 fdd=0.2648249504
 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=69.7247791494
 p0=1.1823996774 b1=-6.1008440394 p1=0.7500000000 ndt=2.0000000000 cr1=-
 6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-
 1.1418272350 rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.56276602 5.57678969 5.56276602 5.57678969 0.00019666 1000.00000000
 1966.63 c/a : 1.59331360 1.58731122 15.47009117 15.41181168 0.00339650
 100.00000000 3396.50 a_{omega} : 8.86570413 8.73254342 1.10821302 1.09156793
 0.00027706 10.00000000 27.71 c_{omega} : 5.39008159 5.32343103 0.67376020
 0.66542888 0.00006941 10.00000000 6.94 a_{4h} : 5.55263546 5.56325146 0.99809176
 1.00000000 0.00000364 1.00000000 0.04 c_{4h} : 18.02391102 17.75908031 1.01491241
 1.00000000 0.00022238 1.00000000 2.22 a_{6h} : 5.54842769 5.54639384 1.00036670
 1.00000000 0.00000013 1.00000000 0.00 c_{6h} : 27.08910587 26.77136353 1.01186874
 1.00000000 0.00014087 1.00000000 1.41 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.83901807 7.88677000 1.11985972
 1.12668143 0.00004654 1.00000000 0.47 DE(o,h) : 0.70288333 -0.63343333
 0.04685889 -0.04222889 0.00793663 3000.00000000 238098.96 DE(4h,h): 1.86685500
 3.17160000 0.00746742 0.01268640 0.00002724 2000.00000000 544.76 DE(6h,h):
 2.81596667 3.72005000 0.01126387 0.01488020 0.00001308 2000.00000000 261.56
 DE(b,h) : 7.38194000 7.63520000 0.07456505 0.07712323 0.00000654 1.00000000
 0.07 DE(f,h) : 4.24119000 4.51880000 0.04284030 0.04564444 0.00000786
 2000.00000000 157.26 c₁₁ : 208.93562758 176.10000000 0.91266163 0.76923077
 0.02057241 100.00000000 20572.41 c₃₃ : 237.98543138 190.50000000 0.96097489
 0.76923077 0.03676581 100.00000000 36765.81 c₄₄ : 54.28185458 50.80000000
 0.82195419 0.76923077 0.00277976 100.00000000 2779.76 c₁₂ : 97.64679227
 86.90000000 0.86436038 0.76923077 0.00904964 100.00000000 9049.64 c₁₃
 : 74.24437438 68.30000000 0.83617946 0.76923077 0.00448213 10.00000000
 448.21 M_{freq0}: 2.82856685 2.85858719 0.20614546 0.20833333 0.00000479
 0.10000000 0.00 M_{freq1}: 2.82856686 2.85858719 0.20614546 0.20833333 0.00000479
 0.10000000 0.00 M_{freq2}: 2.82856686 2.85858719 0.20614546 0.20833333 0.00000479
 0.10000000 0.00 M_{freq3}: 2.82856687 2.85858719 0.20614546 0.20833333 0.00000479

0.10000000 0.00 M_{freq4}: 6.02957369 5.66706047 0.22166010 0.20833333 0.00017760
 0.10000000 0.18 M_{freq5}: 6.02957369 5.66706047 0.22166010 0.20833333 0.00017760
 0.10000000 0.18 H_{freq0}: 4.01647120 4.80643423 0.17409264 0.20833333 0.00117242
 0.10000000 1.17 H_{freq1}: 4.01647120 5.58010025 0.14995516 0.20833333 0.00340801
 0.10000000 3.41 H_{freq2}: 6.59737209 5.65316738 0.24312963 0.20833333 0.00121078
 0.10000000 1.21 H_{freq3}: 6.59737209 6.36651842 0.21588762 0.20833333 0.00005707
 0.10000000 0.06 H_{freq4}: 8.27795011 6.40050186 0.26944339 0.20833333 0.00373444
 0.10000000 3.73 H_{freq5}: 8.27795011 7.64082373 0.22570511 0.20833333 0.00030178
 0.10000000 0.30 bandw. G: 5.09125222 5.87085872 1.44534569 1.66666667
 0.04898297 15.00000000 7347.45 bandw. K: 6.26406339 4.97424321 1.14481798
 0.90909091 0.05556725 15.00000000 8335.09 bandw. M: 7.03142476 7.78109872
 1.50609081 1.66666667 0.02578461 15.00000000 3867.69 bandw. L: 5.78242168
 6.34433701 1.51905068 1.66666667 0.02179048 15.00000000 3268.57 bandw.
 H: 4.79736914 9.70902614 0.44919486 0.90909091 0.21150437 5.00000000 10575.22
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 105.23589358 0.00000000 105.23589358 0.00000000 11074.59329851
 0.00000000 0.00 E_{prisf}: 94.86005764 220.00000000 94.86005764 220.00000000
 15660.00517479 0.00100000 15660.05

PARAMETERS b2=1000000.0000000000 m2=-12.0000000000 p2=0.0000000000
 fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849
 b0=55.0000000000 p0=1.0500000000 b1=-6.9791271873 p1=0.6629981150 ndt=2.0000000000
 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000
 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18 VARGS -vb2=1000000.0000000000
 -vm2=-12.0000000000 -vp2=0.0000000000 -vfdd=0.2648249504 -vqdds=0.5697753882
 -vqddp=0.5648597117 -vqddd=0.8213593849 -vb0=55.0000000000 -vp0=1.0500000000
 -vb1=-6.9791271873 -vp1=0.6629981150 -vndt=2.0000000000 -vcr1=-6.0000000000
 -vcr2=3.2217589360 -vr1dd=6.5000000000 -vrdd=10.0000000000 -vcr3=-1.1418272350
 -vrmaxhm=10.1000000000

a_{hcp} : 5.58686494 5.57678969 5.58686494 5.57678969 0.00010151 1000.00000000
 1015.11 c/a : 1.58301742 1.58731122 15.37012160 15.41181168 0.00173806
 100.00000000 1738.06 a_{omega} : 8.91730311 8.73254342 1.11466289 1.09156793
 0.00053338 10.00000000 53.34 c_{omega} : 5.40664954 5.32343103 0.67583119
 0.66542888 0.00010821 10.00000000 10.82 a_{4h} : 5.58766385 5.56325146 1.00438815
 1.00000000 0.00001926 1.00000000 0.19 c_{4h} : 18.06717880 17.75908031 1.01734879
 1.00000000 0.00030098 1.00000000 3.01 a_{6h} : 5.58217511 5.54639384 1.00645127
 1.00000000 0.00004162 1.00000000 0.42 c_{6h} : 27.18237891 26.77136353 1.01535280
 1.00000000 0.00023571 1.00000000 2.36 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.88330413 7.88677000 1.12618630
 1.12668143 0.00000025 1.00000000 0.00 DE(o,h) : -0.60419667 -0.63343333 -
 0.04027978 -0.04222889 0.00000380 3000.00000000 113.97 DE(4h,h): 2.29304250

3.17160000 0.00917217 0.01268640 0.00001235 2000.00000000 247.00 DE(6h,h):
 3.37653833 3.72005000 0.01350615 0.01488020 0.00000189 2000.00000000 37.76
 DE(b,h) : 7.21744000 7.63520000 0.07290343 0.07712323 0.00001781 1.00000000
 0.18 DE(f,h) : 5.04380000 4.51880000 0.05094747 0.04564444 0.00002812
 2000.00000000 562.44 c₁₁ : 210.19151749 176.10000000 0.91814755 0.76923077
 0.02217621 100.00000000 22176.21 c₃₃ : 273.40612781 190.50000000 1.10400213
 0.76923077 0.11207186 100.00000000 112071.86 c₄₄ : 60.02683608 50.80000000
 0.90894664 0.76923077 0.01952052 100.00000000 19520.52 c₁₂ : 115.11424042
 86.90000000 1.01898062 0.76923077 0.06237499 100.00000000 62374.99 c₁₃
 : 81.44035229 68.30000000 0.91722438 0.76923077 0.02190211 10.00000000
 2190.21 M_{freq0}: 2.97521129 2.85858719 0.21683288 0.20833333 0.00007224
 0.10000000 0.07 M_{freq1}: 2.97521130 2.85858719 0.21683288 0.20833333 0.00007224
 0.10000000 0.07 M_{freq2}: 2.97521130 2.85858719 0.21683288 0.20833333 0.00007224
 0.10000000 0.07 M_{freq3}: 2.97521131 2.85858719 0.21683288 0.20833333 0.00007224
 0.10000000 0.07 M_{freq4}: 6.93944416 5.66706047 0.25510889 0.20833333 0.00218795
 0.10000000 2.19 M_{freq5}: 6.93944416 5.66706047 0.25510889 0.20833333 0.00218795
 0.10000000 2.19 H_{freq0}: 4.09232153 4.80643423 0.17738035 0.20833333 0.00095809
 0.10000000 0.96 H_{freq1}: 4.09232153 5.58010025 0.15278704 0.20833333 0.00308539
 0.10000000 3.09 H_{freq2}: 7.87058136 5.65316738 0.29005058 0.20833333 0.00667771
 0.10000000 6.68 H_{freq3}: 7.87058136 6.36651842 0.25755120 0.20833333 0.00242240
 0.10000000 2.42 H_{freq4}: 9.73498160 6.40050186 0.31686908 0.20833333 0.01178001
 0.10000000 11.78 H_{freq5}: 9.73498160 7.64082373 0.26543227 0.20833333 0.00326029
 0.10000000 3.26 bandw. G: 4.99737290 5.87085872 1.41869448 1.66666667
 0.06149021 15.00000000 9223.53 bandw. K: 6.15657837 4.97424321 1.12517406
 0.90909091 0.04669193 15.00000000 7003.79 bandw. M: 6.93890601 7.78109872
 1.48627382 1.66666667 0.03254158 15.00000000 4881.24 bandw. L: 5.68990293
 6.34433701 1.49474587 1.66666667 0.02955676 15.00000000 4433.51 bandw.
 H: 4.72389837 9.70902614 0.44231553 0.90909091 0.21787925 5.00000000 10893.96
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 103.15991133 0.00000000 103.15991133 0.00000000 10641.96730619
 0.00000000 0.00 E_{prisf}: 95.95221364 220.00000000 95.95221364 220.00000000
 15387.85330116 1.00000000 153878533.01

PARAMETERS b2=882360794.4857044220 m2=-15.9301709745 p2=0.0000000000
 fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849
 b0=58.1772788164 p0=1.0825332663 b1=-5.7757114024 p1=0.6494870700 ndt=2.0000000000
 cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000
 cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18 VARGS -vb2=882360794.4857044220
 -vm2=-15.9301709745 -vp2=0.0000000000 -vfdd=0.2648249504 -vqdds=0.5697753882
 -vqddp=0.5648597117 -vqddd=0.8213593849 -vb0=58.1772788164 -vp0=1.0825332663
 -vb1=-5.7757114024 -vp1=0.6494870700 -vndt=2.0000000000 -vcr1=-6.0000000000

```

-vcr2=3.2217589360 -vr1dd=6.5000000000 -vrcdd=10.0000000000 -vcr3=-1.1418272350
-vm axhm=10.1000000000
a_hcp : 5.59857402 5.57678969 5.59857402 5.57678969 0.00047456 1000.00000000
4745.57 c/a : 1.57804675 1.58731122 15.32185948 15.41181168 0.00809140
100.00000000 8091.40 a_omega : 8.95536748 8.73254342 1.11942094 1.09156793
0.00077579 10.00000000 77.58 c_omega : 5.41277400 5.32343103 0.67659675
0.66542888 0.00012472 10.00000000 12.47 a_4h : 5.59749065 5.56325146 1.00615453
1.00000000 0.00003788 1.00000000 0.38 c_4h : 18.11347665 17.75908031 1.01995578
1.00000000 0.00039823 1.00000000 3.98 a_6h : 5.59241840 5.54639384 1.00829810
1.00000000 0.00006886 1.00000000 0.69 c_6h : 27.24642715 26.77136353 1.01774522
1.00000000 0.00031489 1.00000000 3.15 a_bcc : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_fcc : 7.89909308 7.88677000 1.12844187
1.12668143 0.00000310 1.00000000 0.03 DE(o,h) : 0.47003833 -0.63343333
0.03133589 -0.04222889 0.00541178 3000.00000000 162353.30 DE(4h,h): 2.25634500
3.17160000 0.00902538 0.01268640 0.00001340 2000.00000000 268.06 DE(6h,h):
3.32505833 3.72005000 0.01330023 0.01488020 0.00000250 2000.00000000 49.93
DE(b,h) : 7.66781500 7.63520000 0.07745268 0.07712323 0.00000011 1.00000000
0.00 DE(f,h) : 4.97086500 4.51880000 0.05021076 0.04564444 0.00002085
2000.00000000 417.02 c_11 : 230.33571937 176.10000000 1.00614039 0.76923077
0.05612617 100.00000000 56126.17 c_33 : 292.55927264 190.50000000 1.18134170
0.76923077 0.16983542 100.00000000 169835.42 c_44 : 65.70154566 50.80000000
0.99487501 0.76923077 0.05091532 100.00000000 50915.32 c_12 : 124.17076871
86.90000000 1.09914817 0.76923077 0.10884549 100.00000000 108845.49 c_13
: 86.21863369 68.30000000 0.97103991 0.76923077 0.04072693 10.00000000
4072.69 M_freq0: 3.13773477 2.85858719 0.22867756 0.20833333 0.00041389
0.10000000 0.41 M_freq1: 3.13773478 2.85858719 0.22867756 0.20833333 0.00041389
0.10000000 0.41 M_freq2: 3.13773478 2.85858719 0.22867756 0.20833333 0.00041389
0.10000000 0.41 M_freq3: 3.13773480 2.85858719 0.22867756 0.20833333 0.00041389
0.10000000 0.41 M_freq4: 7.20450402 5.66706047 0.26485307 0.20833333 0.00319448
0.10000000 3.19 M_freq5: 7.20450402 5.66706047 0.26485307 0.20833333 0.00319448
0.10000000 3.19 H_freq0: 4.41794310 4.80643423 0.19149431 0.20833333 0.00028355
0.10000000 0.28 H_freq1: 4.41794310 5.58010025 0.16494414 0.20833333 0.00188262
0.10000000 1.88 H_freq2: 8.14379965 5.65316738 0.30011935 0.20833333 0.00842467
0.10000000 8.42 H_freq3: 8.14379965 6.36651842 0.26649180 0.20833333 0.00338241
0.10000000 3.38 H_freq4: 10.01582142 6.40050186 0.32601029 0.20833333 0.01384787
0.10000000 13.85 H_freq5: 10.01582142 7.64082373 0.27308960 0.20833333 0.00419337
0.10000000 4.19 bandw. G: 4.95247410 5.87085872 1.40594824 1.66666667
0.06797410 15.00000000 10196.11 bandw. K: 6.10759786 4.97424321 1.11622240
0.90909091 0.04290345 15.00000000 6435.52 bandw. M: 6.89400721 7.78109872
1.47665676 1.66666667 0.03610377 15.00000000 5415.56 bandw. L: 5.64772527

```


6.34433701 1.48366574 1.66666667 0.03348934 15.00000000 5023.40 bandw.
H: 4.68852355 9.70902614 0.43900326 0.90909091 0.22098240 5.00000000 11049.12
DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
0.00 DOSerr_o: 88.86184701 0.00000000 88.86184701 0.00000000 7896.42785360
0.00000000 0.00 E_{prif}: 143.82708839 220.00000000 143.82708839 220.00000000
5802.31246266 0.01000000 580231.25

1.2 2019-10-02

fdd=0.2641098014 qdds=0.5701344799 qddp=0.5633017594 qddd=0.8240574383
b0=79.4637950931 p0=1.1406018027 b1=-7.0728554466 p1=0.6935028458 b2=1131252297.3968353271
m2=-16.9865244006 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
cr2=3.4990362148 cr3=-1.2277604496 r1dd=6.5000000000 rcdd=10.0000000000
rmaxhm=10.1000000000 npar=18 VARGS -vfdd=0.2641098014 -vqdds=0.5701344799
-vqddp=0.5633017594 -vqddd=0.8240574383 -vb0=79.4637950931 -vp0=1.1406018027
-vb1=-7.0728554466 -vp1=0.6935028458 -vb2=1131252297.3968353271 -vm2=-
16.9865244006 -vp2=0.0000000000 -vndt=2.0000000000 -vcr1=-6.0000000000
-vcr2=3.4990362148 -vcr3=-1.2277604496 -vr1dd=6.5000000000 -vrccd=10.0000000000
-vr maxhm=10.1000000000

Quantity predicted target norm_{pred} norm_{tar} sq diff. weight objective *
100²

a_{hcp} : 5.62199218 5.57678969 5.62199218 5.57678969 0.00204327 1000.00000000
20432.66 c/a : 1.60753125 1.58731122 15.60813574 15.41181168 0.03854314
100.00000000 38543.14 a_{omega} : 8.97016280 8.73254342 1.12127035 1.09156793
0.00088223 10.00000000 88.22 c_{omega} : 5.43316702 5.32343103 0.67914588
0.66542888 0.00018816 10.00000000 18.82 a_{4h} : 5.61896314 5.56325146 1.01001423
1.00000000 0.00010028 1.00000000 1.00 c_{4h} : 18.19413529 17.75908031 1.02449761
1.00000000 0.00060013 1.00000000 6.00 a_{6h} : 5.61400090 5.54639384 1.01218937
1.00000000 0.00014858 1.00000000 1.49 c_{6h} : 27.36524006 26.77136353 1.02218328
1.00000000 0.00049210 1.00000000 4.92 a_{bcc} : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.92990077 7.88677000 1.13284297
1.12668143 0.00003796 1.00000000 0.38 DE(o,h) : 1.19939667 -0.63343333
0.07995978 -0.04222889 0.01493007 3000.00000000 447902.11 DE(4h,h): 1.84805750
3.17160000 0.00739223 0.01268640 0.00002803 2000.00000000 560.56 DE(6h,h):
2.80304833 3.72005000 0.01121219 0.01488020 0.00001345 2000.00000000 269.09
DE(b,h) : 8.38611000 7.63520000 0.08470818 0.07712323 0.00005753 1.00000000
0.58 DE(f,h) : 4.32071000 4.51880000 0.04364354 0.04564444 0.00000400
2000.00000000 80.07 c₁₁ : 241.35639056 176.10000000 1.05428031 0.76923077
0.08125324 100.00000000 81253.24 c₃₃ : 292.76698939 190.50000000 1.18218045

0.76923077 0.17052744 100.00000000 170527.44 c_{44} : 61.89145344 50.80000000
 0.93718131 0.76923077 0.02820738 100.00000000 28207.38 c_{12} : 132.40515660
 86.90000000 1.17203821 0.76923077 0.16225383 100.00000000 162253.83 c_{13}
 : 83.51234151 68.30000000 0.94056022 0.76923077 0.02935378 10.00000000
 2935.38 $M_{\text{freq}0}$: 3.20761831 2.85858719 0.23377066 0.20833333 0.00064706
 0.10000000 0.65 $M_{\text{freq}1}$: 3.20761832 2.85858719 0.23377066 0.20833333 0.00064706
 0.10000000 0.65 $M_{\text{freq}2}$: 3.20761832 2.85858719 0.23377066 0.20833333 0.00064706
 0.10000000 0.65 $M_{\text{freq}3}$: 3.20761834 2.85858719 0.23377066 0.20833333 0.00064706
 0.10000000 0.65 $M_{\text{freq}4}$: 7.16063337 5.66706047 0.26324029 0.20833333 0.00301477
 0.10000000 3.01 $M_{\text{freq}5}$: 7.16063337 5.66706047 0.26324029 0.20833333 0.00301477
 0.10000000 3.01 $H_{\text{freq}0}$: 4.65063388 4.80643423 0.20158022 0.20833333 0.00004560
 0.10000000 0.05 $H_{\text{freq}1}$: 4.65063388 5.58010025 0.17363166 0.20833333 0.00120421
 0.10000000 1.20 $H_{\text{freq}2}$: 8.12856296 5.65316738 0.29955784 0.20833333 0.00832191
 0.10000000 8.32 $H_{\text{freq}3}$: 8.12856296 6.36651842 0.26599320 0.20833333 0.00332466
 0.10000000 3.32 $H_{\text{freq}4}$: 9.91381764 6.40050186 0.32269011 0.20833333 0.01307747
 0.10000000 13.08 $H_{\text{freq}5}$: 9.91381764 7.64082373 0.27030838 0.20833333 0.00384091
 0.10000000 3.84 bandw. G : 5.09805507 5.87085872 1.44727694 1.66666667
 0.04813185 15.00000000 7219.78 bandw. K : 6.14841496 4.97424321 1.12368212
 0.90909091 0.04604939 15.00000000 6907.41 bandw. M : 7.01781906 7.78109872
 1.50317655 1.66666667 0.02672902 15.00000000 4009.35 bandw. L : 5.78242168
 6.34433701 1.51905068 1.66666667 0.02179048 15.00000000 3268.57 bandw. H :
 4.74294635 9.70902614 0.44409906 0.90909091 0.21621742 1.00000000 2162.17
 DOSerr_h : 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o : 80.73691198 0.00000000 80.73691198 0.00000000 6518.44895674
 0.00000000 0.00 E_{prisf} : 207.40167229 220.00000000 207.40167229 220.00000000
 158.71786117 0.00100000 1587.18

PARAMETERS $b_2=423563676.7901006937$ $m_2=-15.4369946222$ $p_2=0.0000000000$
 $\text{fdd}=0.2648249504$ $\text{qdds}=0.5697753882$ $\text{qddp}=0.5648597117$ $\text{qddd}=0.8213593849$
 $b_0=55.6054749404$ $p_0=1.0942563497$ $b_1=-5.44$ 80628159 $p_1=0.6610373676$
 $\text{ndt}=2.0000000000$ $\text{cr}_1=-6.0000000000$ $\text{cr}_2=3.2217589360$ $\text{r}_1\text{dd}=6.5000000000$
 $\text{rcdd}=10.0000000000$ $\text{cr}_3=-1.1418272350$ $\text{rmaxhm}=10.1000000000$ $\text{npar}=18$
 VARGS $\text{-vb}_2=423563676.7901006937$ $\text{-vm}_2=-15.4369946222$ $\text{-vp}_2=0.0000000000$
 $\text{-vfdd}=0.2648249504$ $\text{-vqdds}=0.5697753882$ $\text{-vqddp}=0.5648597117$ $\text{-vqddd}=0.8213593849$
 $\text{-vb}_0=55.6054749404$ $\text{-vp}_0=1.0942563497$ $\text{-vb}_1=-5.44$ 80628159 $\text{-vp}_1=0.6610373676$
 $\text{-vndt}=2.0000000000$ $\text{-vcr}_1=-6.0000000000$ $\text{-vcr}_2=3.2217589360$ $\text{-vr}_1\text{dd}=6.5000000000$
 $\text{-vr}_2\text{dd}=10.0000000000$ $\text{-vcr}_3=-1.1418272350$ $\text{-vrm axhm}=10.1000000000$ a_{hcp}
 : 5.56698674 5.57678969 5.56698674 5.57678969 0.00009610 1000.00000000
 960.98 c/a : 1.59150388 1.58731122 15.45251985 15.41181168 0.00165716
 100.00000000 1657.16 a_{omega} : 8.90548357 8.73254342 1.11318545 1.09156793
 0.00046732 10.00000000 46.73 c_{omega} : 5.39005450 5.32343103 0.67375681

0.66542888 0.00006935 10.00000000 6.94 a_{4h} : 5.56258735 5.56325146 0.99988063
 1.00000000 0.00000001 1.00000000 0.00 c_{4h} : 18.01739503 17.75908031 1.01454550
 1.00000000 0.00021157 1.00000000 2.12 a_{6h} : 5.55784434 5.54639384 1.00206449
 1.00000000 0.00000426 1.00000000 0.04 c_{6h} : 27.09392166 26.77136353 1.01204863
 1.00000000 0.00014517 1.00000000 1.45 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.85057096 7.88677000 1.12151014
 1.12668143 0.00002674 1.00000000 0.27 DE(o,h) : 0.99867333 -0.63343333
 0.06657822 -0.04222889 0.01183899 3000.00000000 355169.62 DE(4h,h): 2.19377750
 3.17160000 0.00877511 0.01268640 0.00001530 2000.00000000 305.96 DE(6h,h):
 3.24562000 3.72005000 0.01298248 0.01488020 0.00000360 2000.00000000 72.03
 DE(b,h) : 7.95722000 7.63520000 0.08037596 0.07712323 0.00001058 1.00000000
 0.11 DE(f,h) : 4.85910000 4.51880000 0.04908182 0.04564444 0.00001182
 2000.00000000 236.31 c_{11} : 229.24614826 176.10000000 1.00138098 0.76923077
 0.05389372 100.00000000 53893.72 c_{33} : 288.03991759 190.50000000 1.16309274
 0.76923077 0.15512725 100.00000000 155127.25 c_{44} : 64.38616481 50.80000000
 0.97495707 0.76923077 0.04232331 100.00000000 42323.31 c_{12} : 112.89339075
 86.90000000 0.99932186 0.76923077 0.05294191 100.00000000 52941.91 c_{13}
 : 85.51354209 68.30000000 0.96309880 0.76923077 0.03758481 10.00000000
 3758.48 M_{freq0} : 3.13786604 2.85858719 0.22868713 0.20833333 0.00041428
 0.10000000 0.41 M_{freq1} : 3.13786605 2.85858719 0.22868713 0.20833333 0.00041428
 0.10000000 0.41 M_{freq2} : 3.13786605 2.85858719 0.22868713 0.20833333 0.00041428
 0.10000000 0.41 M_{freq3} : 3.13786607 2.85858719 0.22868713 0.20833333 0.00041428
 0.10000000 0.41 M_{freq4} : 7.07999599 5.66706047 0.26027588 0.20833333 0.00269803
 0.10000000 2.70 M_{freq5} : 7.07999599 5.66706047 0.26027588 0.20833333 0.00269803
 0.10000000 2.70 H_{freq0} : 4.36658308 4.80643423 0.18926813 0.20833333 0.00036348
 0.10000000 0.36 H_{freq1} : 4.36658308 5.58010025 0.16302661 0.20833333 0.00205270
 0.10000000 2.05 H_{freq2} : 7.91746806 5.65316738 0.29177847 0.20833333 0.00696309
 0.10000000 6.96 H_{freq3} : 7.91746806 6.36651842 0.25908549 0.20833333 0.00257578
 0.10000000 2.58 H_{freq4} : 9.80196341 6.40050186 0.31904931 0.20833333 0.01225803
 0.10000000 12.26 H_{freq5} : 9.80196341 7.64082373 0.26725858 0.20833333 0.00347218
 0.10000000 3.47 bandw. G: 5.07492538 5.87085872 1.44071070 1.66666667
 0.05105610 15.00000000 7658.41 bandw. K: 6.24501541 4.97424321 1.14133678
 0.90909091 0.05393815 15.00000000 8090.72 bandw. M: 7.01645849 7.78109872
 1.50288512 1.66666667 0.02682440 15.00000000 4023.66 bandw. L: 5.76609484
 6.34433701 1.51476160 1.66666667 0.02307515 15.00000000 3461.27 bandw.
 H: 4.78376344 9.70902614 0.44792091 0.90909091 0.21267777 5.00000000 10633.89
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 89.69636402 0.00000000 89.69636402 0.00000000 8045.43771884
 0.00000000 0.00 E_{prisf}: 149.66676941 220.00000000 149.66676941 220.00000000
 4946.76332459 0.00100000 49467.63

PARAMETERS b2=130679778.1946621835 m2=-15.3111362455 p2=0.0000000000
fdd=0.2648249504 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849
b0=48.8761303111 p0=1.0940394499 b1=-5.5045229932 p1=0.7069982325 ndt=2.0000000000
cr1=-6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000
cr3=-1.1418272350 rmaxhm=10.1000000000 npar=18 VARGS -vb2=130679778.1946621835
-vm2=-15.3111362455 -vp2=0.0000000000 -vfdd=0.2648249504 -vqdds=0.5697753882
-vqddp=0.5648597117 -vqddd=0.8213593849 -vb0=48.8761303111 -vp0=1.0940394499
-vb1=-5.5045229932 -vp1=0.7069982325 -vndt=2.0000000000 -vcr1=-6.0000000000
-vcr2=3.2217589360 -vr1dd=6.5000000000 -vrdd=10.0000000000 -vcr3=-1.1418272350
-vrm axhm=10.1000000000

Quantity predicted target norm_{pred} norm_{tar} sq diff. weight objective *
100²

a_{hcp} : 5.59394485 5.57678969 5.59394485 5.57678969 0.00029430 1000.00000000
2943.00 c/a : 1.61957050 1.58731122 15.72502939 15.41181168 0.09810533
100.00000000 98105.33 a_{omega} : 8.91852283 8.73254342 1.11481535 1.09156793
0.00054044 10.00000000 54.04 c_{omega} : 5.42487248 5.32343103 0.67810906
0.66542888 0.00016079 10.00000000 16.08 a_{4h} : 5.58776045 5.56325146 1.00440552
1.00000000 0.00001941 1.00000000 0.19 c_{4h} : 18.10977036 17.75908031 1.01974708
1.00000000 0.00038995 1.00000000 3.90 a_{6h} : 5.58284146 5.54639384 1.00657141
1.00000000 0.00004318 1.00000000 0.43 c_{6h} : 27.22998269 26.77136353 1.01713096
1.00000000 0.00029347 1.00000000 2.93 a_{bcc} : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.88599981 7.88677000 1.12657140
1.12668143 0.00000001 1.00000000 0.00 DE(o,h) : -0.16436500 -0.63343333 -
0.01095767 -0.04222889 0.00097789 3000.00000000 29336.68 DE(4h,h): 1.92960000
3.17160000 0.00771840 0.01268640 0.00002468 2000.00000000 493.62 DE(6h,h):
2.89581667 3.72005000 0.01158327 0.01488020 0.00001087 2000.00000000 217.40
DE(b,h) : 7.08288500 7.63520000 0.07154429 0.07712323 0.00003112 1.00000000
0.31 DE(f,h) : 4.35564500 4.51880000 0.04399641 0.04564444 0.00000272
2000.00000000 54.32 c₁₁ : 185.11668534 176.10000000 0.80861698 0.76923077
0.00155127 100.00000000 1551.27 c₃₃ : 212.84704018 190.50000000 0.85946715
0.76923077 0.00814260 100.00000000 8142.60 c₄₄ : 49.02224879 50.80000000
0.74231146 0.76923077 0.00072465 100.00000000 724.65 c₁₂ : 88.29471524
86.90000000 0.78157666 0.76923077 0.00015242 100.00000000 152.42 c₁₃ :
68.20905158 68.30000000 0.76820646 0.76923077 0.00000105 10.00000000 0.10
M_{freq0}: 2.66125192 2.85858719 0.19395157 0.20833333 0.00020684 0.10000000
0.21 M_{freq1}: 2.66125193 2.85858719 0.19395157 0.20833333 0.00020683 0.10000000
0.21 M_{freq2}: 2.66125193 2.85858719 0.19395157 0.20833333 0.00020683 0.10000000
0.21 M_{freq3}: 2.66125194 2.85858719 0.19395158 0.20833333 0.00020683 0.10000000
0.21 M_{freq4}: 5.73420882 5.66706047 0.21080185 0.20833333 0.00000609 0.10000000

0.01 M_{freq5}: 5.73420882 5.66706047 0.21080185 0.20833333 0.00000609 0.10000000
 0.01 H_{freq0}: 3.68634494 4.80643423 0.15978343 0.20833333 0.00235709 0.10000000
 2.36 H_{freq1}: 3.68634494 5.58010025 0.13762988 0.20833333 0.00499898 0.10000000
 5.00 H_{freq2}: 6.27448914 5.65316738 0.23123059 0.20833333 0.00052428 0.10000000
 0.52 H_{freq3}: 6.27448914 6.36651842 0.20532183 0.20833333 0.00000907 0.10000000
 0.01 H_{freq4}: 7.93614996 6.40050186 0.25831796 0.20833333 0.00249846 0.10000000
 2.50 H_{freq5}: 7.93614996 7.64082373 0.21638565 0.20833333 0.00006484 0.10000000
 0.06 bandw. G: 4.97016150 5.87085872 1.41096949 1.66666667 0.06538105
 15.00000000 9807.16 bandw. K: 6.12664584 4.97424321 1.11970360 0.90909091
 0.04435771 15.00000000 6653.66 bandw. M: 6.91169462 7.78109872 1.48044530
 1.66666667 0.03467840 15.00000000 5201.76 bandw. L: 5.64364356 6.34433701
 1.48259347 1.66666667 0.03388294 15.00000000 5082.44 bandw. H: 4.70348982
 9.70902614 0.44040461 0.90909091 0.21966685 5.00000000 10983.34 DOS_{errh}:
 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00
 DOS_{errc}: 107.73527467 0.00000000 107.73527467 0.00000000 11606.88940800
 0.00000000 0.00 E_{prisf}: 70.96500541 220.00000000 70.96500541 220.00000000
 22211.42961214 0.00100000 222114.30

1.3 2019-10-07

PARAMETERS fdd=0.2261942778 qdds=0.5664527218 qddp=0.5712409615
 qddd=0.8090890053 b0=54.99305039 p0=1.056186014 b1=-6.938531357 p1=0.6609658271
 b2=1000000.001 m2=-11.99023426 cr2=3.21797029 cr3=-1.138783313 p2=0.0
 cr1=-6.0 ndt=2.0 r1dd=6.5 rcdd=10. rmaxhm=10.001 VARGS -vfdd=0.2261942778
 -vqdds=0.5664527218 -vqddp=0.5712409615 -vqddd=0.8090890053 -vb0=54.99305039
 -vp0=1.056186014 -vb1=-6.938531357 -vp1=0.6609658271 -vb2=1000000.001
 -vm2=-11.99023426 -vcr2=3.21797029 -vcr3=-1.138783313 -vp2=0.0 -vcr1=-
 6.0 -vndt=2.0 -vr1dd=6.5 -vrdd=10. -vrmaxhm=10.001
 a_{hcp}: 5.58591188 5.57678969 5.58591188 5.57678969 0.00008321 1000.00000000
 832.14 c/a : 1.58342293 1.58731122 15.37405881 15.41181168 0.00142528
 100.00000000 1425.28 a_{omega}: 8.92927545 8.73254342 1.11615943 1.09156793
 0.00060474 10.00000000 60.47 c_{omega}: 5.39273370 5.32343103 0.67409171
 0.66542888 0.00007504 10.00000000 7.50 a_{4h}: 5.58700970 5.56325146 1.00427057
 1.00000000 0.00001824 1.00000000 0.18 c_{4h}: 18.06580652 17.75908031 1.01727151
 1.00000000 0.00029831 1.00000000 2.98 a_{6h}: 5.58286246 5.54639384 1.00657519
 1.00000000 0.00004323 1.00000000 0.43 c_{6h}: 27.17218246 26.77136353 1.01497193
 1.00000000 0.00022416 1.00000000 2.24 a_{bcc}: 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc}: 7.88407433 7.88677000 1.12629633
 1.12668143 0.00000015 1.00000000 0.00 DE(o,h): -0.57202167 -0.63343333 -
 0.03813478 -0.04222889 0.00001676 3000.00000000 502.85 DE(4h,h): 2.19219750

3.17160000 0.00876879 0.01268640 0.00001535 2000.00000000 306.95 DE(6h,h):
 3.22577000 3.72005000 0.01290308 0.01488020 0.00000391 2000.00000000 78.18
 DE(b,h) : 6.00302500 7.63520000 0.06063662 0.07712323 0.00027181 1.00000000
 2.72 DE(f,h) : 4.81109500 4.51880000 0.04859692 0.04564444 0.00000872
 2000.00000000 174.34 c_{11} : 195.72594081 176.10000000 0.85495977 0.76923077
 0.00734946 100.00000000 7349.46 c_{33} : 258.13627281 190.50000000 1.04234312
 0.76923077 0.07459035 100.00000000 74590.35 c_{44} : 57.53149355 50.80000000
 0.87116132 0.76923077 0.01038984 100.00000000 10389.84 c_{12} : 119.83029939
 86.90000000 1.06072674 0.76923077 0.08496990 100.00000000 84969.90 c_{13}
 : 77.31249136 68.30000000 0.87073422 0.76923077 0.01030295 10.00000000
 1030.30 $M_{\text{freq}0}$: 2.92665742 2.85858719 0.21329428 0.20833333 0.00002461
 0.10000000 0.02 $M_{\text{freq}1}$: 2.92665743 2.85858719 0.21329428 0.20833333 0.00002461
 0.10000000 0.02 $M_{\text{freq}2}$: 2.92665743 2.85858719 0.21329428 0.20833333 0.00002461
 0.10000000 0.02 $M_{\text{freq}3}$: 2.92665744 2.85858719 0.21329428 0.20833333 0.00002461
 0.10000000 0.02 $M_{\text{freq}4}$: 7.04526852 5.66706047 0.25899923 0.20833333 0.00256703
 0.10000000 2.57 $M_{\text{freq}5}$: 7.04526852 5.66706047 0.25899923 0.20833333 0.00256703
 0.10000000 2.57 $H_{\text{freq}0}$: 4.10916401 4.80643423 0.17811038 0.20833333 0.00091343
 0.10000000 0.91 $H_{\text{freq}1}$: 4.10916401 5.58010025 0.15341585 0.20833333 0.00301593
 0.10000000 3.02 $H_{\text{freq}2}$: 8.03266476 5.65316738 0.29602375 0.20833333 0.00768961
 0.10000000 7.69 $H_{\text{freq}3}$: 8.03266476 6.36651842 0.26285510 0.20833333 0.00297262
 0.10000000 2.97 $H_{\text{freq}4}$: 9.85602686 6.40050186 0.32080905 0.20833333 0.01265079
 0.10000000 12.65 $H_{\text{freq}5}$: 9.85602686 7.64082373 0.26873267 0.20833333 0.00364808
 0.10000000 3.65 bandw. G: 4.23273267 5.87085872 1.20162225 1.66666667
 0.21626631 15.00000000 32439.95 bandw. K: 5.27765028 4.97424321 0.96454148
 0.90909091 0.00307477 15.00000000 461.21 bandw. M: 5.92256037 7.78109872
 1.26857842 1.66666667 0.15847425 15.00000000 23771.14 bandw. L: 4.82321996
 6.34433701 1.26706698 1.66666667 0.15967991 15.00000000 23951.99 bandw.
 H: 4.03681062 9.70902614 0.37798104 0.90909091 0.28207769 5.00000000 14103.88
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 122.59561685 220.00000000 122.59561685 220.00000000
 9487.61385619 0.00500000 474380.69
 ———— E_{prismaticfault} ————
 tbe: 122.596 mJ/m² DFT: 250.000 mJ/m² [Benoit 2012] DFT: 233.000
 mJ/m² [Ackland 1999]
 ———— E_{Basalfault} I2 ————
 tbe: 285.525 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]
 fdd=0.2515488168 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849
 b0=46.3898409291 p0=1.0722677474 b1=-5.6805371975 p1=0.6950452201 b2=960581.6752016575
 m2=-12.0000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000

```

cr2=3.2217589360 cr3=-1.1418272350 r1dd=6.5000000000 rcdd=10.0000000000
rmaxhm=10.1000000000 npar=18
    fdd=0.2515488168 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849
b0=46.3898409291 p0=1.0722677474 b1=-5.6805371975 p1=0.6950452201 b2=960581.6752016575
m2=-12.0000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
cr2=3.2217589360 cr3=-1.1418272350 r1dd=6.5000000000 rcdd=10.0000000000
rmaxhm=10.1000000000 npar=18
    fdd=0.2449247182502603 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849
b0=44.11762729189705 p0=1.0722677474 b1=-5.498594119584881 p1=0.6950452201
b2=864579.3223157182 m2=-12.0000000000 p2=0.0000000000 ndt=2.0000000000
cr1=-6.0000000000 cr2=3.22250077 cr3=-1.12845174 r1dd=6.45 rcdd=9.95
rmaxhm=9.96 npar=18
    fdd=0.2449247182502603 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849
b0=44.11762729189705 p0=1.0722677474 b1=-5.498594119584881 p1=0.6950452201
b2=864579.3223157182 m2=-12.0000000000 p2=0.0000000000 ndt=2.0000000000
cr1=-6.0000000000 cr2=3.22250077 cr3=-1.12845174 r1dd=6.45 rcdd=9.95
rmaxhm=9.96 npar=18

```

```

ahcp : 5.62362601 5.57678969 5.62362601 5.57678969 0.00219364 1000.00000000
21936.41 c/a : 1.60683364 1.58731122 15.60136234 15.41181168 0.03592945
100.00000000 35929.45 aomega : 8.96530627 8.73254342 1.12066328 1.09156793
0.00084654 10.00000000 84.65 comega : 5.44545760 5.32343103 0.68068220
0.66542888 0.00023266 10.00000000 23.27 a4h : 5.61947656 5.56325146 1.01010652
1.00000000 0.00010214 1.00000000 1.02 c4h : 18.20047945 17.75908031 1.02485484
1.00000000 0.00061776 1.00000000 6.18 a6h : 5.61467225 5.54639384 1.01231041
1.00000000 0.00015155 1.00000000 1.52 c6h : 27.37307845 26.77136353 1.02247607
1.00000000 0.00050517 1.00000000 5.05 abcc : 6.20079768 6.17948863 0.88582824
0.88278409 0.0000927 1.00000000 0.09 afcc : 7.93028587 7.88677000 1.13289798
1.12668143 0.00003865 1.00000000 0.39 DE(o,h) : -0.44450000 -0.63343333 -
0.02963333 -0.04222889 0.00015865 3000.00000000 4759.44 DE(4h,h): 1.87517500
3.17160000 0.00750070 0.01268640 0.00002689 2000.00000000 537.83 DE(6h,h):
2.80478500 3.72005000 0.01121914 0.01488020 0.00001340 2000.00000000 268.07
DE(b,h) : 6.71875000 7.63520000 0.06786616 0.07712323 0.00008569 1.00000000
0.86 DE(f,h) : 4.21450000 4.51880000 0.04257071 0.04564444 0.00000945
2000.00000000 188.96 c11 : 177.59548914 176.10000000 0.77576329 0.76923077
0.00004267 100.00000000 42.67 c33 : 207.27557549 190.50000000 0.83696982
0.76923077 0.00458858 100.00000000 4588.58 c44 : 46.83138756 50.80000000
0.70913670 0.76923077 0.00361130 100.00000000 3611.30 c12 : 92.58911362
86.90000000 0.81959028 0.76923077 0.00253608 100.00000000 2536.08 c13
: 65.11602787 68.30000000 0.73337119 0.76923077 0.00128591 10.00000000

```

128.59 M_{freq0}: 2.60924783 2.85858719 0.19016152 0.20833333 0.00033021
 0.10000000 0.33 M_{freq1}: 2.60924784 2.85858719 0.19016153 0.20833333 0.00033021
 0.10000000 0.33 M_{freq2}: 2.60924784 2.85858719 0.19016153 0.20833333 0.00033021
 0.10000000 0.33 M_{freq3}: 2.60924785 2.85858719 0.19016153 0.20833333 0.00033021
 0.10000000 0.33 M_{freq4}: 5.74942187 5.66706047 0.21136112 0.20833333 0.00000917
 0.10000000 0.01 M_{freq5}: 5.74942187 5.66706047 0.21136112 0.20833333 0.00000917
 0.10000000 0.01 H_{freq0}: 3.68898659 4.80643423 0.15989793 0.20833333 0.00234599
 0.10000000 2.35 H_{freq1}: 3.68898659 5.58010025 0.13772851 0.20833333 0.00498504
 0.10000000 4.99 H_{freq2}: 6.37014102 5.65316738 0.23475560 0.20833333 0.00069814
 0.10000000 0.70 H_{freq3}: 6.37014102 6.36651842 0.20845188 0.20833333 0.00000001
 0.10000000 0.00 H_{freq4}: 7.97198243 6.40050186 0.25948429 0.20833333 0.00261642
 0.10000000 2.62 H_{freq5}: 7.97198243 7.64082373 0.21736265 0.20833333 0.00008153
 0.10000000 0.08 bandw. G: 4.61369221 5.87085872 1.30977211 1.66666667
 0.12737372 15.00000000 19106.06 bandw. K: 5.69806635 4.97424321 1.04137657
 0.90909091 0.01749950 15.00000000 2624.92 bandw. M: 6.45726430 7.78109872
 1.38310894 1.66666667 0.08040499 15.00000000 12060.75 bandw. L: 5.24635717
 6.34433701 1.37822575 1.66666667 0.08319816 15.00000000 12479.72 bandw.
 H: 4.38375592 9.70902614 0.41046678 0.90909091 0.24862603 1.00000000 2486.26
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 71.63846063 220.00000000 71.63846063 220.00000000
 22011.14636552 0.00100000 22011.146

1.4 Old Model 2019-03-09

fdd=0.2035564745 cr1=-6.0 cr2=4.024019531 cr3=-1.036884044 qdds=0.5795947819
 qddp=0.5074989694 qddd=0.6628469935 b0=112.9273696 p0=1.563016808
 ndt=1.982104151 r1=5.398570666 rc=7.489291495

1.5 2019-10-10

PARAMETERS fdd=0.2478914348 qdds=0.5723805692 qddp=0.5630575383
 qddd=0.8242396486 b0=61.1218169232 p0=1.1591391821 b1=-4.9392678163
 p1=0.7150006285 b2=335658824.3278234601 m2=-17.73 72494877 p2=0.0000000000
 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.0800670723 cr3=-1.1641220819
 r1dd=6.5000000000 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18
 VARGS -vfdd=0.2478914348 -vqdds=0.5723805692 -vqddp=0.5630575383 -
 vqddd=0.8242396486 -vb0=61.1218169232 -vp0=1.1591391821 -vb1=-4.9392678163
 -vp1=0.7150006285 -vb2=335658824. 3278234601 -vm2=-17.7372494877 -
 vp2=0.0000000000 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.0800670723

-vcr3=-1.1641220819 -vr1dd=6.5000000000 -vrcdd=10.0000000000 -vrm axhm=10.1000000000
 a_{hcp} : 5.66474394 5.57678969 5.66474394 5.57678969 0.00773595 1000.00000000
 77359.50 c/a : 1.58940952 1.58731122 15.43218494 15.41181168 0.00041507
 100.00000000 415.07 a_{omega} : 9.02970550 8.73254342 1.12871319 1.09156793
 0.00137977 10.00000000 137.98 c_{omega} : 5.47185464 5.32343103 0.68398183
 0.66542888 0.00034421 10.00000000 34.42 a_{4h} : 5.65712368 5.56325146 1.01687363
 1.00000000 0.00028472 1.00000000 2.85 c_{4h} : 18.34959344 17.75908031 1.03325133
 1.00000000 0.00110565 1.00000000 11.06 a_{6h} : 5.65344314 5.54639384 1.01930070
 1.00000000 0.00037252 1.00000000 3.73 c_{6h} : 27.58068315 26.77136353 1.03023080
 1.00000000 0.00091390 1.00000000 9.14 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.98650991 7.88677000 1.14092999
 1.12668143 0.00020302 1.00000000 2.03 DE(o,h) : -0.21705167 -0.63343333 -
 0.01447011 -0.04222889 0.00077055 3000.00000000 23116.49 DE(4h,h): 1.73339500
 3.17160000 0.00693358 0.01268640 0.00003309 2000.00000000 661.90 DE(6h,h):
 2.61423000 3.72005000 0.01045692 0.01488020 0.00001957 2000.00000000 391.31
 DE(b,h) : 6.58034500 7.63520000 0.06646813 0.07712323 0.00011353 1.00000000
 1.14 DE(f,h) : 3.94049500 4.51880000 0.03980298 0.04564444 0.00003412
 2000.00000000 682.45 c₁₁ : 173.23939280 176.10000000 0.75673522 0.76923077
 0.00015614 100.00000000 156.14 c₃₃ : 191.81249380 190.50000000 0.77453056
 0.76923077 0.00002809 100.00000000 28.09 c₄₄ : 45.70455006 50.80000000
 0.69207374 0.76923077 0.00595321 100.00000000 5953.21 c₁₂ : 96.20344238
 86.90000000 0.85158398 0.76923077 0.00678205 100.00000000 6782.05 c₁₃
 : 64.10074478 68.30000000 0.72193653 0.76923077 0.00223674 10.00000000
 223.67 M_{freq0}: 2.51985659 2.85858719 0.18364671 0.20833333 0.00060943
 0.10000000 0.61 M_{freq1}: 2.51985660 2.85858719 0.18364671 0.20833333 0.00060943
 0.10000000 0.61 M_{freq2}: 2.51985660 2.85858719 0.18364671 0.20833333 0.00060943
 0.10000000 0.61 M_{freq3}: 2.51985661 2.85858719 0.18364671 0.20833333 0.00060943
 0.10000000 0.61 M_{freq4}: 5.54530787 5.66706047 0.20385745 0.20833333 0.00002003
 0.10000000 0.02 M_{freq5}: 5.54530787 5.66706047 0.20385745 0.20833333 0.00002003
 0.10000000 0.02 H_{freq0}: 3.77465002 4.80643423 0.16361098 0.20833333 0.00200009
 0.10000000 2.00 H_{freq1}: 3.77465002 5.58010025 0.14092675 0.20833333 0.00454365
 0.10000000 4.54 H_{freq2}: 6.09045606 5.65316738 0.22444851 0.20833333 0.00025970
 0.10000000 0.26 H_{freq3}: 6.09045606 6.36651842 0.19929967 0.20833333 0.00008161
 0.10000000 0.08 H_{freq4}: 7.57838063 6.40050186 0.24667273 0.20833333 0.00146991
 0.10000000 1.47 H_{freq5}: 7.57838063 7.64082373 0.20663077 0.20833333 0.00000290
 0.10000000 0.00 bandw. G: 4.29531888 5.87085872 1.21938972 1.66666667
 0.20005666 15.00000000 30008.50 bandw. K: 5.33887592 4.97424321 0.97573105
 0.90909091 0.00444091 15.00000000 666.14 bandw. M: 6.08446818 7.78109872
 1.30325815 1.66666667 0.13206575 15.00000000 19809.86 bandw. L: 4.91029643
 6.34433701 1.28994210 1.66666667 0.14192140 15.00000000 21288.21 bandw.

H: 4.11980537 9.70902614 0.38575214 0.90909091 0.27388347 1.00000000 2738.83
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 71.46811807 220.00000000 71.46811807 220.00000000
 22061.71994819 0.00100000 220617.20
 PARAMETERS fdd=0.2151013501 qdds=0.5666199051 qddp=0.5703036385
 qddd=0.7886982335 b0=55.5349940695 p0=1.0444219716 b1=-7.4709376307
 p1=0.6559635325 b2=695593.0193127145 m2=-11.62483 95708 p2=0.0000000000
 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2788469049 cr3=-1.0671505847
 r1dd=6.5000000000 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18
 VARGS -vfdd=0.2151013501 -vqdds=0.5666199051 -vqddp=0.5703036385 -
 vqddd=0.7886982335 -vb0=55.5349940695 -vp0=1.0444219716 -vb1=-7.4709376307
 -vp1=0.6559635325 -vb2=695593.019 3127145 -vm2=-11.6248395708 -vp2=0.0000000000
 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.2788469049 -vcr3=-1.0671505847
 -vr1dd=6.5000000000 -vrcdd=10.0000000000 -vrmaxh m=10.1000000000
 a_{hcp}: 5.56698674 5.57678969 5.56698674 5.57678969 0.00009610 1000.00000000
 960.98 c/a : 1.59150388 1.58731122 15.45251985 15.41181168 0.00165716
 100.00000000 1657.16 a_{omega}: 8.90180505 8.73254342 1.11272563 1.09156793
 0.00044765 10.00000000 44.76 c_{omega}: 5.37893446 5.32343103 0.67236681
 0.66542888 0.00004813 10.00000000 4.81 a_{4h}: 5.56958507 5.56325146 1.00113847
 1.00000000 0.00000130 1.00000000 0.01 c_{4h}: 17.99600023 17.75908031 1.01334078
 1.00000000 0.00017798 1.00000000 1.78 a_{6h}: 5.56465381 5.54639384 1.00329222
 1.00000000 0.00001084 1.00000000 0.11 c_{6h}: 27.07486744 26.77136353 1.01133689
 1.00000000 0.00012852 1.00000000 1.29 a_{bcc}: 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc}: 7.85731014 7.88677000 1.12247288
 1.12668143 0.00001771 1.00000000 0.18 DE(o,h): -0.23007667 -0.63343333 -
 0.01533844 -0.04222889 0.00072310 3000.00000000 21692.88 DE(4h,h): 2.19581250
 3.17160000 0.00878325 0.01268640 0.00001523 2000.00000000 304.69 DE(6h,h):
 3.22734000 3.72005000 0.01290936 0.01488020 0.00000388 2000.00000000 77.68
 DE(b,h): 6.35131000 7.63520000 0.06415465 0.07712323 0.00016818 1.00000000
 1.68 DE(f,h): 4.81041000 4.51880000 0.04859000 0.04564444 0.00000868
 2000.00000000 173.53 c₁₁: 201.21117275 176.10000000 0.87892007 0.76923077
 0.01203174 100.00000000 12031.74 c₃₃: 282.98882144 190.50000000 1.14269663
 0.76923077 0.13947675 100.00000000 139476.75 c₄₄: 61.86278193 50.80000000
 0.93674715 0.76923077 0.02806174 100.00000000 28061.74 c₁₂: 118.89036883
 86.90000000 1.05240656 0.76923077 0.08018853 100.00000000 80188.53 c₁₃
 : 79.47820909 68.30000000 0.89512568 0.76923077 0.01584953 10.00000000
 1584.95 M_{freq0}: 3.05776487 2.85858719 0.22284937 0.20833333 0.00021072
 0.10000000 0.21 M_{freq1}: 3.05776488 2.85858719 0.22284937 0.20833333 0.00021072
 0.10000000 0.21 M_{freq2}: 3.05776488 2.85858719 0.22284937 0.20833333 0.00021072

0.10000000 0.21 M_{freq3}: 3.05776489 2.85858719 0.22284937 0.20833333 0.00021072
 0.10000000 0.21 M_{freq4}: 7.42734007 5.66706047 0.27304500 0.20833333 0.00418760
 0.10000000 4.19 M_{freq5}: 7.42734007 5.66706047 0.27304500 0.20833333 0.00418760
 0.10000000 4.19 H_{freq0}: 4.19663169 4.80643423 0.18190164 0.20833333 0.00069863
 0.10000000 0.70 H_{freq1}: 4.19663169 5.58010025 0.15668146 0.20833333 0.00266792
 0.10000000 2.67 H_{freq2}: 8.51190520 5.65316738 0.31368496 0.20833333 0.01109897
 0.10000000 11.10 H_{freq3}: 8.51190520 6.36651842 0.27853742 0.20833333 0.00492861
 0.10000000 4.93 H_{freq4}: 10.42571059 6.40050186 0.33935199 0.20833333 0.01716589
 0.10000000 17.17 H_{freq5}: 10.42571059 7.64082373 0.28426556 0.20833333 0.00576570
 0.10000000 5.77 bandw. G: 4.13885335 5.87085872 1.17497103 1.66666667
 0.24176460 15.00000000 36264.69 bandw. K: 5.11574247 4.97424321 0.93495126
 0.90909091 0.00066876 15.00000000 100.31 bandw. M: 5.73752287 7.78109872
 1.22894445 1.66666667 0.19160074 15.00000000 28740.11 bandw. L: 4.70348982
 6.34433701 1.23561370 1.66666667 0.18580666 15.00000000 27871.00 bandw.
 H: 3.91163819 9.70902614 0.36626070 0.90909091 0.29466463 1.00000000 2946.65
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 151.38581994 220.00000000 151.38581994 220.00000000
 4707.90570585 0.00500000 235395.29

PARAMETERS fdd=0.2243711367 qdds=0.5653512020 qddp=0.5721196188
 qddd=0.8143953019 b0=52.3247601320 p0=1.0668199432 b1=-6.3005518996
 p1=0.6642213490 b2=1690361.2028581987 m2=-11.8088480025 p2=0.0000000000
 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.4750555290 cr3=-1.0037421668
 r1dd=6.5000000000 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18
 VARGS -vfdd=0.2243711367 -vqdds=0.5653512020 -vqddp=0.5721196188 -
 vqddd=0.8143953019 -vb0=52.3247601320 -vp0=1.0668199432 -vb1=-6.3005518996
 -vp1=0.6642213490 -vb2=1690361.2028581987 -vm2=-11.8088480025 -vp2=0.0000000000
 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.4750555290 -vcr3=-1.0037421668
 -vr1dd=6.5000000000 -vrcdd=10.0000000000 -vrmax hm=10.1000000000

a_{hcp} : 5.59830172 5.57678969 5.59830172 5.57678969 0.00046277 1000.00000000
 4627.67 c/a : 1.61769241 1.58731122 15.70679431 15.41181168 0.08701475
 100.00000000 87014.75 a_{omega} : 8.95229597 8.73254342 1.11903700 1.09156793
 0.00075455 10.00000000 75.45 c_{omega} : 5.40810121 5.32343103 0.67601265
 0.66542888 0.00011202 10.00000000 11.20 a_{4h} : 5.59669837 5.56325146 1.00601212
 1.00000000 0.00003615 1.00000000 0.36 c_{4h} : 18.11607854 17.75908031 1.02010229
 1.00000000 0.00040410 1.00000000 4.04 a_{6h} : 5.59174945 5.54639384 1.00817749
 1.00000000 0.00006687 1.00000000 0.67 c_{6h} : 27.24862578 26.77136353 1.01782734
 1.00000000 0.00031781 1.00000000 3.18 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.89870798 7.88677000 1.12838685
 1.12668143 0.00000291 1.00000000 0.03 DE(o,h) : 0.63388833 -0.63343333

0.04225922 -0.04222889 0.00713824 3000.00000000 214147.23 DE(4h,h): 2.04125750
 3.17160000 0.00816503 0.01268640 0.00002044 2000.00000000 408.86 DE(6h,h):
 2.96233167 3.72005000 0.01184933 0.01488020 0.00000919 2000.00000000 183.72
 DE(b,h) : 6.77016500 7.63520000 0.06838551 0.07712323 0.00007635 1.00000000
 0.76 DE(f,h) : 4.41522500 4.51880000 0.04459823 0.04564444 0.00000109
 2000.00000000 21.89 c₁₁ : 207.65376176 176.10000000 0.90706225 0.76923077
 0.01899752 100.00000000 18997.52 c₃₃ : 268.62634307 190.50000000 1.08470157
 0.76923077 0.09952182 100.00000000 99521.82 c₄₄ : 58.45068406 50.80000000
 0.88508001 0.76923077 0.01342105 100.00000000 13421.05 c₁₂ : 116.05395320
 86.90000000 1.02729887 0.76923077 0.06659914 100.00000000 66599.14 c₁₃
 : 76.95347435 68.30000000 0.86669078 0.76923077 0.00949845 10.00000000
 949.85 M_{freq0}: 3.03927381 2.85858719 0.22150174 0.20833333 0.00017341
 0.10000000 0.17 M_{freq1}: 3.03927382 2.85858719 0.22150174 0.20833333 0.00017341
 0.10000000 0.17 M_{freq2}: 3.03927382 2.85858719 0.22150174 0.20833333 0.00017341
 0.10000000 0.17 M_{freq3}: 3.03927383 2.85858719 0.22150174 0.20833333 0.00017341
 0.10000000 0.17 M_{freq4}: 7.03885403 5.66706047 0.25876342 0.20833333 0.00254319
 0.10000000 2.54 M_{freq5}: 7.03885403 5.66706047 0.25876342 0.20833333 0.00254319
 0.10000000 2.54 H_{freq0}: 4.32899865 4.80643423 0.18763904 0.20833333 0.00042825
 0.10000000 0.43 H_{freq1}: 4.32899865 5.58010025 0.16162339 0.20833333 0.00218182
 0.10000000 2.18 H_{freq2}: 7.99516633 5.65316738 0.29464184 0.20833333 0.00744916
 0.10000000 7.45 H_{freq3}: 7.99516633 6.36651842 0.26162803 0.20833333 0.00284032
 0.10000000 2.84 H_{freq4}: 9.77982943 6.40050186 0.31832886 0.20833333 0.01209902
 0.10000000 12.10 H_{freq5}: 9.77982943 7.64082373 0.26665508 0.20833333 0.00340143
 0.10000000 3.40 bandw. G: 4.31300629 5.87085872 1.22441097 1.66666667
 0.19559010 15.00000000 29338.52 bandw. K: 5.32935193 4.97424321 0.97399045
 0.90909091 0.00421195 15.00000000 631.79 bandw. M: 6.00963684 7.78109872
 1.28722970 1.66666667 0.14397241 15.00000000 21595.86 bandw. L: 4.89941187
 6.34433701 1.28708271 1.66666667 0.14408398 15.00000000 21612.60 bandw.
 H: 4.08579113 9.70902614 0.38256726 0.90909091 0.27722715 1.00000000 2772.27
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 183.97074239 220.00000000 183.97074239 220.00000000
 1298.10740414 0.00500000 64905.37

fdd=0.2280981517 qdds=0.5663999501 qddp=0.5712979200 qddd=0.7958377449
 b0=55.8948852278 p0=1.0311770126 b1=-8.3348062528 p1=0.6672269668 b2=869260.9536906204
 m2=-11.6635538235 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
 cr2=3.4490441369 cr3=-1.1322198342 r1dd=6.5000000000 rcdd=10.0000000000
 rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.60701545 5.57678969 5.60701545 5.57678969 0.00091360 1000.00000000

9135.97 c/a : 1.61394499 1.58731122 15.67040917 15.41181168 0.06687266
 100.00000000 66872.66 a_{omega} : 8.95826615 8.73254342 1.11978327 1.09156793
 0.00079611 10.00000000 79.61 c_{omega} : 5.41481999 5.32343103 0.67685250
 0.66542888 0.00013050 10.00000000 13.05 a_{4h} : 5.61000069 5.56325146 1.00840322
 1.00000000 0.00007061 1.00000000 0.71 c_{4h} : 18.12679473 17.75908031 1.02070571
 1.00000000 0.00042873 1.00000000 4.29 a_{6h} : 5.60488746 5.54639384 1.01054624
 1.00000000 0.00011122 1.00000000 1.11 c_{6h} : 27.27752577 26.77136353 1.01890685
 1.00000000 0.00035747 1.00000000 3.57 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.91488202 7.88677000 1.13069743
 1.12668143 0.00001613 1.00000000 0.16 $DE(o,h)$: -0.30625667 -0.63343333 -
 0.02041711 -0.04222889 0.00047575 3000.00000000 14272.61 $DE(4h,h)$: 2.08756000
 3.17160000 0.00835024 0.01268640 0.00001880 2000.00000000 376.05 $DE(6h,h)$:
 3.09943000 3.72005000 0.01239772 0.01488020 0.00000616 2000.00000000 123.25
 $DE(b,h)$: 6.89060000 7.63520000 0.06960202 0.07712323 0.00005657 1.00000000
 0.57 $DE(f,h)$: 4.64386000 4.51880000 0.04690768 0.04564444 0.00000160
 2000.00000000 31.92 c_{11} : 204.01698509 176.10000000 0.89117628 0.76923077
 0.01487071 100.00000000 14870.71 c_{33} : 276.62832250 190.50000000 1.11701321
 0.76923077 0.12095263 100.00000000 120952.63 c_{44} : 59.70541492 50.80000000
 0.90407957 0.76923077 0.01818420 100.00000000 18184.20 c_{12} : 124.20099527
 86.90000000 1.09941573 0.76923077 0.10902211 100.00000000 109022.11 c_{13}
 : 77.17820459 68.30000000 0.86922181 0.76923077 0.00999821 10.00000000
 999.82 $M_{\text{freq}0}$: 3.06693012 2.85858719 0.22351733 0.20833333 0.00023055
 0.10000000 0.23 $M_{\text{freq}1}$: 3.06693013 2.85858719 0.22351733 0.20833333 0.00023055
 0.10000000 0.23 $M_{\text{freq}2}$: 3.06693013 2.85858719 0.22351733 0.20833333 0.00023055
 0.10000000 0.23 $M_{\text{freq}3}$: 3.06693015 2.85858719 0.22351733 0.20833333 0.00023055
 0.10000000 0.23 $M_{\text{freq}4}$: 7.24323456 5.66706047 0.26627688 0.20833333 0.00335745
 0.10000000 3.36 $M_{\text{freq}5}$: 7.24323456 5.66706047 0.26627688 0.20833333 0.00335745
 0.10000000 3.36 $H_{\text{freq}0}$: 4.27628506 4.80643423 0.18535419 0.20833333 0.00052804
 0.10000000 0.53 $H_{\text{freq}1}$: 4.27628506 5.58010025 0.15965533 0.20833333 0.00236955
 0.10000000 2.37 $H_{\text{freq}2}$: 8.33964444 5.65316738 0.30733672 0.20833333 0.00980167
 0.10000000 9.80 $H_{\text{freq}3}$: 8.33964444 6.36651842 0.27290048 0.20833333 0.00416892
 0.10000000 4.17 $H_{\text{freq}4}$: 10.17262803 6.40050186 0.33111427 0.20833333 0.01507516
 0.10000000 15.08 $H_{\text{freq}5}$: 10.17262803 7.64082373 0.27736506 0.20833333 0.00476538
 0.10000000 4.77 bandw. G : 4.36062623 5.87085872 1.23792970 1.66666667
 0.18381538 15.00000000 27572.31 bandw. K : 5.34703934 4.97424321 0.97722300
 0.90909091 0.00464198 15.00000000 696.30 bandw. M : 6.05453564 7.78109872
 1.29684677 1.66666667 0.13676676 15.00000000 20515.01 bandw. L : 4.94703182
 6.34433701 1.29959254 1.66666667 0.13474342 15.00000000 20211.51 bandw. H :
 4.10619968 9.70902614 0.38447819 0.90909091 0.27521851 1.00000000 2752.19
 $DO\text{Serr}_h$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000

0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00 E_{prisf}: 170.78297893 220.00000000 170.78297893 220.00000000
2422.31516302 0.00500000 121115.76
fdd=0.2179244771 qdds=0.5675512492 qddp=0.5721116911 qddd=0.8122937636
b0=52.4993185997 p0=1.0505764293 b1=-6.6866077393 p1=0.6593593831 b2=1135940.9163906001
m2=-11.5928 912764 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
cr2=3.6148353355 cr3=-1.1034803781 r1dd=6.5000000000 rcdd=10.0000000000
rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.64105348 5.57678969 5.64105348 5.57678969 0.00412983 1000.00000000
41298.34 c/a : 1.59941757 1.58731122 15.52935688 15.41181168 0.01381687
100.00000000 13816.87 a_{omega} : 9.01440247 8.73254342 1.12680031 1.09156793
0.00124132 10.00000000 124.13 c_{omega} : 5.44493846 5.32343103 0.68061731
0.66542888 0.00023069 10.00000000 23.07 a_{4h} : 5.64258030 5.56325146 1.01425944
1.00000000 0.00020333 1.00000000 2.03 c_{4h} : 18.24656808 17.75908031 1.02745006
1.00000000 0.00075351 1.00000000 7.54 a_{6h} : 5.63716653 5.54639384 1.01636607
1.00000000 0.00026785 1.00000000 2.68 c_{6h} : 27.45537609 26.77136353 1.02555016
1.00000000 0.00065281 1.00000000 6.53 a_{bcc} : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.96263395 7.88677000 1.13751914
1.12668143 0.00011746 1.00000000 1.17 DE(o,h) : 0.28163500 -0.63343333
0.01877567 -0.04222889 0.00372156 3000.00000000 111646.67 DE(4h,h): 1.82146250
3.17160000 0.00728585 0.01268640 0.00002917 2000.00000000 583.32 DE(6h,h):
2.68946833 3.72005000 0.01075787 0.01488020 0.00001699 2000.00000000 339.87
DE(b,h) : 7.24713500 7.63520000 0.07320338 0.07712323 0.00001537 1.00000000
0.15 DE(f,h) : 4.05937500 4.51880000 0.04100379 0.04564444 0.00002154
2000.00000000 430.71 c₁₁ : 203.07933917 176.10000000 0.88708050 0.76923077
0.01388856 100.00000000 13888.56 c₃₃ : 259.89718138 190.50000000 1.04945359
0.76923077 0.07852483 100.00000000 78524.83 c₄₄ : 55.71591863 50.80000000
0.84366927 0.76923077 0.00554109 100.00000000 5541.09 c₁₂ : 124.21148843
86.90000000 1.09950862 0.76923077 0.10908346 100.00000000 109083.46 c₁₃
: 75.80169292 68.30000000 0.85371881 0.76923077 0.00713823 10.00000000
713.82 M_{freq0}: 3.01663413 2.85858719 0.21985177 0.20833333 0.00013267
0.10000000 0.13 M_{freq1}: 3.01663414 2.85858719 0.21985177 0.20833333 0.00013267
0.10000000 0.13 M_{freq2}: 3.01663414 2.85858719 0.21985177 0.20833333 0.00013267
0.10000000 0.13 M_{freq3}: 3.01663416 2.85858719 0.21985177 0.20833333 0.00013267
0.10000000 0.13 M_{freq4}: 6.94463708 5.66706047 0.25529980 0.20833333 0.00220585
0.10000000 2.21 M_{freq5}: 6.94463708 5.66706047 0.25529980 0.20833333 0.00220585
0.10000000 2.21 H_{freq0}: 4.32293638 4.80643423 0.18737628 0.20833333 0.00043920
0.10000000 0.44 H_{freq1}: 4.32293638 5.58010025 0.16139705 0.20833333 0.00220301
0.10000000 2.20 H_{freq2}: 7.99648440 5.65316738 0.29469042 0.20833333 0.00745755

0.10000000 7.46 H_{freq3}: 7.99648440 6.36651842 0.26167116 0.20833333 0.00284492
 0.10000000 2.84 H_{freq4}: 9.69925048 6.40050186 0.31570605 0.20833333 0.01152890
 0.10000000 11.53 H_{freq5}: 9.69925048 7.64082373 0.26445803 0.20833333 0.00314998
 0.10000000 3.15 bandw. G: 4.12660822 5.87085872 1.17149478 1.66666667
 0.24519519 15.00000000 36779.28 bandw. K: 5.03138714 4.97424321 0.91953451
 0.90909091 0.00010907 15.00000000 16.36 bandw. M: 5.74296515 7.78109872
 1.23011016 1.66666667 0.19058158 15.00000000 28587.24 bandw. L: 4.69396583
 6.34433701 1.23311173 1.66666667 0.18796988 15.00000000 28195.48 bandw.
 H: 3.87762395 9.70902614 0.36307583 0.90909091 0.29813247 1.00000000 2981.32
 DOS_{errh}: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOS_{erro}: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 176.06714740 220.00000000 176.06714740 220.00000000
 1930.09553743 0.00500000 96504.78
 fdd=0.2214704157 qdds=0.5665716666 qddp=0.5715531079 qddd=0.8133669546
 b0=52.9290130950 p0=1.0450911218 b1=-7.4164544044 p1=0.6616600838 b2=1409254.9498441222
 m2=-11.5044596990 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
 cr2=3.1563387155 cr3=-1.0184485093 r1dd=6.5000000000 rcdd=10.0000000000
 rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.57706199 5.57678969 5.57706199 5.57678969 0.00000007 1000.00000000
 0.74 c/a : 1.58719496 1.58731122 15.41068294 15.41181168 0.00000127 100.00000000
 1.27 a_{omega} : 8.93521859 8.73254342 1.11690232 1.09156793 0.00064183 10.00000000
 64.18 c_{omega} : 5.37877063 5.32343103 0.67234633 0.66542888 0.00004785
 10.00000000 4.79 a_{4h} : 5.57599268 5.56325146 1.00229025 1.00000000 0.00000525
 1.00000000 0.05 c_{4h} : 18.04985410 17.75908031 1.01637325 1.00000000 0.00026808
 1.00000000 2.68 a_{6h} : 5.57213737 5.54639384 1.00464149 1.00000000 0.00002154
 1.00000000 0.22 c_{6h} : 27.14019153 26.77136353 1.01377696 1.00000000 0.00018980
 1.00000000 1.90 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409 0.00000927
 1.00000000 0.09 a_{fcc} : 7.87059596 7.88677000 1.12437085 1.12668143 0.00000534
 1.00000000 0.05 DE(o,h) : 0.55550667 -0.63343333 0.03703378 -0.04222889
 0.00628257 3000.00000000 188477.11 DE(4h,h): 2.30046500 3.17160000 0.00920186
 0.01268640 0.00001214 2000.00000000 242.84 DE(6h,h): 3.33150500 3.72005000
 0.01332602 0.01488020 0.00000242 2000.00000000 48.31 DE(b,h) : 6.12225000
 7.63520000 0.06184091 0.07712323 0.00023355 1.00000000 2.34 DE(f,h) :
 4.94694000 4.51880000 0.04996909 0.04564444 0.00001870 2000.00000000 374.05
 c₁₁ : 218.56863705 176.10000000 0.95474004 0.76923077 0.03441369 100.00000000
 34413.69 c₃₃ : 292.25608870 190.50000000 1.18011746 0.76923077 0.16882787
 100.00000000 168827.87 c₄₄ : 66.08167373 50.80000000 1.00063104 0.76923077
 0.05354608 100.00000000 53546.08 c₁₂ : 131.38136144 86.90000000 1.16297567
 0.76923077 0.15503505 100.00000000 155035.05 c₁₃ : 87.17956371 68.30000000

0.98186241 0.76923077 0.04521222 10.00000000 4521.22 M_{freq0} : 3.15842625
 2.85858719 0.23018555 0.20833333 0.00047752 0.10000000 0.48 M_{freq1} : 3.15842627
 2.85858719 0.23018555 0.20833333 0.00047752 0.10000000 0.48 M_{freq2} : 3.15842627
 2.85858719 0.23018555 0.20833333 0.00047752 0.10000000 0.48 M_{freq3} : 3.15842628
 2.85858719 0.23018555 0.20833333 0.00047752 0.10000000 0.48 M_{freq4} : 7.62204688
 5.66706047 0.28020284 0.20833333 0.00516523 0.10000000 5.17 M_{freq5} : 7.62204688
 5.66706047 0.28020284 0.20833333 0.00516523 0.10000000 5.17 H_{freq0} : 4.53961676
 4.80643423 0.19676822 0.20833333 0.00013375 0.10000000 0.13 H_{freq1} : 4.53961676
 5.58010025 0.16948683 0.20833333 0.00150905 0.10000000 1.51 H_{freq2} : 8.66752201
 5.65316738 0.31941983 0.20833333 0.01234021 0.10000000 12.34 H_{freq3} : 8.66752201
 6.36651842 0.28362971 0.20833333 0.00566954 0.10000000 5.67 H_{freq4} : 10.57540158
 6.40050186 0.34422436 0.20833333 0.01846637 0.10000000 18.47 H_{freq5} : 10.57540158
 7.64082373 0.28834701 0.20833333 0.00640219 0.10000000 6.40 bandw. G:
 4.11300253 5.87085872 1.16763229 1.66666667 0.24903531 15.00000000 37355.30
 bandw. K: 5.17016527 4.97424321 0.94489755 0.90909091 0.00128212 15.00000000
 192.32 bandw. M: 5.77970054 7.78109872 1.23797867 1.66666667 0.18377340
 15.00000000 27566.01 bandw. L: 4.68716298 6.34433701 1.23132461 1.66666667
 0.18952270 15.00000000 28428.41 bandw. H: 3.94973415 9.70902614 0.36982776
 0.90909091 0.29080474 1.00000000 2908.05 DOSerr_h : 0.00000000 0.00000000
 0.00000000 0.00000000 0.00000000 1.00000000 0.00 DOSerr_o : 0.00000000
 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00 E_{prisf} : 191.05208713
 220.00000000 191.05208713 220.00000000 837.98165942 0.00500000 41899.08
 ———— $E_{\text{Basalfault}}$ I2 ————
 tbe: 300.214 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]

1.6 2019-10-14

fdd=0.2209703447 qdds=0.5665716666 qddp=0.5715531079 qddd=0.8133669546
 b0=52.1569460578 p0=1.0570892971 b1=-8.0295431356 p1=0.6999146363 b2=1366555.8524337406
 m2=-11.5000 000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
 cr2=3.1563387155 cr3=-1.0184485093 r1dd=6.5000000000 rcdd=10.0000000000
 rmaxhm=10.1000000000 npar=18
 fdd=0.2209703447 qdds=0.5665716666 qddp=0.5715531079 qddd=0.8133669546
 b0=52.1569460578 p0=1.0570892971 b1=-8.0295431356 p1=0.6999146363 b2=1366555.8524337406
 m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
 cr2=3.1563387155 cr3=-1.0184485093 r1dd=6.5000000000 rcdd=10.0000000000
 rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.62158373 5.57678969 5.62158373 5.57678969 0.00200651 1000.00000000
 20065.06 c/a : 1.60770572 1.58731122 15.60982971 15.41181168 0.03921114

100.00000000 39211.14 a_{omega} : 9.00227859 8.73254342 1.12528482 1.09156793
 0.00113683 10.00000000 113.68 c_{omega} : 5.41389459 5.32343103 0.67673682
 0.66542888 0.00012787 10.00000000 12.79 a_{4h} : 5.61716947 5.56325146 1.00969182
 1.00000000 0.00009393 1.00000000 0.94 c_{4h} : 18.20877007 17.75908031 1.02532168
 1.00000000 0.00064119 1.00000000 6.41 a_{6h} : 5.61399550 5.54639384 1.01218840
 1.00000000 0.00014856 1.00000000 1.49 c_{6h} : 27.37027744 26.77136353 1.02237144
 1.00000000 0.00050048 1.00000000 5.00 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.93144116 7.88677000 1.13306302
 1.12668143 0.00004072 1.00000000 0.41 DE(o,h) : 0.60823000 -0.63343333
 0.04054867 -0.04222889 0.00685212 3000.00000000 205563.71 DE(4h,h): 2.00746500
 3.17160000 0.00802986 0.01268640 0.00002168 2000.00000000 433.67 DE(6h,h):
 2.94281333 3.72005000 0.01177125 0.01488020 0.00000967 2000.00000000 193.31
 DE(b,h) : 5.83790000 7.63520000 0.05896869 0.07712323 0.00032959 1.00000000
 3.30 DE(f,h) : 4.38214000 4.51880000 0.04426404 0.04564444 0.00000191
 2000.00000000 38.11 c_{11} : 202.11202443 176.10000000 0.88285513 0.76923077
 0.01291049 100.00000000 12910.49 c_{33} : 248.75262036 190.50000000 1.00445233
 0.76923077 0.05532918 100.00000000 55329.18 c_{44} : 58.01670497 50.80000000
 0.87850856 0.76923077 0.01194163 100.00000000 11941.63 c_{12} : 124.99839096
 86.90000000 1.10647421 0.76923077 0.11373314 100.00000000 113733.14 c_{13}
 : 76.61971559 68.30000000 0.86293181 0.76923077 0.00877989 10.00000000
 877.99 $M_{\text{freq}0}$: 2.96073909 2.85858719 0.21577815 0.20833333 0.00005543
 0.10000000 0.06 $M_{\text{freq}1}$: 2.96073910 2.85858719 0.21577815 0.20833333 0.00005543
 0.10000000 0.06 $M_{\text{freq}2}$: 2.96073910 2.85858719 0.21577815 0.20833333 0.00005543
 0.10000000 0.06 $M_{\text{freq}3}$: 2.96073911 2.85858719 0.21577815 0.20833333 0.00005543
 0.10000000 0.06 $M_{\text{freq}4}$: 6.94050619 5.66706047 0.25514794 0.20833333 0.00219161
 0.10000000 2.19 $M_{\text{freq}5}$: 6.94050619 5.66706047 0.25514794 0.20833333 0.00219161
 0.10000000 2.19 $H_{\text{freq}0}$: 4.44087055 4.80643423 0.19248809 0.20833333 0.00025107
 0.10000000 0.25 $H_{\text{freq}1}$: 4.44087055 5.58010025 0.16580013 0.20833333 0.00180907
 0.10000000 1.81 $H_{\text{freq}2}$: 7.83486022 5.65316738 0.28873416 0.20833333 0.00646429
 0.10000000 6.46 $H_{\text{freq}3}$: 7.83486022 6.36651842 0.25638229 0.20833333 0.00230870
 0.10000000 2.31 $H_{\text{freq}4}$: 9.53237976 6.40050186 0.31027449 0.20833333 0.01039200
 0.10000000 10.39 $H_{\text{freq}5}$: 9.53237976 7.64082373 0.25990816 0.20833333 0.00265996
 0.10000000 2.66 bandw. G: 3.96470042 5.87085872 0.96474094 1.42857143
 0.21513872 15.00000000 32270.81 bandw. K: 4.99873347 4.97424321 0.83743618
 0.83333333 0.00001683 15.00000000 2.53 bandw. M: 5.62595615 7.78109872
 1.03289786 1.42857143 0.15655757 15.00000000 23483.64 bandw. L: 4.52525518
 6.34433701 1.01896388 1.42857143 0.16777834 15.00000000 25166.75 bandw.
 H: 3.83272515 9.70902614 0.35887179 0.90909091 0.30274108 1.00000000 3027.41
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000

0.00000000 0.00 E_{prsf}: 183.30407754 220.00000000 183.30407754 220.00000000
 1346.59072537 0.00500000 67329.54
 fdd=0.2209703447 qdds=0.5665716666 qddp=0.5715531079 qddd=0.8133669546
 b0=52.1569460578 p0=1.0570892971 b1=-8.0295431356 p1=0.6999146363 b2=1366555.8524337406
 m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
 cr2=3.1563387155 cr3=-1.0184485093 r1dd=6.35 rcdd=9.85 rmaxhm=9.86
 npar=18
 a=5.6426873025, c=8.7998008103 c/a=1.5595053099
 C11 = 211.2138 C33 = 249.2500 C' = 27.0534 C'' = 77.6569 C44 =
 58.1521
 E_{omega} - E_{hcp} = -0.236090 E_{fcc} - E_{hcp} = 4.212010
 ———— E_{prismaticfault} ————
 tbe: 151.945 mJ/m² DFT: 250.000 mJ/m² [Benoit 2012] DFT: 233.000
 mJ/m² [Ackland 1999]
 ———— E_{Basalfault} I2 ————
 tbe: 270.320 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]
 fdd=0.2460323705 qdds=0.5968645554 qddp=0.5488210525 qddd=0.8092725812
 b0=59.5270918 p0=1.1327333 b1=-4.490946307 p1=0.6549840155 cr2=3.168195467
 cr3=-1.191602401 p2=0.0 cr1=-6.0 ndt=2.0 r1dd=6.5 rcdd=10. rmaxhm=10.001

a_{hcp} : 5.57978504 5.57678969 5.57978504 5.57678969 0.00000897 1000.00000000
 89.72 c/a : 1.58603306 1.58731122 15.39940161 15.41181168 0.00015401 100.00000000
 154.01 a_{omega} : 8.87205515 8.73254342 1.10900689 1.09156793 0.00030412
 10.00000000 30.41 c_{omega} : 5.42124300 5.32343103 0.67765537 0.66542888
 0.00014949 10.00000000 14.95 a_{4h} : 5.58177886 5.56325146 1.00333032 1.00000000
 0.00001109 1.00000000 0.11 c_{4h} : 18.01884423 17.75908031 1.01462710 1.00000000
 0.00021395 1.00000000 2.14 a_{6h} : 5.57412314 5.54639384 1.00499952 1.00000000
 0.00002500 1.00000000 0.25 c_{6h} : 27.12692717 26.77136353 1.01328149 1.00000000
 0.00017640 1.00000000 1.76 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409
 0.00000927 1.00000000 0.09 a_{fcc} : 7.87136615 7.88677000 1.12448088 1.12668143
 0.00000484 1.00000000 0.05 DE(o,h) : 0.76756333 -0.63343333 0.05117089 -
 0.04222889 0.00872352 3000.00000000 261705.55 DE(4h,h): 1.14033500 3.17160000
 0.00456134 0.01268640 0.00006602 2000.00000000 1320.33 DE(6h,h): 1.93413000
 3.72005000 0.00773652 0.01488020 0.00005103 2000.00000000 1020.64 DE(b,h)
 : 7.53434000 7.63520000 0.07610444 0.07712323 0.00000104 1.00000000 0.01
 DE(f,h) : 3.23856000 4.51880000 0.03271273 0.04564444 0.00016723 2000.00000000
 3344.59 c₁₁ : 190.00221183 176.10000000 0.82995768 0.76923077 0.00368776
 100.00000000 3687.76 c₃₃ : 231.62335859 190.50000000 0.93528511 0.76923077
 0.02757405 100.00000000 27574.05 c₄₄ : 50.44091880 50.80000000 0.76379344
 0.76923077 0.00002956 100.00000000 29.56 c₁₂ : 95.35312741 86.90000000

0.84405707 0.76923077 0.00559898 100.00000000 5598.98 c_{13} : 74.23368754
 68.30000000 0.83605910 0.76923077 0.00446603 10.00000000 446.60 M_{freq0} :
 2.92319720 2.85858719 0.21304210 0.20833333 0.00002217 0.10000000 0.02
 M_{freq1} : 2.92319721 2.85858719 0.21304210 0.20833333 0.00002217 0.10000000
 0.02 M_{freq2} : 2.92319721 2.85858719 0.21304210 0.20833333 0.00002217 0.10000000
 0.02 M_{freq3} : 2.92319723 2.85858719 0.21304210 0.20833333 0.00002217 0.10000000
 0.02 M_{freq4} : 6.45319960 5.66706047 0.23723350 0.20833333 0.00083522 0.10000000
 0.84 M_{freq5} : 6.45319960 5.66706047 0.23723350 0.20833333 0.00083522 0.10000000
 0.84 H_{freq0} : 3.96266778 4.80643423 0.17176055 0.20833333 0.00133757 0.10000000
 1.34 H_{freq1} : 3.96266778 5.58010025 0.14794641 0.20833333 0.00364658 0.10000000
 3.65 H_{freq2} : 7.35229474 5.65316738 0.27095042 0.20833333 0.00392090 0.10000000
 3.92 H_{freq3} : 7.35229474 6.36651842 0.24059116 0.20833333 0.00104057 0.10000000
 1.04 H_{freq4} : 9.03031093 6.40050186 0.29393238 0.20833333 0.00732720 0.10000000
 7.33 H_{freq5} : 9.03031093 7.64082373 0.24621884 0.20833333 0.00143531 0.10000000
 1.44 bandw. G: 4.56471170 5.87085872 1.29586713 1.66666667 0.13749230
 15.00000000 20623.84 bandw. K: 5.27356857 4.97424321 0.96379550 0.90909091
 0.00299259 15.00000000 448.89 bandw. M: 6.08310761 7.78109872 1.30296672
 1.66666667 0.13227765 15.00000000 19841.65 bandw. L: 5.17288640 6.34433701
 1.35892487 1.66666667 0.09470501 15.00000000 14205.75 bandw. H: 4.10347854
 9.70902614 0.38422340 0.90909091 0.27548590 5.00000000 13774.30 DOSerr_h :
 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00
 DOSerr_o : 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00 E_{prisf} : 109.63086340 220.00000000 109.63086340 220.00000000 12181.34631403
 0.00500000 609067.32
 b2=979360405.8982486725 m2=-15.9232689476 p2=0.0000000000 fdd=0.2648249504
 qdds=0.5697753882 qddp=0.5648597117 qddd=0.8213593849 b0=59.9169943713
 p0=1.0751867605 b1=-5.6073622378 p1=0.6278659006 ndt=2.0000000000 cr1=-
 6.0000000000 cr2=3.2217589360 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-
 1.1418272350 rmaxhm=10.1000000000 npar=18
 a_{hcp} : 5.62498753 5.57678969 5.62498753 5.57678969 0.00232303 1000.00000000
 23230.32 c/a : 1.60625260 1.58731122 15.59572085 15.41181168 0.03382258
 100.00000000 33822.58 a_{omega} : 8.99992908 8.73254342 1.12499113 1.09156793
 0.00111711 10.00000000 111.71 c_{omega} : 5.43109984 5.32343103 0.67888748
 0.66542888 0.00018113 10.00000000 18.11 a_{4h} : 5.62654514 5.56325146 1.01137710
 1.00000000 0.00012944 1.00000000 1.29 c_{4h} : 18.19194529 17.75908031 1.02437429
 1.00000000 0.00059411 1.00000000 5.94 a_{6h} : 5.62159443 5.54639384 1.01355846
 1.00000000 0.00018383 1.00000000 1.84 c_{6h} : 27.37250217 26.77136353 1.02245454
 1.00000000 0.00050421 1.00000000 5.04 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.93952818 7.88677000 1.13421831
 1.12668143 0.00005680 1.00000000 0.57 $\text{DE}(o,h)$: 0.06124333 -0.63343333

0.00408289 -0.04222889 0.00214478 3000.00000000 64343.42 DE(4h,h): 2.33537250
 3.17160000 0.00934149 0.01268640 0.00001119 2000.00000000 223.77 DE(6h,h):
 3.42632833 3.72005000 0.01370531 0.01488020 0.00000138 2000.00000000 27.61
 DE(b,h) : 7.83458000 7.63520000 0.07913717 0.07712323 0.00000406 1.00000000
 0.04 DE(f,h) : 5.11296000 4.51880000 0.05164606 0.04564444 0.00003602
 2000.00000000 720.39 c₁₁ : 227.69156320 176.10000000 0.99459033 0.76923077
 0.05078693 100.00000000 50786.93 c₃₃ : 294.38012507 190.50000000 1.18869423
 0.76923077 0.17594959 100.00000000 175949.59 c₄₄ : 65.30471301 50.80000000
 0.98886604 0.76923077 0.04823965 100.00000000 48239.65 c₁₂ : 133.30344523
 86.90000000 1.17998978 0.76923077 0.16872296 100.00000000 168722.96 c₁₃
 : 84.98994819 68.30000000 0.95720180 0.76923077 0.03533311 10.00000000
 3533.31 M_{freq0}: 3.18654457 2.85858719 0.23223481 0.20833333 0.00057128
 0.10000000 0.57 M_{freq1}: 3.18654459 2.85858719 0.23223481 0.20833333 0.00057128
 0.10000000 0.57 M_{freq2}: 3.18654459 2.85858719 0.23223481 0.20833333 0.00057128
 0.10000000 0.57 M_{freq3}: 3.18654460 2.85858719 0.23223481 0.20833333 0.00057128
 0.10000000 0.57 M_{freq4}: 7.41549130 5.66706047 0.27260941 0.20833333 0.00413141
 0.10000000 4.13 M_{freq5}: 7.41549130 5.66706047 0.27260941 0.20833333 0.00413141
 0.10000000 4.13 H_{freq0}: 4.51506755 4.80643423 0.19570414 0.20833333 0.00015950
 0.10000000 0.16 H_{freq1}: 4.51506755 5.58010025 0.16857028 0.20833333 0.00158110
 0.10000000 1.58 H_{freq2}: 8.47327422 5.65316738 0.31226131 0.20833333 0.01080102
 0.10000000 10.80 H_{freq3}: 8.47327422 6.36651842 0.27727328 0.20833333 0.00475272
 0.10000000 4.75 H_{freq4}: 10.35099862 6.40050186 0.33692015 0.20833333 0.01653457
 0.10000000 16.53 H_{freq5}: 10.35099862 7.64082373 0.28222848 0.20833333 0.00546049
 0.10000000 5.46 bandw. G: 4.85179193 5.87085872 1.37736578 1.66666667
 0.08369500 15.00000000 12554.25 bandw. K: 5.99331000 4.97424321 1.09533519
 0.90909091 0.03468693 15.00000000 5203.04 bandw. M: 6.79332504 7.78109872
 1.45509122 1.66666667 0.04476417 15.00000000 6714.63 bandw. L: 5.51847114
 6.34433701 1.44971049 1.66666667 0.04706998 15.00000000 7060.50 bandw.
 H: 4.61097107 9.70902614 0.43174174 0.90909091 0.22786222 5.00000000 11393.11
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 181.83831141 220.00000000 181.83831141 220.00000000
 1456.31447590 0.01000000 145631.45
 -vfdd=0.2515488168 -vqdds=0.5697753882 -vqddp=0.5648597117 -vqddd=0.8213593849
 -vb0=46.3898409291 -vp0=1.0722677474 -vb1=-5.6805371975 -vp1=0.6950452201
 -vb2=960581.6752016575 -vm2=-12.0000000000 -vp2=0.0000000000 -vndt=2.0000000000
 -vcr1=-6.0000000000 -vcr2=3.2217589360 -vcr3=-1.1418272350 -vr1dd=6.5000000000
 -vridd=10.0000000000 -vrmaxhm=10.1000000000 -vahcp=5.62362601 -vq=1.60683364

1.7 2019-10-16

fdd=0.2140672778 qdds=0.5665716666 qddp=0.5715531079 qddd=0.8133669546
b0=50.8874806903 p0=1.0275177064 b1=-8.0064171217 p1=0.6715816626 b2=859594.4816890366
m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
cr2=3.1563387155 cr3=-1.0184485093 r1dd=6.5000000000 rcdd=10.0000000000
rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.60674315 5.57678969 5.60674315 5.57678969 0.00089721 1000.00000000
8972.10 c/a : 1.61406192 1.58731122 15.67154450 15.41181168 0.06746114
100.00000000 67461.14 a_{omega} : 8.97344123 8.73254342 1.12168015 1.09156793
0.00090675 10.00000000 90.67 c_{omega} : 5.40174192 5.32343103 0.67521774
0.66542888 0.00009582 10.00000000 9.58 a_{4h} : 5.60784723 5.56325146 1.00801613
1.00000000 0.00006426 1.00000000 0.64 c_{4h} : 18.14091306 17.75908031 1.02150071
1.00000000 0.00046228 1.00000000 4.62 a_{6h} : 5.60375180 5.54639384 1.01034149
1.00000000 0.00010695 1.00000000 1.07 c_{6h} : 27.28368854 26.77136353 1.01913705
1.00000000 0.00036623 1.00000000 3.66 a_{bcc} : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.91526712 7.88677000 1.13075245
1.12668143 0.00001657 1.00000000 0.17 DE(o,h) : -0.48212667 -0.63343333 -
0.03214178 -0.04222889 0.00010175 3000.00000000 3052.49 DE(4h,h): 2.15130750
3.17160000 0.00860523 0.01268640 0.00001666 2000.00000000 333.12 DE(6h,h):
3.12456667 3.72005000 0.01249827 0.01488020 0.00000567 2000.00000000 113.47
DE(b,h) : 5.36737000 7.63520000 0.05421586 0.07712323 0.00052475 1.00000000
5.25 DE(f,h) : 4.63445000 4.51880000 0.04681263 0.04564444 0.00000136
2000.00000000 27.29 c₁₁ : 186.96209568 176.10000000 0.81667800 0.76923077
0.00225124 100.00000000 2251.24 c₃₃ : 246.89937852 190.50000000 0.99696902
0.76923077 0.05186471 100.00000000 51864.71 c₄₄ : 55.81265006 50.80000000
0.84513401 0.76923077 0.00576130 100.00000000 5761.30 c₁₂ : 123.56433205
86.90000000 1.09378005 0.76923077 0.10533223 100.00000000 105332.23 c₁₃
: 74.20404116 68.30000000 0.83572521 0.76923077 0.00442151 10.00000000
442.15 M_{freq0}: 2.90044289 2.85858719 0.21138377 0.20833333 0.00000931
0.10000000 0.01 M_{freq1}: 2.90044291 2.85858719 0.21138377 0.20833333 0.00000931
0.10000000 0.01 M_{freq2}: 2.90044291 2.85858719 0.21138377 0.20833333 0.00000931
0.10000000 0.01 M_{freq3}: 2.90044292 2.85858719 0.21138377 0.20833333 0.00000931
0.10000000 0.01 M_{freq4}: 7.05148055 5.66706047 0.25922759 0.20833333 0.00259023
0.10000000 2.59 M_{freq5}: 7.05148055 5.66706047 0.25922759 0.20833333 0.00259023
0.10000000 2.59 H_{freq0}: 4.20444148 4.80643423 0.18224015 0.20833333 0.00068085
0.10000000 0.68 H_{freq1}: 4.20444148 5.58010025 0.15697304 0.20833333 0.00263788
0.10000000 2.64 H_{freq2}: 8.05973032 5.65316738 0.29702119 0.20833333 0.00786554
0.10000000 7.87 H_{freq3}: 8.05973032 6.36651842 0.26374077 0.20833333 0.00306998

0.10000000 3.07 H_{freq4} : 9.82646428 6.40050186 0.31984680 0.20833333 0.01243525
 0.10000000 12.44 H_{freq5} : 9.82646428 7.64082373 0.26792662 0.20833333 0.00355136
 0.10000000 3.55 bandw. G: 3.88442680 5.87085872 0.94520775 1.42857143
 0.23364045 15.00000000 35046.07 bandw. K: 4.89396959 4.97424321 0.81988512
 0.83333333 0.00018085 15.00000000 27.13 bandw. M: 5.49398088 7.78109872
 1.00866785 1.42857143 0.17631902 15.00000000 26447.85 bandw. L: 4.42865472
 6.34433701 0.99721209 1.42857143 0.18607087 15.00000000 27910.63 bandw.
 H: 3.74700925 9.70902614 0.35084590 0.90909091 0.31163749 1.00000000 3116.37
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 152.13844679 220.00000000 152.13844679 220.00000000
 4605.19040432 0.00500000 230259.52
 fdd=0.2228781141 qdds=0.5665716666 qddp=0.5715531079 qddd=0.8133669546
 b0=50.9848615755 p0=1.0367421832 b1=-7.0846900618 p1=0.6533512918 b2=1076726.9089723818
 m2=-11.5000 000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
 cr2=3.1563387155 cr3=-1.0184485093 r1dd=6.5000000000 rcdd=10.0000000000
 rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.56698674 5.57678969 5.56698674 5.57678969 0.00009610 1000.00000000
 960.98 c/a : 1.59150388 1.58731122 15.45251985 15.41181168 0.00165716
 100.00000000 1657.16 a_{omega} : 8.91450492 8.73254342 1.11431311 1.09156793
 0.00051734 10.00000000 51.73 c_{omega} : 5.37410763 5.32343103 0.67176345
 0.66542888 0.00004013 10.00000000 4.01 a_{4h} : 5.56724969 5.56325146 1.00071869
 1.00000000 0.00000052 1.00000000 0.01 c_{4h} : 18.00856273 17.75908031 1.01404816
 1.00000000 0.00019735 1.00000000 1.97 a_{6h} : 5.56315391 5.54639384 1.00302180
 1.00000000 0.00000913 1.00000000 0.09 c_{6h} : 27.08175231 26.77136353 1.01159406
 1.00000000 0.00013442 1.00000000 1.34 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.85711759 7.88677000 1.12244537
 1.12668143 0.00001794 1.00000000 0.18 DE(o,h): -0.04491667 -0.63343333 -
 0.00299444 -0.04222889 0.00153934 3000.00000000 46180.25 DE(4h,h): 2.35324250
 3.17160000 0.00941297 0.01268640 0.00001072 2000.00000000 214.31 DE(6h,h):
 3.40459667 3.72005000 0.01361839 0.01488020 0.00000159 2000.00000000 31.84
 DE(b,h): 6.06623000 7.63520000 0.06127505 0.07712323 0.00025116 1.00000000
 2.51 DE(f,h): 5.05529000 4.51880000 0.05106354 0.04564444 0.00002937
 2000.00000000 587.33 c_{11} : 203.76796153 176.10000000 0.89008851 0.76923077
 0.01460659 100.00000000 14606.59 c_{33} : 278.24209018 190.50000000 1.12352954
 0.76923077 0.12552762 100.00000000 125527.62 c_{44} : 61.86278193 50.80000000
 0.93674715 0.76923077 0.02806174 100.00000000 28061.74 c_{12} : 121.08618827
 86.90000000 1.07184375 0.76923077 0.09157462 100.00000000 91574.62 c_{13}
 : 82.54845896 68.30000000 0.92970446 0.76923077 0.02575181 10.00000000

2575.18 M_{freq0}: 3.05562828 2.85858719 0.22269365 0.20833333 0.00020622
 0.10000000 0.21 M_{freq1}: 3.05562829 2.85858719 0.22269365 0.20833333 0.00020622
 0.10000000 0.21 M_{freq2}: 3.05562829 2.85858719 0.22269365 0.20833333 0.00020622
 0.10000000 0.21 M_{freq3}: 3.05562830 2.85858719 0.22269366 0.20833333 0.00020622
 0.10000000 0.21 M_{freq4}: 7.45331153 5.66706047 0.27399976 0.20833333 0.00431208
 0.10000000 4.31 M_{freq5}: 7.45331153 5.66706047 0.27399976 0.20833333 0.00431208
 0.10000000 4.31 H_{freq0}: 4.29471116 4.80643423 0.18615286 0.20833333 0.00049197
 0.10000000 0.49 H_{freq1}: 4.29471116 5.58010025 0.16034326 0.20833333 0.00230305
 0.10000000 2.30 H_{freq2}: 8.47282337 5.65316738 0.31224470 0.20833333 0.01079757
 0.10000000 10.80 H_{freq3}: 8.47282337 6.36651842 0.27725853 0.20833333 0.00475068
 0.10000000 4.75 H_{freq4}: 10.39201763 6.40050186 0.33825530 0.20833333 0.01687972
 0.10000000 16.88 H_{freq5}: 10.39201763 7.64082373 0.28334689 0.20833333 0.00562703
 0.10000000 5.63 bandw. G: 4.17286760 5.87085872 1.01539480 1.42857143
 0.17071492 15.00000000 25607.24 bandw. K: 5.24091490 4.97424321 0.87800875
 0.83333333 0.00199589 15.00000000 299.38 bandw. M: 5.84908960 7.78109872
 1.07386406 1.42857143 0.12581732 15.00000000 18872.60 bandw. L: 4.74974919
 6.34433701 1.06951380 1.42857143 0.12892238 15.00000000 19338.36 bandw.
 H: 4.00143580 9.70902614 0.37466877 0.90909091 0.28560702 1.00000000 2856.07
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 153.49123069 220.00000000 153.49123069 220.00000000
 4423.41639481 0.00500000 221170.82

fdd=0.2108451653 qdds=0.5665716666 qddp=0.5715531079 qddd=0.8133669546
 b0=45.8686333415 p0=1.0476021633 b1=-7.2512696921 p1=0.6952246832 b2=1073970.8829916473
 m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
 cr2=3.1563387155 cr3=-1.0184485093 r1dd=6.5000000000 rcdd=10.0000000000
 rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.57270513 5.57678969 5.57270513 5.57678969 0.00001668 1000.00000000
 166.84 c/a : 1.58905637 1.58731122 15.42875602 15.41181168 0.00028711
 100.00000000 287.11 a_{omega} : 8.92179103 8.73254342 1.11522388 1.09156793
 0.00055960 10.00000000 55.96 c_{omega} : 5.37765605 5.32343103 0.67220701
 0.66542888 0.00004594 10.00000000 4.59 a_{4h} : 5.56806496 5.56325146 1.00086523
 1.00000000 0.00000075 1.00000000 0.01 c_{4h} : 18.04548947 17.75908031 1.01612748
 1.00000000 0.00026010 1.00000000 2.60 a_{6h} : 5.56465904 5.54639384 1.00329317
 1.00000000 0.00001084 1.00000000 0.11 c_{6h} : 27.12570313 26.77136353 1.01323577
 1.00000000 0.00017519 1.00000000 1.75 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.86096856 7.88677000 1.12299551
 1.12668143 0.00001359 1.00000000 0.14 DE(o,h) : 0.45685833 -0.63343333
 0.03045722 -0.04222889 0.00528327 3000.00000000 158498.12 DE(4h,h): 1.97939750

3.17160000 0.00791759 0.01268640 0.00002274 2000.00000000 454.83 DE(6h,h):
 2.89579333 3.72005000 0.01158317 0.01488020 0.00001087 2000.00000000 217.41
 DE(b,h) : 5.60077500 7.63520000 0.05657348 0.07712323 0.00042229 1.00000000
 4.22 DE(f,h) : 4.31236500 4.51880000 0.04355924 0.04564444 0.00000435
 2000.00000000 86.96 c₁₁ : 190.31131027 176.10000000 0.83130787 0.76923077
 0.00385357 100.00000000 3853.57 c₃₃ : 238.74569902 190.50000000 0.96404482
 0.76923077 0.03795251 100.00000000 37952.51 c₄₄ : 55.14444230 50.80000000
 0.83501578 0.76923077 0.00432767 100.00000000 4327.67 c₁₂ : 107.72009667
 86.90000000 0.95352834 0.76923077 0.03396559 100.00000000 33965.59 c₁₃
 : 75.61395373 68.30000000 0.85160439 0.76923077 0.00678541 10.00000000
 678.54 M_{freq0}: 2.85601825 2.85858719 0.20814611 0.20833333 0.00000004
 0.10000000 0.00 M_{freq1}: 2.85601826 2.85858719 0.20814611 0.20833333 0.00000004
 0.10000000 0.00 M_{freq2}: 2.85601826 2.85858719 0.20814611 0.20833333 0.00000004
 0.10000000 0.00 M_{freq3}: 2.85601827 2.85858719 0.20814611 0.20833333 0.00000004
 0.10000000 0.00 M_{freq4}: 6.71192549 5.66706047 0.24674482 0.20833333 0.00147544
 0.10000000 1.48 M_{freq5}: 6.71192549 5.66706047 0.24674482 0.20833333 0.00147544
 0.10000000 1.48 H_{freq0}: 4.13084812 4.80643423 0.17905027 0.20833333 0.00085750
 0.10000000 0.86 H_{freq1}: 4.13084812 5.58010025 0.15422543 0.20833333 0.00292767
 0.10000000 2.93 H_{freq2}: 7.53514722 5.65316738 0.27768899 0.20833333 0.00481021
 0.10000000 4.81 H_{freq3}: 7.53514722 6.36651842 0.24657470 0.20833333 0.00146240
 0.10000000 1.46 H_{freq4}: 9.25844799 6.40050186 0.30135814 0.20833333 0.00865361
 0.10000000 8.65 H_{freq5}: 9.25844799 7.64082373 0.25243919 0.20833333 0.00194533
 0.10000000 1.95 bandw. G: 3.92796503 5.87085872 0.95580202 1.42857143
 0.22351091 15.00000000 33526.64 bandw. K: 4.93886840 4.97424321 0.82740700
 0.83333333 0.00003512 15.00000000 5.27 bandw. M: 5.51575000 7.78109872
 1.01266455 1.42857143 0.17297853 15.00000000 25946.78 bandw. L: 4.47627466
 6.34433701 1.00793481 1.42857143 0.17693517 15.00000000 26540.28 bandw.
 H: 3.77149950 9.70902614 0.35313901 0.90909091 0.30908251 1.00000000 3090.83
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 138.88172002 220.00000000 138.88172002 220.00000000
 6580.17534686 0.00500000 329008.77

1.8 2019-10-18

fdd=0.2133933543 qdds=0.5665716666 qddp=0.5715531079 qddd=0.8133669546
 b0=57.0099791242 p0=1.0676109997 b1=-8.2660331461 p1=0.6992076690 b2=965487.3545493595
 m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
 cr2=3.1563387155 cr3=-1.0184485093 r1dd=6.5000000000 rcdd=10.0000000000
 rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.63370126 5.57678969 5.63370126 5.57678969 0.00323893 1000.00000000
32389.27 c/a : 1.60254063 1.58731122 15.55967986 15.41181168 0.02186500
100.00000000 21865.00 a_{omega} : 9.01829172 8.73254342 1.12728646 1.09156793
0.00127581 10.00000000 127.58 c_{omega} : 5.41962382 5.32343103 0.67745298
0.66542888 0.00014458 10.00000000 14.46 $a_{4\text{h}}$: 5.63038746 5.56325146 1.01206776
1.00000000 0.00014563 1.00000000 1.46 $c_{4\text{h}}$: 18.24603866 17.75908031 1.02742025
1.00000000 0.00075187 1.00000000 7.52 $a_{6\text{h}}$: 5.62701645 5.54639384 1.01453604
1.00000000 0.00021130 1.00000000 2.11 $c_{6\text{h}}$: 27.43037636 26.77136353 1.02461633
1.00000000 0.00060596 1.00000000 6.06 a_{bcc} : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.94992578 7.88677000 1.13570368
1.12668143 0.00008140 1.00000000 0.81 DE(o,h) : 0.28538333 -0.63343333
0.01902556 -0.04222889 0.00375211 3000.00000000 112563.21 DE(4h,h) : 1.96250000
3.17160000 0.00785000 0.01268640 0.00002339 2000.00000000 467.82 DE(6h,h) :
2.87275500 3.72005000 0.01149102 0.01488020 0.00001149 2000.00000000 229.73
 DE(b,h) : 5.53596000 7.63520000 0.05591879 0.07712323 0.00044963 1.00000000
4.50 DE(f,h) : 4.27181000 4.51880000 0.04314960 0.04564444 0.00000622
2000.00000000 124.49 c_{11} : 196.80382177 176.10000000 0.85966812 0.76923077
0.00817891 100.00000000 8178.91 c_{33} : 246.24441607 190.50000000 0.99432431
0.76923077 0.05066710 100.00000000 50667.10 c_{44} : 56.44711885 50.80000000
0.85474135 0.76923077 0.00731206 100.00000000 7312.06 c_{12} : 129.68241447
86.90000000 1.14793675 0.76923077 0.14341822 100.00000000 143418.22 c_{13}
: 74.54117180 68.30000000 0.83952215 0.76923077 0.00494088 10.00000000
494.09 M_{freq0} : 2.92500829 2.85858719 0.21317409 0.20833333 0.00002343
0.10000000 0.02 M_{freq1} : 2.92500830 2.85858719 0.21317409 0.20833333 0.00002343
0.10000000 0.02 M_{freq2} : 2.92500830 2.85858719 0.21317409 0.20833333 0.00002343
0.10000000 0.02 M_{freq3} : 2.92500831 2.85858719 0.21317409 0.20833333 0.00002343
0.10000000 0.02 M_{freq4} : 6.93807696 5.66706047 0.25505863 0.20833333 0.00218325
0.10000000 2.18 M_{freq5} : 6.93807696 5.66706047 0.25505863 0.20833333 0.00218325
0.10000000 2.18 H_{freq0} : 4.42754941 4.80643423 0.19191069 0.20833333 0.00026970
0.10000000 0.27 H_{freq1} : 4.42754941 5.58010025 0.16530279 0.20833333 0.00185163
0.10000000 1.85 H_{freq2} : 7.88407442 5.65316738 0.29054783 0.20833333 0.00675922
0.10000000 6.76 H_{freq3} : 7.88407442 6.36651842 0.25799274 0.20833333 0.00246606
0.10000000 2.47 H_{freq4} : 9.55383477 6.40050186 0.31097284 0.20833333 0.01053487
0.10000000 10.53 H_{freq5} : 9.55383477 7.64082373 0.26049315 0.20833333 0.00272065
0.10000000 2.72 bandw. G : 3.79190805 5.87085872 0.92269492 1.42857143
0.25591104 15.00000000 38386.66 bandw. K : 4.78512401 4.97424321 0.80165026
0.83333333 0.00100382 15.00000000 150.57 bandw. M : 5.39601985 7.78109872
0.99068269 1.42857143 0.19174655 15.00000000 28761.98 bandw. L : 4.33477540
6.34433701 0.97607304 1.42857143 0.20475479 15.00000000 30713.22 bandw.

H: 3.67217791 9.70902614 0.34383918 0.90909091 0.31950952 1.00000000 3195.10
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prsf}: 183.05812252 220.00000000 183.05812252 220.00000000
 1364.70231173 0.00500000 68235.12

1.9 2019-10-19

PARAMETERS fdd=0.2373568526 qdds=0.5721313058 qddp=0.5652404895
 qddd=0.8290761169 b0=73.7884191068 p0=1.1375788554 b1=-4.4963531029
 p1=0.6070238105 b2=514034776.3068868518 m2=-17.9331967319 p2=0.0000000000
 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.1927668481 cr3=-1.1996137401
 r1dd=6.5000000000 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18
 VARGS -vfdd=0.2373568526 -vqdds=0.5721313058 -vqddp=0.5652404895 -
 vqddd=0.8290761169 -vb0=73.7884191068 -vp0=1.1375788554 -vb1=-4.4963531029
 -vp1=0.6070238105 -vb2=514034776.3068868518 -vm2=-17.9331967319 -vp2=0.0000000000
 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.1927668481 -vcr3=-1.1996137401
 -vr1dd=6.5000000000 -vrccd=10.0000000000 -vrm axhm=10.1000000000
 a_{hcp} : 5.64187039 5.57678969 5.64187039 5.57678969 0.00423550 1000.00000000
 42354.98 c/a : 1.59907106 1.58731122 15.52599254 15.41181168 0.01303727
 100.00000000 13037.27 a_{omega} : 9.00869668 8.73254342 1.12608708 1.09156793
 0.00119157 10.00000000 119.16 c_{omega} : 5.43898359 5.32343103 0.67987295
 0.66542888 0.00020863 10.00000000 20.86 a_{4h} : 5.64534416 5.56325146 1.01475625
 1.00000000 0.00021775 1.00000000 2.18 c_{4h} : 18.24449689 17.75908031 1.02733343
 1.00000000 0.00074712 1.00000000 7.47 a_{6h} : 5.64048670 5.54639384 1.01696469
 1.00000000 0.00028780 1.00000000 2.88 c_{6h} : 27.45586778 26.77136353 1.02556852
 1.00000000 0.00065375 1.00000000 6.54 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.96609982 7.88677000 1.13801426
 1.12668143 0.00012843 1.00000000 1.28 DE(o,h) : -0.65481000 -0.63343333 -
 0.04365400 -0.04222889 0.00000203 3000.00000000 60.93 DE(4h,h): 2.12175500
 3.17160000 0.00848702 0.01268640 0.00001763 2000.00000000 352.70 DE(6h,h):
 3.11138833 3.72005000 0.01244555 0.01488020 0.00000593 2000.00000000 118.55
 DE(b,h) : 6.70316000 7.63520000 0.06770869 0.07712323 0.00008863 1.00000000
 0.89 DE(f,h) : 4.63432000 4.51880000 0.04681131 0.04564444 0.00000136
 2000.00000000 27.23 c₁₁ : 205.12787921 176.10000000 0.89602883 0.76923077
 0.01607775 100.00000000 16077.75 c₃₃ : 273.50916253 190.50000000 1.10441818
 0.76923077 0.11235060 100.00000000 112350.60 c₄₄ : 59.15080084 50.80000000
 0.89568142 0.76923077 0.01598977 100.00000000 15989.77 c₁₂ : 137.35969396
 86.90000000 1.21589532 0.76923077 0.19950922 100.00000000 199509.22 c₁₃
 : 76.58816117 68.30000000 0.86257643 0.76923077 0.00871341 10.00000000

871.34 M_{freq0}: 3.03817005 2.85858719 0.22142130 0.20833333 0.00017129
 0.10000000 0.17 M_{freq1}: 3.03817006 2.85858719 0.22142130 0.20833333 0.00017129
 0.10000000 0.17 M_{freq2}: 3.03817006 2.85858719 0.22142130 0.20833333 0.00017129
 0.10000000 0.17 M_{freq3}: 3.03817007 2.85858719 0.22142130 0.20833333 0.00017129
 0.10000000 0.17 M_{freq4}: 7.23221436 5.66706047 0.26587176 0.20833333 0.00331067
 0.10000000 3.31 M_{freq5}: 7.23221436 5.66706047 0.26587176 0.20833333 0.00331067
 0.10000000 3.31 H_{freq0}: 4.38573130 4.80643423 0.19009810 0.20833333 0.00033252
 0.10000000 0.33 H_{freq1}: 4.38573130 5.58010025 0.16374151 0.20833333 0.00198843
 0.10000000 1.99 H_{freq2}: 8.37910370 5.65316738 0.30879089 0.20833333 0.01009172
 0.10000000 10.09 H_{freq3}: 8.37910370 6.36651842 0.27419172 0.20833333 0.00433733
 0.10000000 4.34 H_{freq4}: 10.15218782 6.40050186 0.33044895 0.20833333 0.01491222
 0.10000000 14.91 H_{freq5}: 10.15218782 7.64082373 0.27680774 0.20833333 0.00468874
 0.10000000 4.69 bandw. G: 4.23953552 5.87085872 1.20355349 1.66666667
 0.21447381 15.00000000 32171.07 bandw. K: 5.23683319 4.97424321 0.95708176
 0.90909091 0.00230312 15.00000000 345.47 bandw. M: 5.95657461 7.78109872
 1.27586408 1.66666667 0.15272666 15.00000000 22909.00 bandw. L: 4.83138338
 6.34433701 1.26921152 1.66666667 0.15797059 15.00000000 23695.59 bandw.
 H: 4.03545005 9.70902614 0.37785365 0.90909091 0.28221303 1.00000000 2822.13
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 170.66064429 220.00000000 170.66064429 220.00000000
 2434.37202179 0.00100000 24343.72

fdd=0.2216269669 qdds=0.5675508195 qddp=0.5720969588 qddd=0.7892712967
 b0=55.3548562714 p0=1.0447774207 b1=-6.8943229861 p1=0.6469895968 b2=607017.7016521859
 m2=-11.5128612989 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
 cr2=3.6855170631 cr3=-1.0757609783 r1dd=6.5000000000 rcdd=10.0000000000
 rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.60892158 5.57678969 5.60892158 5.57678969 0.00103246 1000.00000000
 10324.59 c/a : 1.61312679 1.58731122 15.66246500 15.41181168 0.06282708
 100.00000000 62827.08 a_{omega} : 8.95409963 8.73254342 1.11926245 1.09156793
 0.00076699 10.00000000 76.70 c_{omega} : 5.42286044 5.32343103 0.67785755
 0.66542888 0.00015447 10.00000000 15.45 a_{4h} : 5.61401412 5.56325146 1.00912464
 1.00000000 0.00008326 1.00000000 0.83 c_{4h} : 18.12359152 17.75908031 1.02052534
 1.00000000 0.00042129 1.00000000 4.21 a_{6h} : 5.60787856 5.54639384 1.01108553
 1.00000000 0.00012289 1.00000000 1.23 c_{6h} : 27.28143813 26.77136353 1.01905299
 1.00000000 0.00036302 1.00000000 3.63 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.91911808 7.88677000 1.13130258
 1.12668143 0.00002136 1.00000000 0.21 DE(o,h) : -0.14413333 -0.63343333 -
 0.00960889 -0.04222889 0.00106406 3000.00000000 31921.93 DE(4h,h): 1.93800500

3.17160000 0.00775202 0.01268640 0.00002435 2000.00000000 486.96 DE(6h,h):
 2.88877500 3.72005000 0.01155510 0.01488020 0.00001106 2000.00000000 221.13
 DE(b,h) : 7.35291000 7.63520000 0.07427182 0.07712323 0.00000813 1.00000000
 0.08 DE(f,h) : 4.38920000 4.51880000 0.04433535 0.04564444 0.00000171
 2000.00000000 34.27 c₁₁ : 204.50321205 176.10000000 0.89330019 0.76923077
 0.01539322 100.00000000 15393.22 c₃₃ : 268.45014957 190.50000000 1.08399011
 0.76923077 0.09907344 100.00000000 99073.44 c₄₄ : 57.17098136 50.80000000
 0.86570232 0.76923077 0.00930676 100.00000000 9306.76 c₁₂ : 121.47614681
 86.90000000 1.07529563 0.76923077 0.09367570 100.00000000 93675.70 c₁₃
 : 82.51177319 68.30000000 0.92929128 0.76923077 0.02561937 10.00000000
 2561.94 M_{freq0}: 3.07386802 2.85858719 0.22402296 0.20833333 0.00024616
 0.10000000 0.25 M_{freq1}: 3.07386803 2.85858719 0.22402296 0.20833333 0.00024616
 0.10000000 0.25 M_{freq2}: 3.07386803 2.85858719 0.22402296 0.20833333 0.00024616
 0.10000000 0.25 M_{freq3}: 3.07386804 2.85858719 0.22402296 0.20833333 0.00024616
 0.10000000 0.25 M_{freq4}: 7.20361262 5.66706047 0.26482030 0.20833333 0.00319078
 0.10000000 3.19 M_{freq5}: 7.20361262 5.66706047 0.26482030 0.20833333 0.00319078
 0.10000000 3.19 H_{freq0}: 4.21400171 4.80643423 0.18265454 0.20833333 0.00065940
 0.10000000 0.66 H_{freq1}: 4.21400171 5.58010025 0.15732997 0.20833333 0.00260134
 0.10000000 2.60 H_{freq2}: 8.32819842 5.65316738 0.30691491 0.20833333 0.00971833
 0.10000000 9.72 H_{freq3}: 8.32819842 6.36651842 0.27252593 0.20833333 0.00412069
 0.10000000 4.12 H_{freq4}: 10.15430032 6.40050186 0.33051771 0.20833333 0.01492902
 0.10000000 14.93 H_{freq5}: 10.15430032 7.64082373 0.27686534 0.20833333 0.00469664
 0.10000000 4.70 bandw. G: 4.35790509 5.87085872 1.23715720 1.66666667
 0.18447838 15.00000000 27671.76 bandw. K: 5.26268401 4.97424321 0.96180625
 0.90909091 0.00277891 15.00000000 416.84 bandw. M: 5.99194943 7.78109872
 1.28344116 1.66666667 0.14686179 15.00000000 22029.27 bandw. L: 4.93750783
 6.34433701 1.29709057 1.66666667 0.13658649 15.00000000 20487.97 bandw.
 H: 4.05041631 9.70902614 0.37925499 0.90909091 0.28072610 1.00000000 2807.26
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 171.18282882 220.00000000 171.18282882 220.00000000
 2383.11620172 0.00500000 119155.81

b2=200000.0000000000 m2=-11.5000000000 p2=0.0000000000 fdd=0.2000000000
 qdds=0.5676884766 qddp=0.5600000000 qddd=0.7740390160 b0=54.6320355636
 p0=1.0263023240 b1=-7.70160 34138 p1=0.6500762614 ndt=2.0000000000
 cr1=-6.0000000000 cr2=3.7700742958 r1dd=6.5000000000 rcdd=10.0000000000
 cr3=-1.2500000000 rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.58849877 5.57678969 5.58849877 5.57678969 0.00013710 1000.00000000
 1371.03 c/a : 1.62192223 1.58731122 15.74786322 15.41181168 0.11293064

100.00000000 112930.64 a_{omega} : 8.90826054 8.73254342 1.11353257 1.09156793
 0.00048245 10.00000000 48.24 c_{omega} : 5.41381819 5.32343103 0.67672727
 0.66542888 0.00012765 10.00000000 12.77 a_{4h} : 5.59810940 5.56325146 1.00626575
 1.00000000 0.00003926 1.00000000 0.39 c_{4h} : 18.02703794 17.75908031 1.01508849
 1.00000000 0.00022766 1.00000000 2.28 a_{6h} : 5.59006656 5.54639384 1.00787407
 1.00000000 0.00006200 1.00000000 0.62 c_{6h} : 27.15843831 26.77136353 1.01445854
 1.00000000 0.00020905 1.00000000 2.09 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.89312409 7.88677000 1.12758916
 1.12668143 0.00000082 1.00000000 0.01 DE(o,h) : -0.29985833 -0.63343333 -
 0.01999056 -0.04222889 0.00049454 3000.00000000 14836.30 DE(4h,h): 1.59495750
 3.17160000 0.00637983 0.01268640 0.00003977 2000.00000000 795.46 DE(6h,h):
 2.52157833 3.72005000 0.01008631 0.01488020 0.00002298 2000.00000000 459.63
 DE(b,h) : 7.30718500 7.63520000 0.07380995 0.07712323 0.00001098 1.00000000
 0.11 DE(f,h) : 3.98875500 4.51880000 0.04029045 0.04564444 0.00002867
 2000.00000000 573.30 c_{11} : 189.12687908 176.10000000 0.82613410 0.76923077
 0.00323799 200.00000000 6475.98 c_{33} : 250.59045959 190.50000000 1.01187345
 0.76923077 0.05887547 200.00000000 117750.94 c_{44} : 54.68921770 50.80000000
 0.82812262 0.76923077 0.00346825 200.00000000 6936.50 c_{12} : 110.34576435
 86.90000000 0.97677051 0.76923077 0.04307274 200.00000000 86145.49 c_{13}
 : 81.81523097 68.30000000 0.92144646 0.76923077 0.02316962 200.00000000
 46339.23 M_{freq0} : 3.06341745 2.85858719 0.22326133 0.20833333 0.00022284
 0.10000000 0.22 M_{freq1} : 3.06341746 2.85858719 0.22326133 0.20833333 0.00022285
 0.10000000 0.22 M_{freq2} : 3.06341746 2.85858719 0.22326133 0.20833333 0.00022285
 0.10000000 0.22 M_{freq3} : 3.06341747 2.85858719 0.22326133 0.20833333 0.00022285
 0.10000000 0.22 M_{freq4} : 7.24797821 5.66706047 0.26645127 0.20833333 0.00337769
 0.10000000 3.38 M_{freq5} : 7.24797821 5.66706047 0.26645127 0.20833333 0.00337769
 0.10000000 3.38 H_{freq0} : 3.98211559 4.80643423 0.17260351 0.20833333 0.00127662
 0.10000000 1.28 H_{freq1} : 3.98211559 5.58010025 0.14867249 0.20833333 0.00355942
 0.10000000 3.56 H_{freq2} : 8.43264838 5.65316738 0.31076415 0.20833333 0.01049207
 0.10000000 10.49 H_{freq3} : 8.43264838 6.36651842 0.27594387 0.20833333 0.00457119
 0.10000000 4.57 H_{freq4} : 10.29419141 6.40050186 0.33507110 0.20833333 0.01606246
 0.10000000 16.06 H_{freq5} : 10.29419141 7.64082373 0.28067958 0.20833333 0.00523398
 0.10000000 5.23 bandw. G: 4.23409324 5.87085872 1.20200850 1.66666667
 0.21590721 15.00000000 32386.08 bandw. K: 4.94975296 4.97424321 0.90461508
 0.90909091 0.00002003 15.00000000 3.00 bandw. M: 5.66813381 7.78109872
 1.21408172 1.66666667 0.20483314 15.00000000 30724.97 bandw. L: 4.78512401
 6.34433701 1.25705912 1.66666667 0.16777834 15.00000000 25166.75 bandw.
 H: 3.82184059 9.70902614 0.35785263 0.90909091 0.30386364 1.00000000 3038.64
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000

0.00000000 0.00 E_{prsf}: 159.02183640 220.00000000 159.02183640 220.00000000
 3718.33643625 0.00500000 185916.82
 fdd=0.2109713175 qdds=0.5674904535 qddp=0.5756255087 qddd=0.7670691708
 b0=60.0241189770 p0=1.0644046612 b1=-6.8574705667 p1=0.6486948127 b2=497874.2212954389
 m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
 cr2=3.4497003840 cr3=-1.1163682882 r1dd=6.5000000000 rcdd=10.0000000000
 rmaxhm=10.1000000000 npar=18
 a_{hcp} : 5.64486574 5.57678969 5.64486574 5.57678969 0.00463435 1000.00000000
 46343.48 c/a : 1.59780141 1.58731122 15.51366495 15.41181168 0.01037409
 100.00000000 10374.09 a_{omega} : 9.02090160 8.73254342 1.12761270 1.09156793
 0.00129923 10.00000000 129.92 c_{omega} : 5.43846597 5.32343103 0.67980825
 0.66542888 0.00020677 10.00000000 20.68 a_{4h} : 5.64894630 5.56325146 1.01540373
 1.00000000 0.00023727 1.00000000 2.37 c_{4h} : 18.25030477 17.75908031 1.02766047
 1.00000000 0.00076510 1.00000000 7.65 a_{6h} : 5.64451553 5.54639384 1.01769108
 1.00000000 0.00031297 1.00000000 3.13 c_{6h} : 27.46316370 26.77136353 1.02584105
 1.00000000 0.00066776 1.00000000 6.68 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.97072097 7.88677000 1.13867442
 1.12668143 0.00014383 1.00000000 1.44 DE(o,h) : -0.52831500 -0.63343333 -
 0.03522100 -0.04222889 0.00004911 3000.00000000 1473.32 DE(4h,h): 1.87802750
 3.17160000 0.00751211 0.01268640 0.00002677 2000.00000000 535.47 DE(6h,h):
 2.84014500 3.72005000 0.01136058 0.01488020 0.00001239 2000.00000000 247.75
 DE(b,h) : 6.71715500 7.63520000 0.06785005 0.07712323 0.00008599 1.00000000
 0.86 DE(f,h) : 4.28790500 4.51880000 0.04331217 0.04564444 0.00000544
 2000.00000000 108.79 c₁₁ : 197.98529610 176.10000000 0.86482897 0.76923077
 0.00913902 200.00000000 18278.03 c₃₃ : 263.41063593 190.50000000 1.06364077
 0.76923077 0.08667725 200.00000000 173354.49 c₄₄ : 57.72591165 50.80000000
 0.87410526 0.76923077 0.01099866 200.00000000 21997.32 c₁₂ : 137.31543329
 86.90000000 1.21550353 0.76923077 0.19915937 200.00000000 398318.75 c₁₃
 : 72.35523892 68.30000000 0.81490302 0.76923077 0.00208595 200.00000000
 4171.91 M_{freq0}: 3.02691595 2.85858719 0.22060110 0.20833333 0.00015050
 0.10000000 0.15 M_{freq1}: 3.02691596 2.85858719 0.22060110 0.20833333 0.00015050
 0.10000000 0.15 M_{freq2}: 3.02691596 2.85858719 0.22060110 0.20833333 0.00015050
 0.10000000 0.15 M_{freq3}: 3.02691597 2.85858719 0.22060111 0.20833333 0.00015050
 0.10000000 0.15 M_{freq4}: 7.16107157 5.66706047 0.26325640 0.20833333 0.00301654
 0.10000000 3.02 M_{freq5}: 7.16107157 5.66706047 0.26325640 0.20833333 0.00301654
 0.10000000 3.02 H_{freq0}: 4.32668314 4.80643423 0.18753868 0.20833333 0.00043242
 0.10000000 0.43 H_{freq1}: 4.32668314 5.58010025 0.16153694 0.20833333 0.00218990
 0.10000000 2.19 H_{freq2}: 8.32634189 5.65316738 0.30684649 0.20833333 0.00970484
 0.10000000 9.70 H_{freq3}: 8.32634189 6.36651842 0.27246518 0.20833333 0.00411289
 0.10000000 4.11 H_{freq4}: 10.05257962 6.40050186 0.32720675 0.20833333 0.01413089

0.10000000 14.13 H_{freq5} : 10.05257962 7.64082373 0.27409184 0.20833333 0.00432418
0.10000000 4.32 bandw. G: 3.86946053 5.87085872 0.94156597 1.42857143
0.23717432 15.00000000 35576.15 bandw. K: 4.74974919 4.97424321 0.79572392
0.83333333 0.00141447 15.00000000 212.17 bandw. M: 5.41506783 7.78109872
0.99417980 1.42857143 0.18869609 15.00000000 28304.41 bandw. L: 4.40824617
6.34433701 0.99261665 1.42857143 0.19005657 15.00000000 28508.49 bandw.
H: 3.65721164 9.70902614 0.34243783 0.90909091 0.32109571 1.00000000 3210.96
DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00 E_{prisf}: 179.69651618 220.00000000 179.69651618 220.00000000
1624.37080837 0.00500000 81218.54

b2=504779.7995565861 m2=-11.5000000000 p2=0.0000000000 fdd=0.2400000000
qdds=0.5750000000 qddp=0.5750000000 qddd=0.7500000000 b0=66.8564029459
p0=1.1850000000 b1=-10.0000000000 p1=0.8500000000 ndt=2.0000000000
cr1=-6.0000000000 cr2=3.0000000000 r1dd=6.5000000000 rcdd=10.0000000000
cr3=-1.2500000000 rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.57461126 5.57678969 5.57461126 5.57678969 0.00000475 1000.00000000
47.46 c/a : 1.62793993 1.58731122 15.80629143 15.41181168 0.15561427 100.00000000
155614.27 a_{omega} : 8.89627075 8.73254342 1.11203384 1.09156793 0.00041885
10.00000000 41.89 c_{omega} : 5.39317771 5.32343103 0.67414721 0.66542888
0.00007601 10.00000000 7.60 a_{4h} : 5.56290615 5.56325146 0.99993793 1.00000000
0.00000000 1.00000000 0.00 c_{4h} : 18.06015038 17.75908031 1.01695302 1.00000000
0.00028740 1.00000000 2.87 a_{6h} : 5.56147284 5.54639384 1.00271870 1.00000000
0.00000739 1.00000000 0.07 c_{6h} : 27.12141943 26.77136353 1.01307576 1.00000000
0.00017098 1.00000000 1.71 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409
0.00000927 1.00000000 0.09 a_{fcc} : 7.85326663 7.88677000 1.12189523 1.12668143
0.00002291 1.00000000 0.23 DE(o,h) : 0.90350500 -0.63343333 0.06023367 -
0.04222889 0.01049858 3000.00000000 314957.26 DE(4h,h): 1.39366250 3.17160000
0.00557465 0.01268640 0.00005058 2000.00000000 1011.54 DE(6h,h): 2.35288167
3.72005000 0.00941153 0.01488020 0.00002991 2000.00000000 598.13 DE(b,h)
: 6.89534500 7.63520000 0.06964995 0.07712323 0.00005585 1.00000000 0.56
DE(f,h) : 3.73991500 4.51880000 0.03777692 0.04564444 0.00006190 2000.00000000
1237.96 c₁₁ : 183.39366296 176.10000000 0.80109056 0.76923077 0.00101505
200.00000000 2030.09 c₃₃ : 189.89794119 190.50000000 0.76679968 0.76923077
0.00000591 200.00000000 11.82 c₄₄ : 48.85821794 50.80000000 0.73982765
0.76923077 0.00086454 200.00000000 1729.09 c₁₂ : 89.06355947 86.90000000
0.78838240 0.76923077 0.00036678 200.00000000 733.57 c₁₃ : 63.83154948
68.30000000 0.71890471 0.76923077 0.00253271 200.00000000 5065.42 M_{freq0}:
2.66005767 2.85858719 0.19386454 0.20833333 0.00020935 0.10000000 0.21

M_{freq1}: 2.66005768 2.85858719 0.19386454 0.20833333 0.00020935 0.10000000
0.21 M_{freq2}: 2.66005768 2.85858719 0.19386454 0.20833333 0.00020935 0.10000000
0.21 M_{freq3}: 2.66005769 2.85858719 0.19386454 0.20833333 0.00020935 0.10000000
0.21 M_{freq4}: 5.53422963 5.66706047 0.20345019 0.20833333 0.00002385 0.10000000
0.02 M_{freq5}: 5.53422963 5.66706047 0.20345019 0.20833333 0.00002385 0.10000000
0.02 H_{freq0}: 3.81185478 4.80643423 0.16522361 0.20833333 0.00185845 0.10000000
1.86 H_{freq1}: 3.81185478 5.58010025 0.14231580 0.20833333 0.00435832 0.10000000
4.36 H_{freq2}: 5.94124541 5.65316738 0.21894973 0.20833333 0.00011271 0.10000000
0.11 H_{freq3}: 5.94124541 6.36651842 0.19441701 0.20833333 0.00019366 0.10000000
0.19 H_{freq4}: 7.45197524 6.40050186 0.24255830 0.20833333 0.00117135 0.10000000
1.17 H_{freq5}: 7.45197524 7.64082373 0.20318422 0.20833333 0.00002651 0.10000000
0.03 bandw. G: 4.28171318 5.87085872 1.21552723 1.66666667 0.20352679
15.00000000 30529.02 bandw. K: 5.27901085 4.97424321 0.96479013 0.90909091
0.00310240 15.00000000 465.36 bandw. M: 5.94705062 7.78109872 1.27382410
1.66666667 0.15432529 15.00000000 23148.79 bandw. L: 4.86539763 6.34433701
1.27814712 1.66666667 0.15094744 15.00000000 22642.12 bandw. H: 4.04633460
9.70902614 0.37887281 0.90909091 0.28113123 1.00000000 2811.31 DOSerr_h:
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00
DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00 E_{prisf}: 106.24862733 220.00000000 106.24862733 220.00000000 12939.37478401
0.00500000 646968.74

1.10 2019-10-23

b2=659516.0443812666 m2=-11.5000000000 p2=0.0000000000 fdd=0.2079280312
qdds=0.5779569377 qddp=0.5500000000 qddd=0.7997346930 b0=61.8713325655
p0=1.1850000000 b1=-6.1749682055 p1=0.7746914774 ndt=2.0000000000 cr1=-
6.0000000000 cr2=3.6778242946 r1dd=6.5000000000 rcdd=10.0000000000 cr3=-
1.2500000000 rmaxhm=10.1000000000 npar=18 VARGS -vb2=659516.0443812666
-vm2=-11.5000000000 -vp2=0.0000000000 -vfdd=0.2079280312 -vqdds=0.5779569377
-vqddp=0.5500000000 -vqddd=0.7997346930 -vb0=61.8713325655 -vp0=1.1850000000
-vb1=-6.1749682055 -vp1=0.7746914774 -vndt=2.0000000000 -vcr1=-6.0000000000
-vcr2=3.6778242946 -vr1dd=6.5000000000 -vrdd=10.0000000000 -vcr3=-1.2500000000
-vrmaxhm=10.1000000000
a_{hcp} : 5.60892158 5.57678969 5.60892158 5.57678969 0.00103246 1000.00000000
10324.59 c/a : 1.61312679 1.58731122 15.66246500 15.41181168 0.06282708
100.00000000 62827.08 a_{omega} : 8.93038665 8.73254342 1.11629833 1.09156793
0.00061159 10.00000000 61.16 c_{omega} : 5.44355140 5.32343103 0.68044393
0.66542888 0.00022545 10.00000000 22.55 a_{4h} : 5.60195654 5.56325146 1.00695728
1.00000000 0.00004840 1.00000000 0.48 c_{4h} : 18.14446401 17.75908031 1.02170066

1.00000000 0.00047092 1.00000000 4.71 a_{6h} : 5.59616500 5.54639384 1.00897361
 1.00000000 0.00008053 1.00000000 0.81 c_{6h} : 27.28498264 26.77136353 1.01918539
 1.00000000 0.00036808 1.00000000 3.68 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.90563971 7.88677000 1.12937710
 1.12668143 0.00000727 1.00000000 0.07 DE(o,h) : 2.52724167 -0.63343333
 0.16848278 -0.04222889 0.04439941 3000.00000000 1331982.19 DE(4h,h): 0.67249250
 3.17160000 0.00268997 0.01268640 0.00009993 2000.00000000 1998.57 DE(6h,h):
 1.31325667 3.72005000 0.00525303 0.01488020 0.00009268 2000.00000000 1853.65
 DE(b,h) : 7.73368500 7.63520000 0.07811803 0.07712323 0.00000099 1.00000000
 0.01 DE(f,h) : 2.37292500 4.51880000 0.02396894 0.04564444 0.00046983
 2000.00000000 9396.55 c_{11} : 188.64224235 176.10000000 0.82401713 0.76923077
 0.00300155 200.00000000 6003.09 c_{33} : 209.41683651 190.50000000 0.84561614
 0.76923077 0.00583472 200.00000000 11669.45 c_{44} : 47.01653541 50.80000000
 0.71194027 0.76923077 0.00328220 200.00000000 6564.40 c_{12} : 88.36706627
 86.90000000 0.78221710 0.76923077 0.00016864 200.00000000 337.29 c_{13} :
 64.20264411 68.30000000 0.72308418 0.76923077 0.00212951 200.00000000
 4259.02 M_{freq0} : 2.90295744 2.85858719 0.21156703 0.20833333 0.00001046
 0.10000000 0.01 M_{freq1} : 2.90295745 2.85858719 0.21156703 0.20833333 0.00001046
 0.10000000 0.01 M_{freq2} : 2.90295745 2.85858719 0.21156703 0.20833333 0.00001046
 0.10000000 0.01 M_{freq3} : 2.90295746 2.85858719 0.21156703 0.20833333 0.00001046
 0.10000000 0.01 M_{freq4} : 5.93116182 5.66706047 0.21804227 0.20833333 0.00009426
 0.10000000 0.09 M_{freq5} : 5.93116182 5.66706047 0.21804227 0.20833333 0.00009426
 0.10000000 0.09 H_{freq0} : 4.08984062 4.80643423 0.17727282 0.20833333 0.00096476
 0.10000000 0.96 H_{freq1} : 4.08984062 5.58010025 0.15269441 0.20833333 0.00309569
 0.10000000 3.10 H_{freq2} : 6.59387549 5.65316738 0.24300078 0.20833333 0.00120183
 0.10000000 1.20 H_{freq3} : 6.59387549 6.36651842 0.21577320 0.20833333 0.00005535
 0.10000000 0.06 H_{freq4} : 8.07363804 6.40050186 0.26279313 0.20833333 0.00296587
 0.10000000 2.97 H_{freq5} : 8.07363804 7.64082373 0.22013437 0.20833333 0.00013926
 0.10000000 0.14 bandw. G: 4.29531888 5.87085872 1.21938972 1.66666667
 0.20005666 15.00000000 30008.50 bandw. K: 4.93206555 4.97424321 0.90138253
 0.90909091 0.00005942 15.00000000 8.91 bandw. M: 5.71031148 7.78109872
 1.22311593 1.66666667 0.19673726 15.00000000 29510.59 bandw. L: 4.84771022
 6.34433701 1.27350061 1.66666667 0.15457955 15.00000000 23186.93 bandw.
 H: 3.83408571 9.70902614 0.35899918 0.90909091 0.30260091 1.00000000 3026.01
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 166.34500821 220.00000000 166.34500821 220.00000000
 2878.85814412 0.00500000 143942.91

————— E_{Basalfault} I2 —————

tbe: 58.453 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]

b2=504779.7995565861 m2=-11.5000000000 p2=0.0000000000 fdd=0.2400000000
 qdds=0.5750000000 qddp=0.5750000000 qddd=0.7500000000 b0=66.8564029459
 p0=1.1850000000 b1=-10.0000000000 p1=0.8500000000 ndt=2.0000000000
 cr1=-6.0000000000 cr2=3.0000000000 ridd=6.5000000000 rcdd=10.0000000000
 cr3=-1.2500000000 rmaxhm=10.1000000000 npar=18 a_{hcp} : 5.57461126 5.57678969
 5.57461126 5.57678969 0.00000475 1000.00000000 47.46 c/a : 1.62793993
 1.58731122 15.80629143 15.41181168 0.15561427 100.00000000 155614.27 a_{omega}
 : 8.89627075 8.73254342 1.11203384 1.09156793 0.00041885 10.00000000 41.89
 c_{omega} : 5.39317771 5.32343103 0.67414721 0.66542888 0.00007601 10.00000000
 7.60 a_{4h} : 5.56290615 5.56325146 0.99993793 1.00000000 0.00000000 1.00000000
 0.00 c_{4h} : 18.06015038 17.75908031 1.01695302 1.00000000 0.00028740 1.00000000
 2.87 a_{6h} : 5.56147284 5.54639384 1.00271870 1.00000000 0.00000739 1.00000000
 0.07 c_{6h} : 27.12141943 26.77136353 1.01307576 1.00000000 0.00017098 1.00000000
 1.71 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409 0.00000927 1.00000000
 0.09 a_{fcc} : 7.85326663 7.88677000 1.12189523 1.12668143 0.00002291 1.00000000
 0.23 DE(o,h) : 0.90350500 -0.63343333 0.06023367 -0.04222889 0.01049858
 3000.00000000 314957.26 DE(4h,h): 1.39366250 3.17160000 0.00557465 0.01268640
 0.00005058 2000.00000000 1011.54 DE(6h,h): 2.35288167 3.72005000 0.00941153
 0.01488020 0.00002991 2000.00000000 598.13 DE(b,h) : 6.89534500 7.63520000
 0.06964995 0.07712323 0.00005585 1.00000000 0.56 DE(f,h) : 3.73991500
 4.51880000 0.03777692 0.04564444 0.00006190 2000.00000000 1237.96 c₁₁ :
 183.39366296 176.10000000 0.80109056 0.76923077 0.00101505 100.00000000
 1015.05 c₃₃ : 189.89794119 190.50000000 0.76679968 0.76923077 0.00000591
 100.00000000 5.91 c₄₄ : 48.85821794 50.80000000 0.73982765 0.76923077
 0.00086454 100.00000000 864.54 c₁₂ : 89.06355947 86.90000000 0.78838240
 0.76923077 0.00036678 100.00000000 366.78 c₁₃ : 63.83154948 68.30000000
 0.71890471 0.76923077 0.00253271 10.00000000 253.27 M_{freq0}: 2.66005767
 2.85858719 0.19386454 0.20833333 0.00020935 0.10000000 0.21 M_{freq1}: 2.66005768
 2.85858719 0.19386454 0.20833333 0.00020935 0.10000000 0.21 M_{freq2}: 2.66005768
 2.85858719 0.19386454 0.20833333 0.00020935 0.10000000 0.21 M_{freq3}: 2.66005769
 2.85858719 0.19386454 0.20833333 0.00020935 0.10000000 0.21 M_{freq4}: 5.53422963
 5.66706047 0.20345019 0.20833333 0.00002385 0.10000000 0.02 M_{freq5}: 5.53422963
 5.66706047 0.20345019 0.20833333 0.00002385 0.10000000 0.02 H_{freq0}: 3.81185478
 4.80643423 0.16522361 0.20833333 0.00185845 0.10000000 1.86 H_{freq1}: 3.81185478
 5.58010025 0.14231580 0.20833333 0.00435832 0.10000000 4.36 H_{freq2}: 5.94124541
 5.65316738 0.21894973 0.20833333 0.00011271 0.10000000 0.11 H_{freq3}: 5.94124541
 6.36651842 0.19441701 0.20833333 0.00019366 0.10000000 0.19 H_{freq4}: 7.45197524
 6.40050186 0.24255830 0.20833333 0.00117135 0.10000000 1.17 H_{freq5}: 7.45197524
 7.64082373 0.20318422 0.20833333 0.00002651 0.10000000 0.03 bandw. G:
 4.28171318 5.87085872 1.21552723 1.66666667 0.20352679 15.00000000 30529.02

bandw. K: 5.27901085 4.97424321 0.96479013 0.90909091 0.00310240 15.00000000
 465.36 bandw. M: 5.94705062 7.78109872 1.27382410 1.66666667 0.15432529
 15.00000000 23148.79 bandw. L: 4.86539763 6.34433701 1.27814712 1.66666667
 0.15094744 15.00000000 22642.12 bandw. H: 4.04633460 9.70902614 0.37887281
 0.90909091 0.28113123 5.00000000 14056.56 DOSerr_h: 0.00000000 0.00000000
 0.00000000 0.00000000 0.00000000 1.00000000 0.00 DOSerr_o: 0.00000000
 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00

————- E_{Basalfault} I2 —————

tbe: 194.019 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]

————- E_{prismaticfault} —————

tbe: 106.249 mJ/m² DFT: 250.000 mJ/m² [Benoit 2012] DFT: 233.000
 mJ/m² [Ackland 1999]

1.11 2019-10-25

PARAMETERS fdd=0.1996748611 qdds=0.5613768169 qddp=0.5668040794
 qddd=0.7729099571 b0=66.4084486262 p0=1.1975965455 b1=-3.9903136673
 p1=0.6875520869 b2=687169.0932117153 m2=-11.5000000000 p2=0.0000000000
 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.3390616081 cr3=-1.2048480891
 r1dd=6.5000000000 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18
 VARGS -vfdd=0.1996748611 -vqdds=0.5613768169 -vqddp=0.5668040794 -
 vqddd=0.7729099571 -vb0=66.4084486262 -vp0=1.1975965455 -vb1=-3.9903136673
 -vp1=0.6875520869 -vb2=687169.093 2117153 -vm2=-11.5000000000 -vp2=0.0000000000
 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.3390616081 -vcr3=-1.2048480891
 -vr1dd=6.5000000000 -vrdd=10.0000000000 -vrmaxh m=10.1000000000
 a_{hcp}: 5.73036925 5.57678969 5.73036925 5.57678969 0.02358668 1000.00000000
 235866.81 c/a : 1.56211819 1.58731122 15.16720300 15.41181168 0.05983341
 100.00000000 59833.41 a_{omega} : 9.15812985 8.73254342 1.14476623 1.09156793
 0.00283006 10.00000000 283.01 c_{omega} : 5.51707646 5.32343103 0.68963456
 0.66542888 0.00058591 10.00000000 58.59 a_{4h} : 5.72210491 5.56325146 1.02855407
 1.00000000 0.00081533 1.00000000 8.15 c_{4h} : 18.56365721 17.75908031 1.04530510
 1.00000000 0.00205255 1.00000000 20.53 a_{6h} : 5.71934406 5.54639384 1.03118246
 1.00000000 0.00097235 1.00000000 9.72 c_{6h} : 27.89917562 26.77136353 1.04212756
 1.00000000 0.00177473 1.00000000 17.75 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 8.07893300 7.88677000 1.15413329
 1.12668143 0.00075360 1.00000000 7.54 DE(o,h) : 0.74893333 -0.63343333
 0.04992889 -0.04222889 0.00849306 300.00000000 25479.17 DE(4h,h): 1.37746500
 3.17160000 0.00550986 0.01268640 0.00005150 2000.00000000 1030.05 DE(6h,h):
 2.16358500 3.72005000 0.00865434 0.01488020 0.00003876 2000.00000000 775.23
 DE(b,h) : 8.46742000 7.63520000 0.08552949 0.07712323 0.00007067 1.00000000

0.71 DE(f,h) : 3.32836000 4.51880000 0.03361980 0.04564444 0.00014459
 20000.00000000 28918.42 c₁₁ : 178.13198086 176.10000000 0.77810676 0.76923077
 0.00007878 200.00000000 157.57 c₃₃ : 198.06934208 190.50000000 0.79979545
 0.76923077 0.00093420 200.00000000 1868.40 c₄₄ : 46.87680969 50.80000000
 0.70982450 0.76923077 0.00352911 200.00000000 7058.21 c₁₂ : 108.27146945
 86.90000000 0.95840904 0.76923077 0.03578842 200.00000000 71576.84 c₁₃
 : 60.82048039 68.30000000 0.68499246 0.76923077 0.00709609 200.00000000
 14192.19 M_{freq0}: 2.65837552 2.85858719 0.19374194 0.20833333 0.00021291
 0.10000000 0.21 M_{freq1}: 2.65837553 2.85858719 0.19374194 0.20833333 0.00021291
 0.10000000 0.21 M_{freq2}: 2.65837553 2.85858719 0.19374194 0.20833333 0.00021291
 0.10000000 0.21 M_{freq3}: 2.65837554 2.85858719 0.19374194 0.20833333 0.00021291
 0.10000000 0.21 M_{freq4}: 5.86567748 5.66706047 0.21563492 0.20833333 0.00005331
 0.10000000 0.05 M_{freq5}: 5.86567748 5.66706047 0.21563492 0.20833333 0.00005331
 0.10000000 0.05 H_{freq0}: 4.08375870 4.80643423 0.17700920 0.20833333 0.00098120
 0.10000000 0.98 H_{freq1}: 4.08375870 5.58010025 0.15246734 0.20833333 0.00312101
 0.10000000 3.12 H_{freq2}: 6.55042546 5.65316738 0.24139953 0.20833333 0.00109337
 0.10000000 1.09 H_{freq3}: 6.55042546 6.36651842 0.21435137 0.20833333 0.00003622
 0.10000000 0.04 H_{freq4}: 7.93335679 6.40050186 0.25822704 0.20833333 0.00248938
 0.10000000 2.49 H_{freq5}: 7.93335679 7.64082373 0.21630949 0.20833333 0.00006362
 0.10000000 0.06 bandw. G: 3.52795751 5.87085872 0.85846714 1.42857143
 0.32501890 20.00000000 65003.78 bandw. K: 4.36334737 4.97424321 0.73099015
 0.83333333 0.01047413 20.00000000 2094.83 bandw. M: 5.02730544 7.78109872
 0.92298853 1.42857143 0.25561406 20.00000000 51122.81 bandw. L: 4.05994030
 6.34433701 0.91418768 1.42857143 0.26459064 20.00000000 52918.13 bandw.
 H: 3.37693426 9.70902614 0.31619446 0.90909091 0.35152620 5.00000000 17576.31
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 119.44084079 220.00000000 119.44084079 220.00000000
 10112.14450048 0.00500000 505607.23
 ———— E_{Basalfault} I2 ————
 tbe: 181.871 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]
 fdd=0.2033496917 qdds=0.5756399625 qddp=0.5588992296 qddd=0.8019668349
 b0=66.7519567809 p0=1.1959305769 b1=-4.7548799880 p1=0.7066840634 b2=809796.5622505632
 m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
 cr2=3.3129621462 cr3=-1.2333907751 r1dd=6.5000000000 rcdd=10.0000000000
 rmaxhm=10.1000000000 npar=18
 a_{hcp} : 5.63969196 5.57678969 5.63969196 5.57678969 0.00395670 1000.00000000
 39566.95 c/a : 1.59999530 1.58731122 15.53496628 15.41181168 0.01516705
 100.00000000 15167.05 a_{omega} : 9.00648433 8.73254342 1.12581054 1.09156793
 0.00117256 10.00000000 117.26 c_{omega} : 5.44776429 5.32343103 0.68097054

0.66542888 0.00024154 10.00000000 24.15 a_{4h} : 5.63333543 5.56325146 1.01259766
 1.00000000 0.00015870 1.00000000 1.59 c_{4h} : 18.26259726 17.75908031 1.02835265
 1.00000000 0.00080387 1.00000000 8.04 a_{6h} : 5.62878054 5.54639384 1.01485410
 1.00000000 0.00022064 1.00000000 2.21 c_{6h} : 27.45757376 26.77136353 1.02563225
 1.00000000 0.00065701 1.00000000 6.57 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.95185126 7.88677000 1.13597875
 1.12668143 0.00008644 1.00000000 0.86 DE(o,h) : 2.06713667 -0.63343333
 0.13780911 -0.04222889 0.03241368 300.00000000 97241.04 DE(4h,h): 1.21707000
 3.17160000 0.00486828 0.01268640 0.00006112 2000.00000000 1222.46 DE(6h,h):
 1.92688500 3.72005000 0.00770754 0.01488020 0.00005145 2000.00000000 1028.94
 DE(b,h) : 6.98348000 7.63520000 0.07054020 0.07712323 0.00004334 1.00000000
 0.43 DE(f,h) : 2.99983000 4.51880000 0.03030131 0.04564444 0.00023541
 20000.00000000 47082.34 c_{11} : 197.87671665 176.10000000 0.86435468 0.76923077
 0.00904856 200.00000000 18097.12 c_{33} : 235.02901939 190.50000000 0.94903703
 0.76923077 0.03233029 200.00000000 64660.58 c_{44} : 50.83851670 50.80000000
 0.76981400 0.76923077 0.00000034 200.00000000 0.68 c_{12} : 103.63233365
 86.90000000 0.91734384 0.76923077 0.02193748 200.00000000 43874.96 c_{13}
 : 62.82860225 68.30000000 0.70760899 0.76923077 0.00379724 200.00000000
 7594.49 M_{freq0} : 2.92168711 2.85858719 0.21293204 0.20833333 0.00002115
 0.10000000 0.02 M_{freq1} : 2.92168712 2.85858719 0.21293205 0.20833333 0.00002115
 0.10000000 0.02 M_{freq2} : 2.92168712 2.85858719 0.21293205 0.20833333 0.00002115
 0.10000000 0.02 M_{freq3} : 2.92168713 2.85858719 0.21293205 0.20833333 0.00002115
 0.10000000 0.02 M_{freq4} : 6.35723654 5.66706047 0.23370569 0.20833333 0.00064376
 0.10000000 0.64 M_{freq5} : 6.35723654 5.66706047 0.23370569 0.20833333 0.00064376
 0.10000000 0.64 H_{freq0} : 4.33622049 4.80643423 0.18795207 0.20833333 0.00041540
 0.10000000 0.42 H_{freq1} : 4.33622049 5.58010025 0.16189302 0.20833333 0.00215670
 0.10000000 2.16 H_{freq2} : 7.16242789 5.65316738 0.26395335 0.20833333 0.00309359
 0.10000000 3.09 H_{freq3} : 7.16242789 6.36651842 0.23437810 0.20833333 0.00067833
 0.10000000 0.68 H_{freq4} : 8.68591775 6.40050186 0.28272255 0.20833333 0.00553376
 0.10000000 5.53 H_{freq5} : 8.68591775 7.64082373 0.23682868 0.20833333 0.00081198
 0.10000000 0.81 bandw. G: 3.77149950 5.87085872 0.91772885 1.42857143
 0.26096014 20.00000000 52192.03 bandw. K: 4.52389461 4.97424321 0.75788658
 0.83333333 0.00569221 20.00000000 1138.44 bandw. M: 5.19193438 7.78109872
 0.95321360 1.42857143 0.22596507 20.00000000 45193.01 bandw. L: 4.28443432
 6.34433701 0.96473760 1.42857143 0.21514182 20.00000000 43028.36 bandw.
 H: 3.49938554 9.70902614 0.32766001 0.90909091 0.33806189 5.00000000 16903.09
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 192.95890747 220.00000000 192.95890747 220.00000000
 731.22068519 0.00500000 36561.03

```

fdd=0.2191492497 qdds=0.5666686522 qddp=0.5740515649 qddd=0.7927877406
b0=61.5223951343 p0=1.1224359712 b1=-8.5854597936 p1=0.7580275313 b2=717811.8061519205
m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
cr2=3.8490348767 cr3=-1.1468894046 r1dd=6.5000000000 rcdd=10.0000000000
rmaxhm=10.1000000000 npar=18 VARGS -vfdd=0.2191492497 -vqdds=0.5666686522
-vqddp=0.5740515649 -vqddd=0.7927877406 -vb0=61.5223951343 -vp0=1.1224359712
-vb1=-8.5854597936 -vp1=0.7580275313 -vb2=717811.806 1519205 -vm2=-
11.5000000000 -vp2=0.0000000000 -vndt=2.0000000000 -vcr1=-6.0000000000
-vcr2=3.8490348767 -vcr3=-1.1468894046 -vr1dd=6.5000000000 -vrcdd=10.0000000000
-vrmaxh m=10.1000000000
a_hcp : 5.55663918 5.57678969 5.55663918 5.57678969 0.00040604 1000.00000000
4060.43 c/a : 1.59594552 1.58731122 15.49564541 15.41181168 0.00702809
100.00000000 7028.09 a_omega : 8.86850776 8.73254342 1.10856347 1.09156793
0.00028885 10.00000000 28.88 c_omega : 5.38457336 5.32343103 0.67307167
0.66542888 0.00005841 10.00000000 5.84 a_4h : 5.55005614 5.56325146 0.99762813
1.00000000 0.00000563 1.00000000 0.06 c_4h : 17.98631929 17.75908031 1.01279565
1.00000000 0.00016373 1.00000000 1.64 a_6h : 5.54499483 5.54639384 0.99974776
1.00000000 0.00000006 1.00000000 0.00 c_6h : 27.04207163 26.77136353 1.01011185
1.00000000 0.00010225 1.00000000 1.02 a_bcc : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_fcc : 7.83247144 7.88677000 1.11892449
1.12668143 0.00006017 1.00000000 0.60 DE(o,h) : 2.18659000 -0.63343333
0.14577267 -0.04222889 0.03534458 300.00000000 106033.75 DE(4h,h): 1.44806500
3.17160000 0.00579226 0.01268640 0.00004753 2000.00000000 950.58 DE(6h,h):
2.25622500 3.72005000 0.00902490 0.01488020 0.00003428 2000.00000000 685.69
DE(b,h) : 8.17231000 7.63520000 0.08254859 0.07712323 0.00002943 1.00000000
0.29 DE(f,h) : 3.52323000 4.51880000 0.03558818 0.04564444 0.00010113
20000.00000000 20225.68 c_11 : 223.84039990 176.10000000 0.97776788 0.76923077
0.04348772 200.00000000 86975.45 c_33 : 261.70835128 190.50000000 1.05676702
0.76923077 0.08267709 200.00000000 165354.19 c_44 : 57.98693676 50.80000000
0.87805779 0.76923077 0.01184332 200.00000000 23686.64 c_12 : 103.36482959
86.90000000 0.91497592 0.76923077 0.02124165 200.00000000 42483.30 c_13 :
75.87982605 68.30000000 0.85459878 0.76923077 0.00728770 200.00000000
14575.40 M_freq0: 3.09053446 2.85858719 0.22523761 0.20833333 0.00028575
0.10000000 0.29 M_freq1: 3.09053447 2.85858719 0.22523761 0.20833333 0.00028575
0.10000000 0.29 M_freq2: 3.09053447 2.85858719 0.22523761 0.20833333 0.00028575
0.10000000 0.29 M_freq3: 3.09053449 2.85858719 0.22523761 0.20833333 0.00028575
0.10000000 0.29 M_freq4: 6.62655638 5.66706047 0.24360647 0.20833333 0.00124419
0.10000000 1.24 M_freq5: 6.62655638 5.66706047 0.24360647 0.20833333 0.00124419
0.10000000 1.24 H_freq0: 4.34189277 4.80643423 0.18819793 0.20833333 0.00040543
0.10000000 0.41 H_freq1: 4.34189277 5.58010025 0.16210479 0.20833333 0.00213708

```

0.10000000 2.14 H_{freq2}: 7.41145816 5.65316738 0.27313074 0.20833333 0.00419870
 0.10000000 4.20 H_{freq3}: 7.41145816 6.36651842 0.24252718 0.20833333 0.00116922
 0.10000000 1.17 H_{freq4}: 9.10573433 6.40050186 0.29638738 0.20833333 0.00775352
 0.10000000 7.75 H_{freq5}: 9.10573433 7.64082373 0.24827532 0.20833333 0.00159536
 0.10000000 1.60 bandw. G: 4.58375968 5.87085872 1.11537825 1.42857143
 0.09808997 20.00000000 19617.99 bandw. K: 5.47221176 4.97424321 0.91675784
 0.83333333 0.00695965 20.00000000 1391.93 bandw. M: 6.19739547 7.78109872
 1.13781131 1.42857143 0.08454145 20.00000000 16908.29 bandw. L: 5.18649210
 6.34433701 1.16785638 1.42857143 0.06797234 20.00000000 13594.47 bandw.
 H: 4.20143956 9.70902614 0.39339584 0.90909091 0.26594140 5.00000000 13297.07
 DOS_{errh}: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOS_{erro}: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 171.98938061 220.00000000 171.98938061 220.00000000
 2305.01957445 0.00500000 115250.98
 fdd=0.2122128374 qdds=0.5802399619 qddp=0.5506218303 qddd=0.7985751886
 b0=73.1365845881 p0=1.2632046664 b1=-4.4547201964 p1=0.7828722693 b2=668037.5062577532
 m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
 cr2=3.3768946881 cr3=-1.1338728535 r1dd=6.5000000000 rcdd=10.0000000000
 rmaxhm=10.1000000000 npar=18
 a_{hcp} : 5.69782890 5.57678969 5.69782890 5.57678969 0.01465049 1000.00000000
 146504.90 c/a : 1.57557204 1.58731122 15.29783152 15.41181168 0.01299148
 100.00000000 12991.48 a_{omega} : 9.07908385 8.73254342 1.13488548 1.09156793
 0.00187641 10.00000000 187.64 c_{omega} : 5.52116211 5.32343103 0.69014526
 0.66542888 0.00061090 10.00000000 61.09 a_{4h} : 5.68808445 5.56325146 1.02243885
 1.00000000 0.00050350 1.00000000 5.04 c_{4h} : 18.44844400 17.75908031 1.03881753
 1.00000000 0.00150680 1.00000000 15.07 a_{6h} : 5.68183863 5.54639384 1.02442033
 1.00000000 0.00059635 1.00000000 5.96 c_{6h} : 27.74184558 26.77136353 1.03625075
 1.00000000 0.00131412 1.00000000 13.14 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 8.02925559 7.88677000 1.14703651
 1.12668143 0.00041433 1.00000000 4.14 DE(o,h) : 2.32915000 -0.63343333
 0.15527667 -0.04222889 0.03900844 300.00000000 117025.33 DE(4h,h): 0.85166250
 3.17160000 0.00340665 0.01268640 0.00008611 2000.00000000 1722.28 DE(6h,h):
 1.45723667 3.72005000 0.00582895 0.01488020 0.00008193 2000.00000000 1638.50
 DE(b,h) : 8.33560000 7.63520000 0.08419798 0.07712323 0.00005005 1.00000000
 0.50 DE(f,h) : 2.42162000 4.51880000 0.02446081 0.04564444 0.00044875
 20000.00000000 89749.29 c₁₁ : 176.99471293 176.10000000 0.77313901 0.76923077
 0.00001527 200.00000000 30.55 c₃₃ : 186.32850615 190.50000000 0.75238646
 0.76923077 0.00028373 200.00000000 567.46 c₄₄ : 42.11490258 50.80000000
 0.63771809 0.76923077 0.01729559 200.00000000 34591.17 c₁₂ : 79.11110984
 86.90000000 0.70028423 0.76923077 0.00475362 200.00000000 9507.25 c₁₃ :

53.23875590 68.30000000 0.59960306 0.76923077 0.02877356 200.00000000
 57547.12 M_{freq0}: 2.66368299 2.85858719 0.19412875 0.20833333 0.00020177
 0.10000000 0.20 M_{freq1}: 2.66368300 2.85858719 0.19412875 0.20833333 0.00020177
 0.10000000 0.20 M_{freq2}: 2.66368300 2.85858719 0.19412875 0.20833333 0.00020177
 0.10000000 0.20 M_{freq3}: 2.66368301 2.85858719 0.19412875 0.20833333 0.00020177
 0.10000000 0.20 M_{freq4}: 5.40698528 5.66706047 0.19877241 0.20833333 0.00009141
 0.10000000 0.09 M_{freq5}: 5.40698528 5.66706047 0.19877241 0.20833333 0.00009141
 0.10000000 0.09 H_{freq0}: 3.95471742 4.80643423 0.17141594 0.20833333 0.00136289
 0.10000000 1.36 H_{freq1}: 3.95471742 5.58010025 0.14764958 0.20833333 0.00368252
 0.10000000 3.68 H_{freq2}: 5.90872297 5.65316738 0.21775120 0.20833333 0.00008870
 0.10000000 0.09 H_{freq3}: 5.90872297 6.36651842 0.19335277 0.20833333 0.00022442
 0.10000000 0.22 H_{freq4}: 7.26013735 6.40050186 0.23631407 0.20833333 0.00078292
 0.10000000 0.78 H_{freq5}: 7.26013735 7.64082373 0.19795361 0.20833333 0.00010774
 0.10000000 0.11 bandw. G: 3.86129711 5.87085872 0.93957954 1.42857143
 0.23911307 20.00000000 47822.61 bandw. K: 4.54566372 4.97424321 0.76153355
 0.83333333 0.00515521 20.00000000 1031.04 bandw. M: 5.30214054 7.78109872
 0.97344691 1.42857143 0.20713833 20.00000000 41427.67 bandw. L: 4.41368845
 6.34433701 0.99384210 1.42857143 0.18898959 20.00000000 37797.92 bandw.
 H: 3.54564492 9.70902614 0.33199144 0.90909091 0.33304380 5.00000000 16652.19
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 105.06064957 220.00000000 105.06064957 220.00000000
 13211.05427625 0.00500000 660552.71
 ———— E_{Basalfault} I2 ————
 tbe: 88.828 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]

1.12 2019-10-28

fdd=0.1947759320 qdds=0.5574317424 qddp=0.5696892318 qddd=0.7755035206
 b0=57.0403256066 p0=1.2033018731 b1=-3.3927882483 p1=0.6832191939 b2=614064.0142907096
 m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
 cr2=3.2639887643 cr3=-1.2458565306 r1dd=6.5000000000 rcdd=10.0000000000
 rmaxhm=10.1000000000 npar=18 VARGS -vfdd=0.1947759320 -vqdds=0.5574317424
 -vqddp=0.5696892318 -vqddd=0.7755035206 -vb0=57.0403256066 -vp0=1.2033018731
 -vb1=-3.3927882483 -vp1=0.6832191939 -vb2=614064.014 2907096 -vm2=-
 11.5000000000 -vp2=0.0000000000 -vndt=2.0000000000 -vcr1=-6.0000000000
 -vcr2=3.2639887643 -vcr3=-1.2458565306 -vr1dd=6.5000000000 -vrcdd=10.0000000000
 -vrmaxh m=10.1000000000
 a_{hcp} : 5.58768186 5.57678969 5.58768186 5.57678969 0.00011864 1000.00000000
 1186.39 c/a : 1.62227538 1.58731122 15.75129214 15.41181168 0.11524698

100.00000000 115246.98 a_{omega} : 8.93247488 8.73254342 1.11655936 1.09156793
 0.00062457 10.00000000 62.46 c_{omega} : 5.39665426 5.32343103 0.67458178
 0.66542888 0.00008378 10.00000000 8.38 a_{4h} : 5.57932240 5.56325146 1.00288877
 1.00000000 0.00000834 1.00000000 0.08 c_{4h} : 18.09815454 17.75908031 1.01909301
 1.00000000 0.00036454 1.00000000 3.65 a_{6h} : 5.57691999 5.54639384 1.00550378
 1.00000000 0.00003029 1.00000000 0.30 c_{6h} : 27.19065397 26.77136353 1.01566190
 1.00000000 0.00024530 1.00000000 2.45 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.87675750 7.88677000 1.12525107
 1.12668143 0.00000205 1.00000000 0.02 DE(o,h) : 0.81603167 -0.63343333
 0.05440211 -0.04222889 0.00933755 3000.00000000 280126.50 DE(4h,h): 1.54928500
 3.17160000 0.00619714 0.01268640 0.00004211 2000.00000000 842.21 DE(6h,h):
 2.42087167 3.72005000 0.00968349 0.01488020 0.00002701 2000.00000000 540.12
 DE(b,h) : 5.89112500 7.63520000 0.05950631 0.07712323 0.00031036 1.00000000
 3.10 DE(f,h) : 3.68590500 4.51880000 0.03723136 0.04564444 0.00007078
 2000.00000000 1415.60 c_{11} : 171.39986242 176.10000000 0.74869988 0.76923077
 0.00042152 200.00000000 843.04 c_{33} : 193.75759266 190.50000000 0.78238479
 0.76923077 0.00017303 200.00000000 346.06 c_{44} : 48.33577790 50.80000000
 0.73191669 0.76923077 0.00139234 200.00000000 2784.68 c_{12} : 90.93886140
 86.90000000 0.80498240 0.76923077 0.00127818 200.00000000 2556.36 c_{13} :
 64.50444044 68.30000000 0.72648317 0.76923077 0.00182736 200.00000000
 3654.71 M_{freq0} : 2.67934359 2.85858719 0.19527009 0.20833333 0.00017065
 0.10000000 0.17 M_{freq1} : 2.67934360 2.85858719 0.19527009 0.20833333 0.00017065
 0.10000000 0.17 M_{freq2} : 2.67934360 2.85858719 0.19527009 0.20833333 0.00017065
 0.10000000 0.17 M_{freq3} : 2.67934361 2.85858719 0.19527009 0.20833333 0.00017065
 0.10000000 0.17 M_{freq4} : 5.94154925 5.66706047 0.21842413 0.20833333 0.00010182
 0.10000000 0.10 M_{freq5} : 5.94154925 5.66706047 0.21842413 0.20833333 0.00010182
 0.10000000 0.10 H_{freq0} : 3.87022016 4.80643423 0.16775344 0.20833333 0.00164673
 0.10000000 1.65 H_{freq1} : 3.87022016 5.58010025 0.14449487 0.20833333 0.00407535
 0.10000000 4.08 H_{freq2} : 6.55198943 5.65316738 0.24145717 0.20833333 0.00109719
 0.10000000 1.10 H_{freq3} : 6.55198943 6.36651842 0.21440255 0.20833333 0.00003684
 0.10000000 0.04 H_{freq4} : 8.09781698 6.40050186 0.26358014 0.20833333 0.00305221
 0.10000000 3.05 H_{freq5} : 8.09781698 7.64082373 0.22079363 0.20833333 0.00015526
 0.10000000 0.16 bandw. G: 3.80551375 5.87085872 0.92600563 1.42857143
 0.25257238 15.00000000 37885.86 bandw. K: 4.73614350 4.97424321 0.79344457
 0.83333333 0.00159111 15.00000000 238.67 bandw. M: 5.30758282 7.78109872
 0.97444608 1.42857143 0.20622983 15.00000000 30934.47 bandw. L: 4.32525142
 6.34433701 0.97392849 1.42857143 0.20670020 15.00000000 31005.03 bandw.
 H: 3.61639455 9.70902614 0.33861598 0.90909091 0.32544164 1.00000000 3254.42
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000

0.00000000 0.00 E_{prsf}: 128.19028679 220.00000000 128.19028679 220.00000000
 8429.02343885 0.00500000 421451.17
 ——— E_{Basalfault} I2 ———
 tbe: 199.455 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]
 ## above model for parameter comparison
 fdd=0.1947759320 qdds=0.5574317424 qddp=0.5696892318 qddd=0.7755035206
 b0=57.0403256066 p0=1.2033018731 b1=-3.3927882483 p1=0.6832191939 b2=614064.0142907096
 m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
 cr2=3.2639887643 cr3=-1.2458565306 r1dd=6.5000000000 rcdd=10.0000000000
 rmaxhm=10.1000000000 npar=18
 ## » Averaged Parameters for below and above model
 fdd=0.19457916745 qdds=0.55787572025 qddp=0.5674206158499999 qddd=0.77550969935
 b0=62.052002964850004 p0=1.2042435259 b1=-3.5371354253 p1=0.6724720237999999
 b2=616290.2350520021 m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000
 cr1=-6.0000000000 cr2=3.15587807505 cr3=-1.2255817141 r1dd=6.5000000000
 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18
 fdd=0.1943824029 qdds=0.5583196981 qddp=0.5651519999 qddd=0.7755158781
 b0=67.0636803231 p0=1.2051851787 b1=-3.6814826023 p1=0.6617248537 b2=618516.4558132945
 m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
 cr2=3.0477673858 cr3=-1.2053068976 r1dd=6.5000000000 rcdd=10.0000000000
 rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.64132578 5.57678969 5.64132578 5.57678969 0.00416491 1000.00000000
 41649.07 c/a : 1.59930205 1.58731122 15.52823532 15.41181168 0.01355446
 100.00000000 13554.46 a_{omega} : 9.02663399 8.73254342 1.12832925 1.09156793
 0.00135139 10.00000000 135.14 c_{omega} : 5.42825585 5.32343103 0.67853198
 0.66542888 0.00017169 10.00000000 17.17 a_{4h} : 5.63523851 5.56325146 1.01293974
 1.00000000 0.00016744 1.00000000 1.67 c_{4h} : 18.27263692 17.75908031 1.02891797
 1.00000000 0.00083625 1.00000000 8.36 a_{6h} : 5.63240115 5.54639384 1.01550689
 1.00000000 0.00024046 1.00000000 2.40 c_{6h} : 27.45989488 26.77136353 1.02571895
 1.00000000 0.00066146 1.00000000 6.61 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.95685751 7.88677000 1.13669393
 1.12668143 0.00010025 1.00000000 1.00 DE(o,h) : 0.55758500 -0.63343333
 0.03717233 -0.04222889 0.00630455 3000.00000000 189136.62 DE(4h,h): 1.64759250
 3.17160000 0.00659037 0.01268640 0.00003716 2000.00000000 743.23 DE(6h,h):
 2.54485333 3.72005000 0.01017941 0.01488020 0.00002210 2000.00000000 441.95
 DE(b,h) : 5.56874500 7.63520000 0.05624995 0.07712323 0.00043569 1.00000000
 4.36 DE(f,h) : 3.85176500 4.51880000 0.03890672 0.04564444 0.00004540
 2000.00000000 907.94 c₁₁ : 180.32787110 176.10000000 0.78769873 0.76923077
 0.00034107 200.00000000 682.13 c₃₃ : 216.36777014 190.50000000 0.87368371

0.76923077 0.01091042 200.00000000 21820.83 c_{44} : 50.47165422 50.80000000
 0.76425885 0.76923077 0.00002472 200.00000000 49.44 c_{12} : 112.37710248
 86.90000000 0.99475173 0.76923077 0.05085970 200.00000000 101719.40 c_{13}
 : 64.58400786 68.30000000 0.72737930 0.76923077 0.00175155 200.00000000
 3503.09 $M_{\text{freq}0}$: 2.73169321 2.85858719 0.19908532 0.20833333 0.00008553
 0.10000000 0.09 $M_{\text{freq}1}$: 2.73169322 2.85858719 0.19908532 0.20833333 0.00008553
 0.10000000 0.09 $M_{\text{freq}2}$: 2.73169322 2.85858719 0.19908532 0.20833333 0.00008553
 0.10000000 0.09 $M_{\text{freq}3}$: 2.73169323 2.85858719 0.19908532 0.20833333 0.00008553
 0.10000000 0.09 $M_{\text{freq}4}$: 6.34014433 5.66706047 0.23307734 0.20833333 0.00061227
 0.10000000 0.61 $M_{\text{freq}5}$: 6.34014433 5.66706047 0.23307734 0.20833333 0.00061227
 0.10000000 0.61 $H_{\text{freq}0}$: 4.14771540 4.80643423 0.17978138 0.20833333 0.00081521
 0.10000000 0.82 $H_{\text{freq}1}$: 4.14771540 5.58010025 0.15485517 0.20833333 0.00285991
 0.10000000 2.86 $H_{\text{freq}2}$: 7.09055226 5.65316738 0.26130456 0.20833333 0.00280595
 0.10000000 2.81 $H_{\text{freq}3}$: 7.09055226 6.36651842 0.23202609 0.20833333 0.00056135
 0.10000000 0.56 $H_{\text{freq}4}$: 8.63042603 6.40050186 0.28091632 0.20833333 0.00526829
 0.10000000 5.27 $H_{\text{freq}5}$: 8.63042603 7.64082373 0.23531565 0.20833333 0.00072805
 0.10000000 0.73 bandw. G : 3.55516890 5.87085872 0.86508856 1.42857143
 0.31751294 15.00000000 47626.94 bandw. K : 4.48307751 4.97424321 0.75104851
 0.83333333 0.00677079 15.00000000 1015.62 bandw. M : 5.05043512 7.78109872
 0.92723503 1.42857143 0.25133818 15.00000000 37700.73 bandw. L : 4.06266144
 6.34433701 0.91480040 1.42857143 0.26396067 15.00000000 39594.10 bandw. H : 3.43407819 9.70902614 0.32154505 0.90909091 0.34521014 1.00000000 3452.10
 DOSerr_h : 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o : 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf} : 152.18611138 220.00000000 152.18611138 220.00000000
 4598.72348944 0.00500000 229936.17

————— $E_{\text{Basalfault}}$ I_2 —————

tbe: 217.755 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]

fdd=0.1998794678 qdds=0.5573467916 qddp=0.5644606130 qddd=0.7764612168

b0=62.4514914041 p0=1.1849342894 b1=-3.8776052011 p1=0.6712307190 b2=555591.5726223444

m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000

cr2=3.2116156837 cr3=-1.1584326850 r1dd=6.5000000000 rcdd=10.0000000000

rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.64895030 5.57678969 5.64895030 5.57678969 0.00520715 1000.00000000

52071.53 c/a : 1.59607222 1.58731122 15.49687567 15.41181168 0.00723588

100.00000000 7235.88 a_{omega} : 9.03093983 8.73254342 1.12886748 1.09156793

0.00139126 10.00000000 139.13 c_{omega} : 5.44232400 5.32343103 0.68029050

0.66542888 0.00022087 10.00000000 22.09 a_{4h} : 5.64260466 5.56325146 1.01426382

1.00000000 0.00020346 1.00000000 2.03 c_{4h} : 18.29615777 17.75908031 1.03024241

1.00000000 0.00091460 1.00000000 9.15 a_{6h} : 5.63991068 5.54639384 1.01686084
 1.00000000 0.00028429 1.00000000 2.84 c_{6h} : 27.49471229 26.77136353 1.02701950
 1.00000000 0.00073005 1.00000000 7.30 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.96648491 7.88677000 1.13806927
 1.12668143 0.00012968 1.00000000 1.30 DE(o,h) : 0.49607167 -0.63343333
 0.03307144 -0.04222889 0.00567014 3000.00000000 170104.21 DE(4h,h): 1.62742750
 3.17160000 0.00650971 0.01268640 0.00003815 2000.00000000 763.03 DE(6h,h):
 2.49639667 3.72005000 0.00998559 0.01488020 0.00002396 2000.00000000 479.14
 DE(b,h) : 6.06889500 7.63520000 0.06130197 0.07712323 0.00025031 1.00000000
 2.50 DE(f,h) : 3.77535500 4.51880000 0.03813490 0.04564444 0.00005639
 2000.00000000 1127.87 c_{11} : 178.19624781 176.10000000 0.77838749 0.76923077
 0.00008385 200.00000000 167.69 c_{33} : 205.26699173 190.50000000 0.82885924
 0.76923077 0.00355555 200.00000000 7111.11 c_{44} : 49.33709794 50.80000000
 0.74707901 0.76923077 0.00049070 200.00000000 981.40 c_{12} : 106.47843654
 86.90000000 0.94253728 0.76923077 0.03003515 200.00000000 60070.29 c_{13}
 : 65.64472379 68.30000000 0.73932564 0.76923077 0.00089432 200.00000000
 1788.63 M_{freq0} : 2.70467695 2.85858719 0.19711638 0.20833333 0.00012582
 0.10000000 0.13 M_{freq1} : 2.70467696 2.85858719 0.19711638 0.20833333 0.00012582
 0.10000000 0.13 M_{freq2} : 2.70467696 2.85858719 0.19711638 0.20833333 0.00012582
 0.10000000 0.13 M_{freq3} : 2.70467697 2.85858719 0.19711638 0.20833333 0.00012582
 0.10000000 0.13 M_{freq4} : 6.14562383 5.66706047 0.22592635 0.20833333 0.00030951
 0.10000000 0.31 M_{freq5} : 6.14562383 5.66706047 0.22592635 0.20833333 0.00030951
 0.10000000 0.31 H_{freq0} : 4.05129137 4.80643423 0.17560191 0.20833333 0.00107135
 0.10000000 1.07 H_{freq1} : 4.05129137 5.58010025 0.15125517 0.20833333 0.00325792
 0.10000000 3.26 H_{freq2} : 6.86608203 5.65316738 0.25303227 0.20833333 0.00199799
 0.10000000 2.00 H_{freq3} : 6.86608203 6.36651842 0.22468069 0.20833333 0.00026724
 0.10000000 0.27 H_{freq4} : 8.38773465 6.40050186 0.27301683 0.20833333 0.00418395
 0.10000000 4.18 H_{freq5} : 8.38773465 7.64082373 0.22869847 0.20833333 0.00041474
 0.10000000 0.41 bandw. G: 3.74292754 5.87085872 0.91077636 1.42857143
 0.26811173 15.00000000 40216.76 bandw. K: 4.67627843 4.97424321 0.78341539
 0.83333333 0.00249180 15.00000000 373.77 bandw. M: 5.29125598 7.78109872
 0.97144856 1.42857143 0.20896132 15.00000000 31344.20 bandw. L: 4.27218919
 6.34433701 0.96198033 1.42857143 0.21770725 15.00000000 32656.09 bandw.
 H: 3.59054372 9.70902614 0.33619547 0.90909091 0.32820918 1.00000000 3282.09
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 136.25032209 220.00000000 136.25032209 220.00000000
 7014.00854936 0.00500000 350700.43

————— E_{Basalfault} I2 —————

tbe: 209.896 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]

```

fdd=0.2223730008 qdds=0.5698125753 qddp=0.5893992814 qddd=0.8181557355
b0=45.9308146269 p0=1.0344656254 b1=-6.4376368057 p1=0.6666749620 b2=574084.9970890016
m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
cr2=3.7870564018 cr3=-1.1484118203 r1dd=6.5000000000 rcdd=10.0000000000
rmaxhm=10.1000000000 npar=18 VARGS -vfdd=0.2223730008 -vqdds=0.5698125753
-vqddp=0.5893992814 -vqddd=0.8181557355 -vb0=45.9308146269 -vp0=1.0344656254
-vb1=-6.4376368057 -vp1=0.6666749620 -vb2=574084.9970890016 -vm2=-
11.5000000000 -vp2=0.0000000000 -vndt=2.0000000000 -vcr1=-6.0000000000
-vcr2=3.7870564018 -vcr3=-1.1484118203 -vr1dd=6.5000000000 -vrcdd=10.0000000000
-vrmaxhm=10.1000000000
a_hcp : 5.61178078 5.57678969 5.61178078 5.57678969 0.00122438 1000.00000000
12243.76 c/a : 1.61190054 1.58731122 15.65055885 15.41181168 0.05700021
100.00000000 57000.21 a_omega : 8.95510642 8.73254342 1.11938830 1.09156793
0.00077397 10.00000000 77.40 c_omega : 5.43080886 5.32343103 0.67885111
0.66542888 0.00018016 10.00000000 18.02 a_4h : 5.61406087 5.56325146 1.00913304
1.00000000 0.00008341 1.00000000 0.83 c_4h : 18.14174156 17.75908031 1.02154736
1.00000000 0.00046429 1.00000000 4.64 a_6h : 5.60832119 5.54639384 1.01116533
1.00000000 0.00012466 1.00000000 1.25 c_6h : 27.29989563 26.77136353 1.01974244
1.00000000 0.00038976 1.00000000 3.90 a_bcc : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_fcc : 7.91988827 7.88677000 1.13141261
1.12668143 0.00002238 1.00000000 0.22 DE(o,h) : -0.55514000 -0.63343333 -
0.03700933 -0.04222889 0.00002724 3000.00000000 817.31 DE(4h,h): 1.89282000
3.17160000 0.00757128 0.01268640 0.00002616 2000.00000000 523.29 DE(6h,h):
2.80150667 3.72005000 0.01120603 0.01488020 0.00001350 2000.00000000 269.99
DE(b,h) : 6.65552000 7.63520000 0.06722747 0.07712323 0.00009793 1.00000000
0.98 DE(f,h) : 4.20863000 4.51880000 0.04251141 0.04564444 0.00000982
2000.00000000 196.32 c_11 : 177.05930978 176.10000000 0.77342118 0.76923077
0.00001756 200.00000000 35.12 c_33 : 228.72305006 190.50000000 0.92357379
0.76923077 0.02382177 200.00000000 47643.54 c_44 : 49.82979139 50.80000000
0.75453954 0.76923077 0.00021583 200.00000000 431.66 c_12 : 99.81205407
86.90000000 0.88352708 0.76923077 0.01306365 200.00000000 26127.29 c_13
: 67.77549049 68.30000000 0.76332347 0.76923077 0.00003490 200.00000000
69.79 M_freq0: 2.75579850 2.85858719 0.20084211 0.20833333 0.00005612 0.10000000
0.06 M_freq1: 2.75579851 2.85858719 0.20084211 0.20833333 0.00005612 0.10000000
0.06 M_freq2: 2.75579851 2.85858719 0.20084211 0.20833333 0.00005612 0.10000000
0.06 M_freq3: 2.75579852 2.85858719 0.20084211 0.20833333 0.00005612 0.10000000
0.06 M_freq4: 6.31576556 5.66706047 0.23218113 0.20833333 0.00056872 0.10000000
0.57 M_freq5: 6.31576556 5.66706047 0.23218113 0.20833333 0.00056872 0.10000000
0.57 H_freq0: 3.78337642 4.80643423 0.16398922 0.20833333 0.00196640 0.10000000
1.97 H_freq1: 3.78337642 5.58010025 0.14125256 0.20833333 0.00449983 0.10000000

```

4.50 $H_{\text{freq}2}$: 7.19523396 5.65316738 0.26516234 0.20833333 0.00322954 0.10000000
 3.23 $H_{\text{freq}3}$: 7.19523396 6.36651842 0.23545162 0.20833333 0.00073540 0.10000000
 0.74 $H_{\text{freq}4}$: 8.86793693 6.40050186 0.28864719 0.20833333 0.00645032 0.10000000
 6.45 $H_{\text{freq}5}$: 8.86793693 7.64082373 0.24179158 0.20833333 0.00111945 0.10000000
 1.12 bandw. G: 4.15790133 5.87085872 1.01175302 1.42857143 0.17373758
 15.00000000 26060.64 bandw. K: 5.11030019 4.97424321 0.85612692 0.83333333
 0.00051955 15.00000000 77.93 bandw. M: 5.80010909 7.78109872 1.06487148
 1.42857143 0.13227765 15.00000000 19841.65 bandw. L: 4.72253780 6.34433701
 1.06338654 1.42857143 0.13336000 15.00000000 20004.00 bandw. H: 3.92524389
 9.70902614 0.36753465 0.90909091 0.29328318 1.00000000 2932.83 DOSerr_h :
 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00
 DOSerr_o : 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00 E_{prisf} : 108.02513676 220.00000000 108.02513676 220.00000000 12538.36999754
 0.00500000 626918.50

————— $E_{\text{Basalfault}}$ I2 —————

tbe: 217.718 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]

1.13 2019-10-29

fdd=0.1981497869 qdds=0.5571936407 qddp=0.5708638551 qddd=0.7755505499
 b0=59.5217870968 p0=1.2317798310 b1=-2.9932745250 p1=0.6809293835 b2=741823.0518046410
 m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
 cr2=3.2770451354 cr3=-1.2487703713 r1dd=6.5000000000 rcdd=10.0000000000
 rmaxhm=10.1000000000 npar=18 VARGS -vfdd=0.1981497869 -vqdds=0.5571936407
 -vqddp=0.5708638551 -vqddd=0.7755505499 -vb0=59.5217870968 -vp0=1.2317798310
 -vb1=-2.9932745250 -vp1=0.6809293835 -vb2=741823.0518046410 -vm2=-
 11.5000000000 -vp2=0.0000000000 -vndt=2.0000000000 -vcr1=-6.0000000000
 -vcr2=3.2770451354 -vcr3=-1.2487703713 -vr1dd=6.5000000000 -vrcdd=10.0000000000
 -vrmaxhm=10.1000000000

a_{hcp} : 5.56453600 5.57678969 5.56453600 5.57678969 0.00015015 1000.00000000
 1501.53 c/a : 1.59255435 1.58731122 15.46271931 15.41181168 0.00259159
 100.00000000 2591.59 a_{omega} : 8.89894657 8.73254342 1.11236832 1.09156793
 0.00043266 10.00000000 43.27 c_{omega} : 5.37839325 5.32343103 0.67229916
 0.66542888 0.00004720 10.00000000 4.72 a_{4h} : 5.55450787 5.56325146 0.99842833
 1.00000000 0.00000247 1.00000000 0.02 c_{4h} : 18.02932378 17.75908031 1.01521720
 1.00000000 0.00023156 1.00000000 2.32 a_{6h} : 5.55261301 5.54639384 1.00112130
 1.00000000 0.00000126 1.00000000 0.01 c_{6h} : 27.07915153 26.77136353 1.01149691
 1.00000000 0.00013218 1.00000000 1.32 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.84209884 7.88677000 1.12029983
 1.12668143 0.00004072 1.00000000 0.41 $\text{DE}(o,h)$: 1.20201333 -0.63343333

0.08013422 -0.04222889 0.01497273 3000.00000000 449181.93 DE(4h,h): 1.56144250
 3.17160000 0.00624577 0.01268640 0.00004148 2000.00000000 829.63 DE(6h,h):
 2.44864500 3.72005000 0.00979458 0.01488020 0.00002586 2000.00000000 517.27
 DE(b,h) : 6.30197000 7.63520000 0.06365626 0.07712323 0.00018136 1.00000000
 1.81 DE(f,h) : 3.73166000 4.51880000 0.03769354 0.04564444 0.00006322
 10000.00000000 6321.70 c_{11} : 183.22750967 176.10000000 0.80036478 0.76923077
 0.00096933 200.00000000 1938.65 c_{33} : 204.37133584 190.50000000 0.82524262
 0.76923077 0.00313733 200.00000000 6274.66 c_{44} : 51.73068964 50.80000000
 0.78332359 0.76923077 0.00019861 200.00000000 397.21 c_{12} : 92.53673893
 86.90000000 0.81912666 0.76923077 0.00248960 200.00000000 4979.20 c_{13} :
 69.44016069 68.30000000 0.78207186 0.76923077 0.00016489 200.00000000
 329.79 $M_{\text{freq}0}$: 2.75379045 2.85858719 0.20069577 0.20833333 0.00005833
 0.10000000 0.06 $M_{\text{freq}1}$: 2.75379046 2.85858719 0.20069577 0.20833333 0.00005833
 0.10000000 0.06 $M_{\text{freq}2}$: 2.75379046 2.85858719 0.20069577 0.20833333 0.00005833
 0.10000000 0.06 $M_{\text{freq}3}$: 2.75379047 2.85858719 0.20069577 0.20833333 0.00005833
 0.10000000 0.06 $M_{\text{freq}4}$: 6.02365259 5.66706047 0.22144243 0.20833333 0.00017185
 0.10000000 0.17 $M_{\text{freq}5}$: 6.02365259 5.66706047 0.22144243 0.20833333 0.00017185
 0.10000000 0.17 $H_{\text{freq}0}$: 3.94643405 4.80643423 0.17105690 0.20833333 0.00138953
 0.10000000 1.39 $H_{\text{freq}1}$: 3.94643405 5.58010025 0.14734032 0.20833333 0.00372015
 0.10000000 3.72 $H_{\text{freq}2}$: 6.60840329 5.65316738 0.24353616 0.20833333 0.00123924
 0.10000000 1.24 $H_{\text{freq}3}$: 6.60840329 6.36651842 0.21624860 0.20833333 0.00006265
 0.10000000 0.06 $H_{\text{freq}4}$: 8.18710820 6.40050186 0.26648653 0.20833333 0.00338179
 0.10000000 3.38 $H_{\text{freq}5}$: 8.18710820 7.64082373 0.22322823 0.20833333 0.00022186
 0.10000000 0.22 bandw. G : 3.94021016 5.87085872 0.95878166 1.42857143
 0.22070243 15.00000000 33105.36 bandw. K : 4.89805130 4.97424321 0.82056893
 0.83333333 0.00016293 15.00000000 24.44 bandw. M : 5.46813005 7.78109872
 1.00392177 1.42857143 0.18032734 15.00000000 27049.10 bandw. L : 4.47627466
 6.34433701 1.00793481 1.42857143 0.17693517 15.00000000 26540.28 bandw. H : 3.73340355 9.70902614 0.34957195 0.90909091 0.31306146 1.00000000 3130.61
 DOSerr_h : 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o : 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf} : 123.68325847 220.00000000 123.68325847 220.00000000
 9276.91469958 0.00500000 463845.73

————— $E_{\text{Basalfault I2}}$ —————

tbe: 203.632 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]

bulk modulus: 115; target: 110 C12 - C66 = 47.1914 | 42.3000 C13 - C44

= 17.7095 | 17.5000

fdd=0.222299836 qdds=0.5694802234 qddp=0.5890968074 qddd=0.8163634071

b0=45.83166545 p0=1.035247743 b1=-6.44286741 p1=0.667994596 b2=573363.0706

cr2=3.785987706 cr3=-1.147452833 m2=-11.5 p2=0.0 cr1=-6.0 ndt=2.0 r1dd=6.5

```

rcdd=10. rmaxhm=10.001 npar=18
fdd=0.222299836 qdds=0.5694802234 qddp=0.5890968074 qddd=0.8163634071
bscl0=0.4583166545 p0=1.035247743 bscl1=-0.644286741 p1=0.667994596
bscl2=0.5733630706 cr2=3.785987706 cr3=-1.147452833 m2=-11.5 p2=0.0
cr1=-6.0 ndt=2.0 r1dd=6.5 rcdd=10. rmaxhm=10.001 VARGS -vfdd=0.222299836
-vqdds=0.5694802234 -vqddp=0.5890968074 -vqddd=0.8163634071 -vbscl0=0.4583166545
-vp0=1.035247743 -vbscl1=-0.644286741 -vp1=0.667994596 -vbscl2=0.5733630706
-vcr2=3.785987706 -vcr3=-1.147452833 -vm2=-11.5 -vp2=0.0 -vcr1=-6.0 -
vndt=2.0 -vr1dd=6.5 -vrcdd=10. -vrmaxhm=10.001
ahcp : 5.60619854 5.57678969 5.60619854 5.57678969 0.00086488 1000.00000000
8648.81 c/a : 1.61429581 1.58731122 15.67381548 15.41181168 0.06864599
125.00000000 85807.48 aomega : 8.94586865 8.73254342 1.11823358 1.09156793
0.00071106 10.00000000 71.11 comega : 5.42663308 5.32343103 0.67832914
0.66542888 0.00016642 10.00000000 16.64 a4h : 5.60816798 5.56325146 1.00807379
1.00000000 0.00006519 1.00000000 0.65 c4h : 18.12261446 17.75908031 1.02047033
1.00000000 0.00041903 1.00000000 4.19 a6h : 5.60237180 5.54639384 1.01009268
1.00000000 0.00010186 1.00000000 1.02 c6h : 27.27105311 26.77136353 1.01866508
1.00000000 0.00034839 1.00000000 3.48 abcc : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 afcc : 7.91141616 7.88677000 1.13020231
1.12668143 0.00001240 1.00000000 0.12 DE(o,h) : -0.50330833 -0.63343333 -
0.03355389 -0.04222889 0.00007526 3000.00000000 2257.67 DE(4h,h): 1.89448250
3.17160000 0.00757793 0.01268640 0.00002610 2000.00000000 521.93 DE(6h,h):
2.80696500 3.72005000 0.01122786 0.01488020 0.00001334 2000.00000000 266.79
DE(b,h) : 6.67165500 7.63520000 0.06739045 0.07712323 0.00009473 1.00000000
0.95 DE(f,h) : 4.21800500 4.51880000 0.04260611 0.04564444 0.00000923
10000.00000000 923.15 c11 : 178.38166085 176.10000000 0.77919740 0.76923077
0.00009933 200.00000000 198.67 c33 : 229.07015846 190.50000000 0.92497540
0.76923077 0.02425639 200.00000000 48512.78 c44 : 50.94869128 50.80000000
0.77148230 0.76923077 0.00000507 200.00000000 10.14 c12 : 99.68009298
86.90000000 0.88235897 0.76923077 0.01279799 200.00000000 25595.98 c13
: 68.82143440 68.30000000 0.77510344 0.76923077 0.00003449 200.00000000
68.98 Mfreq0: 2.76038540 2.85858719 0.20117640 0.20833333 0.00005122 0.10000000
0.05 Mfreq1: 2.76038541 2.85858719 0.20117641 0.20833333 0.00005122 0.10000000
0.05 Mfreq2: 2.76038541 2.85858719 0.20117641 0.20833333 0.00005122 0.10000000
0.05 Mfreq3: 2.76038542 2.85858719 0.20117641 0.20833333 0.00005122 0.10000000
0.05 Mfreq4: 6.31949645 5.66706047 0.23231828 0.20833333 0.00057528 0.10000000
0.58 Mfreq5: 6.31949645 5.66706047 0.23231828 0.20833333 0.00057528 0.10000000
0.58 Hfreq0: 3.77497077 4.80643423 0.16362488 0.20833333 0.00199885 0.10000000
2.00 Hfreq1: 3.77497077 5.58010025 0.14093873 0.20833333 0.00454203 0.10000000
4.54 Hfreq2: 7.19023621 5.65316738 0.26497816 0.20833333 0.00320864 0.10000000

```


3.21 $H_{\text{freq}3}$: 7.19023621 6.36651842 0.23528808 0.20833333 0.00072656 0.10000000
 0.73 $H_{\text{freq}4}$: 8.87191820 6.40050186 0.28877678 0.20833333 0.00647115 0.10000000
 6.47 $H_{\text{freq}5}$: 8.87191820 7.64082373 0.24190013 0.20833333 0.00112673 0.10000000
 1.13 bandw. G: 4.18239159 5.87085872 1.18733101 1.66666667 0.22976267
 15.00000000 34464.40 bandw. K: 5.13751159 4.97424321 0.93892978 0.90909091
 0.00089036 15.00000000 133.55 bandw. M: 5.82595991 7.78109872 1.24788716
 1.66666667 0.17537628 15.00000000 26306.44 bandw. L: 4.74838863 6.34433701
 1.24740868 1.66666667 0.17577726 15.00000000 26366.59 bandw. H: 3.94429187
 9.70902614 0.36931818 0.90909091 0.29135460 5.00000000 14567.73 DOSerr_h :
 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00
 DOSerr_o : 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00 E_{prisf} : 108.34044163 220.00000000 108.34044163 220.00000000 12467.85697601
 0.00500000 623392.85
 ———- $E_{\text{Basalfault}}$ I2 ———-
 tbe: 217.029 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]
 fdd=0.222299836 qdds=0.5694802234 qddp=0.5890968074 qddd=0.8163634071
 b0=46.3166545 p0=1.035247743 b1=-6.44286741 p1=0.667994596 b2=573363.0706
 cr2=3.785987706 cr3=-1.157452833 m2=-11.5 p2=0.0 cr1=-6.0 ndt=2.0 r1dd=6.5
 rdd=10.0 rmaxhm=10.001 npar=18
 a_{hcp} : 5.64132578 5.57678969 5.64132578 5.57678969 0.00416491 1000.00000000
 41649.07 c/a : 1.59930205 1.58731122 15.52823532 15.41181168 0.01355446
 100.00000000 13554.46 a_{omega} : 9.00268216 8.73254342 1.12533527 1.09156793
 0.00114023 10.00000000 114.02 c_{omega} : 5.45251944 5.32343103 0.68156493
 0.66542888 0.00026037 10.00000000 26.04 a_{4h} : 5.64348381 5.56325146 1.01442185
 1.00000000 0.00020799 1.00000000 2.08 c_{4h} : 18.23946323 17.75908031 1.02704999
 1.00000000 0.00073170 1.00000000 7.32 a_{6h} : 5.63794259 5.54639384 1.01650599
 1.00000000 0.00027245 1.00000000 2.72 c_{6h} : 27.44832595 26.77136353 1.02528681
 1.00000000 0.00063942 1.00000000 6.39 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.96186376 7.88677000 1.13740911
 1.12668143 0.00011508 1.00000000 1.15 $\text{DE}(o,h)$: -0.69722833 -0.63343333 -
 0.04648189 -0.04222889 0.00001809 3000.00000000 542.64 $\text{DE}(4h,h)$: 1.83117250
 3.17160000 0.00732469 0.01268640 0.00002875 2000.00000000 574.96 $\text{DE}(6h,h)$:
 2.72116000 3.72005000 0.01088464 0.01488020 0.00001596 2000.00000000 319.29
 $\text{DE}(b,h)$: 6.80692500 7.63520000 0.06875682 0.07712323 0.00007000 1.00000000
 0.70 $\text{DE}(f,h)$: 4.09507500 4.51880000 0.04136439 0.04564444 0.00001832
 2000.00000000 366.38 c_{11} : 176.93212224 176.10000000 0.77286560 0.76923077
 0.00001321 100.00000000 13.21 c_{33} : 221.91218797 190.50000000 0.89607183
 0.76923077 0.01608865 100.00000000 16088.65 c_{44} : 49.43737064 50.80000000
 0.74859737 0.76923077 0.00042574 100.00000000 425.74 c_{12} : 105.65600443
 86.90000000 0.93525719 0.76923077 0.02756477 100.00000000 27564.77 c_{13}

: 65.82310124 68.30000000 0.74133462 0.76923077 0.00077819 10.00000000
77.82 M_{freq0}: 2.71899697 2.85858719 0.19816002 0.20833333 0.00010350 0.10000000
0.10 M_{freq1}: 2.71899698 2.85858719 0.19816002 0.20833333 0.00010350 0.10000000
0.10 M_{freq2}: 2.71899698 2.85858719 0.19816002 0.20833333 0.00010350 0.10000000
0.10 M_{freq3}: 2.71899699 2.85858719 0.19816002 0.20833333 0.00010350 0.10000000
0.10 M_{freq4}: 6.19358665 5.66706047 0.22768957 0.20833333 0.00037466 0.10000000
0.37 M_{freq5}: 6.19358665 5.66706047 0.22768957 0.20833333 0.00037466 0.10000000
0.37 H_{freq0}: 3.81166720 4.80643423 0.16521548 0.20833333 0.00185915 0.10000000
1.86 H_{freq1}: 3.81166720 5.58010025 0.14230879 0.20833333 0.00435924 0.10000000
4.36 H_{freq2}: 7.07704092 5.65316738 0.26080663 0.20833333 0.00275345 0.10000000
2.75 H_{freq3}: 7.07704092 6.36651842 0.23158396 0.20833333 0.00054059 0.10000000
0.54 H_{freq4}: 8.68271096 6.40050186 0.28261817 0.20833333 0.00551824 0.10000000
5.52 H_{freq5}: 8.68271096 7.64082373 0.23674124 0.20833333 0.00080701 0.10000000
0.81 bandw. G: 4.07082486 5.87085872 1.15565855 1.66666667 0.26112929
15.00000000 39169.39 bandw. K: 5.01097860 4.97424321 0.91580466 0.90909091
0.00004507 15.00000000 6.76 bandw. M: 5.71167205 7.78109872 1.22340736
1.66666667 0.19647882 15.00000000 29471.82 bandw. L: 4.63682190 6.34433701
1.21809994 1.66666667 0.20121211 15.00000000 30181.82 bandw. H: 3.85585483
9.70902614 0.36103751 0.90909091 0.30036253 5.00000000 15018.13 DOSerr_h:
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00
DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00

————- E_{prismaticfault} —————

tbe: 103.159 mJ/m² DFT: 250.000 mJ/m² [Benoit 2012] DFT: 233.000
mJ/m² [Ackland 1999]

————- E_{Basalfault} I2 —————

tbe: 217.363 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]

————- E_{vacancyformation} —————

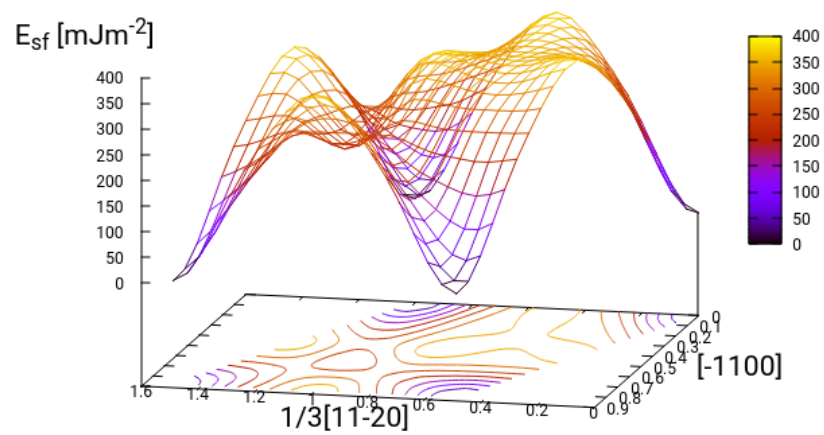
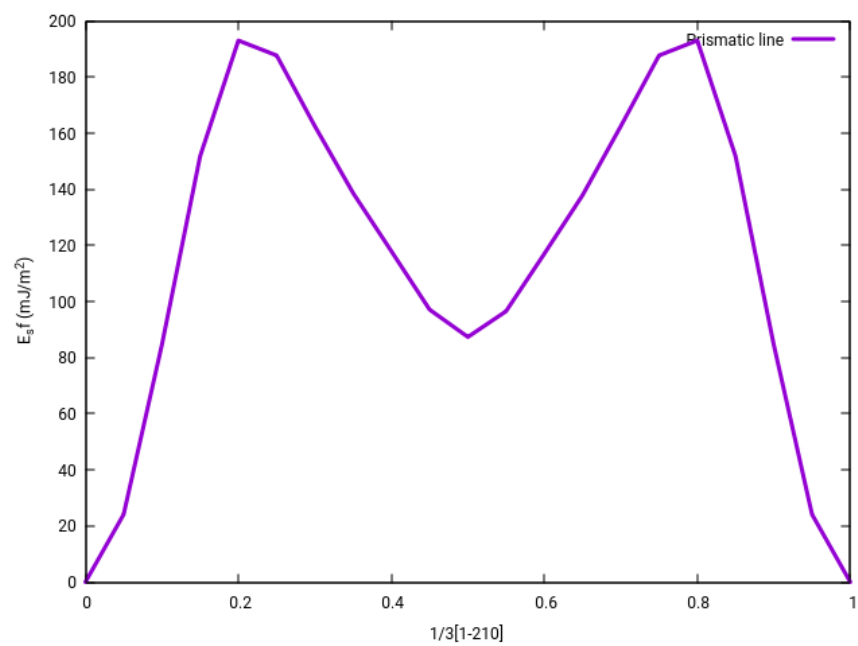
tbe: 2.431 eV | (588 atoms) tbe: 2.429 eV | (896 atoms) DFT: 1.950 eV
| GGA-PAW: Angsten (2013) exp: 1.270 eV | Hashimoto (1984)

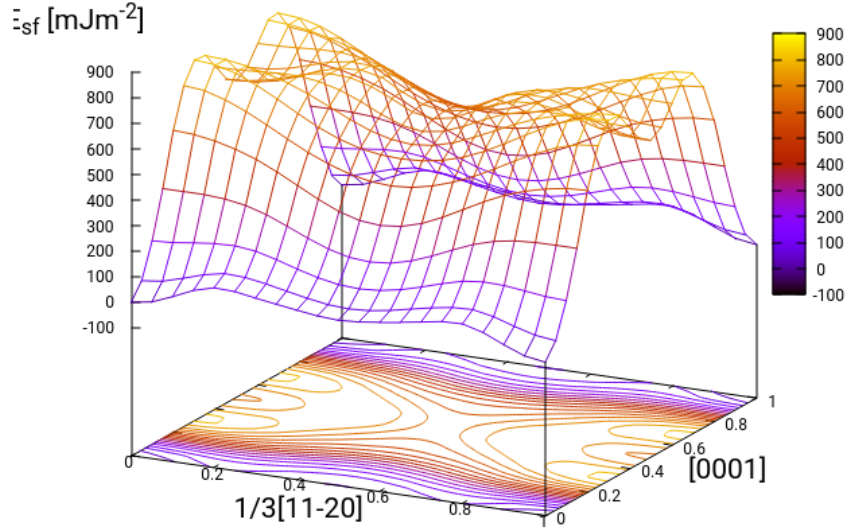
————- E_{tet} - E_{oct} —————

> Note: Preference for tetrahedral oxygen to go into hexahedral site

» ($E_{\text{hexahedral}} - E_{\text{octahedral}}$) tbe: 1.123 eV

» ($E_{\text{tetrahedral}} - E_{\text{octahedral}}$) tbe: 1.552 eV





PARAMETERS fdd=0.1962030050 qdds=0.5603385291 qddp=0.5641791446
 qddd=0.7778812828 b0=67.9784821273 p0=1.2469553135 b1=-3.6289856489
 p1=0.7094094608 b2=624676.8745963273 m2=-11.5000000000 p2=0.0000000000
 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.0990417700 cr3=-1.2615960922
 r1dd=6.5000000000 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18
 VARGS -vfdd=0.1962030050 -vqdds=0.5603385291 -vqddp=0.5641791446 -
 vqddd=0.7778812828 -vb0=67.9784821273 -vp0=1.2469553135 -vb1=-3.6289856489
 -vp1=0.7094094608 -vb2=624676.8745963273 -vm2=-11.5000000000 -vp2=0.0000000000
 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.0990417700 -vcr3=-1.2615960922
 -vr1dd=6.5000000000 -vrdd=10.0000000000 -vrmaxhm=10.1000000000
 a_{hcp} : 5.60402011 5.57678969 5.60402011 5.57678969 0.00074150 1000.00000000
 7414.96 c/a : 1.61523185 1.58731122 15.68290380 15.41181168 0.07349094
 100.00000000 73490.94 a_{omega} : 8.95981987 8.73254342 1.11997748 1.09156793
 0.00080710 10.00000000 80.71 c_{omega} : 5.40668491 5.32343103 0.67583561
 0.66542888 0.00010830 10.00000000 10.83 a_{4h} : 5.59368514 5.56325146 1.00547048
 1.00000000 0.00002993 1.00000000 0.30 c_{4h} : 18.15985408 17.75908031 1.02256726
 1.00000000 0.00050928 1.00000000 5.09 a_{6h} : 5.59157694 5.54639384 1.00814639

1.00000000 0.00006636 1.00000000 0.66 c_{6h} : 27.27780679 26.77136353 1.01891735
 1.00000000 0.00035787 1.00000000 3.58 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.89832289 7.88677000 1.12833184
 1.12668143 0.00000272 1.00000000 0.03 DE(o,h) : 1.25287667 -0.63343333
 0.08352511 -0.04222889 0.01581407 3000.00000000 474422.06 DE(4h,h): 1.46745750
 3.17160000 0.00586983 0.01268640 0.00004647 2000.00000000 929.31 DE(6h,h):
 2.31466000 3.72005000 0.00925864 0.01488020 0.00003160 2000.00000000 632.04
 DE(b,h) : 5.80761000 7.63520000 0.05866273 0.07712323 0.00034079 1.00000000
 3.41 DE(f,h) : 3.53419000 4.51880000 0.03569889 0.04564444 0.00009891
 2000.00000000 1978.28 c_{11} : 177.23443618 176.10000000 0.77418615 0.76923077
 0.00002456 200.00000000 49.11 c_{33} : 197.90379005 190.50000000 0.79912695
 0.76923077 0.00089378 200.00000000 1787.56 c_{44} : 48.54104332 50.80000000
 0.73502488 0.76923077 0.00117004 200.00000000 2340.09 c_{12} : 95.17756142
 86.90000000 0.84250298 0.76923077 0.00536882 200.00000000 10737.63 c_{13}
 : 64.55714847 68.30000000 0.72707679 0.76923077 0.00177696 200.00000000
 3553.92 M_{freq0} : 2.70772104 2.85858719 0.19733823 0.20833333 0.00012089
 0.10000000 0.12 M_{freq1} : 2.70772105 2.85858719 0.19733824 0.20833333 0.00012089
 0.10000000 0.12 M_{freq2} : 2.70772105 2.85858719 0.19733824 0.20833333 0.00012089
 0.10000000 0.12 M_{freq3} : 2.70772106 2.85858719 0.19733824 0.20833333 0.00012089
 0.10000000 0.12 M_{freq4} : 5.97614537 5.66706047 0.21969596 0.20833333 0.00012911
 0.10000000 0.13 M_{freq5} : 5.97614537 5.66706047 0.21969596 0.20833333 0.00012911
 0.10000000 0.13 H_{freq0} : 4.02537315 4.80643423 0.17447849 0.20833333 0.00114615
 0.10000000 1.15 H_{freq1} : 4.02537315 5.58010025 0.15028752 0.20833333 0.00336932
 0.10000000 3.37 H_{freq2} : 6.56901955 5.65316738 0.24208477 0.20833333 0.00113916
 0.10000000 1.14 H_{freq3} : 6.56901955 6.36651842 0.21495983 0.20833333 0.00004391
 0.10000000 0.04 H_{freq4} : 8.07809150 6.40050186 0.26293809 0.20833333 0.00298168
 0.10000000 2.98 H_{freq5} : 8.07809150 7.64082373 0.22025580 0.20833333 0.00014215
 0.10000000 0.14 bandw. G: 3.71843728 5.87085872 0.90481708 1.42857143
 0.27431861 15.00000000 41147.79 bandw. K: 4.63137962 4.97424321 0.77589351
 0.83333333 0.00329933 15.00000000 494.90 bandw. M: 5.20417951 7.78109872
 0.95546174 1.42857143 0.22383277 15.00000000 33574.92 bandw. L: 4.22592982
 6.34433701 0.95156398 1.42857143 0.22753610 15.00000000 34130.42 bandw.
 H: 3.54292378 9.70902614 0.33173665 0.90909091 0.33333794 1.00000000 3333.38
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 145.53612884 220.00000000 145.53612884 220.00000000
 5544.86810749 0.00500000 277243.41

———— E_{Basalfault} I2 ————
 tbe: 191.483 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]
 ———— E_{vacancyformation} ————

tbe: 2.418 eV | DFT: 1.950 eV | GGA-PAW: Angsten (2013) exp: 1.270 eV | Hashimoto (1984)

^^ Modification of the above model to have a slightly higher repulsion term b2

PARAMETERS fdd=0.1962030050 qdds=0.5603385291 qddp=0.5641791446 qddd=0.7778812828 b0=67.9784821273 p0=1.2469553135 b1=-3.6289856489 p1=0.7094094608 b2=626000.0 m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.0990417700 cr3=-1.2615960922 r1dd=6.5000000000 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18 VARGS -vfdd=0.1962030050 -vqdds=0.5603385291 -vqddp=0.5641791446 -vqddd=0.7778812828 -vb0=67.9784821273 -vp0=1.2469553135 -vb1=-3.6289856489 -vp1=0.7094094608 -vb2=626000.0 -vm2=-11.5000000000 -vp2=0.0000000000 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.0990417700 -vcr3=-1.2615960922 -vr1dd=6.5000000000 -vrcdd=10.0000000000 -vrmaxhm=10.1000000000

a_{hcp} : 5.60402011 5.57678969 5.60402011 5.57678969 0.00074150 1000.00000000 7414.96 c/a : 1.57574189 1.58731122 15.29948069 15.41181168 0.01261825 100.00000000 12618.25 a_{omega} : 8.96039623 8.73254342 1.12004953 1.09156793 0.00081120 10.00000000 81.12 c_{omega} : 5.40699833 5.32343103 0.67587479 0.66542888 0.00010912 10.00000000 10.91 a_{4h} : 5.59371954 5.56325146 1.00547667 1.00000000 0.00002999 1.00000000 0.30 c_{4h} : 18.16124146 17.75908031 1.02264538 1.00000000 0.00051281 1.00000000 5.13 a_{6h} : 5.59170678 5.54639384 1.00816980 1.00000000 0.00006675 1.00000000 0.67 c_{6h} : 27.27831362 26.77136353 1.01893628 1.00000000 0.00035858 1.00000000 3.59 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.89832289 7.88677000 1.12833184 1.12668143 0.00000272 1.00000000 0.03 DE(o,h) : 1.25366500 -0.63343333 0.08357767 -0.04222889 0.01582729 3000.00000000 474818.68 DE(4h,h): 1.46735750 3.17160000 0.00586943 0.01268640 0.00004647 2000.00000000 929.42 DE(6h,h): 2.31450833 3.72005000 0.00925803 0.01488020 0.00003161 2000.00000000 632.18 DE(b,h) : 5.80790500 7.63520000 0.05866571 0.07712323 0.00034068 1.00000000 3.41 DE(f,h) : 3.53398500 4.51880000 0.03569682 0.04564444 0.00009896 2000.00000000 1979.11 c₁₁ : 182.18207480 176.10000000 0.79579817 0.76923077 0.00070583 100.00000000 705.83 c₃₃ : 202.88615634 190.50000000 0.81924553 0.76923077 0.00250148 100.00000000 2501.48 c₄₄ : 49.68618188 50.80000000 0.75236496 0.76923077 0.00028446 100.00000000 284.46 c₁₂ : 98.12235223 86.90000000 0.86856999 0.76923077 0.00986828 100.00000000 9868.28 c₁₃ : 65.28413049 68.30000000 0.73526445 0.76923077 0.00115371 10.00000000 115.37 M_{freq0}: 2.70822081 2.85858719 0.19737466 0.20833333 0.00012009 0.10000000 0.12 M_{freq1}: 2.70822082 2.85858719 0.19737466 0.20833333 0.00012009 0.10000000 0.12 M_{freq2}: 2.70822082 2.85858719 0.19737466 0.20833333 0.00012009 0.10000000 0.12 M_{freq3}: 2.70822083 2.85858719 0.19737466 0.20833333 0.00012009

0.10000000 0.12 M_{freq4} : 5.97747622 5.66706047 0.21974488 0.20833333 0.00013022
 0.10000000 0.13 M_{freq5} : 5.97747622 5.66706047 0.21974488 0.20833333 0.00013022
 0.10000000 0.13 H_{freq0} : 4.02620227 4.80643423 0.17451443 0.20833333 0.00114372
 0.10000000 1.14 H_{freq1} : 4.02620227 5.58010025 0.15031847 0.20833333 0.00336572
 0.10000000 3.37 H_{freq2} : 6.57039365 5.65316738 0.24213541 0.20833333 0.00114258
 0.10000000 1.14 H_{freq3} : 6.57039365 6.36651842 0.21500480 0.20833333 0.00004451
 0.10000000 0.04 H_{freq4} : 8.07961869 6.40050186 0.26298780 0.20833333 0.00298711
 0.10000000 2.99 H_{freq5} : 8.07961869 7.64082373 0.22029744 0.20833333 0.00014314
 0.10000000 0.14 bandw. G: 3.71843728 5.87085872 1.05561993 1.66666667
 0.37337811 15.00000000 56006.72 bandw. K: 4.63137962 4.97424321 0.84642928
 0.90909091 0.00392648 15.00000000 588.97 bandw. M: 5.20417951 7.78109872
 1.11470537 1.66666667 0.30466128 15.00000000 45699.19 bandw. L: 4.24497780
 6.34433701 1.11516191 1.66666667 0.30415749 15.00000000 45623.62 bandw.
 H: 3.54292378 9.70902614 0.33173665 0.90909091 0.33333794 5.00000000 16666.90
 DOS err_h : 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOS err_o : 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00

————— $E_{\text{Basalfault I2}}$ —————

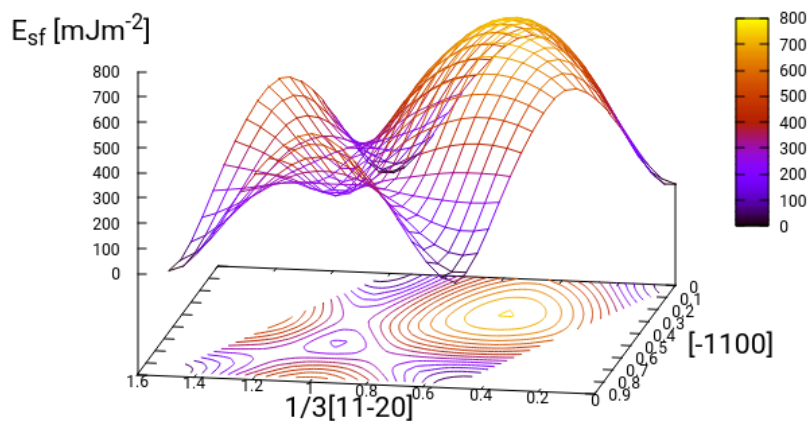
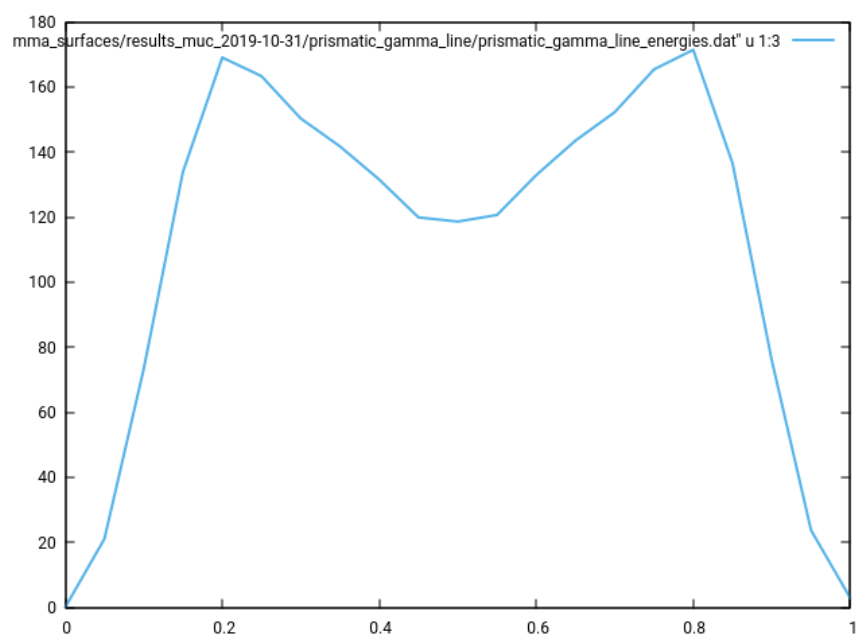
tbe: 193.074 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]

————— $E_{\text{prismaticfault}}$ —————

tbe: 125.532 mJ/m² DFT: 250.000 mJ/m² [Benoit 2012] DFT: 233.000 mJ/m² [Ackland 1999]

————— $E_{\text{vacancyformation}}$ —————

tbe: 2.317 eV | DFT: 1.950 eV | GGA-PAW: Angsten (2013) exp: 1.270 eV | Hashimoto (1984)



1.14 2019-10-30

fdd=0.1976382626 qdds=0.5584066236 qddp=0.5698965104 qddd=0.7754582525
b0=64.5618663617 p0=1.1999708862 b1=-3.9078942413 p1=0.6795447525 b2=746090.0453785007
m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
cr2=3.2372151957 cr3=-1.2470946611 r1dd=6.5000000000 rcdd=10.0000000000
rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.64595495 5.57678969 5.64595495 5.57678969 0.00478383 1000.00000000
47838.34 c/a : 1.59734005 1.58731122 15.50918543 15.41181168 0.00948165
100.00000000 9481.65 a_{omega} : 9.03046888 8.73254342 1.12880861 1.09156793
0.00138687 10.00000000 138.69 c_{omega} : 5.43895641 5.32343103 0.67986955
0.66542888 0.00020853 10.00000000 20.85 a_{4h} : 5.63901520 5.56325146 1.01361861
1.00000000 0.00018547 1.00000000 1.85 c_{4h} : 18.28808079 17.75908031 1.02978761
1.00000000 0.00088730 1.00000000 8.87 a_{6h} : 5.63669087 5.54639384 1.01628031
1.00000000 0.00026505 1.00000000 2.65 c_{6h} : 27.47942256 26.77136353 1.02644837
1.00000000 0.00069952 1.00000000 7.00 a_{bcc} : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.96147866 7.88677000 1.13735409
1.12668143 0.00011391 1.00000000 1.14 DE(o,h) : 0.81686500 -0.63343333
0.05445767 -0.04222889 0.00934829 3000.00000000 280448.70 DE(4h,h): 1.57130250
3.17160000 0.00628521 0.01268640 0.00004098 2000.00000000 819.50 DE(6h,h):
2.44685500 3.72005000 0.00978742 0.01488020 0.00002594 2000.00000000 518.73
DE(b,h) : 6.15719500 7.63520000 0.06219389 0.07712323 0.00022289 1.00000000
2.23 DE(f,h) : 3.72858500 4.51880000 0.03766247 0.04564444 0.00006371
10000.00000000 6371.18 c₁₁ : 181.50184248 176.10000000 0.79282681 0.76923077
0.00055677 200.00000000 1113.55 c₃₃ : 209.75817789 190.50000000 0.84699446
0.76923077 0.00604719 200.00000000 12094.38 c₄₄ : 50.40945127 50.80000000
0.76331695 0.76923077 0.00003497 200.00000000 69.95 c₁₂ : 107.04106317
86.90000000 0.94751760 0.76923077 0.03178619 200.00000000 63572.39 c₁₃
: 65.53222165 68.30000000 0.73805858 0.76923077 0.00097171 200.00000000
1943.41 M_{freq0}: 2.74261358 2.85858719 0.19988120 0.20833333 0.00007144
0.10000000 0.07 M_{freq1}: 2.74261359 2.85858719 0.19988120 0.20833333 0.00007144
0.10000000 0.07 M_{freq2}: 2.74261359 2.85858719 0.19988120 0.20833333 0.00007144
0.10000000 0.07 M_{freq3}: 2.74261360 2.85858719 0.19988120 0.20833333 0.00007144
0.10000000 0.07 M_{freq4}: 6.20327588 5.66706047 0.22804577 0.20833333 0.00038858
0.10000000 0.39 M_{freq5}: 6.20327588 5.66706047 0.22804577 0.20833333 0.00038858
0.10000000 0.39 H_{freq0}: 4.12125379 4.80643423 0.17863441 0.20833333 0.00088203
0.10000000 0.88 H_{freq1}: 4.12125379 5.58010025 0.15386722 0.20833333 0.00296656
0.10000000 2.97 H_{freq2}: 6.90963868 5.65316738 0.25463744 0.20833333 0.00214407
0.10000000 2.14 H_{freq3}: 6.90963868 6.36651842 0.22610601 0.20833333 0.00031587

0.10000000 0.32 H_{freq4} : 8.42924307 6.40050186 0.27436791 0.20833333 0.00436057
 0.10000000 4.36 H_{freq5} : 8.42924307 7.64082373 0.22983023 0.20833333 0.00046212
 0.10000000 0.46 bandw. G: 3.66401449 5.87085872 0.89157424 1.42857143
 0.28836598 15.00000000 43254.90 bandw. K: 4.57967797 4.97424321 0.76723195
 0.83333333 0.00436939 15.00000000 655.41 bandw. M: 5.18104982 7.78109872
 0.95121525 1.42857143 0.22786892 15.00000000 34180.34 bandw. L: 4.18103102
 6.34433701 0.94145400 1.42857143 0.23728339 15.00000000 35592.51 bandw.
 H: 3.51299124 9.70902614 0.32893396 0.90909091 0.33658209 1.00000000 3365.82
 DOSerr_h : 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o : 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf} : 148.51250795 220.00000000 148.51250795 220.00000000
 5110.46151942 0.00500000 255523.08
 ———- $E_{\text{Basalfault}}$ I2 ———-
 tbe: 205.635 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]
 PARAMETERS fdd=0.1969062176 qdds=0.5579049959 qddp=0.5715888469
 qddd=0.7756363005 b0=69.0416992007 p0=1.2429294342 b1=-3.1372571918
 p1=0.6764606786 b2=757176.2759877006 m2=-11.5000000000 p2=0.0000000000
 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.1799239250 cr3=-1.2499925082
 r1dd=6.5000000000 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18
 VARGS -vfdd=0.1969062176 -vqdds=0.5579049959 -vqddp=0.5715888469 -
 vqddd=0.7756363005 -vb0=69.0416992007 -vp0=1.2429294342 -vb1=-3.1372571918
 -vp1=0.6764606786 -vb2=757176.2759877006 -vm2=-11.5000000000 -vp2=0.0000000000
 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.1799239250 -vcr3=-1.2499925082
 -vr1dd=6.5000000000 -vrcdd=10.0000000000 -vrmaxh m=10.1000000000
 a_{hcp} : 5.66515240 5.57678969 5.66515240 5.57678969 0.00780797 1000.00000000
 78079.68 c/a: 1.58923770 1.58731122 15.43051669 15.41181168 0.00034988
 100.00000000 349.88 a_{omega} : 9.06355897 8.73254342 1.13294487 1.09156793
 0.00171205 10.00000000 171.21 c_{omega} : 5.45388891 5.32343103 0.68173611
 0.66542888 0.00026593 10.00000000 26.59 a_{4h} : 5.65642066 5.56325146 1.01674726
 1.00000000 0.00028047 1.00000000 2.80 c_{4h} : 18.35650968 17.75908031 1.03364078
 1.00000000 0.00113170 1.00000000 11.32 a_{6h} : 5.65411986 5.54639384 1.01942271
 1.00000000 0.00037724 1.00000000 3.77 c_{6h} : 27.57854157 26.77136353 1.03015080
 1.00000000 0.00090907 1.00000000 9.09 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.98728011 7.88677000 1.14104002
 1.12668143 0.00020617 1.00000000 2.06 $\text{DE}(o,h)$: 0.75642167 -0.63343333
 0.05042811 -0.04222889 0.00858532 3000.00000000 257559.59 $\text{DE}(4h,h)$: 1.53899750
 3.17160000 0.00615599 0.01268640 0.00004265 2000.00000000 852.93 $\text{DE}(6h,h)$:
 2.41363167 3.72005000 0.00965453 0.01488020 0.00002731 2000.00000000 546.15
 $\text{DE}(b,h)$: 6.19483500 7.63520000 0.06257409 0.07712323 0.00021168 1.00000000
 2.12 $\text{DE}(f,h)$: 3.68273500 4.51880000 0.03719934 0.04564444 0.00007132

10000.00000000 7131.97 c_{11} : 175.23524635 176.10000000 0.76545340 0.76923077
 0.00001427 200.00000000 28.54 c_{33} : 200.93943349 190.50000000 0.81138475
 0.76923077 0.00177696 200.00000000 3553.92 c_{44} : 47.68657259 50.80000000
 0.72208620 0.76923077 0.00222261 200.00000000 4445.22 c_{12} : 103.05424411
 86.90000000 0.91222665 0.76923077 0.02044782 200.00000000 40895.64 c_{13}
 : 59.89207874 68.30000000 0.67453631 0.76923077 0.00896704 200.00000000
 17934.08 $M_{\text{freq}0}$: 2.62695805 2.85858719 0.19145224 0.20833333 0.00028497
 0.10000000 0.28 $M_{\text{freq}1}$: 2.62695806 2.85858719 0.19145224 0.20833333 0.00028497
 0.10000000 0.28 $M_{\text{freq}2}$: 2.62695806 2.85858719 0.19145224 0.20833333 0.00028497
 0.10000000 0.28 $M_{\text{freq}3}$: 2.62695807 2.85858719 0.19145224 0.20833333 0.00028497
 0.10000000 0.28 $M_{\text{freq}4}$: 5.92942676 5.66706047 0.21797848 0.20833333 0.00009303
 0.10000000 0.09 $M_{\text{freq}5}$: 5.92942676 5.66706047 0.21797848 0.20833333 0.00009303
 0.10000000 0.09 $H_{\text{freq}0}$: 4.01662631 4.80643423 0.17409936 0.20833333 0.00117196
 0.10000000 1.17 $H_{\text{freq}1}$: 4.01662631 5.58010025 0.14996095 0.20833333 0.00340733
 0.10000000 3.41 $H_{\text{freq}2}$: 6.52587072 5.65316738 0.24049463 0.20833333 0.00103435
 0.10000000 1.03 $H_{\text{freq}3}$: 6.52587072 6.36651842 0.21354786 0.20833333 0.00002719
 0.10000000 0.03 $H_{\text{freq}4}$: 7.98336637 6.40050186 0.25985483 0.20833333 0.00265446
 0.10000000 2.65 $H_{\text{freq}5}$: 7.98336637 7.64082373 0.21767304 0.20833333 0.00008723
 0.10000000 0.09 bandw. G : 3.55244777 5.87085872 0.86442642 1.42857143
 0.31825959 15.00000000 47738.94 bandw. K : 4.47627466 4.97424321 0.74990883
 0.83333333 0.00695965 15.00000000 1043.95 bandw. M : 5.06812253 7.78109872
 0.93048235 1.42857143 0.24809273 15.00000000 37213.91 bandw. L : 4.06810372
 6.34433701 0.91602586 1.42857143 0.26270296 15.00000000 39405.44 bandw. H :
 3.43543876 9.70902614 0.32167244 0.90909091 0.34506046 1.00000000 3450.60
 DOSerr_h : 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o : 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf} : 127.68536380 220.00000000 127.68536380 220.00000000
 8521.99205731 0.00500000 426099.60

1.15 2019-11-04

PARAMETERS fdd=0.1922822098 qdds=0.5564637163 qddp=0.5682189695
 qddd=0.7783922326 b0=57.0677821986 p0=1.1917944528 b1=-3.5209507363
 p1=0.6753260279 b2=537715.3415722760 m2=-11.5000000000 p2=0.0000000000
 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.1308141671 cr3=-1.2221014245
 r1dd=6.5000000000 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18
 VARGS -vfdd=0.1922822098 -vqdds=0.5564637163 -vqddp=0.5682189695 -
 vqddd=0.7783922326 -vb0=57.0677821986 -vp0=1.1917944528 -vb1=-3.5209507363
 -vp1=0.6753260279 -vb2=537715.3415722760 -vm2=-11.5000000000 -vp2=0.0000000000
 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.1308141671 -vcr3=-1.2221014245

```

-vr1dd=6.5000000000 -vrdd=10.0000000000 -vrmaxh m=10.1000000000 hcp
: 5.60156937 5.57678969 5.60156937 5.57678969 0.00061403 1000.00000000
6140.33 c/a : 1.57677852 1.58731122 15.30954576 15.41181168 0.01045832
100.00000000 10458.32 aomega : 8.95958244 8.73254342 1.11994780 1.09156793
0.00080542 10.00000000 80.54 comega : 5.40050460 5.32343103 0.67506307
0.66542888 0.00009282 10.00000000 9.28 a4h : 5.59436001 5.56325146 1.00559179
1.00000000 0.00003127 1.00000000 0.31 c4h : 18.14476546 17.75908031 1.02171763
1.00000000 0.00047166 1.00000000 4.72 a6h : 5.59177170 5.54639384 1.00818151
1.00000000 0.00006694 1.00000000 0.67 c6h : 27.26286848 26.77136353 1.01835935
1.00000000 0.00033707 1.00000000 3.37 abcc : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 afcc : 7.89832289 7.88677000 1.12833184
1.12668143 0.00000272 1.00000000 0.03 DE(o,h) : 0.39843333 -0.63343333
0.02656222 -0.04222889 0.00473222 3000.00000000 141966.51 DE(4h,h): 1.62832250
3.17160000 0.00651329 0.01268640 0.00003811 2000.00000000 762.15 DE(6h,h):
2.52232333 3.72005000 0.01008929 0.01488020 0.00002295 2000.00000000 459.06
DE(b,h) : 5.29244000 7.63520000 0.05345899 0.07712323 0.00056000 1.00000000
5.60 DE(f,h) : 3.82166000 4.51880000 0.03860263 0.04564444 0.00004959
2000.00000000 991.74 c11 : 171.11082746 176.10000000 0.74743733 0.76923077
0.00047495 200.00000000 949.91 c33 : 200.84439599 190.50000000 0.81100099
0.76923077 0.00174475 200.00000000 3489.50 c44 : 47.64707517 50.80000000
0.72148812 0.76923077 0.00227936 200.00000000 4558.72 c12 : 98.26505555
86.90000000 0.86983319 0.76923077 0.01012085 200.00000000 20241.69 c13
: 63.57333846 68.30000000 0.71599660 0.76923077 0.00283388 200.00000000
5667.75 Mfreq0: 2.61427219 2.85858719 0.19052770 0.20833333 0.00031704
0.10000000 0.32 Mfreq1: 2.61427220 2.85858719 0.19052770 0.20833333 0.00031704
0.10000000 0.32 Mfreq2: 2.61427220 2.85858719 0.19052770 0.20833333 0.00031704
0.10000000 0.32 Mfreq3: 2.61427221 2.85858719 0.19052770 0.20833333 0.00031704
0.10000000 0.32 Mfreq4: 5.98250391 5.66706047 0.21992971 0.20833333 0.00013448
0.10000000 0.13 Mfreq5: 5.98250391 5.66706047 0.21992971 0.20833333 0.00013448
0.10000000 0.13 Hfreq0: 3.85890832 4.80643423 0.16726313 0.20833333 0.00168676
0.10000000 1.69 Hfreq1: 3.85890832 5.58010025 0.14407254 0.20833333 0.00412945
0.10000000 4.13 Hfreq2: 6.61042226 5.65316738 0.24361057 0.20833333 0.00124448
0.10000000 1.24 Hfreq3: 6.61042226 6.36651842 0.21631467 0.20833333 0.00006370
0.10000000 0.06 Hfreq4: 8.14790524 6.40050186 0.26521049 0.20833333 0.00323501
0.10000000 3.24 Hfreq5: 8.14790524 7.64082373 0.22215933 0.20833333 0.00019116
0.10000000 0.19 bandw. G: 3.66265392 5.87085872 0.89124317 1.42857143
0.28872166 15.00000000 43308.25 bandw. K: 4.60824993 4.97424321 0.77201860
0.83333333 0.00375950 15.00000000 563.92 bandw. M: 5.15792014 7.78109872
0.94696875 1.42857143 0.23194114 15.00000000 34791.17 bandw. L: 4.18239159
6.34433701 0.94176036 1.42857143 0.23698501 15.00000000 35547.75 bandw.

```

H: 3.51707295 9.70902614 0.32931614 0.90909091 0.33613878 1.00000000 3361.39
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prsf}: 102.00174503 220.00000000 102.00174503 220.00000000
 13923.58817555 0.00500000 696179.41
 PARAMETERS fdd=0.2023488497 qdds=0.5565157927 qddp=0.5689860518
 qddd=0.7798989561 b0=57.3192892630 p0=1.1628351457 b1=-3.6641201316
 p1=0.6537721271 b2=616842.8875572776 m2=-11.5000000000 p2=0.0000000000
 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.1384275133 cr3=-1.1762014635
 r1dd=6.5000000000 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18
 VARGS -vfdd=0.2023488497 -vqdds=0.5565157927 -vqddp=0.5689860518 -
 vqddd=0.7798989561 -vb0=57.3192892630 -vp0=1.1628351457 -vb1=-3.6641201316
 -vp1=0.6537721271 -vb2=616842.8875572776 -vm2=-11.5000000000 -vp2=0.0000000000
 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.1384275133 -vcr3=-1.1762014635
 -vr1dd=6.5000000000 -vrccd=10.0000000000 -vrmaxh m=10.1000000000
 a_{hcp}: 5.66663305 5.57678969 5.66663305 5.57678969 0.00807183 1000.00000000
 80718.30 c/a: 1.57885166 1.58731122 15.32967466 15.41181168 0.00674649
 100.00000000 6746.49 a_{omega}: 9.06547942 8.73254342 1.13318493 1.09156793
 0.00173197 10.00000000 173.20 c_{omega}: 5.45110369 5.32343103 0.68138796
 0.66542888 0.00025469 10.00000000 25.47 a_{4h}: 5.66203141 5.56325146 1.01775580
 1.00000000 0.00031527 1.00000000 3.15 c_{4h}: 18.35046679 17.75908031 1.03330051
 1.00000000 0.00110892 1.00000000 11.09 a_{6h}: 5.65874115 5.54639384 1.02025592
 1.00000000 0.00041030 1.00000000 4.10 c_{6h}: 27.58301293 26.77136353 1.03031782
 1.00000000 0.00091917 1.00000000 9.19 a_{bcc}: 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc}: 7.99363419 7.88677000 1.14194774
 1.12668143 0.00023306 1.00000000 2.33 DE(o,h): -0.22313500 -0.63343333 -
 0.01487567 -0.04222889 0.00074820 3000.00000000 22445.96 DE(4h,h): 1.73528500
 3.17160000 0.00694114 0.01268640 0.00003301 2000.00000000 660.16 DE(6h,h):
 2.66296667 3.72005000 0.01065187 0.01488020 0.00001788 2000.00000000 357.58
 DE(b,h): 5.88565500 7.63520000 0.05945106 0.07712323 0.00031231 1.00000000
 3.12 DE(f,h): 4.01464500 4.51880000 0.04055197 0.04564444 0.00002593
 2000.00000000 518.67 c₁₁: 171.26007888 176.10000000 0.74808928 0.76923077
 0.00044696 200.00000000 893.93 c₃₃: 204.34896099 190.50000000 0.82515228
 0.76923077 0.00312721 200.00000000 6254.43 c₄₄: 47.61806049 50.80000000
 0.72104877 0.76923077 0.00232151 200.00000000 4643.01 c₁₂: 111.39257489
 86.90000000 0.98603678 0.76923077 0.04700485 200.00000000 94009.69 c₁₃
 : 62.17165804 68.30000000 0.70021014 0.76923077 0.00476385 200.00000000
 9527.70 M_{freq0}: 2.59534163 2.85858719 0.18914804 0.20833333 0.00036808
 0.10000000 0.37 M_{freq1}: 2.59534164 2.85858719 0.18914804 0.20833333 0.00036808
 0.10000000 0.37 M_{freq2}: 2.59534164 2.85858719 0.18914804 0.20833333 0.00036808

0.10000000 0.37 M_{freq3} : 2.59534165 2.85858719 0.18914805 0.20833333 0.00036808
 0.10000000 0.37 M_{freq4} : 6.05074064 5.66706047 0.22243824 0.20833333 0.00019895
 0.10000000 0.20 M_{freq5} : 6.05074064 5.66706047 0.22243824 0.20833333 0.00019895
 0.10000000 0.20 H_{freq0} : 3.94456725 4.80643423 0.17097599 0.20833333 0.00139557
 0.10000000 1.40 H_{freq1} : 3.94456725 5.58010025 0.14727062 0.20833333 0.00372865
 0.10000000 3.73 H_{freq2} : 6.75120377 5.65316738 0.24879872 0.20833333 0.00163745
 0.10000000 1.64 H_{freq3} : 6.75120377 6.36651842 0.22092150 0.20833333 0.00015846
 0.10000000 0.16 H_{freq4} : 8.25023881 6.40050186 0.26854140 0.20833333 0.00362501
 0.10000000 3.63 H_{freq5} : 8.25023881 7.64082373 0.22494954 0.20833333 0.00027610
 0.10000000 0.28 bandw. G: 3.65585107 5.87085872 0.88958782 1.42857143
 0.29050333 15.00000000 43575.50 bandw. K: 4.63137962 4.97424321 0.77589351
 0.83333333 0.00329933 15.00000000 494.90 bandw. M: 5.23275148 7.78109872
 0.96070742 1.42857143 0.21889673 15.00000000 32834.51 bandw. L: 4.20824241
 6.34433701 0.94758126 1.42857143 0.23135154 15.00000000 34702.73 bandw.
 H: 3.55244777 9.70902614 0.33262841 0.90909091 0.33230901 1.00000000 3323.09
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 104.53788408 220.00000000 104.53788408 220.00000000
 13331.50021321 0.00500000 666575.01

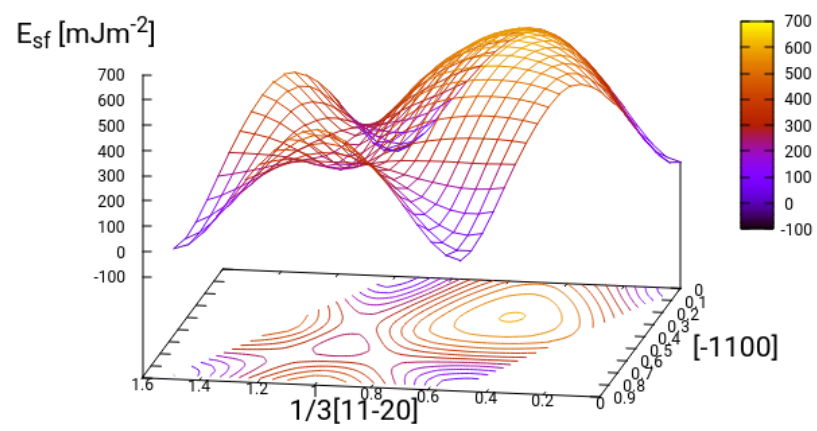
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 qddd=0.7745947522 b0=58.0906936439 p0=1.2185323579 b1=-3.2299188646
 p1=0.6862915307 b2=593519.1134129359 m2=-11.5000000000 p2=0.0000000000
 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.0474400934 cr3=-1.2317472193
 r1dd=6.5000000000 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18
 VARGS -vfdd=0.1958363809 -vqdds=0.5591275855 -vqddp=0.5690351902 -
 vqddd=0.7745947522 -vb0=58.0906936439 -vp0=1.2185323579 -vb1=-3.2299188646
 -vp1=0.6862915307 -vb2=593519.1134129359 -vm2=-11.5000000000 -vp2=0.0000000000
 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.0474400934 -vcr3=-1.2317472193
 -vr1dd=6.5000000000 -vrcdd=10.0000000000 -vrmaxhm=10.1000000000

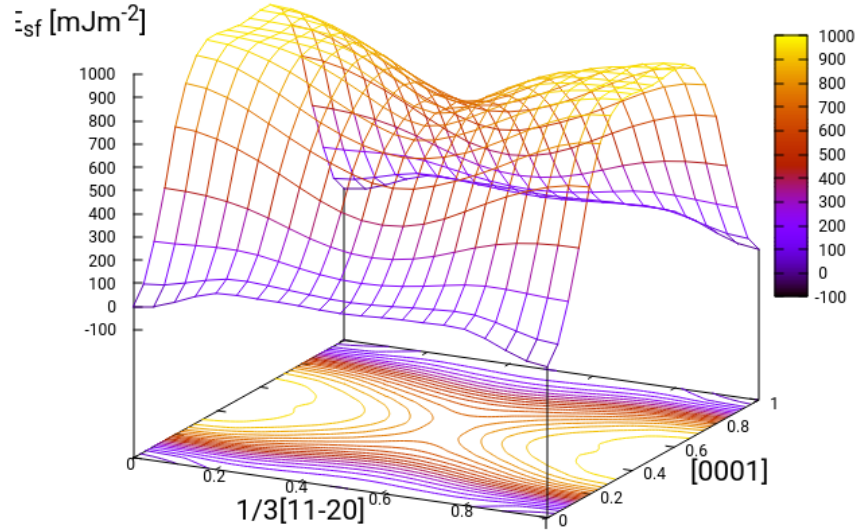
a_{hcp}: 5.58523112 5.57678969 5.58523112 5.57678969 0.00007126 1000.00000000
 712.58 c/a : 1.58371266 1.58731122 15.37687193 15.41181168 0.00122079
 100.00000000 1220.79 a_{omega}: 8.93475285 8.73254342 1.11684411 1.09156793
 0.00063889 10.00000000 63.89 c_{omega}: 5.38726911 5.32343103 0.67340864
 0.66542888 0.00006368 10.00000000 6.37 a_{4h}: 5.57584691 5.56325146 1.00226404
 1.00000000 0.00000513 1.00000000 0.05 c_{4h}: 18.09810672 17.75908031 1.01909031
 1.00000000 0.00036444 1.00000000 3.64 a_{6h}: 5.57365569 5.54639384 1.00491524
 1.00000000 0.00002416 1.00000000 0.24 c_{6h}: 27.18378460 26.77136353 1.01540531
 1.00000000 0.00023732 1.00000000 2.37 a_{bcc}: 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc}: 7.87290654 7.88677000 1.12470093
 1.12668143 0.00000392 1.00000000 0.04 DE(o,h) : 0.58764167 -0.63343333

0.03917611 -0.04222889 0.00662677 3000.00000000 198803.22 DE(4h,h): 1.58019500
 3.17160000 0.00632078 0.01268640 0.00004052 2000.00000000 810.42 DE(6h,h):
 2.48264833 3.72005000 0.00993059 0.01488020 0.00002450 2000.00000000 489.97
 DE(b,h) : 5.35128500 7.63520000 0.05405338 0.07712323 0.00053222 1.00000000
 5.32 DE(f,h) : 3.78088500 4.51880000 0.03819076 0.04564444 0.00005556
 10000.00000000 5555.74 c_{11} : 171.60928873 176.10000000 0.74961468 0.76923077
 0.00038479 200.00000000 769.58 c_{33} : 198.90063708 190.50000000 0.80315218
 0.76923077 0.00115066 200.00000000 2301.32 c_{44} : 47.42549704 50.80000000
 0.71813290 0.76923077 0.00261099 200.00000000 5221.98 c_{12} : 94.65941969
 86.90000000 0.83791644 0.76923077 0.00471772 200.00000000 9435.44 c_{13} :
 61.22624060 68.30000000 0.68956234 0.76923077 0.00634706 200.00000000
 12694.12 $M_{\text{freq}0}$: 2.59341377 2.85858719 0.18900754 0.20833333 0.00037349
 0.10000000 0.37 $M_{\text{freq}1}$: 2.59341378 2.85858719 0.18900754 0.20833333 0.00037349
 0.10000000 0.37 $M_{\text{freq}2}$: 2.59341378 2.85858719 0.18900754 0.20833333 0.00037349
 0.10000000 0.37 $M_{\text{freq}3}$: 2.59341379 2.85858719 0.18900754 0.20833333 0.00037349
 0.10000000 0.37 $M_{\text{freq}4}$: 5.85272461 5.66706047 0.21515875 0.20833333 0.00004659
 0.10000000 0.05 $M_{\text{freq}5}$: 5.85272461 5.66706047 0.21515875 0.20833333 0.00004659
 0.10000000 0.05 $H_{\text{freq}0}$: 3.82320403 4.80643423 0.16571554 0.20833333 0.00181628
 0.10000000 1.82 $H_{\text{freq}1}$: 3.82320403 5.58010025 0.14273952 0.20833333 0.00430255
 0.10000000 4.30 $H_{\text{freq}2}$: 6.40288977 5.65316738 0.23596248 0.20833333 0.00076337
 0.10000000 0.76 $H_{\text{freq}3}$: 6.40288977 6.36651842 0.20952352 0.20833333 0.00000142
 0.10000000 0.00 $H_{\text{freq}4}$: 7.92857431 6.40050186 0.25807137 0.20833333 0.00247387
 0.10000000 2.47 $H_{\text{freq}5}$: 7.92857431 7.64082373 0.21617909 0.20833333 0.00006156
 0.10000000 0.06 bandw. G: 3.69394702 5.87085872 0.89885780 1.42857143
 0.28059652 15.00000000 42089.48 bandw. K: 4.65178817 4.97424321 0.77931255
 0.83333333 0.00291825 15.00000000 437.74 bandw. M: 5.19329495 7.78109872
 0.95346339 1.42857143 0.22572765 15.00000000 33859.15 bandw. L: 4.21232412
 6.34433701 0.94850035 1.42857143 0.23046824 15.00000000 34570.24 bandw.
 H: 3.54700549 9.70902614 0.33211883 0.90909091 0.33289678 1.00000000 3328.97
 DOS $\epsilon_{\text{err}h}$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOS $\epsilon_{\text{err}o}$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf} : 98.95340236 220.00000000 98.95340236 220.00000000
 14652.27879997 0.00500000 732613.94

————— $E_{\text{Basalfault}}$ I2 —————

tbe: 211.658 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]





1.16 2019-11-08

PARAMETERS fdd=0.1985170314 qdds=0.5599973417 qddp=0.5688092470
 qddd=0.7747313173 b0=67.1449079591 p0=1.2485674461 b1=-3.0306254918
 p1=0.6883503780 b2=656837.4154963284 m2=-11.5000000000 p2=0.0000000000
 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.2375414409 cr3=-1.2352888306
 r1dd=6.5000000000 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18
 VARGS -vfdd=0.1985170314 -vqdds=0.5599973417 -vqddp=0.5688092470 -
 vqddd=0.7747313173 -vb0=67.1449079591 -vp0=1.2485674461 -vb1=-3.0306254918
 -vp1=0.6883503780 -vb2=656837.415 4963284 -vm2=-11.5000000000 -vp2=0.0000000000
 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.2375414409 -vcr3=-1.2352888306
 -vr1dd=6.5000000000 -vrcdd=10.0000000000 -vrmaxh m=10.1000000000
 a_{hcp} : 5.65630251 5.57678969 5.65630251 5.57678969 0.00632229 1000.00000000
 63222.89 c/a : 1.59296599 1.58731122 15.46671608 15.41181168 0.00301449
 100.00000000 3014.49 a_{omega} : 9.04033772 8.73254342 1.13004221 1.09156793
 0.00148027 10.00000000 148.03 c_{omega} : 5.45616542 5.32343103 0.68202068
 0.66542888 0.00027529 10.00000000 27.53 a_{4h} : 5.64703239 5.56325146 1.01505971

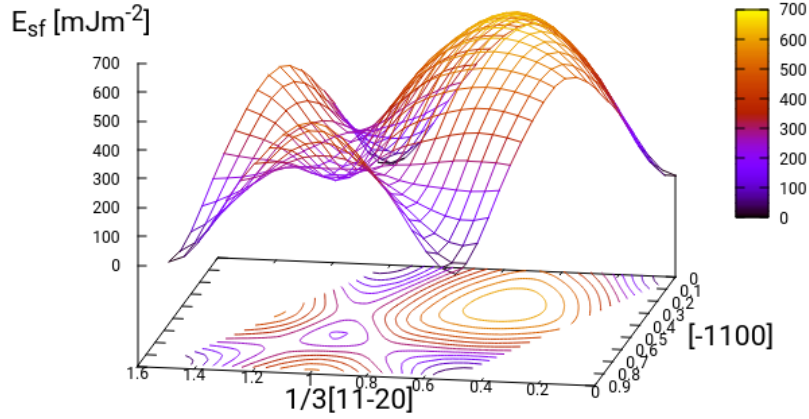
1.00000000 0.00022679 1.00000000 2.27 c_{4h} : 18.32517456 17.75908031 1.03187633
1.00000000 0.00101610 1.00000000 10.16 a_{6h} : 5.64471540 5.54639384 1.01772711
1.00000000 0.00031425 1.00000000 3.14 c_{6h} : 27.53180793 26.77136353 1.02840514
1.00000000 0.00080685 1.00000000 8.07 a_{bcc} : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.97303155 7.88677000 1.13900451
1.12668143 0.00015186 1.00000000 1.52 DE(o,h) : 0.91598667 -0.63343333
0.06106578 -0.04222889 0.01066979 3000.00000000 320093.64 DE(4h,h): 1.44762250
3.17160000 0.00579049 0.01268640 0.00004755 2000.00000000 951.07 DE(6h,h):
2.27979500 3.72005000 0.00911918 0.01488020 0.00003319 2000.00000000 663.79
DE(b,h) : 6.34536000 7.63520000 0.06409455 0.07712323 0.00016975 1.00000000
1.70 DE(f,h) : 3.48966000 4.51880000 0.03524909 0.04564444 0.00010806
10000.00000000 10806.34 c_{11} : 170.36444545 176.10000000 0.74417702 0.76923077
0.00062769 200.00000000 1255.38 c_{33} : 187.75296179 190.50000000 0.75813835
0.76923077 0.00012304 200.00000000 246.08 c_{44} : 45.39492860 50.80000000
0.68738535 0.76923077 0.00669867 200.00000000 13397.34 c_{12} : 93.75627563
86.90000000 0.82992189 0.76923077 0.00368341 200.00000000 7366.82 c_{13} :
61.00093051 68.30000000 0.68702478 0.76923077 0.00675782 200.00000000
13515.65 M_{freq0} : 2.60486873 2.85858719 0.18984238 0.20833333 0.00034192
0.10000000 0.34 M_{freq1} : 2.60486874 2.85858719 0.18984238 0.20833333 0.00034192
0.10000000 0.34 M_{freq2} : 2.60486874 2.85858719 0.18984238 0.20833333 0.00034192
0.10000000 0.34 M_{freq3} : 2.60486875 2.85858719 0.18984238 0.20833333 0.00034192
0.10000000 0.34 M_{freq4} : 5.72079247 5.66706047 0.21030864 0.20833333 0.00000390
0.10000000 0.00 M_{freq5} : 5.72079247 5.66706047 0.21030864 0.20833333 0.00000390
0.10000000 0.00 H_{freq0} : 3.90610849 4.80643423 0.16930901 0.20833333 0.00152290
0.10000000 1.52 H_{freq1} : 3.90610849 5.58010025 0.14583476 0.20833333 0.00390607
0.10000000 3.91 H_{freq2} : 6.27293595 5.65316738 0.23117335 0.20833333 0.00052167
0.10000000 0.52 H_{freq3} : 6.27293595 6.36651842 0.20527101 0.20833333 0.00000938
0.10000000 0.01 H_{freq4} : 7.71555746 6.40050186 0.25113778 0.20833333 0.00183222
0.10000000 1.83 H_{freq5} : 7.71555746 7.64082373 0.21037101 0.20833333 0.00000415
0.10000000 0.00 bandw. G: 3.64632708 5.87085872 0.88727032 1.42857143
0.29300689 15.00000000 43951.03 bandw. K: 4.54430315 4.97424321 0.76130562
0.83333333 0.00518799 15.00000000 778.20 bandw. M: 5.15519900 7.78109872
0.94646916 1.42857143 0.23242259 15.00000000 34863.39 bandw. L: 4.16334361
6.34433701 0.93747128 1.42857143 0.24117936 15.00000000 36176.90 bandw.
H: 3.49122212 9.70902614 0.32689564 0.90909091 0.33895133 1.00000000 3389.51
DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00 E_{prisf}: 119.24169745 220.00000000 119.24169745 220.00000000
10152.23553276 0.00500000 507611.78
PARAMETERS fdd=0.1948454463 qdds=0.5589640802 qddp=0.5693084671

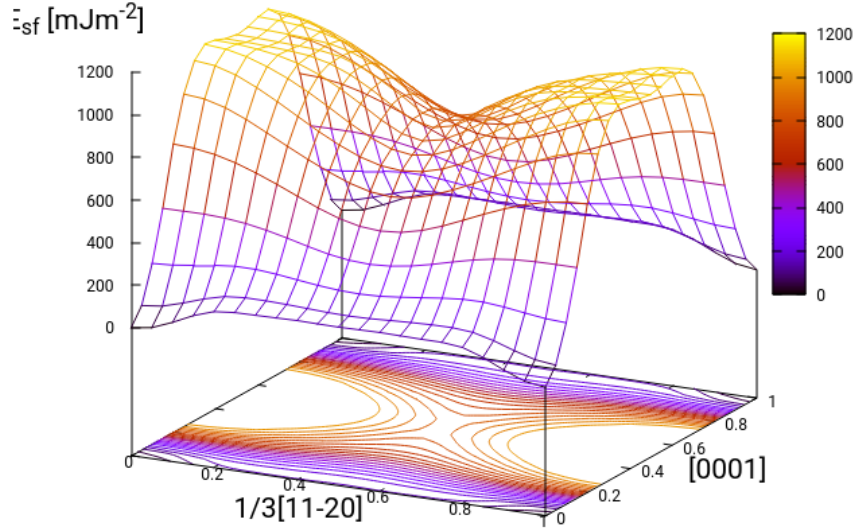
qddd=0.7748730693 b0=58.7994745523 p0=1.1531371547 b1=-3.9117460958
p1=0.6480960332 b2=522504.0614029730 m2=-11.5000000000 p2=0.0000000000
ndt=2.0000000000 cr1=-6.0000000000 cr2=3.4525563800 cr3=-1.2567506668
r1dd=6.5000000000 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18
VARGS -vfdd=0.1948454463 -vqdds=0.5589640802 -vqddp=0.5693084671 -
vqddd=0.7748730693 -vb0=58.7994745523 -vp0=1.1531371547 -vb1=-3.9117460958
-vp1=0.6480960332 -vb2=522504.0614029730 -vm2=-11.5000000000 -vp2=0.0000000000
-vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.4525563800 -vcr3=-1.2567506668
-vr1dd=6.5000000000 -vrdd=10.0000000000 -vrmaxhm=10.1000000000
a_{hcp} : 5.66018285 5.57678969 5.66018285 5.57678969 0.00695442 1000.00000000
69544.19 c/a : 1.59132985 1.58731122 15.45083010 15.41181168 0.00152244
100.00000000 1522.44 a_{omega} : 9.04224617 8.73254342 1.13028077 1.09156793
0.00149868 10.00000000 149.87 c_{omega} : 5.45729411 5.32343103 0.68216176
0.66542888 0.00027999 10.00000000 28.00 a_{4h} : 5.65808661 5.56325146 1.01704671
1.00000000 0.00029059 1.00000000 2.91 c_{4h} : 18.31639427 17.75908031 1.03138192
1.00000000 0.00098482 1.00000000 9.85 a_{6h} : 5.65433822 5.54639384 1.01946208
1.00000000 0.00037877 1.00000000 3.79 c_{6h} : 27.54417628 26.77136353 1.02886714
1.00000000 0.00083331 1.00000000 8.33 a_{bcc} : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.98535463 7.88677000 1.14076495
1.12668143 0.00019835 1.00000000 1.98 DE(o,h) : 0.27998500 -0.63343333
0.01866567 -0.04222889 0.00370815 3000.00000000 111244.41 DE(4h,h): 1.53640250
3.17160000 0.00614561 0.01268640 0.00004278 2000.00000000 855.64 DE(6h,h):
2.38561333 3.72005000 0.00954245 0.01488020 0.00002849 2000.00000000 569.83
DE(b,h) : 6.70516500 7.63520000 0.06772894 0.07712323 0.00008825 1.00000000
0.88 DE(f,h) : 3.63886500 4.51880000 0.03675621 0.04564444 0.00007900
2000.00000000 1580.01 c₁₁ : 178.55891012 176.10000000 0.77997165 0.76923077
0.00011537 200.00000000 230.73 c₃₃ : 216.05201952 190.50000000 0.87240872
0.76923077 0.01064569 200.00000000 21291.38 c₄₄ : 50.21922256 50.80000000
0.76043644 0.76923077 0.00007734 200.00000000 154.68 c₁₂ : 108.89042033
86.90000000 0.96388794 0.76923077 0.03789141 200.00000000 75782.83 c₁₃
: 63.50930696 68.30000000 0.71527545 0.76923077 0.00291118 200.00000000
5822.35 M_{freq0}: 2.76609238 2.85858719 0.20159233 0.20833333 0.00004544
0.10000000 0.05 M_{freq1}: 2.76609239 2.85858719 0.20159233 0.20833333 0.00004544
0.10000000 0.05 M_{freq2}: 2.76609239 2.85858719 0.20159233 0.20833333 0.00004544
0.10000000 0.05 M_{freq3}: 2.76609240 2.85858719 0.20159233 0.20833333 0.00004544
0.10000000 0.05 M_{freq4}: 6.25152012 5.66706047 0.22981933 0.20833333 0.00046165
0.10000000 0.46 M_{freq5}: 6.25152012 5.66706047 0.22981933 0.20833333 0.00046165
0.10000000 0.46 H_{freq0}: 4.03482958 4.80643423 0.17488838 0.20833333 0.00111856
0.10000000 1.12 H_{freq1}: 4.03482958 5.58010025 0.15064057 0.20833333 0.00332845
0.10000000 3.33 H_{freq2}: 7.10258591 5.65316738 0.26174803 0.20833333 0.00285313

0.10000000 2.85 $H_{\text{freq}3}$: 7.10258591 6.36651842 0.23241987 0.20833333 0.00058016
 0.10000000 0.58 $H_{\text{freq}4}$: 8.63246455 6.40050186 0.28098267 0.20833333 0.00527793
 0.10000000 5.28 $H_{\text{freq}5}$: 8.63246455 7.64082373 0.23537123 0.20833333 0.00073105
 0.10000000 0.73 bandw. G: 3.69530759 5.87085872 0.89918888 1.42857143
 0.28024589 15.00000000 42036.88 bandw. K: 4.54566372 4.97424321 0.76153355
 0.83333333 0.00515521 15.00000000 773.28 bandw. M: 5.18104982 7.78109872
 0.95121525 1.42857143 0.22786892 15.00000000 34180.34 bandw. L: 4.21368469
 6.34433701 0.94880672 1.42857143 0.23017418 15.00000000 34526.13 bandw.
 H: 3.49802497 9.70902614 0.32753261 0.90909091 0.33821005 1.00000000 3382.10
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 144.13939923 220.00000000 144.13939923 220.00000000
 5754.83074961 0.00500000 287741.54

———— E_{Basalfault} I2 —————

tbe: 193.082 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]





fdd=0.1952063508 qdds=0.5595656099 qddp=0.5720819509 qddd=0.7767751764
 b0=50.9323750568 p0=1.0807578496 b1=-5.9463572586 p1=0.6739426146 b2=767976.5243575326
 m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
 cr2=3.3787908974 cr3=-1.2240415092 r1dd=6.5000000000 rcdd=10.0000000000
 rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.63288435 5.57678969 5.63288435 5.57678969 0.00314661 1000.00000000
 31466.11 c/a : 1.60288814 1.58731122 15.56305396 15.41181168 0.02287423
 100.00000000 22874.23 a_{omega} : 9.00703954 8.73254342 1.12587994 1.09156793
 0.00117731 10.00000000 117.73 c_{omega} : 5.42934710 5.32343103 0.67866839
 0.66542888 0.00017528 10.00000000 17.53 a_{4h} : 5.63168065 5.56325146 1.01230022
 1.00000000 0.00015130 1.00000000 1.51 c_{4h} : 18.22597130 17.75908031 1.02629027
 1.00000000 0.00069118 1.00000000 6.91 a_{6h} : 5.62820060 5.54639384 1.01474954
 1.00000000 0.00021755 1.00000000 2.18 c_{6h} : 27.40641078 26.77136353 1.02372114
 1.00000000 0.00056269 1.00000000 5.63 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.94838539 7.88677000 1.13548363
 1.12668143 0.00007748 1.00000000 0.77 DE(o,h) : 0.07058833 -0.63343333

0.00470589 -0.04222889 0.00220287 3000.00000000 66086.20 DE(4h,h): 1.69426000
 3.17160000 0.00677704 0.01268640 0.00003492 2000.00000000 698.41 DE(6h,h):
 2.58955833 3.72005000 0.01035823 0.01488020 0.00002045 2000.00000000 408.96
 DE(b,h) : 6.05460500 7.63520000 0.06115763 0.07712323 0.00025490 1.00000000
 2.55 DE(f,h) : 3.91807500 4.51880000 0.03957652 0.04564444 0.00003682
 10000.00000000 3681.98 c₁₁ : 179.57715080 176.10000000 0.78441948 0.76923077
 0.00023070 200.00000000 461.39 c₃₃ : 221.99166520 190.50000000 0.89639275
 0.76923077 0.01617017 200.00000000 32340.34 c₄₄ : 51.00011242 50.80000000
 0.77226094 0.76923077 0.00000918 200.00000000 18.36 c₁₂ : 112.11320549
 86.90000000 0.99241573 0.76923077 0.04981153 200.00000000 99623.06 c₁₃ :
 67.45149382 68.30000000 0.75967444 0.76923077 0.00009132 200.00000000
 182.65 M_{freq0}: 2.80682835 2.85858719 0.20456116 0.20833333 0.00001423
 0.10000000 0.01 M_{freq1}: 2.80682837 2.85858719 0.20456116 0.20833333 0.00001423
 0.10000000 0.01 M_{freq2}: 2.80682837 2.85858719 0.20456116 0.20833333 0.00001423
 0.10000000 0.01 M_{freq3}: 2.80682838 2.85858719 0.20456116 0.20833333 0.00001423
 0.10000000 0.01 M_{freq4}: 6.50650151 5.66706047 0.23919299 0.20833333 0.00095232
 0.10000000 0.95 M_{freq5}: 6.50650151 5.66706047 0.23919299 0.20833333 0.00095232
 0.10000000 0.95 H_{freq0}: 4.06668772 4.80643423 0.17626926 0.20833333 0.00102810
 0.10000000 1.03 H_{freq1}: 4.06668772 5.58010025 0.15183000 0.20833333 0.00319263
 0.10000000 3.19 H_{freq2}: 7.40494486 5.65316738 0.27289071 0.20833333 0.00416765
 0.10000000 4.17 H_{freq3}: 7.40494486 6.36651842 0.24231405 0.20833333 0.00115469
 0.10000000 1.15 H_{freq4}: 9.01135858 6.40050186 0.29331549 0.20833333 0.00722197
 0.10000000 7.22 H_{freq5}: 9.01135858 7.64082373 0.24570209 0.20833333 0.00139642
 0.10000000 1.40 bandw. G: 3.69666816 5.87085872 0.89951995 1.42857143
 0.27989547 15.00000000 41984.32 bandw. K: 4.58375968 4.97424321 0.76791576
 0.83333333 0.00427946 15.00000000 641.92 bandw. M: 5.18785267 7.78109872
 0.95246422 1.42857143 0.22667808 15.00000000 34001.71 bandw. L: 4.20824241
 6.34433701 0.94758126 1.42857143 0.23135154 15.00000000 34702.73 bandw.
 H: 3.51571238 9.70902614 0.32918875 0.90909091 0.33628652 1.00000000 3362.87
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 149.10486599 220.00000000 149.10486599 220.00000000
 5026.12002569 0.00500000 251306.00
 fdd=0.1948303739 qdds=0.5599306995 qddp=0.5718611144 qddd=0.7773545073
 b0=50.5503194662 p0=1.0758879693 b1=-5.9475113962 p1=0.6728267224 b2=755196.3434726764
 m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
 cr2=3.4625598554 cr3=-1.2169594563 r1dd=6.5000000000 rcdd=10.0000000000
 rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.65820864 5.57678969 5.65820864 5.57678969 0.00662905 1000.00000000

66290.46 c/a : 1.59216199 1.58731122 15.45890972 15.41181168 0.00221822
100.00000000 2218.22 a_{omega} : 9.04491543 8.73254342 1.13061443 1.09156793
0.00152463 10.00000000 152.46 c_{omega} : 5.45215752 5.32343103 0.68151969
0.66542888 0.00025891 10.00000000 25.89 a_{4h} : 5.65749922 5.56325146 1.01694113
1.00000000 0.00028700 1.00000000 2.87 c_{4h} : 18.30757352 17.75908031 1.03088523
1.00000000 0.00095390 1.00000000 9.54 a_{6h} : 5.65361570 5.54639384 1.01933181
1.00000000 0.00037372 1.00000000 3.74 c_{6h} : 27.53347395 26.77136353 1.02846737
1.00000000 0.00081039 1.00000000 8.10 a_{bcc} : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.98439188 7.88677000 1.14062741
1.12668143 0.00019449 1.00000000 1.94 DE(o,h) : -0.00912667 -0.63343333 -
0.00060844 -0.04222889 0.00173226 3000.00000000 51967.84 DE(4h,h): 1.61635500
3.17160000 0.00646542 0.01268640 0.00003870 2000.00000000 774.01 DE(6h,h):
2.47645333 3.72005000 0.00990581 0.01488020 0.00002474 2000.00000000 494.89
DE(b,h) : 6.50639000 7.63520000 0.06572111 0.07712323 0.00013001 1.00000000
1.30 DE(f,h) : 3.75517000 4.51880000 0.03793101 0.04564444 0.00005950
10000.00000000 5949.71 c₁₁ : 179.37685698 176.10000000 0.78354456 0.76923077
0.00020488 200.00000000 409.77 c₃₃ : 220.63352230 190.50000000 0.89090863
0.76923077 0.01480550 200.00000000 29611.00 c₄₄ : 50.58870959 50.80000000
0.76603134 0.76923077 0.00001024 200.00000000 20.47 c₁₂ : 114.73413137
86.90000000 1.01561593 0.76923077 0.06070565 200.00000000 121411.29 c₁₃
: 64.26403498 68.30000000 0.72377559 0.76923077 0.00206617 200.00000000
4132.35 M_{freq0}: 2.78569973 2.85858719 0.20302131 0.20833333 0.00002822
0.10000000 0.03 M_{freq1}: 2.78569974 2.85858719 0.20302131 0.20833333 0.00002822
0.10000000 0.03 M_{freq2}: 2.78569974 2.85858719 0.20302131 0.20833333 0.00002822
0.10000000 0.03 M_{freq3}: 2.78569975 2.85858719 0.20302131 0.20833333 0.00002822
0.10000000 0.03 M_{freq4}: 6.39363545 5.66706047 0.23504379 0.20833333 0.00071345
0.10000000 0.71 M_{freq5}: 6.39363545 5.66706047 0.23504379 0.20833333 0.00071345
0.10000000 0.71 H_{freq0}: 4.06082551 4.80643423 0.17601516 0.20833333 0.00104446
0.10000000 1.04 H_{freq1}: 4.06082551 5.58010025 0.15161113 0.20833333 0.00321741
0.10000000 3.22 H_{freq2}: 7.30620632 5.65316738 0.26925195 0.20833333 0.00371108
0.10000000 3.71 H_{freq3}: 7.30620632 6.36651842 0.23908300 0.20833333 0.00094554
0.10000000 0.95 H_{freq4}: 8.86241503 6.40050186 0.28846745 0.20833333 0.00642148
0.10000000 6.42 H_{freq5}: 8.86241503 7.64082373 0.24164102 0.20833333 0.00110940
0.10000000 1.11 bandw. G: 3.66265392 5.87085872 0.89124317 1.42857143
0.28872166 15.00000000 43308.25 bandw. K: 4.51981290 4.97424321 0.75720277
0.83333333 0.00579586 15.00000000 869.38 bandw. M: 5.14567501 7.78109872
0.94472061 1.42857143 0.23411162 15.00000000 35116.74 bandw. L: 4.17694931
6.34433701 0.94053491 1.42857143 0.23817964 15.00000000 35726.95 bandw.
H: 3.47625586 9.70902614 0.32549429 0.90909091 0.34058501 1.00000000 3405.85
DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000

0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00 E_{prisf}: 146.41793427 220.00000000 146.41793427 220.00000000
5414.32039774 0.00500000 270716.02
fdd=0.1921275626 qdds=0.5569515913 qddp=0.5669410627 qddd=0.7790109943
b0=55.0364608200 p0=1.1118288046 b1=-4.5595968409 p1=0.6409600863 b2=547934.5929577192
m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000 cr1=-6.0000000000
cr2=3.3980670998 cr3=-1.2170893463 r1dd=6.5000000000 rcdd=10.0000000000
rmaxhm=10.1000000000 npar=18

a_{hcp} : 5.64663571 5.57678969 5.64663571 5.57678969 0.00487847 1000.00000000
48784.67 c/a : 1.59705179 1.58731122 15.50638661 15.41181168 0.00894442
100.00000000 8944.42 a_{omega} : 9.02562197 8.73254342 1.12820275 1.09156793
0.00134211 10.00000000 134.21 c_{omega} : 5.44172642 5.32343103 0.68021580
0.66542888 0.00021865 10.00000000 21.87 a_{4h} : 5.64692001 5.56325146 1.01503950
1.00000000 0.00022619 1.00000000 2.26 c_{4h} : 18.26710869 17.75908031 1.02860668
1.00000000 0.00081834 1.00000000 8.18 a_{6h} : 5.64309685 5.54639384 1.01743529
1.00000000 0.00030399 1.00000000 3.04 c_{6h} : 27.47497658 26.77136353 1.02628230
1.00000000 0.00069076 1.00000000 6.91 a_{bcc} : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.96918058 7.88677000 1.13845437
1.12668143 0.00013860 1.00000000 1.39 DE(o,h) : -0.10589500 -0.63343333 -
0.00705967 -0.04222889 0.00123687 3000.00000000 37106.23 DE(4h,h): 1.69815000
3.17160000 0.00679260 0.01268640 0.00003474 2000.00000000 694.74 DE(6h,h):
2.57937667 3.72005000 0.01031751 0.01488020 0.00002082 2000.00000000 416.36
DE(b,h) : 6.23829500 7.63520000 0.06301308 0.07712323 0.00019910 1.00000000
1.99 DE(f,h) : 3.89144500 4.51880000 0.03930753 0.04564444 0.00004016
2000.00000000 803.13 c₁₁ : 179.66359732 176.10000000 0.78479709 0.76923077
0.00024231 200.00000000 484.62 c₃₃ : 224.81816276 190.50000000 0.90780603
0.76923077 0.01920310 200.00000000 38406.20 c₄₄ : 51.77737289 50.80000000
0.78403048 0.76923077 0.00021903 200.00000000 438.06 c₁₂ : 115.69901106
86.90000000 1.02415695 0.76923077 0.06498736 200.00000000 129974.72 c₁₃
: 65.67394369 68.30000000 0.73965473 0.76923077 0.00087474 200.00000000
1749.48 M_{freq0}: 2.81185437 2.85858719 0.20492745 0.20833333 0.00001160
0.10000000 0.01 M_{freq1}: 2.81185438 2.85858719 0.20492745 0.20833333 0.00001160
0.10000000 0.01 M_{freq2}: 2.81185438 2.85858719 0.20492745 0.20833333 0.00001160
0.10000000 0.01 M_{freq3}: 2.81185440 2.85858719 0.20492746 0.20833333 0.00001160
0.10000000 0.01 M_{freq4}: 6.53573109 5.66706047 0.24026753 0.20833333 0.00101979
0.10000000 1.02 M_{freq5}: 6.53573109 5.66706047 0.24026753 0.20833333 0.00101979
0.10000000 1.02 H_{freq0}: 4.06603923 4.80643423 0.17624115 0.20833333 0.00102991
0.10000000 1.03 H_{freq1}: 4.06603923 5.58010025 0.15180579 0.20833333 0.00319536
0.10000000 3.20 H_{freq2}: 7.48528085 5.65316738 0.27585129 0.20833333 0.00455867

0.10000000 4.56 H_{freq3}: 7.48528085 6.36651842 0.24494290 0.20833333 0.00134026
 0.10000000 1.34 H_{freq4}: 9.08667284 6.40050186 0.29576694 0.20833333 0.00764464
 0.10000000 7.64 H_{freq5}: 9.08667284 7.64082373 0.24775560 0.20833333 0.00155411
 0.10000000 1.55 bandw. G: 3.68986532 5.87085872 0.89786459 1.42857143
 0.28164975 15.00000000 42247.46 bandw. K: 4.56471170 4.97424321 0.76472465
 0.83333333 0.00470715 15.00000000 706.07 bandw. M: 5.17832868 7.78109872
 0.95071566 1.42857143 0.22834614 15.00000000 34251.92 bandw. L: 4.20688184
 6.34433701 0.94727490 1.42857143 0.23164635 15.00000000 34746.95 bandw.
 H: 3.50618839 9.70902614 0.32829698 0.90909091 0.33732158 1.00000000 3373.22
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf}: 149.13058461 220.00000000 149.13058461 220.00000000
 5022.47403807 0.00500000 251123.70
 PARAMETERS fdd=0.1970300483 qdds=0.5598089474 qddp=0.5699757259
 qddd=0.7759962216 b0=62.7171369456 p0=1.1648866123 b1=-4.7597467477
 p1=0.6770535066 b2=807138.5831859903 m2=-11.5000000000 p2=0.0000000000
 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.1538210130 cr3=-1.2077076968
 r1dd=6.5000000000 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18
 VARGS -vfdd=0.1970300483 -vqdds=0.5598089474 -vqddp=0.5699757259 -
 vqddd=0.7759962216 -vb0=62.7171369456 -vp0=1.1648866123 -vb1=-4.7597467477
 -vp1=0.6770535066 -vb2=807138.5831859903 -vm2=-11.5000000000 -vp2=0.0000000000
 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.1538210130 -vcr3=-1.2077076968
 -vr1dd=6.5000000000 -vrcdd=10.0000000000 -vrmaxhm=10.1000000000
 a_{hcp} : 5.62471523 5.57678969 5.62471523 5.57678969 0.00229686 1000.00000000
 22968.57 c/a : 1.60636879 1.58731122 15.59684893 15.41181168 0.03423878
 100.00000000 34238.78 a_{omega} : 9.00162511 8.73254342 1.12520314 1.09156793
 0.00113133 10.00000000 113.13 c_{omega} : 5.41522759 5.32343103 0.67690345
 0.66542888 0.00013167 10.00000000 13.17 a_{4h} : 5.61929025 5.56325146 1.01007303
 1.00000000 0.00010147 1.00000000 1.01 c_{4h} : 18.21643517 17.75908031 1.02575330
 1.00000000 0.00066323 1.00000000 6.63 a_{6h} : 5.61657519 5.54639384 1.01265351
 1.00000000 0.00016011 1.00000000 1.60 c_{6h} : 27.37506548 26.77136353 1.02255029
 1.00000000 0.00050852 1.00000000 5.09 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.93375174 7.88677000 1.13339311
 1.12668143 0.00004505 1.00000000 0.45 DE(o,h) : 0.75773833 -0.63343333
 0.05051589 -0.04222889 0.00860159 3000.00000000 258047.81 DE(4h,h): 1.69540000
 3.17160000 0.00678160 0.01268640 0.00003487 2000.00000000 697.33 DE(6h,h):
 2.60711167 3.72005000 0.01042845 0.01488020 0.00001982 2000.00000000 396.36
 DE(b,h) : 5.71313500 7.63520000 0.05770843 0.07712323 0.00037693 1.00000000
 3.77 DE(f,h) : 3.94745500 4.51880000 0.03987328 0.04564444 0.00003331
 2000.00000000 666.13 c₁₁ : 188.96232394 176.10000000 0.82541530 0.76923077

0.00315670 100.00000000 3156.70 c_{33} : 228.43905973 190.50000000 0.92242705
 0.76923077 0.02346910 100.00000000 23469.10 c_{44} : 53.12007965 50.80000000
 0.80436220 0.76923077 0.00123422 100.00000000 1234.22 c_{12} : 115.91544768
 86.90000000 1.02607283 0.76923077 0.06596784 100.00000000 65967.84 c_{13}
 : 69.33267364 68.30000000 0.78086129 0.76923077 0.00013527 10.00000000
 13.53 $M_{\text{freq}0}$: 2.84737254 2.85858719 0.20751601 0.20833333 0.00000067 0.10000000
 0.00 $M_{\text{freq}1}$: 2.84737255 2.85858719 0.20751601 0.20833333 0.00000067 0.10000000
 0.00 $M_{\text{freq}2}$: 2.84737255 2.85858719 0.20751601 0.20833333 0.00000067 0.10000000
 0.00 $M_{\text{freq}3}$: 2.84737256 2.85858719 0.20751601 0.20833333 0.00000067 0.10000000
 0.00 $M_{\text{freq}4}$: 6.60368808 5.66706047 0.24276578 0.20833333 0.00118559 0.10000000
 1.19 $M_{\text{freq}5}$: 6.60368808 5.66706047 0.24276578 0.20833333 0.00118559 0.10000000
 1.19 $H_{\text{freq}0}$: 4.26991916 4.80643423 0.18507826 0.20833333 0.00054080 0.10000000
 0.54 $H_{\text{freq}1}$: 4.26991916 5.58010025 0.15941765 0.20833333 0.00239274 0.10000000
 2.39 $H_{\text{freq}2}$: 7.42123707 5.65316738 0.27349112 0.20833333 0.00424554 0.10000000
 4.25 $H_{\text{freq}3}$: 7.42123707 6.36651842 0.24284718 0.20833333 0.00119121 0.10000000
 1.19 $H_{\text{freq}4}$: 9.02306185 6.40050186 0.29369643 0.20833333 0.00728686 0.10000000
 7.29 $H_{\text{freq}5}$: 9.02306185 7.64082373 0.24602119 0.20833333 0.00142037 0.10000000
 1.42 bandw. G: 3.64496651 5.87085872 1.03476246 1.66666667 0.39930293
 15.00000000 59895.44 bandw. K: 4.57559626 4.97424321 0.83623434 0.90909091
 0.00530808 15.00000000 796.21 bandw. M: 5.14975672 7.78109872 1.10304832
 1.66666667 0.31766564 15.00000000 47649.85 bandw. L: 4.15518019 6.34433701
 1.09157195 1.66666667 0.33073393 15.00000000 49610.09 bandw. H: 3.50346725
 9.70902614 0.32804219 0.90909091 0.33761761 5.00000000 16880.88 DOSerr_h :
 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00
 DOSerr_o : 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00

———— $E_{\text{prismaticfault}}$ ————
 tbe: 173.252 mJ/m² DFT: 250.000 mJ/m² [Benoit 2012] DFT: 233.000
 mJ/m² [Ackland 1999]
 ———— $E_{\text{Basalfault}}$ I2 ————
 tbe: 220.655 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]

1.17 Current Best

1.17.1 oo

fdd=0.222299836 qdds=0.5694802234 qddp=0.5890968074 qddd=0.8163634071
 b0=46.3166545 p0=1.035247743 b1=-6.44286741 p1=0.667994596 b2=573363.0706
 cr2=3.785987706 cr3=-1.157452833 m2=-11.5 p2=0.0 cr1=-6.0 ndt=2.0 r1dd=6.5
 redd=10.0 rmaxhm=10.001 npar=18

a_{hcp} : 5.64132578 5.57678969 5.64132578 5.57678969 0.00416491 1000.00000000
41649.07 c/a : 1.59930205 1.58731122 15.52823532 15.41181168 0.01355446
100.00000000 13554.46 a_{ω} : 9.00268216 8.73254342 1.12533527 1.09156793
0.00114023 10.00000000 114.02 c_{ω} : 5.45251944 5.32343103 0.68156493
0.66542888 0.00026037 10.00000000 26.04 a_{4h} : 5.64348381 5.56325146 1.01442185
1.00000000 0.00020799 1.00000000 2.08 c_{4h} : 18.23946323 17.75908031 1.02704999
1.00000000 0.00073170 1.00000000 7.32 a_{6h} : 5.63794259 5.54639384 1.01650599
1.00000000 0.00027245 1.00000000 2.72 c_{6h} : 27.44832595 26.77136353 1.02528681
1.00000000 0.00063942 1.00000000 6.39 a_{bcc} : 6.20079768 6.17948863 0.88582824
0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.96186376 7.88677000 1.13740911
1.12668143 0.00011508 1.00000000 1.15 $DE(o,h)$: -0.69722833 -0.63343333 -
0.04648189 -0.04222889 0.00001809 3000.00000000 542.64 $DE(4h,h)$: 1.83117250
3.17160000 0.00732469 0.01268640 0.00002875 2000.00000000 574.96 $DE(6h,h)$:
2.72116000 3.72005000 0.01088464 0.01488020 0.00001596 2000.00000000 319.29
 $DE(b,h)$: 6.80692500 7.63520000 0.06875682 0.07712323 0.00007000 1.00000000
0.70 $DE(f,h)$: 4.09507500 4.51880000 0.04136439 0.04564444 0.00001832
2000.00000000 366.38 c_{11} : 176.93212224 176.10000000 0.77286560 0.76923077
0.00001321 100.00000000 13.21 c_{33} : 221.91218797 190.50000000 0.89607183
0.76923077 0.01608865 100.00000000 16088.65 c_{44} : 49.43737064 50.80000000
0.74859737 0.76923077 0.00042574 100.00000000 425.74 c_{12} : 105.65600443
86.90000000 0.93525719 0.76923077 0.02756477 100.00000000 27564.77 c_{13}
: 65.82310124 68.30000000 0.74133462 0.76923077 0.00077819 10.00000000
77.82 M_{freq0} : 2.71899697 2.85858719 0.19816002 0.20833333 0.00010350 0.10000000
0.10 M_{freq1} : 2.71899698 2.85858719 0.19816002 0.20833333 0.00010350 0.10000000
0.10 M_{freq2} : 2.71899698 2.85858719 0.19816002 0.20833333 0.00010350 0.10000000
0.10 M_{freq3} : 2.71899699 2.85858719 0.19816002 0.20833333 0.00010350 0.10000000
0.10 M_{freq4} : 6.19358665 5.66706047 0.22768957 0.20833333 0.00037466 0.10000000
0.37 M_{freq5} : 6.19358665 5.66706047 0.22768957 0.20833333 0.00037466 0.10000000
0.37 H_{freq0} : 3.81166720 4.80643423 0.16521548 0.20833333 0.00185915 0.10000000
1.86 H_{freq1} : 3.81166720 5.58010025 0.14230879 0.20833333 0.00435924 0.10000000
4.36 H_{freq2} : 7.07704092 5.65316738 0.26080663 0.20833333 0.00275345 0.10000000
2.75 H_{freq3} : 7.07704092 6.36651842 0.23158396 0.20833333 0.00054059 0.10000000
0.54 H_{freq4} : 8.68271096 6.40050186 0.28261817 0.20833333 0.00551824 0.10000000
5.52 H_{freq5} : 8.68271096 7.64082373 0.23674124 0.20833333 0.00080701 0.10000000
0.81 $bandw.$ G : 4.07082486 5.87085872 1.15565855 1.66666667 0.26112929
15.00000000 39169.39 $bandw.$ K : 5.01097860 4.97424321 0.91580466 0.90909091
0.00004507 15.00000000 6.76 $bandw.$ M : 5.71167205 7.78109872 1.22340736
1.66666667 0.19647882 15.00000000 29471.82 $bandw.$ L : 4.63682190 6.34433701
1.21809994 1.66666667 0.20121211 15.00000000 30181.82 $bandw.$ H : 3.85585483
9.70902614 0.36103751 0.90909091 0.30036253 5.00000000 15018.13 $DOSerr_h$:

0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000 0.00
DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00

————- E_{prismaticfault} —————

tbe: 103.159 mJ/m² DFT: 250.000 mJ/m² [Benoit 2012] DFT: 233.000
mJ/m² [Ackland 1999]

————- E_{Basalfault} I2 —————

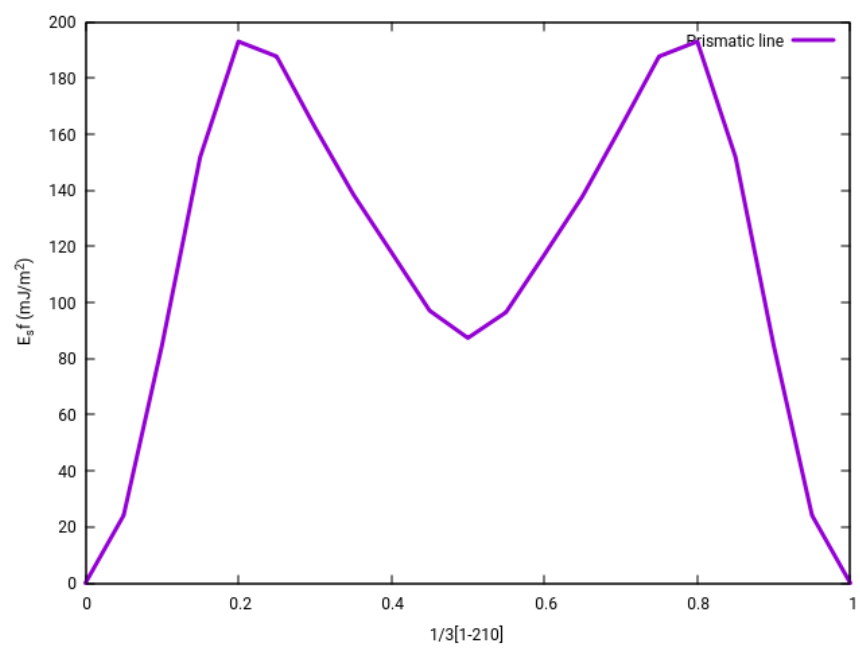
tbe: 217.363 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]

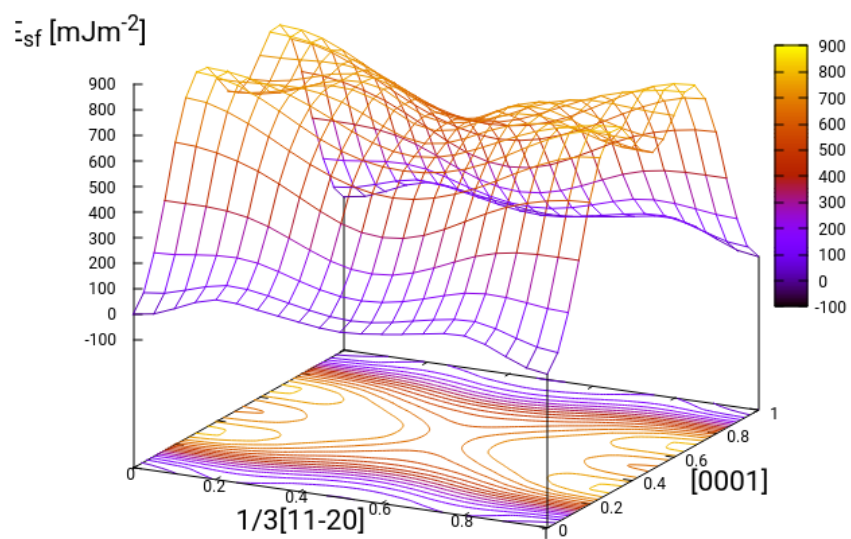
————- E_{vacancyformation} —————

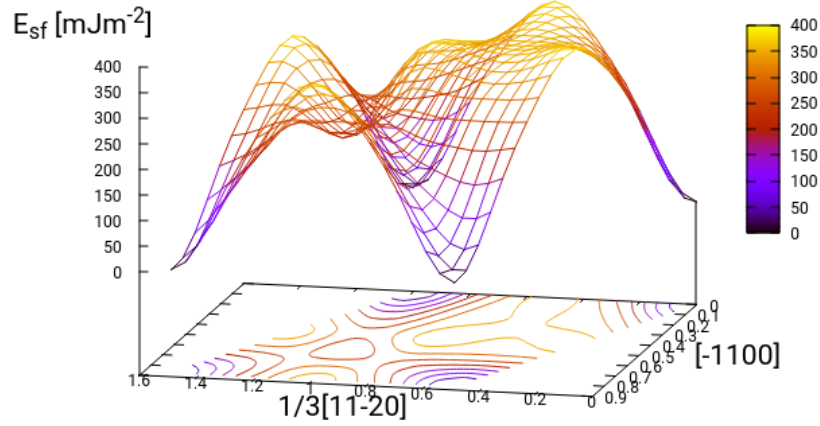
tbe: 2.431 eV | (588 atoms) tbe: 2.429 eV | (896 atoms) DFT: 1.950 eV
| GGA-PAW: Angsten (2013) exp: 1.270 eV | Hashimoto (1984)

————- E_{tet} - E_{oct} —————

- > Note: Preference for tetrahedral oxygen to go into hexahedral site
- » (E_{hexahedral} - E_{octahedral}) tbe: 1.123 eV
- » (E_{tetrahedral} - E_{octahedral}) tbe: 1.552 eV







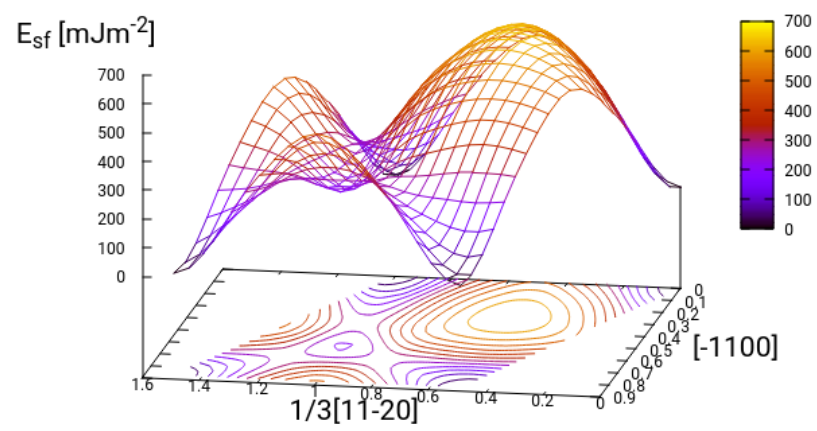
1.17.2 noo pris

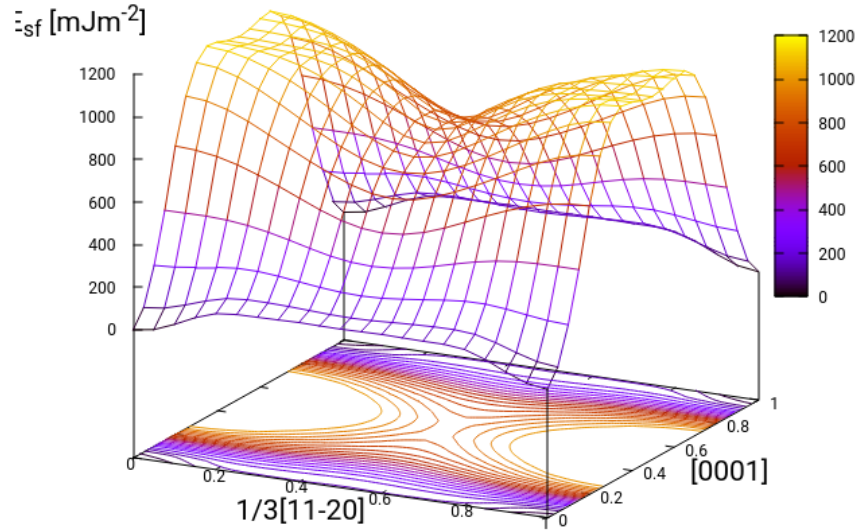
PARAMETERS fdd=0.1948454463 qdds=0.5589640802 qddp=0.5693084671
 qddd=0.7748730693 b0=58.7994745523 p0=1.1531371547 b1=-3.9117460958
 p1=0.6480960332 b2=522504.0614029730 m2=-11.5000000000 p2=0.0000000000
 ndt=2.0000000000 cr1=-6.0000000000 cr2=3.4525563800 cr3=-1.2567506668
 r1dd=6.5000000000 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18
 VARGS -vfdd=0.1948454463 -vqdds=0.5589640802 -vqddp=0.5693084671 -
 vqddd=0.7748730693 -vb0=58.7994745523 -vp0=1.1531371547 -vb1=-3.9117460958
 -vp1=0.6480960332 -vb2=522504.0614029730 -vm2=-11.5000000000 -vp2=0.0000000000
 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.4525563800 -vcr3=-1.2567506668
 -vr1dd=6.5000000000 -vrdd=10.0000000000 -vrmaxhm=10.1000000000
 a_{hcp} : 5.66018285 5.57678969 5.66018285 5.57678969 0.00695442 1000.00000000
 69544.19 c/a : 1.59132985 1.58731122 15.45083010 15.41181168 0.00152244
 100.00000000 1522.44 a_{omega} : 9.04224617 8.73254342 1.13028077 1.09156793
 0.00149868 10.00000000 149.87 c_{omega} : 5.45729411 5.32343103 0.68216176
 0.66542888 0.00027999 10.00000000 28.00 a_{4h} : 5.65808661 5.56325146 1.01704671
 1.00000000 0.00029059 1.00000000 2.91 c_{4h} : 18.31639427 17.75908031 1.03138192
 1.00000000 0.00098482 1.00000000 9.85 a_{6h} : 5.65433822 5.54639384 1.01946208
 1.00000000 0.00037877 1.00000000 3.79 c_{6h} : 27.54417628 26.77136353 1.02886714
 1.00000000 0.00083331 1.00000000 8.33 a_{bcc} : 6.20079768 6.17948863 0.88582824

0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.98535463 7.88677000 1.14076495
 1.12668143 0.00019835 1.00000000 1.98 $DE(o,h)$: 0.27998500 -0.63343333
 0.01866567 -0.04222889 0.00370815 3000.00000000 111244.41 $DE(4h,h)$: 1.53640250
 3.17160000 0.00614561 0.01268640 0.00004278 2000.00000000 855.64 $DE(6h,h)$:
 2.38561333 3.72005000 0.00954245 0.01488020 0.00002849 2000.00000000 569.83
 $DE(b,h)$: 6.70516500 7.63520000 0.06772894 0.07712323 0.00008825 1.00000000
 0.88 $DE(f,h)$: 3.63886500 4.51880000 0.03675621 0.04564444 0.00007900
 2000.00000000 1580.01 c_{11} : 178.55891012 176.10000000 0.77997165 0.76923077
 0.00011537 200.00000000 230.73 c_{33} : 216.05201952 190.50000000 0.87240872
 0.76923077 0.01064569 200.00000000 21291.38 c_{44} : 50.21922256 50.80000000
 0.76043644 0.76923077 0.00007734 200.00000000 154.68 c_{12} : 108.89042033
 86.90000000 0.96388794 0.76923077 0.03789141 200.00000000 75782.83 c_{13}
 : 63.50930696 68.30000000 0.71527545 0.76923077 0.00291118 200.00000000
 5822.35 M_{freq0} : 2.76609238 2.85858719 0.20159233 0.20833333 0.00004544
 0.10000000 0.05 M_{freq1} : 2.76609239 2.85858719 0.20159233 0.20833333 0.00004544
 0.10000000 0.05 M_{freq2} : 2.76609239 2.85858719 0.20159233 0.20833333 0.00004544
 0.10000000 0.05 M_{freq3} : 2.76609240 2.85858719 0.20159233 0.20833333 0.00004544
 0.10000000 0.05 M_{freq4} : 6.25152012 5.66706047 0.22981933 0.20833333 0.00046165
 0.10000000 0.46 M_{freq5} : 6.25152012 5.66706047 0.22981933 0.20833333 0.00046165
 0.10000000 0.46 H_{freq0} : 4.03482958 4.80643423 0.17488838 0.20833333 0.00111856
 0.10000000 1.12 H_{freq1} : 4.03482958 5.58010025 0.15064057 0.20833333 0.00332845
 0.10000000 3.33 H_{freq2} : 7.10258591 5.65316738 0.26174803 0.20833333 0.00285313
 0.10000000 2.85 H_{freq3} : 7.10258591 6.36651842 0.23241987 0.20833333 0.00058016
 0.10000000 0.58 H_{freq4} : 8.63246455 6.40050186 0.28098267 0.20833333 0.00527793
 0.10000000 5.28 H_{freq5} : 8.63246455 7.64082373 0.23537123 0.20833333 0.00073105
 0.10000000 0.73 $bandw.$ G : 3.69530759 5.87085872 0.89918888 1.42857143
 0.28024589 15.00000000 42036.88 $bandw.$ K : 4.54566372 4.97424321 0.76153355
 0.83333333 0.00515521 15.00000000 773.28 $bandw.$ M : 5.18104982 7.78109872
 0.95121525 1.42857143 0.22786892 15.00000000 34180.34 $bandw.$ L : 4.21368469
 6.34433701 0.94880672 1.42857143 0.23017418 15.00000000 34526.13 $bandw.$
 H : 3.49802497 9.70902614 0.32753261 0.90909091 0.33821005 1.00000000 3382.10
 $DOSerr_h$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 $DOSerr_o$: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00 E_{prisf} : 144.13939923 220.00000000 144.13939923 220.00000000
 5754.83074961 0.00500000 287741.54

———— $E_{Basalfault}$ $I2$ ————

tbe: 193.082 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]





1.17.3 noo

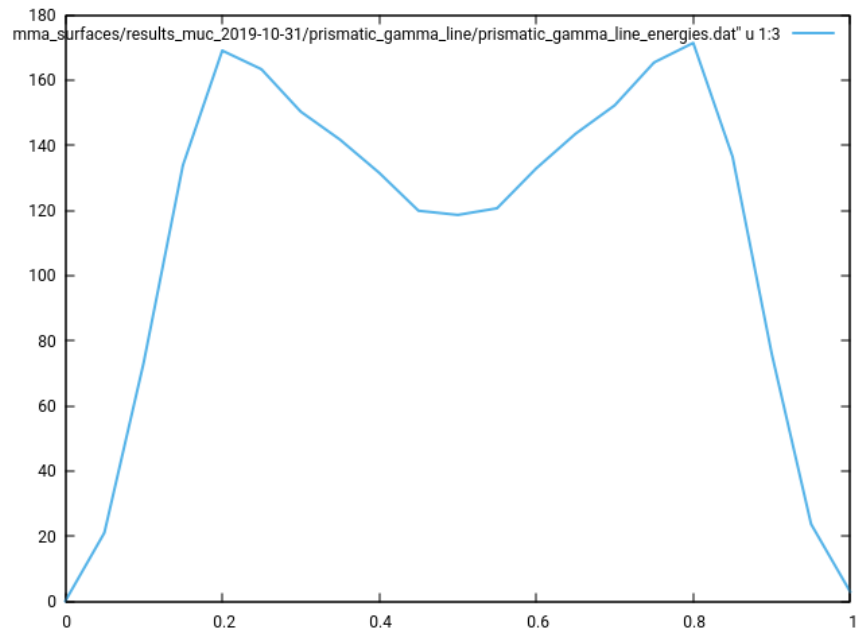
PARAMETERS fdd=0.1962030050 qdds=0.5603385291 qddp=0.5641791446
 qddd=0.7778812828 b0=67.9784821273 p0=1.2469553135 b1=-3.6289856489
 p1=0.7094094608 b2=626000.0 m2=-11.5000000000 p2=0.0000000000 ndt=2.0000000000
 cr1=-6.0000000000 cr2=3.0990417700 cr3=-1.2615960922 r1dd=6.5000000000
 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18 VARGS -vfdd=0.1962030050
 -vqdds=0.5603385291 -vqddp=0.5641791446 -vqddd=0.7778812828 -vb0=67.9784821273
 -vp0=1.2469553135 -vb1=-3.6289856489 -vp1=0.7094094608 -vb2=626000.0
 -vm2=-11.5000000000 -vp2=0.0000000000 -vndt=2.0000000000 -vcr1=-6.0000000000
 -vcr2=3.0990417700 -vcr3=-1.2615960922 -vr1dd=6.5000000000 -vrcdd=10.0000000000
 -vrmaxhm=10.1000000000
 a_{hcp} : 5.60402011 5.57678969 5.60402011 5.57678969 0.00074150 1000.00000000
 7414.96 c/a : 1.57574189 1.58731122 15.29948069 15.41181168 0.01261825
 100.00000000 12618.25 a_{ω} : 8.96039623 8.73254342 1.12004953 1.09156793
 0.00081120 10.00000000 81.12 c_{ω} : 5.40699833 5.32343103 0.67587479
 0.66542888 0.00010912 10.00000000 10.91 a_{4h} : 5.59371954 5.56325146 1.00547667

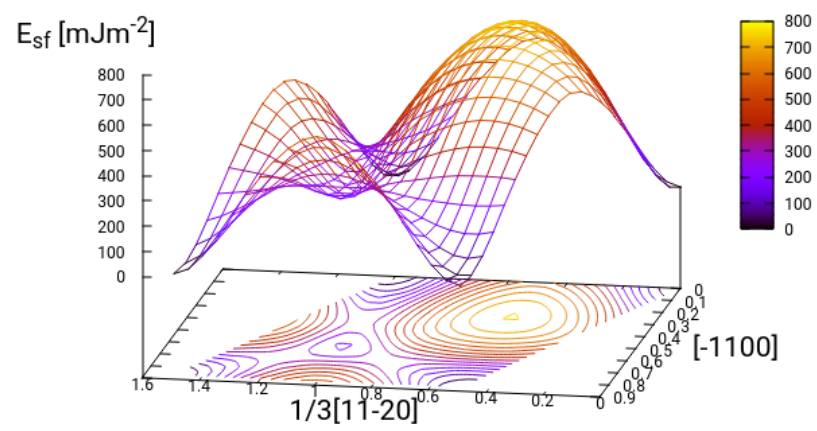
1.00000000 0.00002999 1.00000000 0.30 c_{4h} : 18.16124146 17.75908031 1.02264538
 1.00000000 0.00051281 1.00000000 5.13 a_{6h} : 5.59170678 5.54639384 1.00816980
 1.00000000 0.00006675 1.00000000 0.67 c_{6h} : 27.27831362 26.77136353 1.01893628
 1.00000000 0.00035858 1.00000000 3.59 a_{bcc} : 6.20079768 6.17948863 0.88582824
 0.88278409 0.00000927 1.00000000 0.09 a_{fcc} : 7.89832289 7.88677000 1.12833184
 1.12668143 0.00000272 1.00000000 0.03 DE(o,h) : 1.25366500 -0.63343333
 0.08357767 -0.04222889 0.01582729 3000.00000000 474818.68 DE(4h,h): 1.46735750
 3.17160000 0.00586943 0.01268640 0.00004647 2000.00000000 929.42 DE(6h,h):
 2.31450833 3.72005000 0.00925803 0.01488020 0.00003161 2000.00000000 632.18
 DE(b,h) : 5.80790500 7.63520000 0.05866571 0.07712323 0.00034068 1.00000000
 3.41 DE(f,h) : 3.53398500 4.51880000 0.03569682 0.04564444 0.00009896
 2000.00000000 1979.11 c_{11} : 182.18207480 176.10000000 0.79579817 0.76923077
 0.00070583 100.00000000 705.83 c_{33} : 202.88615634 190.50000000 0.81924553
 0.76923077 0.00250148 100.00000000 2501.48 c_{44} : 49.68618188 50.80000000
 0.75236496 0.76923077 0.00028446 100.00000000 284.46 c_{12} : 98.12235223
 86.90000000 0.86856999 0.76923077 0.00986828 100.00000000 9868.28 c_{13}
 : 65.28413049 68.30000000 0.73526445 0.76923077 0.00115371 10.00000000
 115.37 M_{freq0} : 2.70822081 2.85858719 0.19737466 0.20833333 0.00012009
 0.10000000 0.12 M_{freq1} : 2.70822082 2.85858719 0.19737466 0.20833333 0.00012009
 0.10000000 0.12 M_{freq2} : 2.70822082 2.85858719 0.19737466 0.20833333 0.00012009
 0.10000000 0.12 M_{freq3} : 2.70822083 2.85858719 0.19737466 0.20833333 0.00012009
 0.10000000 0.12 M_{freq4} : 5.97747622 5.66706047 0.21974488 0.20833333 0.00013022
 0.10000000 0.13 M_{freq5} : 5.97747622 5.66706047 0.21974488 0.20833333 0.00013022
 0.10000000 0.13 H_{freq0} : 4.02620227 4.80643423 0.17451443 0.20833333 0.00114372
 0.10000000 1.14 H_{freq1} : 4.02620227 5.58010025 0.15031847 0.20833333 0.00336572
 0.10000000 3.37 H_{freq2} : 6.57039365 5.65316738 0.24213541 0.20833333 0.00114258
 0.10000000 1.14 H_{freq3} : 6.57039365 6.36651842 0.21500480 0.20833333 0.00004451
 0.10000000 0.04 H_{freq4} : 8.07961869 6.40050186 0.26298780 0.20833333 0.00298711
 0.10000000 2.99 H_{freq5} : 8.07961869 7.64082373 0.22029744 0.20833333 0.00014314
 0.10000000 0.14 bandw. G: 3.71843728 5.87085872 1.05561993 1.66666667
 0.37337811 15.00000000 56006.72 bandw. K: 4.63137962 4.97424321 0.84642928
 0.90909091 0.00392648 15.00000000 588.97 bandw. M: 5.20417951 7.78109872
 1.11470537 1.66666667 0.30466128 15.00000000 45699.19 bandw. L: 4.24497780
 6.34433701 1.11516191 1.66666667 0.30415749 15.00000000 45623.62 bandw.
 H: 3.54292378 9.70902614 0.33173665 0.90909091 0.33333794 5.00000000 16666.90
 DOSerr_h: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 1.00000000
 0.00 DOSerr_o: 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
 0.00000000 0.00

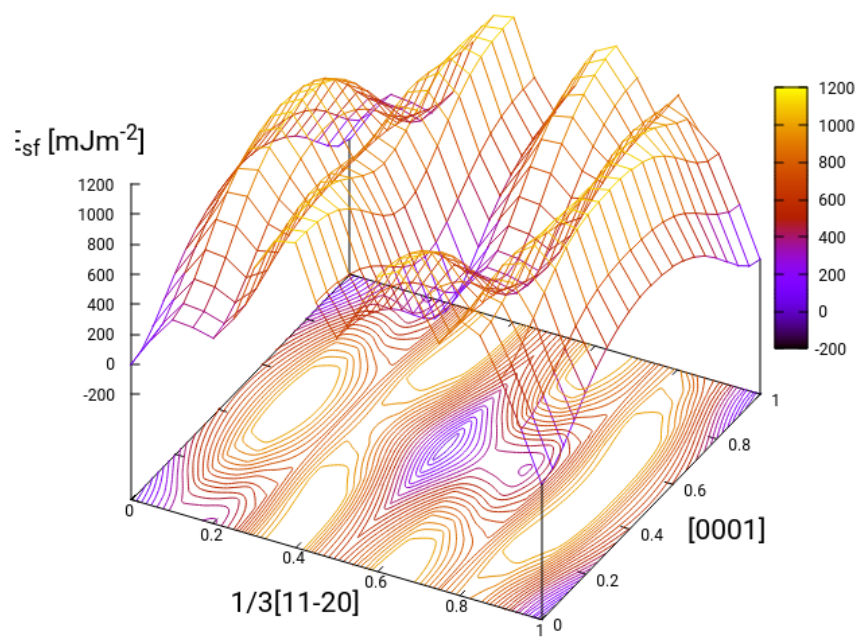
————— E_{Basalfault} I2 —————

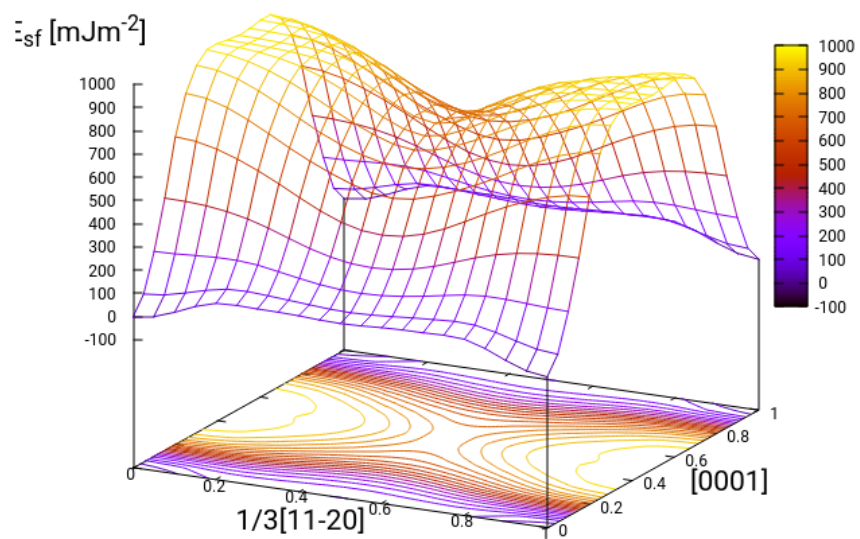
tbe: 193.074 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]

———- $E_{\text{prismaticfault}}$ ———-
 tbe: 125.532 mJ/m² DFT: 250.000 mJ/m² [Benoit 2012] DFT: 233.000
 mJ/m² [Ackland 1999]
 ———- $E_{\text{vacancyformation}}$ ———-
 tbe: 2.317 eV | DFT: 1.950 eV | GGA-PAW: Angsten (2013) exp: 1.270
 eV | Hashimoto (1984)

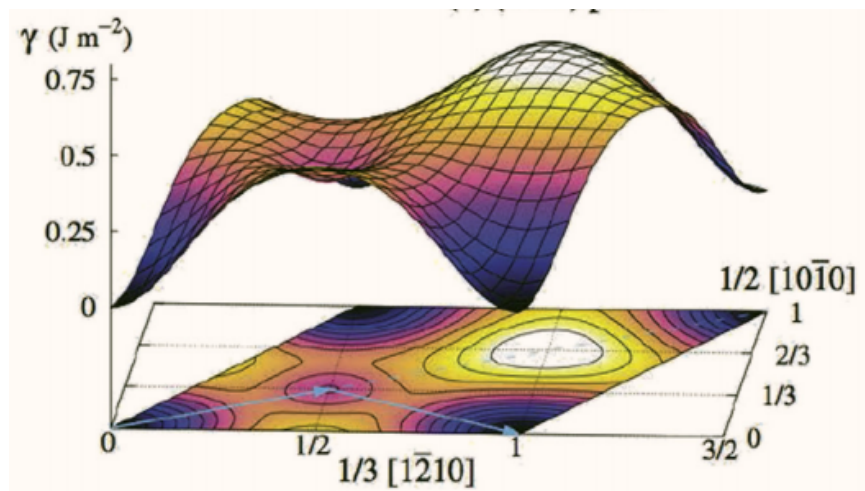


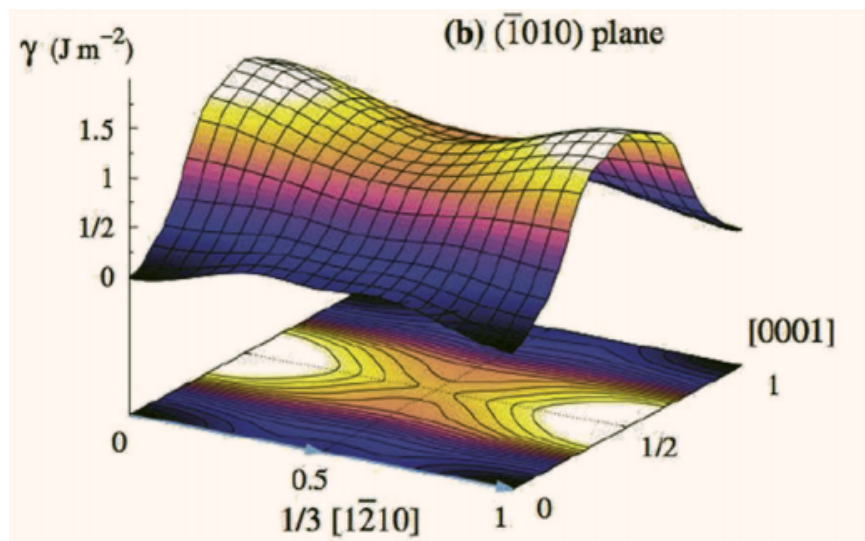


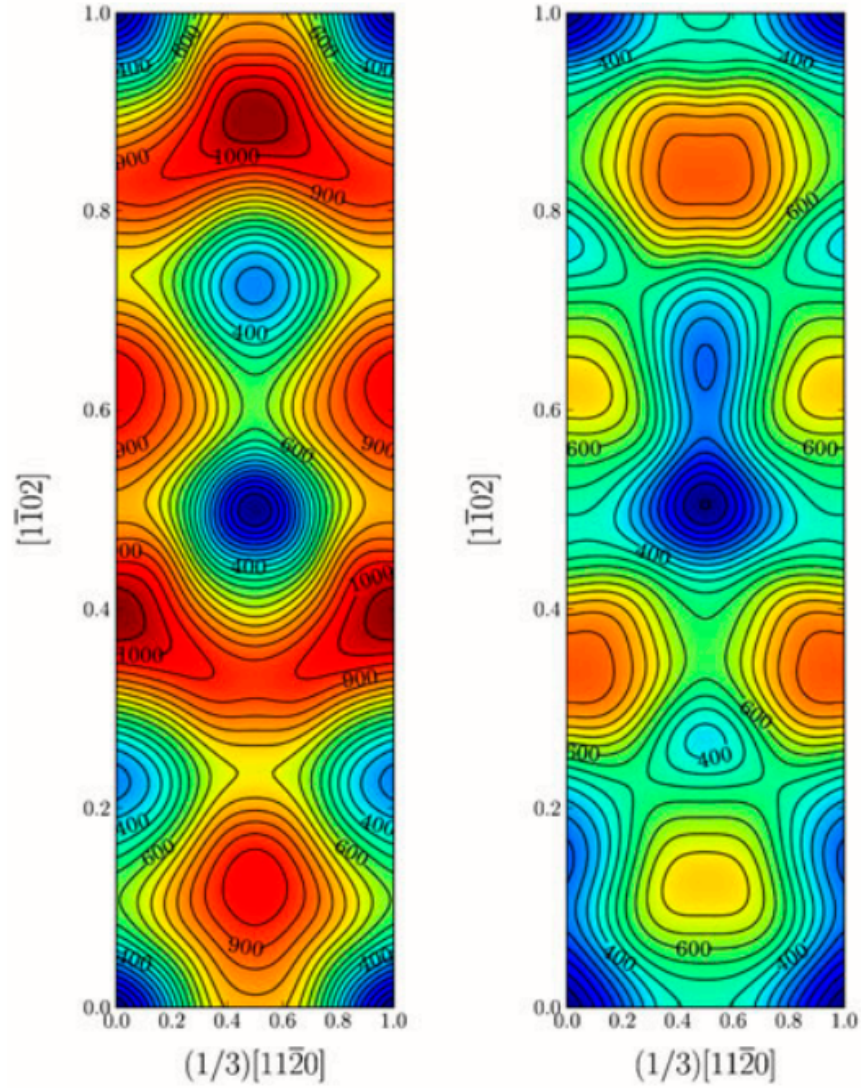




Figures from DFT for comparison







1.17.4 noo alat

1. Objective Function

PARAMETERS fdd=0.1958363809 qdds=0.5591275855 qddp=0.5690351902
qddd=0.7745947522 b0=58.0906936439 p0=1.2185323579 b1=-3.2299188646
p1=0.6862915307 b2=593519.1134129359 m2=-11.5000000000 p2=0.0000000000
ndt=2.0000000000 cr1=-6.0000000000 cr2=3.0474400934 cr3=-1.2317472193
r1dd=6.5000000000 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18

VARGS -vfdd=0.1958363809 -vqdds=0.5591275855 -vqddp=0.5690351902
 -vqddd=0.7745947522 -vb0=58.0906936439 -vp0=1.2185323579 -vb1=-
 3.2299188646 -vp1=0.6862915307 -vb2=593519.1134129359 -vm2=-11.5000000000
 -vp2=0.0000000000 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.0474400934
 -vcr3=-1.2317472193 -vr1dd=6.5000000000 -vrdd=10.0000000000 -vrmaxhm=10.1000000000

 a_{hcp} : 5.58523112 5.57678969 5.58523112 5.57678969 0.00007126 1000.00000000
 712.58 c/a : 1.58371266 1.58731122 15.37687193 15.41181168 0.00122079
 100.00000000 1220.79 a_{omega} : 8.93475285 8.73254342 1.11684411 1.09156793
 0.00063889 10.00000000 63.89 c_{omega} : 5.38726911 5.32343103 0.67340864
 0.66542888 0.00006368 10.00000000 6.37 a_{4h} : 5.57584691 5.56325146
 1.00226404 1.00000000 0.00000513 1.00000000 0.05 c_{4h} : 18.09810672
 17.75908031 1.01909031 1.00000000 0.00036444 1.00000000 3.64 a_{6h} :
 5.57365569 5.54639384 1.00491524 1.00000000 0.00002416 1.00000000
 0.24 c_{6h} : 27.18378460 26.77136353 1.01540531 1.00000000 0.00023732
 1.00000000 2.37 a_{bcc} : 6.20079768 6.17948863 0.88582824 0.88278409
 0.00000927 1.00000000 0.09 a_{fcc} : 7.87290654 7.88677000 1.12470093
 1.12668143 0.00000392 1.00000000 0.04 DE(o,h) : 0.58764167 -0.63343333
 0.03917611 -0.04222889 0.00662677 3000.00000000 198803.22 DE(4h,h):
 1.58019500 3.17160000 0.00632078 0.01268640 0.00004052 2000.00000000
 810.42 DE(6h,h): 2.48264833 3.72005000 0.00993059 0.01488020 0.00002450
 2000.00000000 489.97 DE(b,h) : 5.35128500 7.63520000 0.05405338
 0.07712323 0.00053222 1.00000000 5.32 DE(f,h) : 3.78088500 4.51880000
 0.03819076 0.04564444 0.00005556 10000.00000000 5555.74 c₁₁ : 171.60928873
 176.10000000 0.74961468 0.76923077 0.00038479 200.00000000 769.58
 c₃₃ : 198.90063708 190.50000000 0.80315218 0.76923077 0.00115066
 200.00000000 2301.32 c₄₄ : 47.42549704 50.80000000 0.71813290 0.76923077
 0.00261099 200.00000000 5221.98 c₁₂ : 94.65941969 86.90000000 0.83791644
 0.76923077 0.00471772 200.00000000 9435.44 c₁₃ : 61.22624060 68.30000000
 0.68956234 0.76923077 0.00634706 200.00000000 12694.12 M_{freq0}: 2.59341377
 2.85858719 0.18900754 0.20833333 0.00037349 0.10000000 0.37 M_{freq1}:
 2.59341378 2.85858719 0.18900754 0.20833333 0.00037349 0.10000000
 0.37 M_{freq2}: 2.59341378 2.85858719 0.18900754 0.20833333 0.00037349
 0.10000000 0.37 M_{freq3}: 2.59341379 2.85858719 0.18900754 0.20833333
 0.00037349 0.10000000 0.37 M_{freq4}: 5.85272461 5.66706047 0.21515875
 0.20833333 0.00004659 0.10000000 0.05 M_{freq5}: 5.85272461 5.66706047
 0.21515875 0.20833333 0.00004659 0.10000000 0.05 H_{freq0}: 3.82320403
 4.80643423 0.16571554 0.20833333 0.00181628 0.10000000 1.82 H_{freq1}:
 3.82320403 5.58010025 0.14273952 0.20833333 0.00430255 0.10000000
 4.30 H_{freq2}: 6.40288977 5.65316738 0.23596248 0.20833333 0.00076337

0.10000000 0.76 $H_{\text{freq}3}$: 6.40288977 6.36651842 0.20952352 0.20833333
0.00000142 0.10000000 0.00 $H_{\text{freq}4}$: 7.92857431 6.40050186 0.25807137
0.20833333 0.00247387 0.10000000 2.47 $H_{\text{freq}5}$: 7.92857431 7.64082373
0.21617909 0.20833333 0.00006156 0.10000000 0.06 bandw. G: 3.69394702
5.87085872 0.89885780 1.42857143 0.28059652 15.00000000 42089.48
bandw. K: 4.65178817 4.97424321 0.77931255 0.83333333 0.00291825
15.00000000 437.74 bandw. M: 5.19329495 7.78109872 0.95346339 1.42857143
0.22572765 15.00000000 33859.15 bandw. L: 4.21232412 6.34433701
0.94850035 1.42857143 0.23046824 15.00000000 34570.24 bandw. H:
3.54700549 9.70902614 0.33211883 0.90909091 0.33289678 1.00000000
3328.97 DOSerr_h : 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
1.00000000 0.00 DOSerr_o : 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 0.00 E_{prist} : 98.95340236 220.00000000 98.95340236
220.00000000 14652.27879997 0.00500000 732613.94

———— $E_{\text{Basalfault}}$ I2 —————

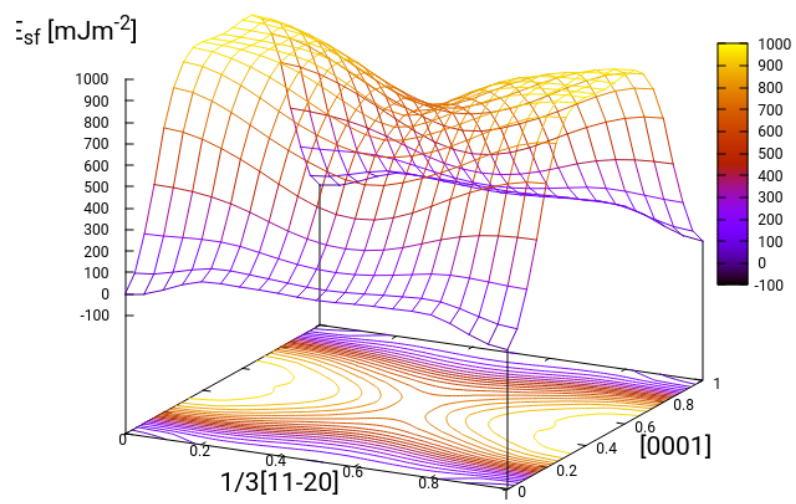
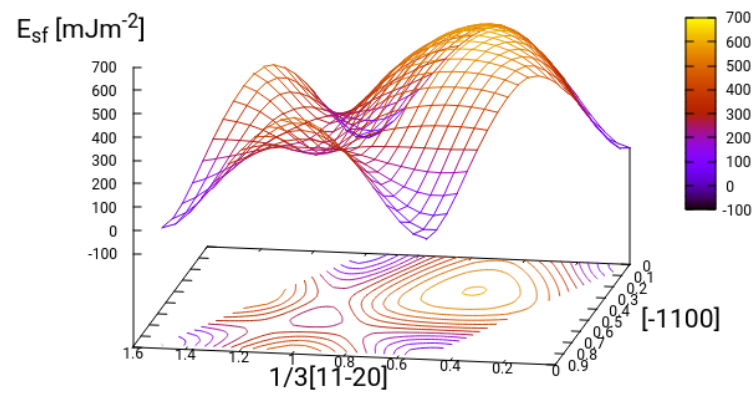
tbe: 211.658 mJ/m² DFT: 260.000 mJ/m² [Benoit 2012]

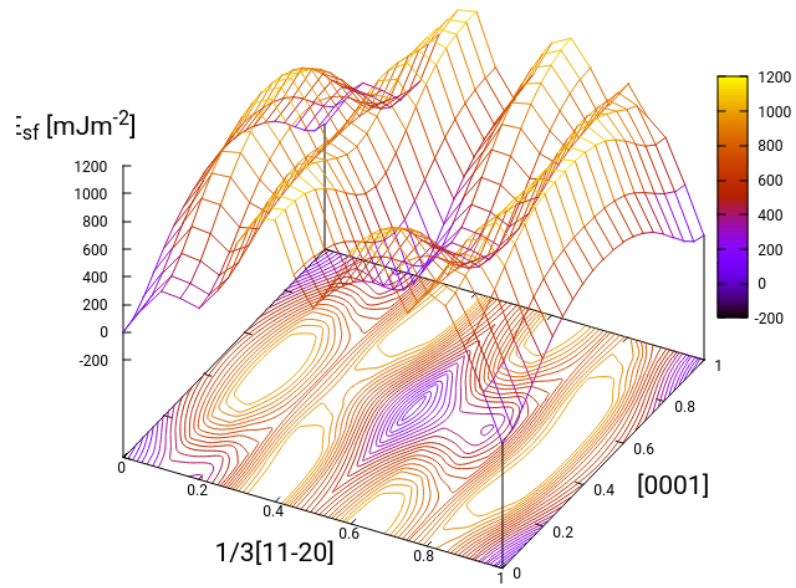
2. Defect Clusters

———— $E_{\text{vacancyformation}}$ —————

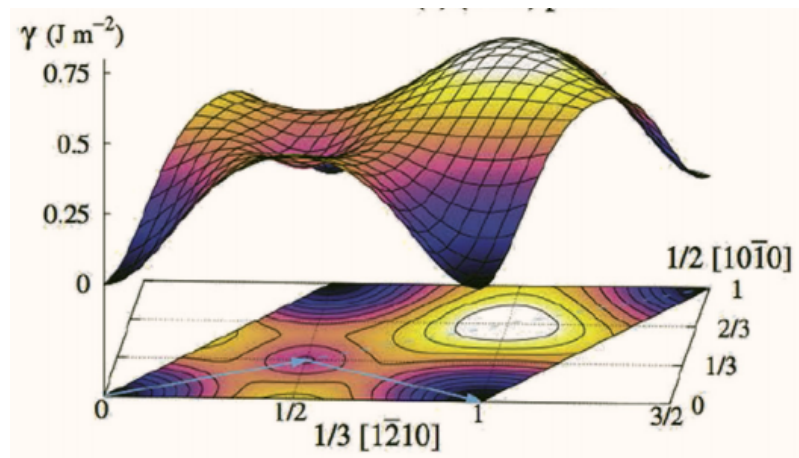
tbe: 2.347 eV | DFT: 1.950 eV | GGA-PAW: Angsten (2013) exp: 1.270
eV | Hashimoto (1984)

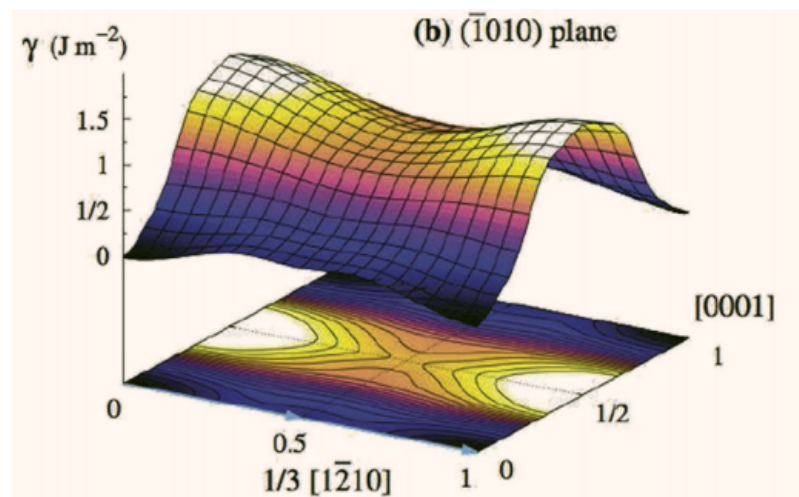
3. Gamma surfaces

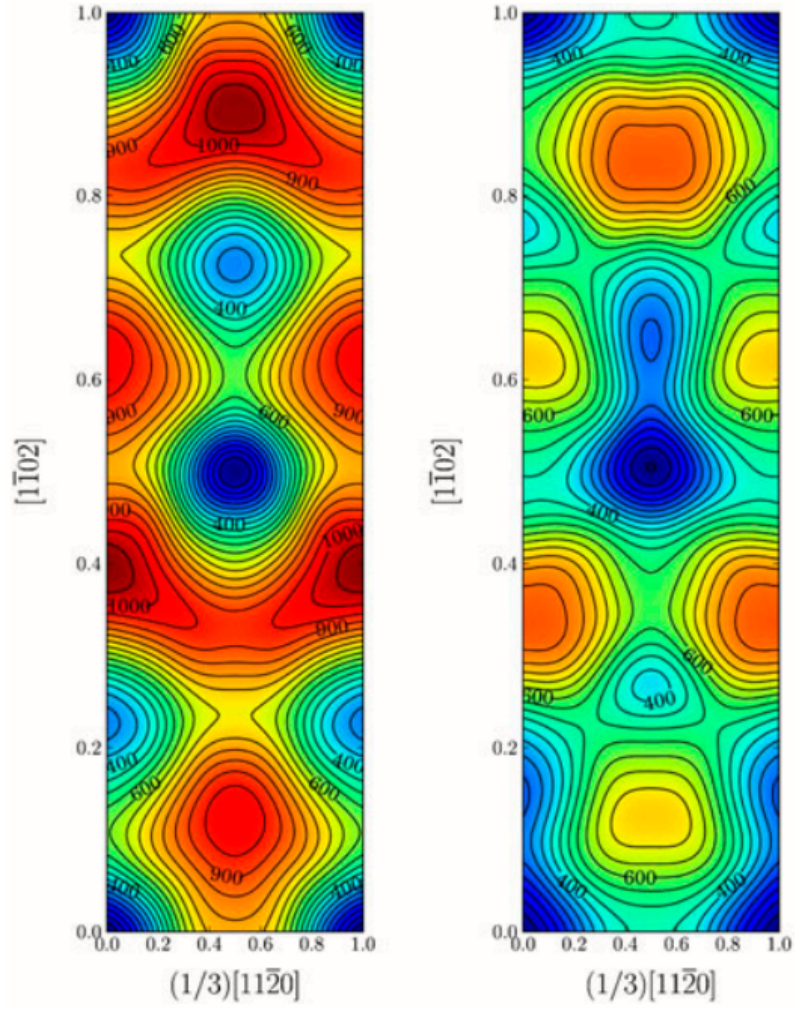




Figures from DFT for comparison

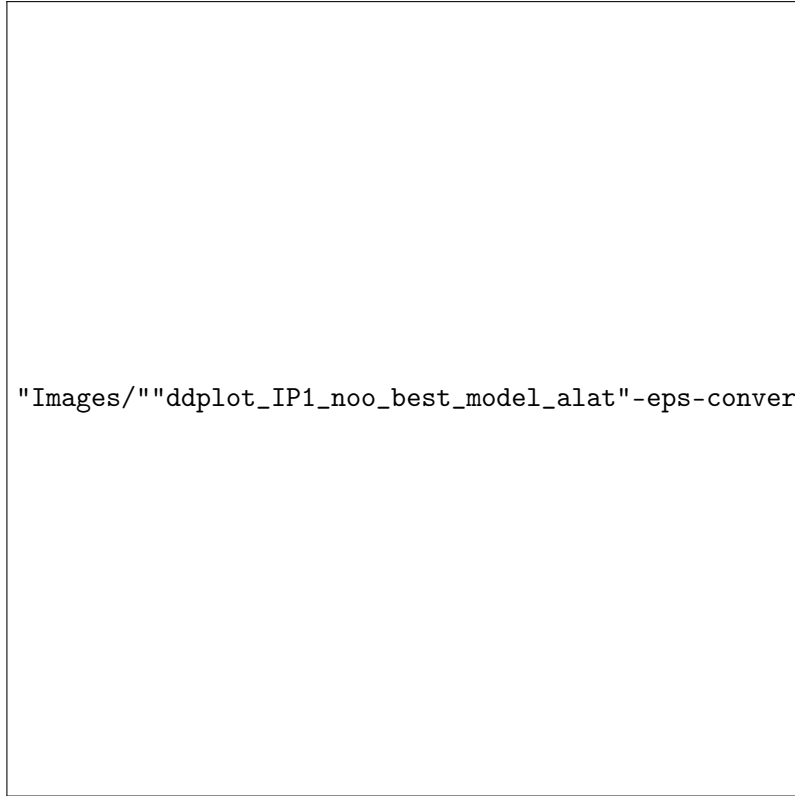




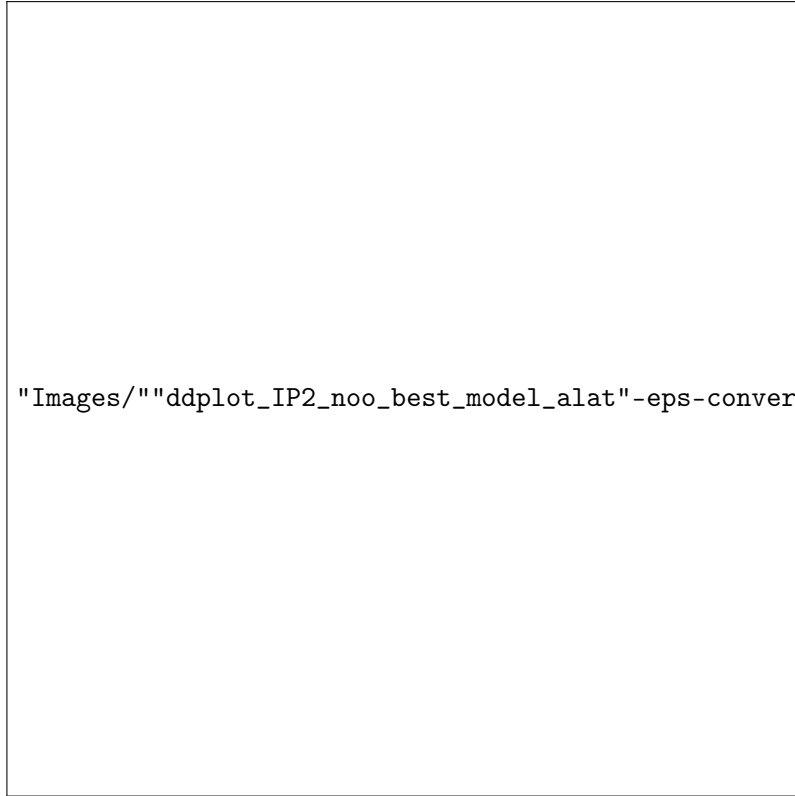


(a) Data $\text{basal}_{\text{gsdata}}$ $\text{prismatic}_{\text{gsdata}}$ $\text{pyramidal}_{\text{gsdata}}$


4. Dislocation core structures



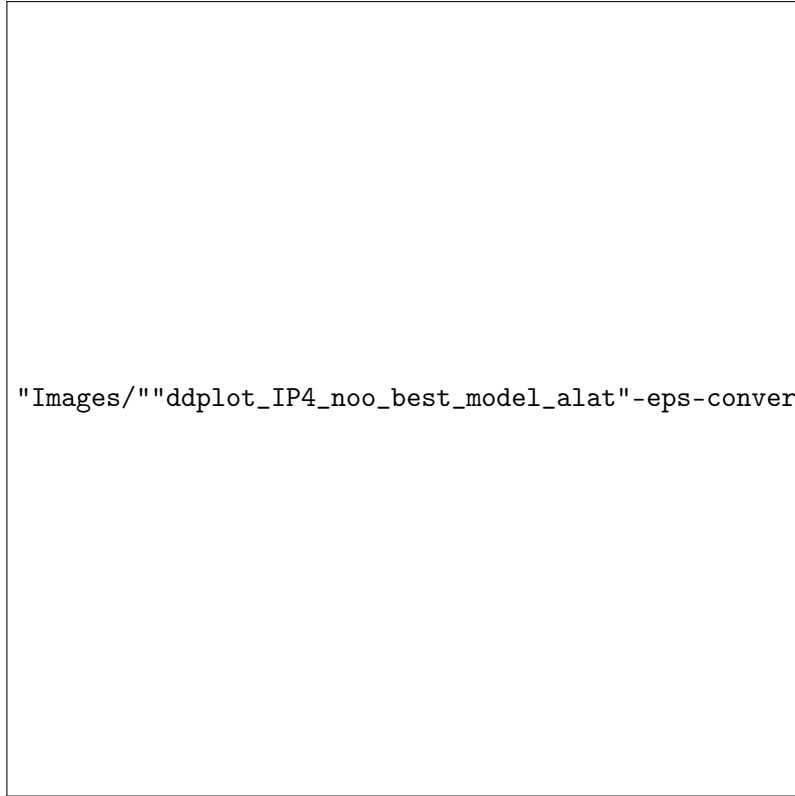
"Images/" "ddplot_IP1_noo_best_model_alat"-eps-converted-to.pdf



"Images/" "ddplot_IP2_noo_best_model_alat"-eps-converted-to.pdf



"Images/" "ddplot_IP3_noo_best_model_alat"-eps-converted-to.pdf



"Images/" "ddplot_IP4_noo_best_model_alat"-eps-converted-to.pdf

"Images/" "ddplot_IP5_noo_best_model_alat"-eps-converted-to.pdf

(a) Data IP1 IP2 IP3 IP4 IP5

5. Directory of the results `file:///home/tigany/Documents/ti/2019-09-11_final_model/tbe/dislocations/2019-11-08_no_omega_ordering_ec_latpar/` `file:///home/tigany/Documents/ti/final_model_2019-11`

6. BOP

(a) 4 recursion levels

$k_B T = 0.1$

» Lattice parameters: $> hcp$ $a = 2.901660$ A $c = 4.747485$ A $etot = -18.342162$ eV

$> omega$ $a = 7.917318$ A $c = 2.749892$ A $etot = -17.458700$ eV

» Elastic Constants in $eV/(A^3)$ in 10^{11} Pa

calc. exp. calc. exp.



C11 1.112 1.099 1.781 1.761 C12 0.461 0.542 0.738 0.868 C13
0.381 0.426 0.611 0.682 C33 1.229 1.189 1.969 1.905 C44 0.178
0.317 0.285 0.508 C66 0.326 0.281 0.522 0.450 K 0.655 0.687 1.050
1.101 R 0.417 0.386 0.669 0.618 H 0.349 0.305 0.558 0.489

(b) 5 recursion levels

kbT = 0.1

Incredibly slow. Probably better to not do.

1.18 Higher Quality DFT energies

Energies were calculated at 26x26x26 grid of k points.

It was a double kappa basis set.

{'Structure': 'hcp', 'a': 5.573445955631, 'c': 8.814165906273, 'Energy (Ry/atom)': -1707.61941055} {'Structure': 'omega', 'a': 8.7038058379, 'c': 5.35245317114, 'Energy (Ry/atom)': -1707.6197605999998} {'Structure': 'bcc', 'a': 6.177301070027708, 'c': 6.177301070027708, 'Energy (Ry/atom)': -1707.6111003} {'Structure': 'fcc', 'a': 7.799738260742188, 'c': 7.799738260742188, 'Energy (Ry/atom)': -1707.6148392}

E(omega - hcp) = -0.350 mRyd per atom E(fcc - hcp) = 4.571 mRyd per atom E(bcc - hcp) = 8.310 mRyd per atom

1.19 Trends I've noticed during the fitting

It seems that there are two things of importance when it comes to accurately obtaining the stacking fault energies of hcp (specifically the basal I_2 and prismatic faults).

From the ANNI model, one finds that the difference in energy between the fcc and hcp titanium polymorphs gives the largest contribution to the basal stacking fault energy.

It seems that when the energy difference between fcc and hcp is around 4 mRyd, (roughly the same as lmt0 calculations with pure titanium), that the basal stacking fault energy of the canonical tight binding model agrees really quite well with the *ab initio* calculations (~260 mRyd for the compared to ~280 mRyd for DFT).

But, when one actually fits for to this, the prismatic stacking fault energy is low (~50 mRyd compared to 230 mRyd). This means that the stacking fault energy for the prismatic splitting is low, and it seems that it gives rise to a very wide spreading of the core, which seemingly doesn't dissociate. The displacement is allowed to spread along the prismatic plane, but the 1/3[1-210] screw dislocation does not dissociate into it's equal, collinear partials

(this may be something to do with how the differential displacement/burger's circuits are calculated in ddplot/ovito, so I will double check this.

One only has to look at the gamma surfaces to see this.

When one tries to rectify this problem, essentially by lowering the tolerance for the basal stacking fault energy, one finds some trends with the lowering of $E(\text{fcc} - \text{hcp})$:

- The basal stacking fault energy decreases, as expected by the ANNNI model.
- The prismatic stacking fault energy can increase, while keeping similar elastic constants
 - C44 gets lower while C12 gets larger
- $E(\text{omega} - \text{hcp})$ can become *positive*, and is more likely to be.
- One can find models with reasonable stacking faults but they are much lower than that of DFT.

1.20 Narrowed Data for Sasha

1. Objective Function

```
PARAMETERS fdd=0.1958363809 qdds=0.5591275855 qddp=0.5690351902
qddd=0.7745947522 b0=58.0906936439 p0=1.2185323579 b1=-3.2299188646
p1=0.6862915307 b2=593519.1134129359 m2=-11.5000000000 p2=0.0000000000
ndt=2.0000000000 cr1=-6.0000000000 cr2=3.0474400934 cr3=-1.2317472193
r1dd=6.5000000000 rcdd=10.0000000000 rmaxhm=10.1000000000 npar=18
VARGS -vfdd=0.1958363809 -vqdds=0.5591275855 -vqddp=0.5690351902
-vqddd=0.7745947522 -vb0=58.0906936439 -vp0=1.2185323579 -vb1=-
3.2299188646 -vp1=0.6862915307 -vb2=593519.1134129359 -vm2=-11.5000000000
-vp2=0.0000000000 -vndt=2.0000000000 -vcr1=-6.0000000000 -vcr2=3.0474400934
-vcr3=-1.2317472193 -vr1dd=6.5000000000 -vrdd=10.0000000000 -vrmaxhm=10.1000000000
```

Quantity	From Model	Target
a _{hcp}	5.58523112	5.57678969
c/a	1.58371266	1.58731122
a _{omega}	8.93475285	8.73254342
c _{omega}	5.38726911	5.32343103
a _{4h}	5.57584691	5.56325146
c _{4h}	18.09810672	17.75908031
a _{6h}	5.57365569	5.54639384
c _{6h}	27.18378460	26.77136353
a _{bcc}	6.20079768	6.17948863
a _{fcc}	7.87290654	7.88677000
DE(o,h)	0.58764167	-0.63343333
DE(4h,h)	1.58019500	3.17160000
DE(6h,h)	2.48264833	3.72005000
DE(b,h)	5.35128500	7.63520000
DE(f,h)	3.78088500	4.51880000
c ₁₁	171.60928873	176.10000000
c ₃₃	198.90063708	190.50000000
c ₄₄	47.42549704	50.80000000
c ₁₂	94.65941969	86.90000000
c ₁₃	61.22624060	68.30000000
M _{freq0}	2.59341377	2.85858719
M _{freq1}	2.59341378	2.85858719
M _{freq2}	2.59341378	2.85858719
M _{freq3}	2.59341379	2.85858719
M _{freq4}	5.85272461	5.66706047
M _{freq5}	5.85272461	5.66706047
H _{freq0}	3.82320403	4.80643423
H _{freq1}	3.82320403	5.58010025
H _{freq2}	6.40288977	5.65316738
H _{freq3}	6.40288977	6.36651842
H _{freq4}	7.92857431	6.40050186
H _{freq5}	7.92857431	7.64082373
bandw. G	3.69394702	5.87085872
bandw. K	4.65178817	4.97424321
bandw. M	5.19329495	7.78109872
bandw. L	4.21232412	6.34433701
bandw. H	3.54700549	9.70902614
DOSerr _h	0.00000000	0.00000000
DOSerr _o	0.00000000	0.00000000
E _{prisf}	98.95340236	220.00000000

————— $E_{\text{prismaticfault}}$ —————

tbe:	98.953	mJ/m ²	
DFT:	250.000	mJ/m ²	[Benoit 2012]
DFT:	233.000	mJ/m ²	[Ackland 1999]

————— $E_{\text{Basalfault I2}}$ —————

tbe:	211.658	mJ/m ²	
DFT:	260.000	mJ/m ²	[Benoit 2012]

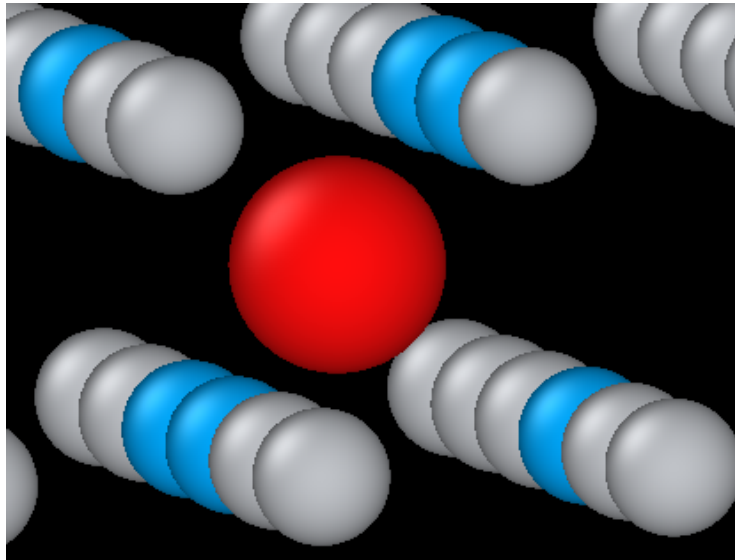
2. Defect Clusters

————— $E_{\text{vacancyformation}}$ —————

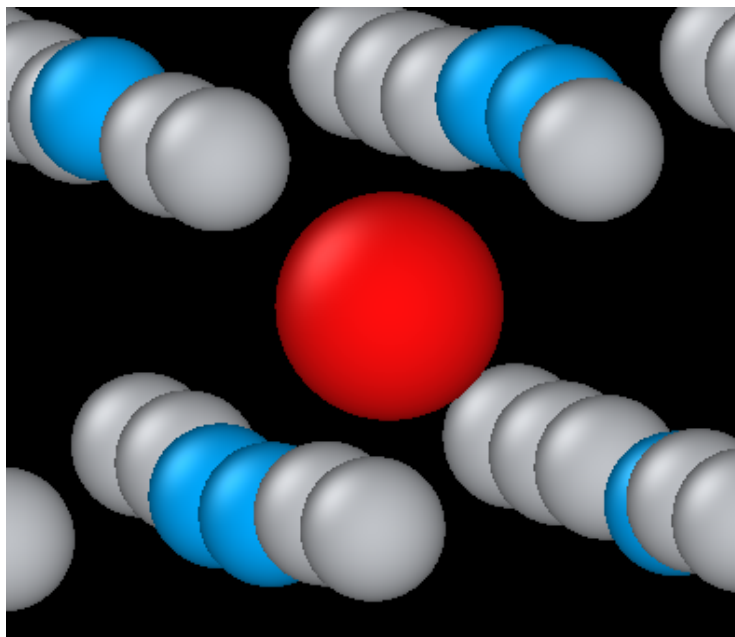
tbe:	2.347 eV	
DFT:	1.950 eV	GGA-PAW: Angsten (2013)
exp:	1.270 eV	Hashimoto (1984)

(a) Octahedral O interstitial relaxation

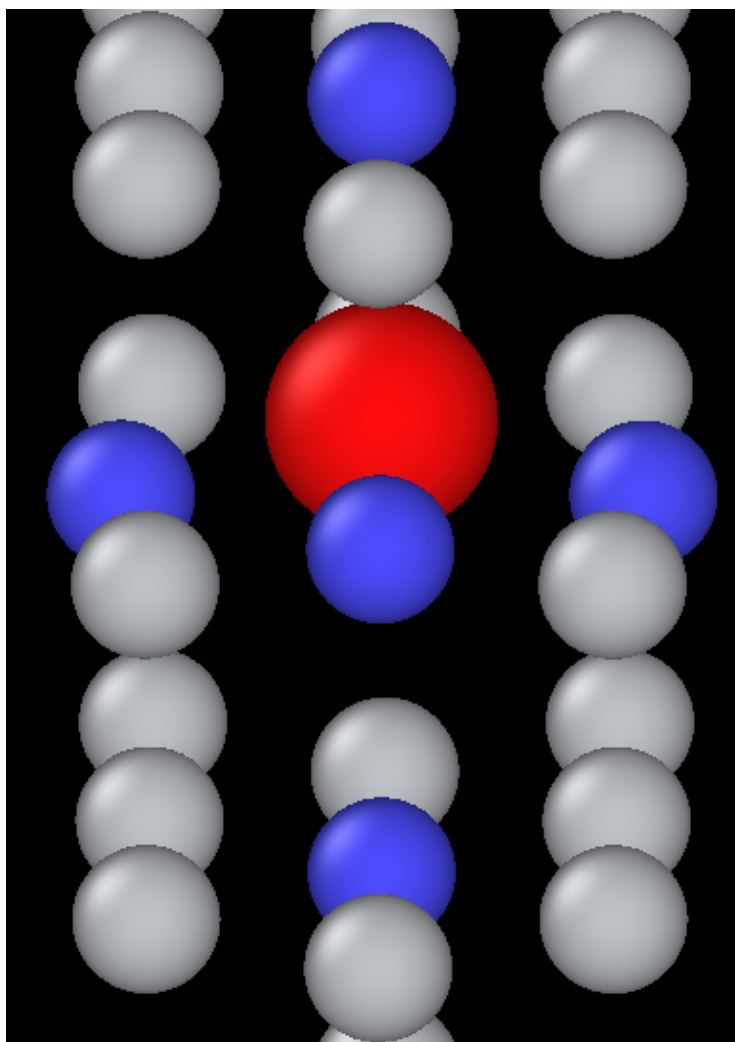
Initial:



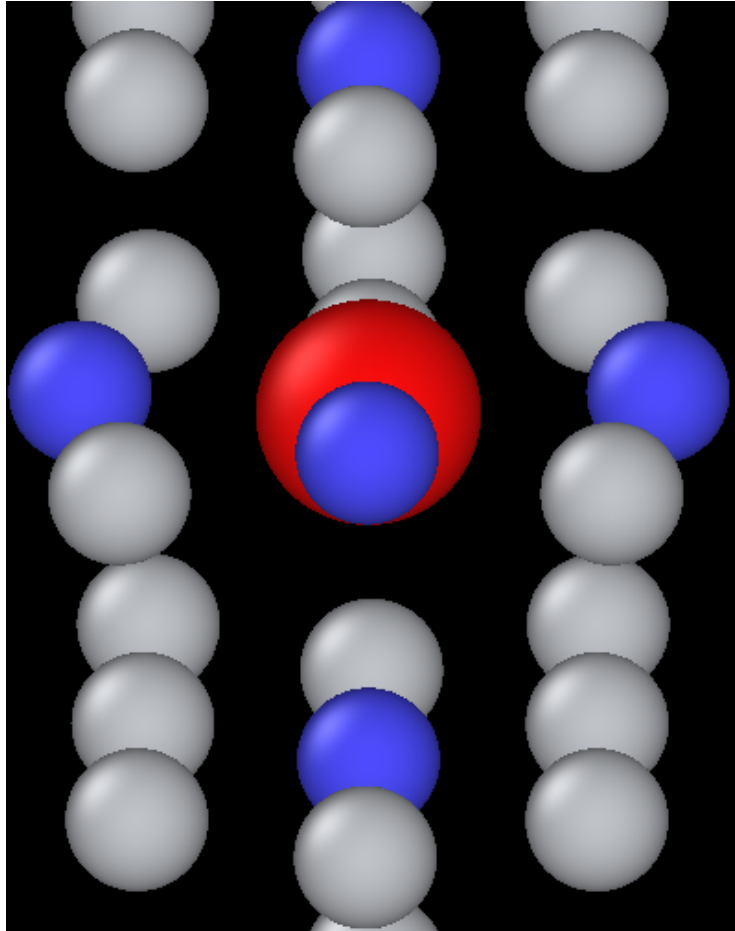
Final:



(b) Tetrahedral O interstitial relaxation
Initial:



Final:



(c) Energies for defects

Relative differences are

» $(E_{\text{tetrahedral}} - E_{\text{octahedral}})$

tbe: 1.65 eV

GGA-DFT: 1.23 eV Kwasniak (2013)

» $(E_{\text{hexahedral}} - E_{\text{octahedral}})$

tbe: 0.90 eV

> Note: Preference for tetrahedral oxygen to go into hexahedral site as seen by images above

All formation energies below use the chemical potential of Akysanov (2013) of value $\mu_{\text{oxygen}} = \frac{5.6}{2} \text{ eV}$.

(d) All formation energies

Quantity	Energy (eV)
E_{Vf}	2.347
E_{Tsol}	- 21.783
$E_{Tdilimp}$	- 28.991
$E_{Tformation}$	- 21.783
$E_{TVformation}$	- 18.905
$E_{Tvacsolbind}$	- 0.530
E_{Osol}	- 23.436
$E_{Odilimp}$	- 30.645
$E_{Oformation}$	- 23.436
$E_{OVformation}$	- 18.905
$E_{Ovacsolbind}$	- 2.183
E_{OOSol}	- 49.606
$E_{OODilimp}$	- 56.814
$E_{OOformation}$	- 46.806
$E_{OOVformation}$	- 41.910
$E_{OOvacsolbind}$	- 2.547
E_{OOOSol}	- 76.037
$E_{OOOdilimp}$	- 83.246
$E_{OOOformation}$	- 70.437
$E_{OOOVformation}$	- 66.013
$E_{OOOvacsolbind}$	- 2.076
$E_{OOOOSol}$	- 102.470
$E_{OOOOdilimp}$	- 109.679
$E_{OOOOformation}$	- 94.070
$E_{OOOOVformation}$	- 88.998
$E_{OOOOvacsolbind}$	- 2.724
$E_{OOOOOSol}$	- 128.781
$E_{OOOOOdilimp}$	- 135.989
$E_{OOOOOformation}$	- 117.581
$E_{OOOOOVformation}$	- 113.649
$E_{OOOOOvacsolbind}$	- 1.583
$E_{OOOOOOSol}$	- 155.148
$E_{OOOOOOdilimp}$	- 162.357
$E_{OOOOOOformation}$	- 141.148
$E_{OOOOOOVformation}$	- 137.110
$E_{OOOOOOvacsolbind}$	- 1.690

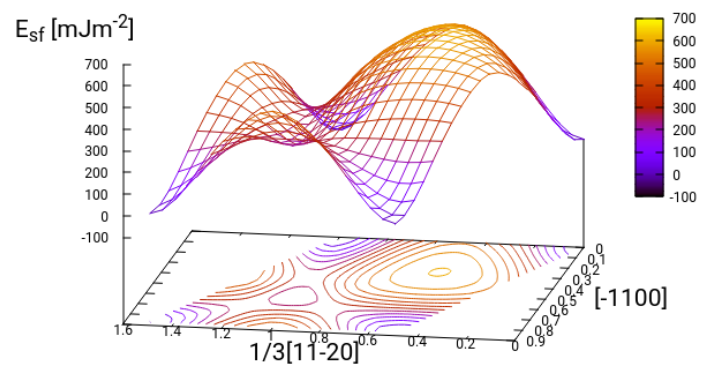
3. Gamma surfaces

Energies are accurate to within 2 mJm^{-2} , comparing the energies of points in the corners which (the zeros of energy). So surface energies might be $\pm 2 \text{ mJm}^{-2}$ off which is reasonable.

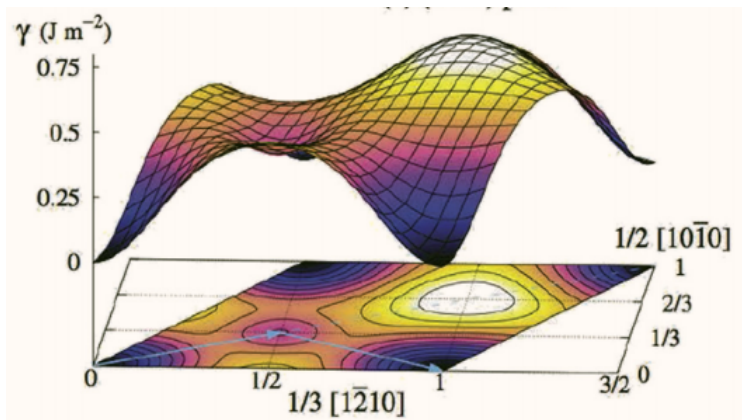
These calculations were done in tight binding with 15 layers for both basal and prismatic with k-points adjusted accordingly. DFT comparisons are used results of Rodney.

The Pyramidal surface was obtained using the same 32 atom cell that Ready used in his paper on the pyramidal gamma surface with DFT pseudopotentials.

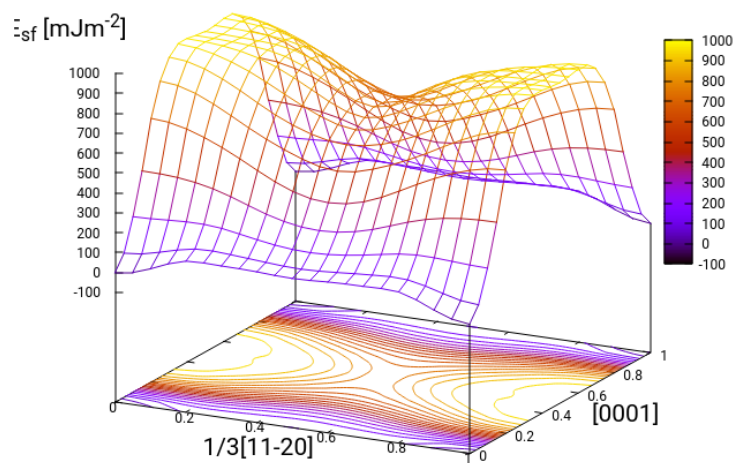
(a) Basal
TBE:



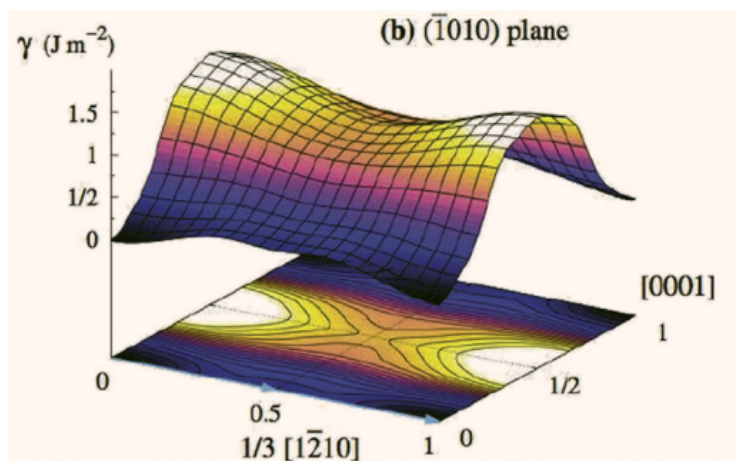
DFT:



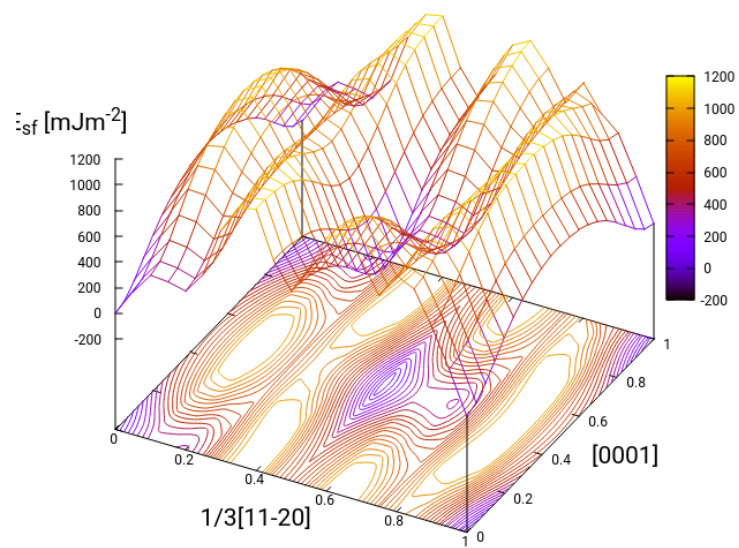
(b) Prismatic
TBE:



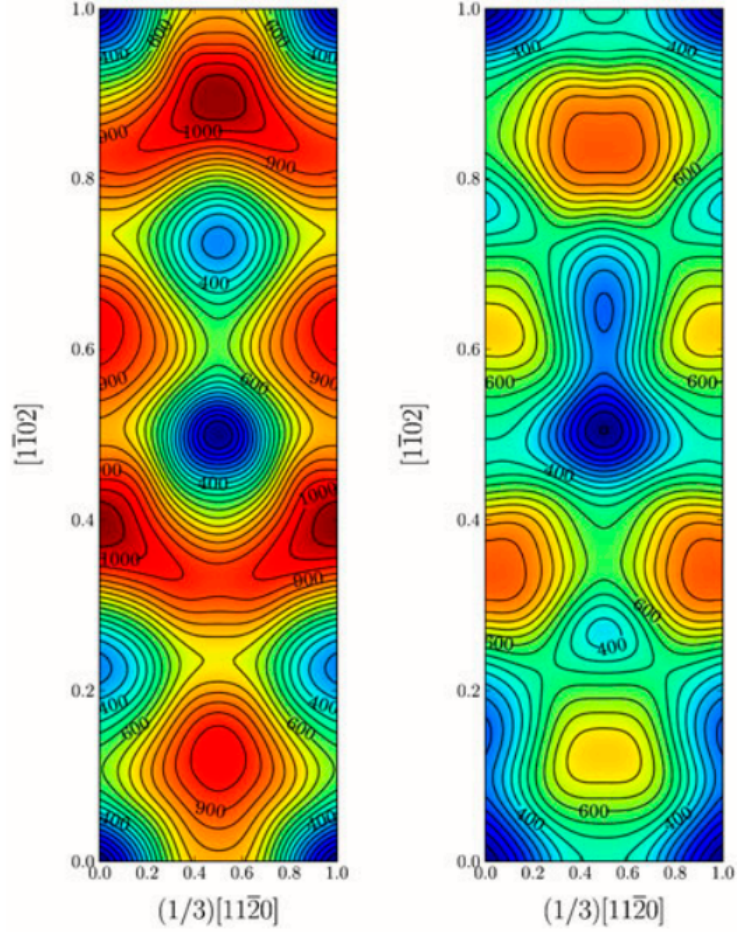
DFT:



(c) Pyramidal first order
TBE:



DFT pseudopot:



(d) Data $\text{basal}_{\text{gsdata}}$ $\text{prismatic}_{\text{gsdata}}$ $\text{pyramidal}_{\text{gsdata}}$

4. Dislocation core structures In the following figures we have the partial differential displacement maps of dislocations in their initial and final state. These were done in different initial positions of the dislocation centre (elastic centre) as following the paper by Clouet.

The partial burger's vector seen here is the $1/6[11\bar{2}0]$ dislocation.

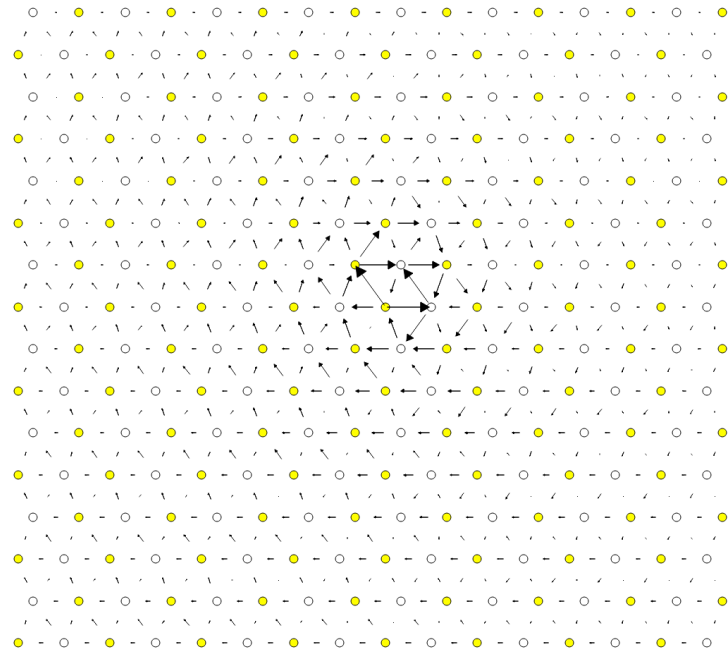
One can see that all of the dislocations have dissociated on the prismatic plane. But there is a difference between initial positions as to upon which prismatic plane they dissociate on, from the original.

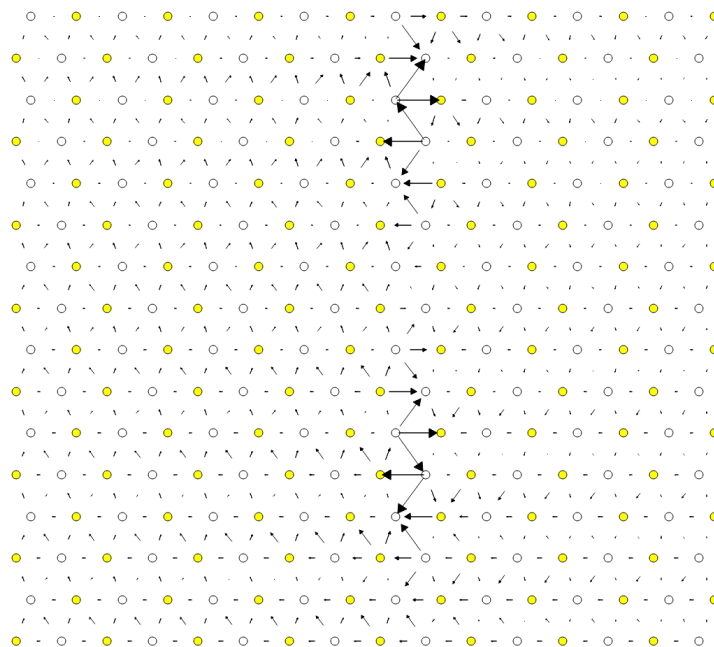
Only initial position 2 actually dissociated on a different prismatic plane to the others.

There does seem to be a large dissociation distance.

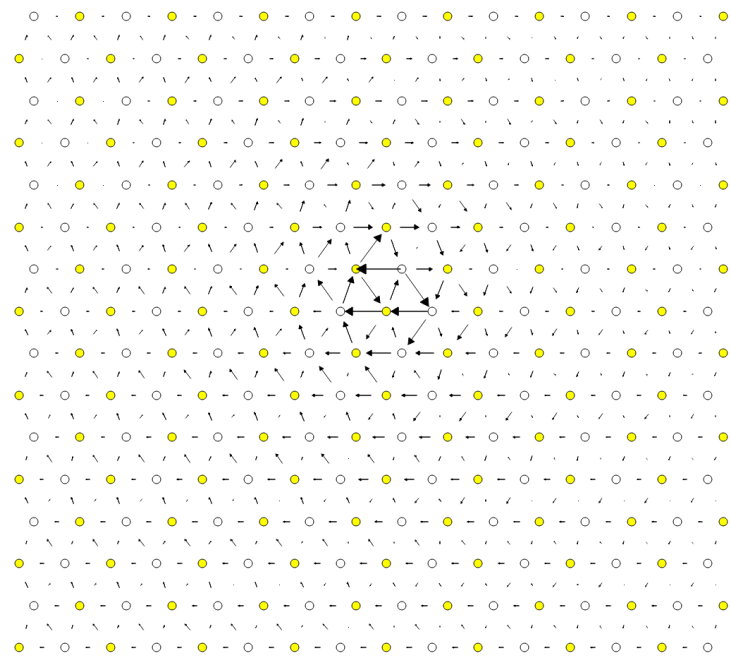
There is a small energy difference between the dip in the prismatic gamma surface along the $1/3[11\bar{2}0]$ direction. This means that along that direction, due to the small relative energy barrier between the trough in the centre of the gamma surface line and the peaks, so to speak, the dislocation can dissociate easily along this direction.

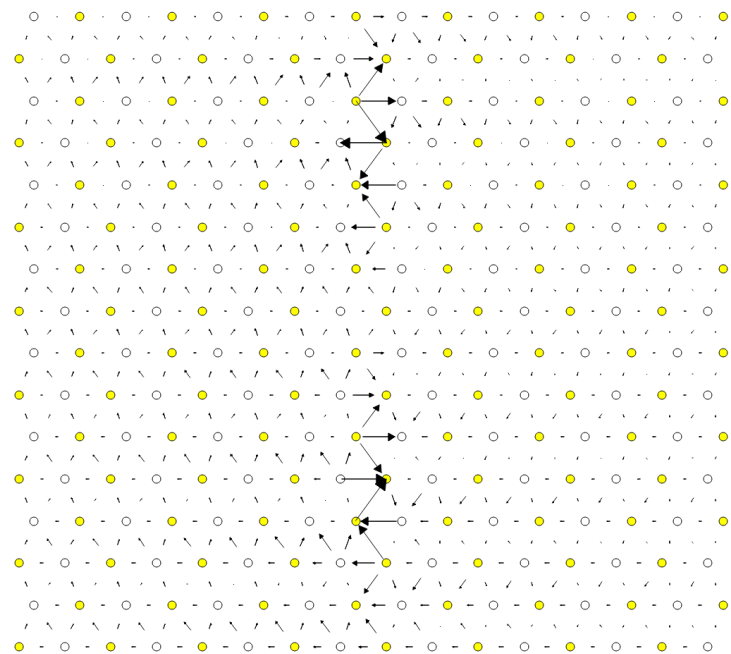
(a) IP1



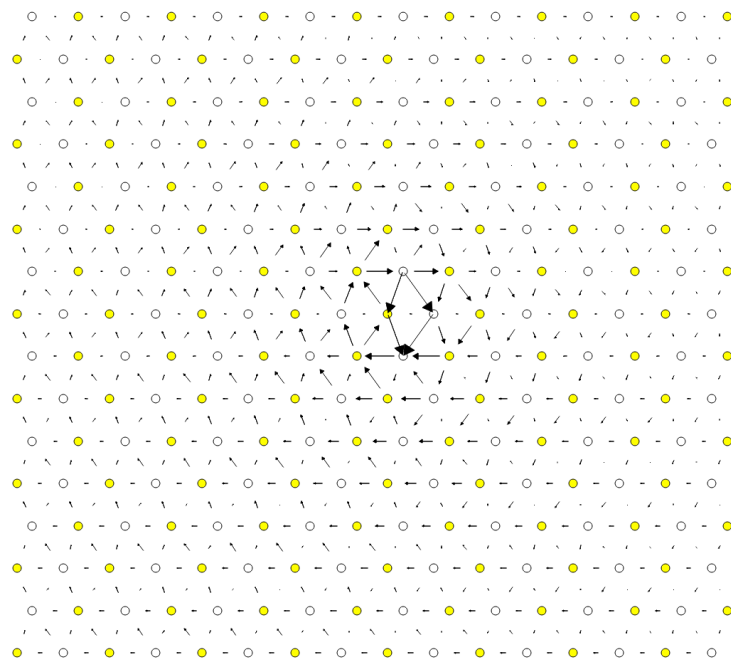


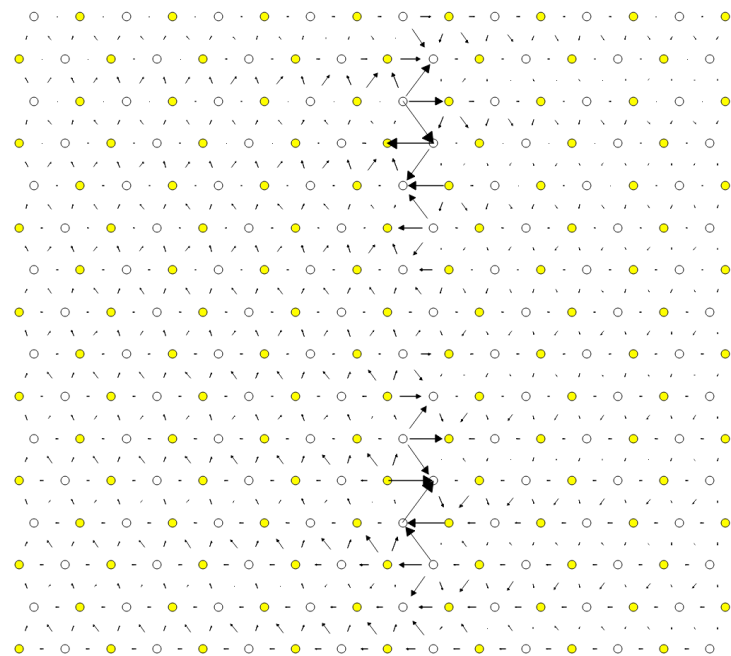
(b) IP2



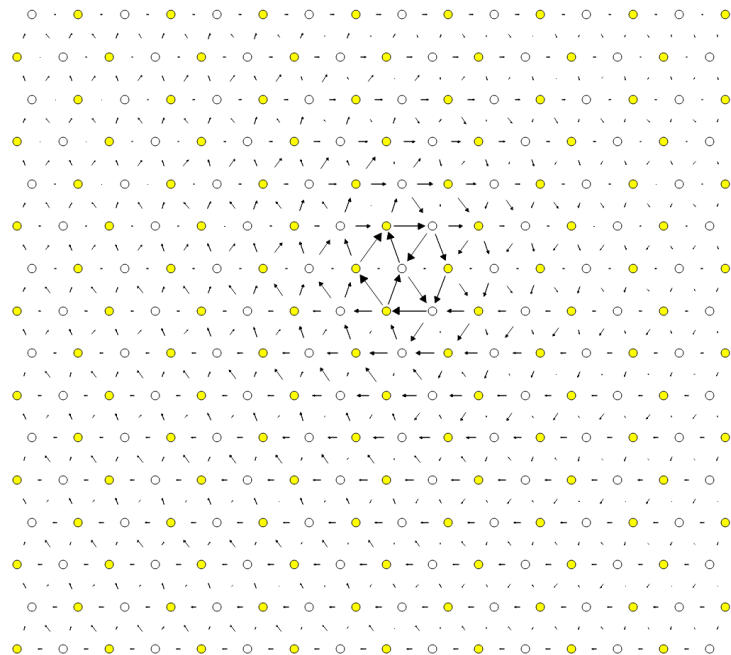


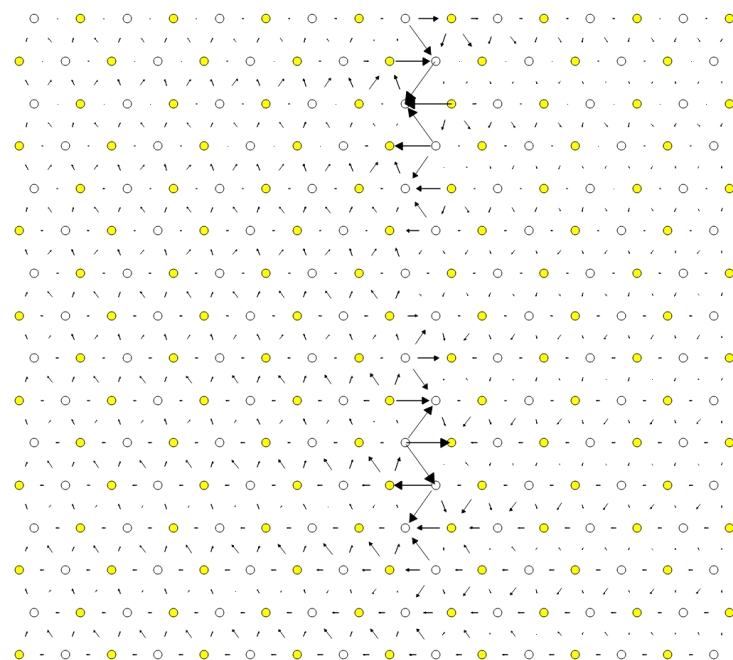
(c) IP3



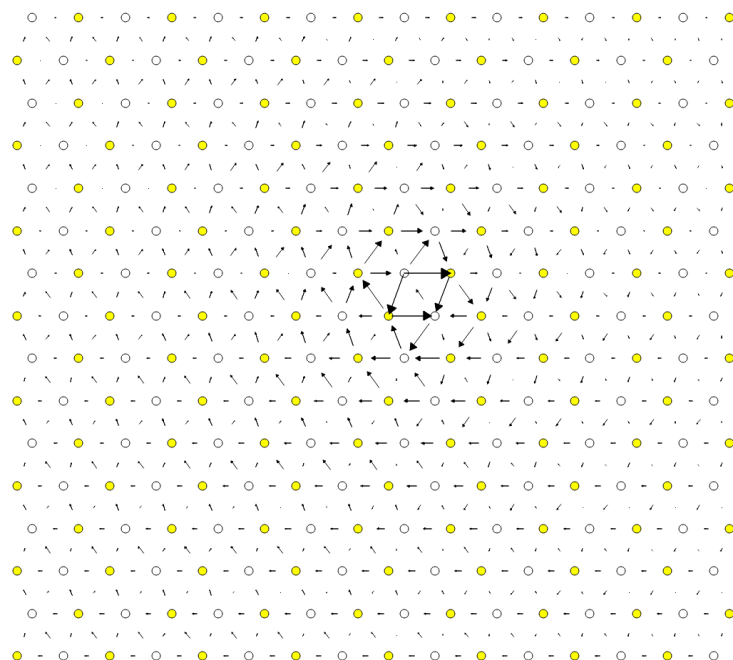


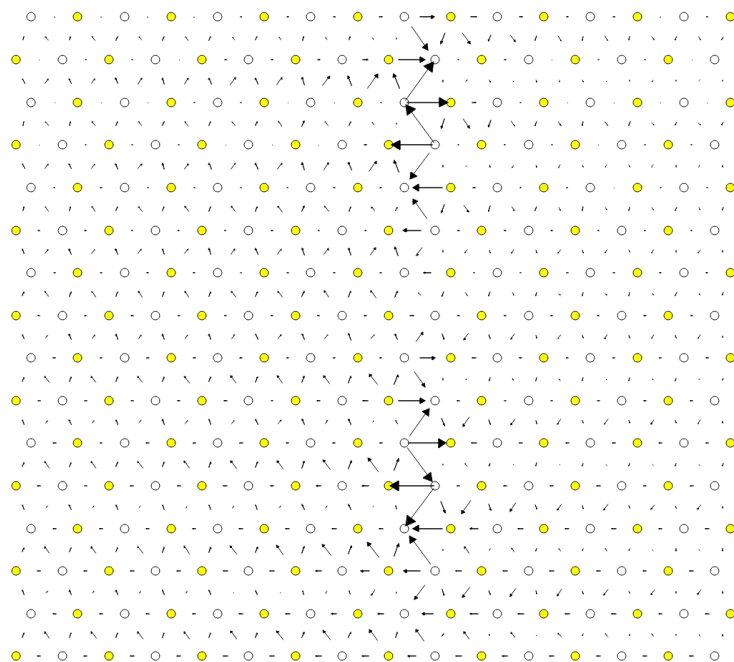
(d) IP4





(e) IP5





(f) Data IP1 IP2 IP3 IP4 IP5

5. Directory of the results `file:///home/tigany/Documents/ti/2019-09-11_final_model/tbe/dislocations/2019-11-08_no_omega_ordering_ec_latpar/` `file:///home/tigany/Documents/ti/final_model_2019-11`

6. BOP

(a) 4 recursion levels

`kbT = 0.1`

» Lattice parameters:

> hcp

```
a    2.901660 Å
c    4.747485 Å
etot -18.342162 eV
```

> omega

```
a    7.917318 Å
c    2.749892 Å
etot -17.458700 eV
```


Omega is still not as stable as hcp as expected from model.

» Elastic Constants

Quantity	calc. (10^{11} Pa)	exp. (10^{11} GPa)
C11	1.781	1.761
C12	0.738	0.868
C13	0.611	0.682
C33	1.969	1.905
C44	0.285	0.508
C66	0.522	0.450
K	1.050	1.101
R	0.669	0.618
H	0.558	0.489