High temperature thermoelectric properties of $Yb_{14}MnSb_{11}$ prepared from direct reaction of the elements

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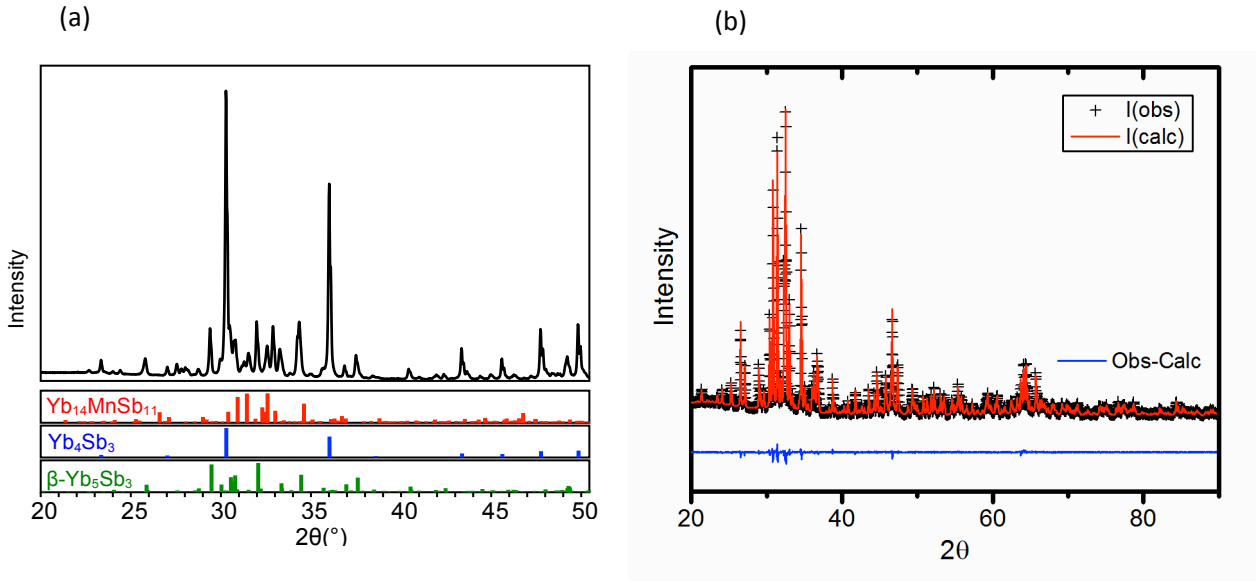
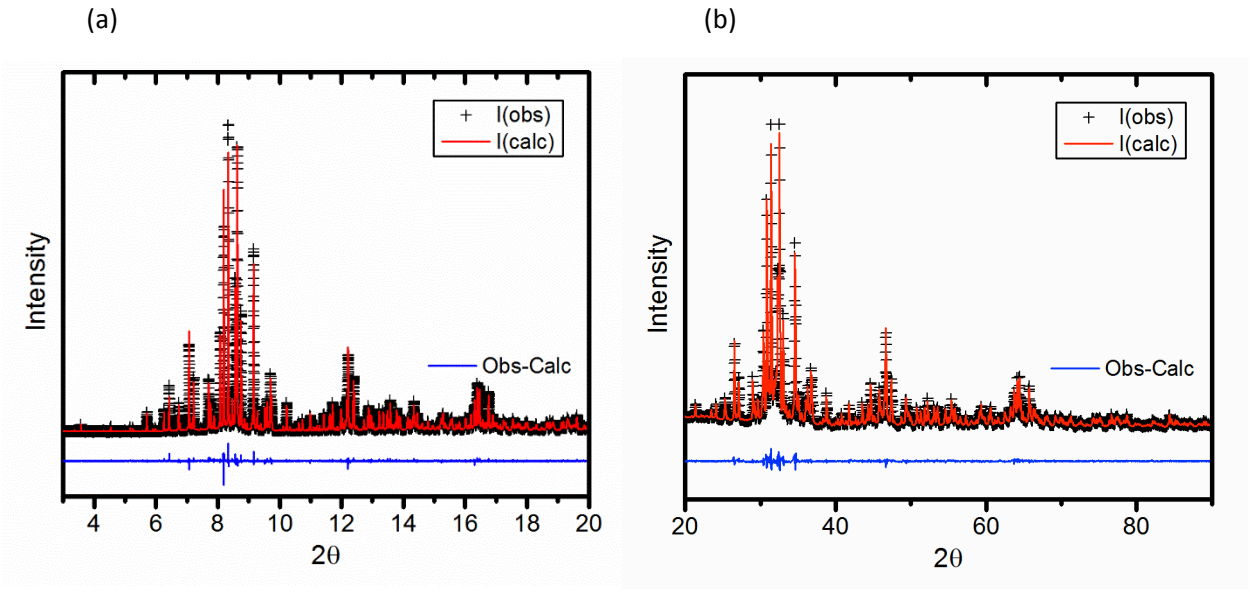
- SUPPORTING INFORMATION

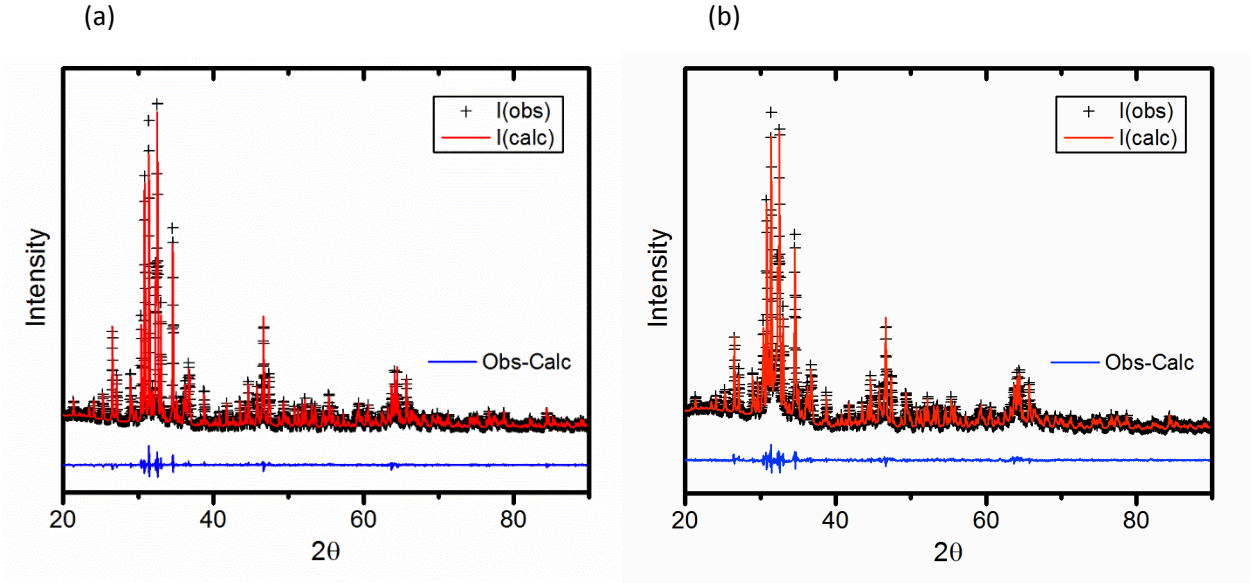
Ball milling Yb filings with elemental Mn and Sb followed by annealing at 1100˚C resulted in a product that consisted mainly of Yb_4Sb_3, as determined by powder X-ray diffraction, shown in SFigure 1(a). This result is attributed to the small amount of Mn present and the ductility on Yb leading to an inhomogeneous distribution of Mn in the mixture.



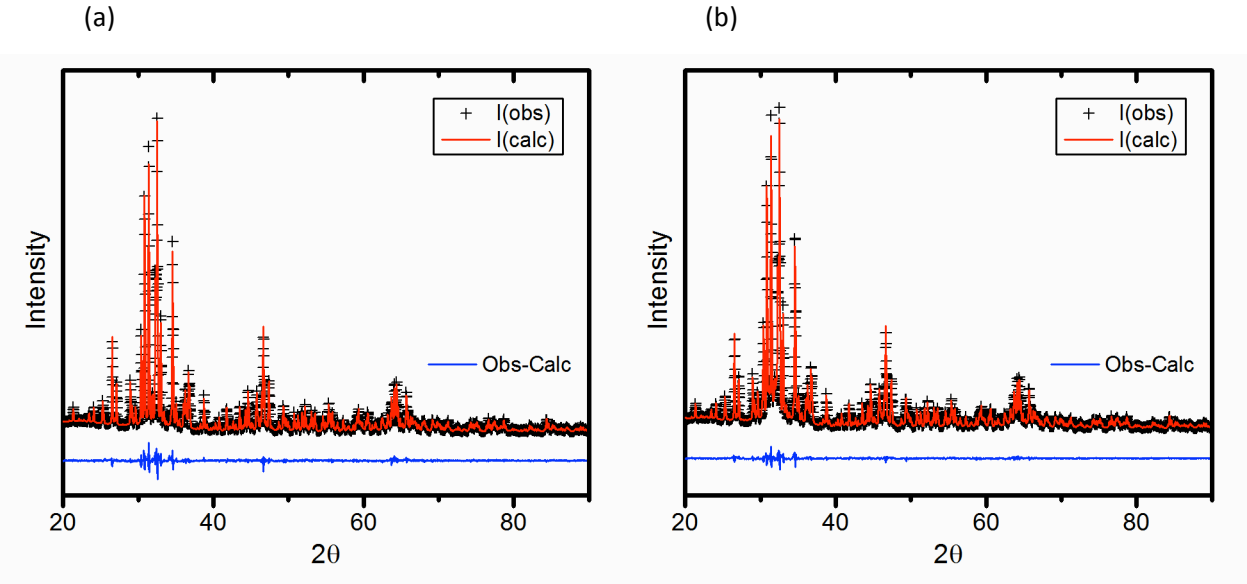
SFigure 1: (a) PXRD of sample produced by ball milling Yb filings and elemental Mn and Sb followed by annealing. (b) PXRD and Rietveld refinement of Mn1-A, a sample produced by ball milling Yb filings, MnSb, and Sb in stoichiometric amounts followed by annealing (see experimental section).



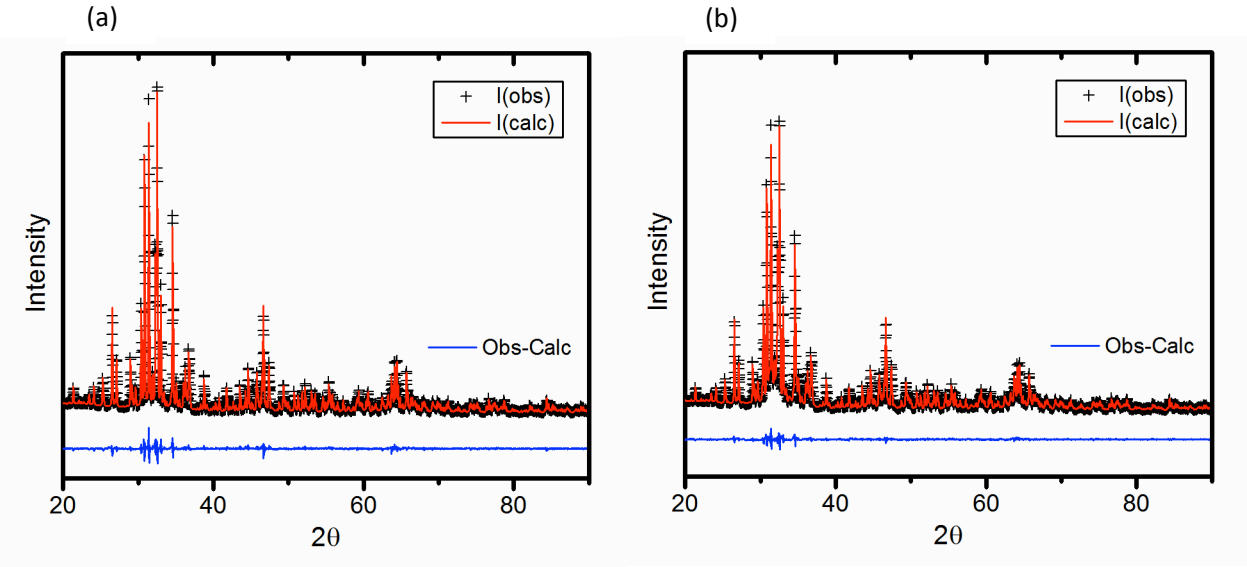
SFigure 2: (a) Synchrotron PXRD and Rietveld refinement of the Mn1-B-SPS pellet. (b) PXRD and Rietveld refinement of the Mn1-B-SPS-HT pellet after 6 hours of annealing at 1273 K.



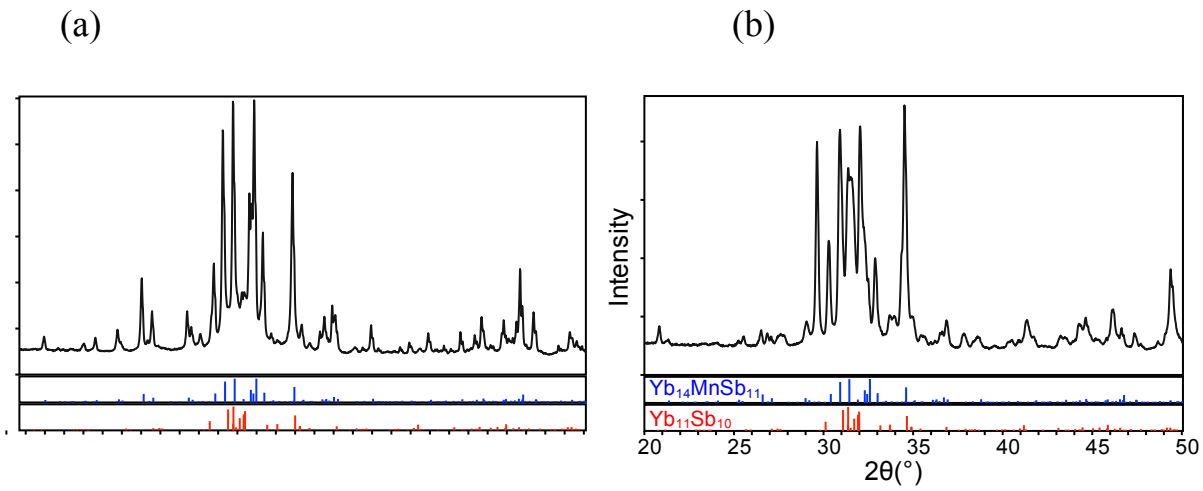
SFigure 3: (a) PXRD and Rietveld refinement of Mn1-C. (b) PXRD and Rietveld refinement of Mn1-C-TE after thermoelectric measurements.



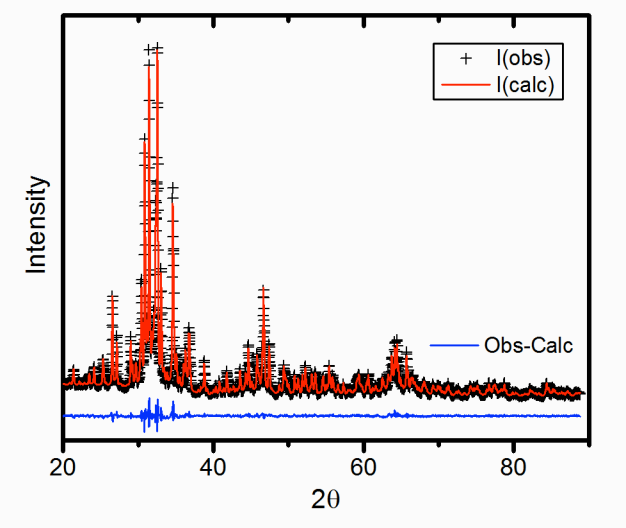
SFigure 4: (a) PXRD and Rietveld refinement of Mn1.05. (b) PXRD and Rietveld refinement of the Mn1.05 after 6 hours of annealing at 1273 K (Mn1.05-HT).



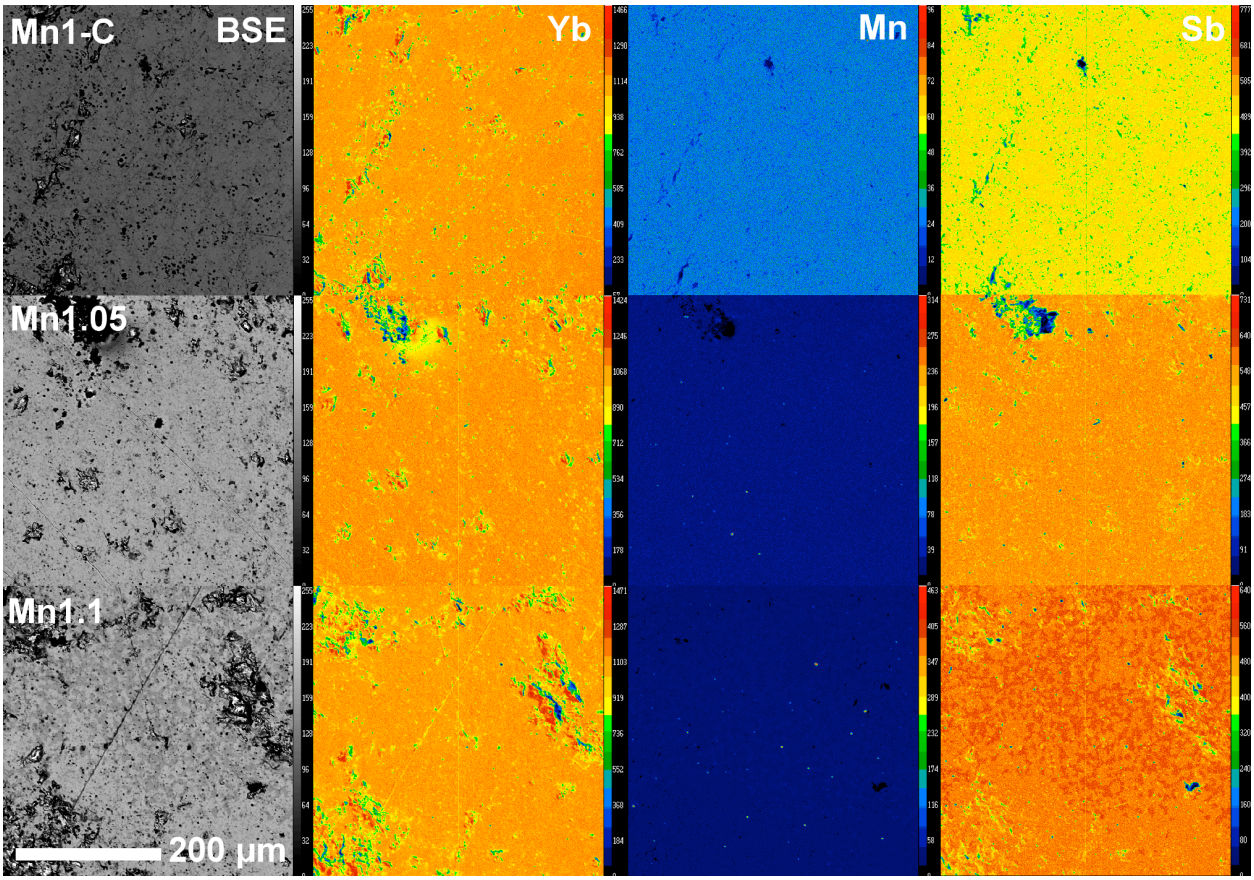
SFigure 5: (a) PXRD and Rietveld refinement of Mn1.1. (b) PXRD and Rietveld refinement of the Mn1.1 pellet after 6 hours of annealing at 1273 K (Mn1.1-HT).



SFigure 6: (a) PXRD of $Yb_{14}MnSb_{11}$ single crystal (from Sn-flux) after TG/DSC. (b) PXRD of cold pressed pellet from ground $Yb_{14}MnSb_{11}$ single crystal after TG/DSC.



SFigure 7: PXRD and Rietveld refinement of JPL ATEC $Yb_{14}MnSb_{11}$.



SFigure 8: Electron microprobe images of Mn1-C, Mn1.05, and Mn1.1, showing BSE Z and elemental maps for Yb, Mn, and Sb.

STable 1: Lattice Parameters, Volume, R_{wp}, and Additional Phases Determined from Rietveld Refinement of PXRD Data for $Yb_{14}MnSb_{11}$ Samples[a]

Sample	a (Å)	c (Å)	Volume (Å^3)	R_{wp}	# of Reflns	Yb_2O_3 (% wt)	$Yb_{11}Sb_{10}$ (% wt)
Mn1-A	16.6226(1)	22.0191(2)	6084.1(1)	0.0313	3404	1.2(1)	
Mn1-B*	16.62399(3)	22.01975(5)	6085.31(3)	0.0894	47481	2.22(5)	
Mn1-B-SPS*	16.62447(4)	22.01678(6)	6084.84(4)	0.0701	47379	1.02(1)	1.47(5)
Mn1-B-SPS-HT	16.6214(2)	22.0186(3)	6083.1(2)	0.0371	3404	1.38(4)	14.6(3)
Mn1-C	16.6214(1)	22.0185(2)	6083.1(1)	0.0402	3404	0.58(4)	
Mn1-C-TE	16.6216(2)	22.0172(3)	6082.9(2)	0.0374	3404	2.3(1)	20(1)
Mn1-D-DSC	16.6193(4)	22.0163(6)	6080.9(4)	0.0537	3889	7.1(3)	39.5(9)
Mn1.05	16.6264(1)	22.0168(2)	6086.3(1)	0.0335	3404	1.16(3)	
Mn1.05-HT	16.6228(2)	22.0190(3)	6084.3(2)	0.0379	3404	1.56(4)	10.9(3)
Mn1.1	16.6205(1)	22.0193(2)	6082.7(1)	0.0358	3404	1.17(3)	
Mn1.1-HT	16.6196(1)	22.0154(2)	6080.9(2)	0.0369	3404	1.54(4)	14.6(3)
ATEC-TE	16.6193(2)	22.0242(4)	6083.1(2)	0.0340	3346	1.38(4)	17.7(3)
Flux[27]	16.6081(2)	21.9883(2)					
Polycrystalline[26]	16.6140(2)	21.9925(3)					

[a] Mn*x* represents samples prepared according to the stoichiometry, $Yb_{14}Mn_xSb_{11}$

[b] A-D indicates different sample batches

[c] –SPS, -DSC, -TE indicate sample measured after SPS, DSC, Thermoelectric Measurements

[d] -HT is a sample annealed at 1000˚C for 6 hours

*Collected on 11-BM

STable 2: Atomic Percentages from Electron Microprobe Elemental Analysis.

	Yb	Mn	Sb
$Yb_{14}MnSb_{11}$ (calc)	53.84615	3.846154	42.30769
Mn1-B-SPS	53.95(8)	3.77(4)	42.3(1)
Mn1-C-TE	53(1)	4.4(5)	42.4(9)
Mn1.05-TE	51.0(7)	3.8(2)	45.1(8)
Mn1.1-TE	52(2)	4.7(7)	43.0(9)

STable 3: Thermal Diffusivity

Mn1-A		Mn1-B		Mn1-C-JPL		Mn1.05		Mn1.05-JPL		Mn1.1-JPL	
Temp (K)	Diff (cm^2/s)	Temp (K)	Diff (cm^2/s)	Temp (K)	Diff (cm^2/s)	Temp (K)	Diff (cm^2/s)	Temp (K)	Diff (cm^2/s)	Temp (K)	Diff (cm^2/s)
322.75	0.00615	319.65	0.00684	299.1	0.00735	371.95	0.00666	297.9	0.00685	302	0.00716
323.15	0.00615	315.75	0.00681	372.9	0.0073	372.65	0.00667	374.5	0.00699	373	0.00742
372.75	0.00607	313.75	0.00675	473.1	0.00716	372.85	0.00668	471.7	0.007	473.1	0.0073
372.75	0.00613	369.45	0.00689	573.2	0.007	421.85	0.00674	578.1	0.00681	574	0.00712
372.75	0.00617	371.35	0.00689	673.5	0.0067	422.35	0.00673	676.7	0.00648	673.8	0.00681
422.75	0.0062	372.35	0.0069	773.8	0.00651	422.65	0.00671	775.6	0.00637	773.9	0.00654
422.85	0.0062	422.75	0.00701	873.5	0.00619	471.55	0.00676	875	0.006	873.6	0.00631
422.85	0.00621	422.75	0.007	973.4	0.0061	472.15	0.00675	974.3	0.00573	973.5	0.00614
472.95	0.00628	422.85	0.00702	1073.3	0.00615	472.45	0.00673	1073.9	0.00556	1073.4	0.00598
472.95	0.00625	470.95	0.00705	1173.3	0.00648	519.45	0.00673	1173.8	0.00553	1173.4	0.00602
472.95	0.00628	471.95	0.00704	1273.3	0.00736	520.45	0.0067	1273.6	0.00567	1273.4	0.00636
523.45	0.00624	472.45	0.007			521.55	0.00669				
523.15	0.00624	522.35	0.00698			571.85	0.00664				
523.05	0.00626	522.75	0.00699			572.15	0.00663				
573.35	0.00618	522.85	0.00698			572.75	0.00663				
573.15	0.00618	573.05	0.00694			623.25	0.00652				
572.95	0.00619	573.15	0.00692			623.15	0.0065				
623.75	0.00611	573.05	0.00692			623.35	0.00651				
623.35	0.00607	623.35	0.00679			674.55	0.00636				
623.05	0.00604	623.35	0.00681			673.95	0.00638				
673.45	0.00598	623.25	0.00678			673.75	0.00638				
673.15	0.00596	673.45	0.00665			724.35	0.00619				
673.05	0.00598	673.25	0.00661			724.25	0.00619				
723.35	0.00585	673.15	0.00664			723.85	0.00621				
723.05	0.00576	723.45	0.00642			775.25	0.00604				
722.95	0.00576	723.25	0.00637			774.45	0.00603				
773.35	0.00563	723.05	0.00639			773.75	0.00602				
773.15	0.00559	773.35	0.00623			824.15	0.0059				
772.95	0.00554	773.15	0.0062			823.85	0.00588				
823.25	0.00551	773.05	0.0062			823.55	0.00586				
823.05	0.00542	823.25	0.00606			874.05	0.00573				
822.85	0.00543	823.15	0.00601			873.75	0.00573				
873.15	0.00522	822.95	0.006			873.45	0.00574				
873.05	0.00518	873.25	0.00581			923.85	0.00557				
872.95	0.0053	873.05	0.00571			923.65	0.00555				
923.15	0.00516	872.95	0.00568			923.35	0.00556				
922.95	0.00508	923.15	0.00552			973.65	0.00544				
922.85	0.005	923.05	0.0055			973.45	0.00545				
972.95	0.00488	922.85	0.00549			973.25	0.00541				
972.85	0.0049	973.15	0.00542			1023.55	0.00537				
1023.15	0.0048	972.95	0.00536			1023.35	0.0053				
1022.85	0.00483	972.85	0.00539			1023.25	0.00539				
1022.95	0.00478	1023.05	0.00529			1073.35	0.0053				
1073.05	0.00472	1022.95	0.00525			1073.25	0.00525				
1072.75	0.00484	1022.85	0.00526			1073.05	0.00528				
1072.85	0.0048	1072.95	0.00529								
		1072.85	0.00527								
		1072.85	0.00522								