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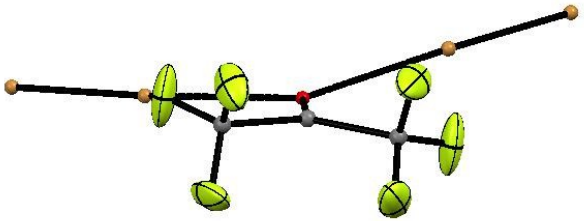
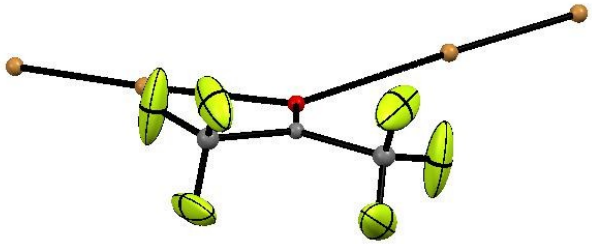
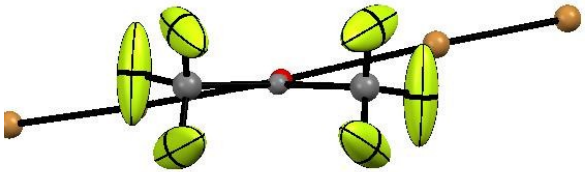
Thermal Ellipsoid plots showing increasing in motion of deuterium atoms with temperature



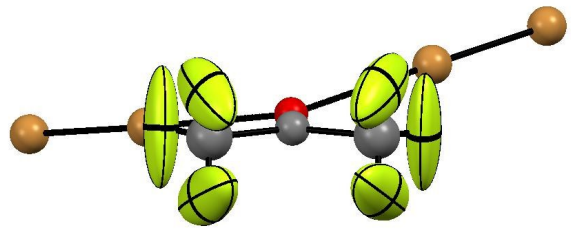
14 K



35 K

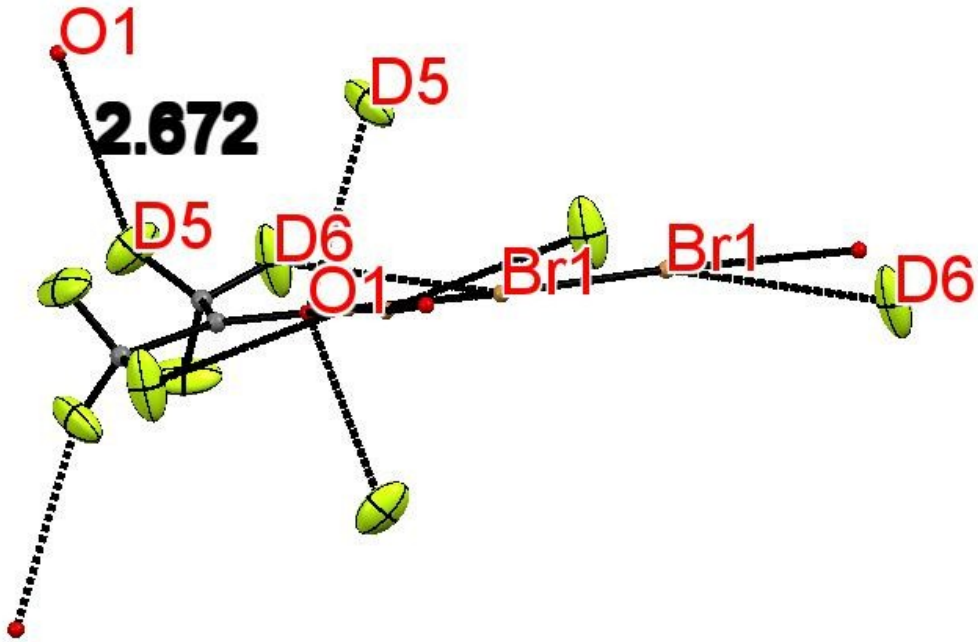


75 K

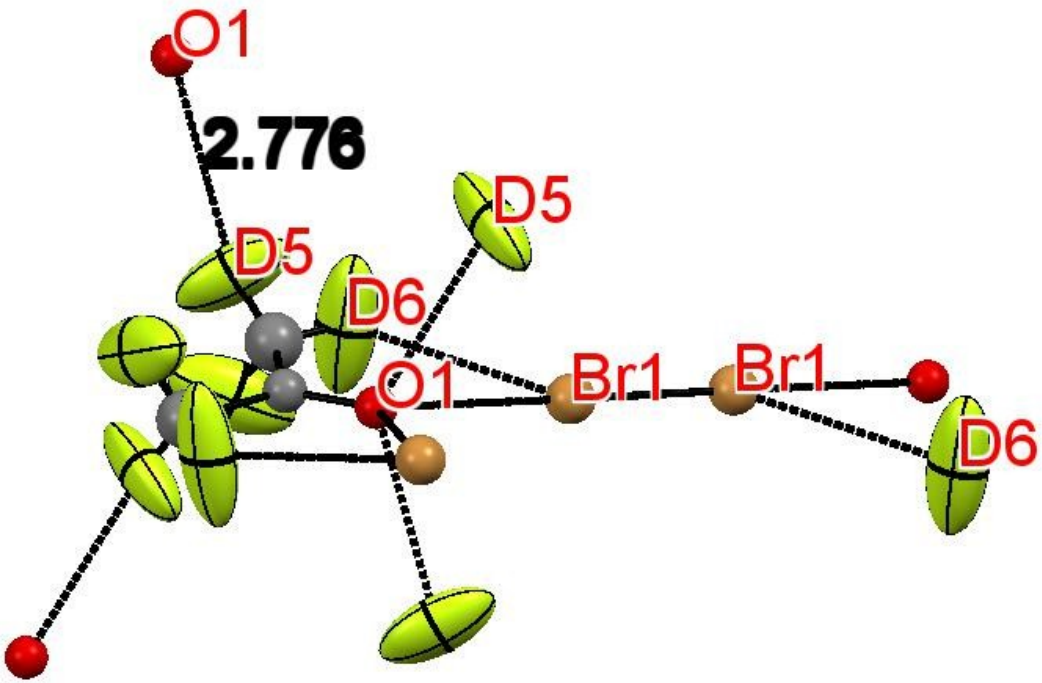


200 K

Selected Thermal Ellipsoid plots (1 4K 200K) showing increse in D5---O1 distance (Å) with temperature



14 K structure



200K structure

Crystallographic data for acetone bromine complex

Compound	$C_3D_6OBr_2$	$C_3D_6OBr_2$	$C_3D_6OBr_2$	$C_3D_6OBr_2$
Temperature /K	14	35	75	200
Radiation	Neutron(TOF)	Neutron(TOF)	Neutron(TOF)	Neutron(TOF)
Crystal System	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space Group	C2/c	C2/c	C2/c	C2/c
a/Å	7.5631(1)	7.5560(1)	7.5643(1)	7.6463(2)
b/Å	7.3561(1)	7.3529(1)	7.3605(2)	7.4306(2)
c/Å	11.8747(2)	11.9119(2)	11.97900(2)	12.2258(3)
β/°	102.169(1)	102.108(1)	102.115(1)	102.997(1)
V/Å^3	645.806(28)	647.084(27)	652.102(30)	676.831(48)
Formula	$C_3D_6OBr_2$	$C_3D_6OBr_2$	$C_3D_6OBr_2$	$C_3D_6OBr_2$
Mw/g mol^{-1}	223.924	223.924	223.924	223.924
D_c / g·cm^{-3}	2.303	2.299	2.281	2.197
Z	4	4	4	4
d_{min}/ Å	0.663	0.663	0.663	0.663
N_{ref}	1574	1537	1548	1605
N Parameters	113	87	86	86
R_{wp}	0.0356	0.0349	0.0341	0.0313
R_p	0.0394	0.0385	0.0382	0.0371
R_{Bragg} (R_Fsqd) * Bank 2θ = 168.33° ! Bank 2θ = 89.58° $ Bank 2θ = 30.00°	0.14807* 0.06869! 0.09397$	0.16710* 0.07390! 0.11684$	0.21801* 0.10065! 0.11227$	0.40627* 0.22181! 0.16337$
CCDC deposition number	1562036	1562265	1562187	1562188

Intra and Interatomic Distances for the acetone and bromine complex

	Temperature /K	Temperature /K	Temperature /K	Temperature /K
Bond / Å	14	35	75	200
Br(1) – Br(1)	2.3208(33)	2.3265(30)	2.3277(34)	2.309(5)
Br(1) – O(1)	2.7368(22)	2.7338(21)	2.7373(24)	2.797(4)
O(1) – C(3)	1.248(4)	1.2425(33)	1.250(4)	1.227(6)
C(3) – C(4)	1.4848(25)	1.4941(20)	1.4991(23)	1.506(4)
C(4) – D(5)	1.0697(28)	1.0444(23)	1.0234(27)	0.968(5)
C(4) – D(6)	1.0827(26)	1.0700(24)	1.0485(30)	0.983(5)
C(4) – D(7)	1.0830(25)	1.0610(22)	1.00330(26)	1.003(5)

Intra and Interatomic Angles for the acetone and bromine complex

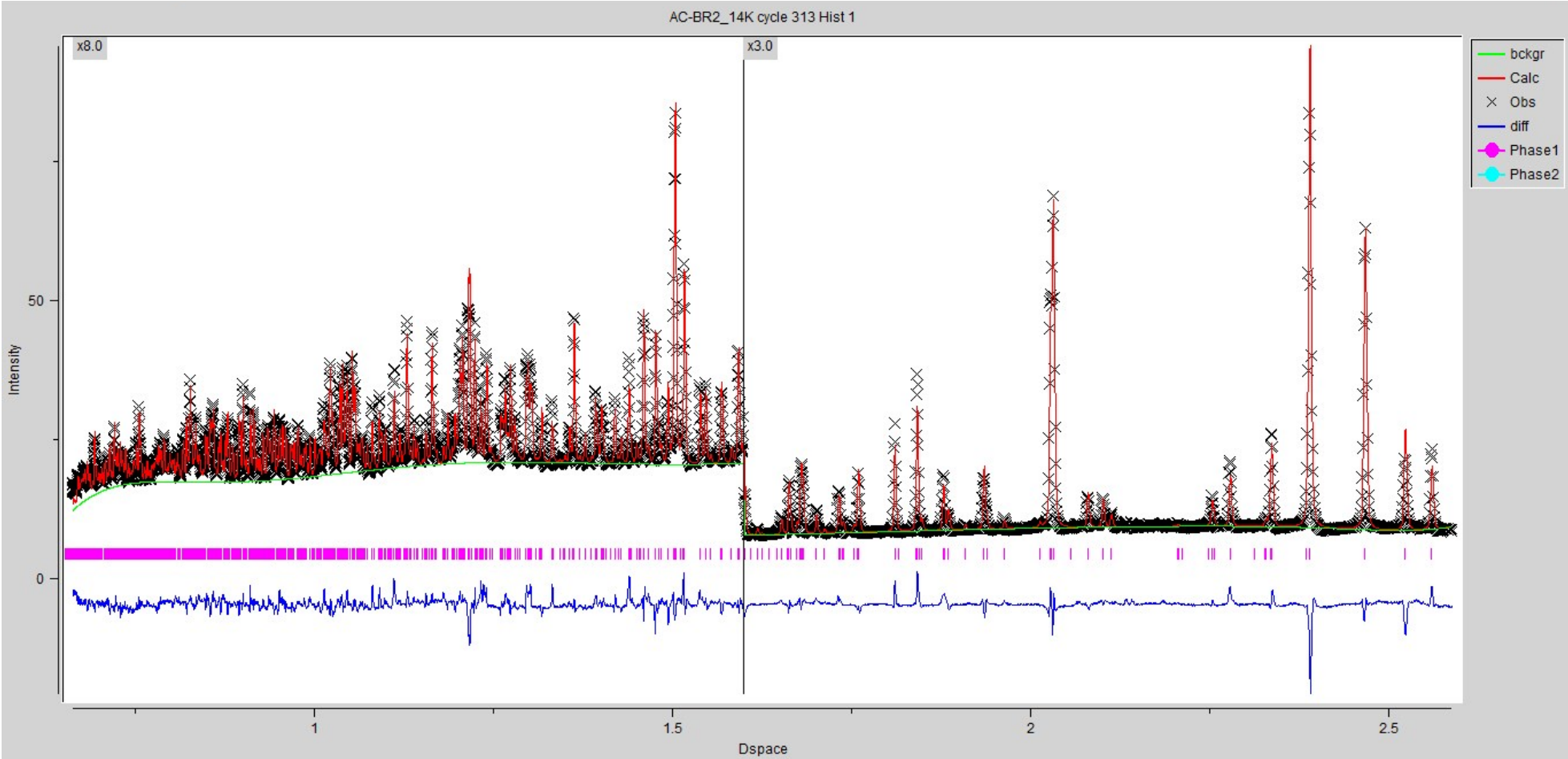
	Temperature /K	Temperature /K	Temperature /K	Temperature /K
Bond / Å	14	35	75	200
Br(1) –Br(1) - O(1)	177.56(10)	178.15(10)	178.24(12)	178.16(19)
Br(1) - O(1) - Br(1)	109.25(13)	109.47(13)	110.08(14)	110.09(20)
Br(1) - O(1) – C(3)	125.37(7)	125.26(6)	124.96(7)	124.96(10)
O(1) – C(3) – C(4)	120.11(14)	120.60(11)	120.52(13)	119.36(28)
C(4) – C(3) – C(4)	119.79(28)	118.79(22)	118.96(27)	121.3(6)
C(3) – C(4) – D(5)	109.50(18)	109.59(17)	109.65(22)	108.4(5)
C(3) – C(4) – D(6)	111.02(25)	109.82(20)	109.26(26)	110.3(5)
C(3) – C(4) – D(7)	108.93(18)	109.54(16)	109.66(21)	108.4(5)
D(5) – C(4) – D(6)	108.90(25)	107.46(23)	105.79(30)	107.4(7)
D(5) – C(4) – D(7)	106.78(28)	107.95(25)	109.32(33)	109.2(7)
D(6) – C(4) – D(8)	111.62(24)	112.41(23)	113.07(31)	113.1(7)

Selected parameters interatomic parameters

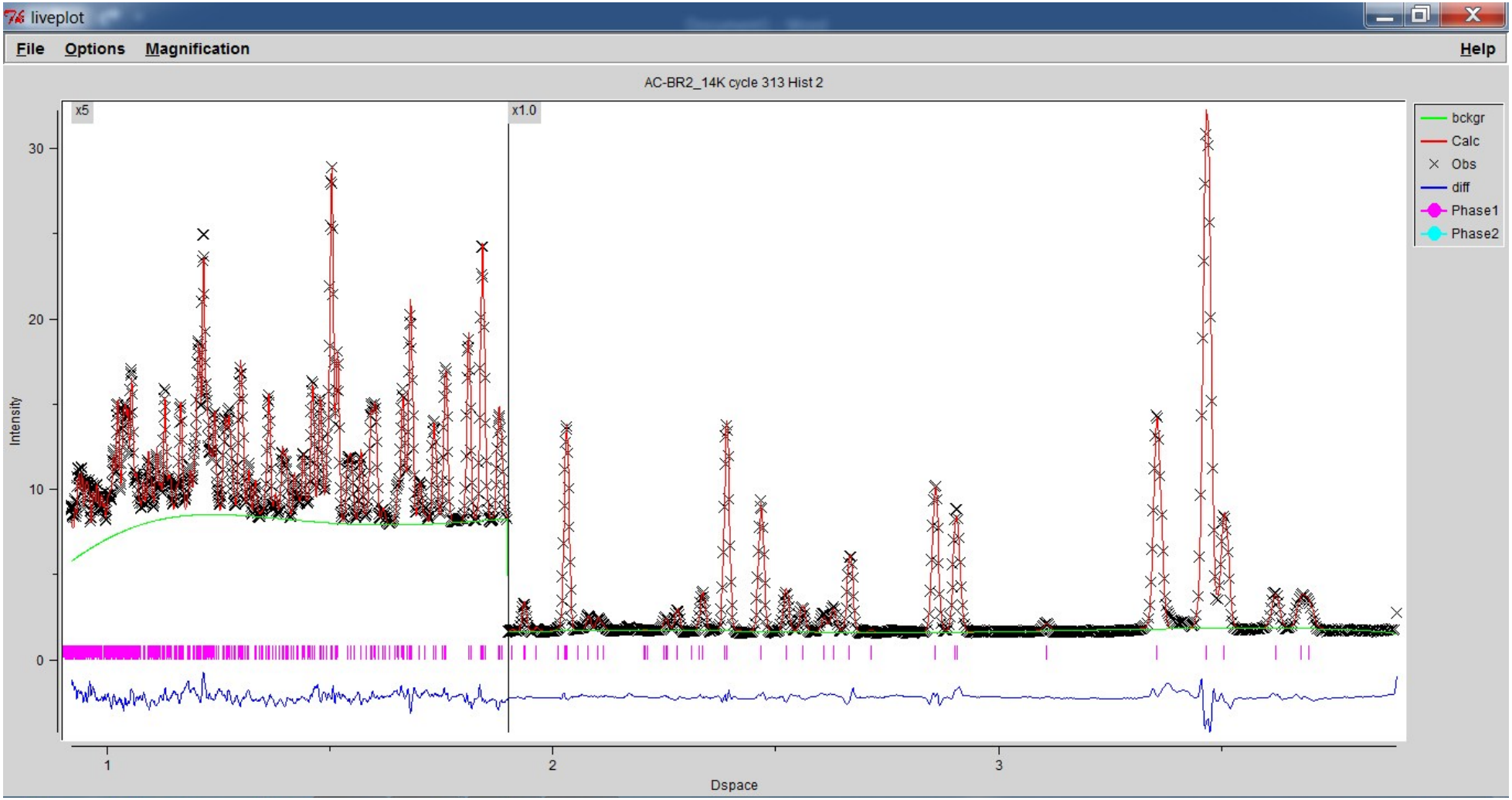
Temperature /K	D6---Br1 / Å	D7---Br1/ Å	D5-O/ Å
14	3.004(3)	3.017(3)	2.672(3)
35	2.994(3)	3.024(3)	2.666(2)
75	2.976(4)	3.049(3)	2.661(3)
200	2.986(7)	3.119(5)	2.777(5)

Rietveld Plots

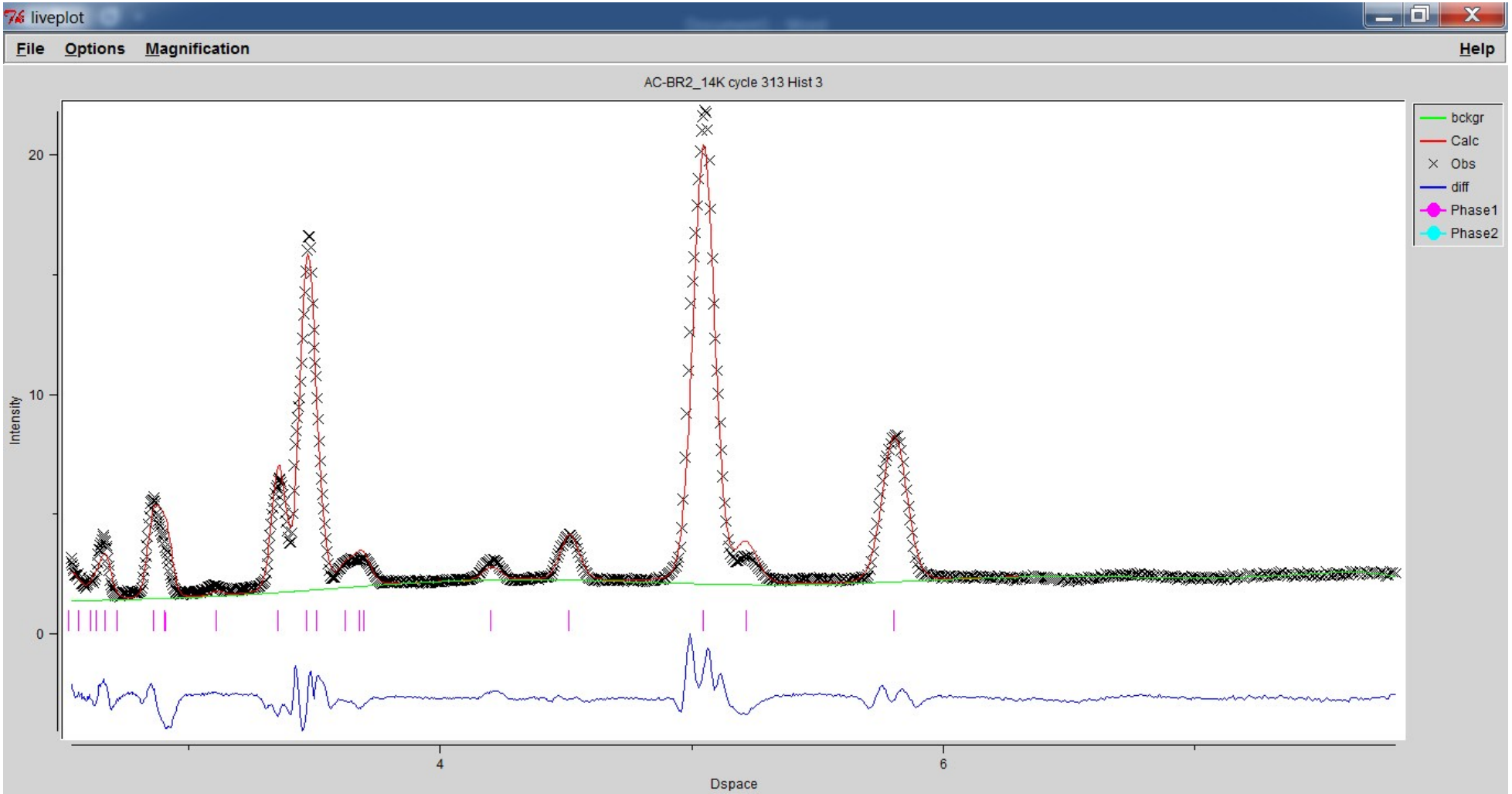
Observed and Difference Plot Acetone Bromine Complex 14K 168.33° Bank



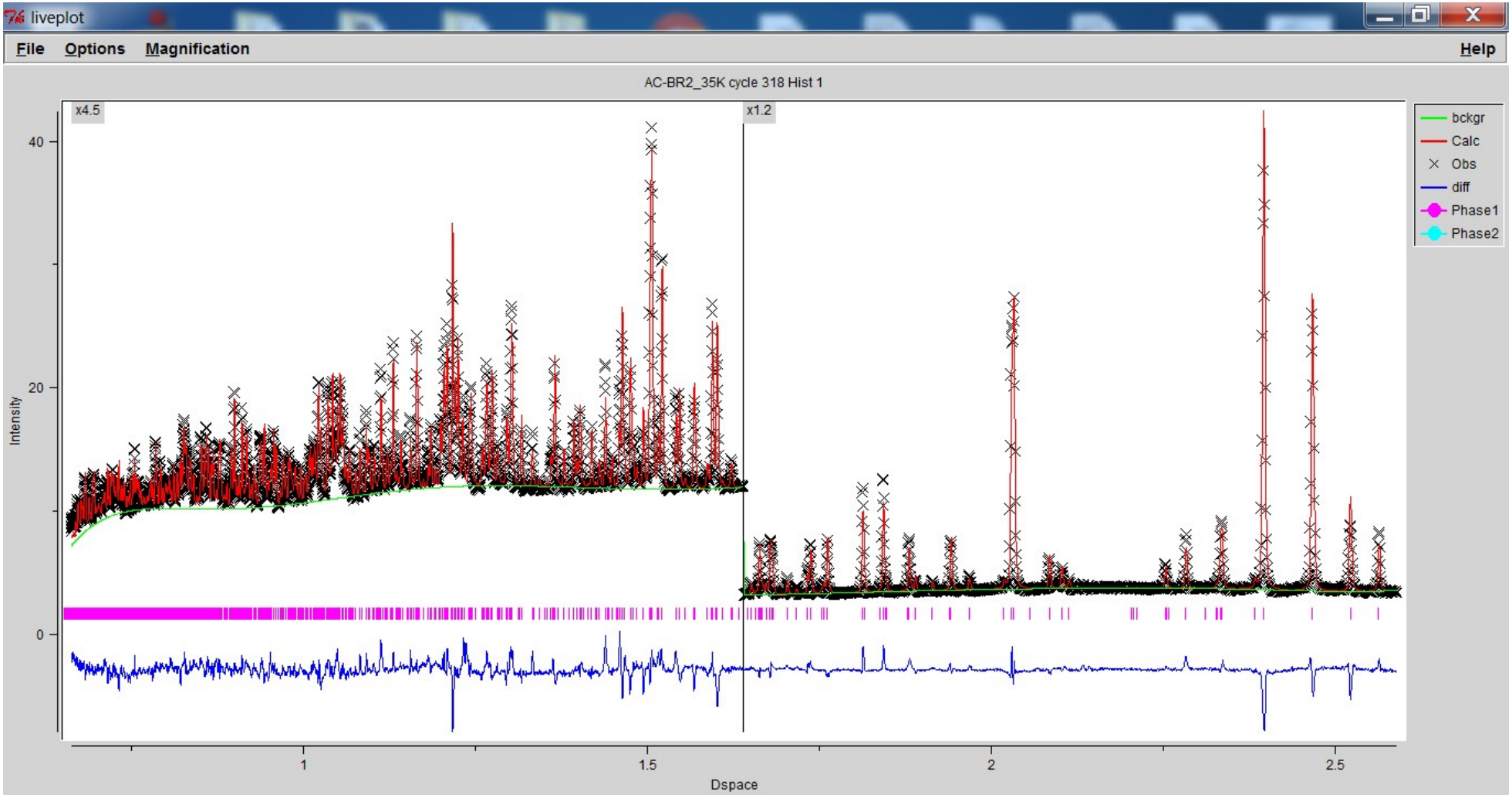
Observed and Difference Plot Acetone Bromine Complex 14K 89.58°Bank



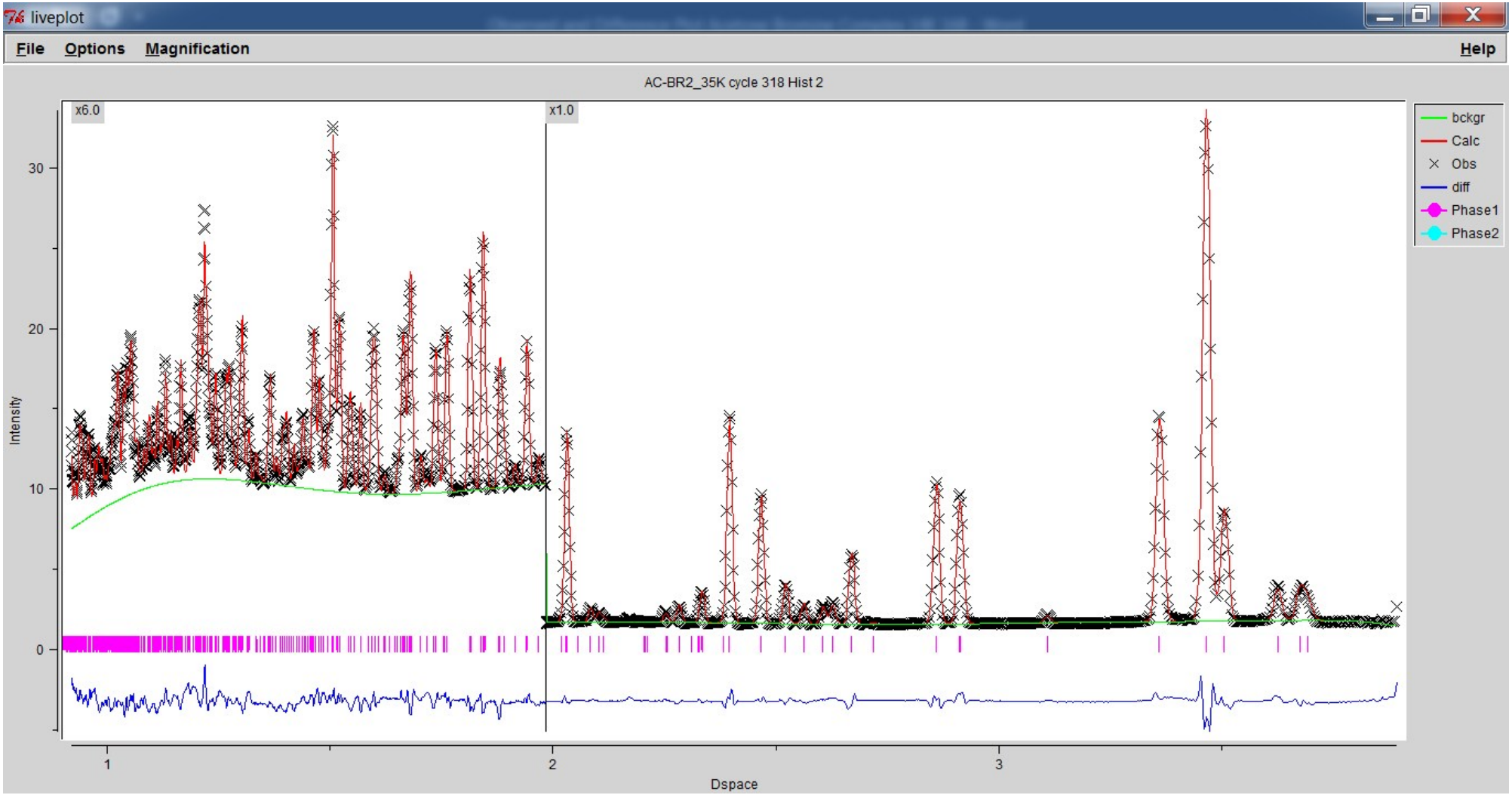
Observed and Difference Plot Acetone Bromine Complex 14K 30.00º Bank



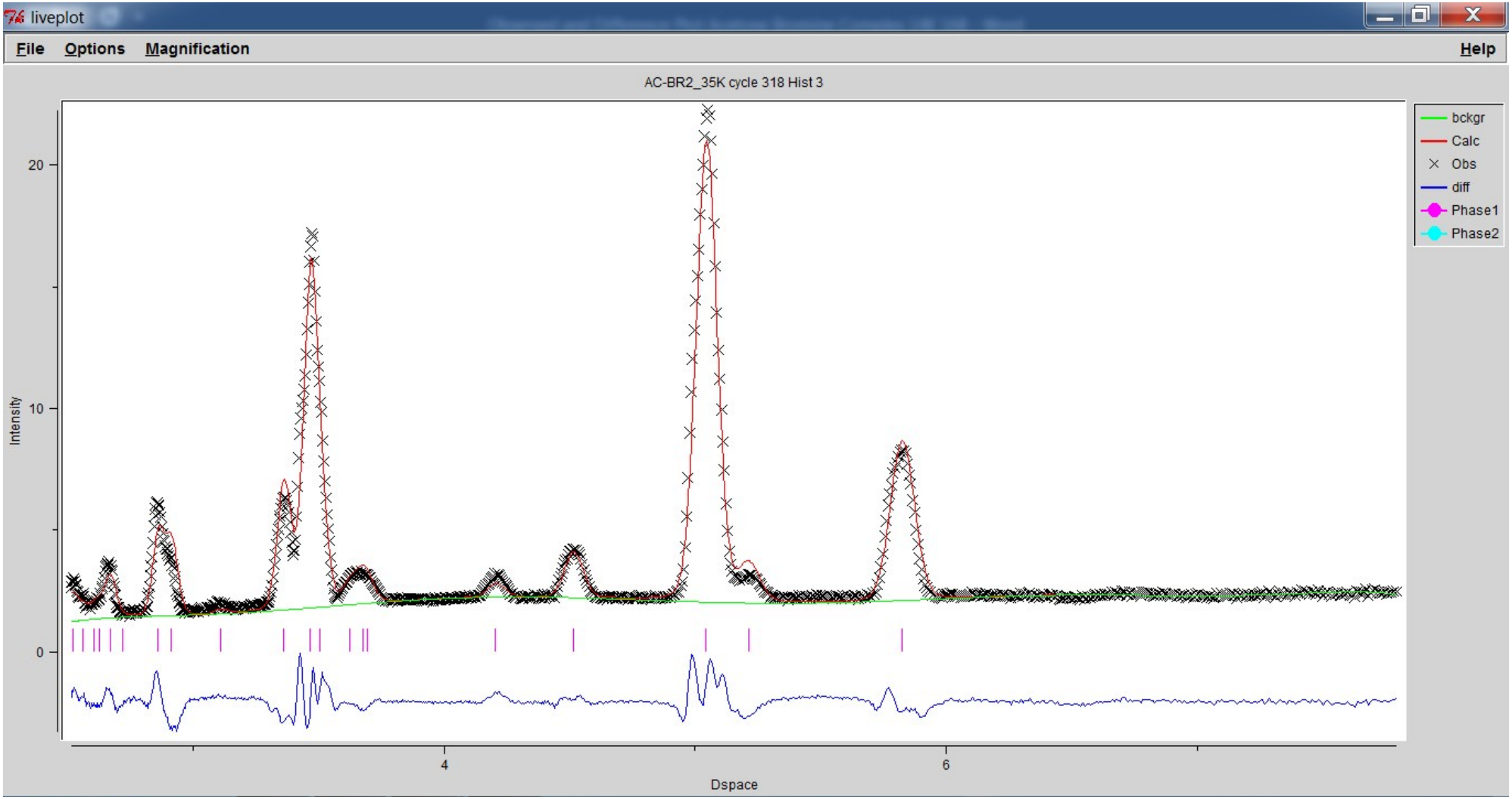
Observed and Difference Plot Acetone Bromine Complex 35K 168.33º Bank



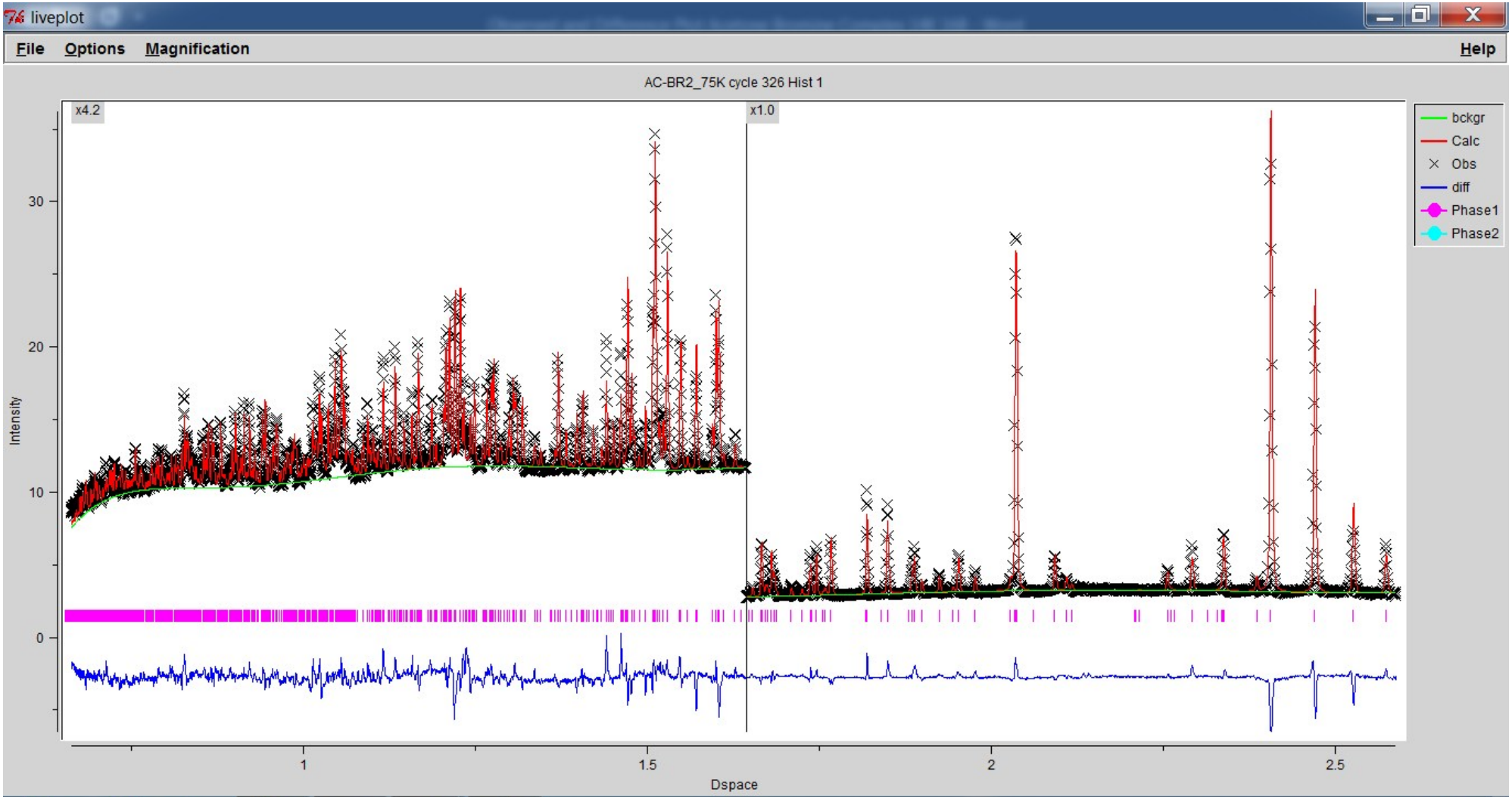
Observed and Difference Plot Acetone Bromine Complex 35K 89.58º Bank



Observed and Difference Plot Acetone Bromine Complex 35K 30.00° Bank

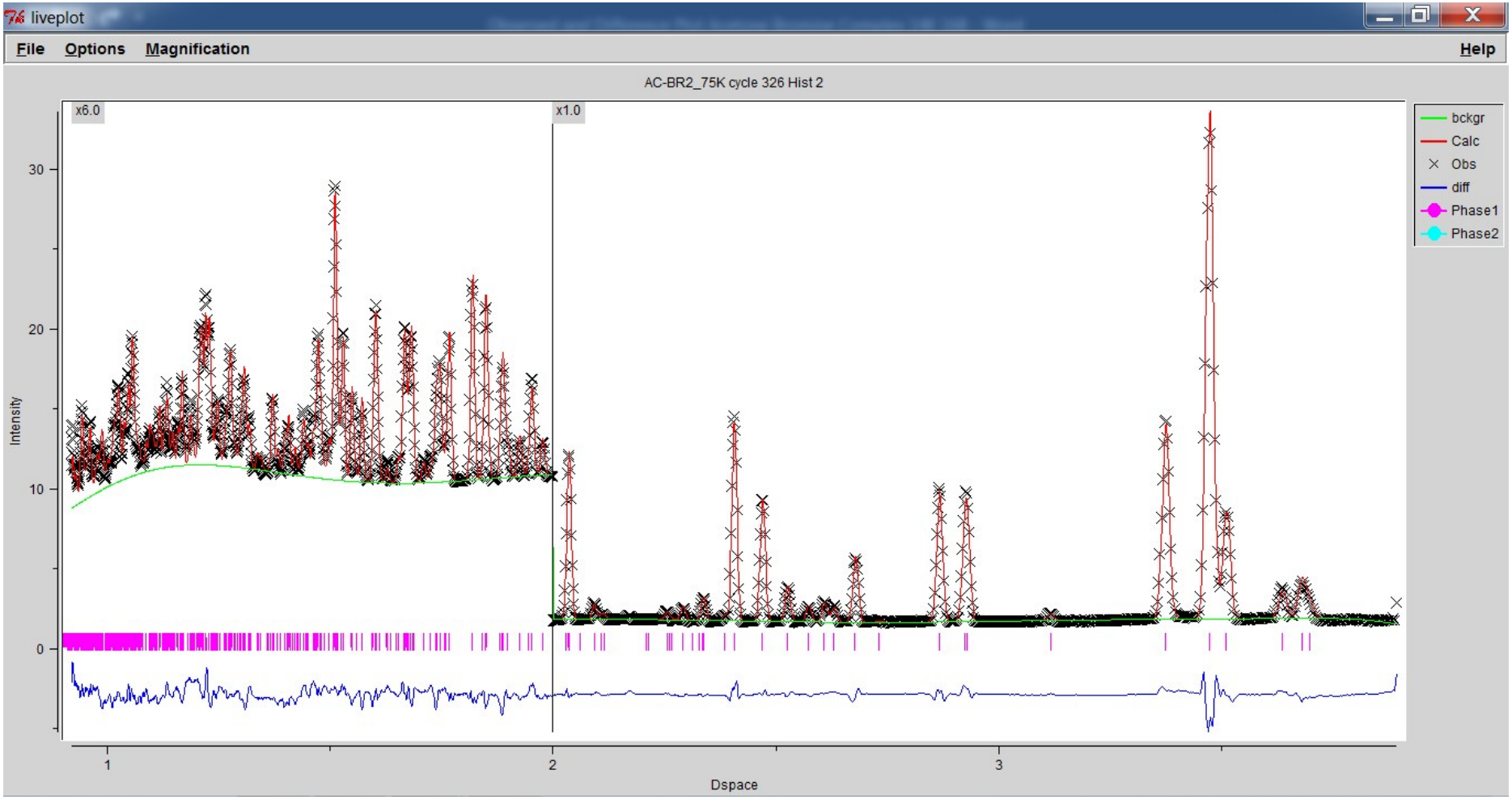


Observed and Difference Plot Acetone Bromine Complex 75K 168.33° Bank

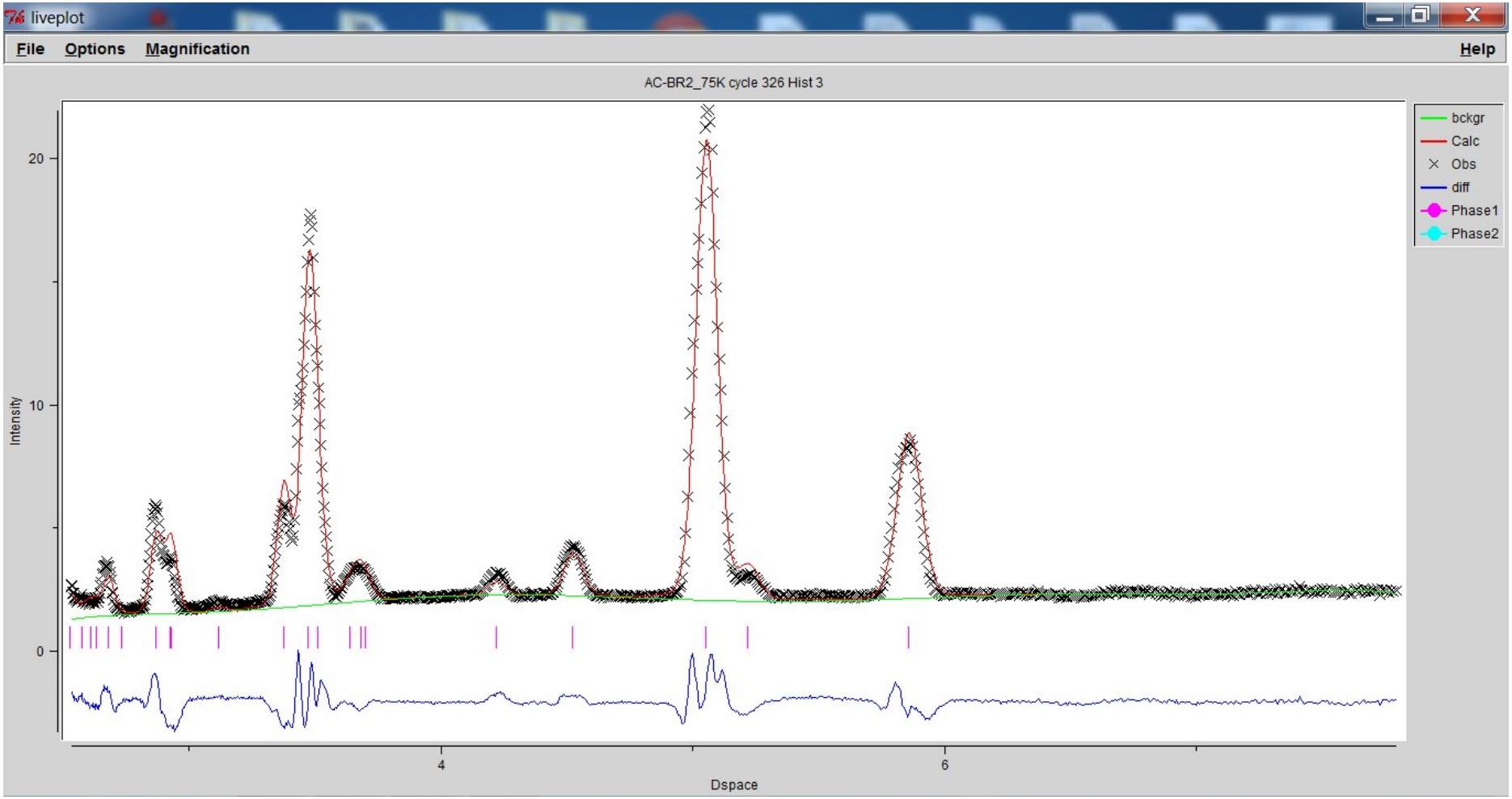


Observed and Difference Plot Acetone Bromine Complex 75K 89.58º Bank

v



Observed and Difference Plot Acetone Bromine Complex 75K 30.00º Bank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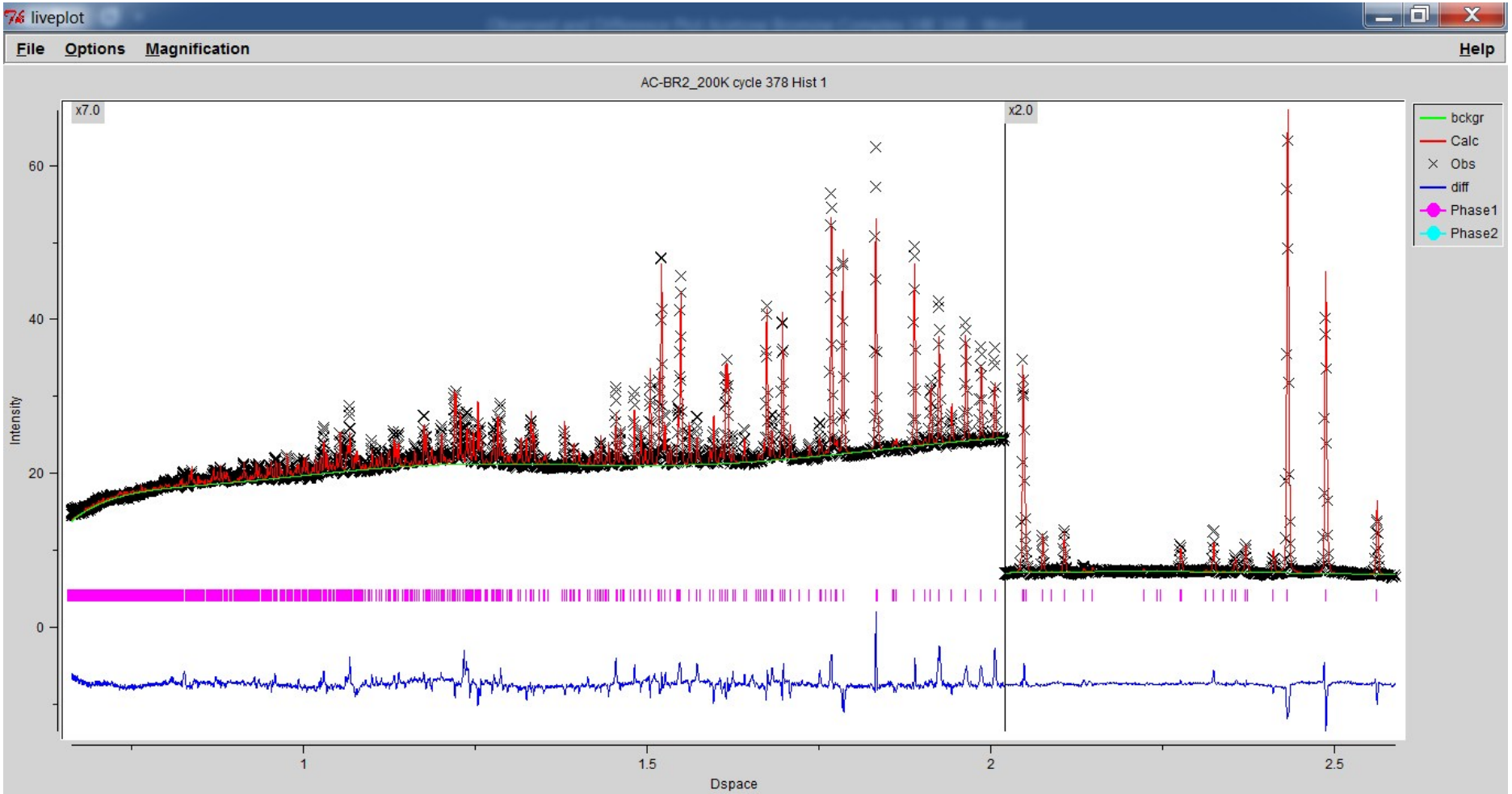
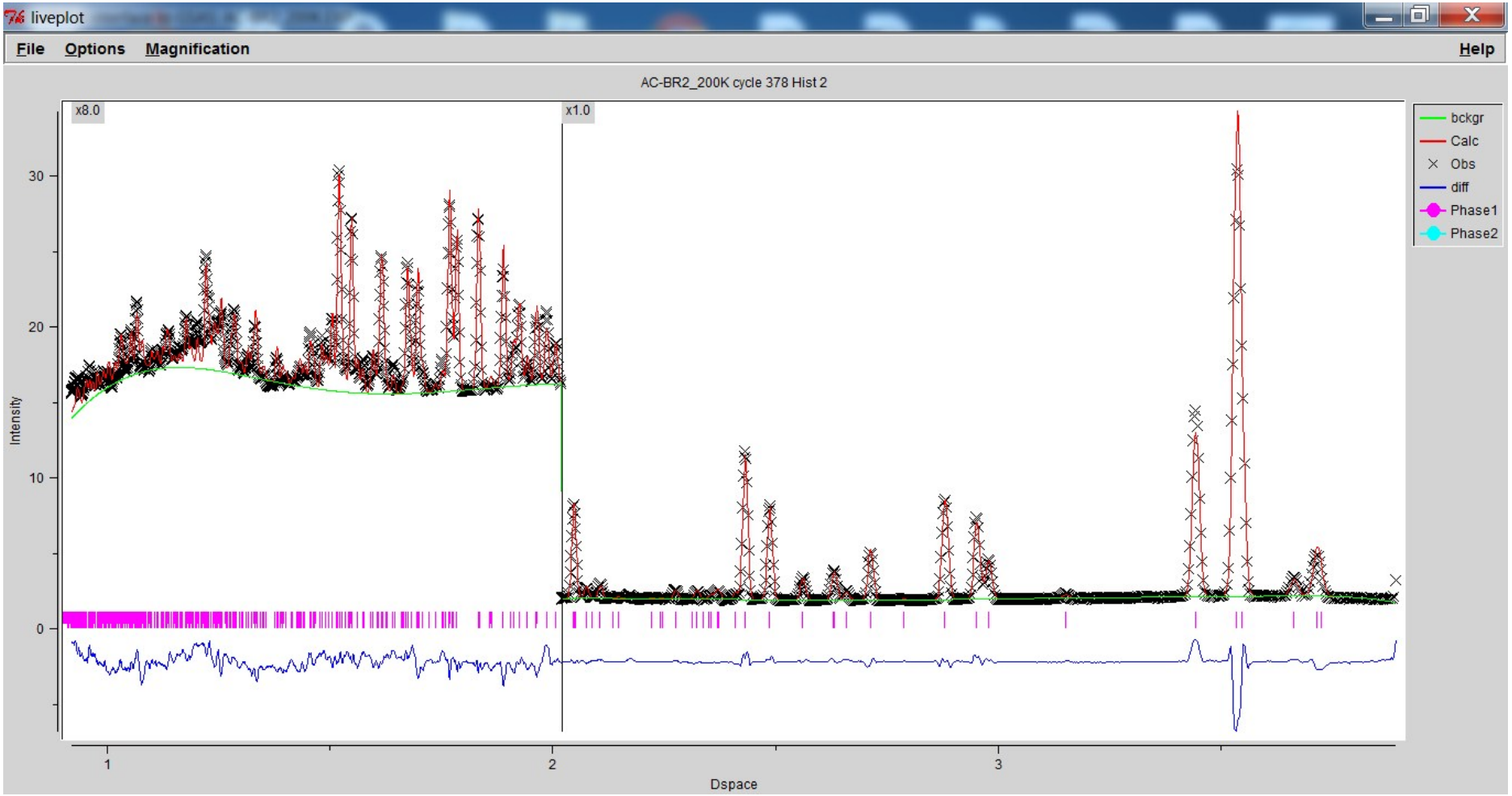
File
Options
Magnification
Help
AC-BR2_75K cycle 326 Hist 3
bckgr
Calc
Obs
diff
Phase1
Phase2
Intensity
20
10
0
4
6
Dspace

Observed and Difference Plot Acetone Bromine Complex 200 K 168.33º Bank



Observed and Difference Plot Acetone Bromine Complex 75K 89.58º Bank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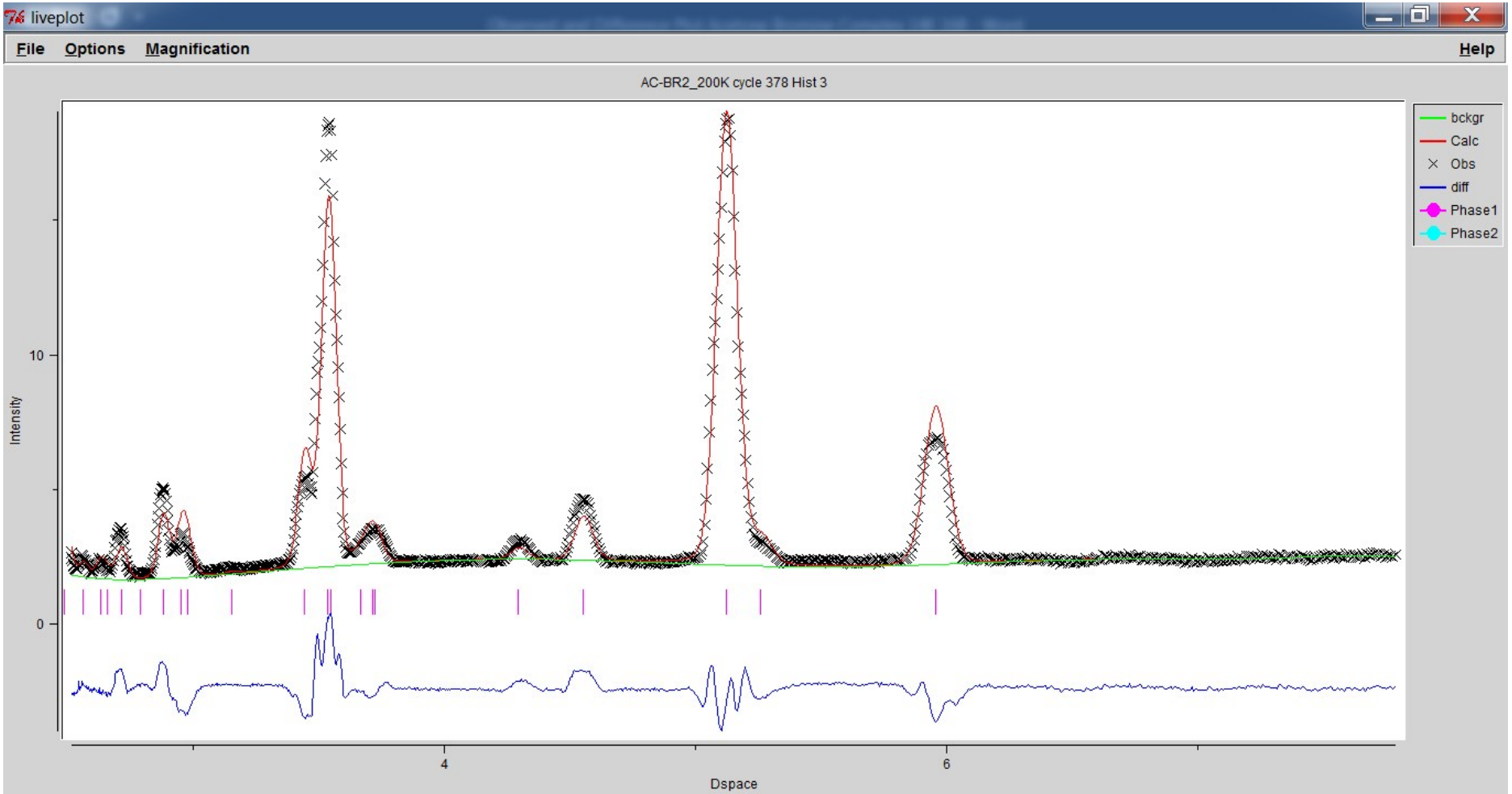
File
Options
Magnification
Help
AC-BR2_200K cycle 378 Hist 2
x8.0
x1.0
bckgr
Calc
Obs
diff
Phase1
Phase2
Intensity
30
20
10
0
1
2
3
Dspace

Observed and Difference Plot Acetone Bromine Complex 30.00º Bank



Data on acetone bound to metals with no filled valence d orbitals

(Groups 1,2,3, Lanthanides, and p block metals)

67 hits (exclusion criteria R<0.05, no disorder)

109 discrete O---M contacts

REFCODE	C=O Distance / Å
DECXEO01	1.234
NASLUO	1.234
FUHCIW	1.233
FUHCIW	1.233
CEMBAY	1.232
FUQHOP	1.232
ODUNUY	1.229
ROJKUW	1.229
BOTHID	1.228
REHBUC	1.228
REHBUC	1.228
IMUGUS	1.227
USARAI	1.227
BOTHEZ	1.226
BOTHEZ	1.226
BOTHEZ	1.226
BOTHID	1.225
BOTHID	1.225
REHBUC	1.225
REHBUC	1.225
TUJSAT	1.225
USARAI	1.225
COTDIZ	1.224
QOTXUU	1.223

ETEVOP	1.222
FEWPUT	1.222
FUHCIW	1.222
ZUHPID	1.222
ODUNAE	1.221
GABXAL	1.22
GIXXES	1.22
HUTBUV	1.22
HUTBUV	1.22
TOKZEA	1.22
TOKZEA	1.22
XOGZOK	1.22
IMUGOM	1.219
XARZUN	1.219
YOKDUY	1.219
DECXEO01	1.218
YOKDUY	1.218
TOKZEA	1.217
TOKZEA	1.217
WOGCUR	1.217
ZUHPID	1.217
MAPMIB	1.216
TUJSAT	1.216
BASTAR	1.215
GIYFUR	1.215
MEHBIK	1.215
TOKZEA	1.215
TOKZEA	1.215
BIGQIT	1.214
DOHVIG	1.214
PORDIL	1.214
RESHAA	1.214

YOGPUH	1.214
HUTBUV	1.213
HUTBUV	1.213
JOBXII	1.213
KCLNLA01	1.213
UNIHEF	1.213
BASTOF	1.212
UNIHEF	1.212
HUTBUV	1.211
HUTBUV	1.211
IMUGOM	1.211
MEHBIK	1.211
QOXSUR	1.211
REHBUC	1.211
RUWTUY	1.211
ZUHPOJ	1.211
RUHFEG	1.21
FUHCIW	1.209
JUZHAN	1.208
RESHAA	1.207
WOTDUG	1.207
ZUDDUZ	1.207
ZUHPOJ	1.207
WOTDUG	1.206
WOTDUG	1.206
YEZPAV	1.206
CAKQIQ	1.205
HUTBUV	1.205
AHIGUV	1.204
MEHBIK	1.204
WOTDUG	1.204
YAPZIZ	1.204

BASVOH	1.202
KAMXUS	1.202
LAFNOX	1.202
GIYFUR01	1.201
HECGEC	1.201
OZOJIX	1.201
APIQAS	1.2
GIXXES	1.2
JOBXAA	1.199
SOVSIF10	1.198
YAPZIZ	1.198
BASVOH	1.197
HUTBUV	1.197
MAPMIB	1.197
GIXXES	1.187
SIKRIO	1.187
HUTBUV	1.186
QILKAX	1.18
DUGJUM	1.174
BOPKAT	1.172
KAKNAO	1.172