

EXCURVE 9.310 >>> 22/08/11 at 17:29:50

Experiment in : f17200.dat

Fit index with K\*\*3 weight: 0.2211E-03 R-factor : 30.9070 Chisqu :  
0.00000 R-exafs : 30.9070 R-distance : 0.0000

&PAR  
LMAX = 25.00000 DLMAX = 25.00000 TLMAX = 9.00000 WP = 0.10000  
NS = 6.00000 E0 = 0.00000 VPI = 0.00000 RMAX = 6.00000  
NO = 1.00 T0 = 1. R0 = 0.00000 A0 = 0.01000  
UN0 = 0. ANG0 = 0.00000 TH0 = 0.00000 PHI0 = 0.00000 CLUS0 =  
-1  
N1 = 1.00 T1 = 3. R1 = 2.05233 A1 = 0.00598  
UN1 = 1. ANG1 = 0.00000 TH1 = 90.00000 PHI1 = 0.00000 CLUS1 =  
1  
N2 = 3.00 T2 = 4. R2 = 2.31856 A2 = 0.00598  
UN2 = 0. ANG2 = 0.00000 TH2 = 90.00000 PHI2 = 0.00000 CLUS2 =  
1  
N3 = 1.00 T3 = 2. R3 = 2.95771 A3 = 0.00840  
UN3 = 1. ANG3 = 238.57245 TH3 = 94.16022 PHI3 = 21.89385 CLUS3 =  
1  
N4 = 1.00 T4 = 2. R4 = 3.10386 A4 = 0.00840  
UN4 = 1. ANG4 = 129.07494 TH4 = 90.08382 PHI4 = 339.96014 CLUS4 =  
1  
N5 = 1.00 T5 = 3. R5 = 4.10659 A5 = 0.00662  
UN5 = 1. ANG5 = 203.63939 TH5 = 94.86033 PHI5 = 11.07169 CLUS5 =  
1  
N6 = 1.00 T6 = 2. R6 = 4.20612 A6 = 0.00662  
UN6 = 1. ANG6 = 163.80774 TH6 = 92.98430 PHI6 = 352.17450 CLUS6 =  
1  
PIV1 = 1.000 PLA1 = 4.000 PLB1 = 3.000 TORA1 = 0.000  
TORB1 = 0.000  
ATOM1 = 30. ION1 = 0. MTR1 = 1.3800 ALF1 = 0.6667 CMAG1 = 0.0000  
ATOM2 = 6. ION2 = 0. MTR2 = 1.1000 ALF2 = 0.6667 CMAG2 = 0.0000  
ATOM3 = 7. ION3 = 0. MTR3 = 1.0000 ALF3 = 0.6667 CMAG3 = 0.0000  
ATOM4 = 16. ION4 = 0. MTR4 = 1.2700 ALF4 = 0.6667 CMAG4 = 0.0000  
OMIN = 1.000 OMAX = 3.000 YMIN = -1.000 YMAX = 1.000  
PLMIN = 0.000 PLMAX = 10.000 ATMAX = 2.000  
XEMIN = 0.000 XEMAX = 120.000 XNP = 50.000 XLMAX = 3.000  
XLOUT = 10.000 XOPT = 1.000 SIZE = 0.300  
WEX = 1.000 WD = 0.000 WA = 0.000 MINANG = -1.000  
ZMIN = 1.000 ZMAX = 1.000  
VX = 0.000 VY = 0.000 VZ = 0.000  
BOND = 0.000 NPARS = 1.000 NIND = 0.000  
ACELL = 1.0000 BCELL = 1.0000 CCELL = 1.0000  
AFAC = 1.0000 AFAC1 = 1.0000 AFAC2 = 1.0000  
AFAC3 = 1.0000 AFAC4 = 1.0000  
EF = -9.2136 EF1 = 0.0000 EF2 = 0.0000  
EF3 = 0.0000 EF4 = 0.0000  
EMIN = 3.0000 EMIN1 = 17.4531 EMIN2 = 3.0000  
EMIN3 = 3.0000 EMIN4 = 3.0000  
EMAX = 915.3892 EMAX1 = 736.1510 EMAX2 = 3000.0000  
EMAX3 = 3000.0000 EMAX4 = 3000.0000  
CW = -1.0000 CW1 = -1.0000 CW2 = -1.0000

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CW3      =  -1.0000 CW4      =  -1.0000
VO       =  -19.3699 FEO    =  -2.7845 RHO0    =   0.5712
POST0    =   1.00000      POST1 =  0.000000E+00 POST2 =  0.000000E+00
POST3    =  0.000000E+00 POST4 =  0.000000E+00 POST5 =  0.000000E+00
POST6    =  0.000000E+00 POST7 =  0.000000E+00 POST8 =  0.000000E+00
PRE0     =  0.000000E+00 PRE1  =  0.000000E+00 PRE2  =  0.000000E+00
POST01   =   1.00000      POST11=  0.000000E+00 POST21=  0.000000E+00
POST31   =  0.000000E+00 POST41=  0.000000E+00 POST51=  0.000000E+00
POST61   =  0.000000E+00 POST71=  0.000000E+00 POST81=  0.000000E+00
PRE01    =  0.000000E+00 PRE11 =  0.000000E+00 PRE21 =  0.000000E+00
OFFSET=   0.010 DWMIN =    0.002 DWMAX =    0.020 TEMP  =  298.000
&END
&ERR
EF                0.64079 R1                0.01389 R2                0.00352 A[1-2]
0.00117
A[3-4]            0.00972 A[5-6]            0.00396
&END
&SET
TITLE ' '
FINAL_STATE = L+1
QUINN = ON
DISORDER = APPROX
WEIGHTING = K3
POLARISATION = OFF
THEORY = SMALL_ATOM
CORRELATION = ON
ATOMIC_ABS = OFF
AVERAGE = OFF
RELCOR = ON
WAVEVEC = CENTRAL
RCOR = OFF
MS = UNITS
MAPSIZE = LARGE
EXCHANGE = HEDIN-LUNDQVIST
DEBUG = OFF
GROUND_STATE = VON_BARTH
CONSTANT = NONE
SYM = ON
SIGMA = OFF
AUTOBACK = OFF
RESTRAINTS = ABS
&END

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