Optimization and evaluation of data quality for charge density studies

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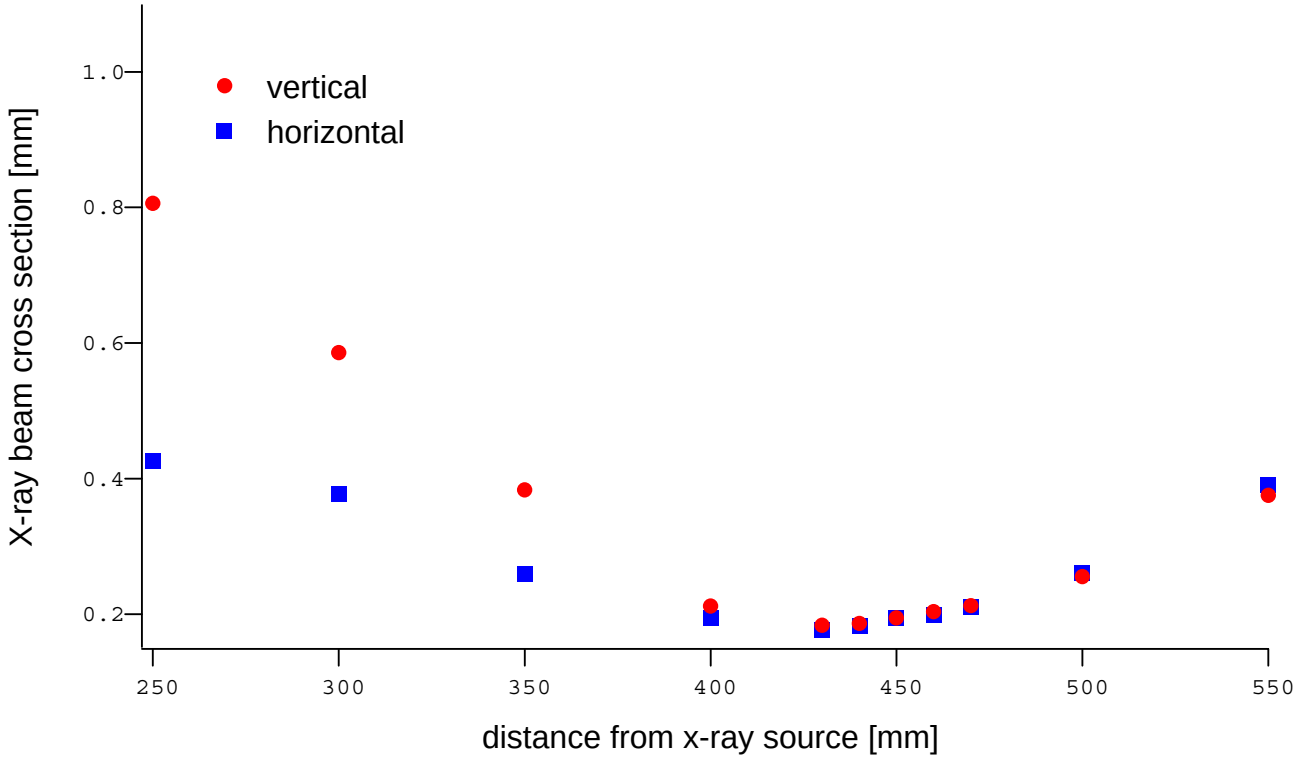
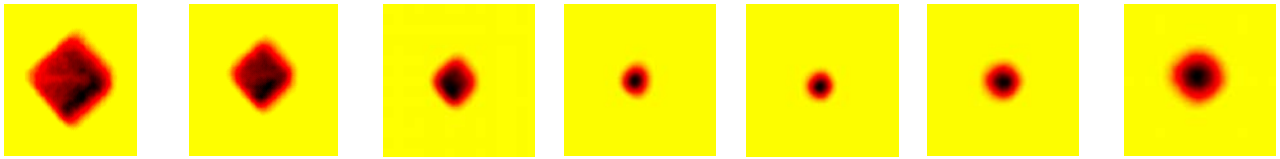
Supplementary Material

Beam profiles
Scale factor and normal probability plots.

X-ray Beam Cross Section of MicroMax-007 + VariMax-Mo

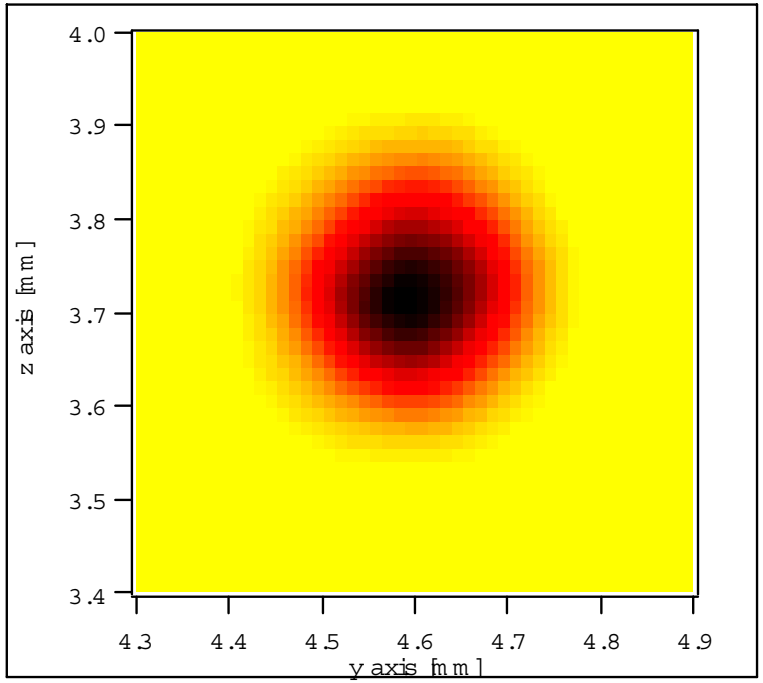


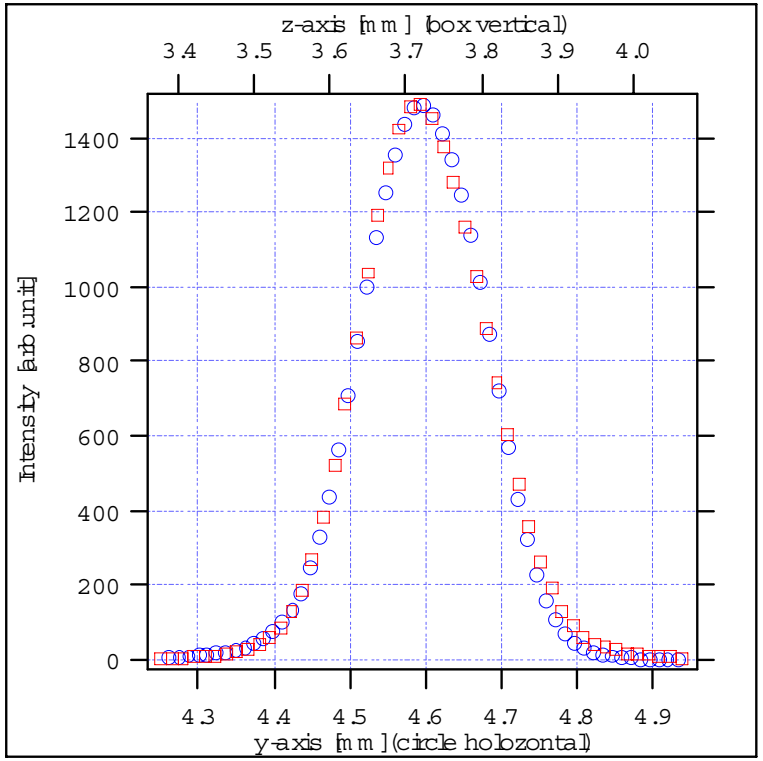


250 mm | 300 mm | 350 mm | 400 mm | 450 mm | 500 mm | 500 mm

Beam Shape of MM007 with VM-Mo

450 mm from X-ray focus

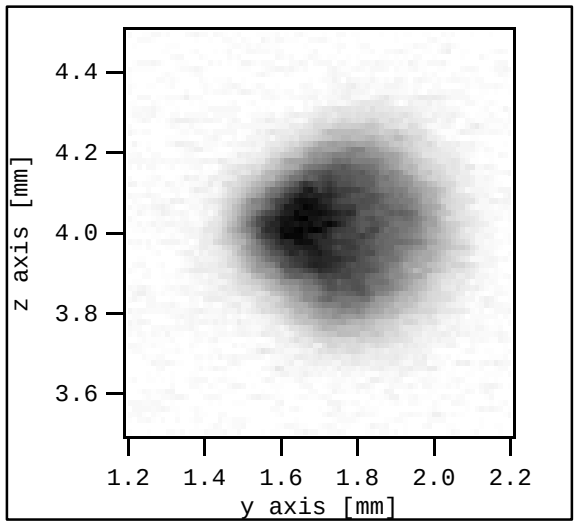


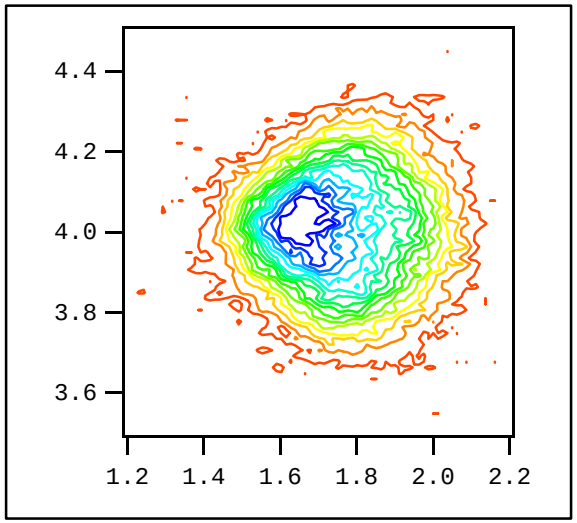


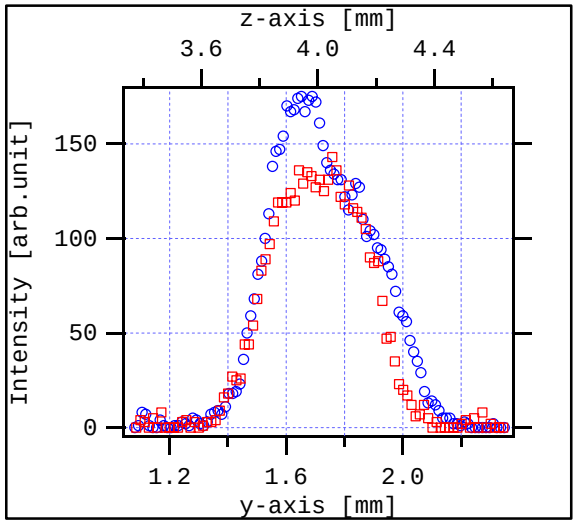
Horizontal **FWHM=0.193 mm**
FW10M=0.334 mm

Vertical **FWHM=0.194 mm**
FW10M=0.346 mm

ultraX + 50kV100mA fine 0.3
mirror adjast to intensty maximum



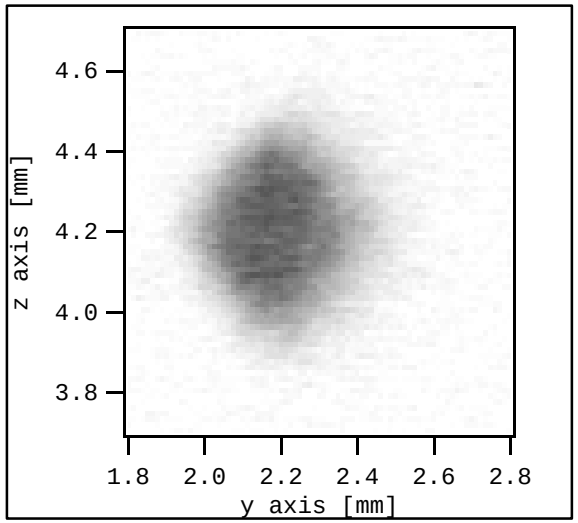


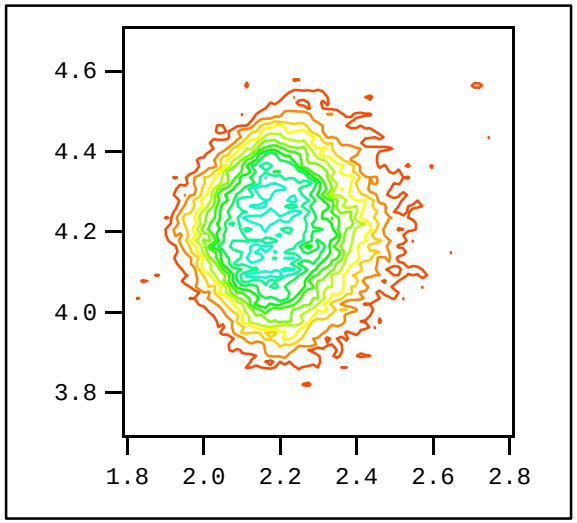


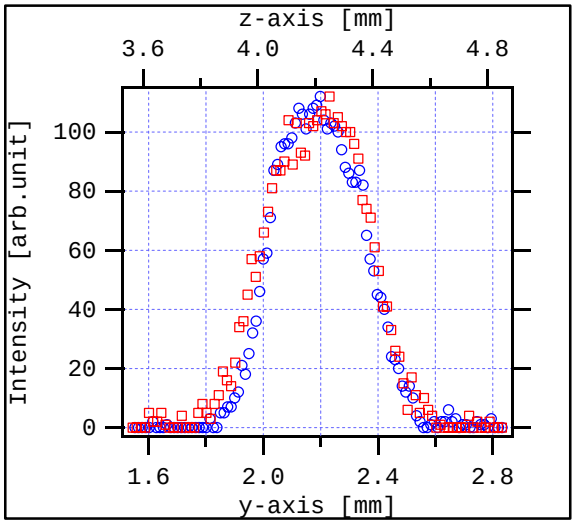
Y direction FWHM=0.427
FW10M=0.674

Z direction FWHM=0.421
FW10M=0.636

ultraX + 50kV100mA fine 0.3
mirror adjast to intensty flat



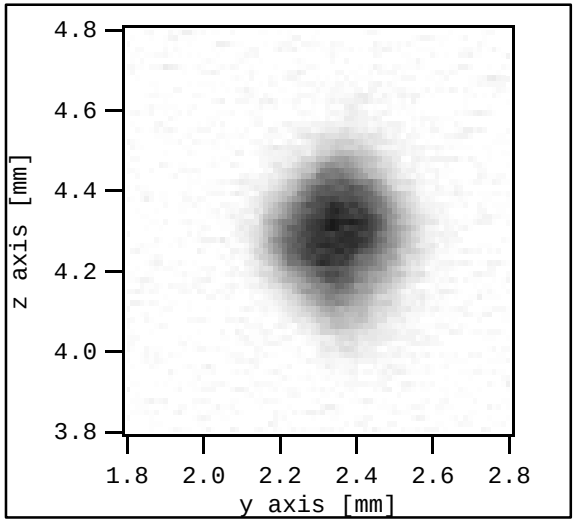


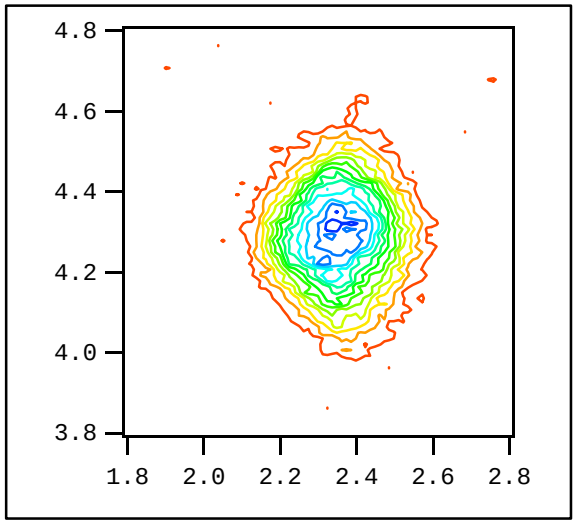


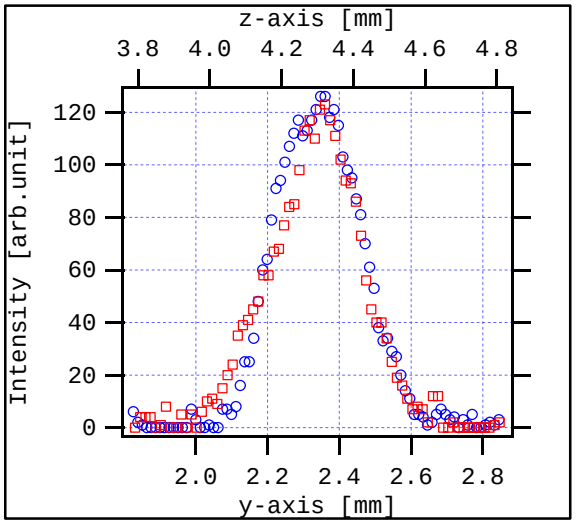
Y direction FWHM=0.376
FW10M=0.609

Z direction FWHM=0.412
FW10M=0.647

ultraX + 50kV24mA 0.1focus



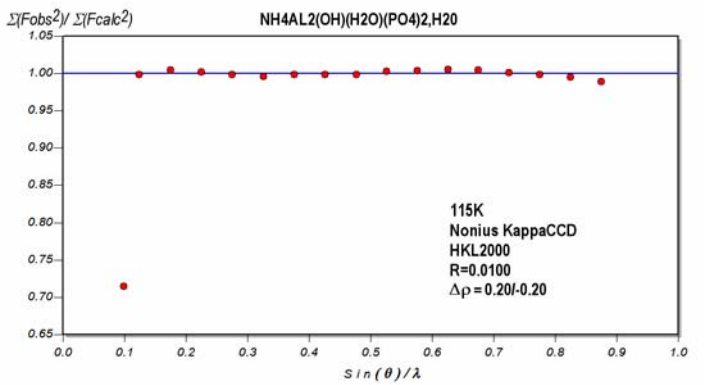


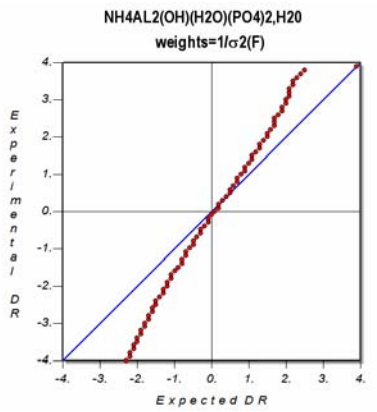


Y direction FWHM=0.286
FW10M=0.47

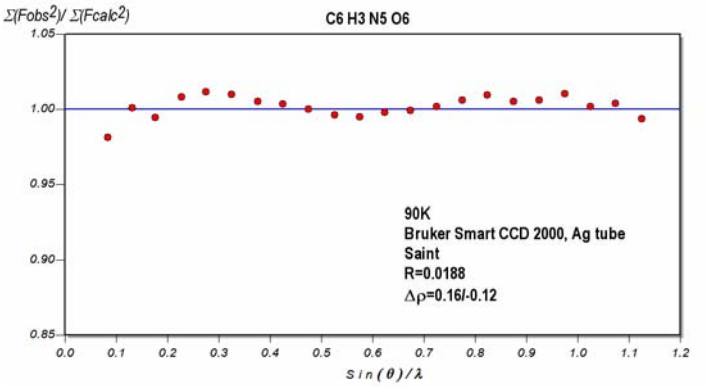
Z direction FWHM=0.284
FW10M=0.517

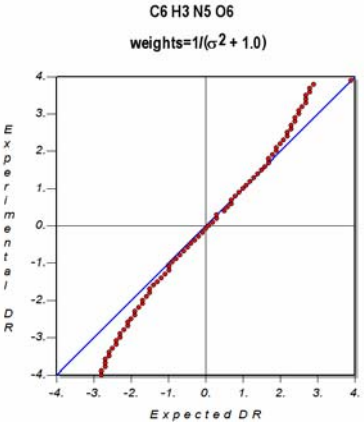
E. Aubert, F. Porcher, Souhassou & C. Lecomte, *Acta Cryst.* (2003) **B59**, 687-700.



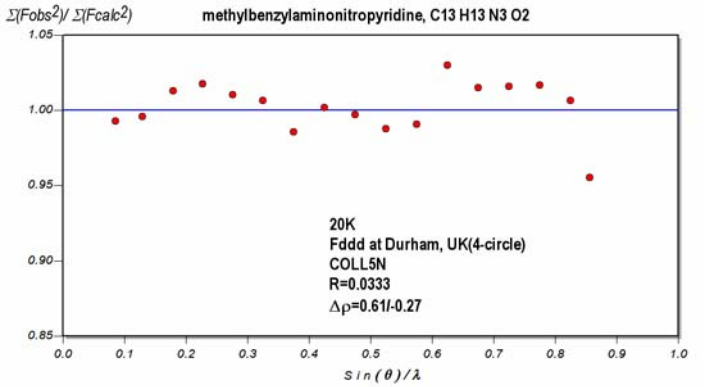


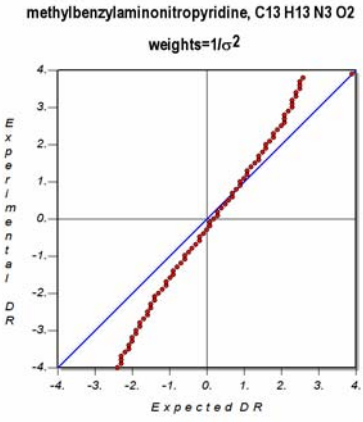
Y.-S. Chen, A.I. Stash & A.A. Pinkerton, *Acta Cryst.* (2007) **B63**, 309-318.



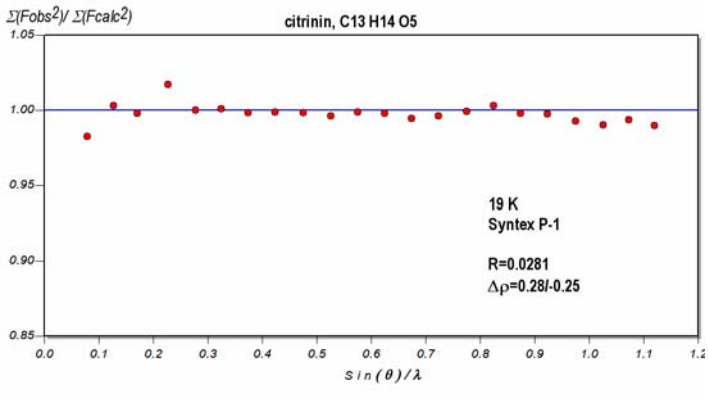


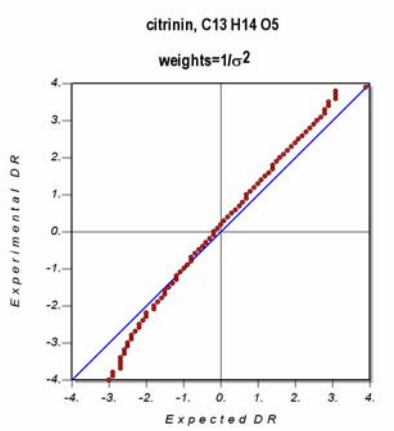
J.M. Cole, A.E. Goeta, J.A.K. Howard & G.J. McIntyre, *Acta Cryst*. (2002) **B58,** 690-700.



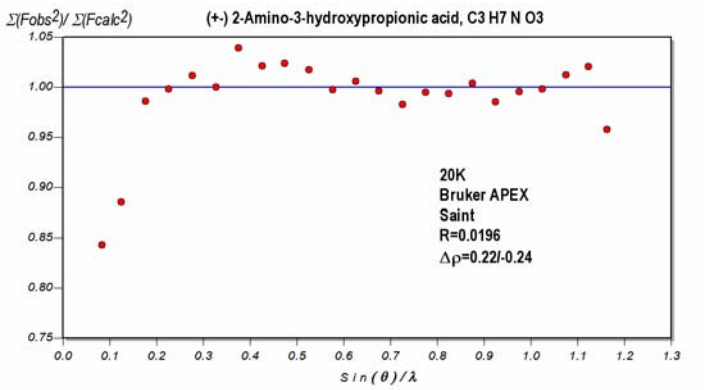


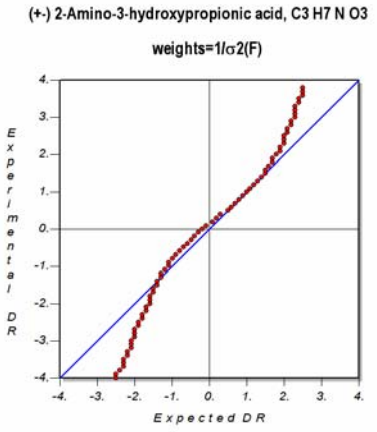
R. Destro, L. Loconte, L.L. Presti, P. Roversi & R. Soave, *Acta Cryst*. (2004) **A60**, 365-370.

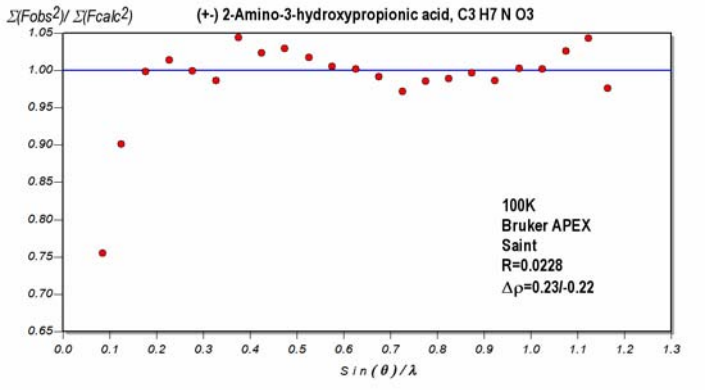


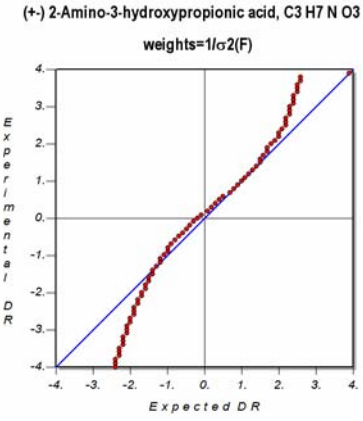


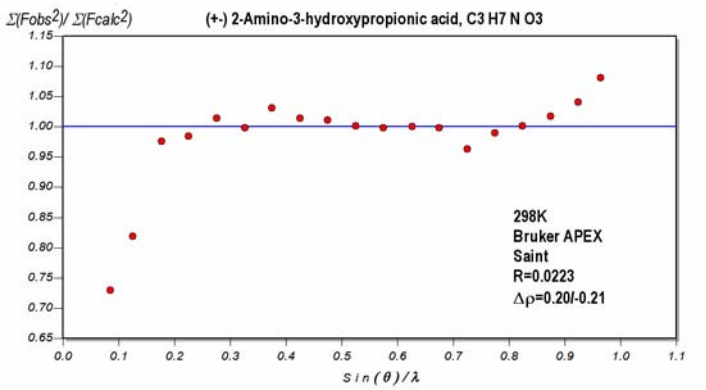
B. Dittrich, C.B. Hübschle, M. Messerschmidt, R. Kalinowski, D. Girnt & P. Luger, *Acta Cryst*. (2005) **A61**, 314-320.

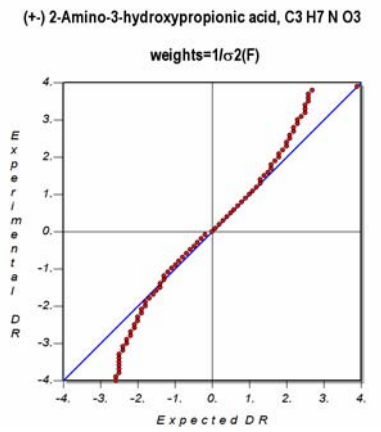




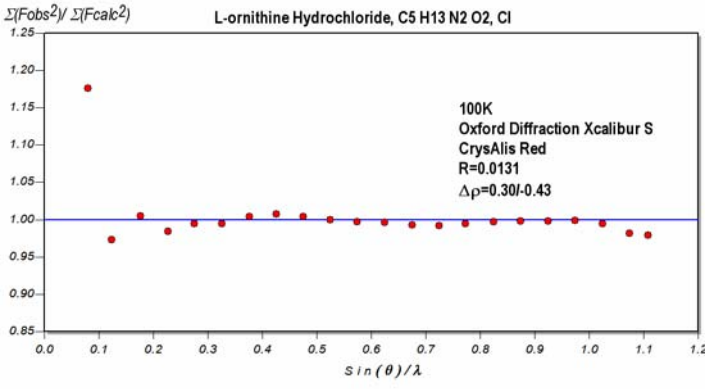


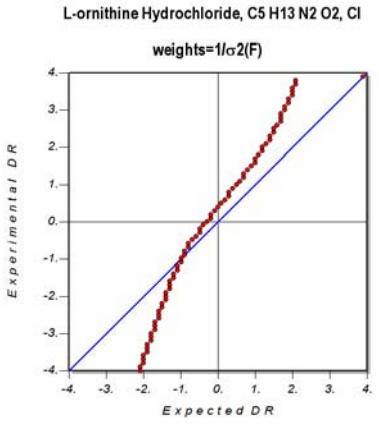




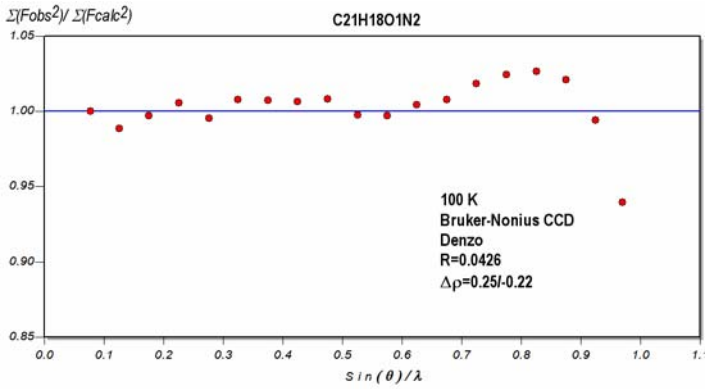


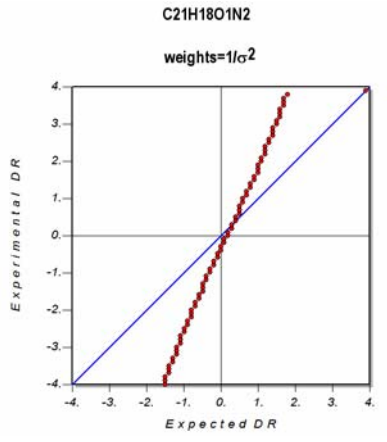
B. Dittrich, P. Munshi & M.A. Spackman *Acta Cryst*. (2007) **B63**, 505-509.

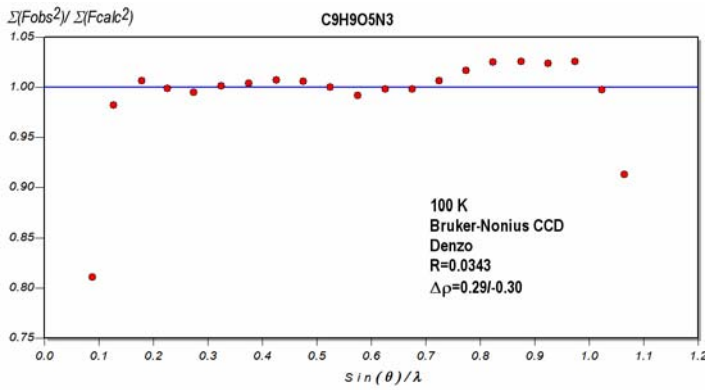


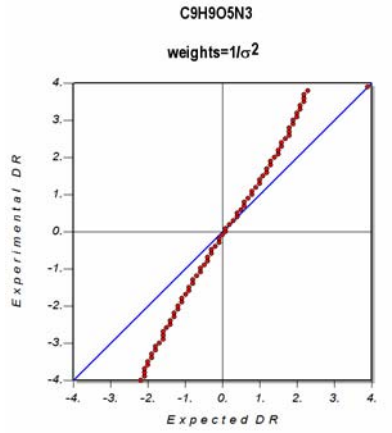


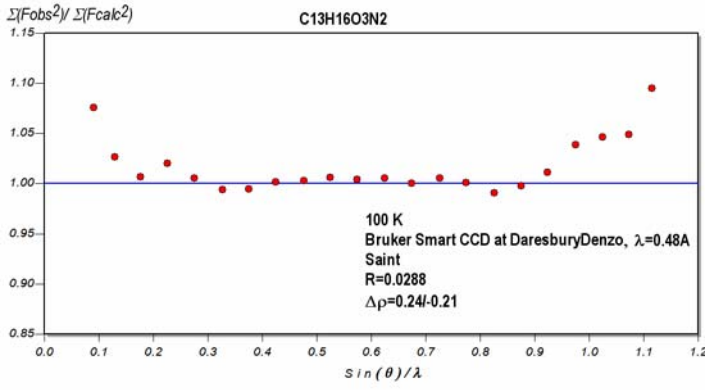
P.M. Dominiak, E. Grech, G. Barr, S. Teat, P. Mallinson & K. Woźniak, *Eur. J. Chem*. (2003) **9**, 963-966.

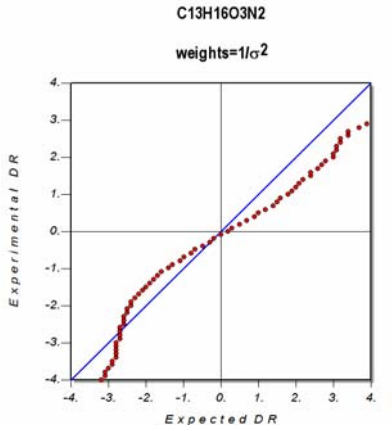




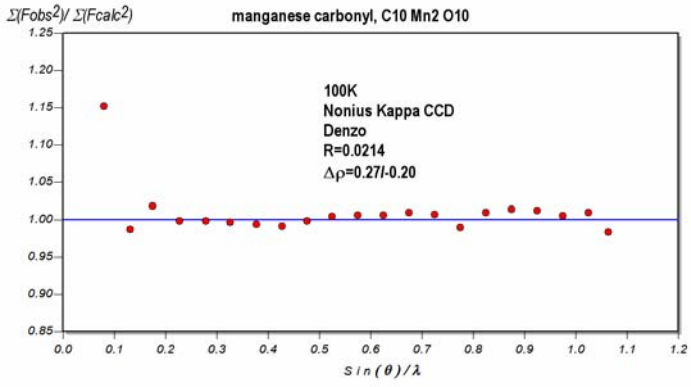


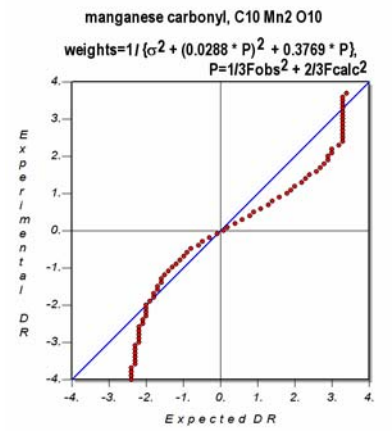




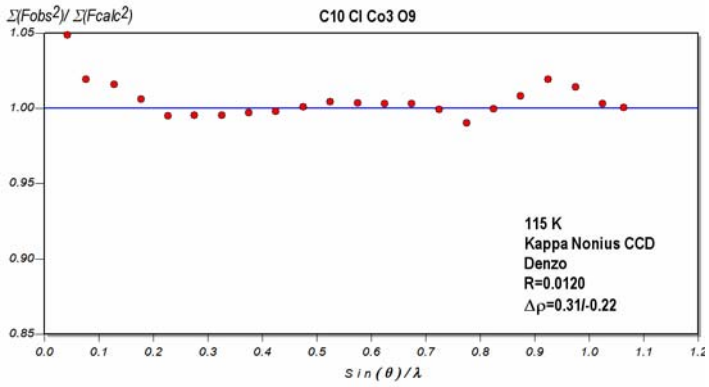


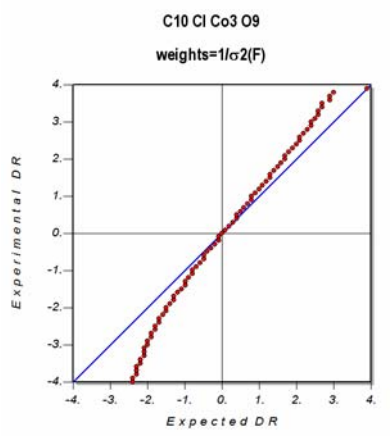
L.J. Farrugia, P.R. Mallinson & B. Stewart, *Acta Cryst.* (2003) **B59**, 234-247.

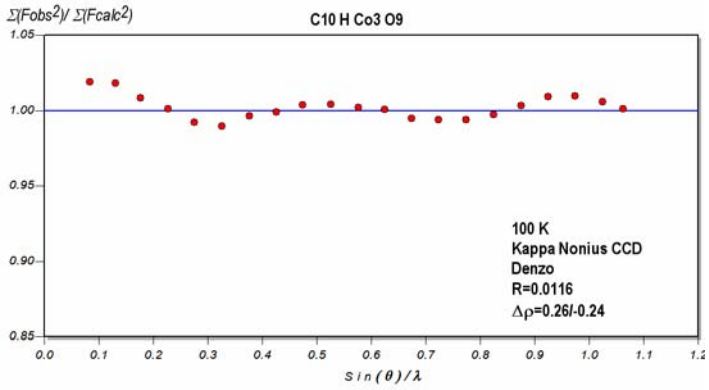


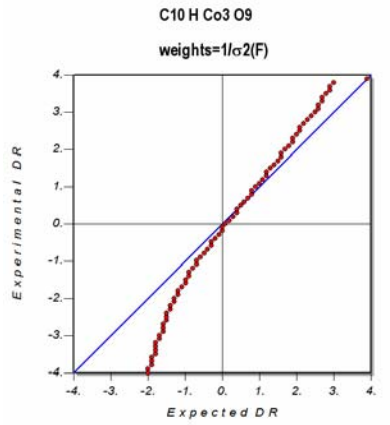


L.J. Farrugia & C. Evans, *C. R. Chimie* (2005) **8**, 1566-1583.

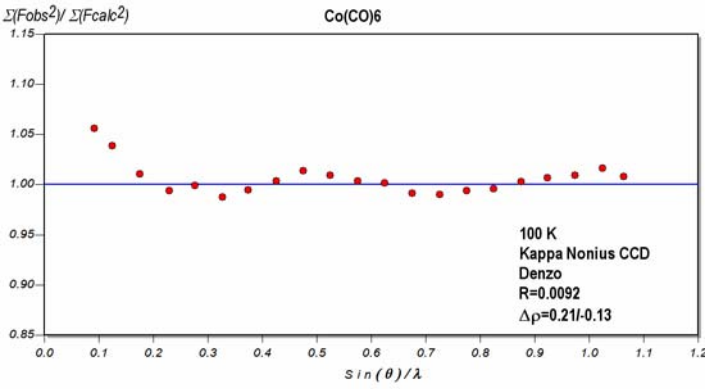


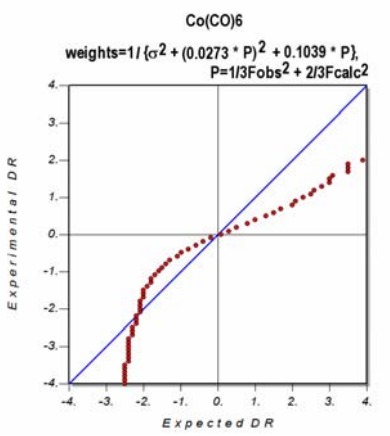


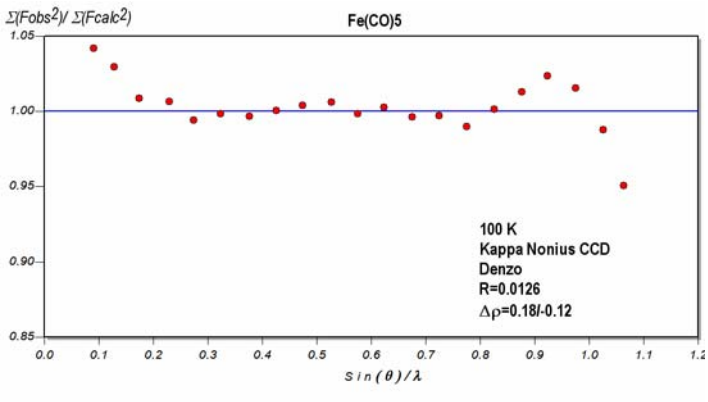


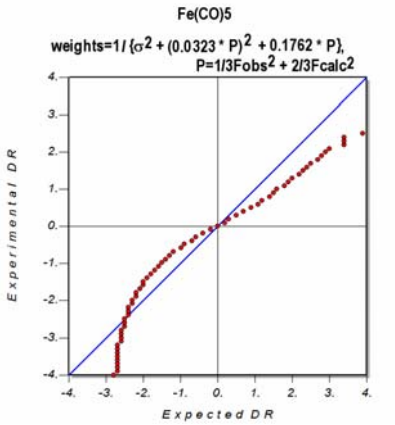


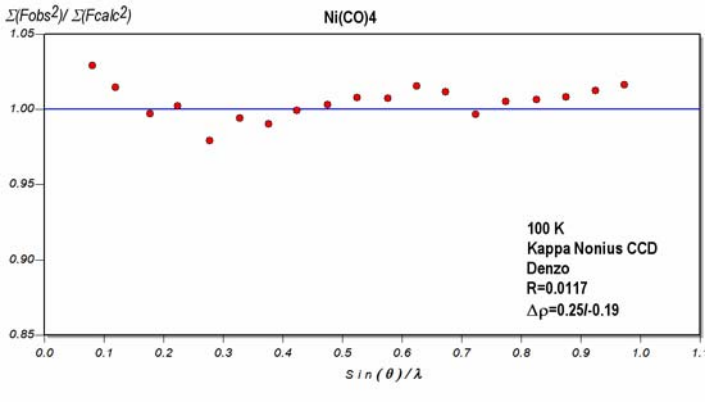
L.J. Farrugia & C. Evans, *J. Phys. Chem.* (2005) **A109**, 8834-8848.

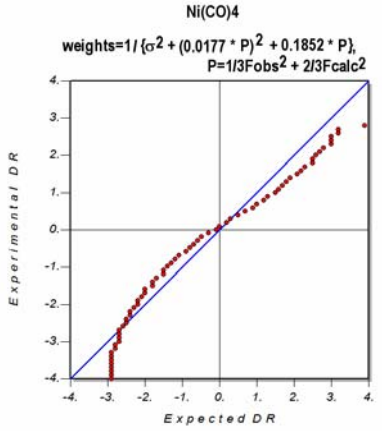




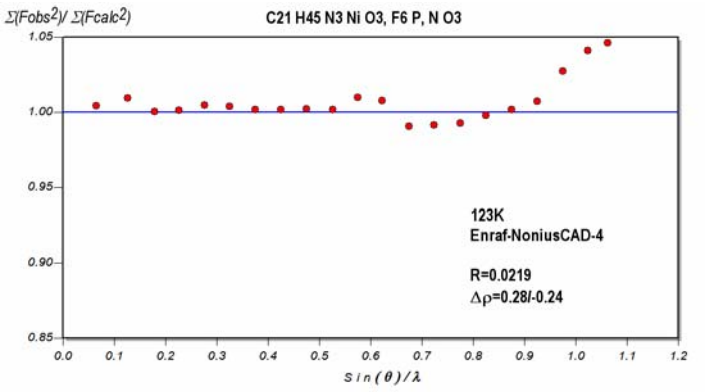


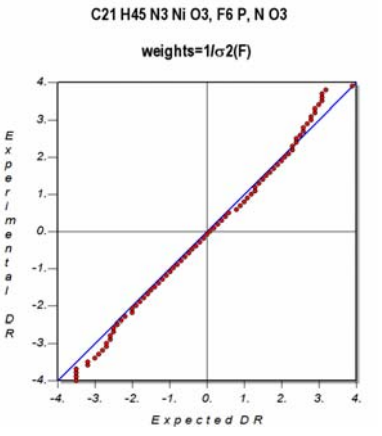




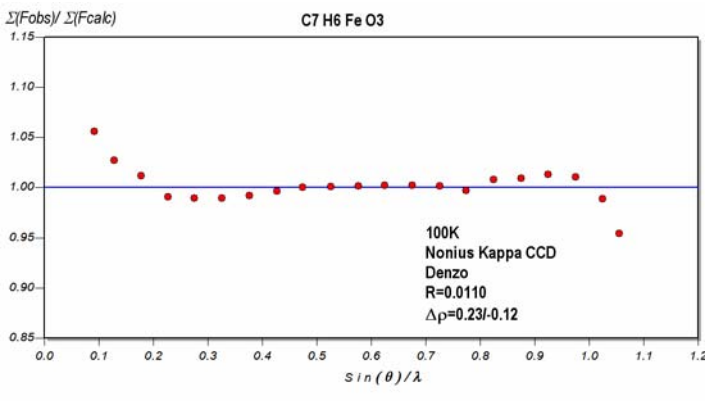


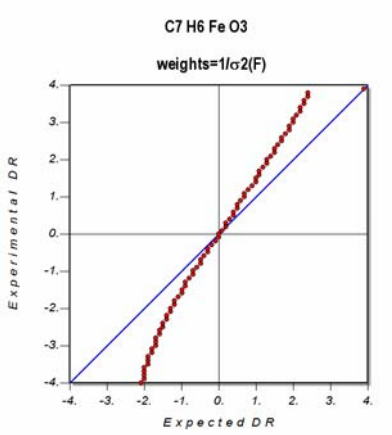
L.J. Farrugia, C.S. Frampton, J.A.K. Howard, P.R. Mallinson, R.D. Peacock, G.T. Smith & B. Stewart, *Acta Cryst.* (2006) **B62**, 236-244.



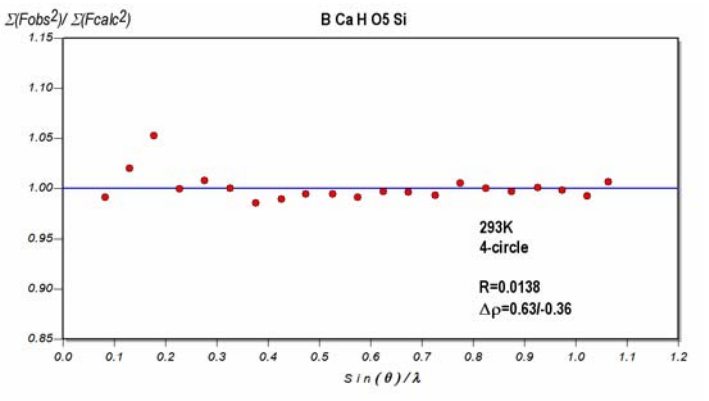


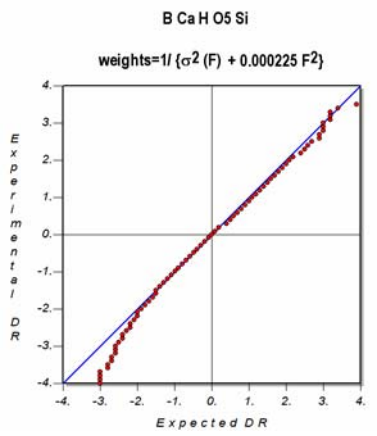
L.J. Farrugia, C. Evans & M. Tegel, *J. Phys. Chem.* (2006) **110**, 7952-7961



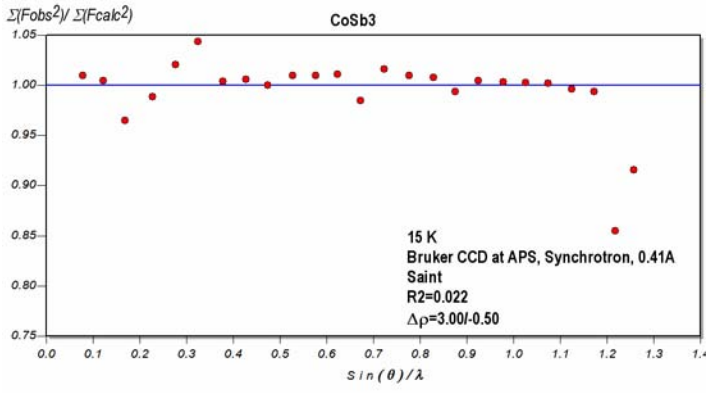


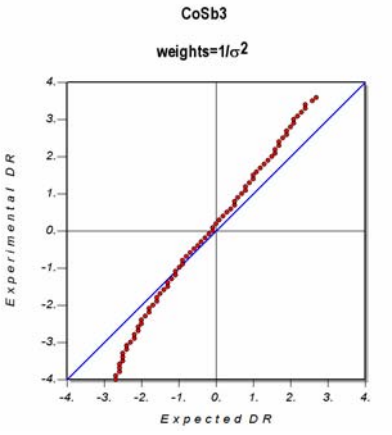
Yu.V. Ivanov & E.L. Belokoneva, *Acta Cryst.* (2007) **B63**, 49-55.

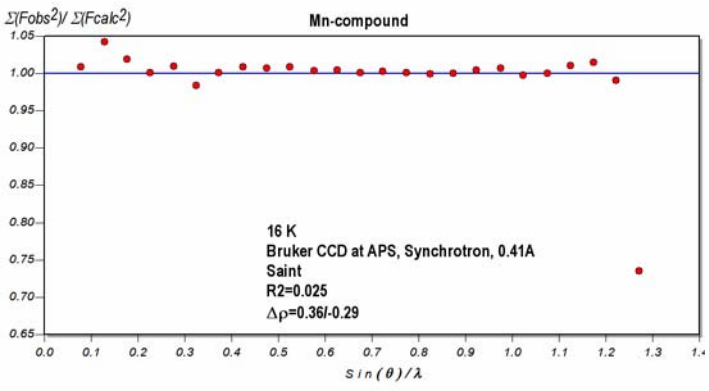


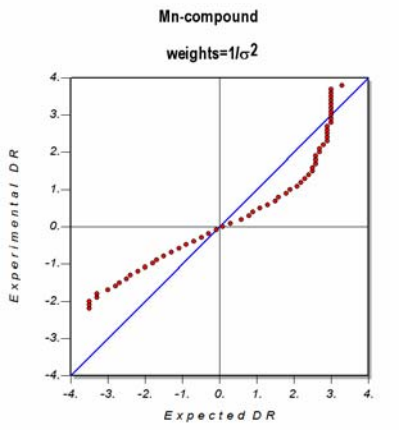


B.B. Iversen & J. Overgaard, personal communication.

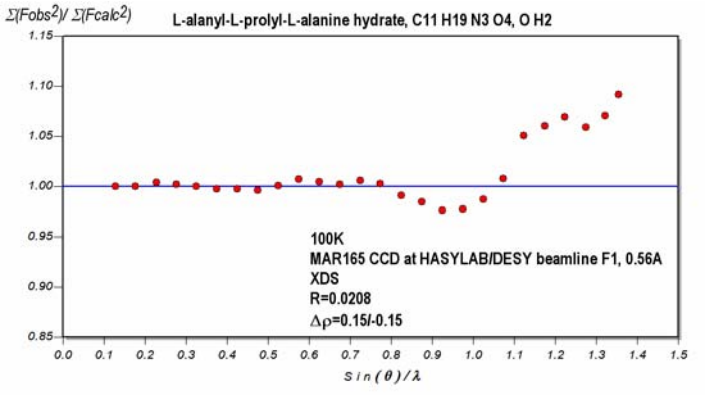


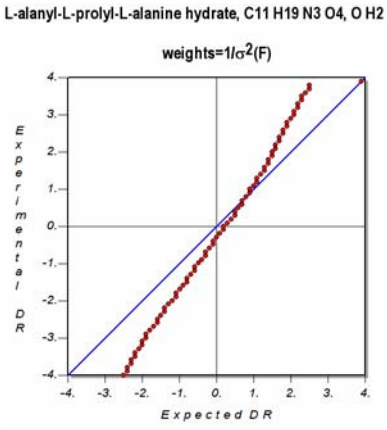




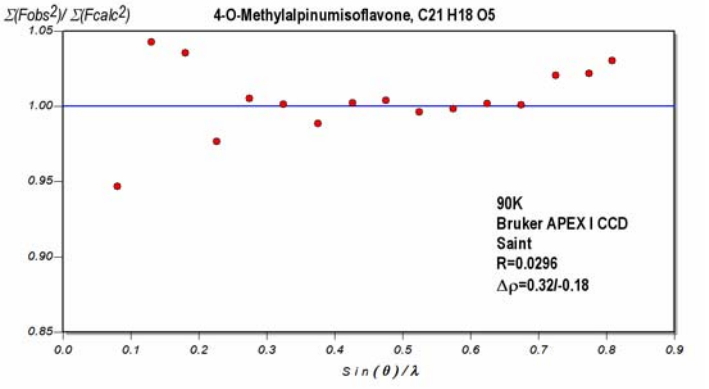


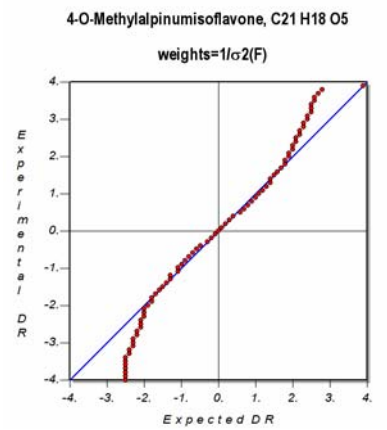
R. Kalinowski & P. Luger, *Acta Cryst. B* (2007) in press.

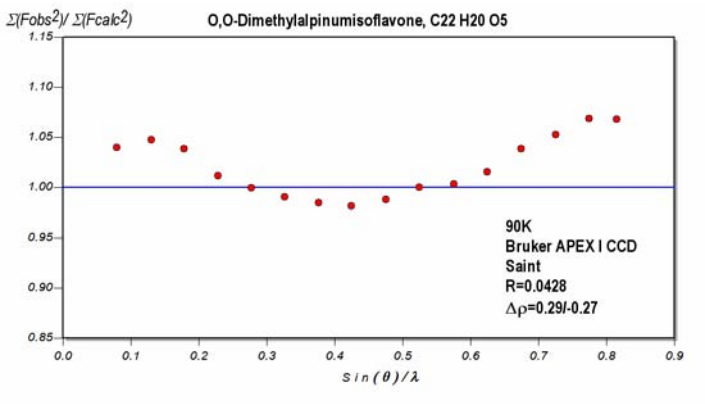


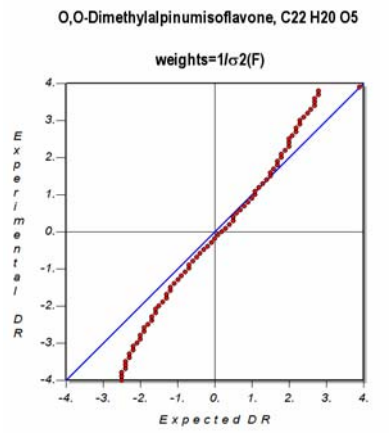


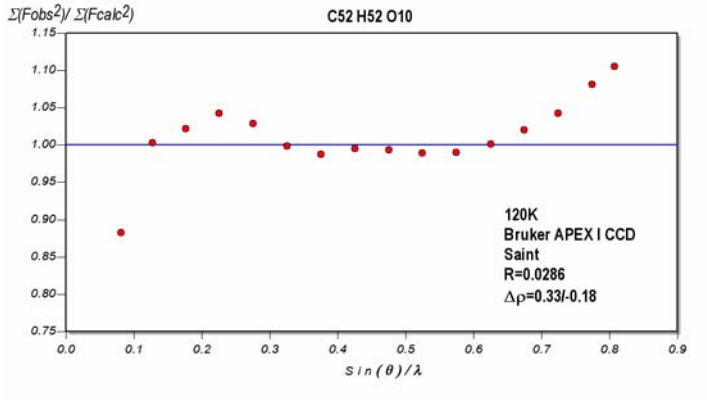
R. Kingsford-Adaboh, B. Dittrich, C.B. Hübschle, W.S.K. Gbewonyo & H. Ishida, *Acta Cryst*. (2006) **B62**, 843-849.

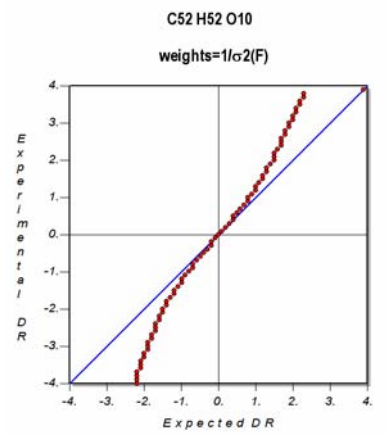




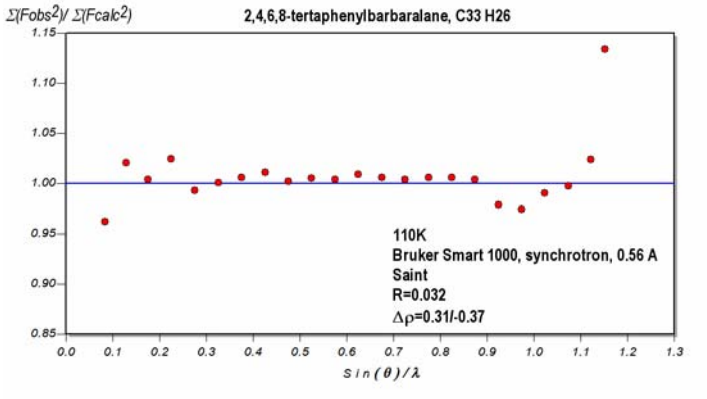


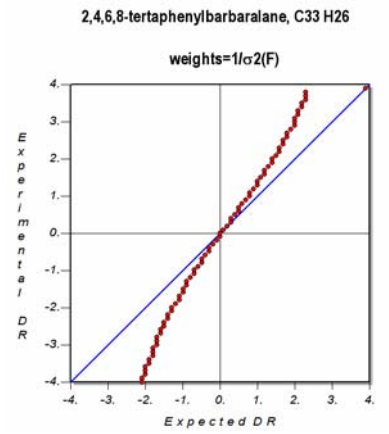




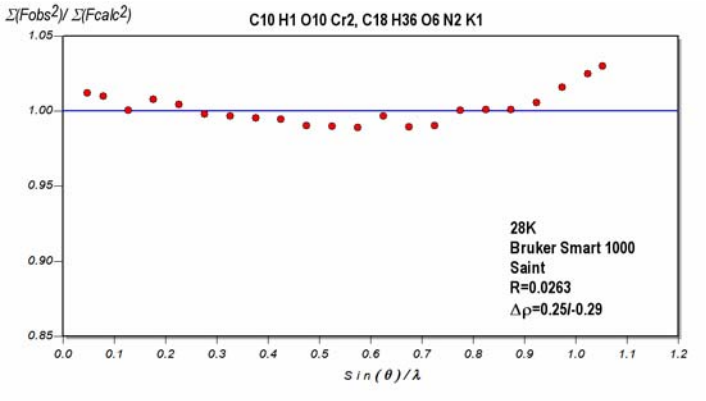


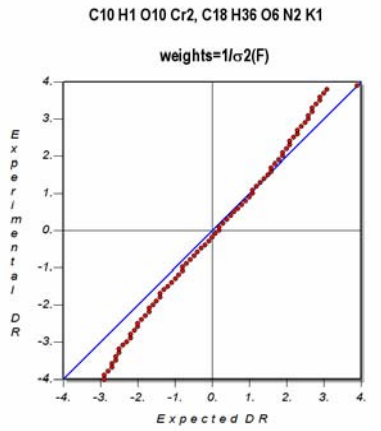
P. Luger, M. Messerschmidt, S. Scheins & A. Wagner, *Acta Cryst* (2004) **A60**, 390-396.



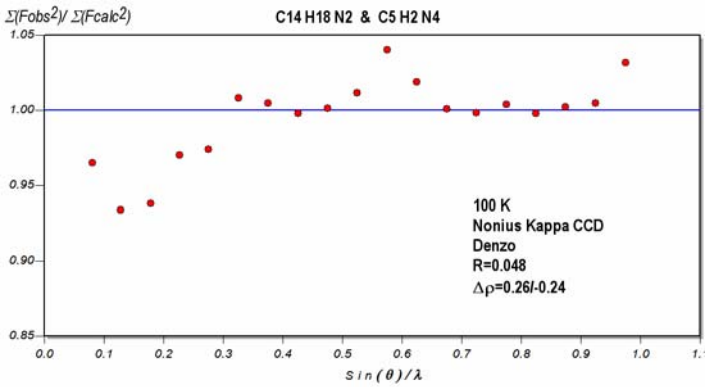


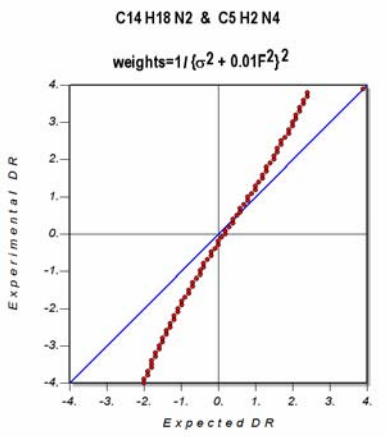
P. Macchi & A. Sironi, *Acta Cryst.* (2004) **A60**, 502-509.

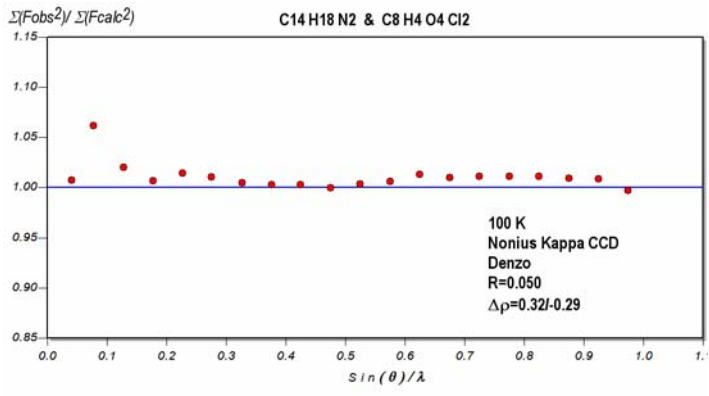


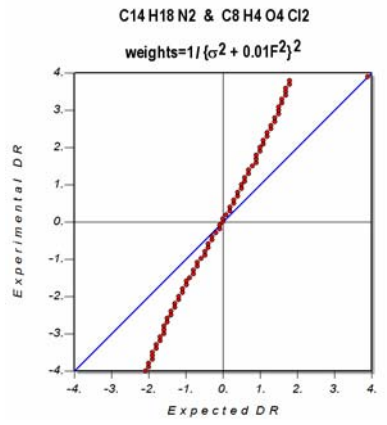


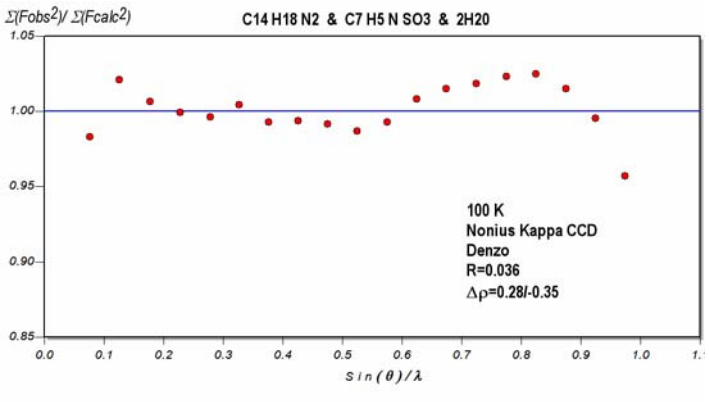
P.R. Mallinson, G.T. Smith, C.C. Wilson, E. Grech & K. Wozniak, *J. Am. Chem. Soc.* (2003) **125**, 4259-4270.

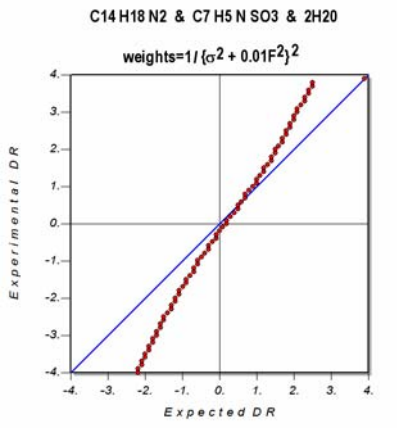


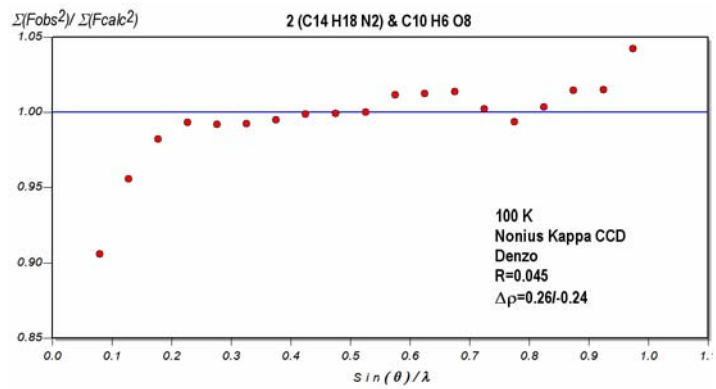


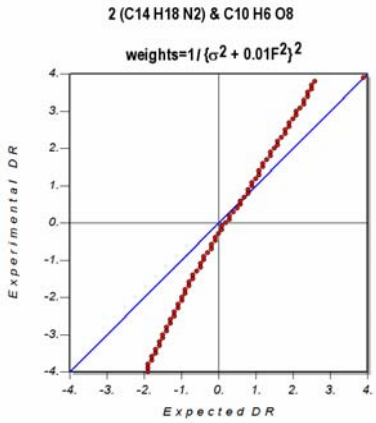




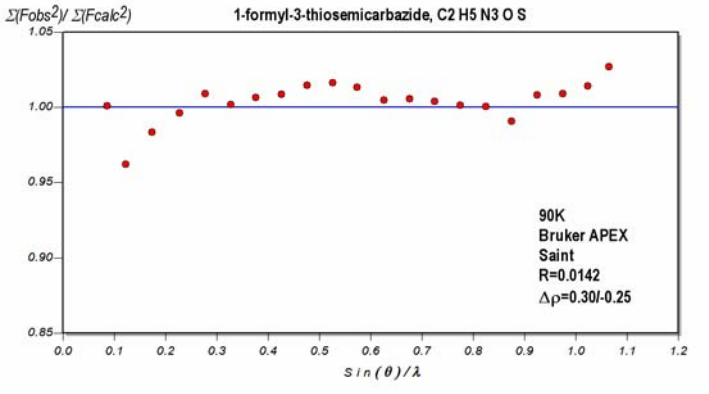


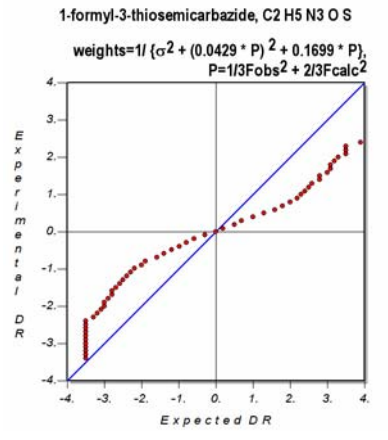


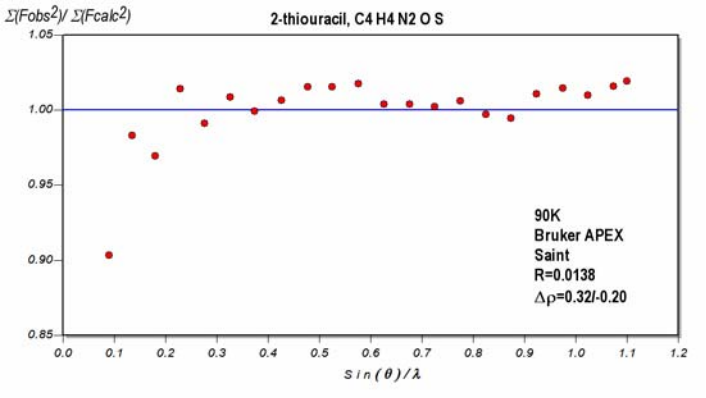


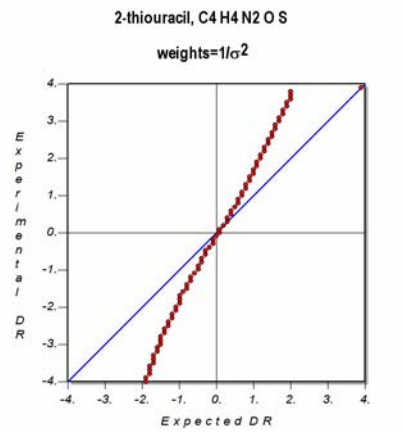


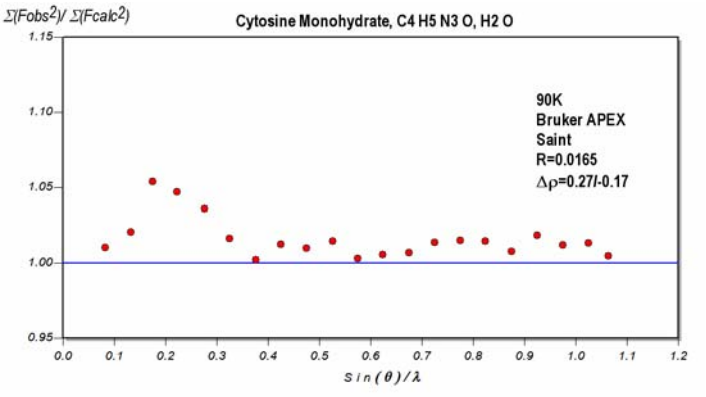
P. Munshi, T.S. Thakur, T.N. Guru Row & G.R. Desiraju, *Acta Cryst* (2006) **B62**, 118-127.

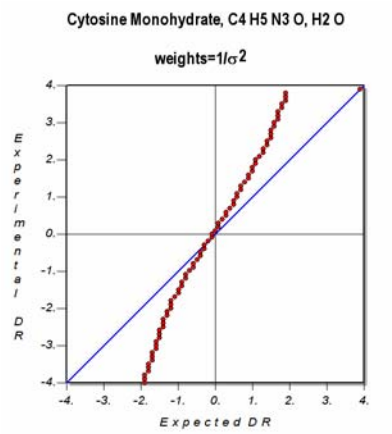


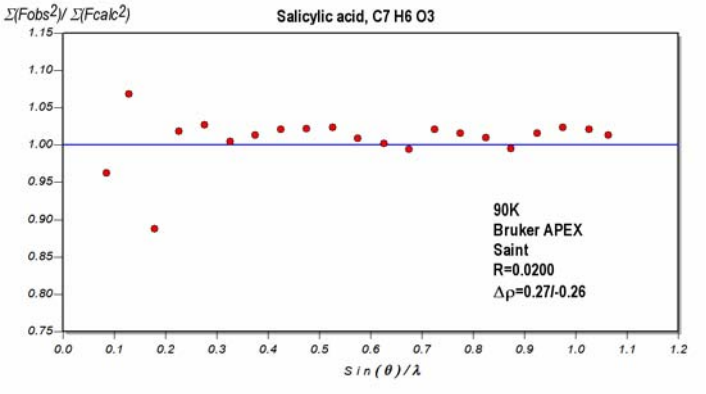


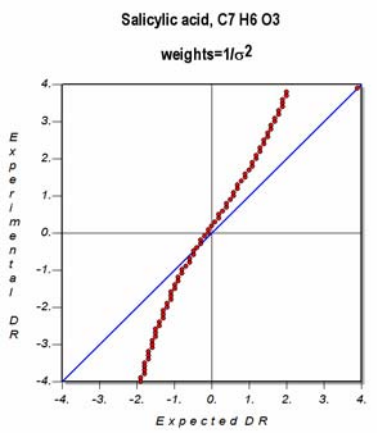

Σ(Fobs²)/ Σ(Fcalc²)
2-thiouracil, C4 H4 N2 O S
90K
Bruker APEX
Saint
R=0.0138
Δρ=0.32/-0.20
Sin(θ)/λ


2-thiouracil, C4 H4 N2 O S
weights=1/σ²
Experimental DR
Expected DR

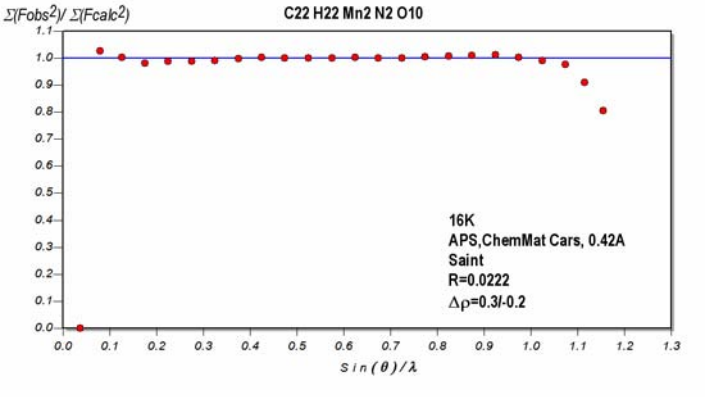

Σ(Fobs²)/ Σ(Fcalc²)
Cytosine Monohydrate, C4 H5 N3 O, H2 O
90K
Bruker APEX
Saint
R=0.0165
Δρ=0.27/-0.17
Sin(θ)/λ

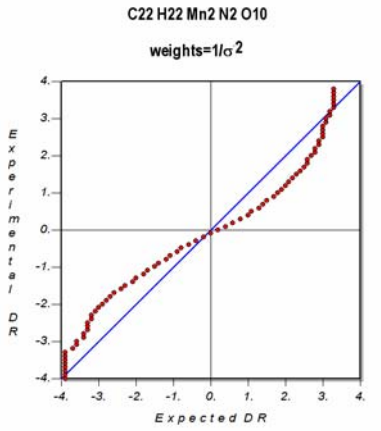

Cytosine Monohydrate, C4 H5 N3 O, H2 O
weights=1/σ²
Experimental DR
Expected DR

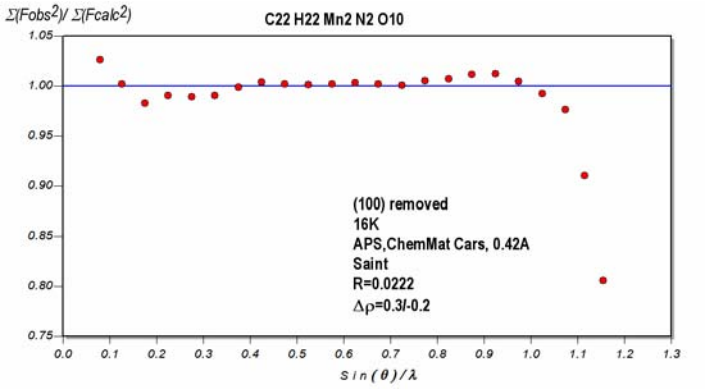

Σ(Fobs²)/ Σ(Fcalc²)
Salicylic acid, C7 H6 O3
90K
Bruker APEX
Saint
R=0.0200
Δρ=0.27/-0.26
Sin(θ)/λ


Salicylic acid, C7 H6 O3
weights=1/σ²
Experimental DR
Expected DR

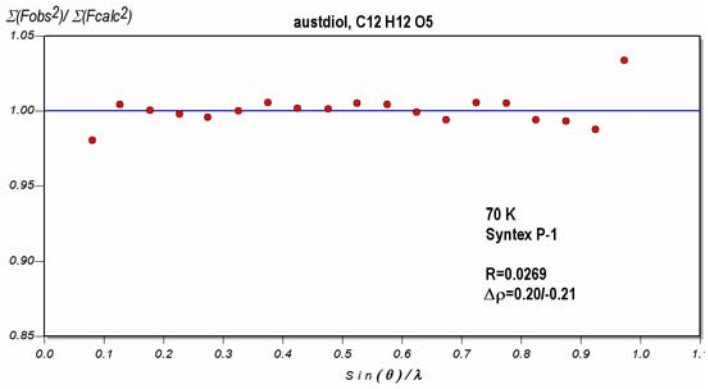
R.D. Poulsen, A. Bentien, T. Graber & B.B. Iversen, *Acta Cryst.* (2004) **A60**, 382-389.

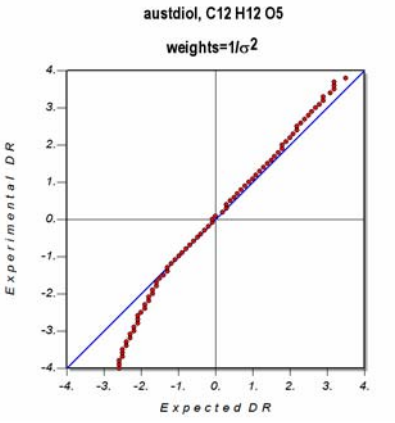




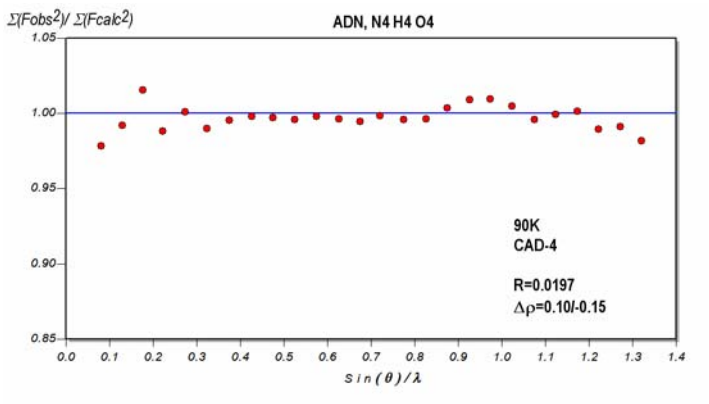


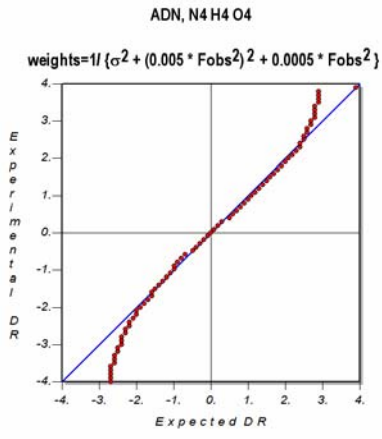
L.L. Presti, R. Soave & R. Destro, *J. Phys. Chem.* (2006) **110**, 6405-6414.



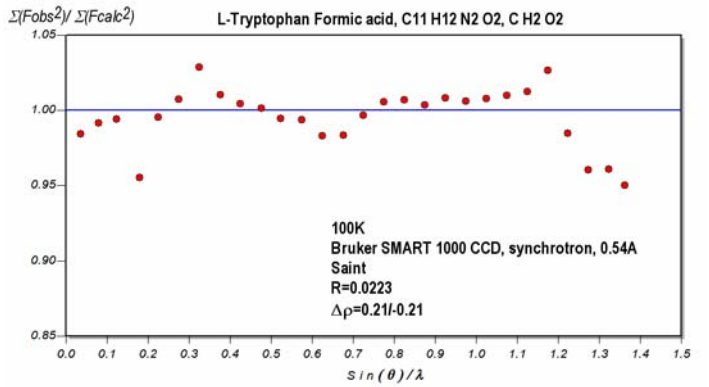


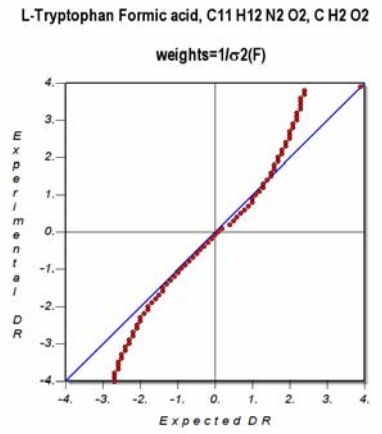
J.P. Ritchie, E.A. Zhurova, A. Martin & A.A. Pinkerton, *J. Phys. Chem.* (2003) **107**, 14576-14589.



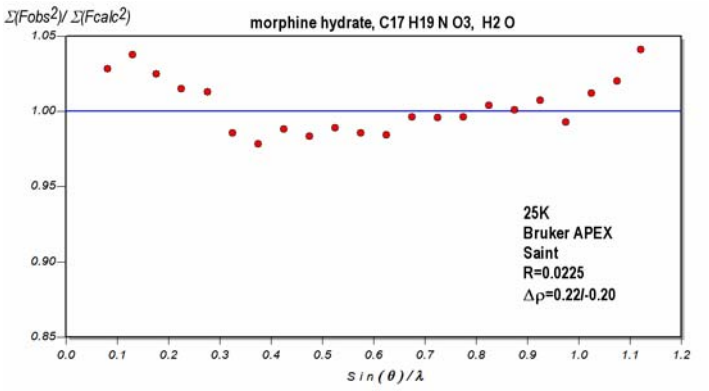


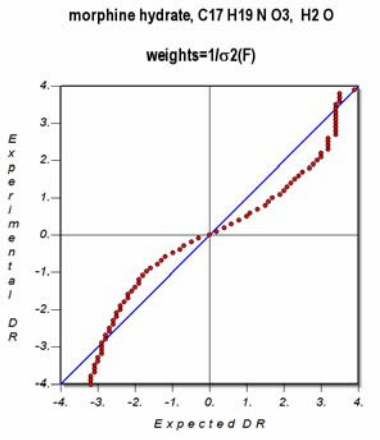
S.Scheins, B. Dittrich, M. Messerschmidt, C. Paulmann & P. Luger, *Acta Cryst.* (2004) **B60**, 184-190.



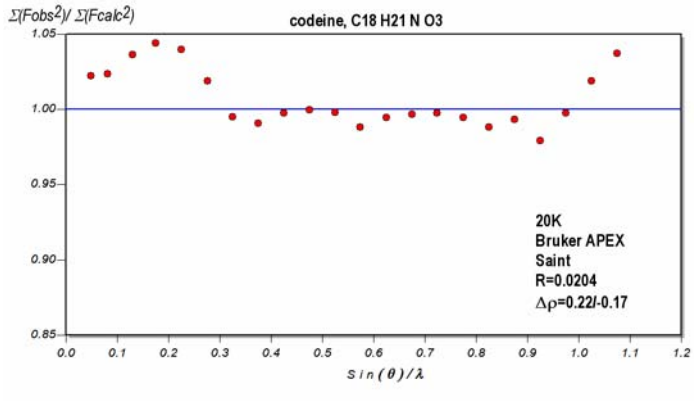


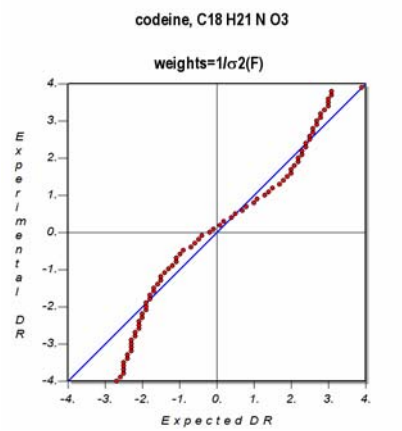
S. Scheins, M. Messerschmidt & P. Luger, *Acta Cryst*. (2005) **B61**, 443-448.

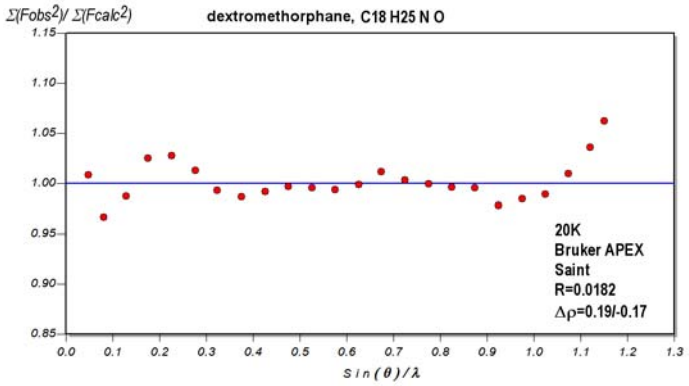


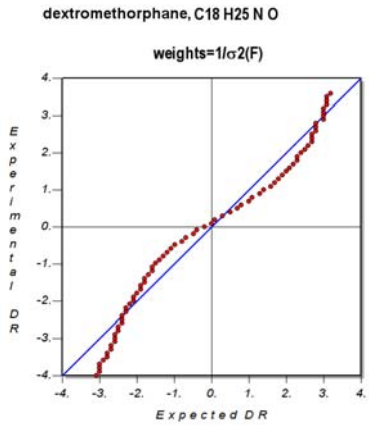


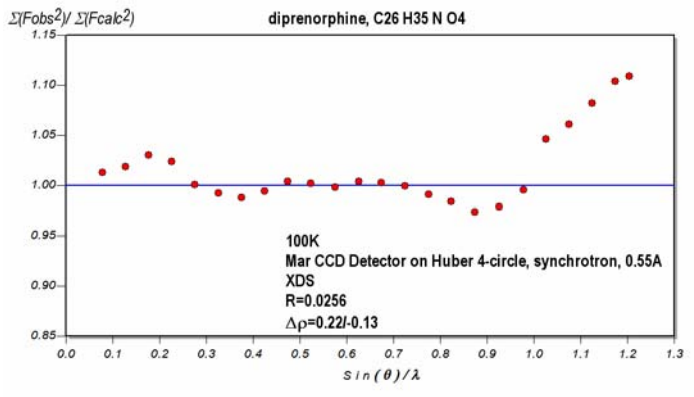
S. Scheins, M. Messerschmidt, W. Morgenroth, C. Paulmann & P. Luger, *J. Phys. Chem. A* (2007) **111**, 5499-5508.

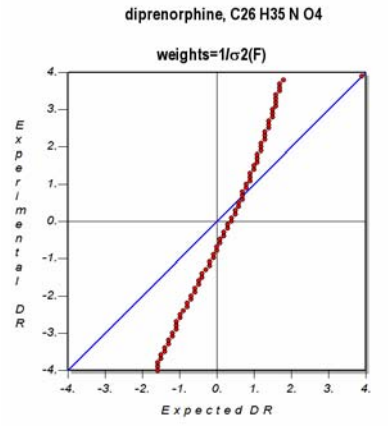


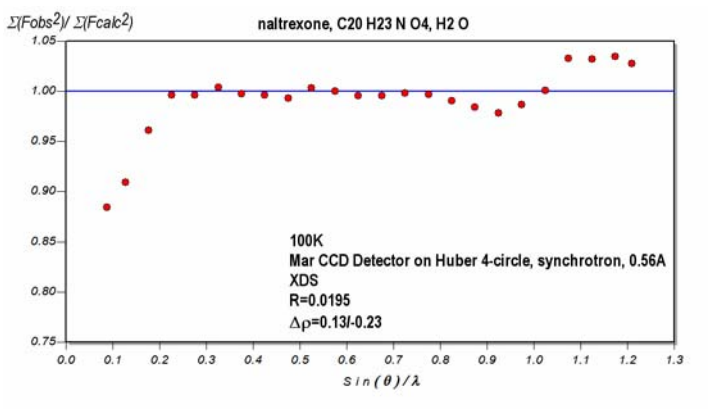


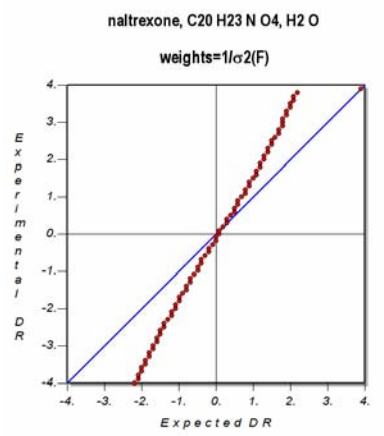


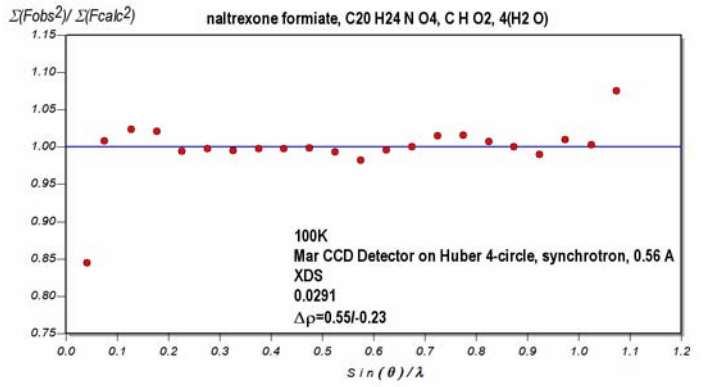


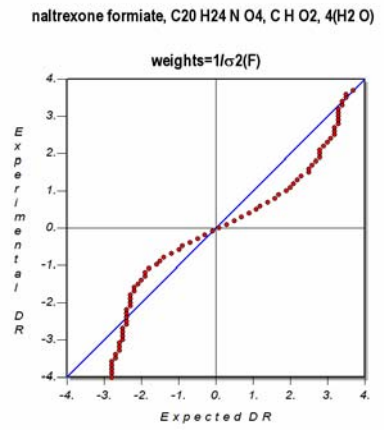




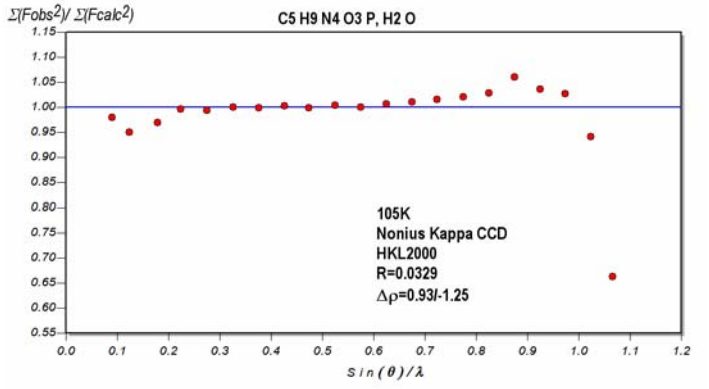


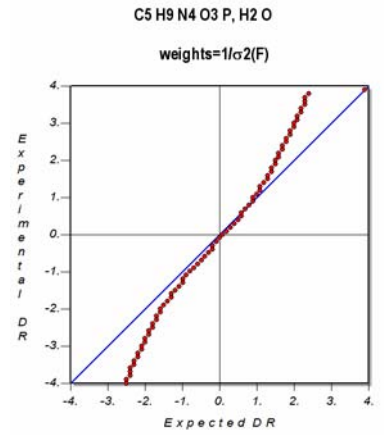




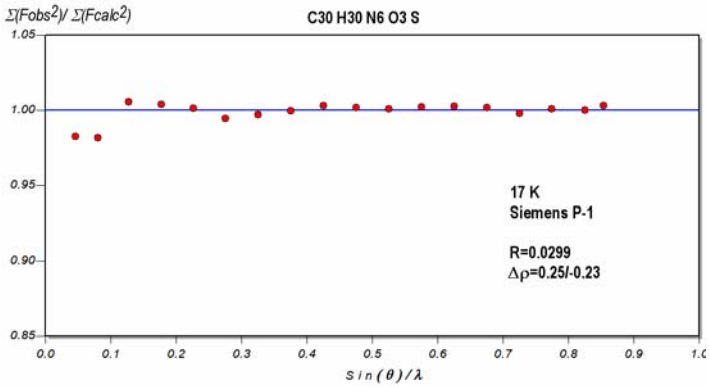


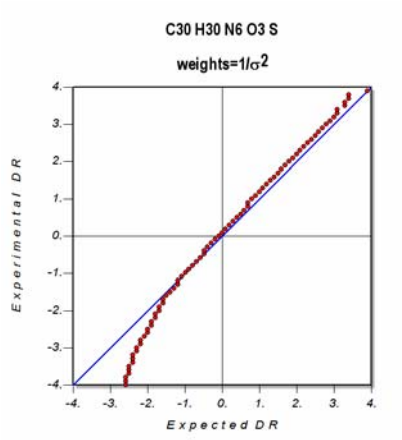
M. Slouf, A. Holy, V. Petricek & I. Cisarova, *Acta Cryst.* (2002) **B58**, 519-529.



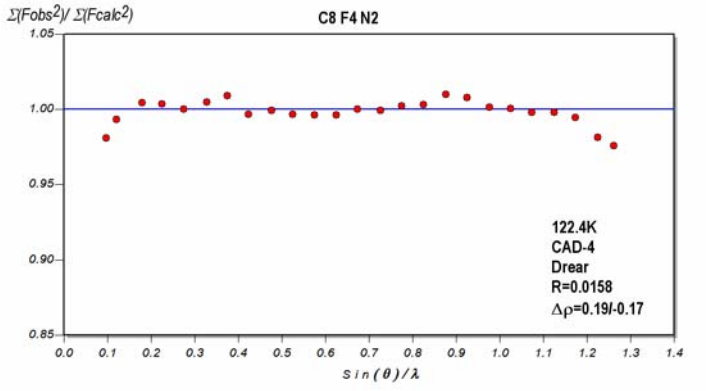


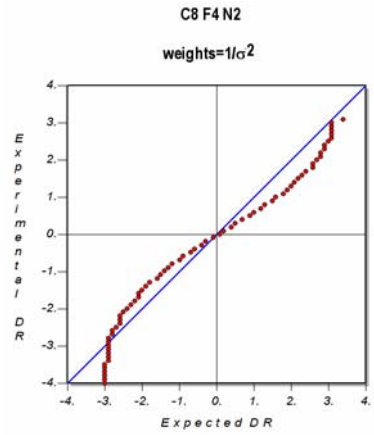
R. Destro, R. Soave, M. Barzaghi & L.L. Presti, Chem. Eur. J. (2005) **11**, 4621-4634; R. Soave, M. Barzaghi & R. Destro, *Chem. Eur. J.* (2007) **13**, 6942-6956.

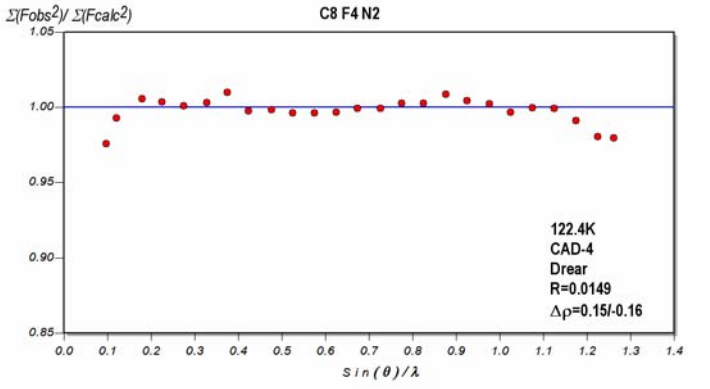


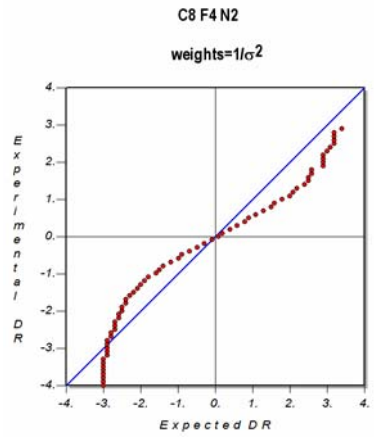


H.O. Sørensen, R.F. Stewart, G.J. McIntyre & S. Larsen, *Acta Cryst.* (2003) **A59**, 540-550.

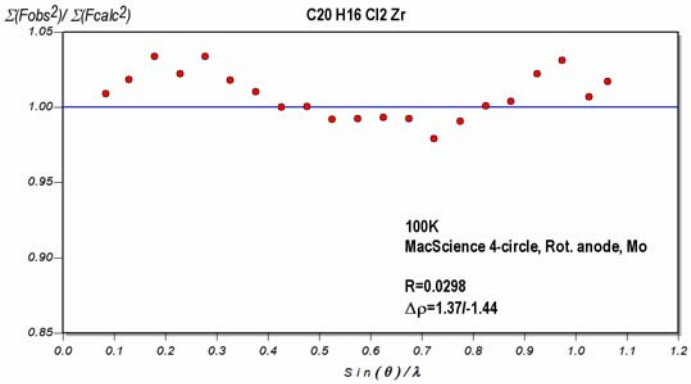


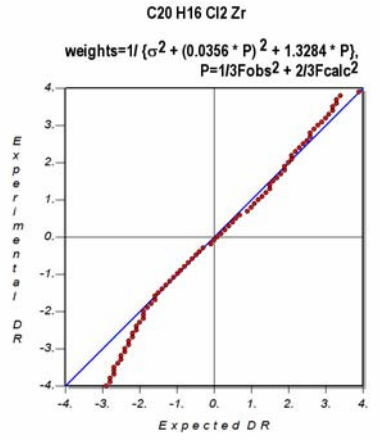




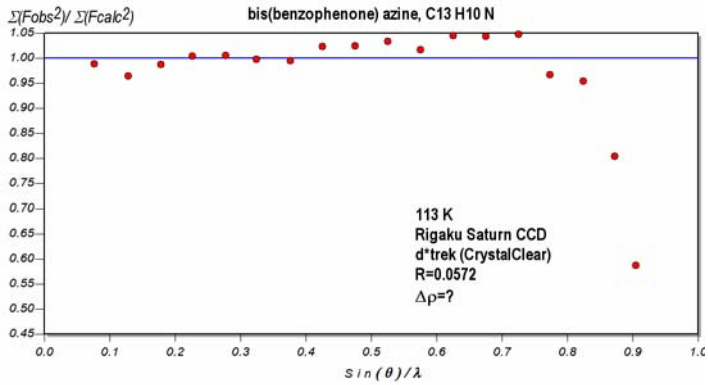


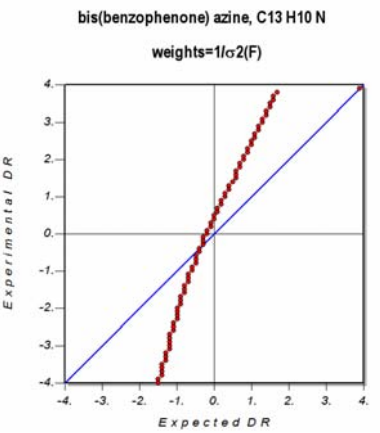
A.I. Stash, K. Tanaka, K.Shiozawa, H. Makino & V.G. Tsirelson, *Acta Cryst*. (2005) **B61**, 418-428.

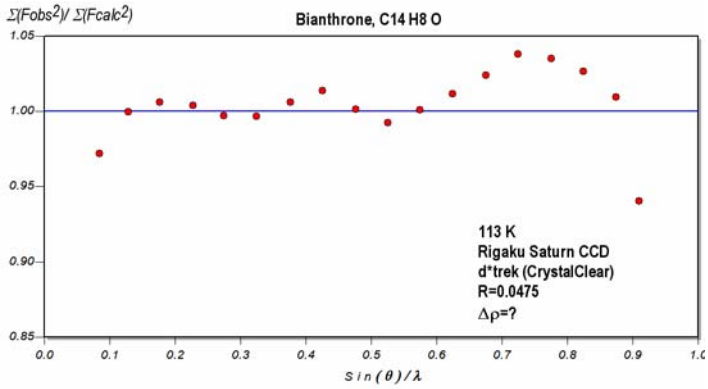


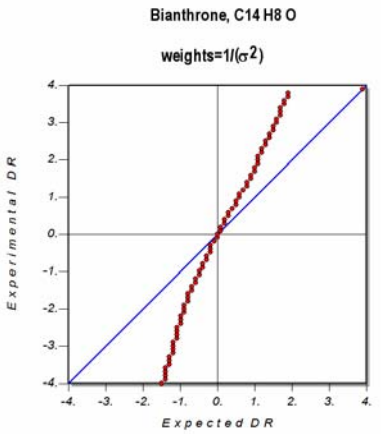


D.J. Wolstenholme & T.S. Cameron, *J. Phys. Chem. A* (2006) **110**, 8970-8978.

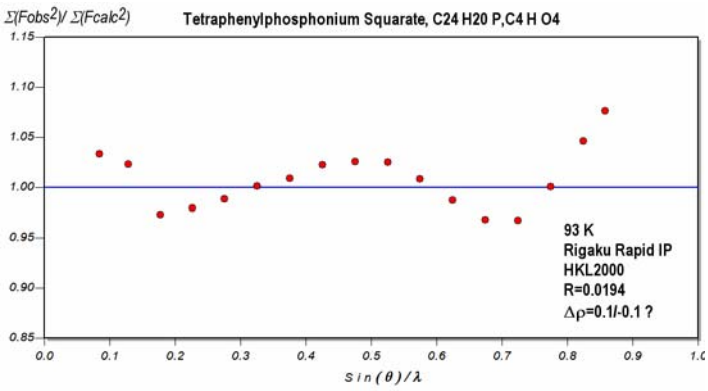


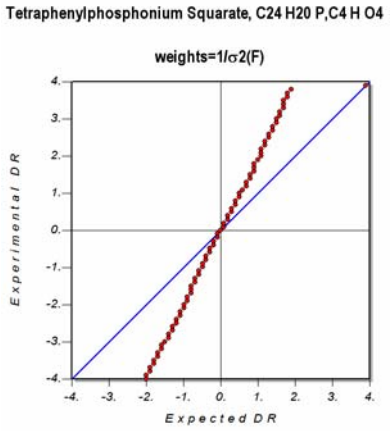




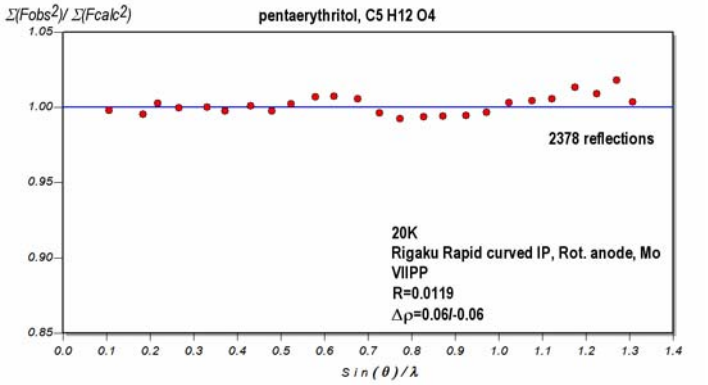


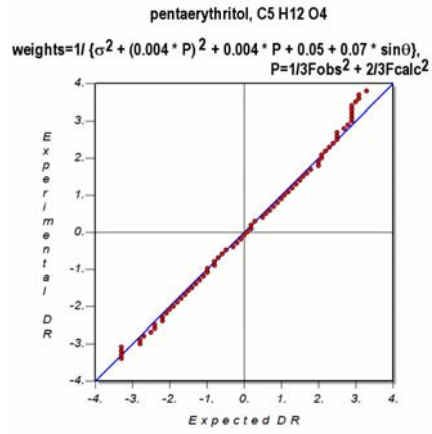
D. Wolstenholme, M.A.S. Aquino, T.S. Cameron, J.D. Ferrara & K.N. Robertson, *Can J. Chem*. (2006) **84**, 804-811.



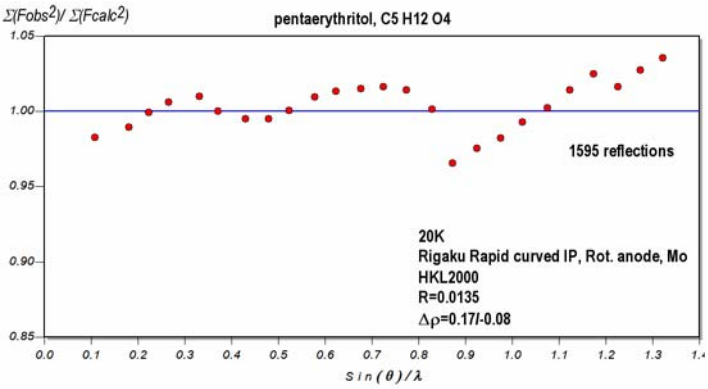


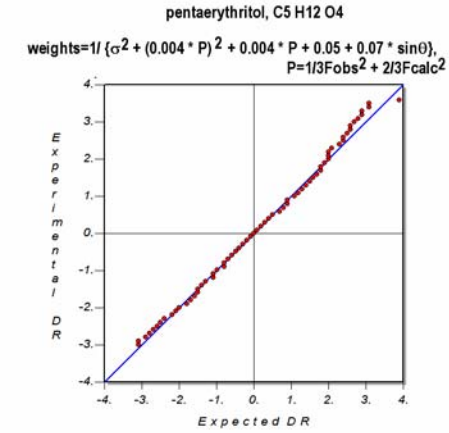
V.V. Zhurov, E.A. Zhurova, Y.-S. Chen & A.A. Pinkerton, *J. Appl. Cryst.* (2005) **38**, 827-829.



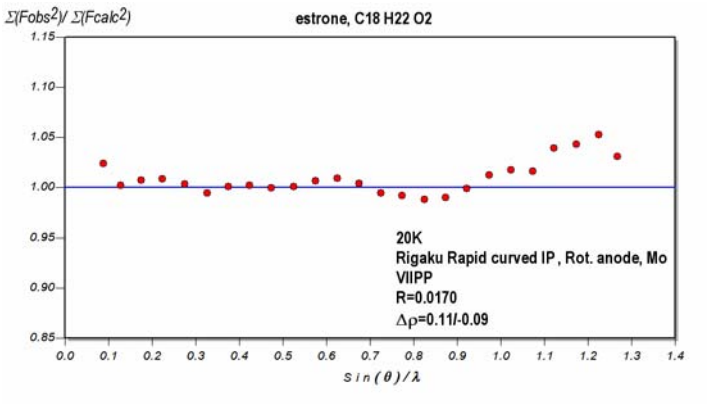


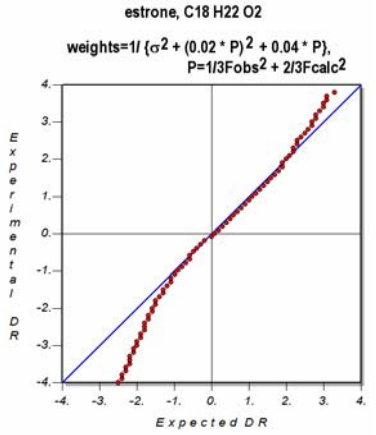
V.V. Zhurov, E.A. Zhurova & A.A. Pinkerton, unpublished results.



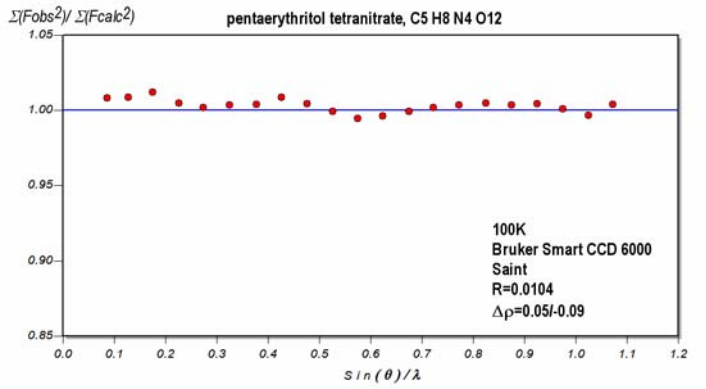


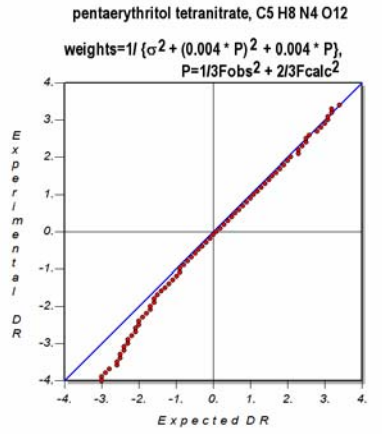
E.A. Zhurova, C.F. Matta, N. Wu, V.V. Zhurov & A.A. Pinkerton, *J. Am. Chem. Soc.* (2006) **128**, 8849-8861.



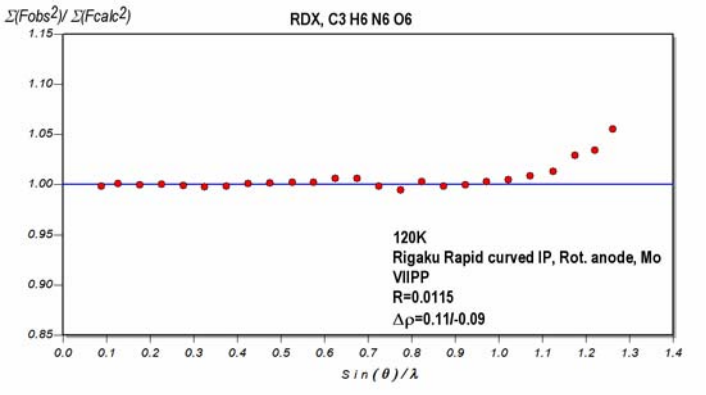


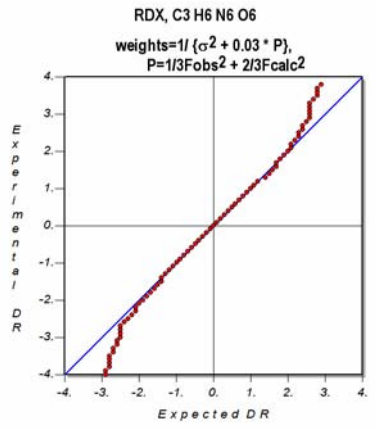
E.A. Zhurova, A.I. Stash, V.G. Tsirelson, V.V. Zhurov, E.V. Bartashevich, V.A. Potemkin & A.A. Pinkerton, *J. Am. Chem. Soc.* (2006) **128**, 14728-14734.

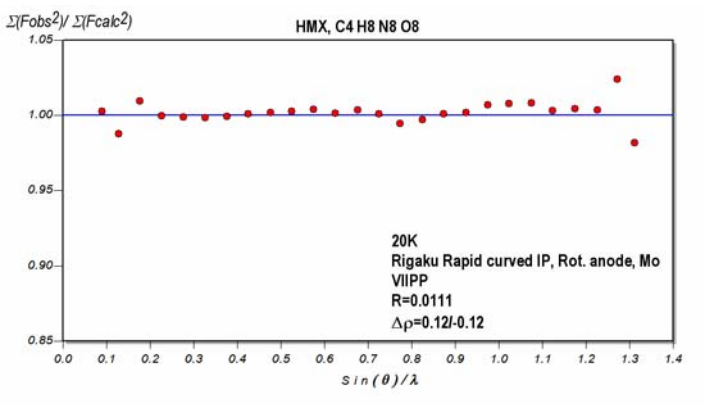


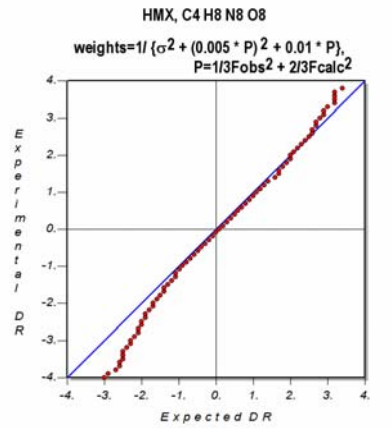


E.A. Zhurova, V.V. Zhurov & A.A. Pinkerton, unpublished results.






Σ(Fobs²)/ Σ(Fcalc²)
HMX, C4 H8 N8 O8
1.05
1.00
0.95
0.90
0.85
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4
Sin(θ)/λ
20K
Rigaku Rapid curved IP, Rot. anode, Mo
VIIPP
R=0.0111
Δρ=0.12/-0.12


HMX, C4 H8 N8 O8
weights=1/ {σ² + (0.005 * P)² + 0.01 * P},
P=1/3Fobs² + 2/3Fcalc²
Experimental DR
4. 3. 2. 1. 0. -1. -2. -3. -4.
-4. -3. -2. -1. 0. 1. 2. 3. 4.
Expected DR