ESRF	Experiment title: Assessing the experimental electron density of phenolic groups at very high resolution and ultra low temperature. Comparison with the to-date dissimilar theoretical results.	**Experiment number**: HC 1176
Beamline:	**Date of experiment**: from: to:	**Date of report**: 16/08/2014
Shifts:	**Local contact(s)**: Jonathan Wright	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Christian Jelsch. DR2 CNRS. CRM2. Université de Lorraine.

* Jonathan Wright, ESRF staff. ID 11 beamline

Report:

The charge density of quercetin dihydrate (Figure 1) was measured on a monocrystal.

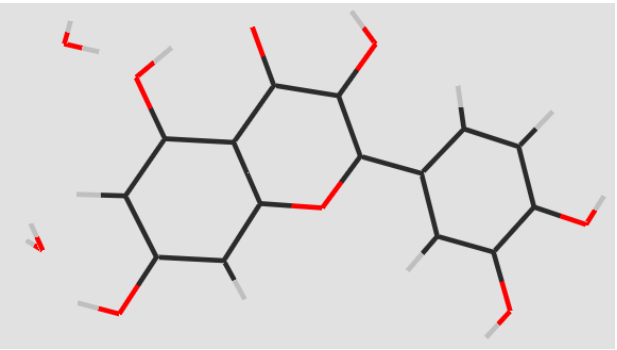

Figure 1

- Beamline: ID11
- Scheduled shifts: 6
- Start date and time: 16 April 2014 at 08:00
- End date and time: 18 April 2014 at 08:00
- This is a **Green** proposal

Temperature : 30 K by helium cryostat.

979397 Reflections were measured, Mean (I/sigma) = 6.55
88449 Reflections after merging [I] 499 outliers were downweighted
Wavelength: 0.15815 Angstrom, Absorption Mu [mm-1]: 0.00
Unit cell: 3.652 12.885 14.832 72.38 85.15 86.92 Vol 662.5
Crystal system: Triclinic Space group: P-1 # 2 [cen] Laue: 1
Formula: C25 H20 O15 Formula weight: 560.42

Z: 1.00 Density: 1.405 At.vol: 16.6 F(000): 290.00

Resolution	#Data	#Theory	%Complete	Mean I	Mean I/s	Rint	Rsigma
Inf - 0.86	2267	2271	99.8	140.3	51.56	0.0137	0.0182
0.86 - 0.68	2364	2364	100.0	42.3	54.95	0.0106	0.0136
0.68 - 0.59	2489	2489	100.0	29.6	57.17	0.0094	0.0129
0.59 - 0.53	2696	2696	100.0	21.2	57.27	0.0090	0.0126
0.53 - 0.49	2759	2759	100.0	11.9	48.01	0.0106	0.0141
0.49 - 0.46	2643	2643	100.0	11.4	46.59	0.0105	0.0149
0.46 - 0.44	2272	2272	100.0	10.9	42.04	0.0109	0.0156
0.44 - 0.42	2606	2606	100.0	6.9	37.27	0.0129	0.0177
0.42 - 0.40	3307	3307	100.0	6.0	32.88	0.0140	0.0194
0.40 - 0.38	3951	3951	100.0	4.4	29.43	0.0168	0.0228
0.38 - 0.37	2371	2371	100.0	3.1	24.80	0.0220	0.0290
0.37 - 0.36	2663	2663	100.0	2.6	21.88	0.0254	0.0331
0.36 - 0.35	2899	2899	100.0	2.5	19.67	0.0272	0.0361
0.35 - 0.34	3257	3257	100.0	2.3	17.43	0.0315	0.0420
0.34 - 0.33	3842	3842	100.0	2.0	13.91	0.0403	0.0551
0.33 - 0.31	2146	3726	57.6	1.2	6.02	0.0893	0.2264
0.40 - 0.31	22885	24465	93.5	2.9	20.55	0.0257	0.0390
Inf - 0.31	44532	46116	96.6	16.4	34.00	0.0132	0.0181

The experimental charge density was refined with software MoPro vs the merged diffraction data.
The figure 2 shows the electron accumulation/depletion in blue/red with 0.05 e/Å^3 contour levels.
The figure on the right shows an exemple of deformation electron density for the lone pairs of a phenol group. The two lobes of the electron lone pairs are in accordance to quantum chemical calculations, contrarily to precedent experiments on other compounds.

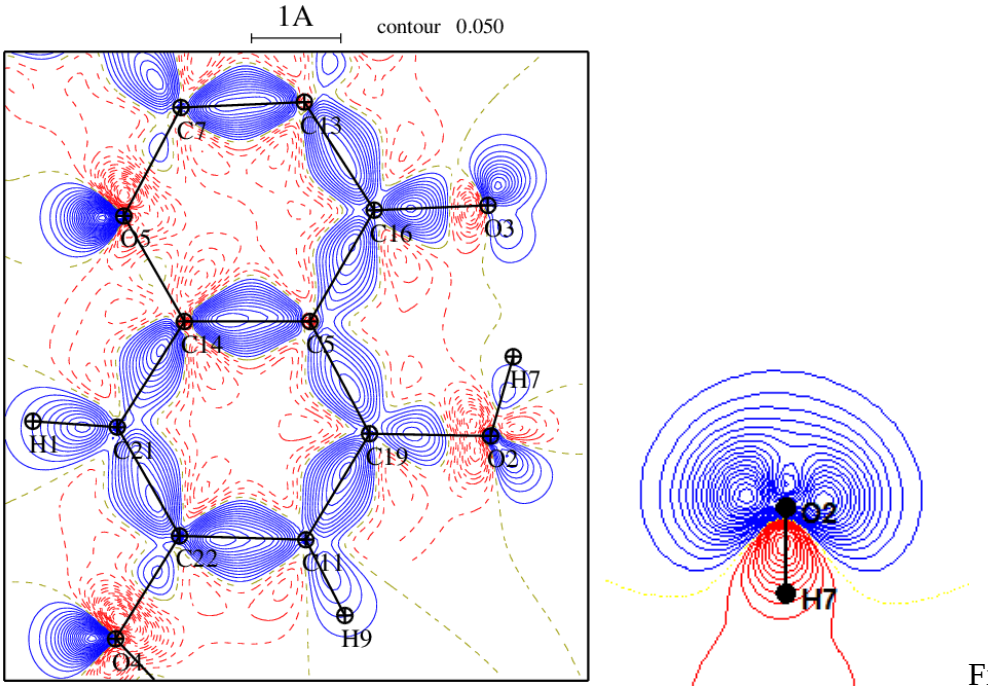

Figure 2.

The diffraction data seem promising and quantum chemical calculations will be carried out to compare the results with experimental charge density. Polarizations of the oxygen and hydrogen atoms will be assessed by both methods.