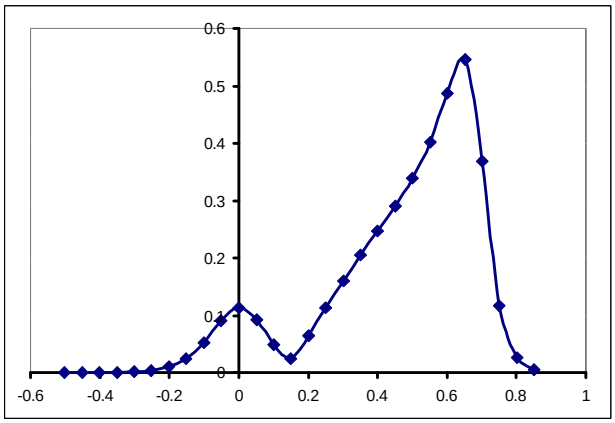
Table S1. Supplementary topological parameters obtained from the experiment.

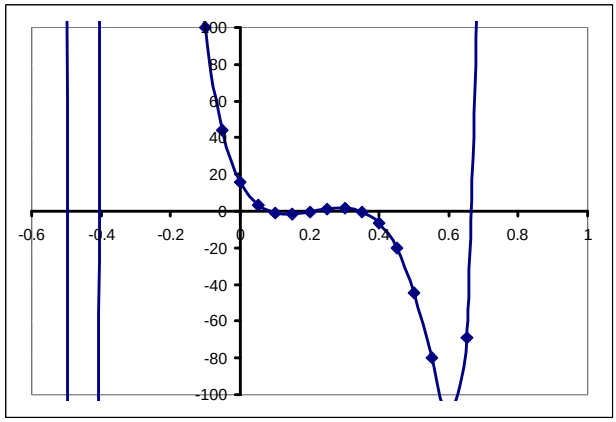
bond	R (Å)	d_1 (Å)	d_2 (Å)	λ_1 (eÅ^{-5})	λ_2(eÅ^{-5})	λ_3 (eÅ^{-5})
P-O(3)	1.5946	0.6353	0.9593	-7.76	-6.98	30.39
P-O(4)	1.5611	0.6291	0.9320	-9.06	-7.55	35.19
P-O(5)	1.5080	0.6127	0.8953	-10.06	-9.58	42.87
P-O(6)	1.5015	0.6045	0.8970	-11.20	-9.91	49.28
O(4)-H(4)	1.0210	0.8001	0.2209	-31.66	-29.97	30.26
O(3)-C(2)	1.4255	0.8676	0.5579	-10.48	-8.65	13.18
C(2)-H(2)	1.1047	0.7172	0.3875	-17.02	-16.12	12.59
C(2)-H(3)	1.1039	0.7178	0.3861	-17.70	-16.56	12.44
C(1)-C(2)	1.5118	0.8188	0.6929	-11.46	-11.16	8.69
O(1)-C(1)	1.3026	0.8438	0.4588	-19.73	-17.38	14.36
O(1)-H(1)	1.0702	0.8164	0.2538	-29.79	-27.66	27.12
O(2)-C(1)	1.2285	0.8057	0.4227	-25.25	-23.16	28.45
H(1)-O(5^{i})	1.4473	0.4543	0.9930	-6.61	-5.64	10.87
H(4)-O(6^{ii})	1.4688	0.4719	0.9969	-6.90	-6.07	10.38
K-O(2)	2.8702	1.4755	1.3947	-0.24	-0.23	1.75
K-O(2^{iii})	2.8002	1.4491	1.3510	-0.29	-0.28	2.06
K-O(4^{v})	2.7527	1.4199	1.3328	-0.34	-0.33	2.40
K-O(5^{i})	2.6948	1.3950	1.2998	-0.39	-0.39	2.75
K-O(6^{vi})	2.7842	1.4399	1.3443	-0.29	-0.29	2.13

R – interatomic distance; d_1 – distance between the first atom and the critical point; d_2 – distance between the critical point and the other atom; λ_1, λ_2 λ_3 – eigenvalues of the Hessian matrix

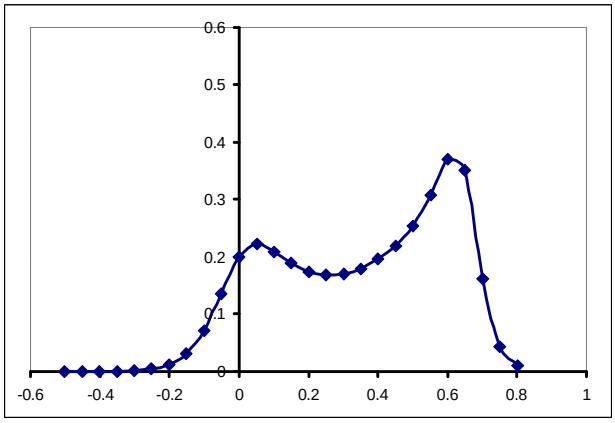
Figure S1. Ellipticity (left column) and Laplacian (right column) profile diagrams calculated with step 0.05 Å along the bond paths of the respective bonds. The *x* axis represents the distance from the bond critical points (*x*=0) in both directions along the bond paths. The Y axis represents the e (dimensionless) or $\nabla^2?_c$ (e·Å^{-5}).

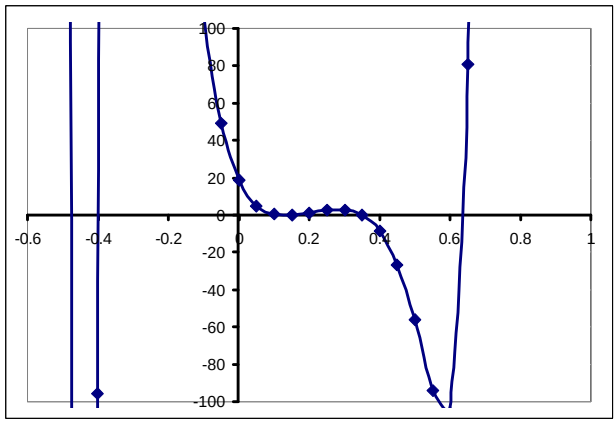
P-O3



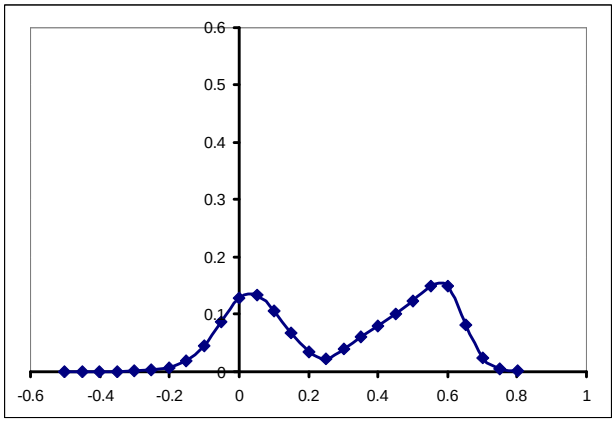


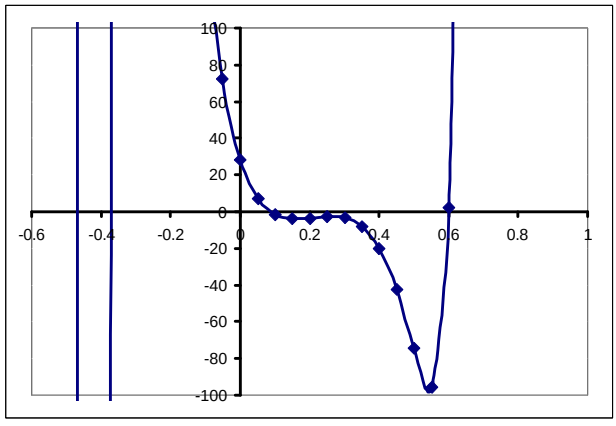
P-O4



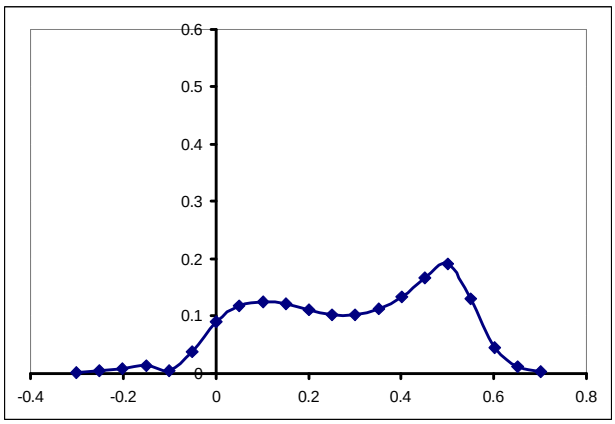


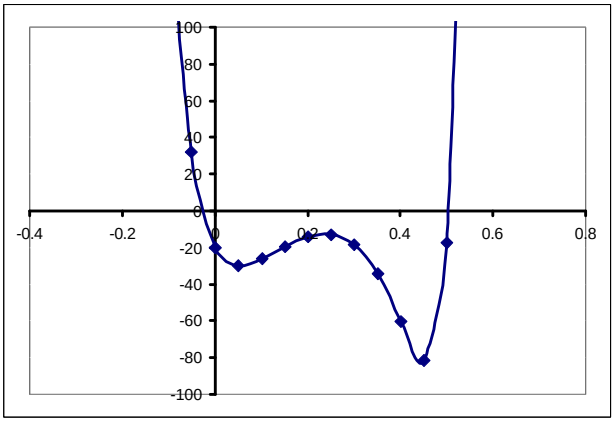
P-O6



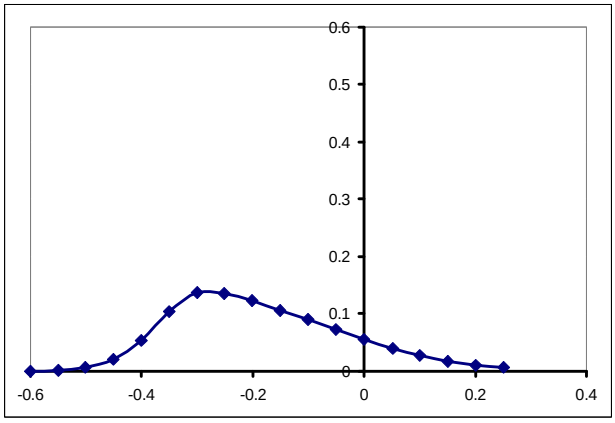


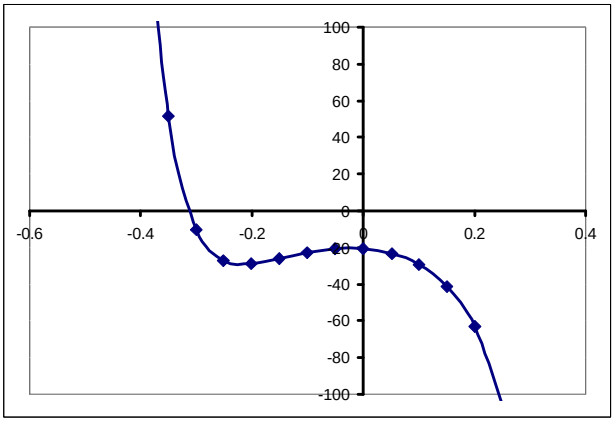
C1-O2



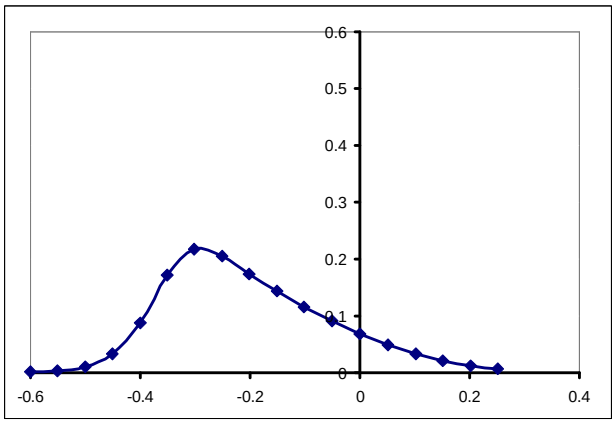


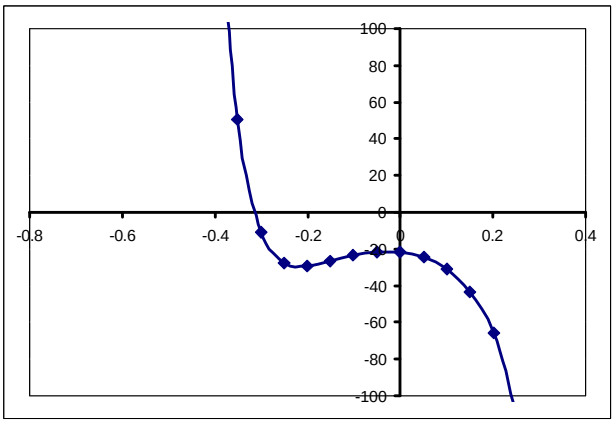
C2-H2



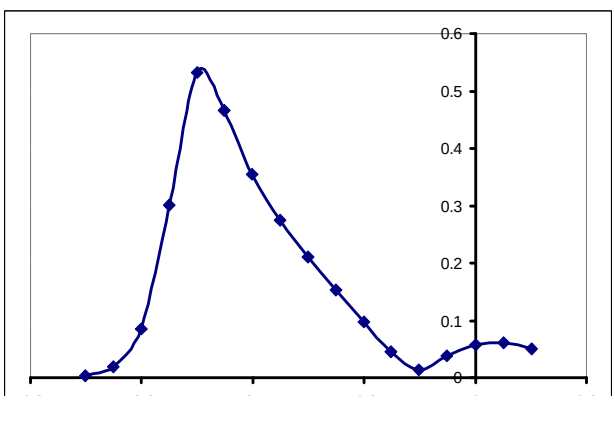


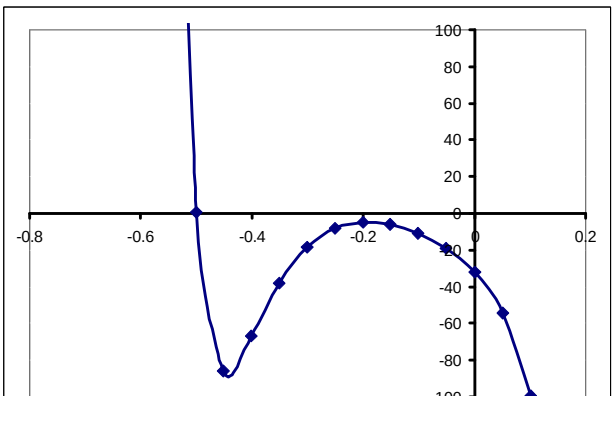
C2-H3





O4-H4





O1-H1

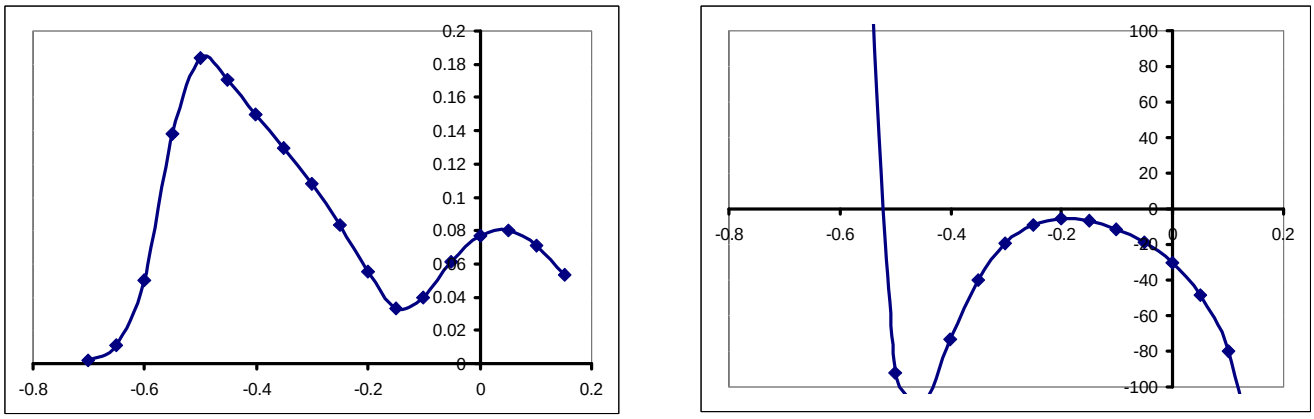
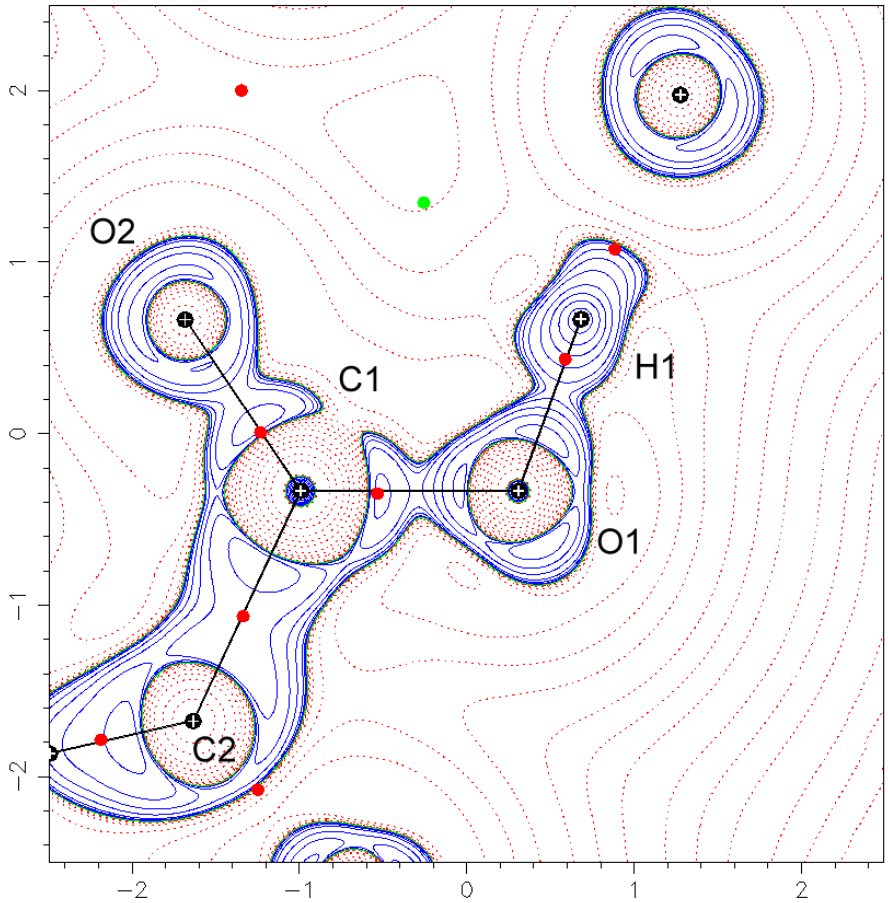
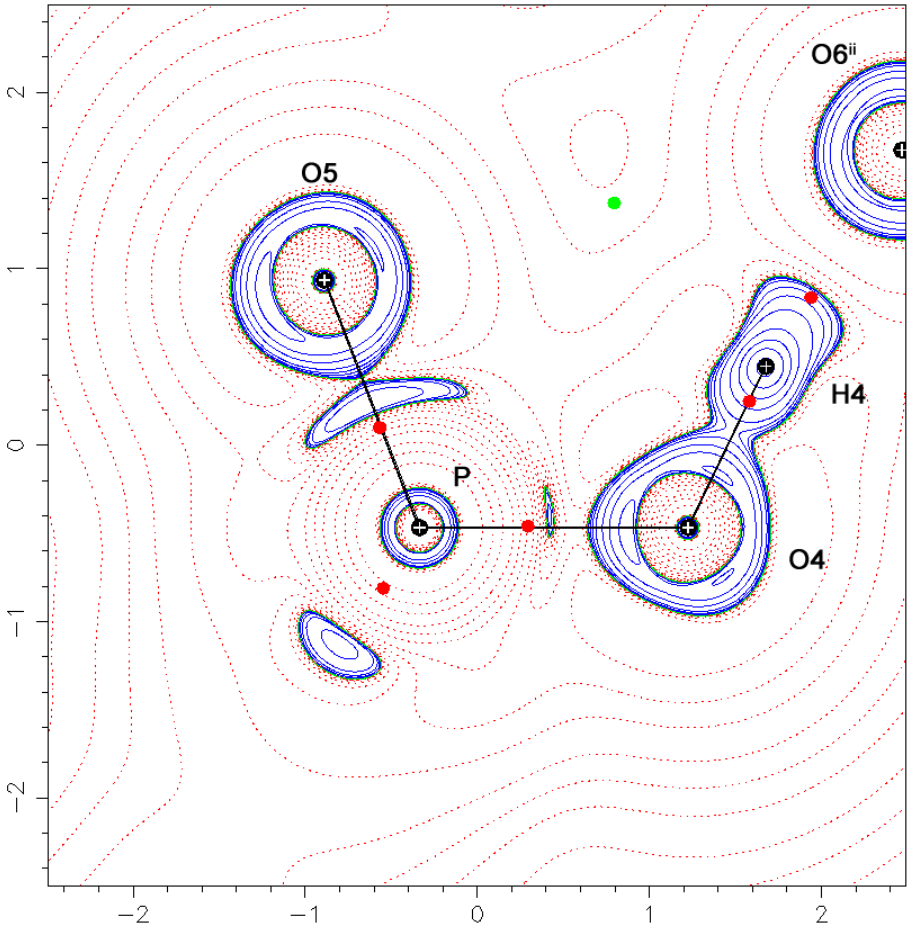


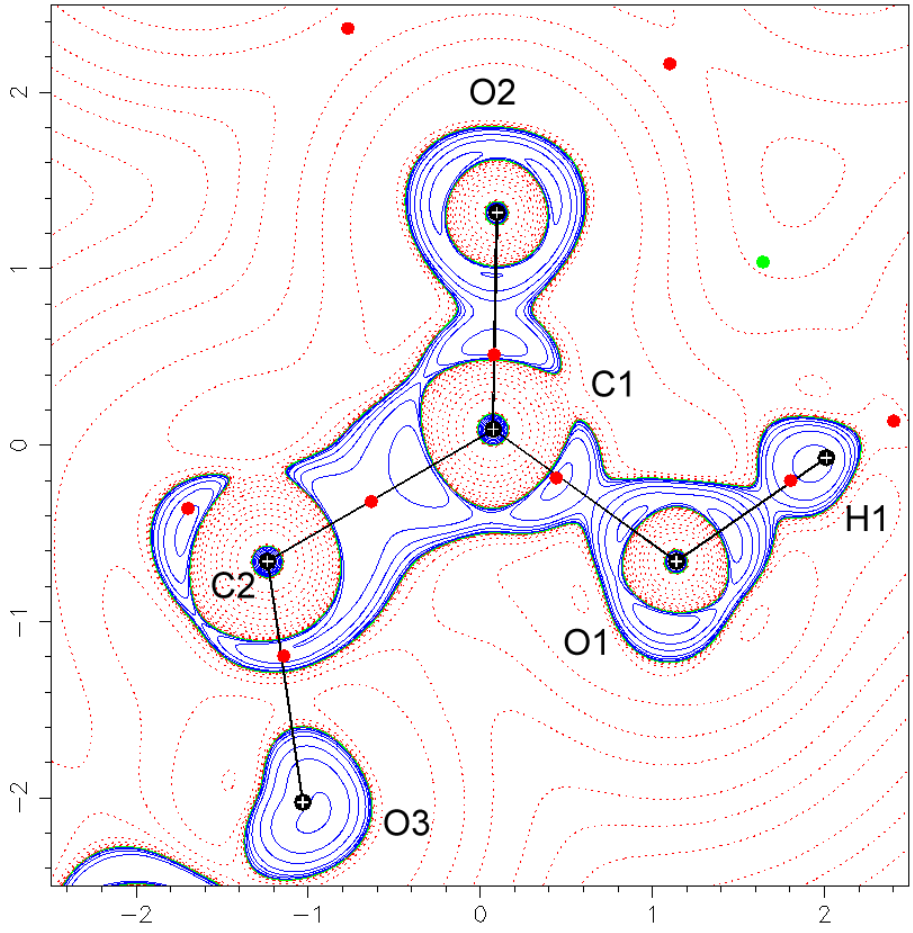
Figure S2. Maps of $-\nabla^2\rho_c$ ($eÅ^{-5}$) in the planes defined by the following atoms: a) C1-O1-H1 b) P-O4-H4 c) C2-C1-O1. The solid contours denote regions of negative Laplacian, whereas the dashed contours indicate areas of positive.



a)



b)



c)