

Supplementary Materials

Experimental and Theoretical charge density analysis of *1,4-bis (5-hexyl-2-thienyl) butane-1,4 dione*: Applications of a virtual atom model.

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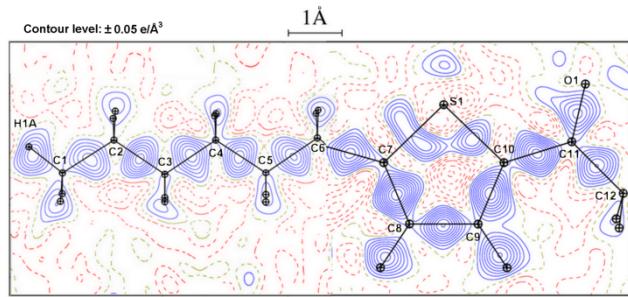


Figure Sup1: Fourier deformation electron density obtained after spherical atom model refinement.

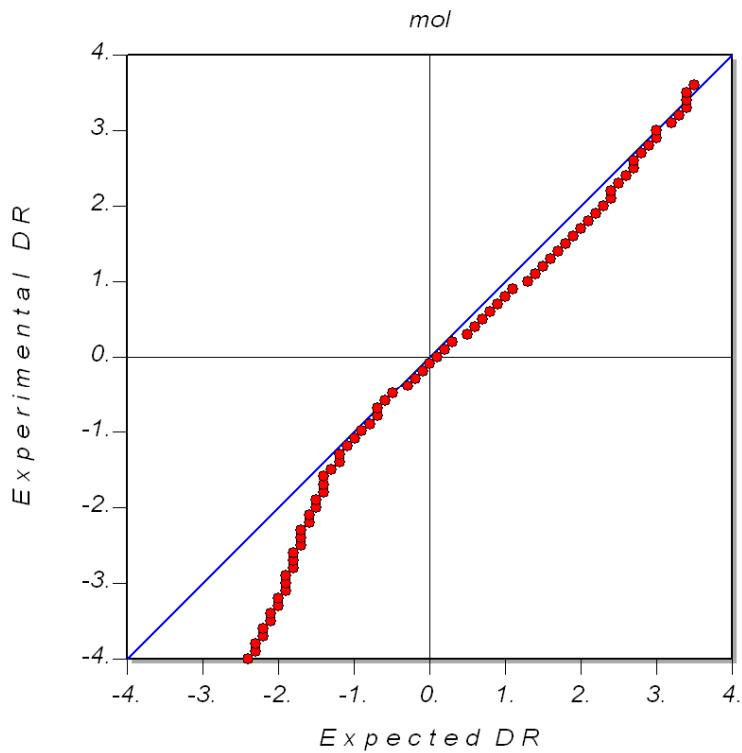


Figure Sup2: An XDRKplot showing the expected and experimental data reduction profile.

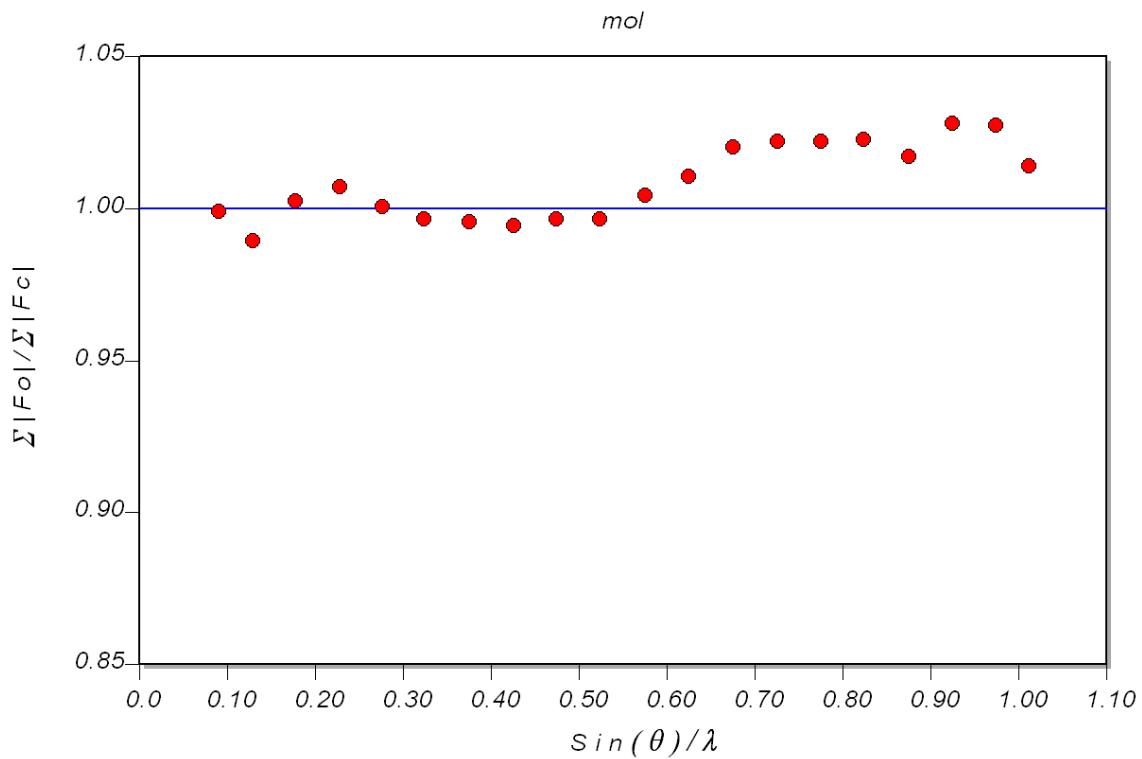


Figure Sup2 : An XDRKplot showing the fit of the diffraction data as a function of resolution.

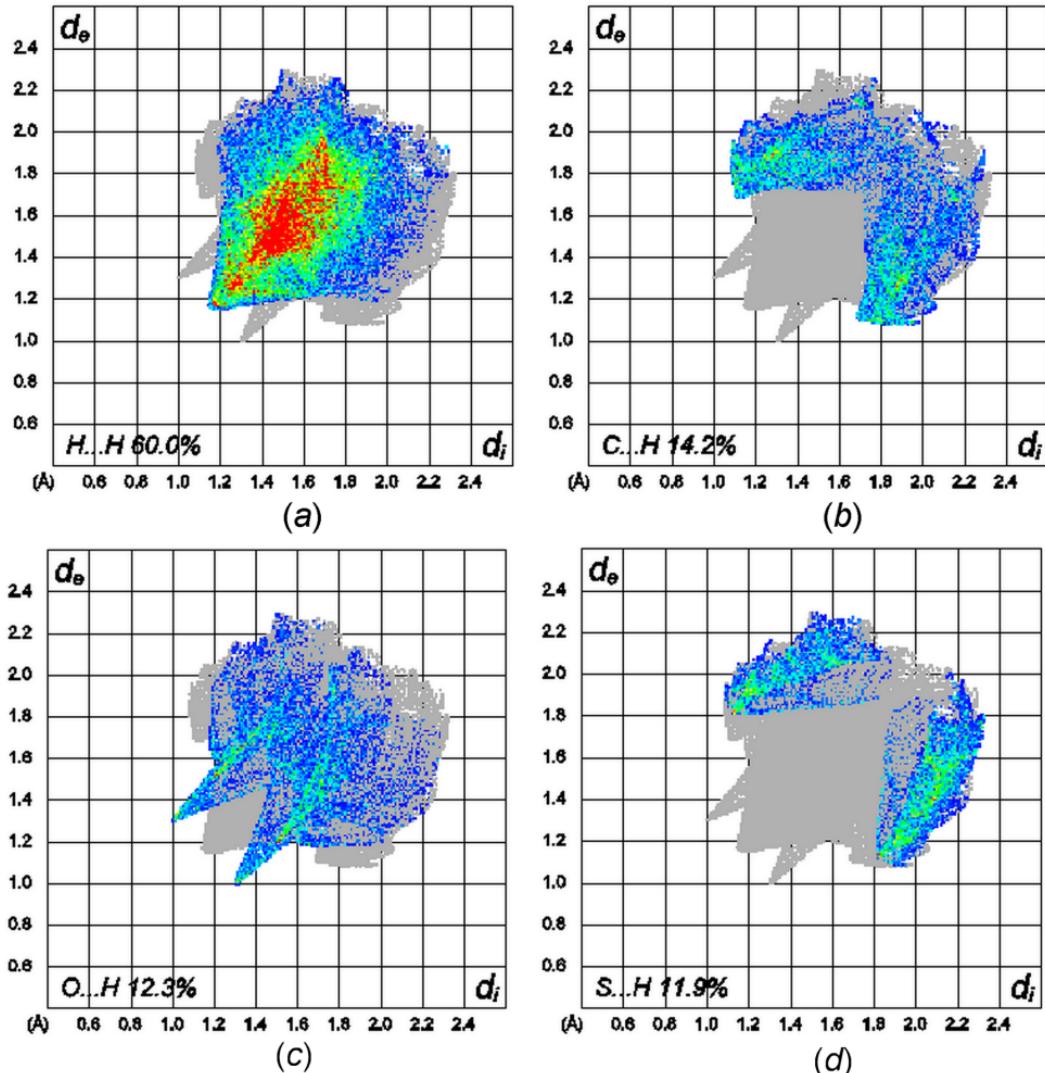


Figure Sup3. Fingerprint plot of the Hirshfeld surface showing the major interactions. The red colour shows the regions where the inter-atomic distances are smaller than the sum of van der Waals radii.

Table SUP1. Topological properties of the intermolecular critical points: interatomic distance, atomic distances to (3,-1) critical point, ρ total electron density, Laplacian of ρ , Hessian ρ eigenvalues, ellipticity.

Top line: experimentat multipolar model.

Middle line: theoretical multipolar with κ -core correction.

Bottom line: virtual atom model refined vs. experimental data.

d_{12} : Internuclear distance. d_{1cp} and d_{2cp} : distance from CP to atoms 1 and 2.

$\rho(\mathbf{r}_{cp})$: density ($e \text{ \AA}^{-3}$) ; $\nabla^2 \rho(\mathbf{r}_{cp})$, $\lambda_1, \lambda_2, \lambda_3$: Laplacian and eigenvalues of Hessian matrix ($e \text{ \AA}^{-5}$)

n.a means that the CP is not available for this model.

Symmetry operators:

- | | | | |
|------------------------|-------------------------|--------------------------|---------------------------|
| (i) $x+1, y-1, z$ | (ii) $x-1, y, z$ | (iii) $x, y-1, z$ | (iv) $-x-1, -y, -z$ |
| (v) $-x-3, -y+3, -z+1$ | (vi) $-x-2, -y+3, -z+1$ | (vii) $-x-3, -y+2, -z+1$ | (viii) $-x-2, -y+2, -y+1$ |
| (ix) $-x-1, -y+1, -z$ | (x) $x, y+1, z$ | | |

Interacting atoms	d_{12} (Å)	d_{1cp} (Å)	d_{2cp} (Å)	$\rho(\mathbf{r}_b)$ ($e/\text{\AA}^3$)	$\nabla^2 \rho(\mathbf{r}_{cp})$ ($e/\text{\AA}^5$)	λ_1 ($e/\text{\AA}^5$)	λ_2 ($e/\text{\AA}^5$)	λ_3 ($e/\text{\AA}^5$)	ε
H1A...H1A ^v	2.723	1.3613	1.3613	0.021	0.26	-0.05	-0.05	0.36	0.07
	2.770	1.3851	1.3851	0.017	0.23	-0.05	-0.04	0.32	0.19
	2.716	1.3580	1.3580	0.016	0.22	-0.05	-0.03	0.30	0.27
H1B...H1B ^{vi}	2.556	1.2782	1.2782	0.022	0.27	-0.06	-0.06	0.38	0.04
	2.576	1.2882	1.2881	0.016	0.24	-0.05	-0.04	0.32	0.12
	2.556	1.2782	1.2782	0.019	0.25	-0.06	-0.06	0.37	0.01
H6A ...H1C ⁱ	2.499	1.2215	1.2781	0.033	0.36	-0.09	-0.07	0.53	0.22
	2.494	1.2354	1.2626	0.024	0.32	-0.06	-0.05	0.44	0.17
	2.503	1.2518	1.2620	0.023	0.32	-0.07	-0.04	0.43	0.46
H2B...H2A ^{vii}	2.470	1.2555	1.2379	0.044	0.50	-0.13	-0.10	0.73	0.28
	2.497	1.2884	1.2618	0.035	0.46	-0.11	-0.09	0.65	0.19
	2.462	1.2721	1.2423	0.028	0.47	-0.08	-0.05	0.59	0.40
H2A...H2A ^{viii}	2.320	1.1599	1.1599	0.050	0.49	-0.16	-0.15	0.80	0.05
	2.287	1.1435	1.1435	0.040	0.53	-0.14	-0.12	0.78	0.16
	2.328	1.1638	1.1638	0.033	0.49	-0.11	-0.08	0.68	0.23
H2B...H3A ⁱⁱ	2.352	1.1793	1.1731	0.047	0.45	-0.14	-0.13	0.71	0.03
	2.337	1.1646	1.1726	0.033	0.45	-0.10	-0.09	0.65	0.06
	2.359	1.1730	1.1857	0.030	0.43	-0.10	-0.08	0.61	0.17
H2A...H4B ^{viii}	2.528	1.2840	1.2478	0.037	0.38	-0.10	-0.07	0.56	0.27
	2.507	1.2653	1.2420	0.028	0.37	-0.08	-0.07	0.52	0.15
	2.535	1.2712	1.2648	0.023	0.33	-0.07	-0.03	0.43	0.50
H2B...H5A ⁱⁱ	2.356	1.1767	1.1790	0.045	0.44	-0.14	-0.13	0.71	0.07
	2.343	1.1642	1.1788	0.033	0.45	-0.10	-0.09	0.64	0.15
	2.366	1.1760	1.1900	0.030	0.42	-0.10	-0.08	0.60	0.19
H4A...H1C ⁱⁱⁱ	2.851	1.4725	1.4218	0.019	0.22	-0.05	-0.03	0.30	0.38
	2.873	1.4919	1.4667	0.015	0.20	-0.04	-0.02	0.26	0.36
	2.843	1.4351	1.4288	0.012	0.18	-0.03	-0.02	0.22	0.30
H4A...H5A ⁱⁱ	2.454	1.2238	1.2304	0.037	0.38	-0.11	-0.10	0.59	0.09
	2.450	1.2159	1.2344	0.028	0.37	-0.08	-0.07	0.52	0.18
	2.467	1.2314	1.2357	0.025	0.35	-0.08	-0.06	0.48	0.25

Table SUPP. 1. (continued).

Interacting atoms	d_{12} (Å)	d_{1cp} (Å)	d_{2cp} (Å)	$\rho(\mathbf{r}_b)$ (e/Å ³)	$\nabla^2\rho(\mathbf{r}_{cp})$ (e/Å ⁵)	λ_1 (e/Å ⁵)	λ_2 (e/Å ⁵)	λ_3 (e/Å ⁵)	ε
H9...H9 ^{ix}	2.891	1.4460	1.4450	0.026	0.29	-0.06	-0.03	0.38	0.52
	2.892	1.4462	1.4459	0.023	0.28	-0.06	-0.04	0.38	0.28
	2.897	1.4492	1.4476	0.021	0.26	-0.04	-0.01	0.31	0.80
H1C...H6B ^x	2.759	1.3811	1.4200	0.024	0.28	-0.06	-0.03	0.37	0.54
	2.773	1.4364	1.4378	0.019	0.25	-0.05	-0.03	0.32	0.46
	2.750	1.3943	1.3628	0.015	0.22	-0.03	-0.02	0.27	0.49
H4B...H2A ^{viii}	2.528	1.2840	1.2478	0.037	0.38	-0.10	-0.07	0.56	0.27
	2.507	1.2653	1.2420	0.028	0.37	-0.08	-0.07	0.52	0.15
	2.535	1.2712	1.2648	0.023	0.33	-0.07	-0.03	0.43	0.50
S1...H3B ⁱ	2.937	1.8231	1.1172	0.058	0.51	-0.14	-0.13	0.79	0.05
	2.929	1.8461	1.0947	0.041	0.51	-0.11	-0.10	0.71	0.08
	2.940	1.8522	1.0879	0.050	0.53	-0.14	-0.13	0.80	0.07
S1...H5A ⁱⁱ	3.285	1.9986	1.2991	0.037	0.38	-0.09	-0.08	0.54	0.13
	3.295	1.9641	1.3548	0.025	0.30	-0.05	-0.05	0.40	0.06
	3.274	2.0179	1.2627	0.028	0.31	-0.06	-0.05	0.42	0.17
S1...H12A ⁱⁱ	2.970	1.8205	1.1673	0.070	0.67	-0.14	-0.10	0.91	0.24
	2.958	1.8044	1.1667	0.055	0.61	-0.11	-0.07	0.79	0.37
	2.971	1.8735	1.0996	0.057	0.65	-0.11	-0.07	0.83	0.34
S1...H1C ⁱ	3.118	1.9486	1.1709	0.041	0.43	-0.10	-0.09	0.61	0.14
	3.101	1.9317	1.1813	0.031	0.38	-0.07	-0.07	0.52	0.08
	3.118	1.9485	1.1696	0.036	0.39	-0.09	-0.08	0.56	0.15
S1...H3A ⁱⁱⁱ	3.442	2.0320	1.4341	0.027	0.27	-0.06	-0.03	0.37	0.47
	3.451	2.0456	1.4458	0.022	0.25	-0.05	-0.03	0.33	0.42
	3.429	2.0928	1.3600	0.022	0.25	-0.04	-0.03	0.32	0.36
S1...H12B ^{iv}	3.153	1.9431	1.2689	0.049	0.50	-0.08	-0.06	0.63	0.29
	3.120	1.9172	1.2761	0.039	0.44	-0.05	-0.05	0.54	0.02
	3.149	1.9722	1.2000	0.038	0.45	-0.06	-0.05	0.56	0.13
O1...H5B ⁱ	2.689	1.5191	1.1705	0.037	0.48	-0.11	-0.11	0.69	0.00
	2.688	1.5820	1.1166	0.028	0.47	-0.08	-0.07	0.62	0.05
	2.689	1.5583	1.1317	0.034	0.50	-0.11	-0.11	0.71	0.03
O1...H8 ⁱⁱⁱ	2.301	1.3466	0.9632	0.090	1.21	-0.32	-0.31	1.85	0.04
	2.310	1.3534	0.9716	0.084	1.23	-0.31	-0.31	1.85	0.02
	2.303	1.3595	0.9479	0.089	1.23	-0.33	-0.28	1.85	0.15
H4A...C7 ⁱⁱ	3.117	1.3113	1.8897	0.028	0.30	-0.06	-0.04	0.40	0.34
	3.117	1.3015	1.9626	0.023	0.28	-0.04	-0.03	0.36	0.20
	n a	n a	n a	n a	n a	n a	n a	n a	n a
H5B...C8 ⁱⁱ	3.109	1.3121	1.8383	0.032	0.34	-0.07	-0.04	0.45	0.48
	n a	n a	n a	n a	n a	n a	n a	n a	n a
	3.121	1.2849	1.8638	0.025	0.31	-0.04	-0.03	0.38	0.20