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Supporting information for article:

Crystal structure and electrostatic properties of prednisolone acetate studied using a transferred multipolar atom model

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Table 1S: Topological properties of (3, -1) CPs on the intermolecular hydrogen bonds: distances (\AA), electron density ($e/\text{\AA}^3$), Laplacian ($e/\text{\AA}^5$), Hessian eigenvalues ($e/\text{\AA}^5$), ellipticity.

Contact	D_{12}	$d_{1\text{cp}}$	$d_{2\text{cp}}$	$\rho(\mathbf{r}_b)$	$\nabla^2\rho(\mathbf{r}_{\text{cp}})$	λ_1	λ_2	λ_3	ε
O1…HO2 ⁱ	1.8835	1.2008	0.6833	0.2314	1.17	-1.44	-1.43	4.03	0.0094
O1…H7B ⁱⁱ	2.6786	1.6192	1.0939	0.0453	0.56	-0.14	-0.1	0.8	0.3455
C2…H6A ⁱⁱ	2.8811	1.7237	1.2332	0.0383	0.6	-0.11	-0.06	0.78	0.7479
C4…H23B ⁱⁱⁱ	2.7242	1.6744	1.0834	0.0523	0.51	-0.17	-0.09	0.77	0.9253
O6…H16B ^{iv}	2.6852	1.5401	1.1455	0.0339	0.53	-0.1	-0.08	0.71	0.2942
O1…HO3 ^v	1.7344	1.1434	0.5912	0.3096	1.16	-2.16	-2.15	5.47	0.0027
O1…H16B ^v	2.4526	1.4401	1.0132	0.0615	0.89	-0.23	-0.14	1.26	0.6039

Symmetry codes: (i) $x, y, z-1$; (ii) $-x, y+1/2, -z+2$; (iii) $x+1, y, z-1$; (iv) $-x+1, y+1/2, -z+1$; (v) $-x+1, y+1/2, -z+2$.