

Selective solvent inclusion as a tool for mapping molecular properties in crystal structures – a diethylstilbestrol example

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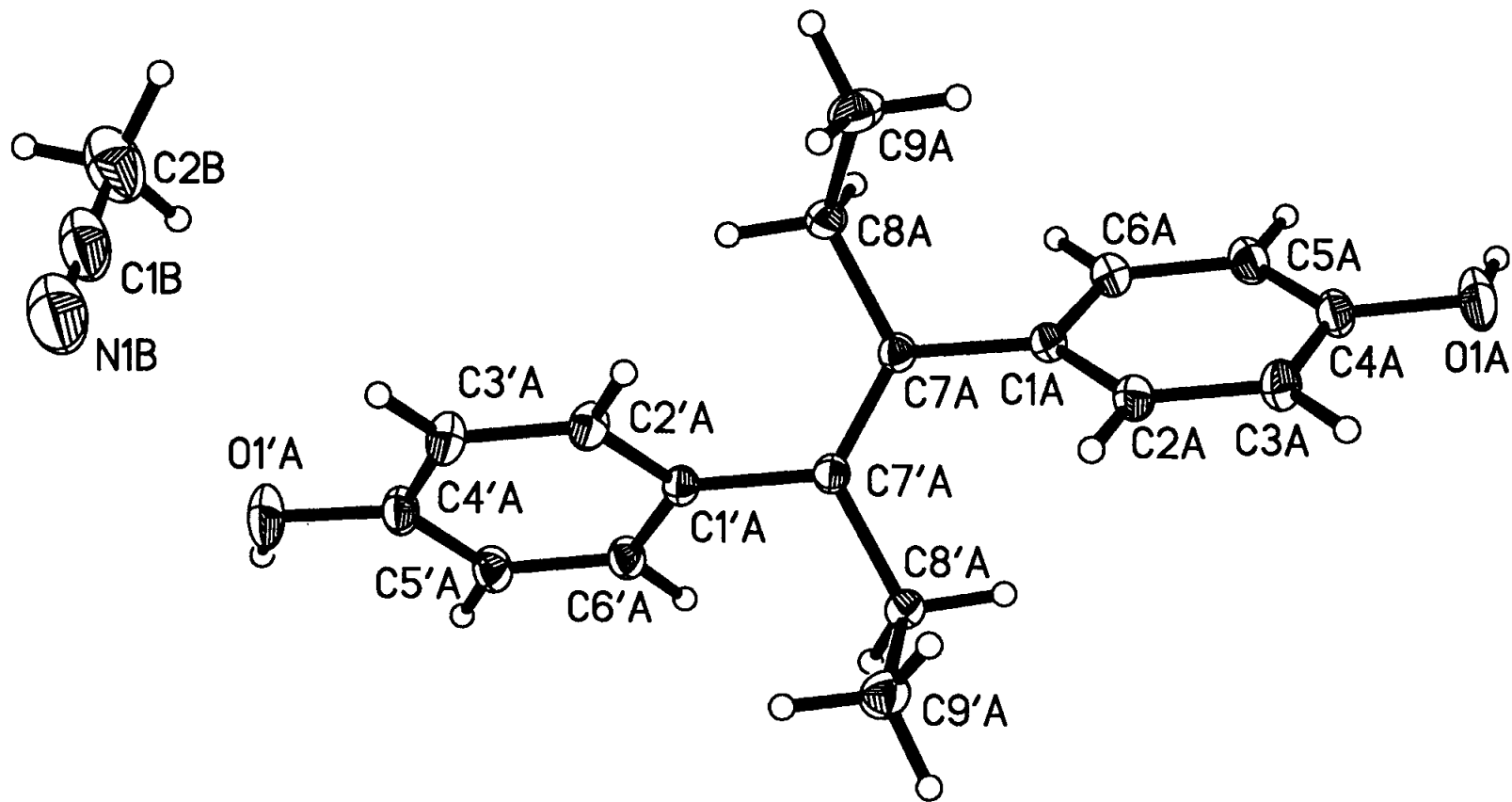
Supplementary material:

Drawings of all molecular structures with atomic numbering. Thermal ellipsoids are at the 50 % probability level. H-atoms are spheres of arbitrary size.

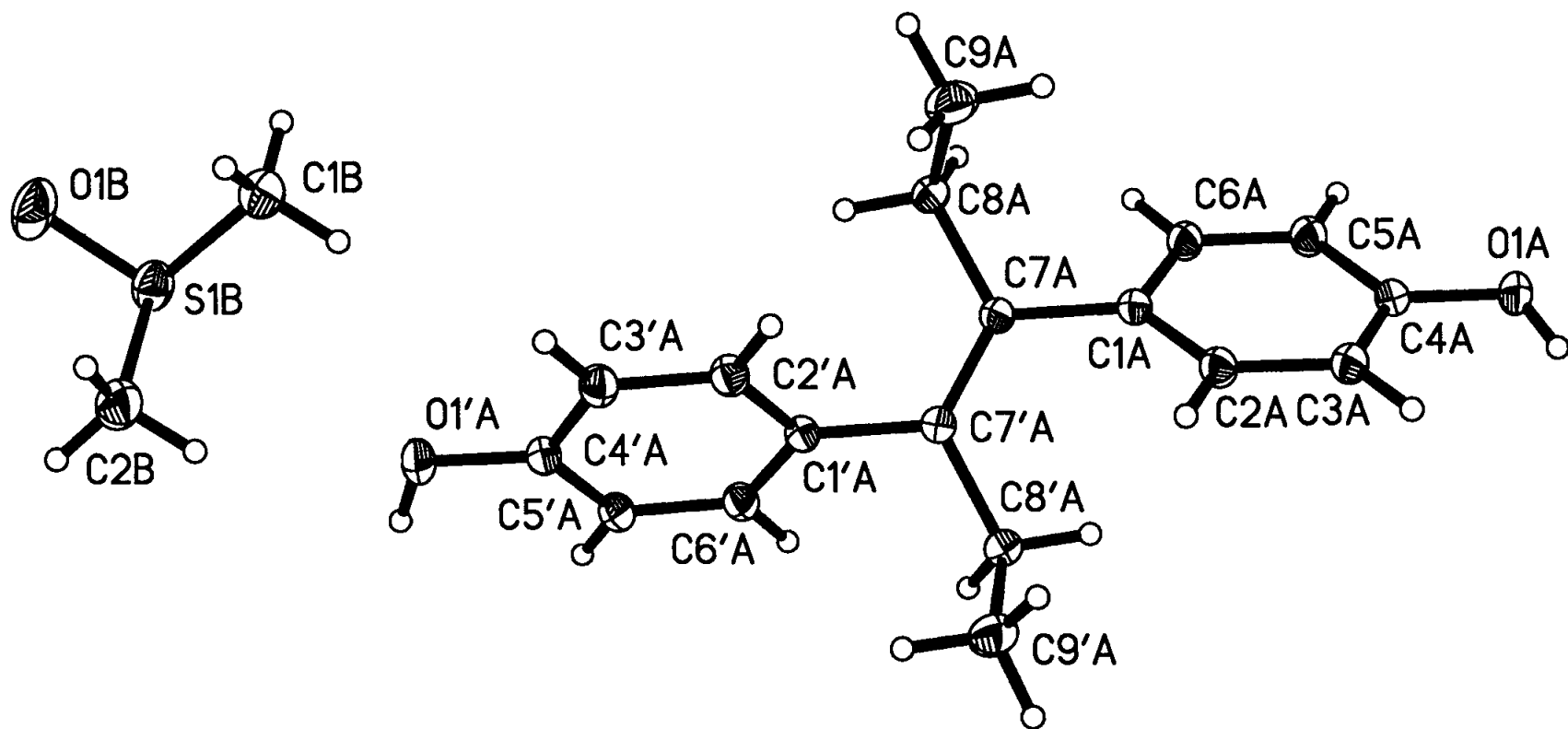
Variable drawing styles for the atoms and bonds have been used to indicate occupancy as follows:

Occupancy	Heavy atom	H-atom	Bond
Full	Shaded elements	Open circle	Solid
0.65 – 1.00	Principal ellipses	Open circle	Open
0.30 – 0.65	Boundary only	Open circle	Open
< 0.30	Dotted circle	Dotted circle	Dashed open

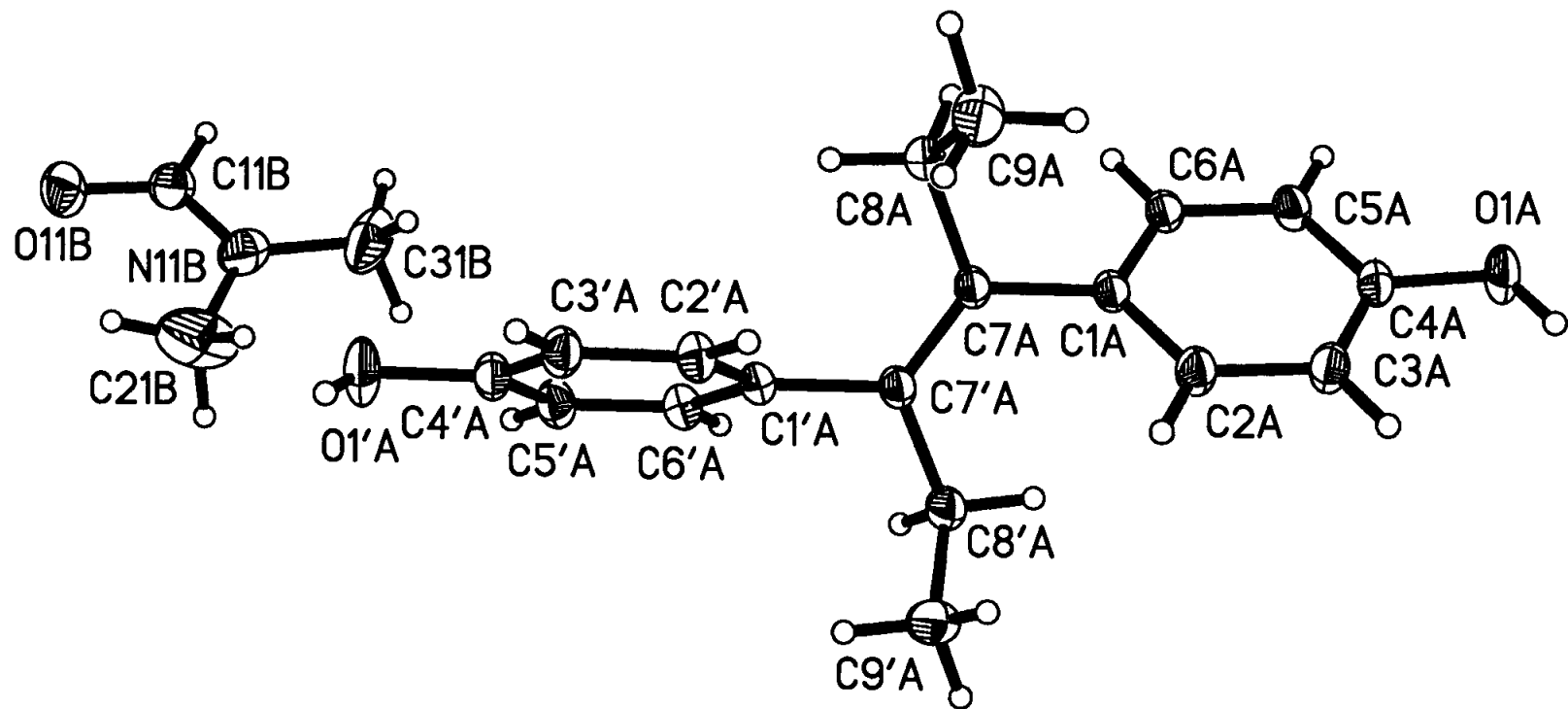
For **d.et.w** and **d.1-pr.w** cross-hatched circles mark H-atoms with occupancy constrained by symmetry to 0.50. For **d.tb** the second major DES-location (atom numbers Cx2, x = 1-9) is shown as a line drawing.



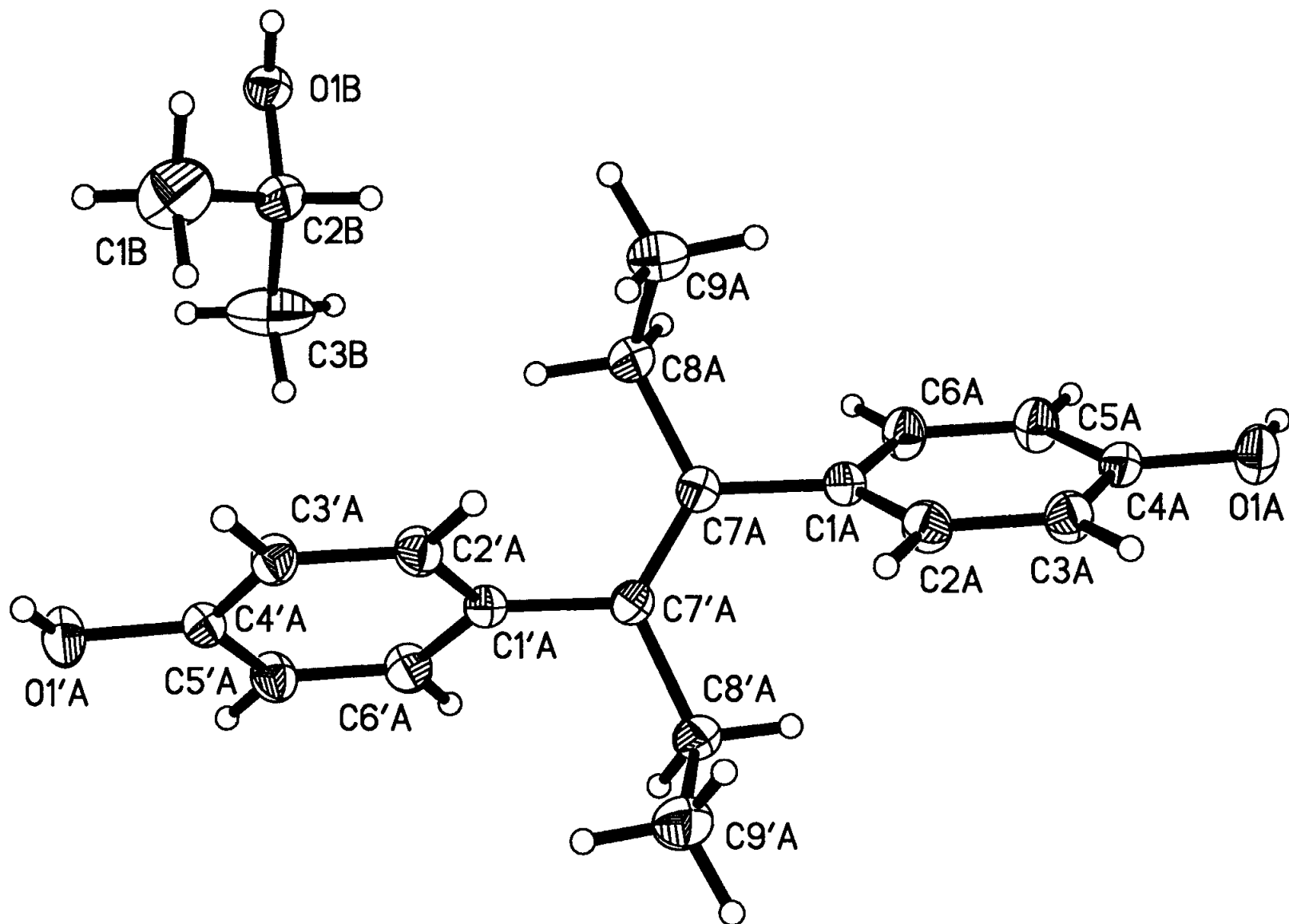
d.acn



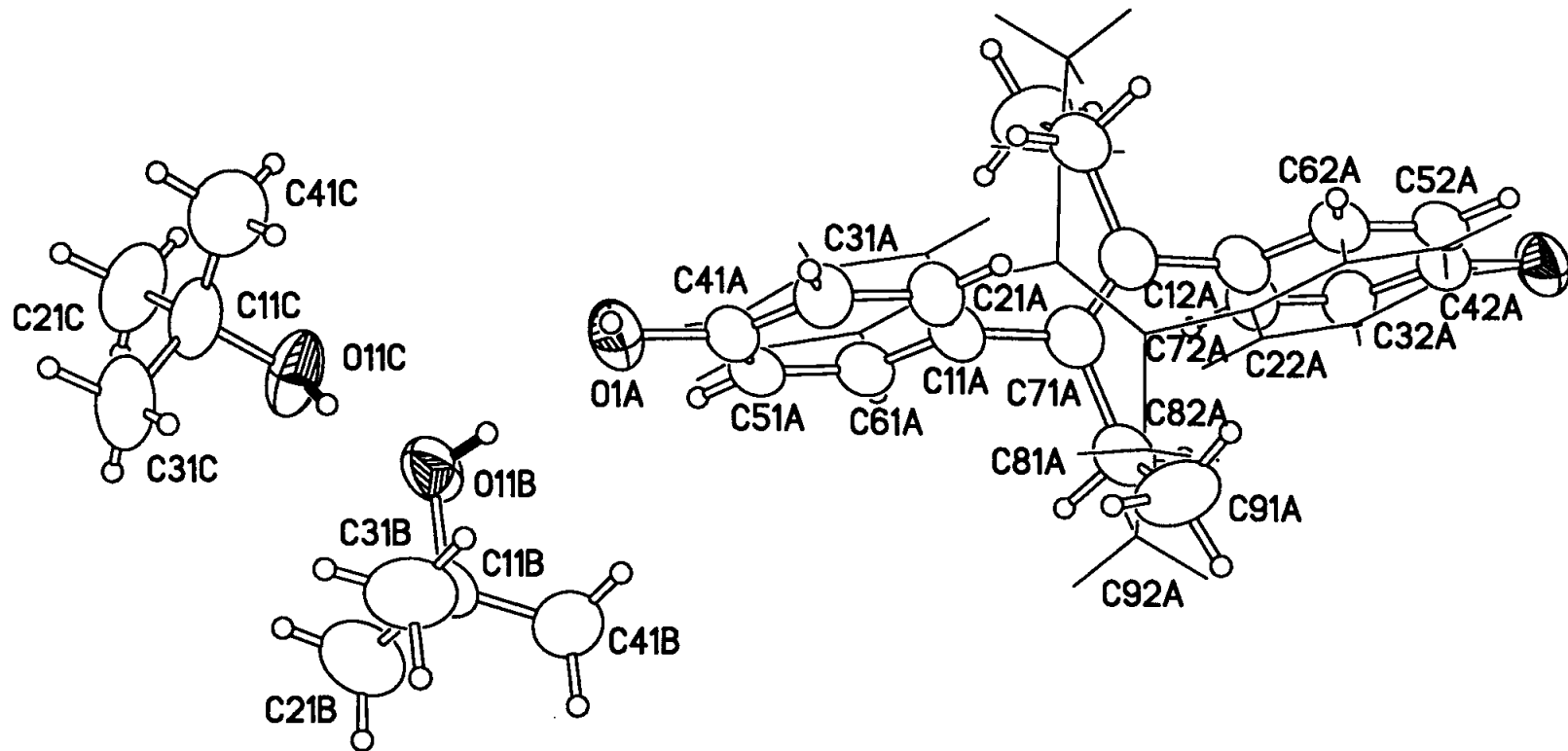
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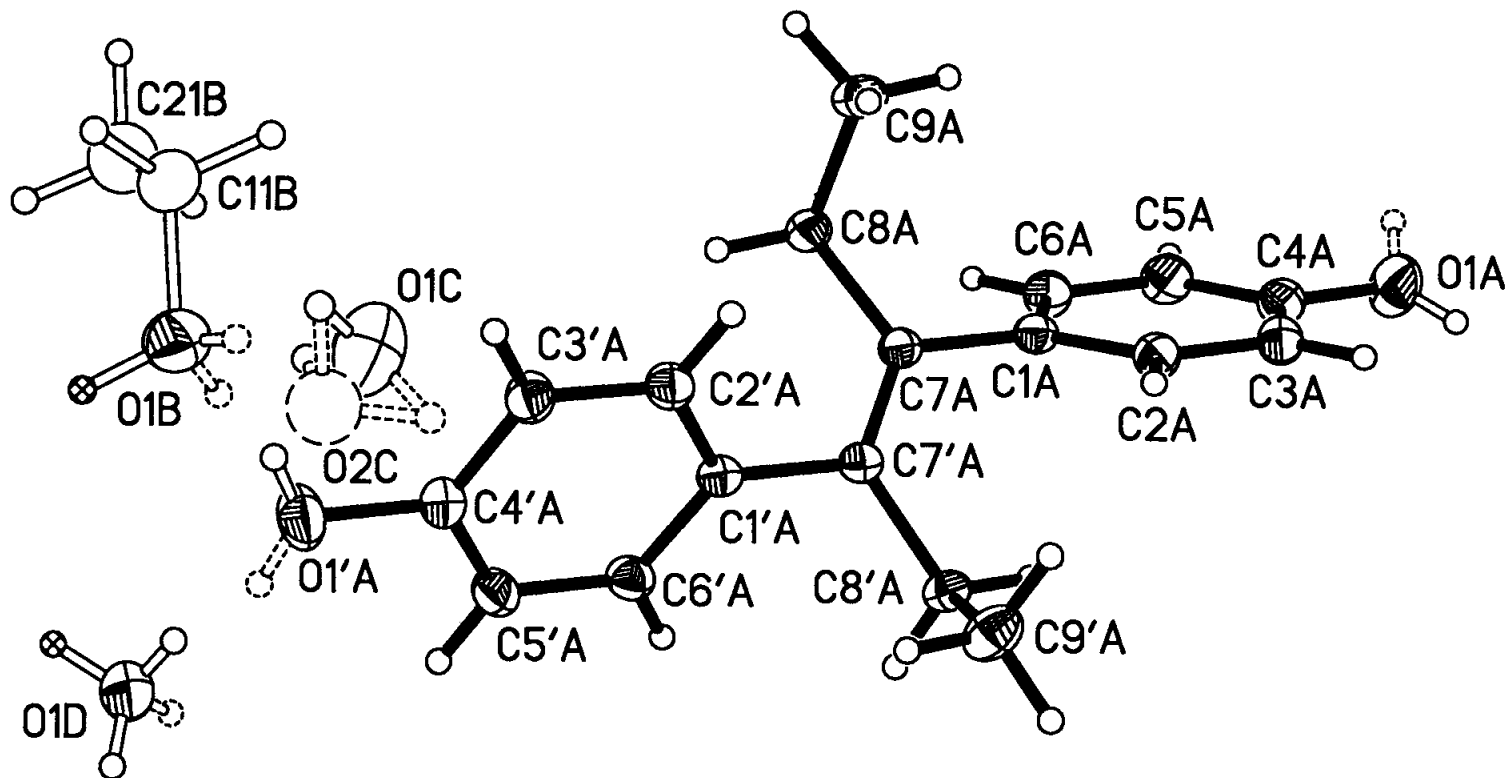
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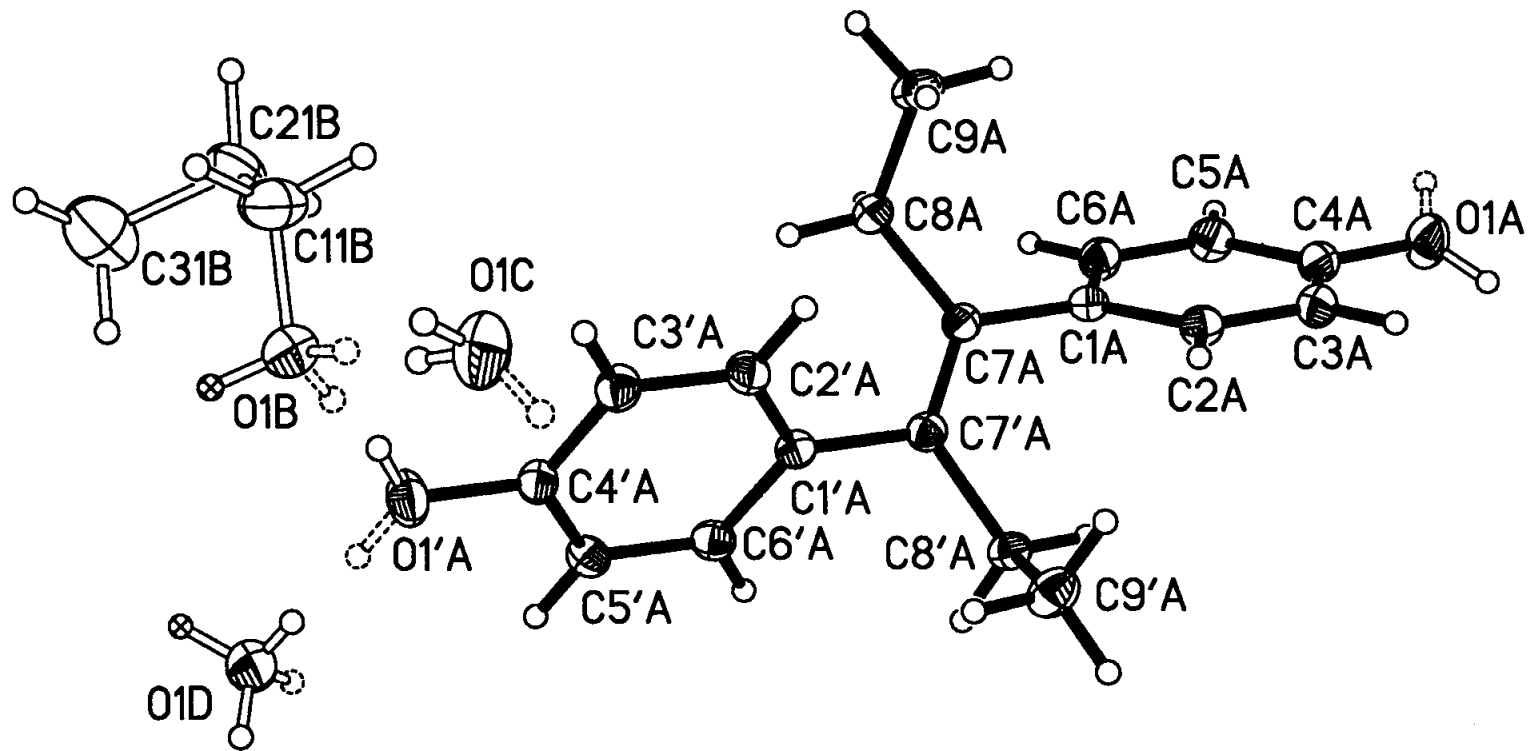
d.2-pr



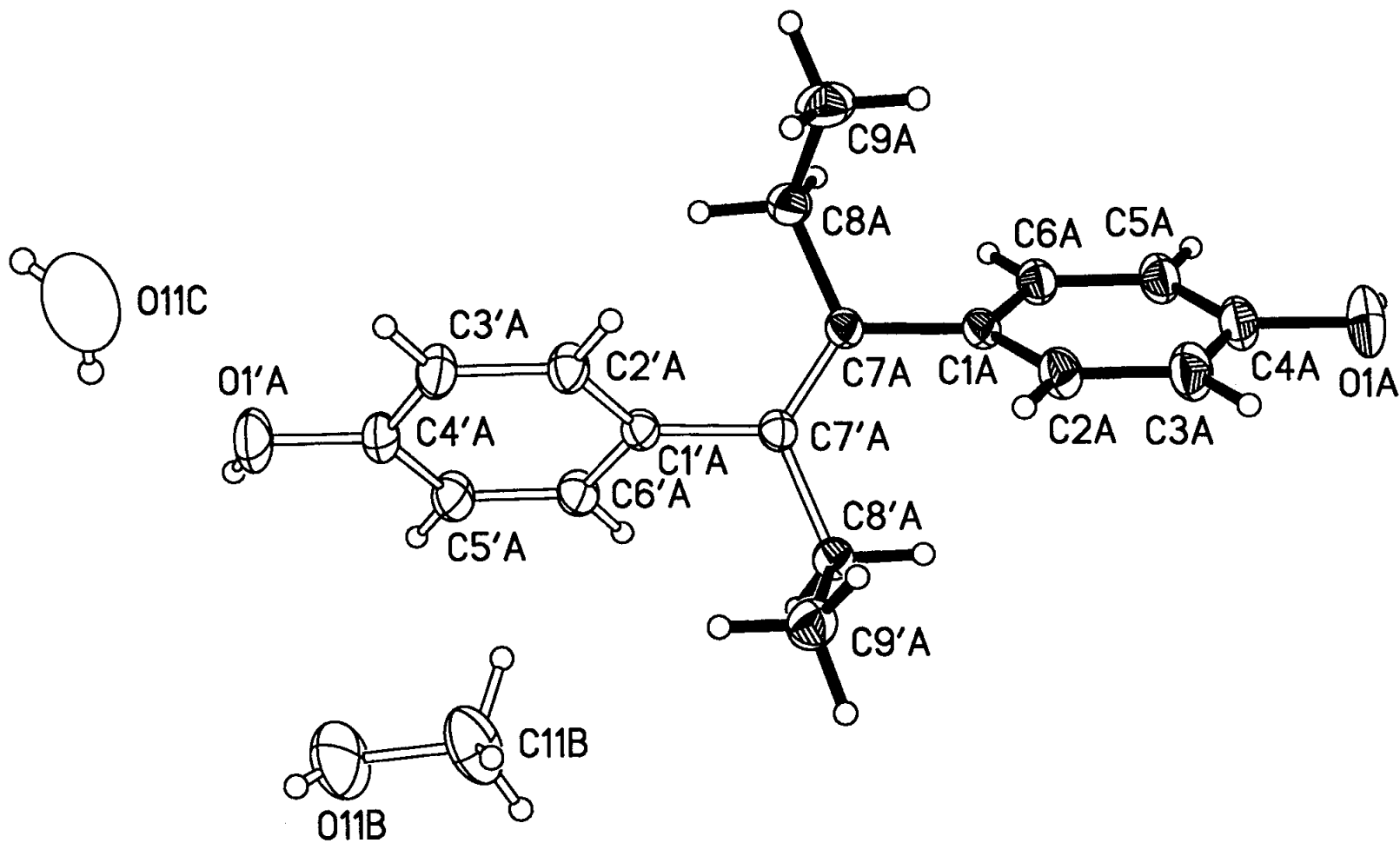
d.tbut



d.et.w



d.1-pr.w



d.met.w