**Supplementary materials**

# Selectivity in guest-host binding in assemblies of *bis*-phenols

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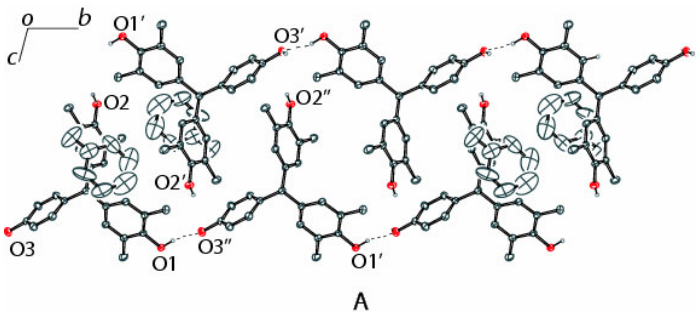
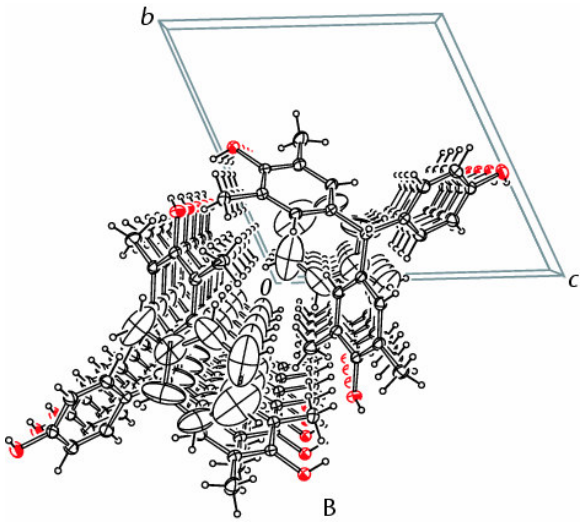


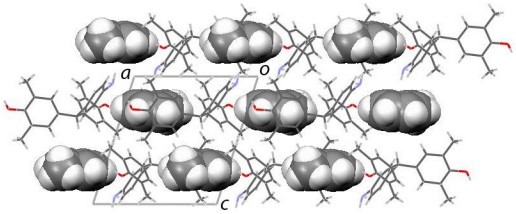

A

Formation of hydrogen-bonded sheets along [100] plane from *bis*(4-hydroxy-3,5-dimethylphenyl)(4-hydroxyphenyl)methane with toluene

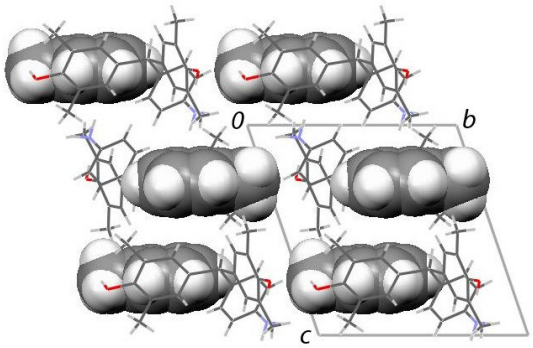



B

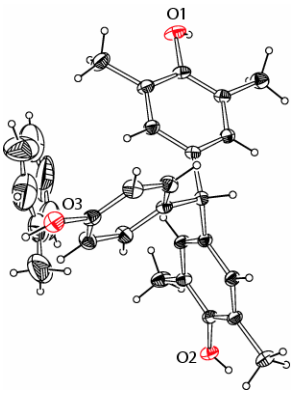
Packing of *bis*(4-hydroxy-3,5-dimethylphenyl)(4-hydroxyphenyl)methane with toluene guest viewed parallel to the *a*-axis



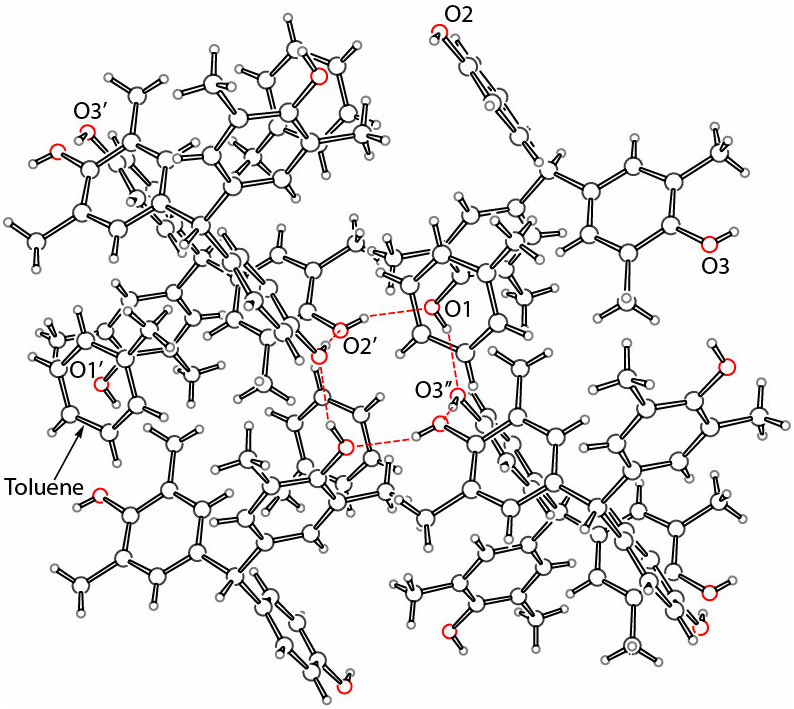

Two-dimensional hydrogen-bonded network in *bis*(4-hydroxy-3,5-dimethylphenyl)(4-aminophenyl)methane with toluene as viewed parallel to [100]




Two-dimensional hydrogen-bonded network in *bis*(4-hydroxy-3,5-dimethylphenyl)(4-aminophenyl)methane with toluene as viewed parallel to [001]



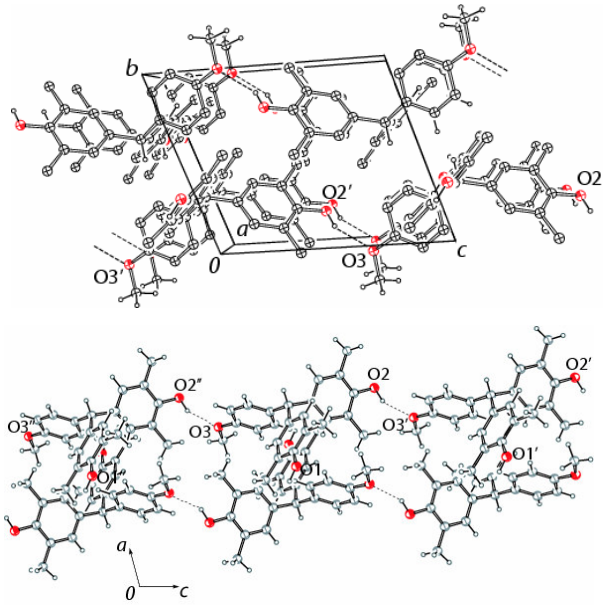

Structure of adduct of *bis* (4-hydroxy-3,5-dimethylphenyl)(4-hydroxyphenyl)methane with toluene



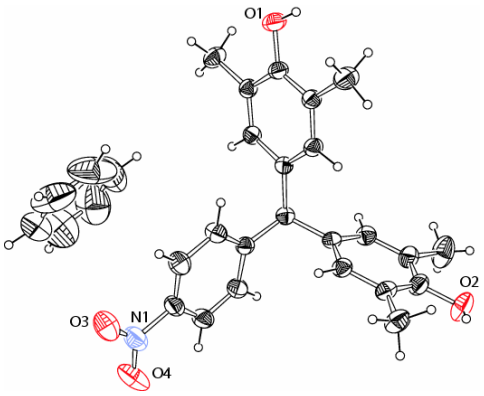

The H-bonding interactions in adduct of *bis*(4-hydroxy-3,5-dimethylphenyl) (4-hydroxyphenyl)methane with toluene showing cyclic hydrogen bonded hexamers generated by intermolecular O–H···O hydrogen-bonding interactions between the hydroxyl groups (thermal ellipsoids drawn to 30% probability)

Table: Important donor acceptor bond distances and angles in adduct of *bis*(4-hydroxy-3,5-dimethylphenyl)(4-hydroxyphenyl)methane with toluene

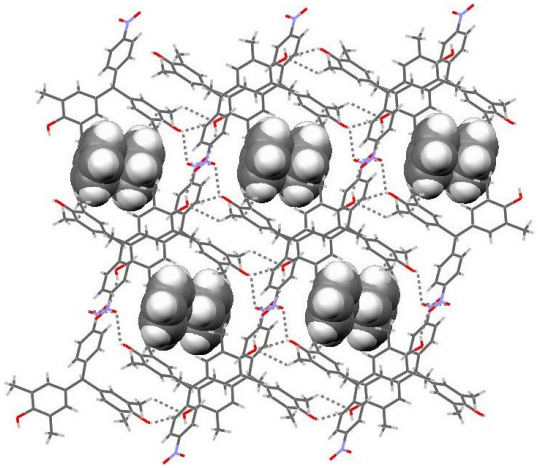
| D–H···A | d (D–H) | d(D···A) | <D–H···A (°) |
|---|---|---|---|
| O1–H1o···O3<br><br>[x, y+1, z] | 0.814 | 2.726 | 150.0 |
| O3–H2o···O2<br><br>[–x+1, –y+1, –z+2] | 0.923 | 2.791 | 173.9 |
| O2–H2o···O1<br><br>[x, y, z+1] | 0.776 | 2.791 | 152.1 |




The hydrogen bonding interactions in the crystal structure of *bis*(4-hydroxy-3,5-dimethylphenyl)(4-methoxyphenyl)methane along two crystallographic direction.



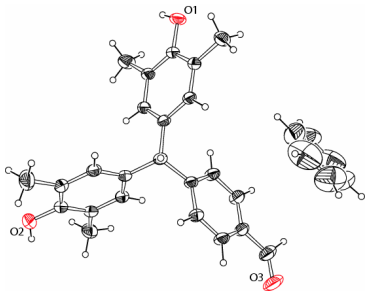

Structure of adduct of bis(4-hydroxy-3,5-dimethylphenyl) (4-nitrophenyl)methane with benzene **(2d)**



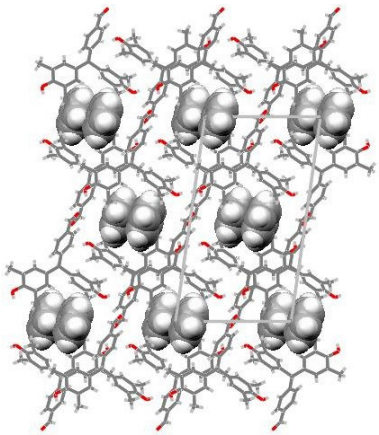
View of the packing of adduct of bis(4-hydroxy-3,5-dimethylphenyl) (4-nitrophenyl)methane with benzene parallel to *b*-axis and the orientation of benzene molecules in the cavities of the lattice

Table: The Donor and acceptor bond distances and angles in bis(4-hydroxy-3,5-dimethylphenyl) (4-nitrophenyl)methane

| D–H···A | d (D–H) | d (D···A) | <D–H···A (°) |
|---|---|---|---|
| O1'–H1o···O4<br>[x-1/2,–y+1/2, z+1/2] | 0.888 | 2.867 | 156.3 |
| O2'–H2o···O3<br>[x+1/2,–y +1/2, z+1/2] | 0.867 | 3.039 | 119.2 |
| O2'–H2o···O1'<br>[x+1, y, z] | 0.867 | 3.214 | 131.9 |



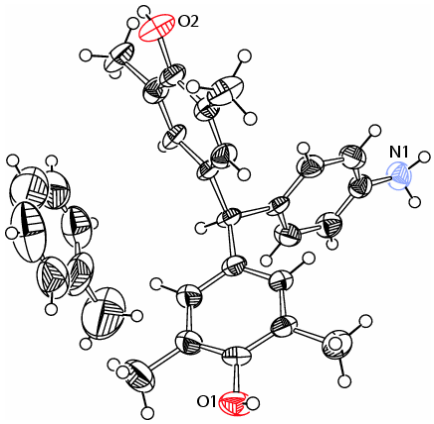

Structure of adduct of *bis*(4-hydroxy-3,5-dimethylphenyl)(4-formylphenyl)-methane (**2e**) with benzene



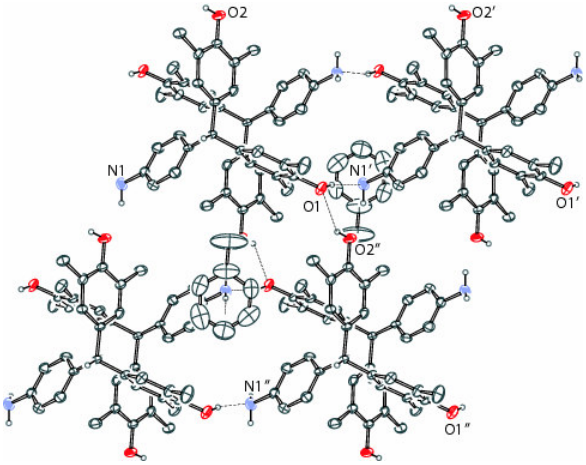
Packing of adduct of *bis*(4-hydroxy-3,5-dimethylphenyl)(4-formylphenyl)-methane (**2e**) with benzene

Table: Donor acceptor distances and angles in *bis*(4-hydroxy-3,5-dimethylphenyl)(4-formylphenyl)-methane **2e**

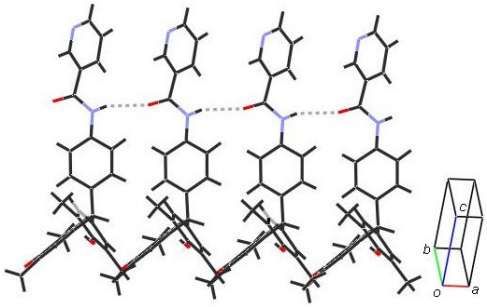
| D–H···A | d(D–H) | d(D···A) | <D–H···A(°) |
|---|---|---|---|
| O1–H1o···O3<br>[x–1/2, -y+3/2, z+1/2] | 0.891 | 2.740 | 145.3 |
| O2–H2o···O1<br>[x+1, y, z] | 0.862 | 2.994 | 164.1 |




Structure of adduct of *bis*(4-hydroxy-3,5-dimethylphenyl)(4-aminophenyl)methane with toluene (**2f**).




Packing adduct of *bis*(4-hydroxy-3,5-dimethylphenyl)(4-aminophenyl)methane with toluene of the molecules that intermolecular hydrogen bonding between the O–H group of the bis-phenol and N–H group (thermal ellipsoids drawn to 50% probability)




Packing of the *bis*{[(4-hydroxy-3,5-dimethylphenyl)methyl]-phenyl}nicotinamide that intermolecular hydrogen bonding between the –OH group of the phenols and C=O group of nicotinamide group