Supporting Information File

Microwave-assisted synthesis, characterization and mesomorphic investigations of novel disubstituted aroylhydrazones

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1. Analytical data of compounds

1.1 *N*-[4-(4'-alkoxy)benzoyloxybenzylidene]-*N'*-[4''-(4'''decyloxy)benzyloxy-benzoyl]hydrazines, ABBH-*n*

1.1.1 *N*-[4-(4'-hexyloxy)benzoyloxybenzylidene]-*N'*-[4''-(4'''decyloxy)benzyloxybenzoyl]hydrazine (ABBH-6) :

Yield: 68%, FT IR (KBr, cm⁻¹): 3215 ν_s (N-H), 2922, 2851 (aliphatic C-H), 1737 (ester, C=O), 1657 (amide-I, C=O), 1548 (amide-II), 1607, 1515 (Ph), 1275, 1256 (OPh); ¹H NMR (300 MHz, CDCl₃, 25°C): δ 11.13 (s, 1H, -NH), 8.37 (s, 1H, -CH=N), 8.12 (d, J(H,H)=8.4 Hz, 2H, -C₆H₄), 7.94 (d, J(H,H)=8.4 Hz, 2H, -C₆H₄), 7.80 (d, J(H,H)=7.5 Hz, 2H, -C₆H₄), 7.34 (d, J(H,H)=8.4 Hz, 2H, -C₆H₄), 7.26 (d, J(H,H)=8.4 Hz, 2H, -C₆H₄), 7.05-6.97 (m, 4H, -C₆H₄), 6.88 (d, J(H,H)=8.4 Hz, 2H, -C₆H₄), 5.06 (s, 2H, Ar-CH₂-O-Ar), 4.08 (t, 2H, -OCH₂), 3.98 (t, 2H, -OCH₂), 1.85-1.25 (m, 24H, -[CH₂]₁₂), 0.88 (m, 6H, [-CH₃]₂); ¹³C NMR (75 MHz, CDCl₃, 25°C): δ_c 165.52, 163.93, 163.50, 162.64, 158.11, 152.20, 146.44, 131.38, 130.98, 128.39, 124.86, 121.06, 116.87, 114.35, 113.43, 71.58, 68.38, 31.58, 29.83, 29.34, 29.18, 25.96, 22.67, 14.11; Elemental analyses: calculated for C₄₄H₅₄N₂O₆ (%), C, 74.76; H, 7.70; N, 3.96; Found, C, 74.83; H, 7.61; N, 4.08.

1.1.2 N-[4-(4'-octyloxy)benzoyloxybenzylidene]-N'-[4''-(4'''-decyloxy)benzyloxybenzoyl]hydrazine (ABBH-8) :

Yield: 74%, FT IR (KBr, cm^{-1}): 3212 ν_{s} (N-H), 2923, 2851 (aliphatic C-H), 1735 (ester, C=O), 1658 (amide-I, C=O), 1546 (amide-II), 1608, 1516 (Ph), 1274, 1257 (OPh); ^1H NMR (300 MHz, CDCl_3 , 25°C): δ 11.14 (s, 1H, -NH), 8.38 (s, 1H, -CH=N), 8.13 (d, $J(\text{H,H})=8.4$ Hz, 2H, $-\text{C}_6\text{H}_4$), 7.95 (d, $J(\text{H,H})=8.4$ Hz, 2H, $-\text{C}_6\text{H}_4$), 7.81 (d, $J(\text{H,H})=7.5$ Hz, 2H, $-\text{C}_6\text{H}_4$), 7.35 (d, $J(\text{H,H})=8.4$ Hz, 2H, $-\text{C}_6\text{H}_4$), 7.04-6.96 (m, 4H, $-\text{C}_6\text{H}_4$), 6.88 (d, $J(\text{H,H})=8.4$ Hz, 2H, $-\text{C}_6\text{H}_4$), 5.06 (s, 2H, Ar- CH_2 -O-Ar), 4.07 (t, 2H, $-\text{OCH}_2$), 3.97 (t, 2H, $-\text{OCH}_2$), 1.84-1.25 (m, 28H, $-\text{[CH}_2\text{]}_{14}$), 0.88 (m, 6H, $-\text{[CH}_3\text{]}_2$); ^{13}C NMR (75 MHz, CDCl_3 , 25°C): δ_{c} 165.53, 163.94, 163.49, 162.68, 158.13, 152.22, 146.48, 131.40, 130.96, 128.37, 124.84, 121.06, 116.86, 114.37, 113.41, 71.59, 68.37, 31.59, 29.83, 29.34, 29.17, 25.96, 22.67, 14.12; Elemental analyses: calculated for $\text{C}_{46}\text{H}_{58}\text{N}_2\text{O}_6$ (%), C, 75.17; H, 7.95; N, 3.81; Found, C, 75.24; H, 7.89; N, 3.78.

1.1.3 N-[4-(4'-dodecyloxy)benzoyloxybenzylidene]-N'-[4''-(4'''-decyloxy)benzyloxybenzoyl]hydrazine (ABBH-12) :

Yield: 84%, FT IR (KBr, cm^{-1}): 3211 ν_{s} (N-H), 2922, 2852 (aliphatic C-H), 1738 (ester, C=O), 1657 (amide-I, C=O), 1547 (amide-II), 1606, 1515 (Ph), 1275, 1257 (OPh); ^1H NMR (300 MHz, CDCl_3 , 25°C): δ 11.20 (s, 1H, -NH), 8.41 (s, 1H, -CH=N), 8.10 (d, $J(\text{H,H})=8.4$ Hz, 2H, $-\text{C}_6\text{H}_4$), 7.93 (d, $J(\text{H,H})=8.4$ Hz, 2H, $-\text{C}_6\text{H}_4$), 7.79 (d, $J(\text{H,H})=7.5$ Hz, 2H, $-\text{C}_6\text{H}_4$), 7.33 (d, $J(\text{H,H})=8.4$ Hz, 2H, $-\text{C}_6\text{H}_4$), 7.24 (d, $J(\text{H,H})=8.4$ Hz, 2H, $-\text{C}_6\text{H}_4$), 7.03-6.97 (m, 4H, $-\text{C}_6\text{H}_4$), 6.89 (d, $J(\text{H,H})=8.4$ Hz, 2H, $-\text{C}_6\text{H}_4$), 5.06 (s, 2H, Ar- CH_2 -O-Ar), 4.06 (t, 2H, $-\text{OCH}_2$), 3.96 (t, 2H, $-\text{OCH}_2$), 1.83-1.27 (m, 36H, $-\text{[CH}_2\text{]}_{18}$), 0.88 (m, 6H, $-\text{[CH}_3\text{]}_2$); ^{13}C NMR (75 MHz, CDCl_3 , 25°C): δ_{c} 165.55, 163.94, 163.49, 162.68, 158.10, 152.20, 146.48, 131.38, 130.97, 128.37, 124.86, 121.08, 116.86, 114.35, 113.41, 71.58, 68.37, 31.58, 29.84, 29.34, 29.19, 25.96, 22.67, 14.10; Elemental analyses: calculated for $\text{C}_{50}\text{H}_{66}\text{N}_2\text{O}_6$ (%), C, 75.91; H, 8.41; N, 3.54; Found, C, 75.98; H, 8.37; N, 3.64.

1.1.4 N-[4-(4'-tetradecyloxy)benzoyloxybenzylidene]-N'-[4''-(4'''-decyloxy)benzyloxy benzoyl]hydrazine (ABBH-14) :

Yield: 78%, FT IR (KBr, cm^{-1}): 3212 ν_{s} (N-H), 2923, 2852 (aliphatic C-H), 1738 (ester, C=O), 1656 (amide-I, C=O), 1546 (amide-II), 1607, 1515 (Ph), 1274, 1256 (OPh); ^1H NMR (300 MHz, CDCl_3 , 25°C): δ 11.18 (s, 1H, -NH), 8.3 (s, 1H, -CH=N), 8.09 (d, $J(\text{H,H})=8.4$ Hz,

2H, -C₆H₄), 7.92 (d, J(H,H)=8.4 Hz, 2H, -C₆H₄), 7.78 (d, J(H,H)=7.5 Hz, 2H, -C₆H₄), 7.32 (d, J(H,H)=8.4 Hz, 2H, -C₆H₄), 7.22 (d, J(H,H)=8.4 Hz, 2H, -C₆H₄), 7.03-6.96 (m, 4H, -C₆H₄), 6.88 (d, J(H,H)=8.4 Hz, 2H, -C₆H₄), 5.04 (s, 2H, Ar-CH₂-O-Ar), 4.05 (t, 2H, -OCH₂), 3.97 (t, 2H, -OCH₂), 1.82-1.26 (m, 40H, -[CH₂]₂₀), 0.88 (m, 6H, [-CH₃]₂); ¹³C NMR (75 MHz, CDCl₃, 25°C): δ_c 165.54, 163.94, 163.47, 162.68, 158.10, 152.22, 146.49, 131.38, 130.96, 128.38, 124.86, 121.06, 116.86, 114.35, 113.42, 71.58, 68.37, 31.59, 29.83, 29.34, 29.17, 25.97, 22.67, 14.10; Elemental analyses: calculated for C₅₂H₇₀N₂O₆ (%), C, 76.25; H, 8.61; N, 3.42; Found, C, 76.35; H, 8.56; N, 3.47.

1.1.5 N-[4-(4'-hexadecyloxy)benzoyloxybenzylidene]-N'-[4''-(4'''-decyloxy)benzyloxy benzoyl]hydrazine (ABBH-16) :

Yield: 82%, FT IR (KBr, cm⁻¹): 3215 ν_s (N-H), 2922, 2852 (aliphatic C-H), 1736 (ester, C=O), 1656 (amide-I, C=O), 1545 (amide-II), 1608, 1516 (Ph), 1274, 1257 (OPh); ¹H NMR (300 MHz, CDCl₃, 25°C): δ 11.19 (s, 1H, -NH), 8.39 (s, 1H, -CH=N), 8.09 (d, J₁(H,H)=8.4 Hz, 2H, -C₆H₄), 7.94 (d, J(H,H)=8.4 Hz, 2H, -C₆H₄), 7.80 (d, J(H,H)=7.5 Hz, 2H, -C₆H₄), 7.33 (d, J(H,H)=8.4 Hz, 2H, -C₆H₄), 7.23 (d, J(H,H)=8.4 Hz, 2H, -C₆H₄), 7.02-6.96 (m, 4H, -C₆H₄), 6.89 (d, J(H,H)=8.4 Hz, 2H, -C₆H₄), 5.05 (s, 2H, Ar-CH₂-O-Ar), 4.03 (t, 2H, -OCH₂), 3.97 (t, 2H, -OCH₂), 1.83-1.27 (m, 44H, -[CH₂]₂₂), 0.88 (m, 6H, [-CH₃]₂); ¹³C NMR (75 MHz, CDCl₃, 25°C): δ_c 165.53, 163.95, 163.48, 162.67, 158.11, 152.21, 146.48, 131.39, 130.96, 128.36, 124.86, 121.05, 116.86, 114.35, 113.43, 71.57, 68.36, 31.58, 29.83, 29.35, 29.17, 25.96, 22.68, 14.10; Elemental analyses: calculated for C₅₄H₇₄N₂O₆ (%), C, 76.56; H, 8.80; N, 3.31; Found, C, 76.68; H, 8.71; N, 3.34.

1.2 N-[4-(4'-alkoxy)benzoyloxy-2-hydroxy-benzylidene]-N'-[4''-(4'''-decyloxy)benzyloxybenzoyl]hydrazines (ABB(OH)H-n)

1.2.1 N-[4-(4'-hexyloxy)benzoyloxy-2-hydroxy-benzylidene]-N'-[4''-(4'''-decyloxy)benzyloxybenzoyl]hydrazine (ABB(OH)H-6)

Yield: 80 %, IR (KBr, cm⁻¹): 3454 ν_s (O-H), 3299 ν_s (N-H), 2923, 2853 (aliphatic C-H), 1730 (ester, C=O), 1655 (amide-I, C=O), 1580 (amide-II), 1608, 1512, 1468 (Ph), 1538, 1281, 1253 (OPh); ¹H NMR (300 MHz, CDCl₃, 25°C): δ 11.12 (s, 1H, -OH), 9.01 (s, 1H, -NH), 8.43 (s, 1H, -CH=N), 8.13 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 7.83 (d, J(H,H)=8.4 Hz, 2H, -C₆H₄), 7.36 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 7.01 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 6.95 (m, 4H, -C₆H₄), 6.90 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 6.82 (s, 1H, C₆H₃), 5.05 (s, 2H, Ar-CH₂-O-Ar),

4.05 (t, 2H, -OCH₂), 3.99 (t, 2H, -OCH₂), 1.78(m, 4H, -OCH₂CH₂), 1.50-1.28 (m, 20H, -[CH₂]₁₀), 0.86 (t, 6H, -CH₃); ¹³C NMR (75 MHz, DMSO-d₆, 25°C): δ_c 166.52, 164.10, 163.72, 163.28, 162.68, 155.41, 152.29, 133.55, 132.32, 131.06, 128.37, 121.13, 121.07, 116.86, 114.37, 113.41, 110.75, 68.37, 52.20, 31.86, 29.54, 29.34, 29.08, 25.96, 22.67, 14.10; Elemental analyses: calculated for C₄₄H₅₄N₂O₇ (%), C, 73.10; H, 7.53; N, 3.88; Found, C, 72.95; H, 7.38; N, 3.59.

1.2.2 N-[4-(4'-octyloxy)benzoyloxy-2-hydroxy-benzylidene]-N'-[4''-(4'''-decyloxy)benzyloxybenzoyl]hydrazine (ABB(OH)H-8)

Yield: 82 %. IR (KBr, cm⁻¹): 3456 ν_s (O-H), 3299 ν_s (N-H), 2923, 2852 (aliphatic C-H), 1731 (ester, C=O), 1658 (amide-I, C=O), 1579 (amide-II), 1606, 1513, 1468 (Ph), 1541, 1280, 1254 (OPh); ¹H NMR (300 MHz, CDCl₃, 25°C): δ 11.10 (s, 1H, -OH), 8.99 (s, 1H, -NH), 8.40 (s, 1H, -CH=N), 8.12 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 7.82 (d, J(H,H)=8.4 Hz, 2H, -C₆H₄), 7.33 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 6.99 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 6.93 (m, 4H, -C₆H₄), 6.88 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 6.79 (s, 1H, C₆H₃), 5.04 (s, 2H, Ar-CH₂-O-Ar), 4.03 (t, 2H, -OCH₂), 3.97 (t, 2H, -OCH₂), 1.77 (m, 4H, -OCH₂CH₂), 1.51-1.28 (m, 24H, -[CH₂]₁₂), 0.86 (t, 6H, -CH₃); ¹³C NMR (75 MHz, DMSO-d₆, 25°C): δ_c 166.56, 164.10, 163.74, 163.28, 162.68, 155.40, 152.29, 133.55, 132.38, 131.10, 128.37, 121.15, 121.10, 116.86, 114.37, 113.43, 110.75, 68.38, 52.19, 31.88, 29.54, 29.34, 29.10, 25.96, 22.67, 14.08; Elemental analyses: calculated for C₄₆H₅₈N₂O₇ (%), C, 73.57; H, 7.78; N, 3.73; Found, C, 73.31; H, 7.59; N, 3.51.

1.2.3 N-[4-(4'-dodecyloxy)benzoyloxy-2-hydroxy-benzylidene]-N'-[4''-(4'''-decyloxy)benzyloxybenzoyl]hydrazine (ABB(OH)H-12)

Yield: 81 %. IR (KBr, cm⁻¹): 3461 ν_s (O-H), 3300 ν_s (N-H), 2922, 2852 (aliphatic C-H), 1728 (ester, C=O), 1654 (amide-I, C=O), 1580 (amide-II), 1606, 1514, 1469 (Ph), 1534, 1280, 1255 (OPh); ¹H NMR (300 MHz, CDCl₃, 25°C): δ 11.08 (s, 1H, -OH), 8.97 (s, 1H, -NH), 8.39 (s, 1H, -CH=N), 8.09 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 7.79 (d, J(H,H)=8.4 Hz, 2H, -C₆H₄), 7.31 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 6.97 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 6.91 (m, 4H, -C₆H₄), 6.86 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 6.78 (s, 1H, C₆H₃), 5.02 (s, 2H, Ar-CH₂-O-Ar), 4.02 (t, 2H, -OCH₂), 3.96 (t, 2H, -OCH₂), 1.76 (m, 4H, -OCH₂CH₂), 1.51-1.28 (m, 32H, -[CH₂]₁₆), 0.87 (t, 6H, -CH₃); ¹³C NMR (75 MHz, DMSO-d₆, 25°C): δ_c 166.55, 164.11, 163.74, 163.27, 162.68, 155.40, 152.29, 133.57, 132.38, 131.06, 128.39, 121.15, 121.07,

116.84, 114.37, 113.42, 110.73, 68.37, 52.19, 31.88, 29.54, 29.35, 29.08, 25.96, 22.67, 14.10;
Elemental analyses: calculated for C₅₀H₆₆N₂O₇ (%), C, 74.41; H, 8.24; N, 3.47; Found, C,
74.07; H, 8.02; N, 3.32.

1.2.4 N-[4-(4'-tetradecyloxy)benzoyloxy-2-hydroxy-benzylidene]-N'-[4''-(4'''-decyloxy)benzyloxybenzoyl]hydrazine (ABB(OH)H-14)

Yield: 83 %. IR (KBr, cm⁻¹): 3463 ν_s (O-H), 3299 ν_s (N-H), 2923, 2852 (aliphatic C-H), 1730 (ester, C=O), 1660 (amide-I, C=O), 1578 (amide-II), 1605, 1514, 1469 (Ph), 1537, 1280, 1255 (OPh); ¹H NMR (300 MHz, CDCl₃, 25°C): δ 11.09 (s, 1H, -OH), 8.98 (s, 1H, -NH), 8.40 (s, 1H, -CH=N), 8.10 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 7.80 (d, J(H,H)=8.4 Hz, 2H, -C₆H₄), 7.32 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 6.98 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 6.92 (m, 4H, -C₆H₄), 6.87 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 6.79 (s, 1H, C₆H₃), 5.03 (s, 2H, Ar-CH₂-O-Ar), 4.03 (t, 2H, -OCH₂), 3.96 (t, 2H, -OCH₂), 1.77 (m, 4H, -OCH₂CH₂), 1.52-1.28 (m, 36H, -[CH₂]₁₈), 0.86 (t, 6H, -CH₃); ¹³C NMR (75 MHz, DMSO-d₆, 25°C): δ_c 166.55, 164.10, 163.74, 163.28, 162.67, 155.42, 152.30, 133.55, 132.40, 131.06, 128.37, 121.17, 121.07, 116.85, 114.37, 113.42, 110.75, 68.36, 52.19, 31.88, 29.54, 29.34, 29.08, 25.96, 22.67, 14.11; Elemental analyses: calculated for C₅₂H₇₀N₂O₇ (%), C, 74.79; H, 8.45; N, 3.35; Found, C, 74.54; H, 8.32; N, 3.19.

1.2.5 N-[4-(4'-hexadecyloxy)benzoyloxy-2-hydroxy-benzylidene]-N'-[4''-(4'''-decyloxy)benzyloxybenzoyl]hydrazine (ABB(OH)H-16)

Yield: 82 %. IR (KBr, cm⁻¹): 3464 ν_s (O-H), 3299 ν_s (N-H), 2922, 2854 (aliphatic C-H), 1729 (ester, C=O), 1655 (amide-I, C=O), 1578 (amide-II), 1605, 1513, 1470 (Ph), 1532, 1280, 1253 (OPh); ¹H NMR (300 MHz, CDCl₃, 25°C): δ 11.09 (s, 1H, -OH), 8.98 (s, 1H, -NH), 8.40 (s, 1H, -CH=N), 8.10 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 7.80 (d, J(H,H)=8.4 Hz, 2H, -C₆H₄), 7.32 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 6.98 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 6.92 (m, 4H, -C₆H₄), 6.87 (d, J(H,H)=8.1 Hz, 2H, -C₆H₄), 6.79 (s, 1H, C₆H₃), 5.03 (s, 2H, Ar-CH₂-O-Ar), 4.03 (t, 2H, -OCH₂), 3.96 (t, 2H, -OCH₂), 1.77 (m, 4H, -OCH₂CH₂), 1.52-1.28 (m, 40H, -[CH₂]₂₀), 0.86 (t, 6H, -CH₃); ¹³C NMR (75 MHz, DMSO-d₆, 25°C): δ_c 166.55, 164.09, 163.74, 163.28, 162.68, 155.41, 152.29, 133.55, 132.37, 131.06, 128.37, 121.17, 121.07, 116.86, 114.37, 113.45, 110.75, 68.37, 52.21, 31.89, 29.54, 29.34, 29.10, 25.96, 22.67, 14.11; Elemental analyses: calculated for C₅₄H₇₄N₂O₇ (%), C, 75.14; H, 8.64; N, 3.25; Found, C, 74.97; H, 8.47; N, 3.11.

Figure SI 1. ^1H NMR spectrum of compound 9

Figure SI 2. ¹³C NMR spectrum of compound 9

Figure SI 3. ^1H NMR spectrum of ABBH-n

Figure SI 4. ^{13}C NMR spectrum of ABBH-n

Figure SI 5. ¹H NMR spectrum of ABB(OH)H-n

Figure SI 6. ^{13}C NMR Spectrum of ABB(OH)H-n

Cartesian Coordinates of ABBH-10 (Keto Form):

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	0.000001056	0.000000427	0.000000519
C	-0.000000269	0.000000761	-0.000000588
C	0.000000216	0.000000553	0.000000950
C	0.000000244	-0.000002302	-0.000001595
C	-0.000001992	0.000000192	-0.000001566
C	-0.000000153	-0.000000988	0.000000913
H	-0.000000024	0.000000296	0.000000590
H	-0.000000279	0.000000856	0.000000409
H	0.000000496	0.000000172	0.000000340
H	0.000000310	0.000000452	0.000000672
C	0.000002435	0.000002659	-0.000000308
H	-0.000000472	-0.000001804	-0.000000054
H	-0.000000209	-0.000000001	0.000000703
O	-0.000002452	-0.000002052	0.000000144
C	0.000002274	0.000000597	-0.000001007
C	-0.000000161	-0.000000353	-0.000000521
C	-0.000000794	0.000000352	-0.000000107
C	-0.000001514	0.000002892	0.000000440
H	-0.000000356	-0.000000338	0.000000406
C	0.000002113	0.000001531	0.000000001
H	-0.000000463	-0.000000120	-0.000000063
C	-0.000000611	-0.000004597	-0.000001207
H	0.000000288	-0.000001821	0.000000465
H	-0.000000434	-0.000000464	-0.000000100
O	0.000000210	0.000001399	0.000001100
C	-0.000003608	0.000000207	-0.000000874
N	0.000001162	-0.000001580	0.000000144
N	-0.000002512	-0.000001234	-0.000000327
H	-0.000000485	-0.000000014	0.000000959
C	0.000005974	0.000001097	-0.000002990
C	0.000002720	0.000001097	0.000001701
C	-0.000001085	-0.000004055	0.000001846
C	0.000008437	0.000007645	-0.000003221
C	0.000000819	0.000000223	0.000001118
H	-0.000001192	0.000001280	-0.000000086
C	-0.000009112	0.000000378	-0.000002290
C	0.000001838	0.000003203	-0.000006420
H	-0.000001493	0.000000026	0.000000498
H	0.000000744	-0.000000751	0.000000340
H	-0.000001297	-0.000000244	0.000000505
O	-0.000000579	-0.000000902	0.000000203
C	0.000002535	0.000000231	0.000000949
C	-0.000001109	0.000000398	-0.000000623
H	-0.000000403	-0.000000213	-0.000000223
H	-0.000000286	-0.000001056	0.000000225
C	0.000000704	-0.000000494	0.000001597

H	-0.000000497	-0.000000424	0.000000599
H	0.000000702	-0.000000432	0.000000296
C	-0.000000733	-0.000000110	-0.000000573
H	0.000000080	-0.000000323	-0.000000572
H	-0.000000477	-0.000000508	0.000000603
H	0.000000007	-0.000000431	0.000000355
H	0.000000155	-0.000000385	0.000000369
C	0.000000644	-0.000000692	0.000000781
C	-0.000000660	-0.000000014	0.000000354
H	-0.000000191	-0.000000404	0.000000525
H	-0.000000075	-0.000000503	0.000000131
C	0.000000597	-0.000000708	0.000000294
H	0.000000043	-0.000000476	0.000000292
H	0.000000106	-0.000000456	0.000000416
C	-0.000000614	-0.000000208	0.000000875
H	-0.000000084	-0.000000622	0.000000454
H	-0.000000146	-0.000000457	0.000000581
H	-0.000000022	-0.000000470	0.000000233
H	0.000000132	-0.000000583	0.000000477
C	0.000000563	-0.000000455	0.000000216
C	-0.000000263	-0.000000329	0.000000656
H	0.000000002	-0.000000679	0.000000565
H	-0.000000076	-0.000000739	0.000000641
H	0.000000089	-0.000000545	0.000000599
H	-0.000000050	-0.000000518	0.000000507
H	-0.000000035	-0.000000614	0.000000635
O	0.000000179	-0.000003907	0.000007154
C	0.000001857	0.000001275	0.000003016
C	-0.000000797	0.000000472	-0.000002194
O	0.000001262	0.000000258	-0.000001435
C	-0.000000030	0.000000483	-0.000001352
C	0.000000085	0.000000130	-0.000001497
C	-0.000000594	0.000001055	-0.000000332
H	0.000000057	-0.000000045	0.000000347
C	-0.000000139	0.000000049	0.000000347
H	-0.000000077	0.000000054	-0.000000131
C	0.000000979	0.000000209	-0.000000852
H	-0.000000251	0.000000041	0.000000863
H	-0.000000036	-0.000000044	0.000000203
O	-0.000000129	0.000000239	0.000000682
C	-0.000000045	0.000000898	-0.000002257
H	-0.000001326	-0.000000888	0.000000092
H	0.000001588	0.000001080	0.000000496
C	-0.000000870	-0.000000463	-0.000000665
C	0.000000777	0.000000431	-0.000000215
H	0.000001391	0.000000632	-0.000000090
H	-0.000001003	0.000000024	-0.000000121
C	-0.000000760	0.000000706	-0.000000377
H	-0.000000013	0.000000189	-0.000000190
H	-0.000000230	0.000000440	-0.000000386
H	0.000000122	0.000000321	-0.000000269
H	0.000000113	0.000000289	-0.000000323
C	0.000000588	0.000000079	0.000000105
C	-0.000000550	0.000000876	-0.000000567
H	-0.000000202	0.000000571	-0.000000353
H	-0.000000056	0.000000162	-0.000000247

C	0.000000480	0.000000022	-0.000000002
H	0.000000078	0.000000264	-0.000000290
H	0.000000145	0.000000380	-0.000000319
H	-0.000000048	0.000000315	-0.000000250
H	-0.000000189	0.000000522	-0.000000377
C	-0.000000474	0.000000876	-0.000000571
C	0.000000325	0.000000022	0.000000030
H	0.000000227	0.000000400	-0.000000362
H	0.000000015	0.000000325	-0.000000302
C	-0.000000528	0.000000750	-0.000000297
H	-0.000000195	0.000000321	-0.000000266
H	0.000000033	0.000000544	-0.000000354
H	0.000000079	0.000000551	-0.000000263
H	0.000000019	0.000000521	-0.000000372
H	0.000000309	0.000000410	-0.000000420
H	-0.000002595	-0.000003300	0.000001083

Cartesian Coordinates of ABB(OH)H-10 (Keto Form):

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-0.000000102	-0.000001166	0.0000000612
C	0.000000222	0.000000418	0.0000000640
C	0.000000956	0.000000040	0.0000000755
C	0.000000222	-0.000000470	0.0000000891
C	0.000000504	-0.000000079	0.0000000861
C	-0.000003705	0.000001432	-0.000000182
H	0.000000705	-0.000001716	-0.000000372
H	-0.000000464	-0.000001292	0.000000226
H	-0.000000540	0.000000766	0.000001027
H	0.000000544	0.000000327	0.000000641
C	-0.000001934	-0.000001971	0.000000113
H	0.000000573	-0.000001466	0.000002023
H	0.000000335	0.000001214	0.000001477
O	0.000003985	0.000000029	0.000000964
C	-0.000005094	0.000000967	0.000000582
C	-0.000000231	0.000000498	-0.000000774
C	-0.000000715	-0.000000142	0.000001485
C	-0.000000049	-0.000000963	0.000000413
H	0.000001374	0.000000356	-0.000000523
C	0.000002296	0.000000796	0.000001966
H	0.000000532	-0.000000348	0.000001366
C	0.000003134	0.000001523	0.000001902
H	-0.000001428	0.000000571	-0.000000712
H	-0.000001475	-0.000000269	0.000001554
O	-0.000000804	0.000003354	0.000002941

C	-0.000003051	-0.000005553	-0.000001633
N	0.000011357	-0.000002451	-0.000005827
N	-0.000005341	0.000006148	0.000001019
H	0.000000038	0.000000562	0.000003479
C	-0.000004091	-0.000002143	0.000002265
C	-0.000000706	-0.000011426	0.000002114
C	-0.000000113	0.000002772	-0.000002003
C	0.000013955	0.000031327	-0.000010639
C	0.000000651	-0.000004194	0.000001506
H	0.000001221	-0.000000711	-0.000001434
C	-0.000004427	-0.000003438	0.000002013
C	0.000008315	0.000001287	0.000000022
H	-0.000001372	0.000000909	-0.000002331
H	-0.000000911	0.000000352	0.000000876
H	0.000001331	0.000000759	-0.000001104
O	0.000002740	-0.000002561	0.000000526
C	-0.000000998	-0.000000357	0.000001666
C	0.000001493	0.000001139	-0.000002335
H	0.000000232	0.000000698	0.000000198
H	-0.000000354	0.000000419	-0.000000638
C	-0.000000817	-0.000001248	0.000002100
H	-0.000000300	-0.000000651	0.000000995
H	-0.000000229	-0.000001156	-0.000000625
C	0.000000194	0.000000746	-0.000001802
H	0.000000314	0.000000575	-0.000000967
H	-0.000000252	0.000001073	0.000000432
H	-0.000000030	-0.000000412	0.000000754
H	-0.000000045	-0.000001136	-0.000000816
C	-0.000000294	-0.000000860	0.000001581
C	0.000000150	0.000000810	-0.000002042
H	-0.000000008	0.000001093	0.000000331
H	0.000000070	0.000000695	-0.000001265
C	0.000000115	-0.000000577	0.000001417
H	0.000000137	-0.000000254	0.000000568
H	-0.000000221	-0.000000899	-0.000000906
C	-0.000000601	0.000000899	-0.000001825
H	-0.000000198	0.000000743	-0.000001344
H	0.000000179	0.000001161	0.000000185
H	0.000000368	-0.000000119	0.000000320
H	-0.000000239	-0.000000648	-0.000000989
C	0.000000984	-0.000000498	0.000001106
C	-0.000001769	0.000000975	-0.000001493
H	0.000000055	0.000001369	0.000000108
H	-0.000000328	0.000000965	-0.000001440
H	0.000000848	0.000000811	-0.000000965
H	0.000000341	-0.000000047	0.000000393
H	0.000000046	-0.000000498	-0.000001144
O	-0.000005911	-0.000001598	-0.000002696
C	0.000002594	0.000002063	0.000002276
C	-0.000001759	0.000000652	-0.000000866
O	-0.000001110	0.000000056	-0.000002475
C	-0.000001478	-0.000000297	-0.000000280
C	0.000000092	0.000001101	0.000001303
C	-0.000000333	0.000000230	-0.000000648
H	0.000001541	0.000000567	-0.000001707
C	0.000000105	-0.000000101	0.000000259

H	0.000000340	-0.000000876	0.000000093
C	0.000006876	-0.000002274	-0.000001608
H	-0.000001364	0.000000750	-0.000001050
H	-0.000001290	-0.000000475	0.000000697
O	-0.000004046	0.000000384	0.000002013
C	0.000001932	0.000001538	-0.000000257
H	-0.000000138	0.000000549	-0.000000625
H	-0.000000618	-0.000001012	-0.000000517
C	-0.000000494	-0.000001203	-0.000001155
C	-0.000000937	0.000000915	0.000000904
H	0.000000128	0.000000410	0.000000358
H	0.000000078	-0.000000531	0.000001124
C	0.000000292	-0.000001432	-0.000001296
H	-0.000000030	0.000000480	-0.000001270
H	0.000000259	-0.000000654	-0.000000581
H	-0.000000023	-0.000000340	0.000001422
H	-0.000000038	0.000000784	0.000000353
C	-0.000000084	0.000001021	0.000000721
C	0.000000126	-0.000001349	-0.000001213
H	0.000000048	-0.000000604	-0.000000630
H	-0.000000028	0.000000333	-0.000001380
C	-0.000000318	0.000001302	0.000000850
H	-0.000000033	-0.000000326	0.000001353
H	0.000000008	0.000000730	0.000000215
H	-0.000000019	0.000000378	-0.000001486
H	0.000000064	-0.000000628	-0.000000644
C	0.000000881	-0.000001203	-0.000001069
C	-0.000000991	0.000001235	0.000000435
H	-0.000000213	0.000000838	0.000000127
H	-0.000000010	-0.000000358	0.000001197
C	0.000001177	-0.000000604	-0.000000155
H	0.000000122	0.000000299	-0.000001472
H	0.000000236	-0.000000566	-0.000000589
H	-0.000000756	-0.000000265	-0.000000423
H	-0.000000352	-0.000000366	0.000000986
H	0.000000310	0.000000826	0.000000015
O	-0.000016753	-0.000017051	0.000006649
H	0.000004639	-0.000002188	0.000002462