

Structure and Conformational Mobility of OLED relevant 1,3,5-Triazine Derivatives

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Analytical data for synthesised compounds

Analytical data for compound *N,N',N''-tris(9-ethyl-9H-carbazol-3-yl)-1,3,5-triazine-2,4,6-triamine* (4):

¹H NMR (600 MHz, DMF-d₇, 223 K, ppm) δ: 50% : 50% mixture of conformers; signals for *propeller* conformer: 10.29 (s, 3H, NH), 9.15 (s, 3H, carbazole-H4), 8.18 (d, J = 7.8 Hz, 3H, carbazole-H5), 7.85-7.80 (m, 3H, carbazole-H2), 7.73-7.68 (m, 6H, carbazole-H1&H8), 7.53-7.49 (m, 3H, carbazole-H7), 7.26-7.22 (m, 3H, carbazole-H6), 4.55 (bs, 6H, CH₂), 1.33 (t, J = 6.8 Hz, 9H, CH₃); ¹³C NMR (151 MHz, DMF-d₇, 223 K) δ 164.4 (triazine-⁴C), 140.3 (carbazole-⁴C), 135.7 (carbazole-⁴C), 132.9 (carbazole-⁴C), 125.8 (carbazole-C6), 122.7 (carbazole-⁴C), 122.4 (carbazole-⁴C), 120.6 (carbazole-C5), 119.4 (carbazole-C2), 118.4 (carbazole-C6), 111.7 (carbazole-4C), 109.1 (carbazole-C1&C8), 37.1 (CH₂), 13.7 (CH₃); signals for *asymmetric* conformer: ¹H NMR (600 MHz, DMF-d₇, 223 K) δ: 10.30 (s, 1H, NH), 9.95 (s, 1H, NH), 9.89 (s, 1H, NH), 9.12 (s, 1H, carbazole-H4), 8.70 (s, 1H, carbazole-H4), 8.59 (s, 1H, carbazole-H4), 8.17 (d, J = 7.8 Hz, 2H, carbazole-H5), 7.95 (d, J = 8.7 Hz, 1H, carbazole-H1), 7.93 (d, J = 8.7 Hz, 1H, carbazole-H1), 7.85-7.79 (m, 2H, carbazole-H5&H1), 7.74-7.68 (m, 3H, carbazole-H8), 7.65 (d, J=8.7 Hz, 1 H, carbazole-H2), 7.62 (d, J=8.7 Hz, 1 H, carbazole-H2), 7.59 (d, J=8.7 Hz, 1 H, carbazole-H2), 7.51 (t, J = 7.6 Hz, 1H, carbazole-H6), 7.45 (t, J = 7.6 Hz, 1H, carbazole-H6), 7.42 (t, J = 7.6 Hz, 1H, carbazole-H6), 7.23 (t, J = 7.6 Hz, 1H, carbazole-H7), 7.00 (t, J = 7.6 Hz, 1H, carbazole-H7), 6.92 (t, J = 7.6 Hz, 1H, carbazole-H7), 4.55 (bs, 2H, CH₂), 4.48 (bs, 2H, CH₂), 4.45 (bs, 2H, CH₂), 1.33 (t, J = 7.4 Hz, 3H, CH₃) 1.26 (t, J = 7.4 Hz, 3H), 1.25 (t, J = 7.4 Hz, 3H); ¹³C NMR (151 MHz, DMF-d₇, 223K) δ 165.3 (triazine-⁴C), 165.2(triazine-⁴C), 164.6 (triazine-⁴C), 140.2 (carbazole-⁴C), 136.2 (carbazole-⁴C), 135.9 (carbazole-⁴C), 135.6 (carbazole-⁴C), 133.0 (carbazole-⁴C), 132.5 (carbazole-⁴C), 132.3 (carbazole-⁴C), 125.8 (carbazole-C6), 122.5 (carbazole-⁴C), 122.4 (carbazole-⁴C), 121.6 (carbazole-C5), 120.5 (carbazole-C1), 118.3 (carbazole-C7), 113.4 (carbazole-C4), 112.5 (carbazole-C4), 111.7 (carbazole-C4), 109.2 (carbazole-C1), 109.1 (carbazole- C8), 37.2 (CH₂), 13.7 (CH₃).

¹H NMR (600 MHz, DMSO-d₆, 393 K, ppm) δ: averaged signals due to fast exchange: 8.58 (s, 1H, NH), 8.48 (d, J = 1.9 Hz, 1H, carbazole-H4), 7.94 (d, J = 7.7 Hz, 1H, carbazole-H5), 7.78 (dd, J = 2.1, 8.7 Hz, 1H, carbazole-H2), 7.51 (d, J = 8.2 Hz, 1H, carbazole-H8), 7.41 (d, J = 8.5 Hz, 1H, carbazole-H1), 7.40 (ddd, J = 1.2, 7.0, 8.2 Hz, 1H, carbazole-H7), 7.05 (ddd, J = 0.6, 7.1, 7.7 Hz, 1H, carbazole-H6), 4.37 (q, J = 7.2 Hz, 2H, CH₂), 1.35 (t, J = 7.1 Hz, 3H, CH₃). ¹³C NMR (151 MHz, DMSO-d₆, 393 K) δ 164.48 (triazine-⁴C), 139.71 and 135.72 (carbazole-C8a and carbazole-C9a), 131.44 (carbazole-C3), 124.69 (carbazole-C7), 122.01 and 121.79 (carbazole-C4a and carbazole-C4b), 120.60 (carbazole-C2), 119.53 (carbazole-C4), 117.51 (carbazole-C6), 112.69 (carbazole-C4), 108.15 (carbazole-C8), 107.76 (carbazole-C1), 36.47 (CH₂), 12.69 (s, CH₃).

Analytical data for compound *N,N',N''-tris(3,5-dimethoxybenzyl)-N,N',N''-tris(9-ethyl-9H-carbazol-3-yl)-1,3,5-triazine-2,4,6-triamine* (5):

¹H NMR (600 MHz, DMF-d₇, 223 K, ppm) δ: 17% : 83% mixture of conformers; signals for major *asymmetric* conformer: 8.45 (s, 1H, carbazole-H4), 8.30 (d, J = 7.7 Hz, 1H, carbazole-H5), 8.29 (s, 1H, carbazole-H4), 8.28 (d, J = 7.7 Hz, 1H, carbazole-H5), 8.20 (s, 1H, carbazole-H4), 7.98 (d, J = 7.7 Hz, 1H, carbazole-H5), 7.68-7.62 (m, 3H, carbazole-H2 & carbazole-H8), 7.57-7.52 (m, 3H, carbazole-H2 & carbazole-H8), 7.47-7.41 (m, 3H, carbazole-H7), 7.20 (dd, J = 7.1, 7.7 Hz, 1H, carbazole-H6), 7.17 (dd, J = 7.1, 7.7 Hz, 1H, carbazole-H6), 7.15 (dd, J = 7.1, 7.7 Hz, 1H, carbazole-H6), 7.09 (d, J = 8.7 Hz, 2H, carbazole-H1), 7.07 (d, J = 8.7 Hz, 1H, carbazole-H1), 6.57 (d, J = 1.9 Hz, 2H, 3,5-dimethoxybenxene-H2), 6.55 (d, J = 1.9 Hz, 2H, 3,5-dimethoxybenxene-H2), 6.40 (t, J = 1.9 Hz, 1H, 3,5-dimethoxybenxene-H4), 6.36 (t, J = 1.9 Hz, 1H, 3,5-dimethoxybenxene-H4), 6.31 (t, J = 1.9 Hz, 1H, 3,5-dimethoxybenxene-H4), 66.19 (d, J = 1.9 Hz, 2H, 3,5-dimethoxybenxene-H2), 5.49 (bs, 2H, benzyl-CH₂), 5.46 (bs, 2H, benzyl-CH₂), 5.05 (bs, 2H, benzyl-CH₂), 4.47 (bs, 4H, -CH₂), 3.99 (bs, 2H, -CH₂), 3.73 (s, 6H, -OMe),

3.72 (s, 6H, -OMe), 3.57 (s, 6H, -OMe), 1.28 (t, $J = 7.1$ Hz, 3H, -CH₃), 0.88 (t, $J = 7.1$ Hz, 3H, -CH₃), 0.87 (t, $J = 7.1$ Hz, 3H, -CH₃). ¹³C NMR (151 MHz, DMF-d₇, 223K) δ 166.4 (triazine-⁴C), 166.3 (triazine-⁴C), 166.3 (triazine-⁴C), 161.0 (3,5-dimethoxybenxene-⁴C3), 160.9 (3,5-dimethoxybenxene-⁴C3), 160.8 (3,5-dimethoxybenxene-⁴C3), 142.5 (3,5-dimethoxybenxene-⁴C1), 142.4 (3,5-dimethoxybenxene-⁴C1), 140.4 (carbazole-⁴C), 140.2 (carbazole-⁴C), 137.7 (carbazole-⁴C), 137.7 (carbazole-⁴C), 137.1 (carbazole-⁴C), 135.1 (carbazole-⁴C), 134.9 (carbazole-⁴C), 126.4 (carbazole-C7), 126.2 (carbazole-C7), 126.1 (carbazole-C2), 125.9 (carbazole-C2), 122.8 (carbazole-⁴C), 122.5 (carbazole-⁴C), 122.2 (carbazole-C5), 122.2 (carbazole-C5), 120.8 (carbazole-C4), 119.6 (carbazole-C4), 118.9 (carbazole-C4), 118.8 (carbazole-C6), 118.7 (carbazole-C6), 109.4 (carbazole-C8), 108.8 (carbazole-C8), 108.1 (carbazole-C1), 105.9 (3,5-dimethoxybenxene-C2), 105.6 (3,5-dimethoxybenxene-C2), 105.3 (3,5-dimethoxybenxene-C2), 97.8 (3,5-dimethoxybenxene-C4), 97.7 (3,5-dimethoxybenxene-C4), 97.6 (3,5-dimethoxybenxene-C4), 54.0 (-OMe), 54.9 (-OMe), 54.8 (-OMe), 53.4 (benzyl-CH₂), 53.2 (benzyl-CH₂), 52.8 (benzyl-CH₂), 37.35 (CH₂), 37.02 (CH₂), 13.85 (CH₃), 13.67 (CH₃). Minor ¹H NMR (600 MHz, DMF-d₇, 223K) δ 8.33 (s, 3H, carbazole-H4), 7.91 (d, $J = 7.7$ Hz, 3H, carbazole-H5), 7.67 (d, $J = 8.8$ Hz, 3H, carbazole-H2), 7.55-7.52 (m, 3H, carbazole-H8), 7.44-7.41 (m, 3H, carbazole-H7), 7.18 (dd, $J = 7.1, 7.7$ Hz, 3H, carbazole-H6), 7.08 (d, $J = 8.7$ Hz, 3H, carbazole-H1), 6.34 (t, $J = 1.9$ Hz, 6H, 3,5-dimethoxybenxene-H4), .26 (d, $J = 1.9$ Hz, 3H, 3,5-dimethoxybenxene-H2), 5.09 (bs, 6H, benzyl-CH₂), 3.99 (bs, 6H, -CH₂), 3.61 (s, 18H, -OMe), 1.26 (t, $J = 7.1$ Hz, 9H, -CH₃). ¹³C NMR (151 MHz, DMF-d₇, 223K) δ 166.1 (triazine-⁴C), 161.0 (3,5-dimethoxybenxene-⁴C3), 142.4 (3,5-dimethoxybenxene-⁴C1), 126.2 (carbazole-C7), 126.1 (carbazole-C2), 122.6 (carbazole-⁴C), 122.2 (carbazole-C5), 121.0 (carbazole-C4), 118.9 (carbazole-C6), 108.8 (carbazole-C8), 108.1 (carbazole-C1), 106.0 (3,5-dimethoxybenxene-C2), 97.6 (3,5-dimethoxybenxene-C4), 54.9 (-OMe), 52.6 (benzyl-CH₂), 37.0 (CH₂), 13.9 (CH₃).

¹H NMR (600 MHz, DMSO-d₆, 403 K, ppm) δ: averaged signals due to fast exchange: 7.90 (d, $J = 1.1$ Hz, 1H, carbazole-H4), 7.86 (d, $J = 7.7$ Hz, 1H, carbazole-H5), 7.43 (d, $J = 8.2$ Hz, 1H, carbazole-H8), 7.38 (ddd, $J = 1.1, 7.1, 8.1$ Hz, 1H, carbazole-H7), 7.25 (dd, $J = 2.0, 8.7$ Hz, 1H, carbazole-H2), 7.12 (d, $J = 8.8$ Hz, 1H, carbazole-H1), 7.09 (ddd, $J = 0.9, 7.0, 7.9$ Hz, 1H, carbazole-H6), 6.30 (d, $J = 2.1$ Hz, 2H, 3,5-dimethoxybenxene-H2 and 3,5-dimethoxybenxene-H6), 6.27 (t, $J = 2.2$ Hz, 1H, 3,5-dimethoxybenxene-H4), 5.06 (s, 2H, benzyl-CH₂), 4.16 (q, $J = 7.0$ Hz, 2H, CH₂), 3.59 (s, 6H, OMe), 1.19 (t, $J = 7.1$ Hz, 3H, CH₃). ¹³C NMR (151 MHz, DMSO-d₆, 403K) δ 165.44 (triazine-⁴C), 159.89 (3,5-dimethoxybenxene-⁴C3 and 3,5-dimethoxybenxene-⁴C5), 140.99 (carbazole-C8a), 139.57 (3,5-dimethoxybenxene-⁴C1), 136.80 (carbazole-C3), 134.61 (carbazole-C8a), 125.06 (carbazole-C2), 124.65 (carbazole-C7), 121.89 and 121.47 (carbazole-C4a and carbazole-C4b), 119.23 (carbazole-C5), 117.81 (carbazole-C4), 117.73 (carbazole-C6), 108.15 (carbazole-C8), 107.27 (carbazole-C1), 105.64 (3,5-dimethoxybenxene-C2 and 3,5-dimethoxybenxene-C6), 98.52 (3,5-dimethoxybenxene-⁴C4), 54.41 (OMe), 52.52 (benzyl-CH₂), 36.32 (CH₂), 12.42 (CH₃).

Analytical data for compound *N,N',N''-tris(9-ethyl-9H-carbazol-3-yl)-N,N',N''-trimethyl-1,3,5-triazine-2,4,6-triamine* (6):

¹H NMR (600 MHz, DMF-d₇, 223 K, ppm) δ: 14% : 86% mixture of conformers; signals for major *asymmetric* conformer: 8.47 (s, 1H, carbazole-H4), 8.37 (d, $J = 7.7$ Hz, 1H, carbazole-H5), 8.33 (d, $J = 7.7$ Hz, 1H, carbazole-H5), 8.27 (d, $J = 7.7$ Hz, 1H, carbazole-H5), 8.21 (s, 1H, carbazole-H4), 8.08 (s, 1H, carbazole-H4), 7.80 (d, $J = 8.8$ Hz, 1H, carbazole-H1), 7.74 (d, $J = 8.5$ Hz, 1H, carbazole-H8), 7.69 (d, $J = 8.8$ Hz, 1H, carbazole-H2), 7.62 (d, $J = 8.5$ Hz, 1H, carbazole-H8), 7.61 (d, $J = 8.8$ Hz, 1H, carbazole-H2), 7.58 (d, $J = 8.5$ Hz, 1H, carbazole-H8), 7.53-7.43 (m, 3H, carbazole-H7), 7.50 (d, $J = 8.8$ Hz, 1H, carbazole-H2), 7.30-7.20 (m, 3H, carbazole-H6), 7.18 (d, $J = 8.7$ Hz, 1H, carbazole-H1), 7.11 (d, $J = 8.7$ Hz, 1H, carbazole-H1), 4.58 (bs, 2H, CH₂), 4.08 (bs, 4H, CH₂), 3.75 (s, 3H, NCH₃), 3.69 (s, 3H, NCH₃), 3.20 (s, 3H, NCH₃), 1.36 (t, $J = 7.6$ Hz, 3H, CH₃), 0.96 (t, $J = 7.6$ Hz, 3H, CH₃), 0.94 (t, $J = 7.6$ Hz, 3H,

CH_3). ^{13}C NMR (151 MHz, DMF-d₇, 223K) δ : 165.9 (triazine-⁴C), 165.6 (triazine-⁴C), 165.3 (triazine-⁴C), 140.5 (carbazole-⁴C), 140.2 (carbazole-⁴C), 140.2 (carbazole-⁴C), 137.8 (carbazole-⁴C), 137.3 (carbazole-⁴C), 137.0 (carbazole-⁴C), 136.9 (carbazole-⁴C), 136.7 (carbazole-⁴C), 125.9 (carbazole-C2), 125.6 (carbazole-C7 & carbazole-C2), 125.5 (carbazole-C2), 122.9 (carbazole-⁴C), 122.8 (carbazole-⁴C), 122.7 (carbazole-⁴C), 122.6 (carbazole-⁴C), 122.2 carbazole-⁴C (), 122.1 (carbazole-⁴C), 120.7 (carbazole-C5), 118.9 (carbazole-C4), 118.8 (carbazole-C6), 118.5 (carbazole-C6), 117.9 (carbazole-C4), 117.6 (carbazole-C4), 109.3 (carbazole-C8), 109.1 (carbazole-C8), 108.7 (carbazole-C1), 107.9 (carbazole-C1), 107.9 (carbazole-C1), 38.1 (NCH₃), 37.9 (NCH₃), 37.4 (NCH₃), 37.2 (CH₂), 36.8 (CH₂), 13.7 (CH₃), 13.5 (CH₃), 13.4 (CH₃); signals for minor *propeller* conformer: ^1H NMR (600 MHz, DMF-d₇, 223K) δ : 8.35 (s, 3H, carbazole-H4), 8.33 (d, J = 7.7 Hz, 3H, carbazole-H5), 7.72 (d, J = 8.7 Hz, 3H, carbazole-H8), 7.58 (d, J = 8.5 Hz, 3H, carbazole-H2), 7.53 (d, J = 8.5 Hz, 3H, carbazole-H1), 4.58 (bs, 6H, CH₂), 3.26 (s, 9H), 1.34 (t, J = 7.6 Hz, 9H, CH₃); ^{13}C NMR (151 MHz, DMF-d₇, 223K) 165.8 (triazine-⁴C), 140.4 (carbazole-⁴C), 137.7 (carbazole-⁴C), 122.9 (carbazole-⁴C), 122.6 (carbazole-⁴C), 120.7 (carbazole-C5), 118.9 (carbazole-C4), 108.7 (carbazole-C1), 37.3 (NCH₃), 13.7 (CH₃).

^1H NMR (600 MHz, DMSO-d₆, 373 K, ppm) δ : averaged signals due to fast exchange: 8.02 (d, J = 7.7 Hz, 1H, carbazole-H5), 7.99 (d, J = 1.9 Hz, 1H, carbazole-H4), 7.48 (td, J = 0.8, 8.3 Hz, 1H, carbazole-H8), 7.41 (ddd, J = 1.2, 7.1, 8.2 Hz, 1H, carbazole-H7), 7.38 (dd, J = 2.1, 8.7 Hz, 1H, carbazole-H2), 7.22 (d, J = 8.6 Hz, 1H, carbazole-H1), 7.12 (ddd, J = 0.9, 7.0, 7.9 Hz, 1H, carbazole-H6), 4.21 (q, J = 7.1 Hz, 2H, CH₂), 3.43 (s, 3H, NCH₃), 1.21 (t, J = 7.1 Hz, 3H, CH₃); ^{13}C NMR (151 MHz, DMSO-d₆, 373K) δ 165.17 (triazine-⁴C), 139.64 (carbazole-C8a), 136.66 (carbazole-C9a), 136.34 (carbazole-³C), 124.89 (carbazole-C7), 124.41 (carbazole-C2), 121.98 and 121.56 (carbazole-C4a and carbazole-C4b), 119.59 (s, carbazole-C5), 117.92 (carbazole-C6), 117.13 (carbazole-C4), 108.38 (carbazole-C8), 107.52 (carbazole-C1), 37.16 (NCH₃), 36.46 (CH₂), 12.78 (CH₃).

Analytical data for compound 2,2',2''-(1,3,5-triazine-2,4,6-triyltriamino)triphenol (11):

^1H NMR (600 MHz, DMF-d₇, 223 K, ppm) δ : 42% : 58% mixture of conformers; signals for major *asymmetric* conformer: 10.71 (s, 3H, -OH), 8.96 (s, 3H, -NH), 7.98 (d, J = 7.8 Hz, 3H, 2-aminophenol-H3), 6.97 (m, 6H, 2-aminophenol-H6 & 2-aminophenol-H5), 6.85 (t, J = 7.7 Hz, 3H, 2-aminophenol-H4). ^{13}C NMR (151 MHz, DMF-d₇, 223K) δ 163.9 (triazine-⁴C), 148.8 (2-aminophenol-⁴C1), 127.2 (2-aminophenol-⁴C2), 124.6 (2-aminophenol-C6), 123.6 (2-aminophenol-C3), 119.3 (2-aminophenol-C5), 116.1 (2-aminophenol-C4); ; signals for minor *propeller* conformer: ^1H NMR (600 MHz, DMF-d₇ 223 K) δ : 10.84 (s, 1H, -OH), 10.63 (s, 1H, -OH), 10.55 (s, 1H, -OH), 9.05 (s, 1H, -NH), 8.54 (s, 1H, -NH), 8.50 (s, 1H, -NH), 8.08 (d, J = 7.8 Hz, 1H, 2-aminophenol-H3), 7.87 (d, J = 7.8 Hz, 1H, 2-aminophenol-H3), 7.82 (d, J = 7.8 Hz, 1H, 2-aminophenol-H3), 6.97 (m, 6H, 2-aminophenol-H6 & 2-aminophenol-H5), 6.85 (t, J = 7.7 Hz, 1H, 2-aminophenol-H4), 6.79 (t, J = 7.7 Hz, 1H, 2-aminophenol-H4), 6.75 (t, J = 7.7 Hz, 1H, 2-aminophenol-H4). ^{13}C NMR (151 MHz, DMF-d₇, 223K) δ 164.6 (triazine-⁴C), 164.5 (triazine-⁴C), 164.2 (triazine-⁴C), 149.6 (2-aminophenol-⁴C1), 148.9 (2-aminophenol-⁴C1), 147.97 (2-aminophenol-⁴C1), 127.8 (2-aminophenol-⁴C2), 126.8 (2-aminophenol-⁴C2), 126.6 (2-aminophenol-⁴C2), 124.8 (2-aminophenol-C6), 124.4 (2-aminophenol-C3), 124.2 (2-aminophenol-C6), 123.8 (2-aminophenol-C6), 123.2 (2-aminophenol-C3), 122.1 (2-aminophenol-C3), 119.4 (2-aminophenol-C5), 118.9 (2-aminophenol-C5), 116.0 (2-aminophenol-C4), 115.5 (2-aminophenol-C4), 115.2 (2-aminophenol-C4)

^1H NMR (600 MHz, DMSO-d₆, 353 K, ppm) δ : averaged signals due to fast exchange: 9.55 (bs, 1H, OH), 8.01 (s, 1H, NH), 7.82 (dd, J = 1.4, 8.0 Hz, 1H, 2-aminophenol-H3), 6.93 (ddd, J = 1.5, 7.3, 7.9 Hz, 1H, 2-aminophenol-H5), 6.88 (dd, J = 1.5, 8.0 Hz, 1H, 2-aminophenol-H6), 6.77 (ddd, J = 1.4, 7.4, 7.8 Hz, 1H, 2-aminophenol-H4). ^{13}C NMR (151 MHz, DMSO-d₆, 353K) δ 163.76 (triazine-⁴C), 147.68 (2-aminophenol-⁴C1), 126.62 (2-aminophenol-⁴C2), 123.47 (2-

aminophenol-C5), 122.53 (2-aminophenol-C3), 118.66 (2-aminophenol-C4), 115.46 (2-aminophenol-C6).

Analytical data for compound 2,2',2''-(1,3,5-triazine-2,4,6-triyltriamino)tris(5-*tert*-butylphenol) (12):

¹H NMR (600 MHz, DMF-*d*₇, 233 K, ppm) δ: 46% : 54% mixture of conformers; signals for major *asymmetric* conformer: 10.17 (s, 3H, -OH), 9.41 (s, 3H, -NH), 7.66 (d, *J* = 2.3 Hz, 3H, 2-amino-5-(*tert*-butyl)phenol-H6), 7.12 (dd, *J* = 2.3, 8.5 Hz, 3H, 2-amino-5-(*tert*-butyl)phenol-H4), 6.91 (d, *J* = 8.5 Hz, 3H, 2-amino-5-(*tert*-butyl)phenol-H3), 1.25 (s, 27H, *t*-Bu-CH₃). ¹³C NMR (151 MHz, DMF-*d*₇, 233K) δ 163.9 (triazine-⁴C), 147.6 (2-amino-5-(*tert*-butyl)phenol-⁴C2), 142.3 (2-amino-5-(*tert*-butyl)phenol-⁴C5), 126.6 (2-amino-5-(*tert*-butyl)phenol-⁴C1), 122.7 (2-amino-5-(*tert*-butyl)phenol-C4), 121.5 (2-amino-5-(*tert*-butyl)phenol-C6), 117.2 (2-amino-5-(*tert*-butyl)phenol-C3), 31.3 (*t*-Bu-CH₃); ; signals for minor *propeller* conformer: ¹H NMR (600 MHz, DMF-*d*₇ 233 K) δ: 10.39 (s, 1H, -OH), 10.11 (s, 1H, -OH), 9.96 (s, 3H, -OH), 9.41 (s, 1H, -NH), 9.10 (s, 1H, -NH), 8.94 (s, 1H, -NH), 7.69 (d, *J* = 2.3 Hz, 1H, 2-amino-5-(*tert*-butyl)phenol-H6), 7.47 (d, *J* = 2.3 Hz, 1H, 2-amino-5-(*tert*-butyl)phenol-H6), 7.40 (d, *J* = 2.3 Hz, 1H, 2-amino-5-(*tert*-butyl)phenol-H6), 7.08 (dd, *J* = 2.3, 8.5 Hz, 1H, 2-amino-5-(*tert*-butyl)phenol-H4), 7.06 (dd, *J* = 2.3, 8.5 Hz, 1H, 2-amino-5-(*tert*-butyl)phenol-H4), 7.00 (dd, *J* = 2.3, 8.5 Hz, 1H, 2-amino-5-(*tert*-butyl)phenol-H4), 6.90 (d, *J* = 8.5 Hz, 1H, 2-amino-5-(*tert*-butyl)phenol-H3), 6.78 (d, *J* = 8.5 Hz, 1H, 2-amino-5-(*tert*-butyl)phenol-H3), 6.77 (d, *J* = 8.5 Hz, 1H, 2-amino-5-(*tert*-butyl)phenol-H3), 1.26 (s, 9H, *t*-Bu-CH₃), 1.15 (s, 9H, *t*-Bu-CH₃), 1.12 (s, 9H, *t*-Bu-CH₃). ¹³C NMR (151 MHz, DMF-*d*₇, 233K) δ 164.9 (triazine-⁴C), 164.6 (triazine-⁴C), 164.2 (triazine-⁴C), 148.7 (2-amino-5-(*tert*-butyl)phenol-⁴C2), 147.8 (2-amino-5-(*tert*-butyl)phenol-⁴C2), 146.8 (2-amino-5-(*tert*-butyl)phenol-⁴C5), 141.9 (2-amino-5-(*tert*-butyl)phenol-⁴C5), 126.0 (2-amino-5-(*tert*-butyl)phenol-⁴C1), 123.3 (2-amino-5-(*tert*-butyl)phenol-C4), 122.4 (2-amino-5-(*tert*-butyl)phenol-C4), 121.5 (2-amino-5-(*tert*-butyl)phenol-C6), 117.5 (2-amino-5-(*tert*-butyl)phenol-C3), 116.4 (2-amino-5-(*tert*-butyl)phenol-C3), 31.3 (*t*-Bu-CH₃), 31.3 (*t*-Bu-CH₃), 31.3 (*t*-Bu-CH₃).

¹H NMR (600 MHz, DMSO-*d*₆, 373 K, ppm) δ: averaged signals due to fast exchange: 9.17 (bs, 1H, OH), 8.07 (bs, 1H, NH), 7.63 (d, *J* = 2.3 Hz, 1H, 2-amino-5-(*tert*-butyl)phenol-H6), 6.96 (dd, *J* = 2.5, 8.4 Hz, 1H, 2-amino-5-(*tert*-butyl)phenol-H4), 6.78 (d, *J* = 8.4 Hz, 1H, 2-amino-5-(*tert*-butyl)phenol-H3), 1.24 (s, 9H, *t*-Bu-CH₃). ¹³C NMR (151 MHz, DMSO-*d*₆, 373K) δ 163.62 (triazine-⁴C), 145.77 (2-amino-5-(*tert*-butyl)phenol-⁴C1), 141.38 (2-amino-5-(*tert*-butyl)phenol-⁴C4), 125.70 (2-amino-5-(*tert*-butyl)phenol-⁴C2), 120.56 (2-amino-5-(*tert*-butyl)phenol-⁴C5), 119.94 (2-amino-5-(*tert*-butyl)phenol-⁴C3), 115.61 (2-amino-5-(*tert*-butyl)phenol-⁴C6), 33.20 (C), 30.83 (*t*-Bu-CH₃).

Analytical data for compound 2,2',2''-[1,3,5-triazine-2,4,6-triyltris(methylimino)]triphenol (13):

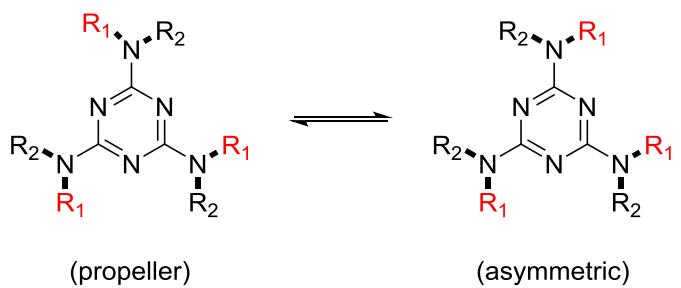
¹H NMR (600 MHz, DMF-*d*₇, 223 K, ppm) δ: 37% : 63% mixture of conformers; signals for major *asymmetric* conformer: ; signals for minor *propeller* conformer: ¹H NMR (600 MHz, DMF-*d*₇ 223 K) δ: 10.05 (s, 3H, -OH), 7.25 (dd, *J* = 1.4, 7.7 Hz, 3H, 2-aminophenol-H3), 7.16 (ddd, *J* = 1.2, 7.7, 7.9 Hz, 3H, 2-aminophenol-H4), 7.01 (dd, *J* = 1.2, 8.1 Hz, 3H, 2-aminophenol-H6), 6.88 (ddd, *J* = 1.4, 7.9, 8.1 Hz, 3H, 2-aminophenol-H5), 3.04 (s, 9H, -CH₃). ¹³C NMR (151 MHz, DMF-*d*₇, 223K) δ 165.47 (triazine-⁴C), 153.59 (2-aminophenol-⁴C1), 132.24 (2-aminophenol-⁴C2), 129.26, 127.80 (2-aminophenol-C4), 127.61 (2-aminophenol-C3), 119.16 (2-aminophenol-C5), 116.78 (2-aminophenol-C6), 35.82 (-NCH₃); signals for minor *propeller* conformer: ¹H NMR (600 MHz, DMF-*d*₇, 223K) δ: 7.35 (dd, *J* = 1.4, 7.7 Hz, 1H, 2-

aminophenol-H3), 7.20 (ddd, $J = 1.2, 7.7, 7.9$ Hz, 1H, 2-aminophenol-H4), 7.18 (d, $J=7.7$ Hz, 1H, 2-aminophenol-H3), 7.07 (d, $J=7.7$ Hz, 1 H, 2-aminophenol-H3), 7.05 (dd, $J = 1.2, 8.1$ Hz, 1H, 2-aminophenol-H6), 7.00-6.95 (m, 2H, 2-aminophenol-H4), 6.92 (ddd, $J = 1.4, 7.9, 8.1$ Hz, 1H, 2-aminophenol-H5), 6.76 (dd, $J = 1.2, 8.1$ Hz, 1H, 2-aminophenol-H6), 6.74 (dd, $J = 1.2, 8.1$ Hz, 1H, 2-aminophenol-H6), 6.71 (ddd, $J = 1.4, 7.9, 8.1$ Hz, 1H, 2-aminophenol-H5), 6.67 (ddd, $J = 1.4, 7.9, 8.1$ Hz, 1H, 2-aminophenol-H5). ^{13}C NMR (151 MHz, DMF-d₇, 223K) δ 165.65 (triazine-⁴C), 165.15 (triazine-⁴C), 164.90 (triazine-⁴C), 153.74 (2-aminophenol-⁴C1), 152.84 (2-aminophenol-⁴C1), 152.82 (2-aminophenol-⁴C1), 132.36 (2-aminophenol-⁴C2), 132.24 (2-aminophenol-⁴C2), 132.06 (2-aminophenol-⁴C2), 129.49 (2-aminophenol-C4), 128.22 (2-aminophenol-C3), 127.80 (2-aminophenol-C3), 126.88 (2-aminophenol-C4), 119.16 (2-aminophenol-C5), 116.69 (2-aminophenol-C6), 37.02 (-NCH₃), 36.41 (-NCH₃), 36.28 (-NCH₃) ^1H NMR (600 MHz, DMSO-d₆, 343 K, ppm) δ : averaged signals due to fast exchange: 7.07 (d, $J = 7.6$ Hz, 1H, 2-aminophenol-H3), 7.02 (t, $J = 7.1$ Hz, 1H, 2-aminophenol-H5), 6.81 (d, $J = 7.8$ Hz, 1H, 2-aminophenol-H6), 6.74 (t, $J = 7.4$ Hz, 1H, 2-aminophenol-H4), 3.17 (s, 1H, -CH₃). ^{13}C NMR (151 MHz, DMSO-d₆, 353K) δ 164.55 (triazine-⁴C), 152.08 (aminophenol-⁴C1), 131.75 (aminophenol-⁴C2), 127.72 (aminophenol-⁴C3), 126.47 (aminophenol-⁴C5), 118.64 (aminophenol-⁴C4), 116.73 (aminophenol-⁴C6), 36.04 (-NCH₃).

Analytical data for compound 2,2',2''-(1,3,5-triazine-2,4,6-triyltriamino)tris(3-methylphenol) (14):

^1H NMR (600 MHz, DMF-d₇, 223 K, ppm) δ : 48% : 52% mixture of conformers; signals for major *asymmetric* conformer: ^1H NMR (600 MHz, DMF-d₇ 223 K) δ : 9.85 (s, 3H, -OH), 9.03 (s, 3H, -NH), 7.05 (dd, $J = 7.4, 8.0$ Hz, 3H, 3-methylphenol-H5), 6.81 (d, $J = 8.0$ Hz, 3H, 3-methylphenol-H6), 6.77 (d, $J = 7.4$ Hz, 3H, 3-methylphenol-H4), 2.25 (s, 9H, -CH₃). ^{13}C NMR (151 MHz, DMF-d₇, 223K) δ 165.18 (triazine-⁴C), 153.26 (3-methylphenol-⁴C1), 136.04 (3-methylphenol-⁴C2), 126.66 (3-methylphenol-C5), 125.91 (3-methylphenol-⁴C3), 121.16 (3-methylphenol-C4), 115.19 (3-methylphenol-C6), 18.29 (-CH₃) ; signals for minor *propeller* conformer: ^1H NMR (600 MHz, DMF-d₇, 223K) δ : 9.77 (s, 1H, -OH), 9.70 (s, 1H, -OH), 9.08 (s, 1H, -NH), 8.93 (s, 1H, -NH), 8.81 (s, 1H, -NH), 7.07 (dd, $J = 7.4, 8.0$ Hz, 1H, 3-methylphenol-H5), 6.91 (dd, $J = 7.4, 8.0$ Hz, 1H, 3-methylphenol-H5), 6.90 (dd, $J = 7.4, 8.0$ Hz, 1H, 3-methylphenol-H5), 6.84 (d, $J = 8.0$ Hz, 1H, 3-methylphenol-H6), 6.79 (d, $J = 7.4$ Hz, 1H, 3-methylphenol-H4), 6.64 (d, $J = 7.4$ Hz, 1H, 3-methylphenol-H4), 6.63-6.59 (m, 3H, 2*3-methylphenol-H6 & 3-methylphenol-H4), 6.61 (d, $J = 7.3$ Hz, 1H), 2.31 (s, 3H, -CH₃), 2.21 (s, 3H, -CH₃), 2.13 (s, 3H, -CH₃). ^{13}C NMR (151 MHz, DMF-d₇, 223K) δ 165.5 (triazine-⁴C), 165.4 (triazine-⁴C), 165.4 (triazine-⁴C), 153.41 (3-methylphenol-⁴C1), 153.28 (3-methylphenol-⁴C1), 153.19 (3-methylphenol-⁴C1), 136.60 (3-methylphenol-⁴C2), 135.25 (3-methylphenol-⁴C2), 135.20 (3-methylphenol-⁴C2), 126.69 (3-methylphenol-C5), 126.49 (3-methylphenol-C5), 126.36 (3-methylphenol-C5), 125.87 (3-methylphenol-⁴C3), 125.61 (3-methylphenol-⁴C3), 125.38 (3-methylphenol-⁴C3), 121.10 (3-methylphenol-C4), 121.02 (3-methylphenol-C4), 120.96 (3-methylphenol-C4), 115.34 (3-methylphenol-C6), 115.26 (3-methylphenol-C6), 114.82 (3-methylphenol-C6), 18.37 (-CH₃), 18.14 (-CH₃), 18.06 (-CH₃).

^1H NMR (600 MHz, DMSO-d₆, 353 K, ppm) δ : averaged signals due to fast exchange: 8.91 (bs, 1H, OH), 7.83 (bs, 1H, NH), 6.92 (t, $J = 7.8$ Hz, 1H, 3-methylphenol-H5), 6.65 (t, $J = 7.5$ Hz, 2H, 3-methylphenol-H4 and 3-methylphenol-H6), 2.16 (s, 3H, -CH₃). ^{13}C NMR (151 MHz, DMSO-d₆, 353K) δ 164.80 (triazine-⁴C), 152.32 (3-methylphenol-⁴C1), 135.28 (3-methylphenol-⁴C3), 125.67 (3-methylphenol-⁴C2), 124.97 (3-methylphenol-⁴C5), 120.44 (3-methylphenol-⁴C4), 114.29 (3-methylphenol-⁴C6), 26.46 (C), 17.74 (CH₃).



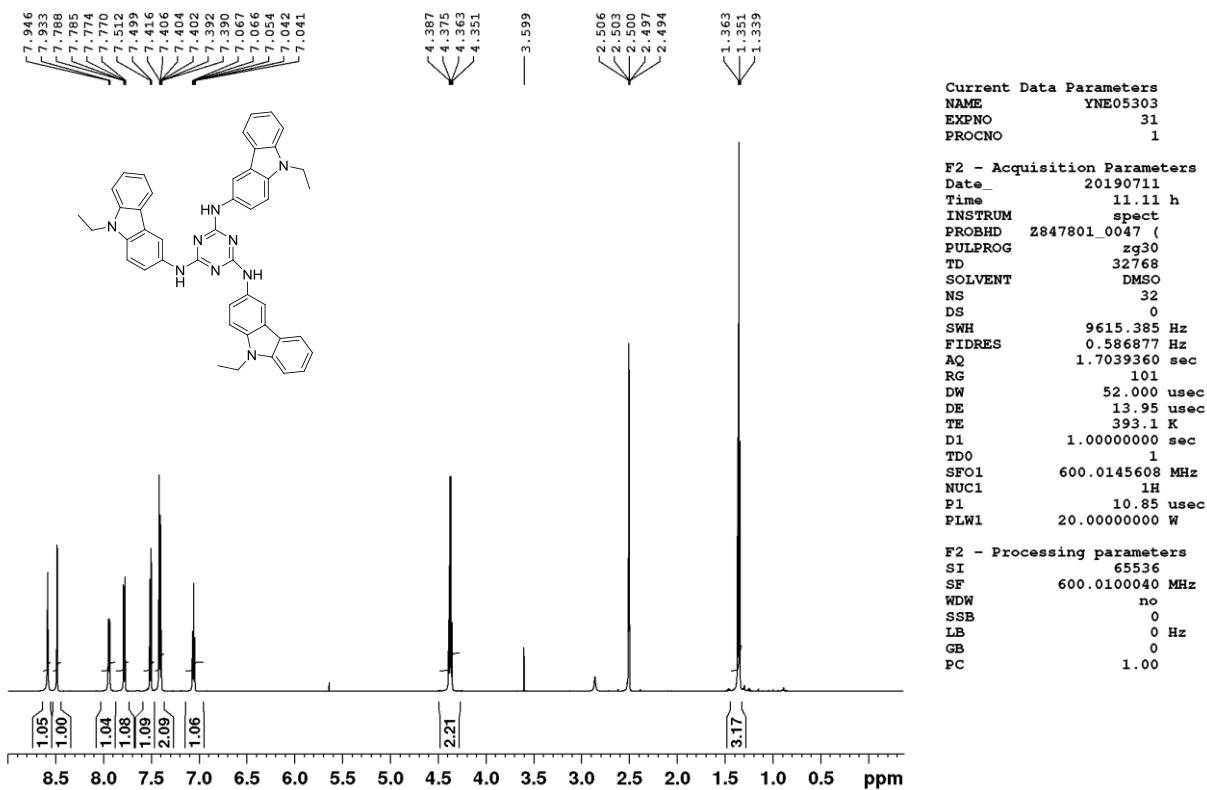
IR typical vibrational frequencies of studied compounds.

Comp.	R ₁	R ₂	ν_{NH}	ν_{OH}	$\nu_{\text{C}H(Ar)}$	$\nu_{\text{C}=\text{N}}$
4	H		3400, 3376	-	3050 3020	1505
5			-	-	3050 3021	1539
6	CH ₃		-	-	3050 3025	1538
11	H		3409, 3396, 3388	3280 (broad)	3050	1510
12	H		3383, 3282, 3189	3280 (broad)	3063	1507
13	CH ₃		-	3247 (broad)	3069	1540
14	H		3359	3274 (broad)	3085	1504

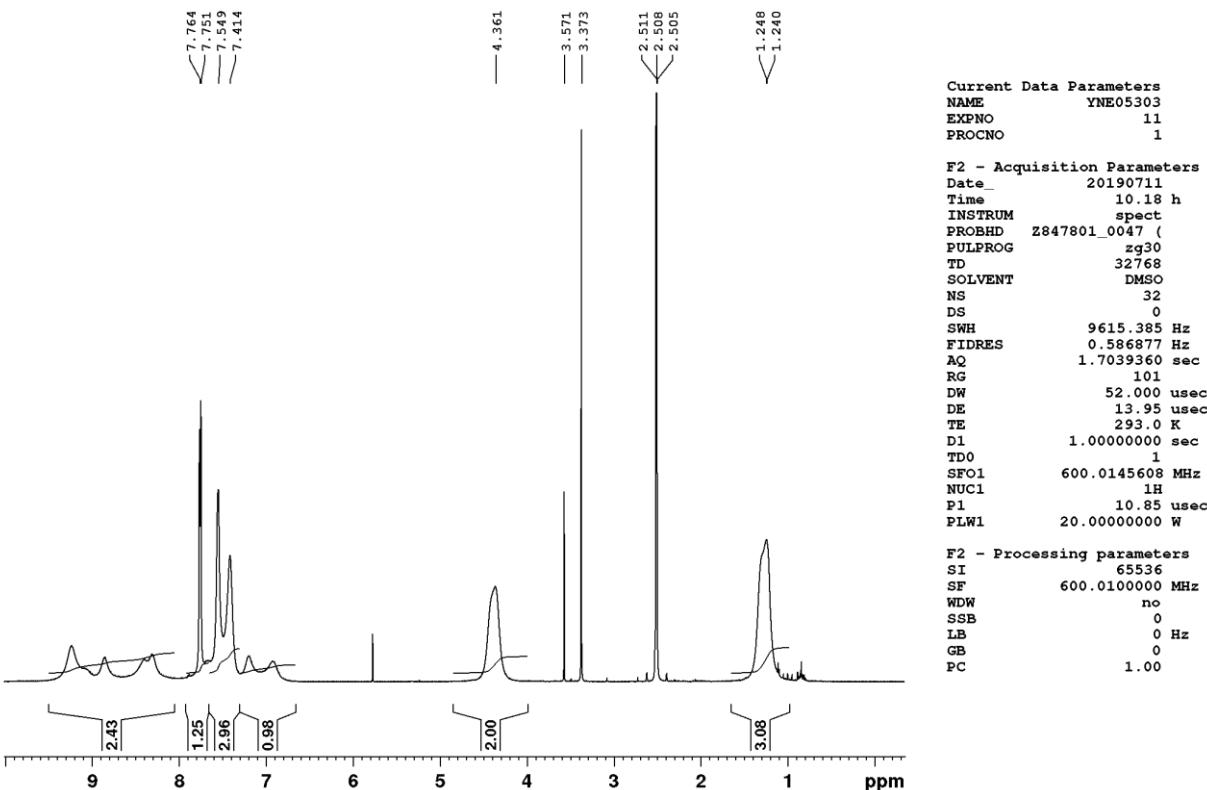
¹H and ¹³C NMR spectra of the studies compounds:

Compound 4:

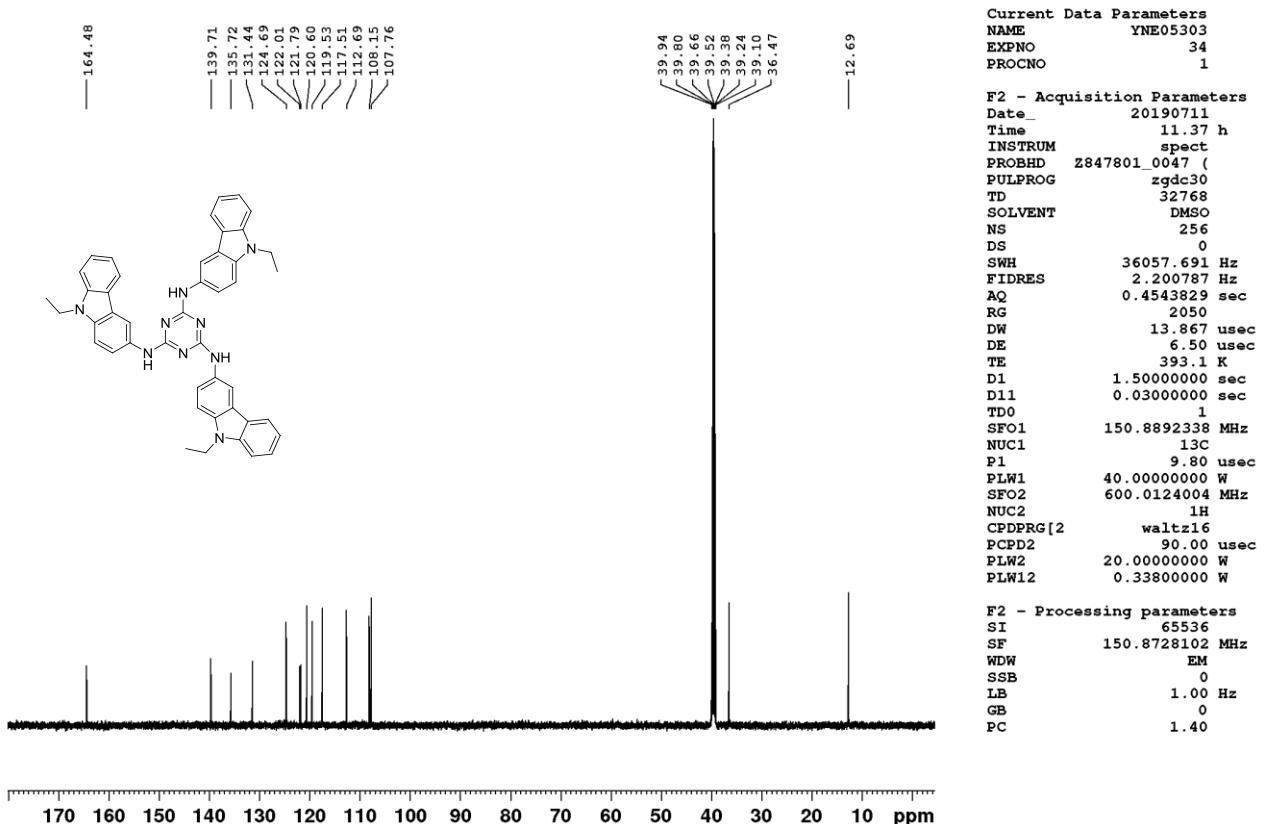
¹H NMR (600 MHz, DMSO-d₆, 393 K):



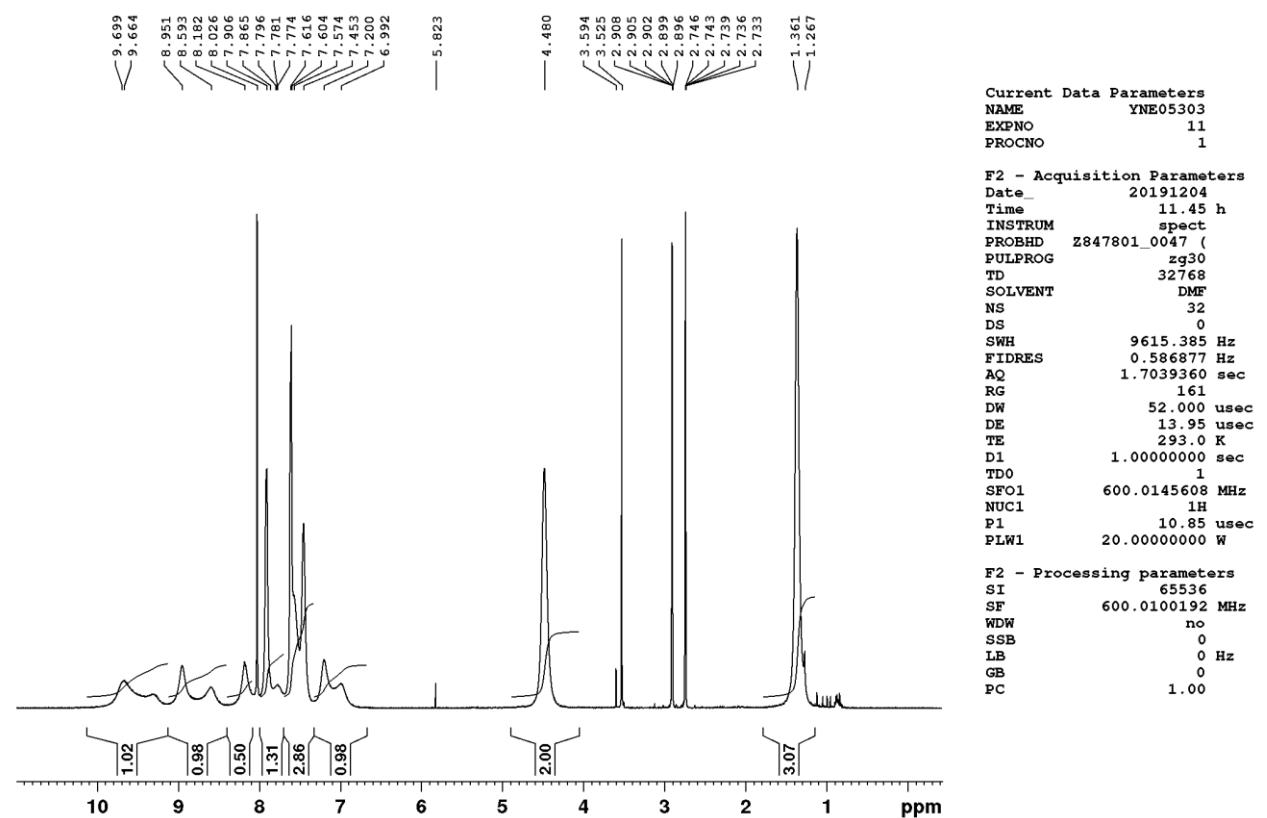
¹H NMR (600 MHz, DMSO-d₆, 293 K):



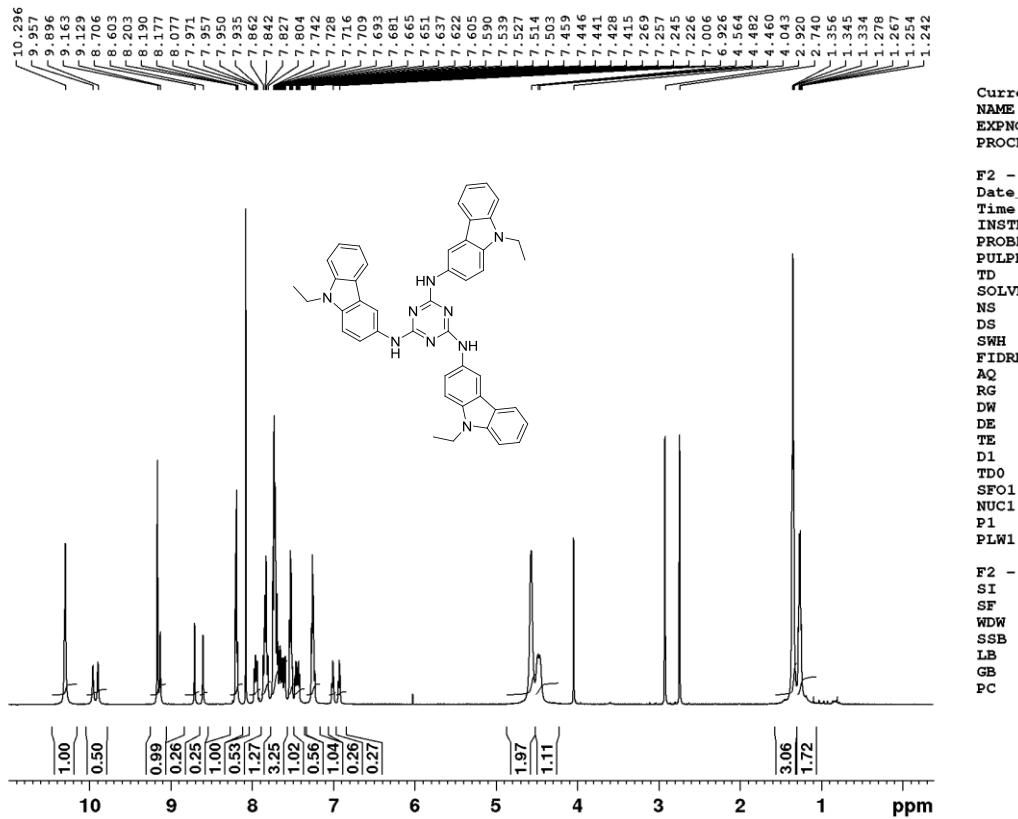
¹³C NMR (150.9 MHz, DMSO-d6, 393 K):



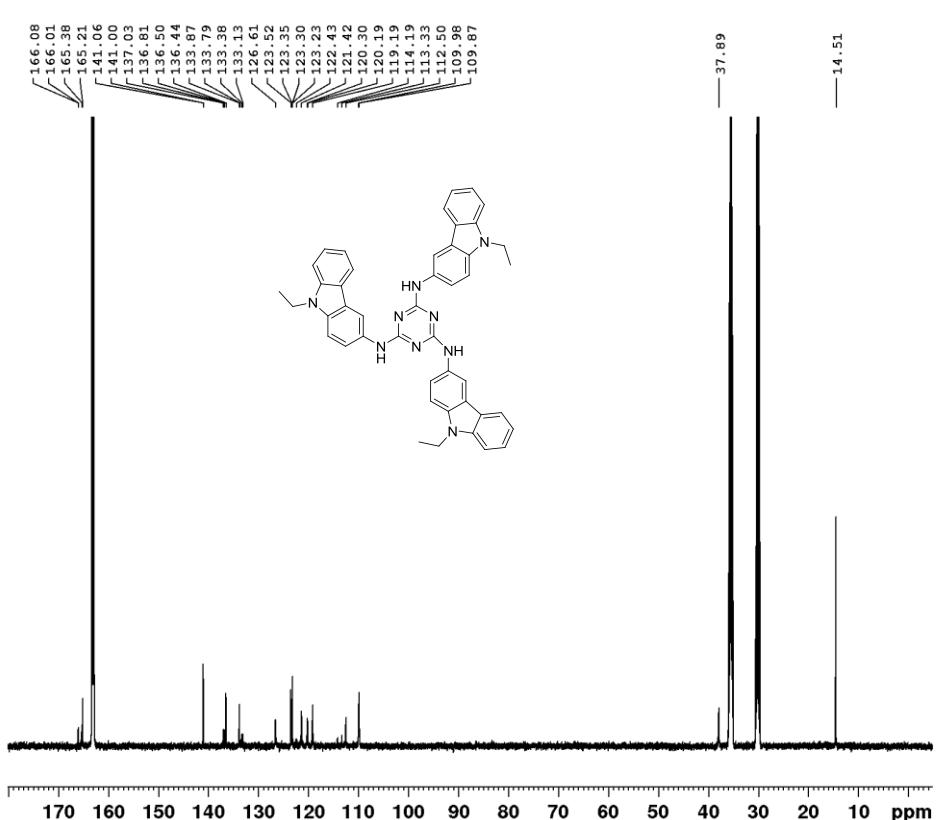
¹H NMR (600 MHz, DMF-d7, 293 K):



¹H NMR (600 MHz, DMF-d₇, 223 K):

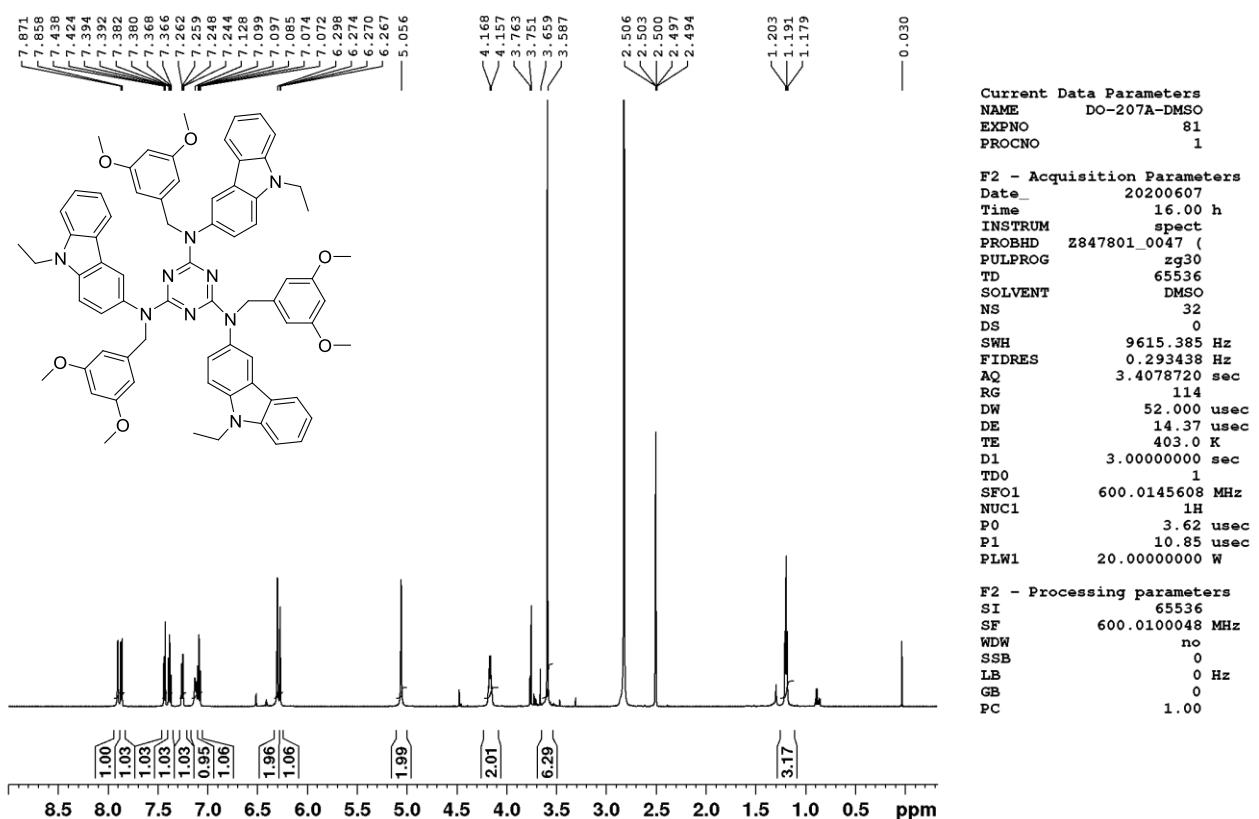


¹³C NMR (150.9 MHz, DMF-d₇, 223 K):

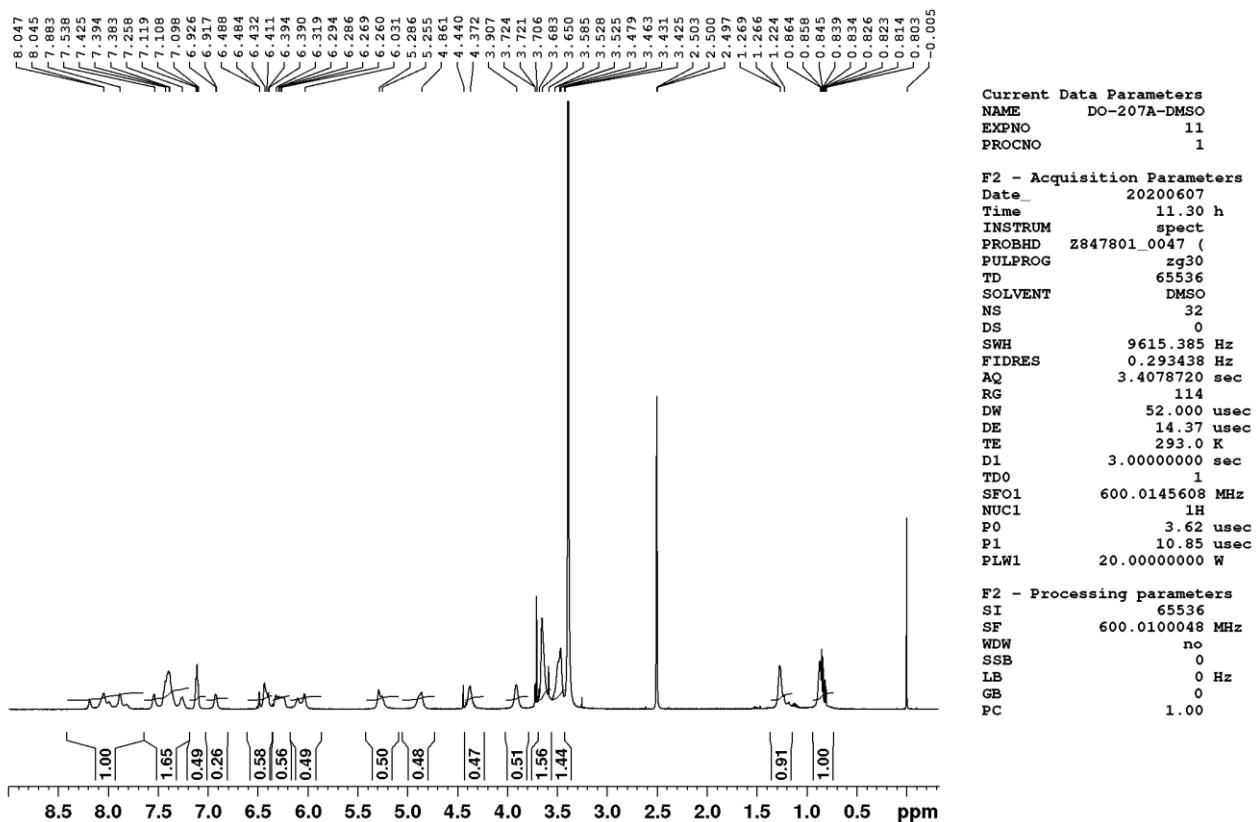


Compound 5:

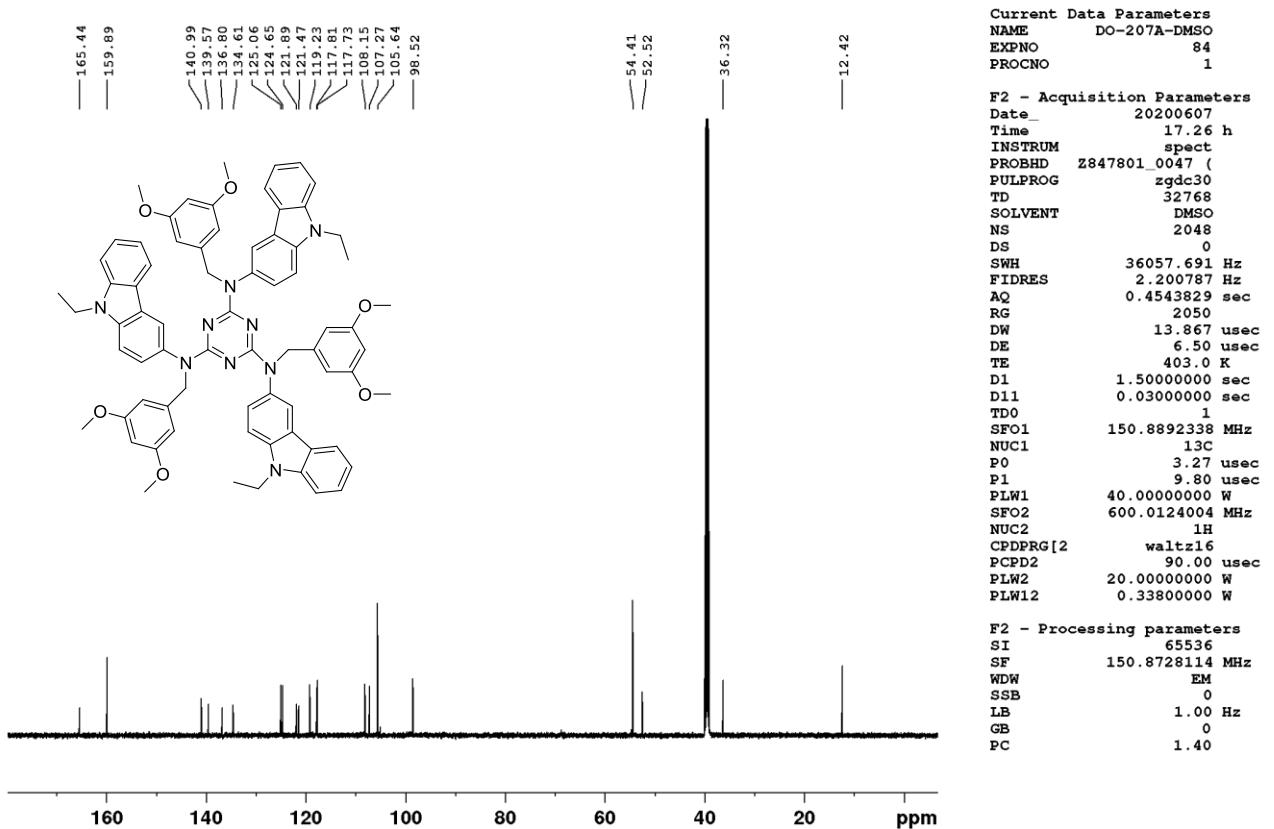
¹H NMR (600 MHz, DMSO-d6, 403 K):



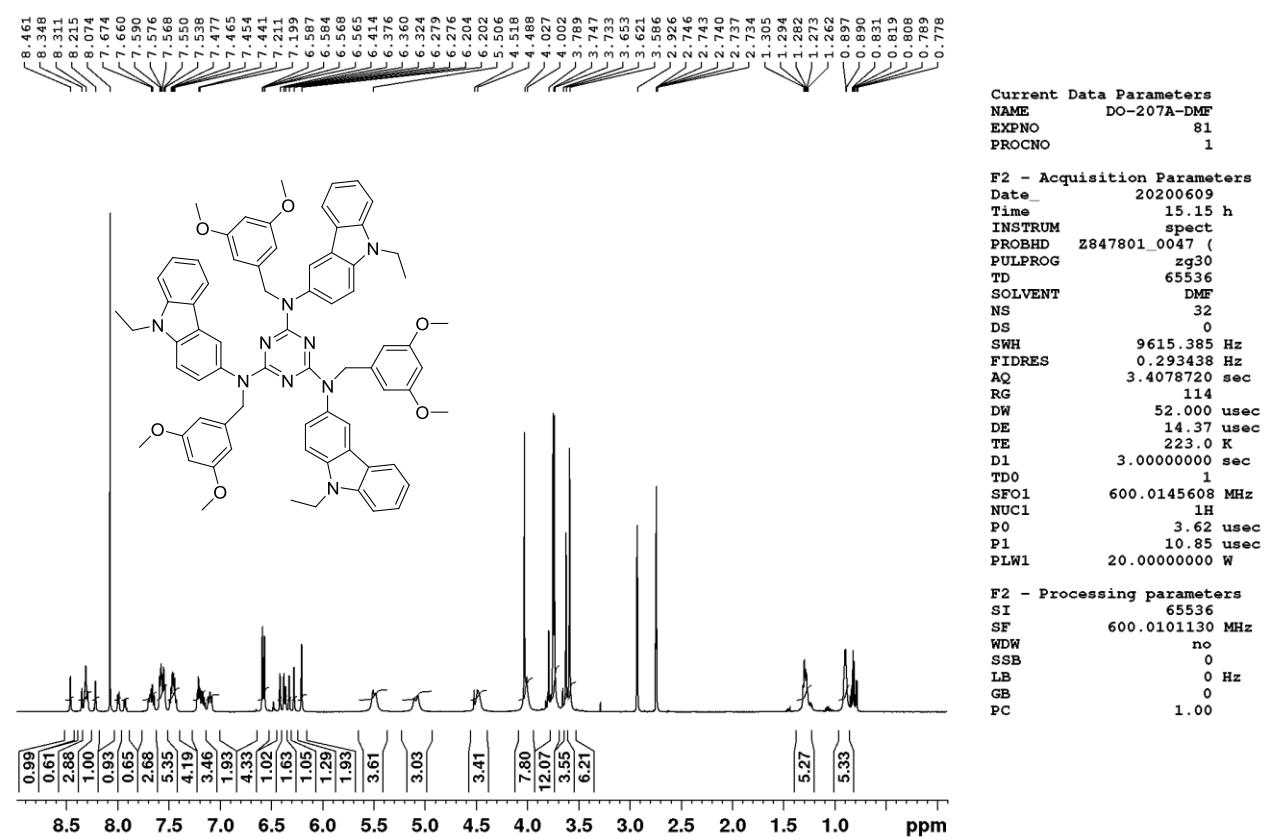
¹H NMR (600 MHz, DMSO-d6, 293 K):



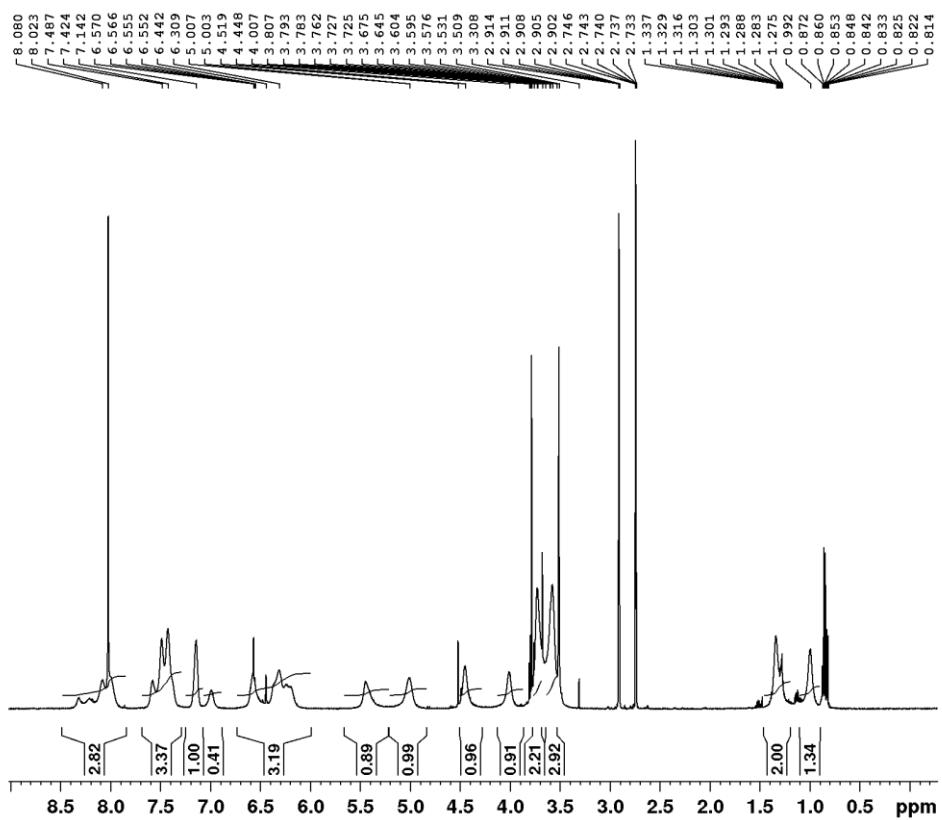
¹³C NMR (150.9 MHz, DMSO-d6, 403 K):



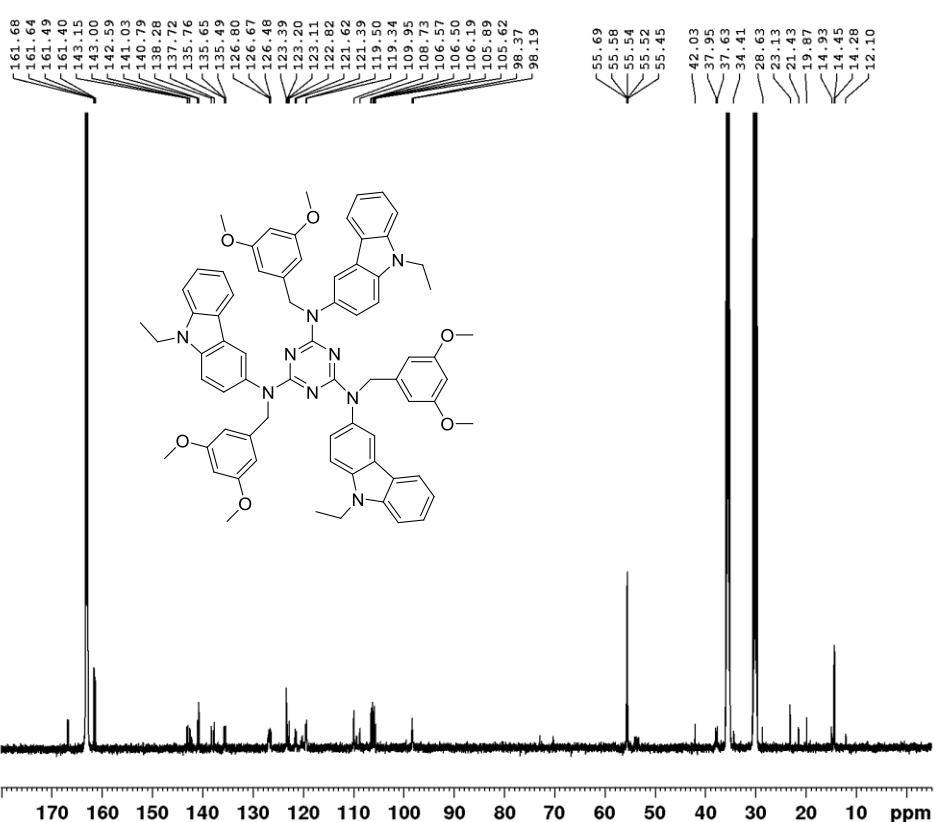
¹H NMR (600 MHz, DMF-d7, 223 K):



¹H NMR (600 MHz, DMF-d7, 293 K):

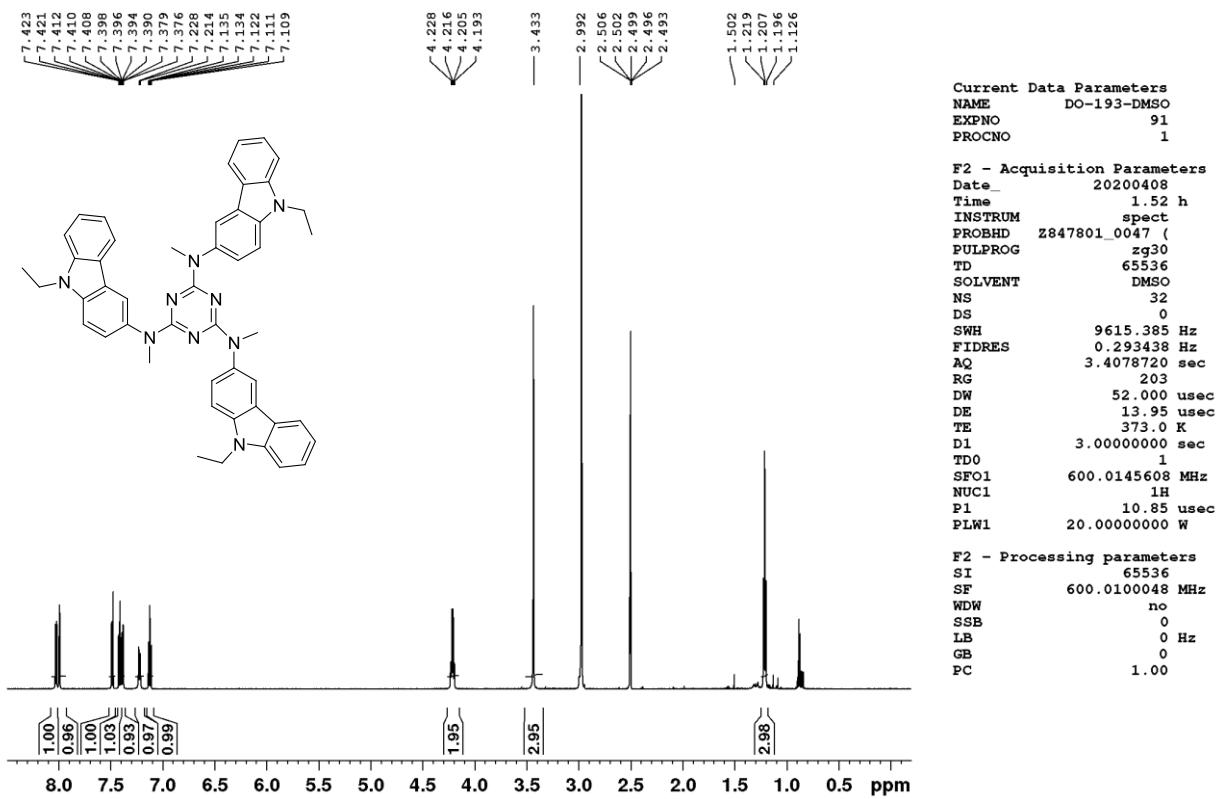


¹³C NMR (150.9 MHz, DMF-d7, 223 K):

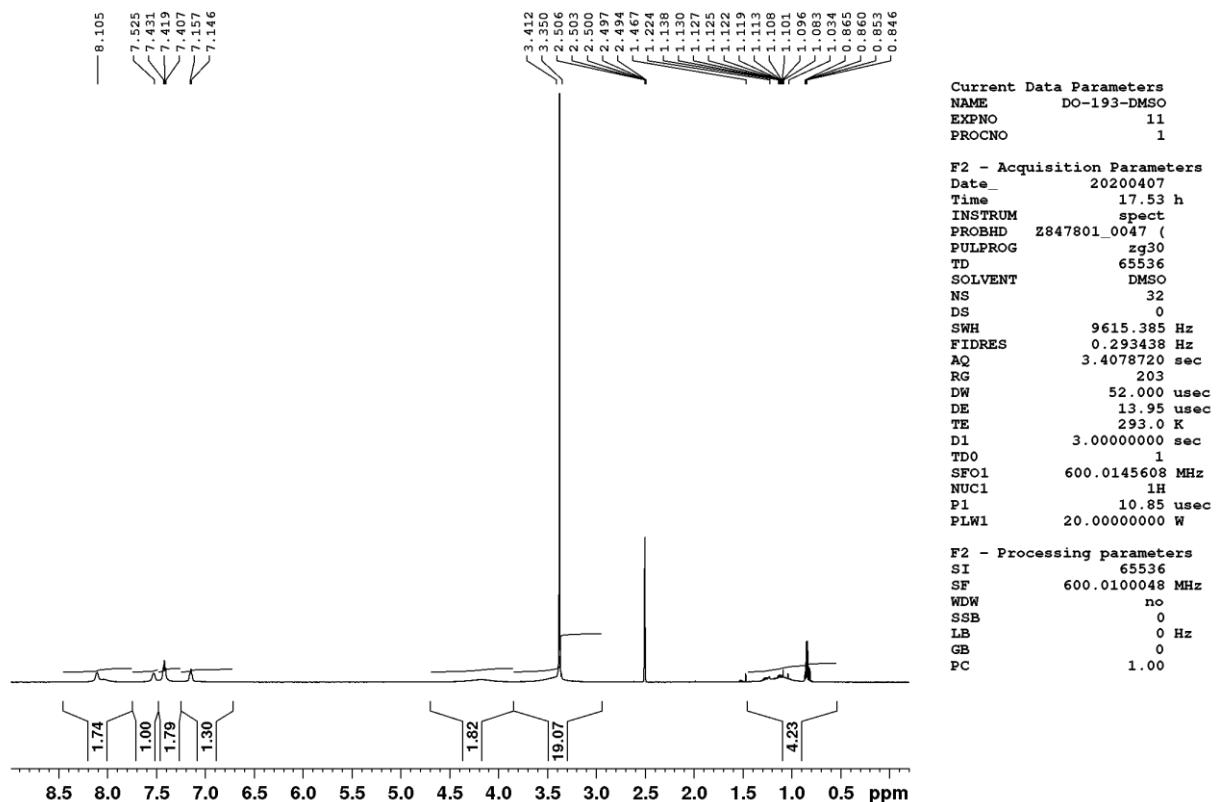


Compound 6:

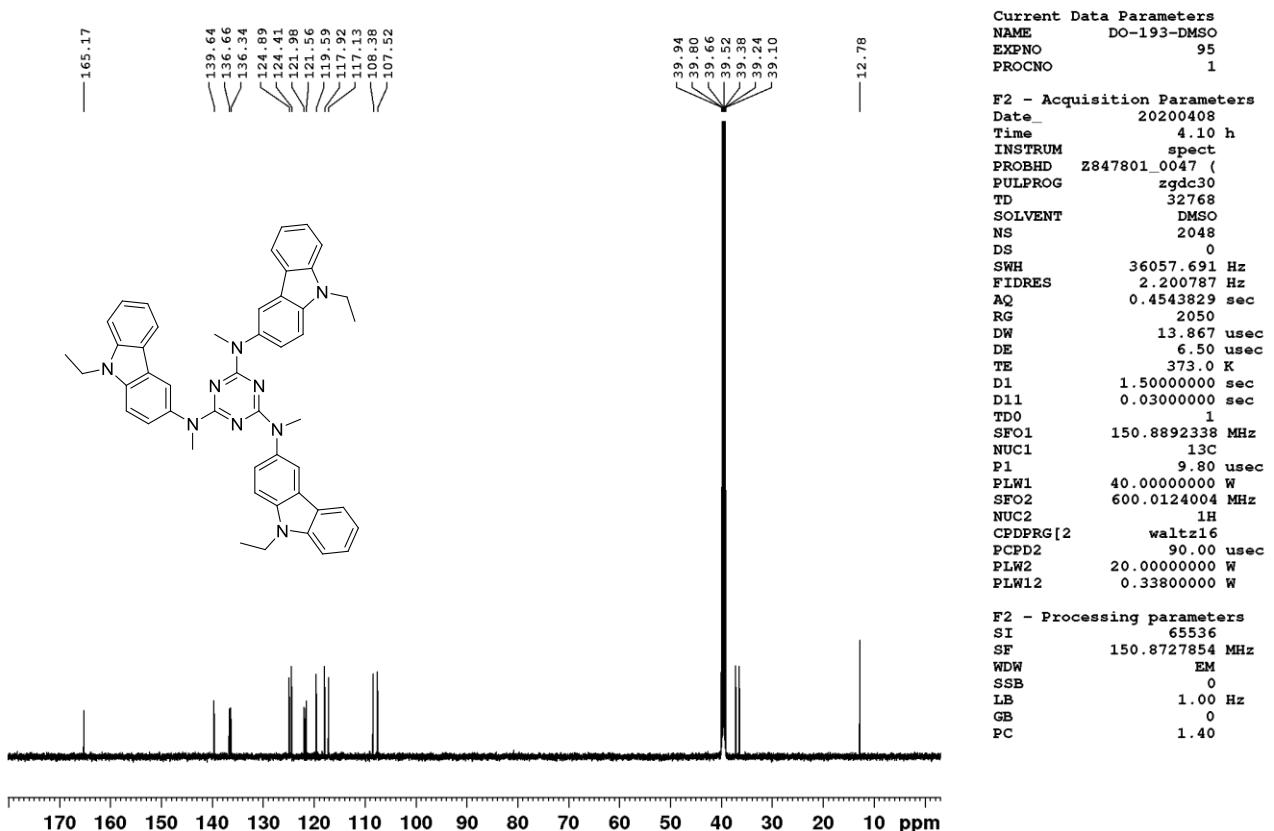
¹H NMR (600 MHz, DMSO-d6, 373 K):



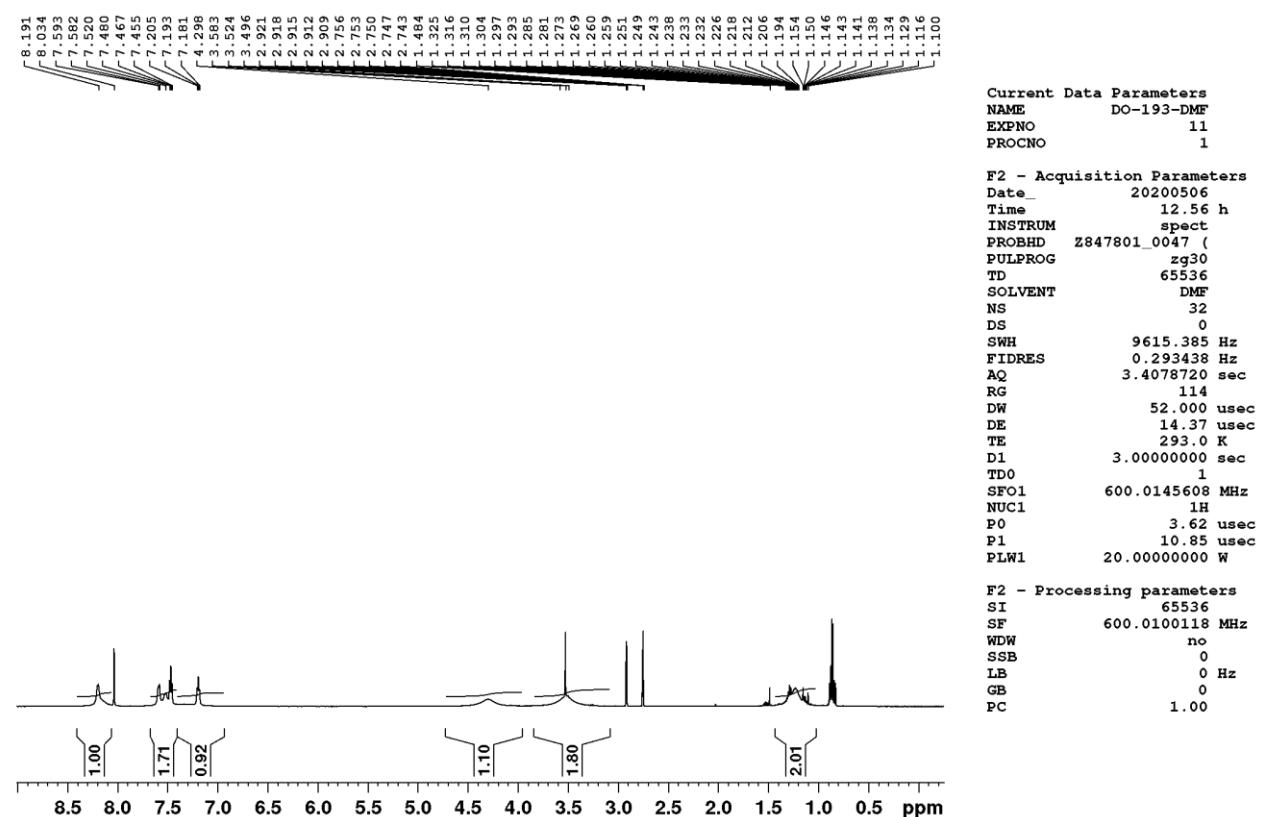
¹H NMR (600 MHz, DMSO-d6, 293 K):



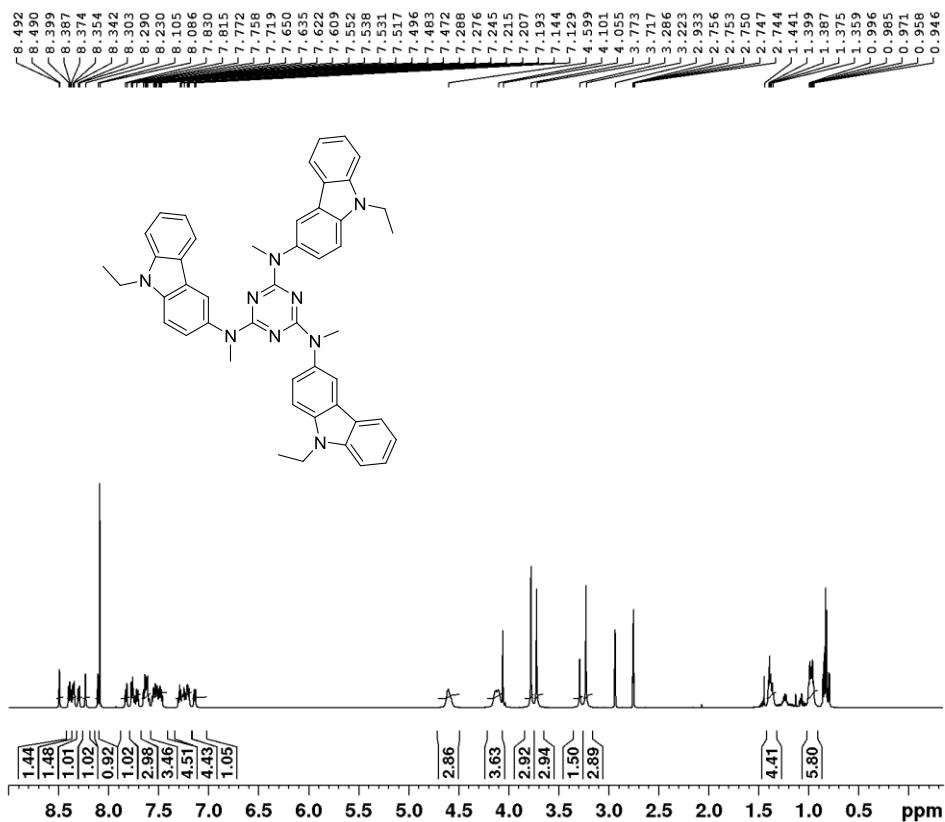
¹³C NMR (150.9 MHz, DMSO-d6, 373 K):



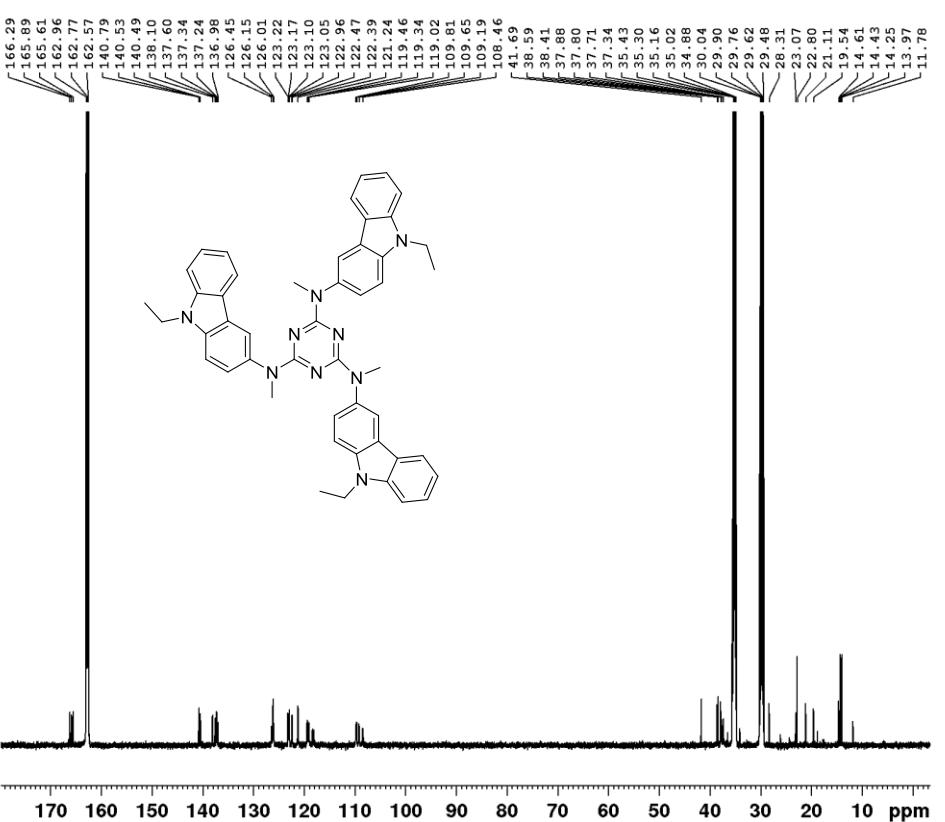
¹H NMR (600 MHz, DMF-d7, 293 K):



¹H NMR (600 MHz, DMF-d7, 223 K):



¹³C NMR (150.9 MHz, DMF-d₇, 223 K):



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F2 - Processing parameters
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Current Data Parameters
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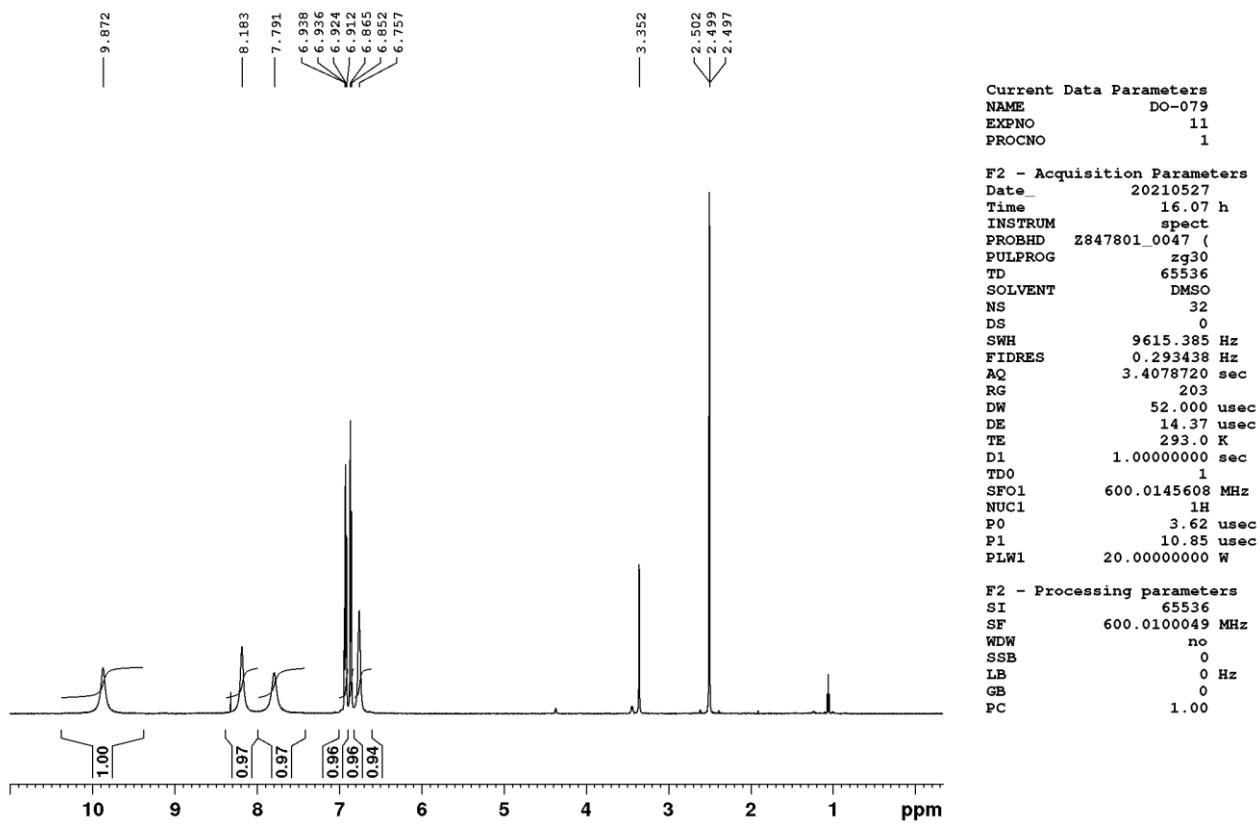
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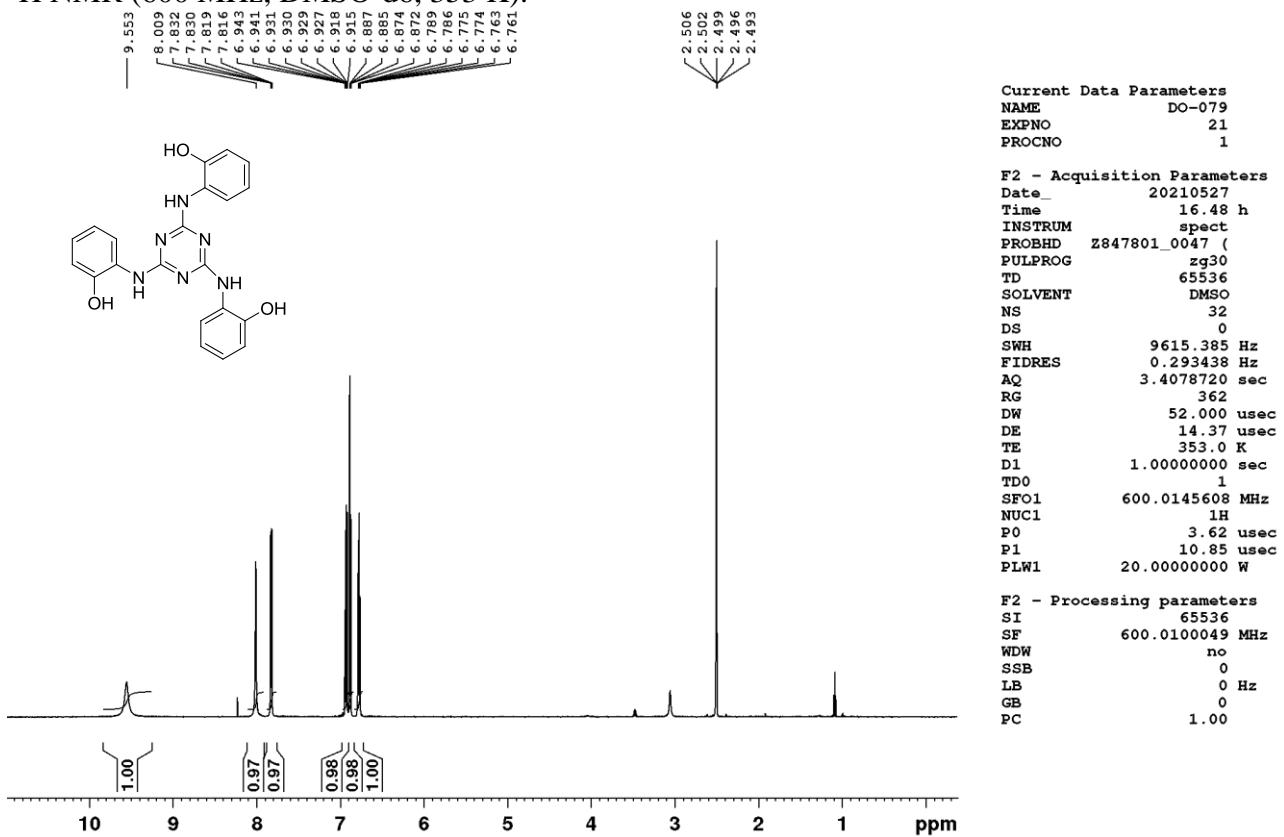
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Compound 11:

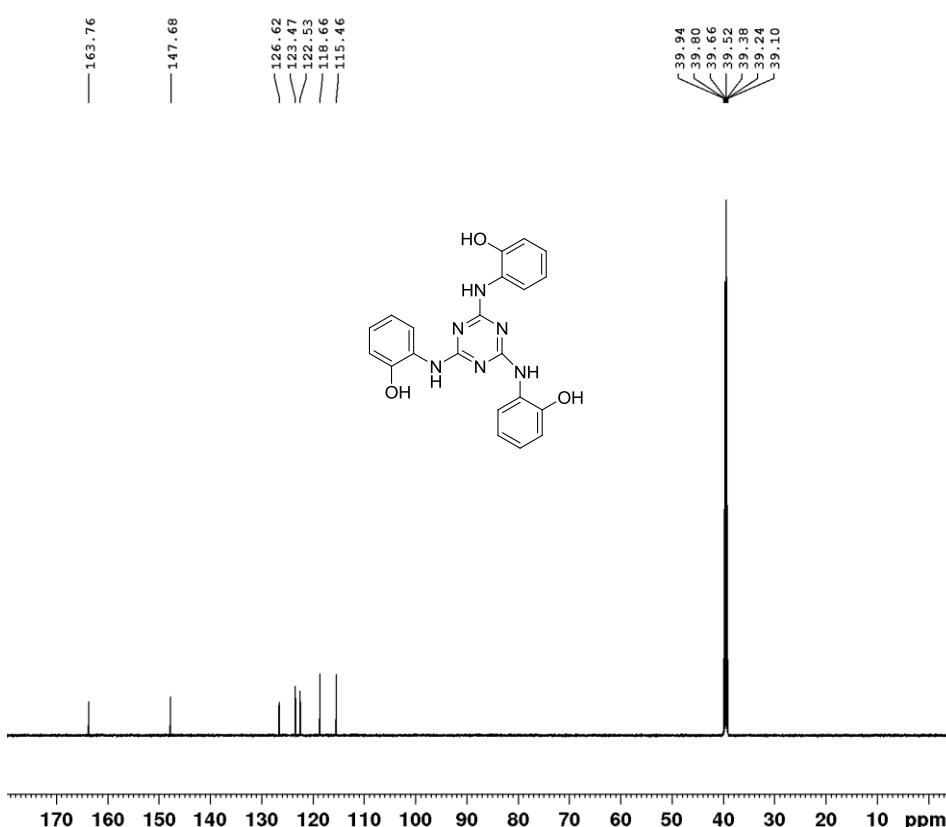
¹H NMR (600 MHz, DMSO-d₆, 293 K):



¹H NMR (600 MHz, DMSO-d₆, 353 K):



¹³C NMR (150.9 MHz, DMSO-d6, 353 K):

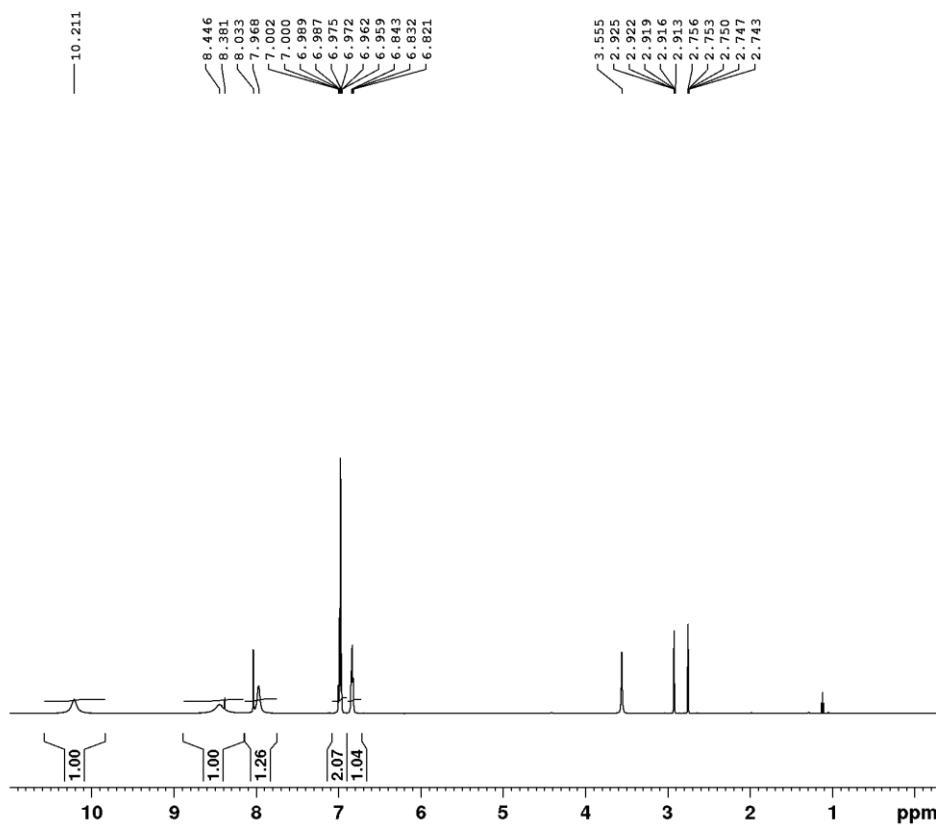


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PROCNO 1

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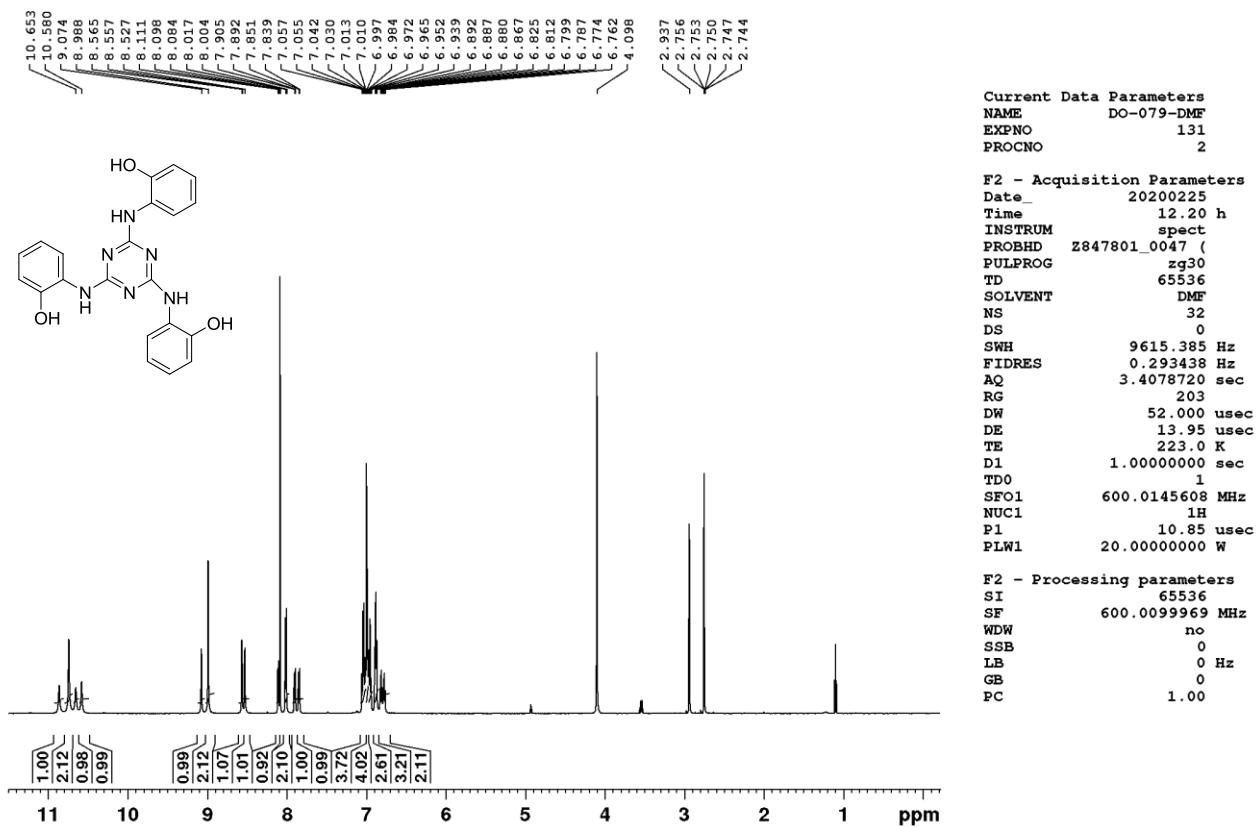


Current Data Parameters
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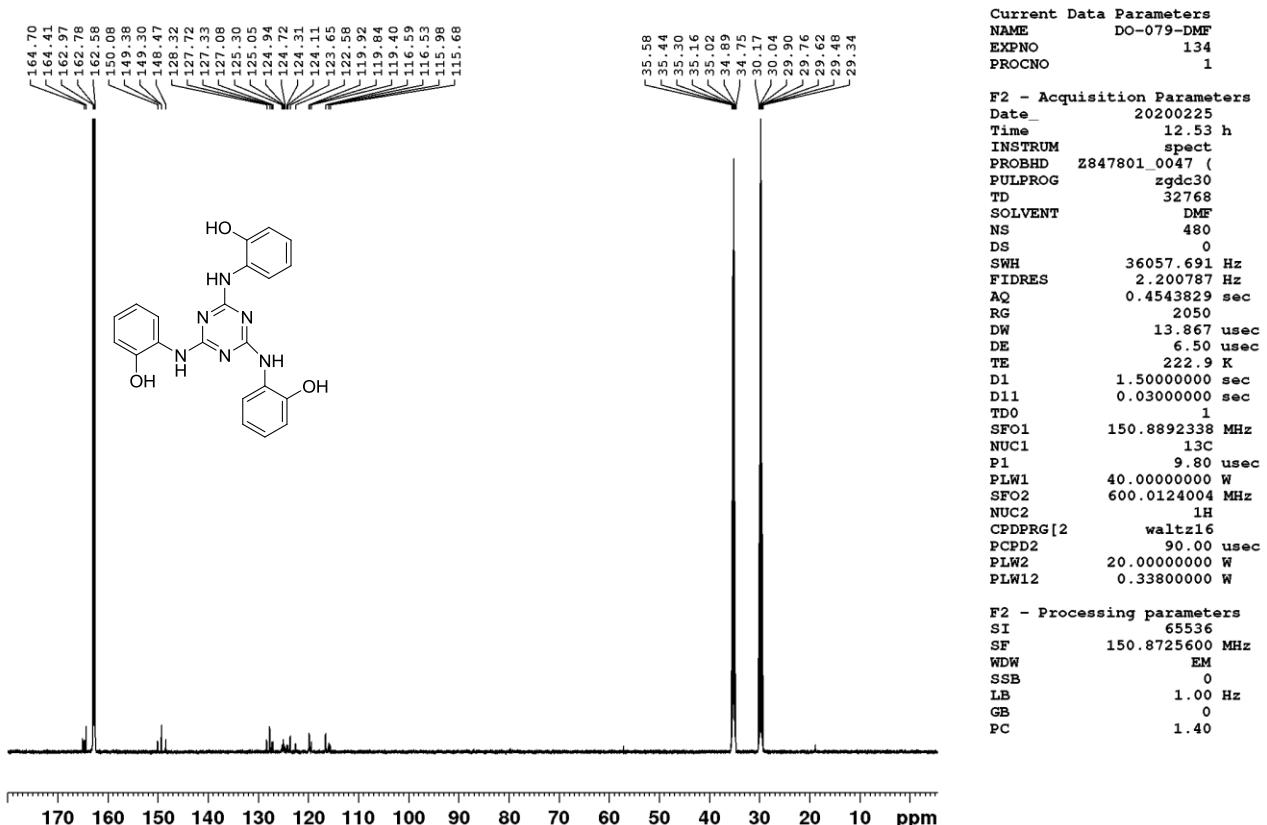
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F2 - Processing parameters
SI 65536
SF 600.0101086 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

¹H NMR (600 MHz, DMF-d₇, 223 K):

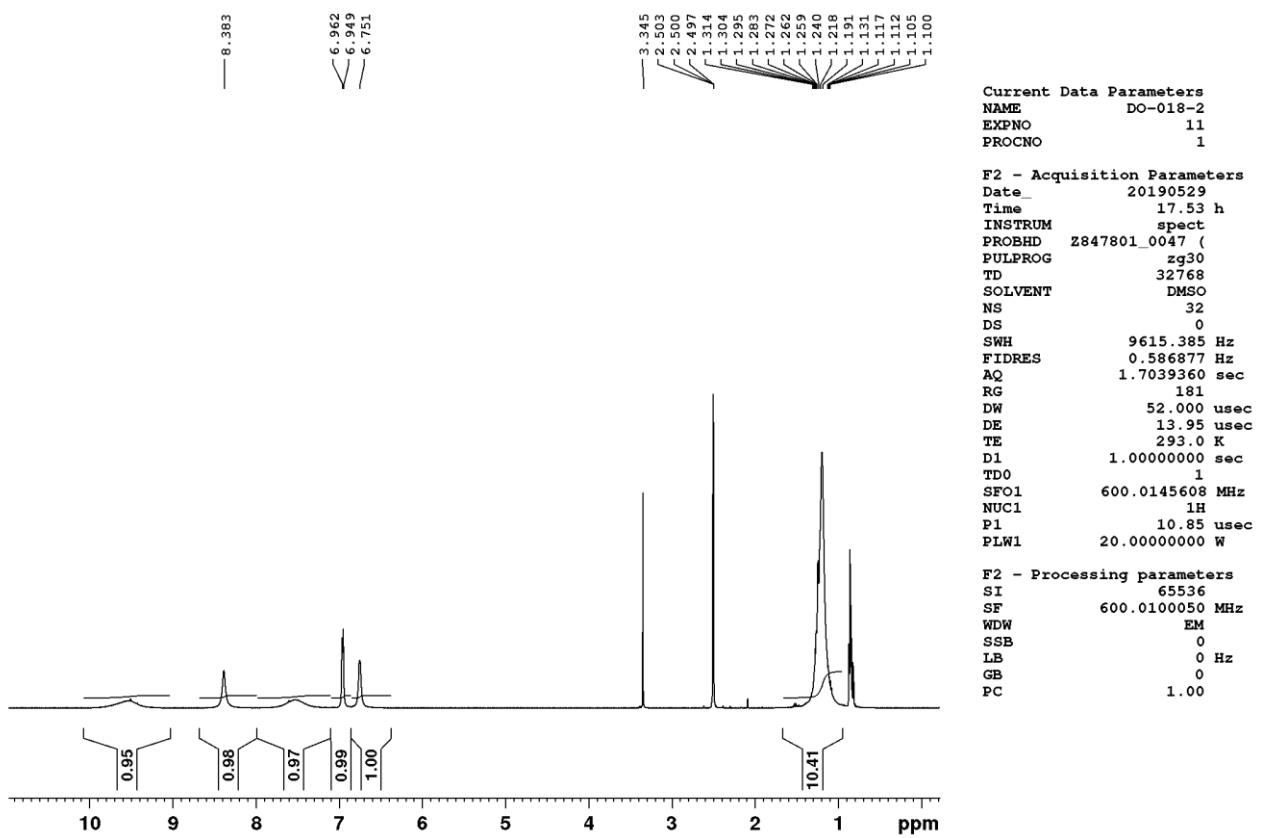


¹³C NMR (150.9 MHz, DMF-d₇, 223 K):

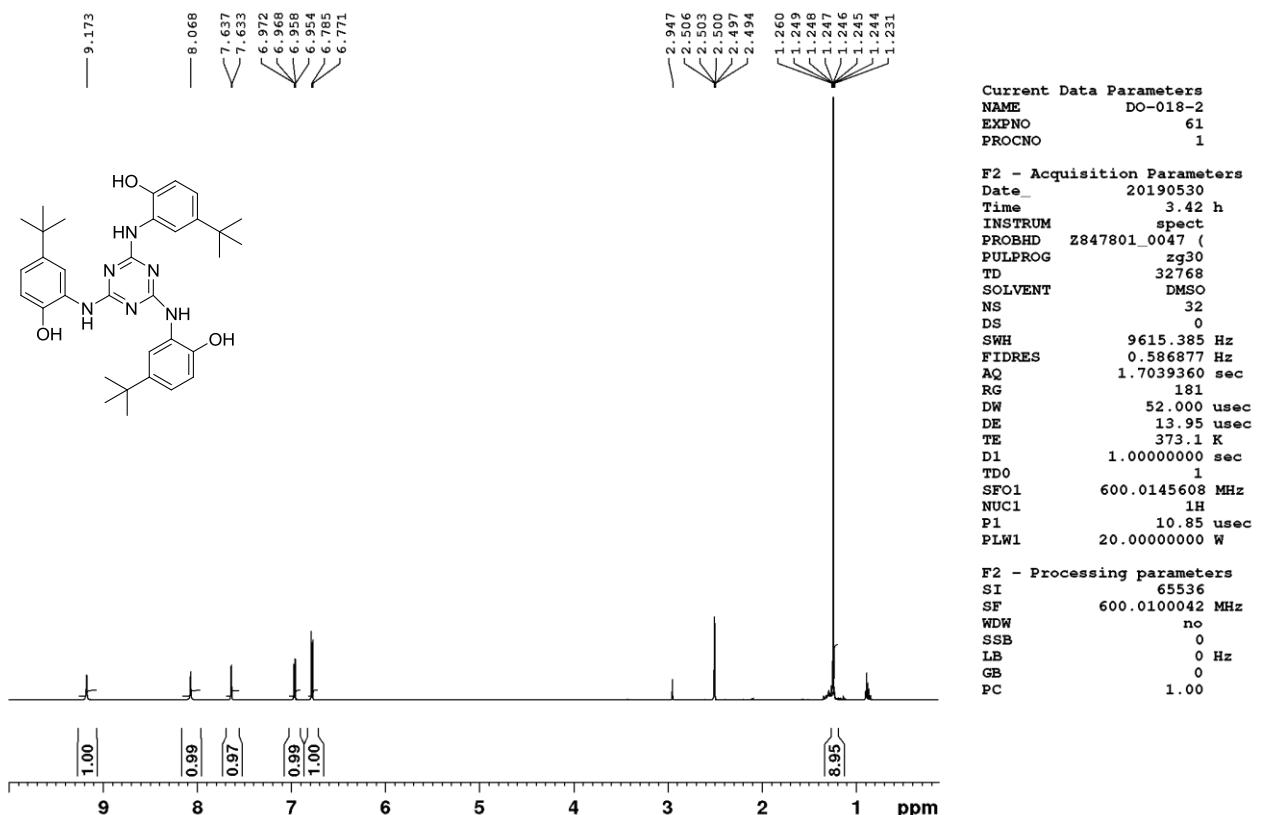


Compound 12:

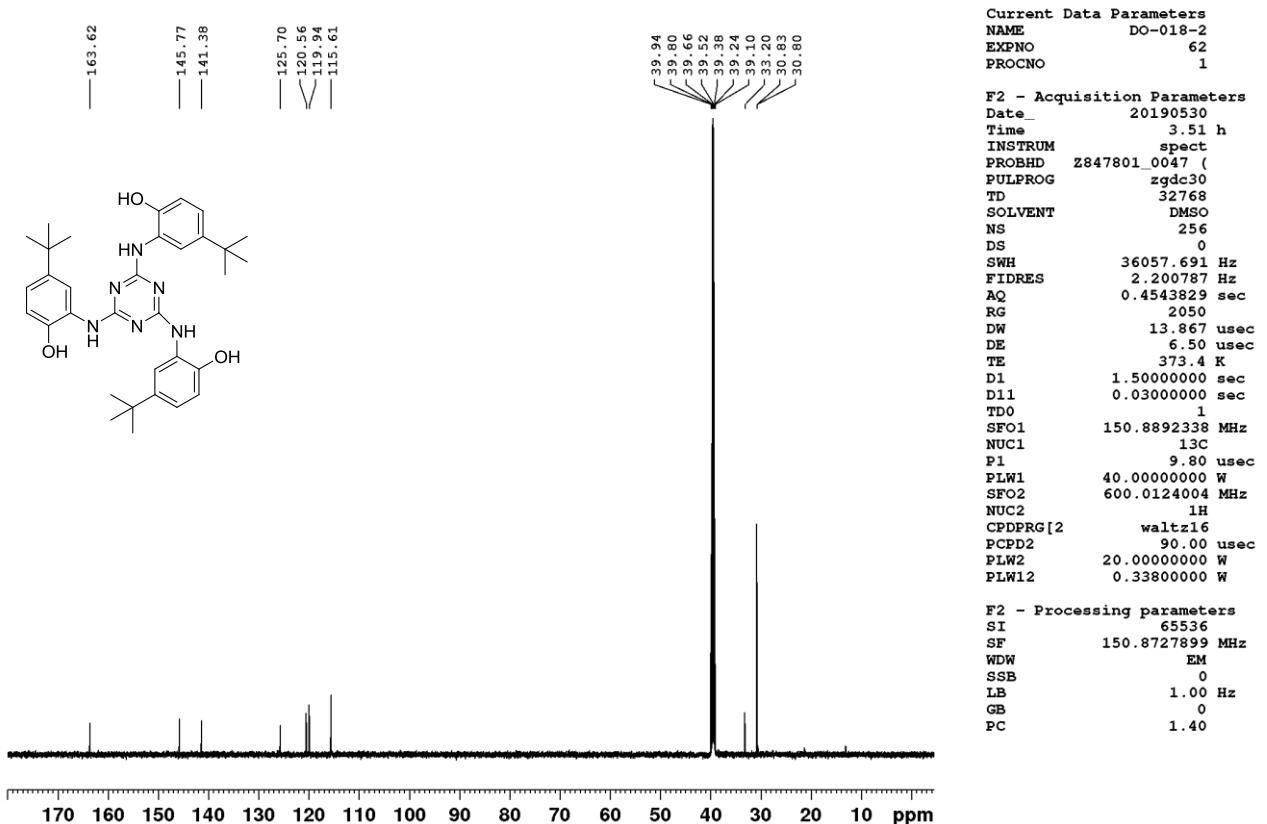
¹H NMR (600 MHz, DMSO-d₆, 293 K):



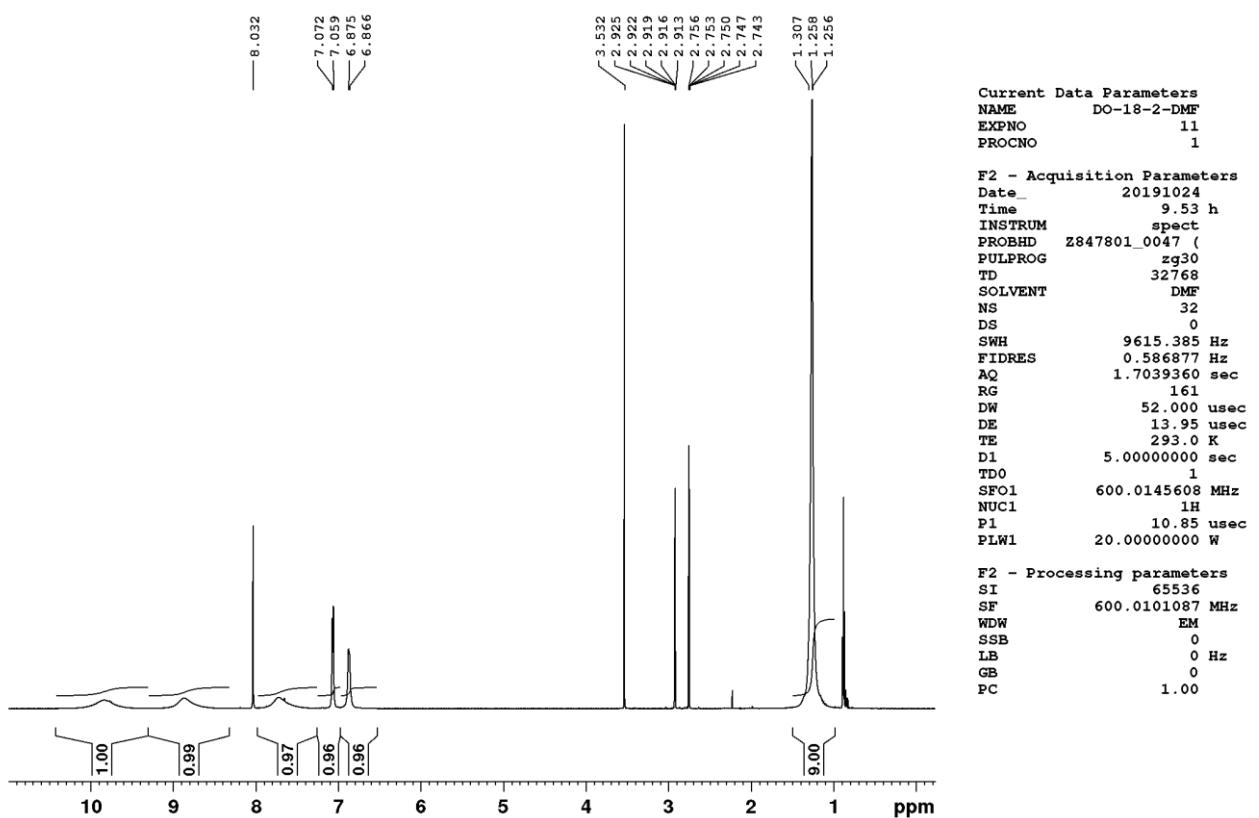
¹H NMR (600 MHz, DMSO-d₆, 373 K):



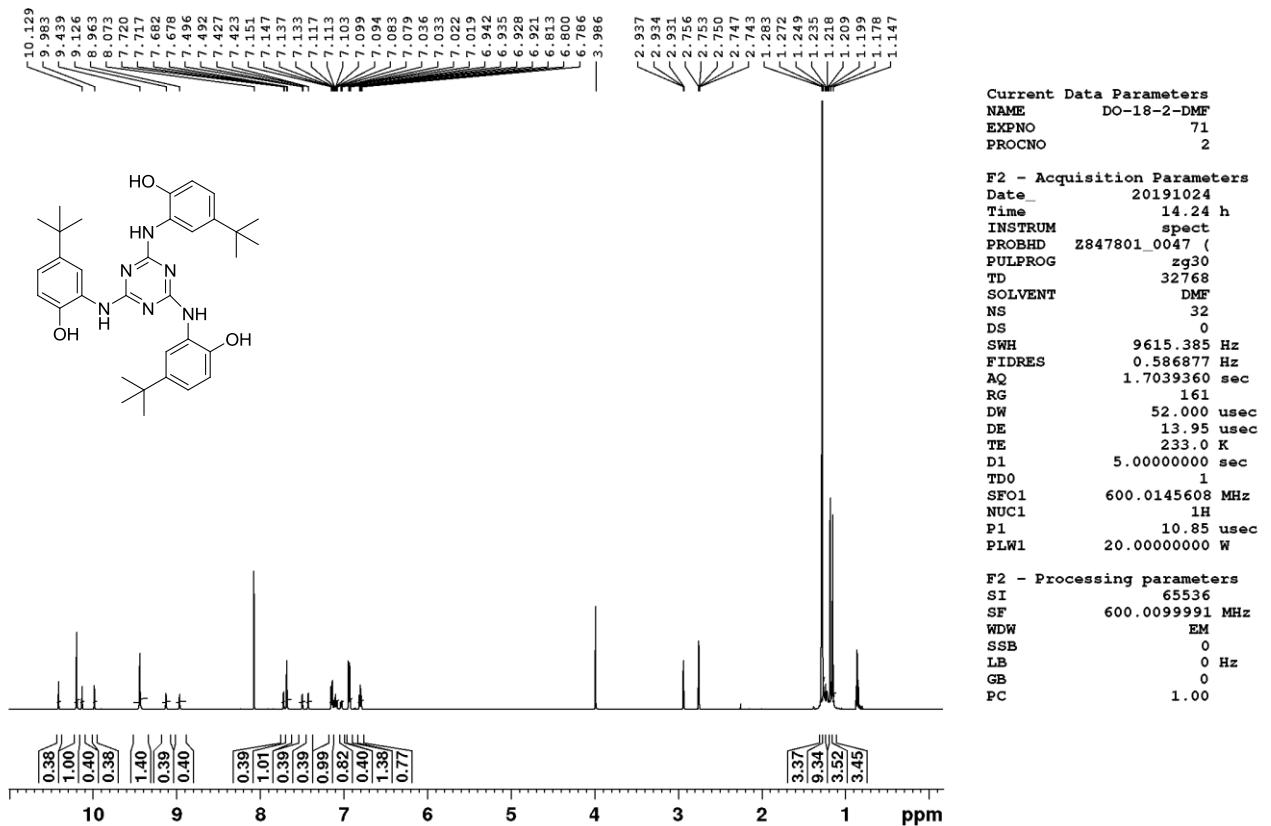
¹³C NMR (150.9 MHz, DMSO-d6, 373 K):



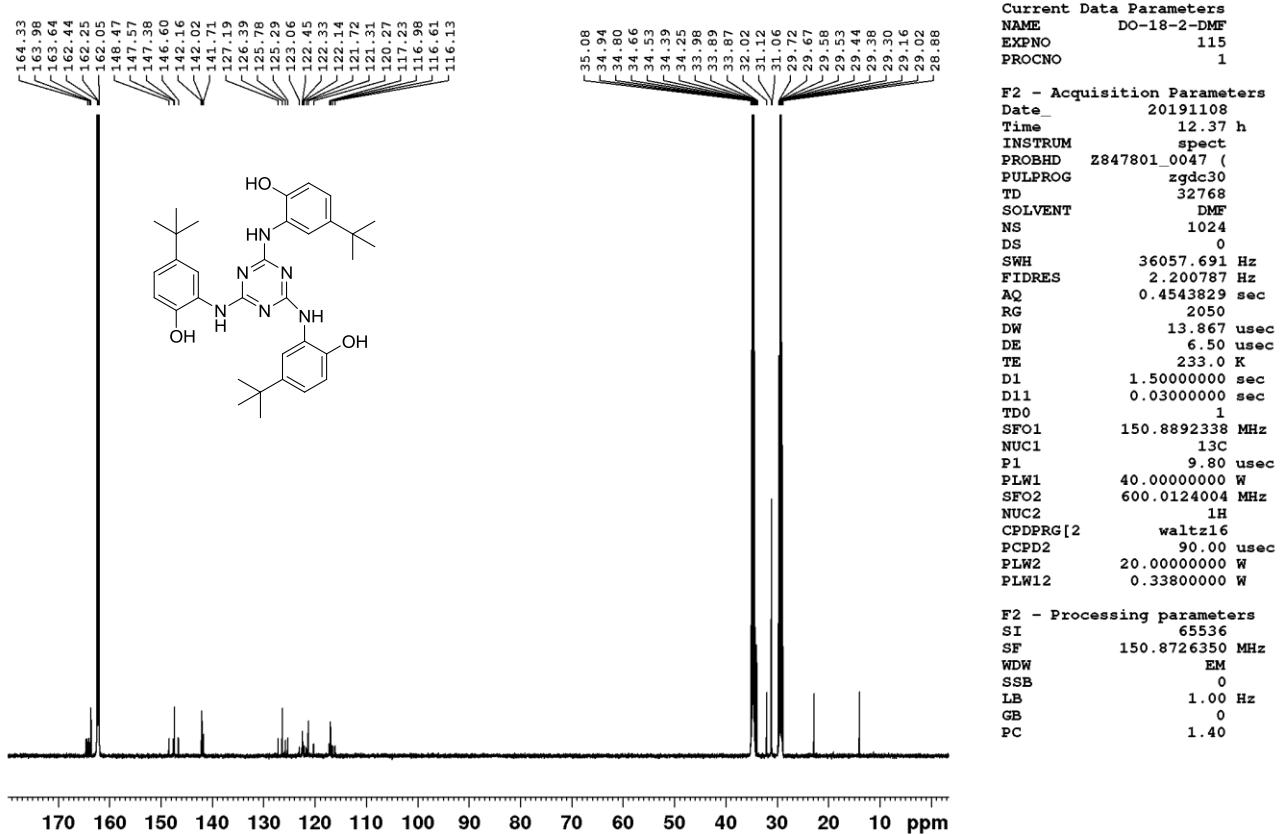
¹H NMR (600 MHz, DMF-d7, 293 K):



¹H NMR (600 MHz, DMF-d7, 233 K):

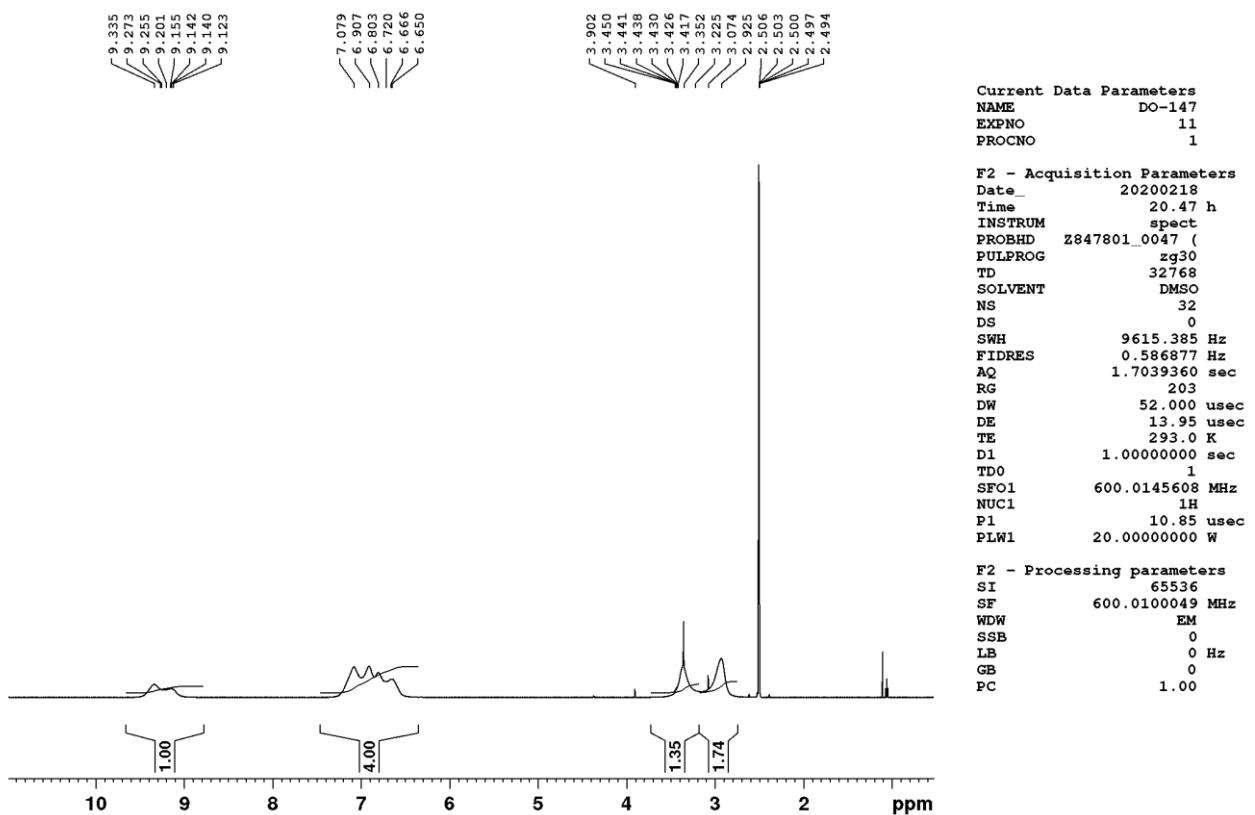


¹³C NMR (150.9 MHz, DMF-d₇, 233 K):

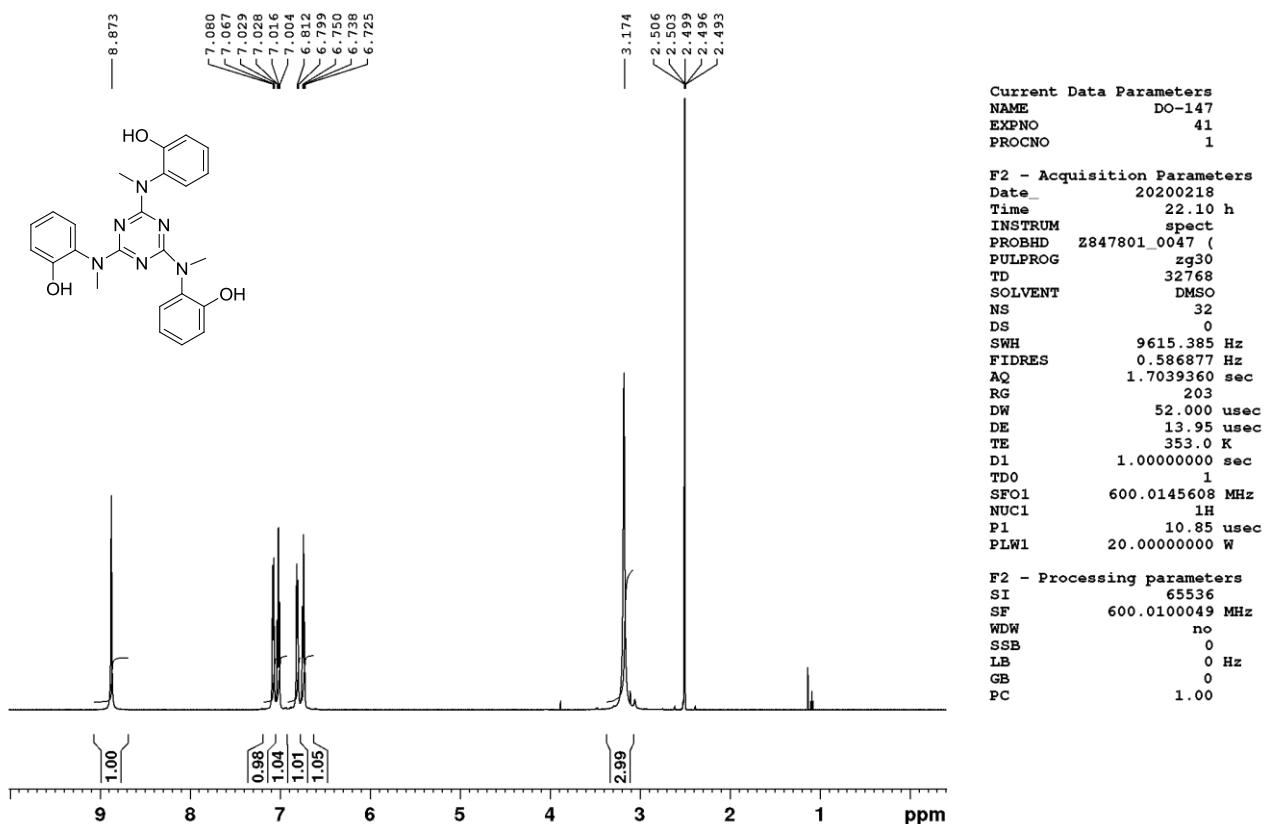


Compound 13:

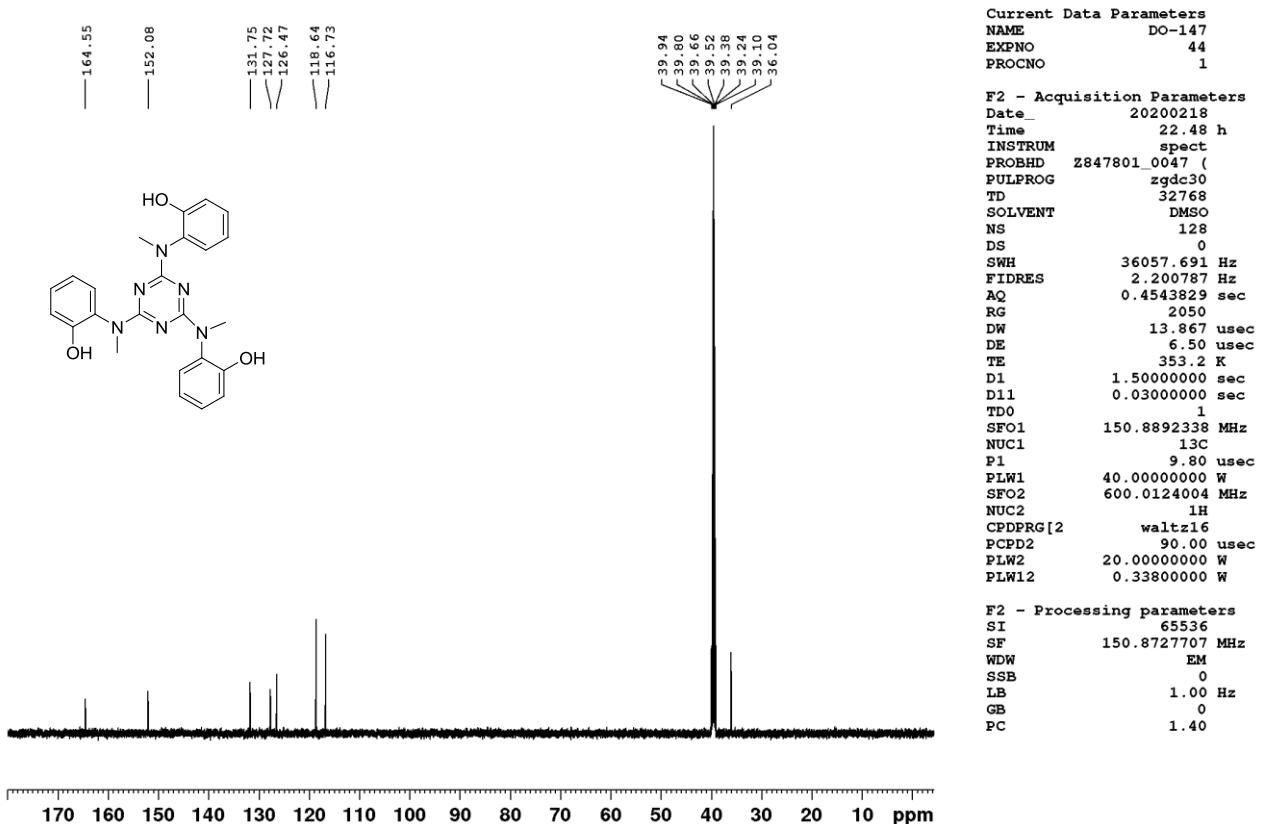
¹H NMR (600 MHz, DMSO-d6, 293 K):



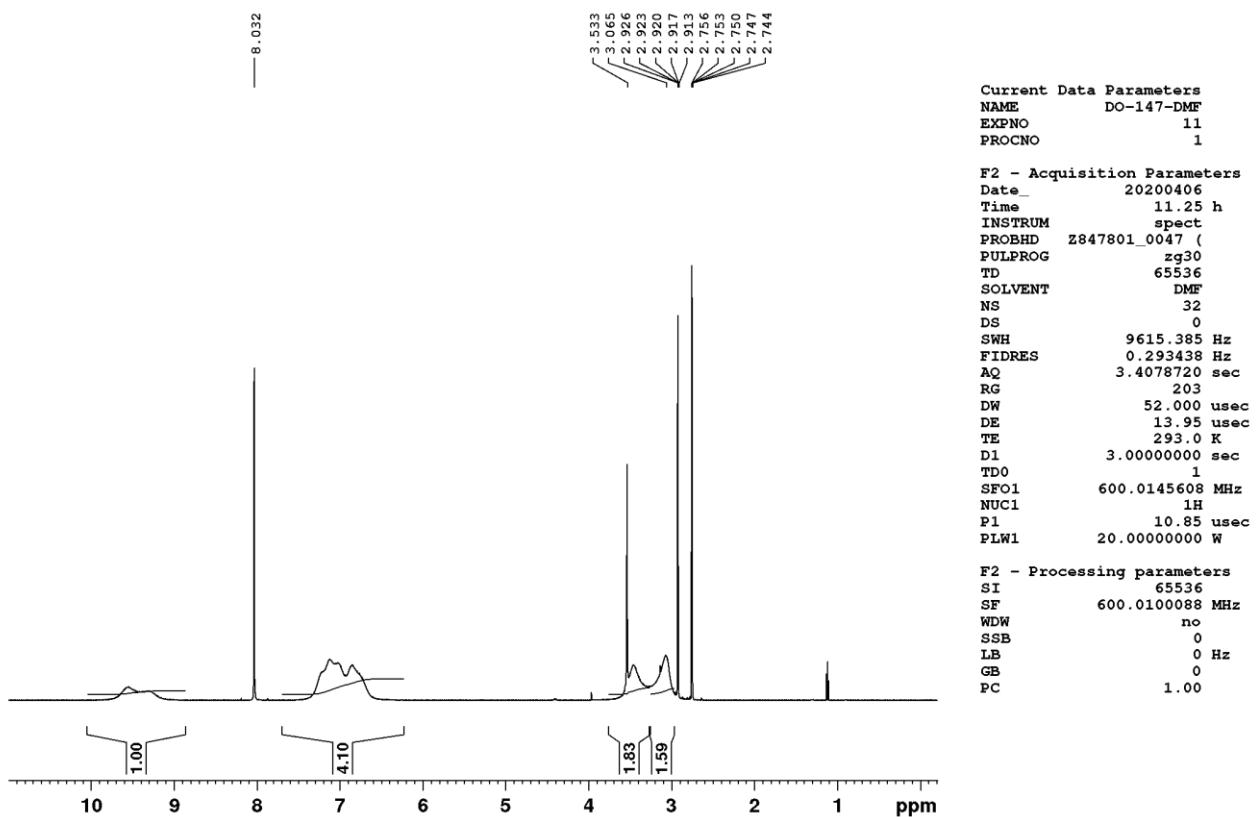
¹H NMR (600 MHz, DMSO-d6, 353 K):



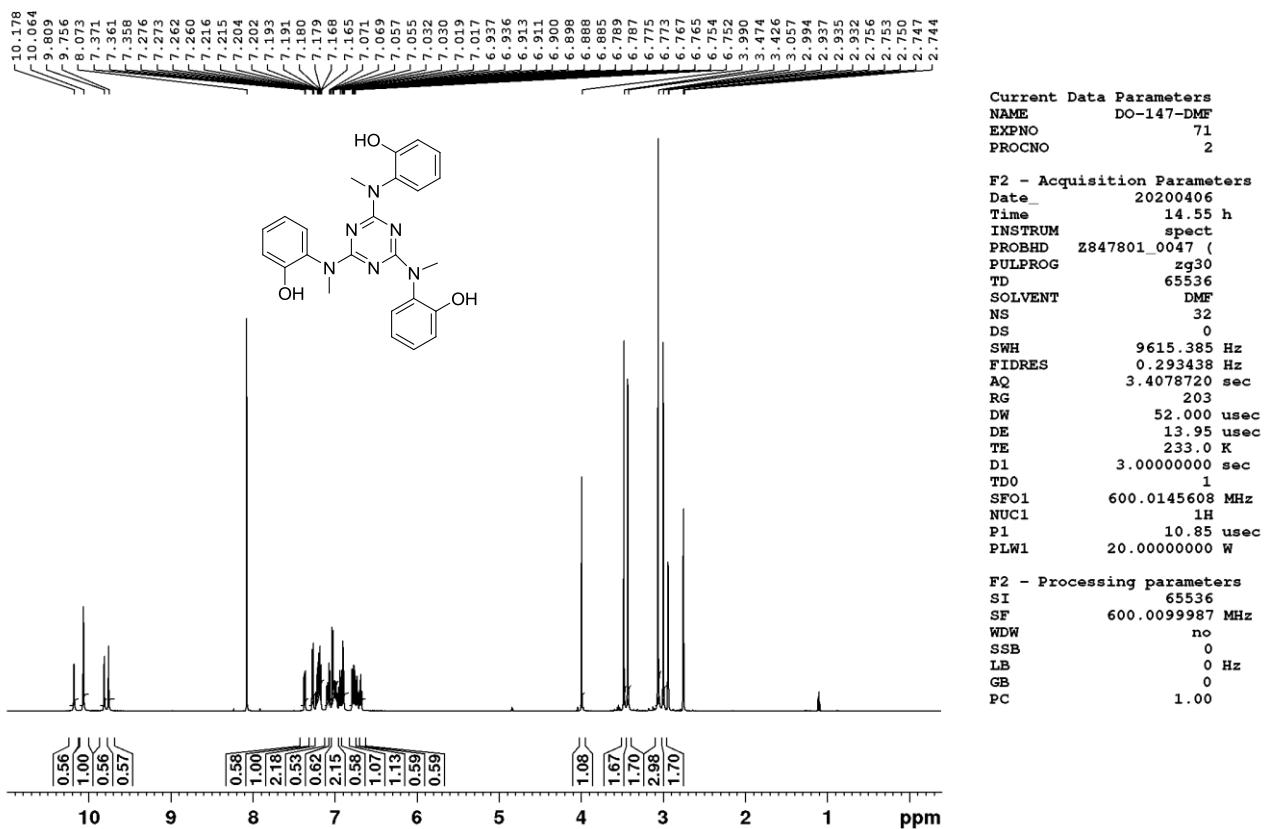
¹³C NMR (150.9 MHz, DMSO-d6, 353 K):



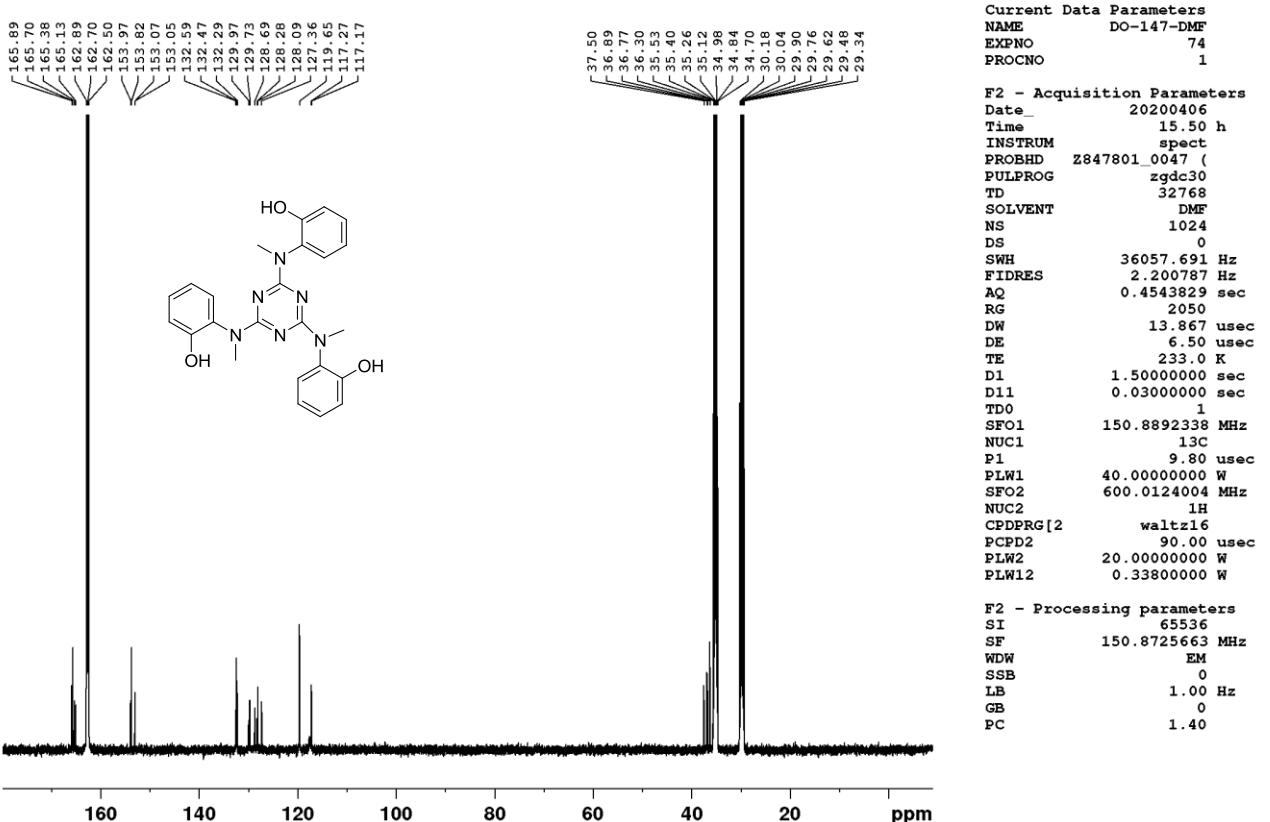
¹H NMR (600 MHz, DMF-d7, 293 K):



¹H NMR (600 MHz, DMF-d₇, 233 K):

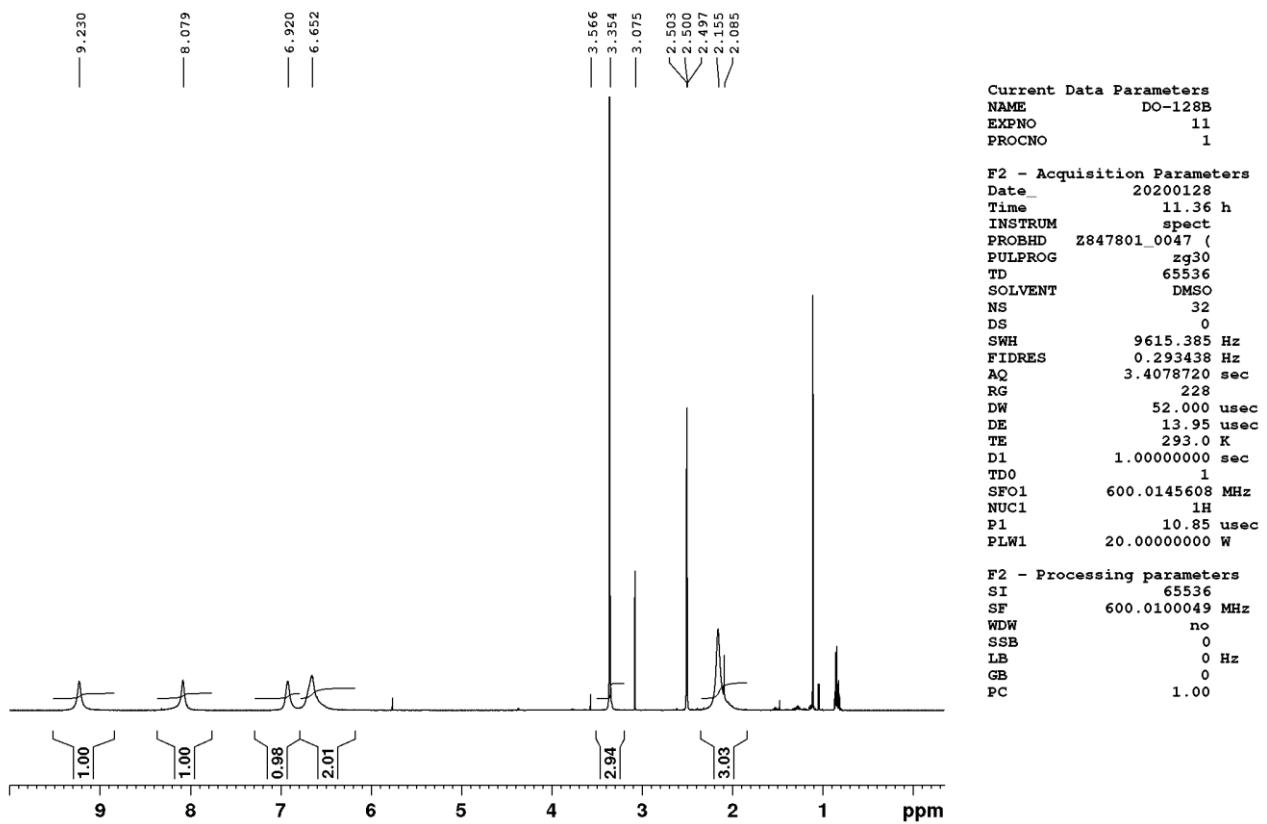


¹³C NMR (150.9 MHz, DMF-d₇, 233 K):

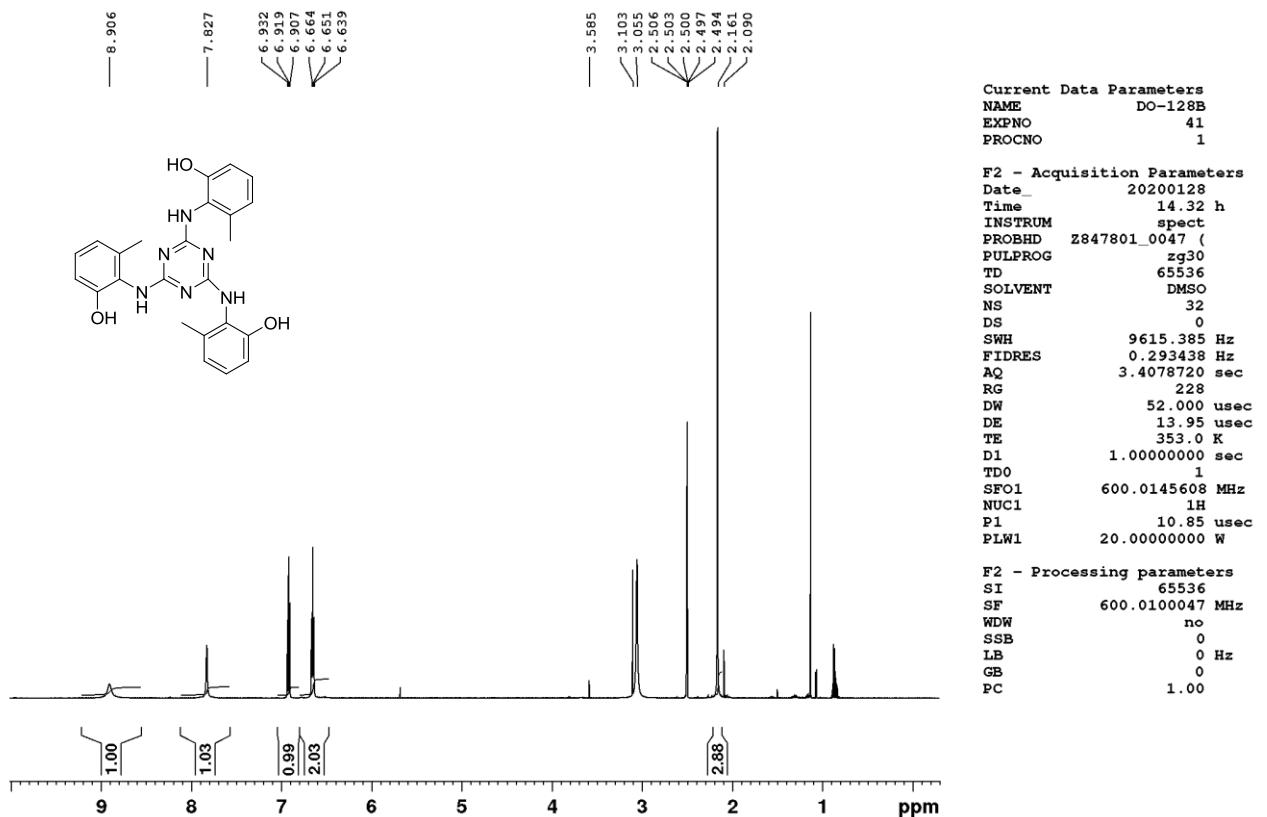


Compound 14:

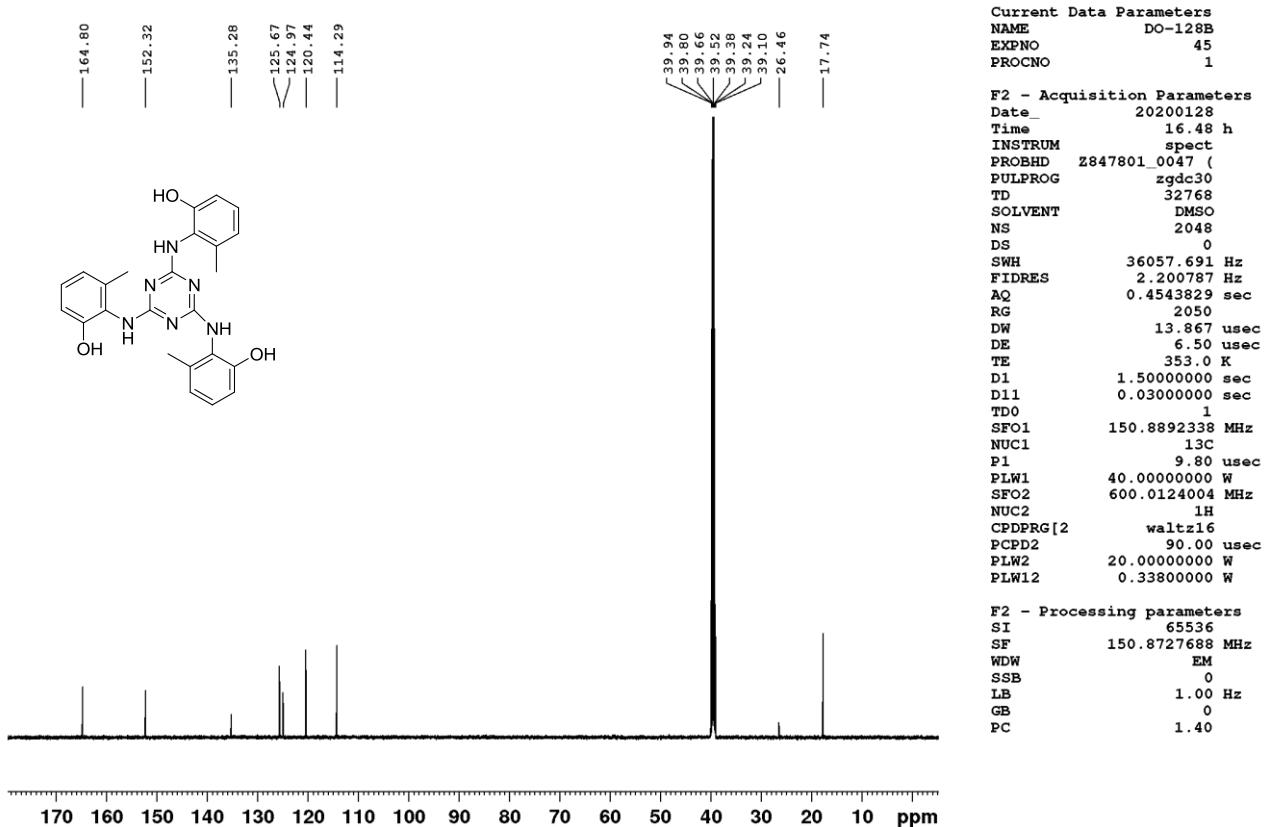
¹H NMR (600 MHz, DMSO-d₆, 293 K):



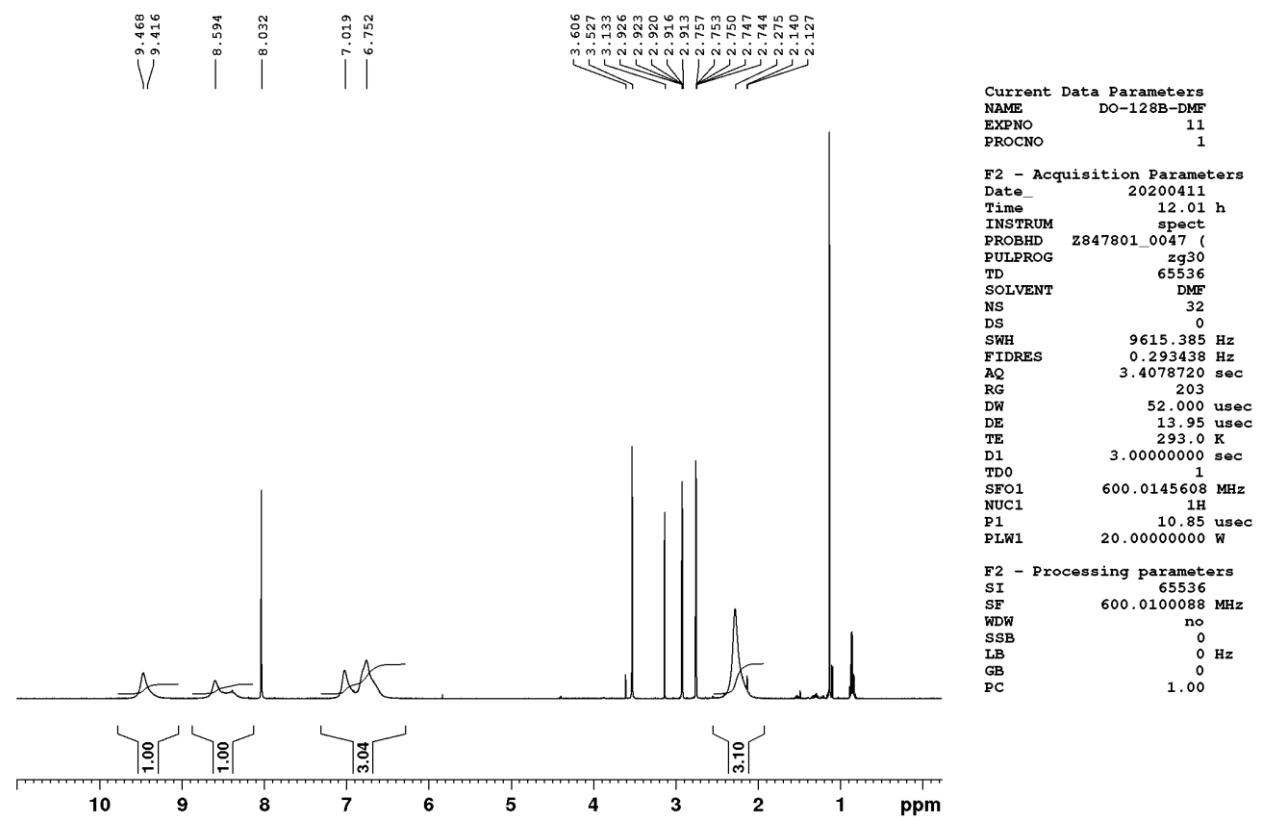
¹H NMR (600 MHz, DMSO-d₆, 353 K):



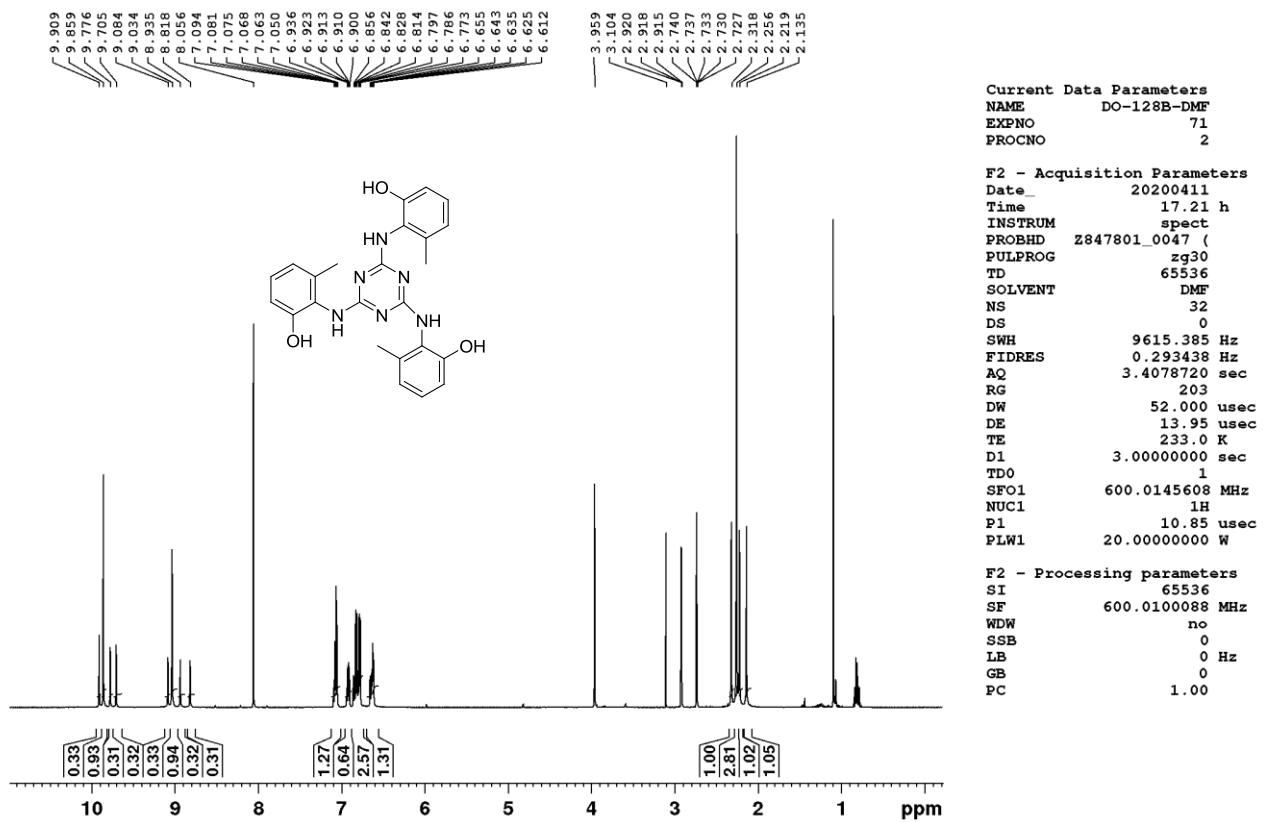
¹³C NMR (150.9 MHz, DMSO-d6, 353 K):



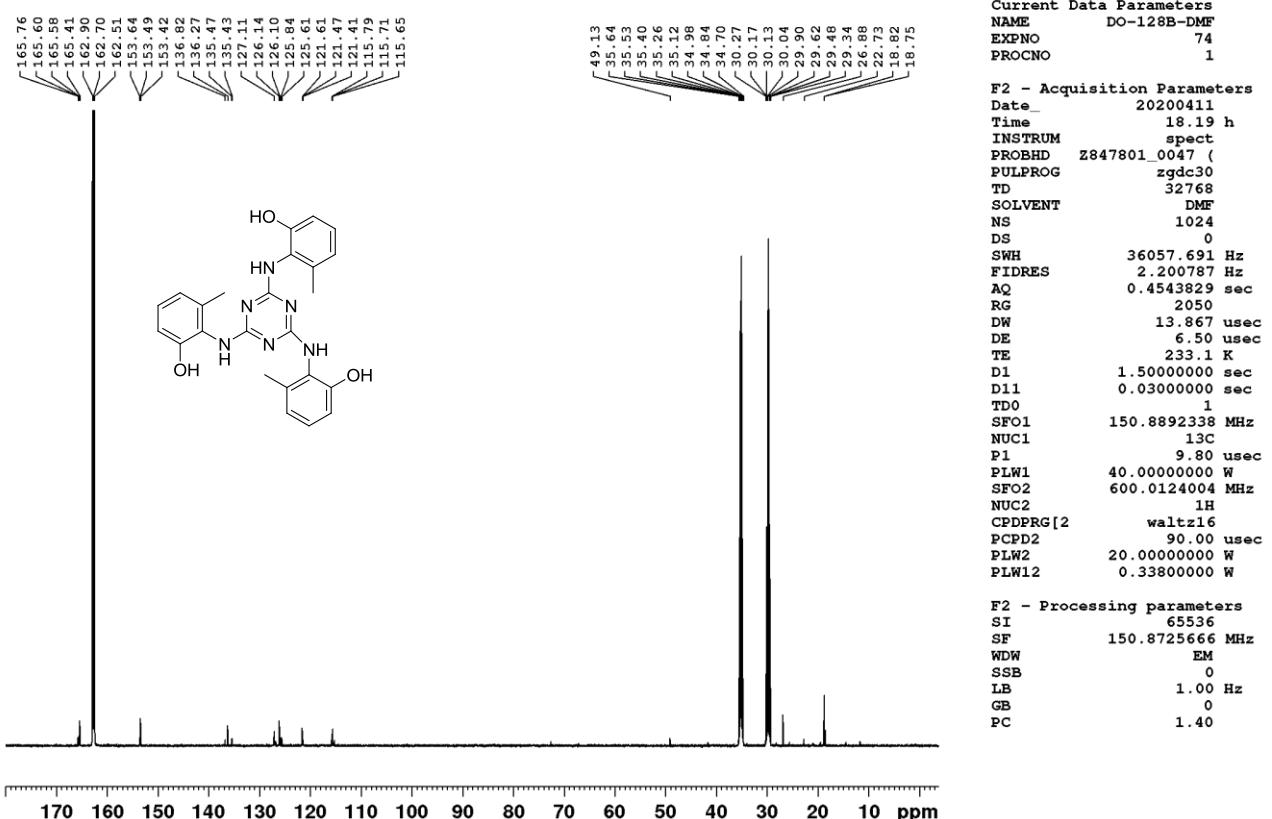
¹H NMR (600 MHz, DMF-d7, 293 K):



¹H NMR (600 MHz, DMF-d7, 233 K):



¹³C NMR (150.9 MHz, DMF-d7, 233 K):



Dynamic NMR spectra

Compound 4

¹H and ¹³C spectra were recorded on a Bruker II+ 600 spectrometer (BBO probe) at 600.13 for ¹H NMR and 150.92 MHz for ¹³C NMR with TMS as internal standard for chemical shifts (δ , ppm). The spectra were recorded in steps of 10 K between 273 and 323 K (0.05M in 600 μ L DMF-d7). Temperature calibration was done with B-VT 3000 unit (it was checked and calibrated with methanol and ethylene glycol reference samples). ¹H NMR spectra were acquired using a spectral width of 10 kHz, an acquisition time of 3.4 s and 32 scans, zero-filled to 64k datapoints (0.15 Hz per point) and processed without apodization.

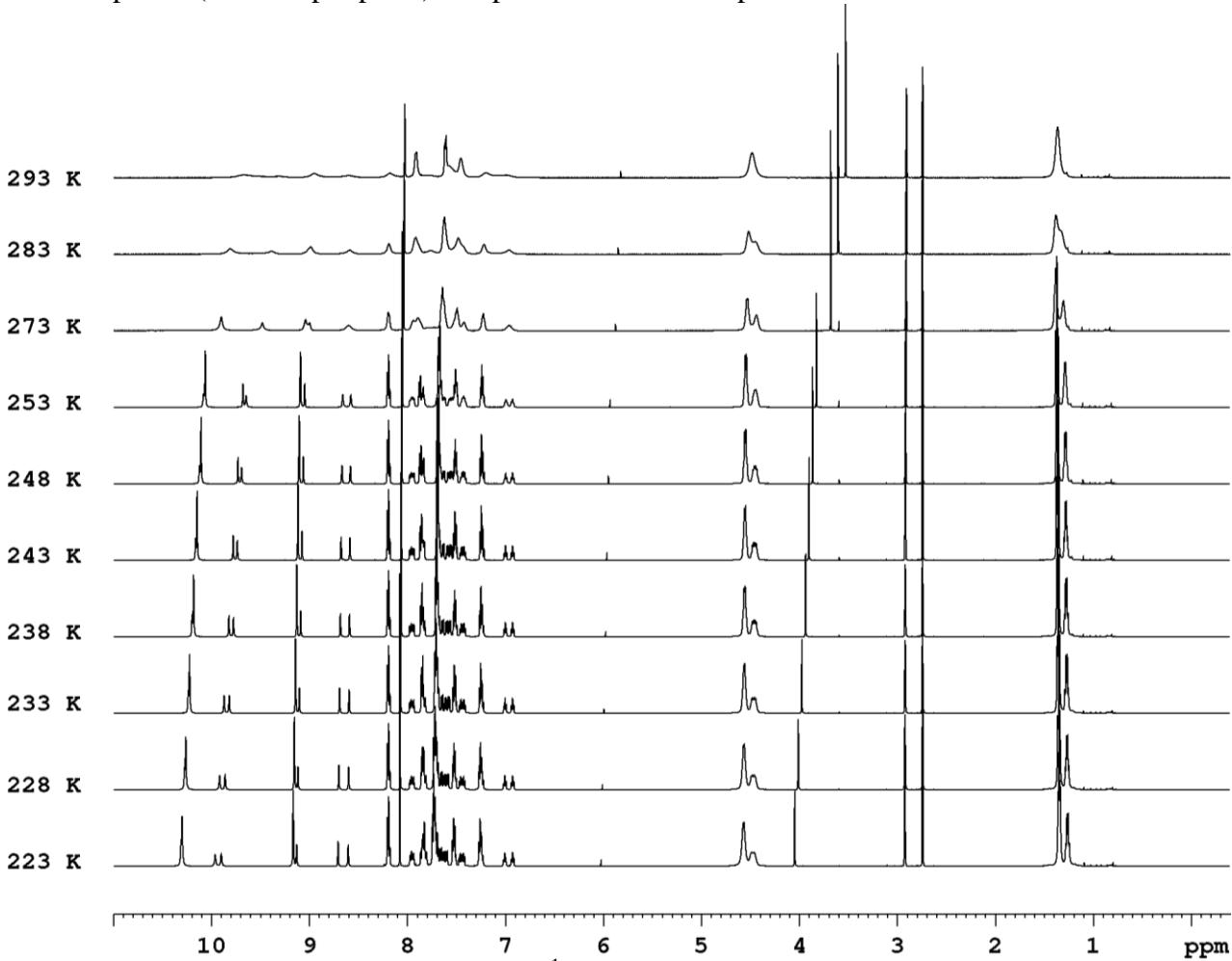


Figure S1. Temperature-dependent ¹H NMR spectra of compound 4 in DMF-d7.

¹H ROESY spectra (roesyph.2) were recorded on a BBO probe in steps of 5 K between 223 and 253 K. The spectra were acquired using a spectral width of 3.0 kHz, 2048 x 256 complex time domain datapoints, mixing times in the range of 0.03 to 0.1 s and 8 scans in about 75 min. The spectra were zero-filled to 4096 x 4096 datapoints and processed with a shifted square sine bell apodization in both dimensions. Populations and exchange rates were obtained from diagonal- and crosspeak integrals using EXSYCalc (MestreLab Research S.L.).

In the ¹H ROESY spectra of **4** the intensity of following peaks were calculated by volume integration in order to obtain the rate constants of *asym* to *sym* exchange:

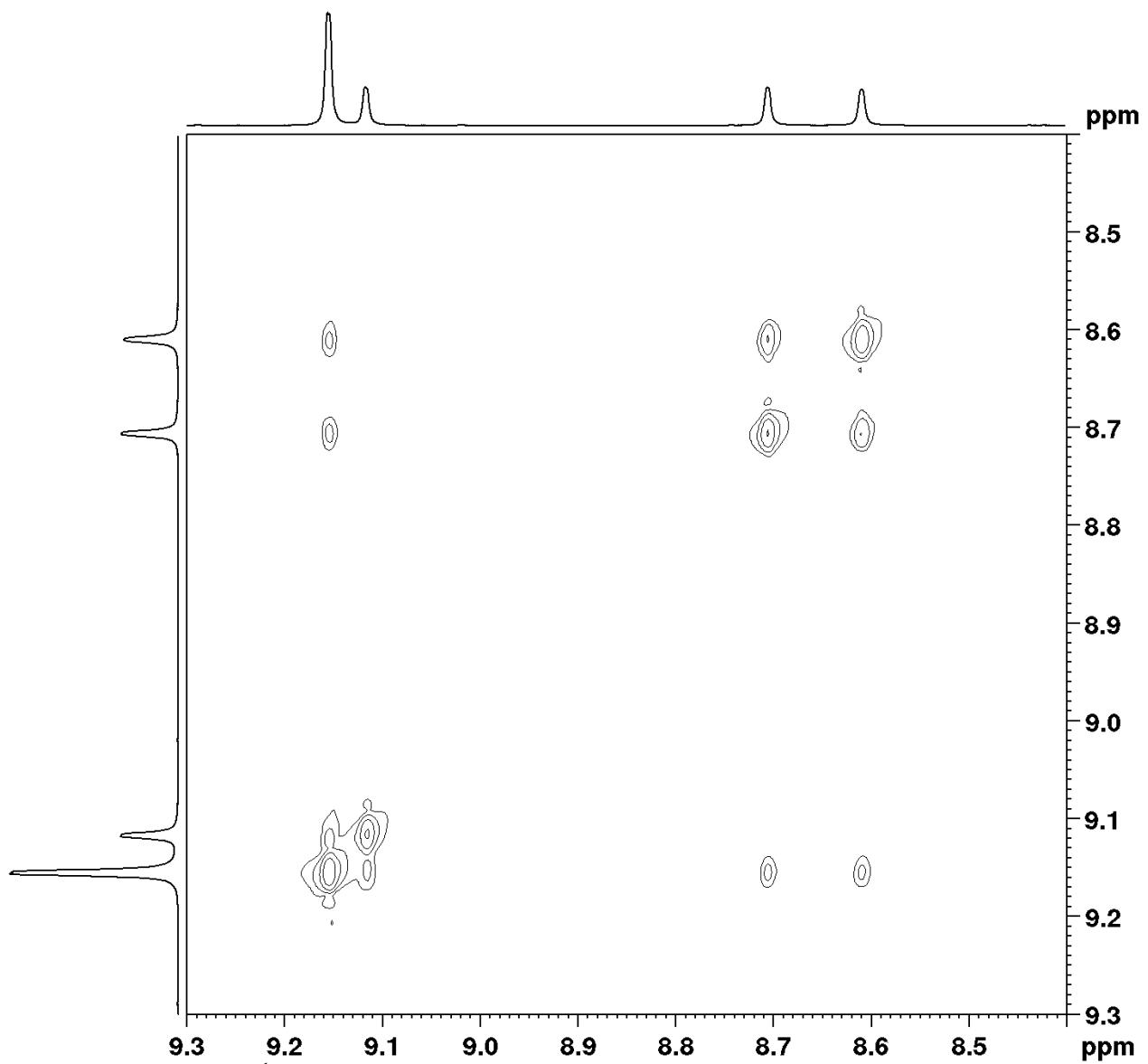


Figure S2. ^1H ROESY spectrum of compound **4** in DMF-d7 at 233K using mixing time of 0.3 s (region of carbazol-H-4 protons).

In the ^1H ROESY spectra of **4** the intensity of following peaks were calculated by volume integration:

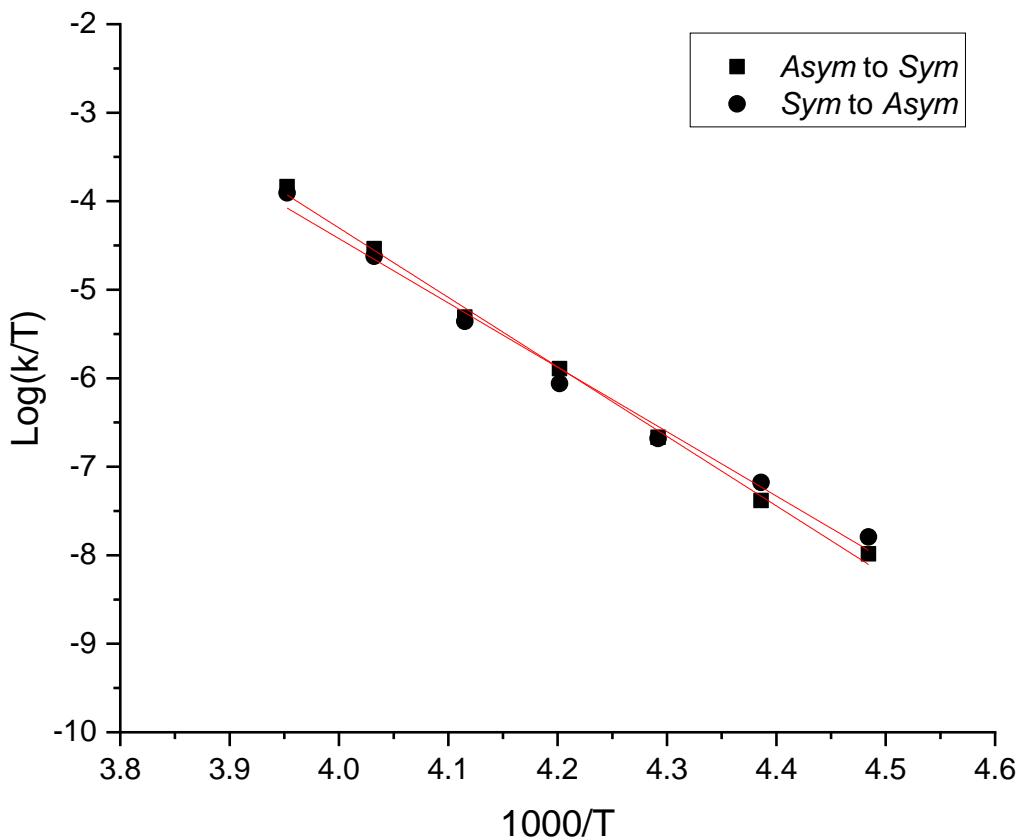
	<i>Sym</i>	<i>Asym</i>	<i>Asym</i>	<i>Asym</i>
<i>Sym</i>	I ₁₁	I ₁₂	I ₁₃	I ₁₄
<i>Asym</i>	I ₂₁	I ₂₂	I ₂₃	I ₂₄
<i>Asym</i>	I ₃₁	I ₃₂	I ₃₃	I ₃₄
<i>Asym</i>	I ₄₁	I ₄₂	I ₄₃	I ₄₄

It can be transformed into:

	<i>Sym</i>	<i>Asym</i>	
<i>Sym</i>	I ₁₁	I ₁₂ + I ₁₃ + I ₁₄	
<i>Asym</i>	I ₂₁ + I ₃₁ + I ₄₁	I ₂₂ + I ₂₃ + I ₂₄ + I ₃₂ + I ₃₃ + I ₃₄ + I ₄₂ + I ₄₃ + I ₄₄	

Table S1. Rate constants of compound **4** calculated from 2D integrals

T, K	Asym to Sym	Sym to Asym
223	0.076	0.092
228	0.142	0.174
233	0.296	0.292
238	0.657	0.555
243	1.202	1.145
248	2.659	2.435
253	5.465	5.086

**Figure S3.** Eyring plot of rate constants of compound **4**

Errors analysis: Usually the presented errors in activation parameters are the statistical errors based on scattering of the data points around the Eyring straight line only. The errors in this analysis are due to inaccuracies in both the calculated rate constants, k , and the measured temperatures, T and are computed according to the error propagation equations of Binsch [1] and Heinzer and Oth [2]. The absolute error in temperature is assumed to be not more than ± 0.5 K. The relative errors in k are estimated to be not more than $\pm 10\%$ at all temperatures according the precision of the volume integration of peaks. The errors analysis was performed using self-made computer program using the cited equations.

Table S2. Experimental thermodynamic parameters of exchange processes in compound **4** in DMF-d7

Exchange	$\Delta H^\neq(298K)$	$\Delta S^\neq(298K)$	$\Delta G^\neq(298K)$	R^2
<i>Asym to Sym</i>	15.6 ± 0.7	6.6 ± 3.1	13.6 ± 0.1	0.998
<i>Sym to Asym</i>	14.4 ± 0.8	1.8 ± 3.0	13.9 ± 0.1	0.995

ΔG^\neq and ΔH^\neq in kcal mol⁻¹ and ΔS^\neq in cal mol⁻¹ K⁻¹

Table S3. Experimental Thermodynamic parameters of compound **4** in DMF-d7

Conformer	$\Delta H^0(298K)$	$\Delta S^0(298K)$	$\Delta G^0(298K)$
<i>Asym</i>	0.00	0.00	0.00
<i>Sym</i>	0.9 ± 0.03	4.0 ± 0.1	-0.31 ± 0.0

$$\Delta H^0 = H^0(\text{Sym}) - H^0(\text{Asym})$$

$$\Delta S^0 = S^0(\text{Sym}) - S^0(\text{Asym})$$

$$\Delta G^0 = G^0(\text{Sym}) - G^0(\text{Asym})$$

ΔG^0 and ΔH^0 in kcal mol⁻¹ and ΔS^0 in cal mol⁻¹ K⁻¹

Compound 5

¹H and ¹³C spectra were recorded on a Bruker II+ 600 spectrometer (BBO probe) at 600.13 for ¹H NMR and 150.92 MHz for ¹³C NMR with TMS as internal standard for chemical shifts (δ , ppm). The spectra were recorded in steps of 10 K between 223 and 293 K (0.025M in 600 μ L DMF-d7). Temperature calibration was done with B-VT 3000 unit (it was checked and calibrated with methanol and ethylene glycol reference samples). ¹H NMR spectra were acquired using a spectral width of 10 kHz, an acquisition time of 3.4 s and 32 scans, zero-filled to 64k datapoints (0.15 Hz per point) and processed without apodization.

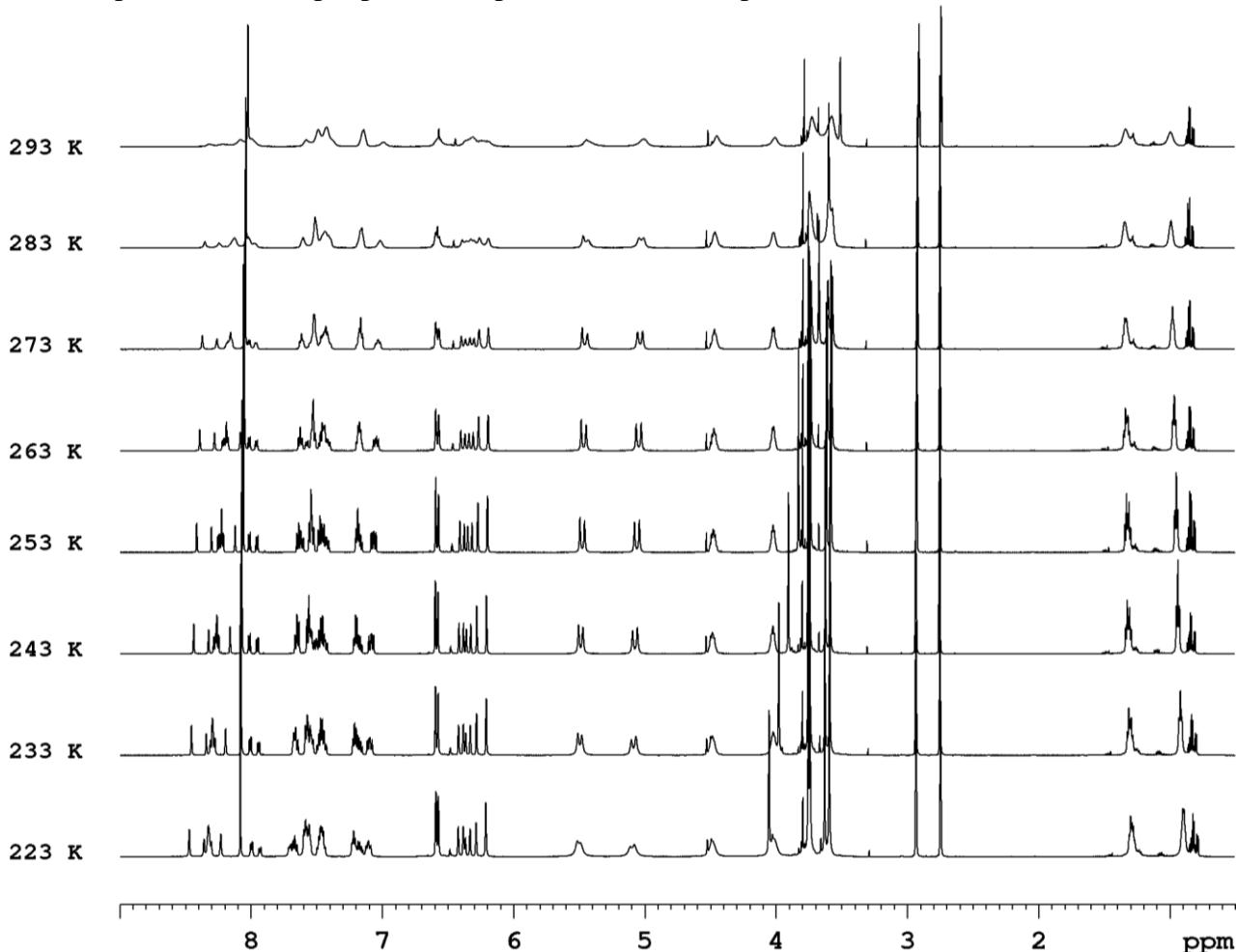


Figure S4. Temperature-dependent ¹H NMR spectra of compound 5 in DMF-d7.

¹H ROESY spectra (roesyph.2) were recorded on a BBO probe in steps of 5 K between 223 and 253 K. The spectra were acquired using a spectral width of 3.0 kHz, 2048 x 256 complex time domain datapoints, mixing times in the range of 0.03 to 0.1 s and 8 scans in about 75 min. The spectra were zero-filled to 4096 x 4096 datapoints and processed with a shifted square sine bell apodization in both dimensions. Populations and exchange rates were obtained from diagonal- and crosspeak integrals using EXSYCalc (MestreLab Research S.L.).

In the ¹H ROESY spectra of **5** the intensity of following peaks were calculated by volume integration in order to obtain the rate constants of *asym* to *sym* exchange:

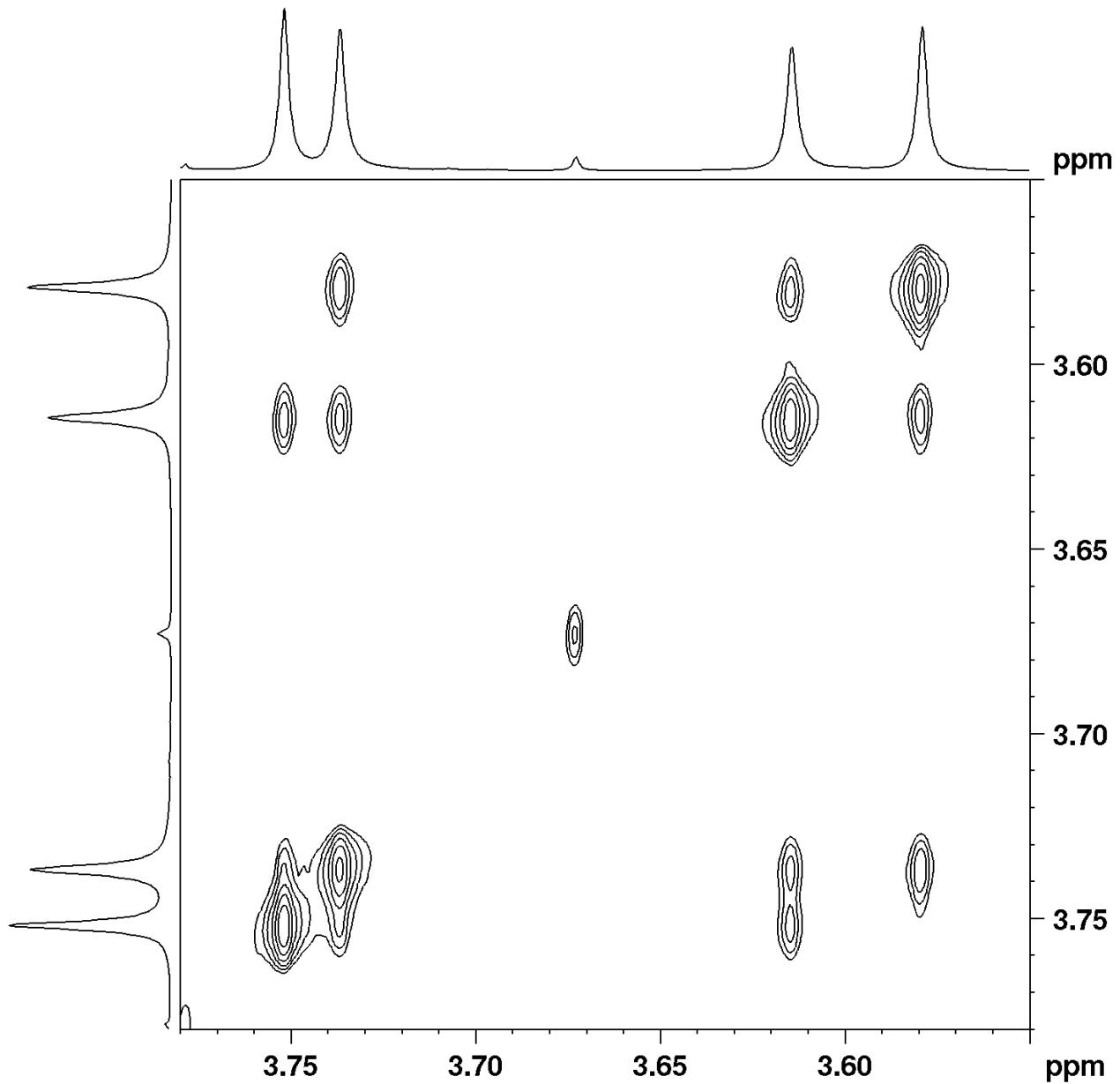


Figure S5. ^1H ROESY spectrum of compound **5** in DMF-d_7 at 253K using mixing time of 0.3 s (region of N-CH_3 protons).

In the ^1H ROESY spectra of **5** the intensity of following peaks were calculated by volume integration:

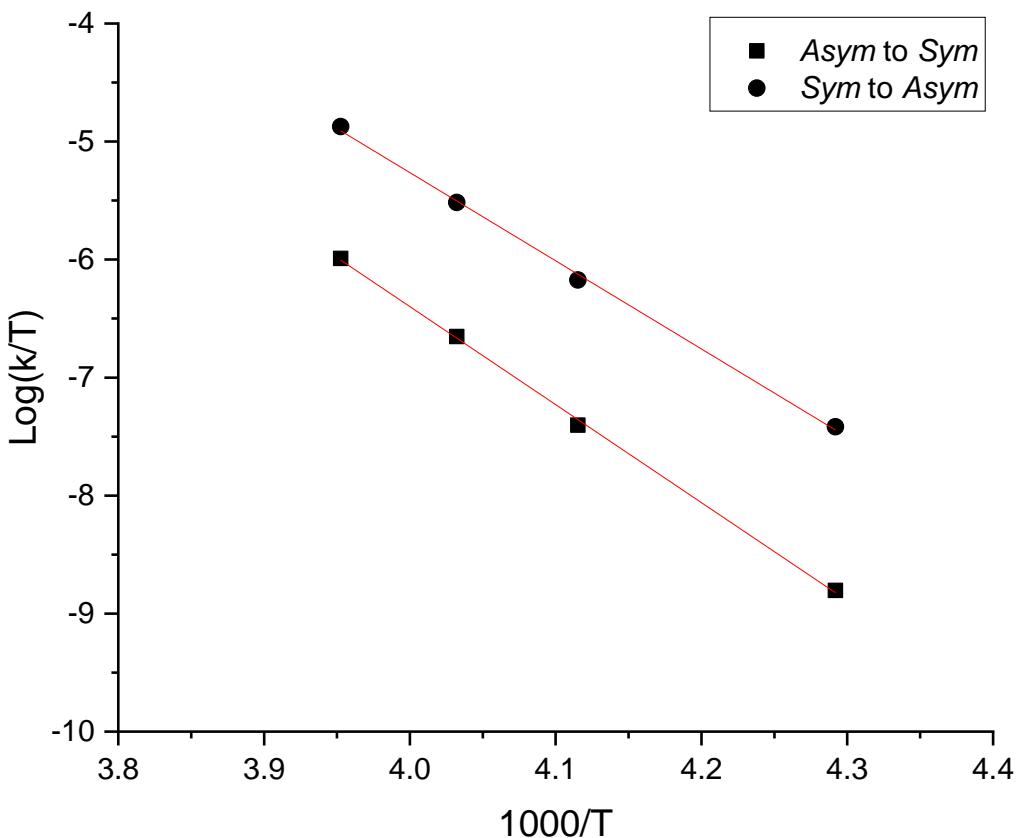
	Asym	Asym	Sym	Asym
Asym	I ₁₁	I ₁₂	I ₁₃	I ₁₄
Asym	I ₂₁	I ₂₂	I ₂₃	I ₂₄
Sym	I ₃₁	I ₃₂	I ₃₃	I ₃₄
Asym	I ₄₁	I ₄₂	I ₄₃	I ₄₄

It can be transformed into:

	Sym	Asym
Sym	I ₃₃	I ₃₁ + I ₃₂ + I ₃₄
Asym	I ₁₃ + I ₂₃ + I ₄₃	I ₁₁ + I ₁₂ + I ₁₄ + I ₂₁ + I ₂₂ + I ₂₄ + I ₄₁ + I ₄₂ + I ₄₄

Table S4. Rate constants of compound **5** calculated from 2D integrals

T, K	Asym to Sym	Sym to Asym
233	0.035	0.140
243	0.148	0.506
248	0.320	0.996
253	0.633	1.935

**Figure S6.** Eyring plot of rate constants of compound **5**

Errors analysis: Usually the presented errors in activation parameters are the statistical errors based on scattering of the data points around the Eyring straight line only. The errors in this analysis are due to inaccuracies in both the calculated rate constants, k , and the measured temperatures, T and are computed according to the error propagation equations of Binsch [1] and Heinzer and Oth [2]. The absolute error in temperature is assumed to be not more than ± 0.5 K. The relative errors in k are estimated to be not more than $\pm 10\%$ at all temperatures according the precision of the volume integration of peaks. The errors analysis was performed using self-made computer program using the cited equations.

Table S5. Experimental thermodynamic parameters of exchange processes in compound **5** in DMF-d7

Exchange	$\Delta H^\neq(298K)$	$\Delta S^\neq(298K)$	$\Delta G^\neq(298K)$	R^2
Asym to Sym	16.5 ± 1.0	6.1 ± 4.4	14.7 ± 0.1	0.9997
Sym to Asym	14.8 ± 1.0	1.7 ± 3.7	14.3 ± 0.1	0.9993

ΔG^\neq and ΔH^\neq in kcal mol⁻¹ and ΔS^\neq in cal mol⁻¹ K⁻¹

Table S6. Experimental Thermodynamic parameters of compound **5** in DMF-d7

Conformer	ΔH^0 (298K)	ΔS^0 (298K)	ΔG^0 (298K)
<i>Asym</i>	0.00	0.00	0.00
<i>Sym</i>	-1.5 ± 0.0	-3.7 ± 0.1	-0.41 ± 0.0

$$\Delta H^0 = H^0(\text{Sym}) - H^0(\text{Asym})$$

$$\Delta S^0 = S^0(\text{Sym}) - S^0(\text{Asym})$$

$$\Delta G^0 = G^0(\text{Sym}) - G^0(\text{Asym})$$

ΔG^0 and ΔH^0 in kcal mol⁻¹ and ΔS^0 in cal mol⁻¹ K⁻¹

Compound 6

¹H and ¹³C spectra were recorded on a Bruker II+ 600 spectrometer (BBO probe) at 600.13 for ¹H NMR and 150.92 MHz for ¹³C NMR with TMS as internal standard for chemical shifts (δ , ppm). The spectra were recorded in steps of 10 K between 223 and 293 K (0.05M in 600 μ L DMF-d7). Temperature calibration was done with B-VT 3000 unit (it was checked and calibrated with methanol and ethylene glycol reference samples). ¹H NMR spectra were acquired using a spectral width of 10 kHz, an acquisition time of 3.4 s and 32 scans, zero-filled to 64k datapoints (0.15 Hz per point) and processed without apodization.

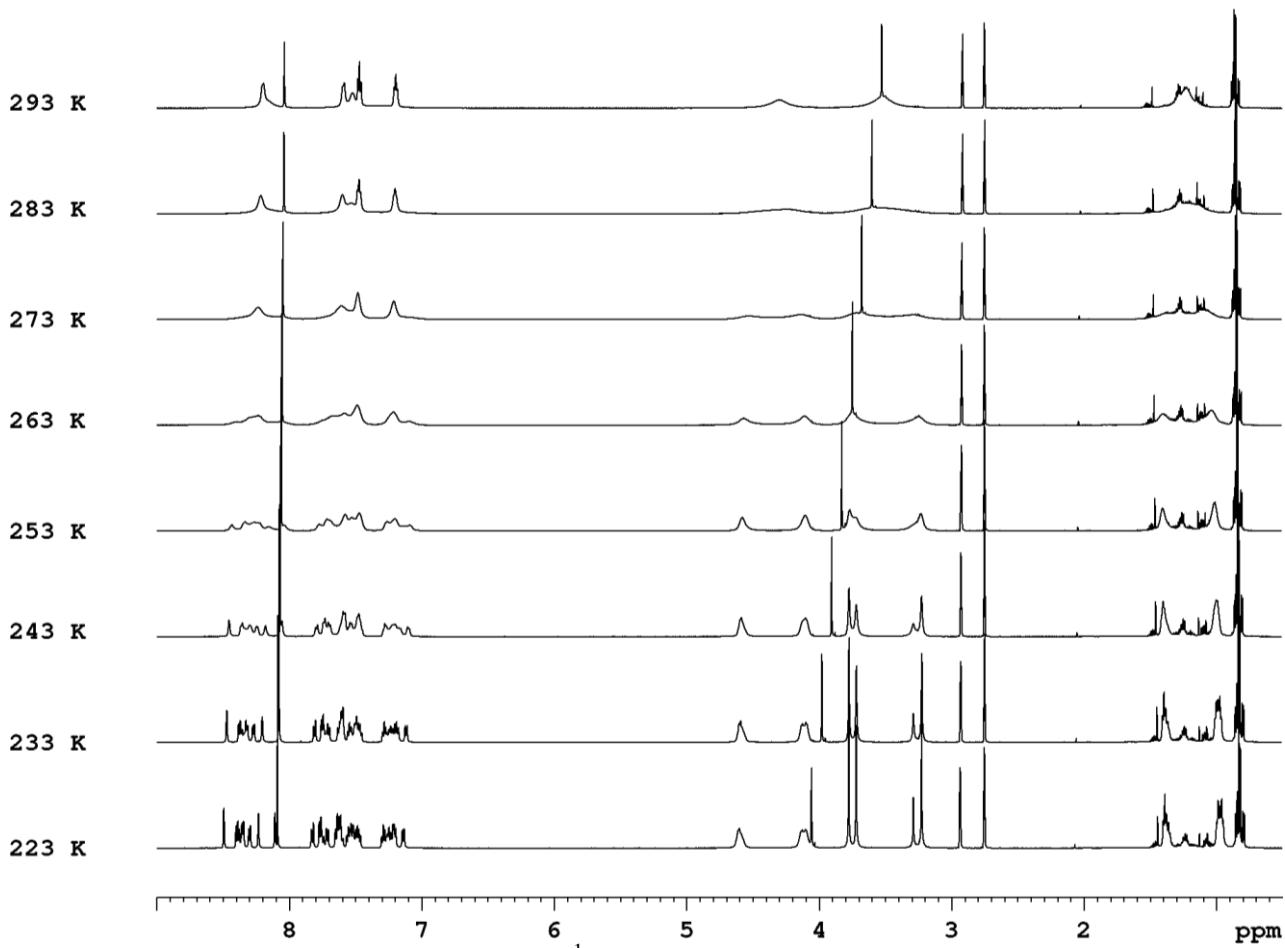


Figure S7. Temperature-dependent ¹H NMR spectra of compound **6** in DMF-d7.

¹H ROESY spectra (roesyph.2) were recorded on a BBO probe in steps of 5 K between 223 and 243 K. The spectra were acquired using a spectral width of 3.0 kHz, 2048 x 256 complex time domain datapoints, mixing times in the range of 0.03 to 0.1 s and 8 scans in about 75 min. The spectra were zero-filled to 4096 x 4096 datapoints and processed with a shifted square sine bell apodization in both dimensions. Populations and exchange rates were obtained from diagonal- and crosspeak integrals using EXSYCalc (MestreLab Research S.L.).

In the ¹H ROESY spectra of **6** the intensity of following peaks were calculated by volume integration in order to obtain the rate constants of *asym* to *sym* exchange:

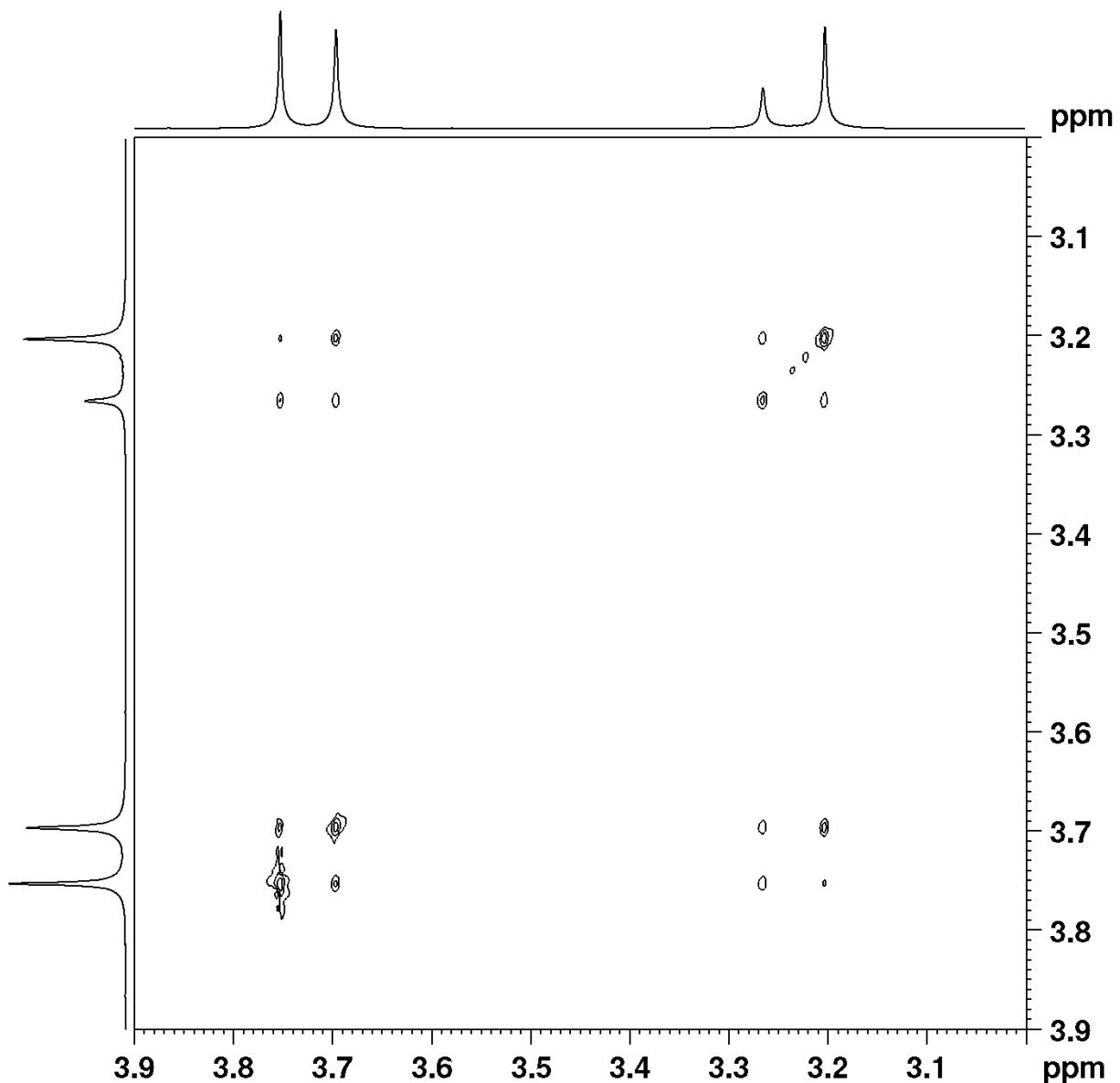


Figure S8. ^1H ROESY spectrum of compound **6** in DMF-d_7 at 223K using mixing time of 0.3 s (region of OCH_3 protons).

In the ^1H ROESY spectra of **6** the intensity of following peaks were calculated by volume integration:

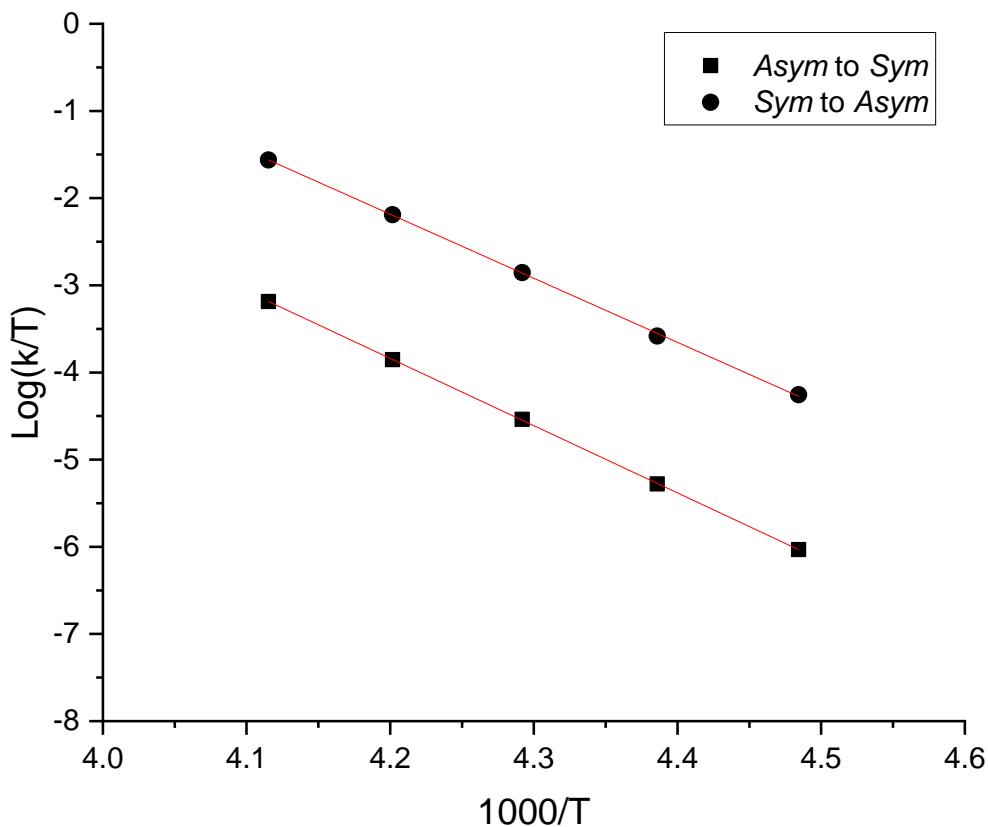
	Asym	Asym	Sym	Asym
Asym	I ₁₁	I ₁₂	I ₁₃	I ₁₄
Asym	I ₂₁	I ₂₂	I ₂₃	I ₂₄
Sym	I ₃₁	I ₃₂	I ₃₃	I ₃₄
Asym	I ₄₁	I ₄₂	I ₄₃	I ₄₄

It can be transformed into:

	Sym	Asym
Sym	I ₃₃	I ₃₁ + I ₃₂ + I ₃₄
Asym	I ₁₃ + I ₂₃ + I ₄₃	I ₁₁ + I ₁₂ + I ₁₄ + I ₂₁ + I ₂₂ + I ₂₄ + I ₄₁ + I ₄₂ + I ₄₄

Table S7. Rate constants of compound **6** calculated from 2D integrals

T, K	Asym to Sym	Sym to Asym
223	0.535	3.160
228	1.161	6.345
233	2.493	13.429
238	5.049	26.646
243	10.029	50.966

**Figure S9.** Eyring plot of rate constants of compound **6**

Errors analysis: Usually the presented errors in activation parameters are the statistical errors based on scattering of the data points around the Eyring straight line only. The errors in this analysis are due to inaccuracies in both the calculated rate constants, k , and the measured temperatures, T and are computed according to the error propagation equations of Binsch [1] and Heinzer and Oth [2]. The absolute error in temperature is assumed to be not more than ± 0.5 K. The relative errors in k are estimated to be not more than $\pm 10\%$ at all temperatures according the precision of the volume integration of peaks. The errors analysis was performed using self-made computer program using the cited equations.

Table S8. Experimental thermodynamic parameters of exchange processes in compound **6** in DMF-d7

Exchange	$\Delta H^\neq(298K)$	$\Delta S^\neq(298K)$	$\Delta G^\neq(298K)$	R^2
Asym to Sym	15.3 ± 1.0	9.6 ± 4.1	12.5 ± 0.1	0.999
Sym to Asym	14.6 ± 0.9	9.8 ± 4.2	11.7 ± 0.1	0.999

ΔG^\neq and ΔH^\neq in kcal mol⁻¹ and ΔS^\neq in cal mol⁻¹ K⁻¹

Table S9. Experimental Thermodynamic parameters of compound **6** in DMF-d7

Conformer	ΔH^0 (298K)	ΔS^0 (298K)	ΔG^0 (298K)
<i>Asym</i>	0.00	0.00	0.00
<i>Sym</i>	-0.6 ± 0.1	0.9 ± 0.4	-0.8 ± 0.0

$$\Delta H^0 = H^0(\text{Sym}) - H^0(\text{Asym})$$

$$\Delta S^0 = S^0(\text{Sym}) - S^0(\text{Asym})$$

$$\Delta G^0 = G^0(\text{Sym}) - G^0(\text{Asym})$$

ΔG^0 and ΔH^0 in kcal mol⁻¹ and ΔS^0 in cal mol⁻¹ K⁻¹

Compound 11

¹H and ¹³C spectra were recorded on a Bruker II+ 600 spectrometer (BBO probe) at 600.13 for ¹H NMR and 150.92 MHz for ¹³C NMR with TMS as internal standard for chemical shifts (δ , ppm). The spectra were recorded in steps of 10 K between 223 and 293 K (0.05M in 600 μ L DMF-d7). Temperature calibration was done with B-VT 3000 unit (it was checked and calibrated with methanol and ethylene glycol reference samples). ¹H NMR spectra were acquired using a spectral width of 10 kHz, an acquisition time of 3.4 s and 32 scans, zero-filled to 64k datapoints (0.15 Hz per point) and processed without apodization.

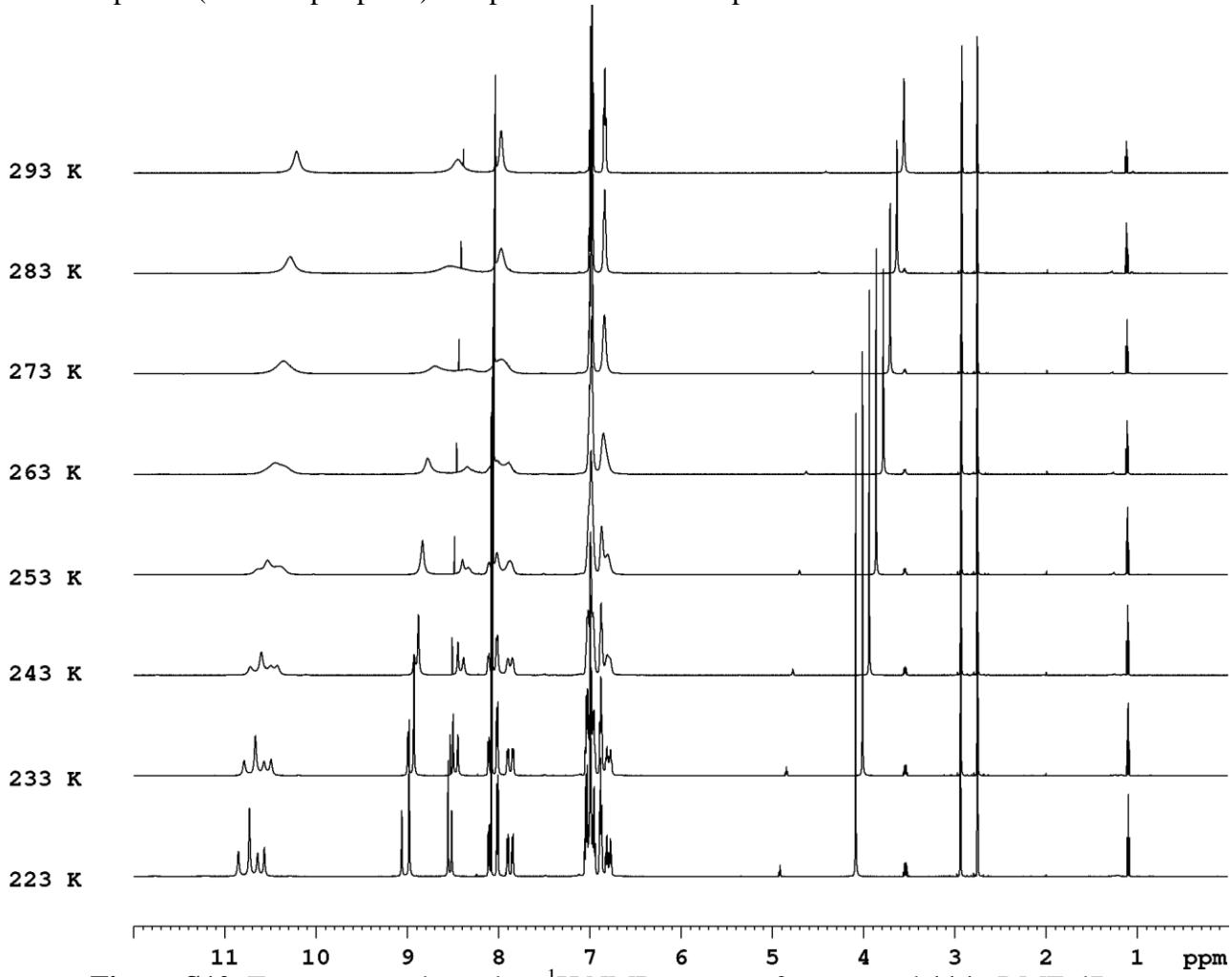


Figure S10. Temperature-dependent ¹H NMR spectra of compound 11 in DMF-d7.

¹H ROESY spectra (roesyph.2) were recorded on a BBO probe in steps of 5 K between 228 and 238 K. The spectra were acquired using a spectral width of 3.0 kHz, 2048 x 256 complex time domain datapoints, mixing times in the range of 0.05 to 0.3 s and 8 scans in about 75 min. The spectra were zero-filled to 4096 x 4096 datapoints and processed with a shifted square sine bell apodization in both dimensions. Populations and exchange rates were obtained from diagonal- and crosspeak integrals using EXSYCalc (MestreLab Research S.L.).

In the ¹H ROESY spectra of **11** the intensity of following peaks were calculated by volume integration in order to obtain the rate constants of *asym* to *sym* exchange:

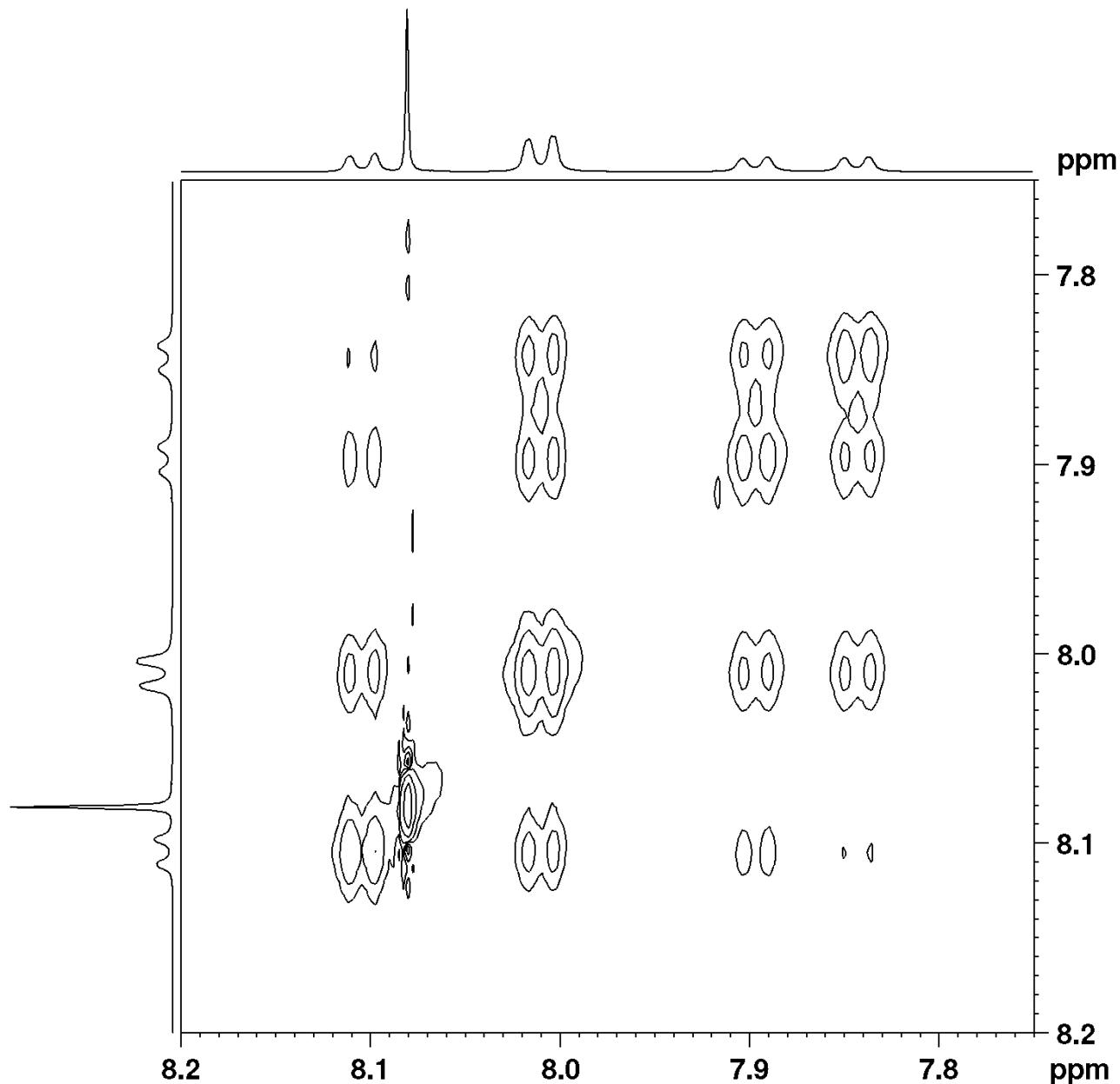


Figure S11. ^1H ROESY spectrum of compound **11** in DMF-d_7 at 223K using mixing time of 0.3 s (region of Ar-H-3 protons).

In the ^1H ROESY spectra of **11** the intensity of following peaks were calculated by volume integration:

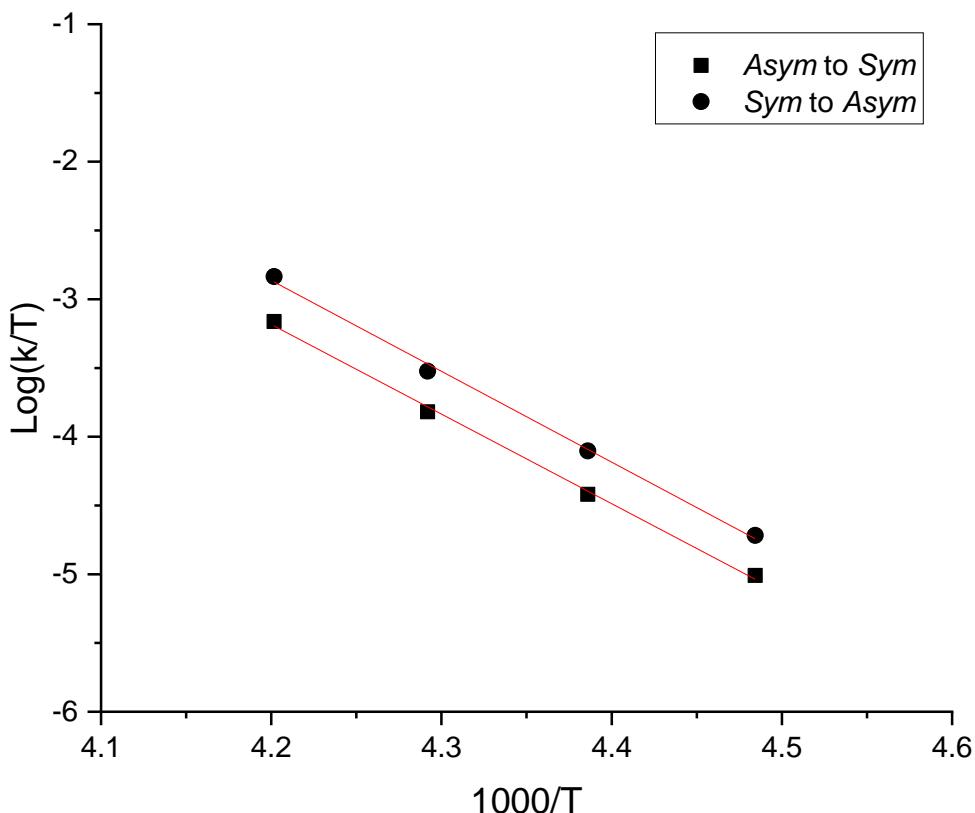
	<i>Asym</i>	<i>Sym</i>	<i>Asym</i>	<i>Asym</i>
<i>Asym</i>	I_{11}	I_{12}	I_{13}	I_{14}
<i>Sym</i>	I_{21}	I_{22}	I_{23}	I_{24}
<i>Asym</i>	I_{31}	I_{32}	I_{33}	I_{34}
<i>Asym</i>	I_{41}	I_{42}	I_{43}	I_{44}

It can be transformed into:

	<i>Sym</i>	<i>Asym</i>
<i>Sym</i>	I_{22}	$I_{21} + I_{23} + I_{24}$
<i>Asym</i>	$I_{12} + I_{32} + I_{42}$	$I_{11} + I_{13} + I_{14} + I_{31} + I_{33} + I_{34} + I_{41} + I_{43} + I_{44}$

Table S10. Rate constants of compound **11** calculated from 2D integrals

T, K	Asym to Sym	Sym to Asym
223	1.488	1.992
228	2.747	3.768
233	5.116	6.875
238	10.077	13.974

**Figure S12.** Eyring plot of rate constants of compound **11**

Errors analysis: Usually the presented errors in activation parameters are the statistical errors based on scattering of the data points around the Eyring straight line only. The errors in this analysis are due to inaccuracies in both the calculated rate constants, k , and the measured temperatures, T and are computed according to the error propagation equations of Binsch [1] and Heinzer and Oth [2]. The absolute error in temperature is assumed to be not more than ± 0.5 K. The relative errors in k are estimated to be not more than $\pm 10\%$ at all temperatures according the precision of the volume integration of peaks. The errors analysis was performed using self-made computer program using the cited equations.

Table S11. Experimental thermodynamic parameters of exchange processes in compound **11** in DMF-d7

Exchange	$\Delta H^\neq(298K)$	$\Delta S^\neq(298K)$	$\Delta G^\neq(298K)$	R^2
Asym to Sym	12.9 ± 1.2	0.8 ± 4.2	12.7 ± 0.1	0.999
Sym to Asym	13.1 ± 1.2	2.2 ± 4.4	12.4 ± 0.1	0.999

ΔG^\neq and ΔH^\neq in kcal mol⁻¹ and ΔS^\neq in cal mol⁻¹ K⁻¹

Table S12. Experimental Thermodynamic parameters of compound **11** in DMF-d7

Conformer	ΔH^0 (298K)	ΔS^0 (298K)	ΔG^0 (298K)
<i>Asym</i>	0.00	0.00	0.00
<i>Sym</i>	0.3 ± 0.1	1.8 ± 0.4	-0.3 ± 0.0

$$\Delta H^0 = H^0(\text{Sym}) - H^0(\text{Asym})$$

$$\Delta S^0 = S^0(\text{Sym}) - S^0(\text{Asym})$$

$$\Delta G^0 = G^0(\text{Sym}) - G^0(\text{Asym})$$

ΔG^0 and ΔH^0 in kcal mol⁻¹ and ΔS^0 in cal mol⁻¹ K⁻¹

Compound 12

¹H and ¹³C spectra were recorded on a Bruker II+ 600 spectrometer (BBO probe) at 600.13 for ¹H NMR and 150.92 MHz for ¹³C NMR with TMS as internal standard for chemical shifts (δ , ppm). The spectra were recorded in steps of 10 K between 233 and 293 K (0.05M in 600 μ L DMF-d7). Temperature calibration was done with B-VT 3000 unit (it was checked and calibrated with methanol and ethylene glycol reference samples). ¹H NMR spectra were acquired using a spectral width of 10 kHz, an acquisition time of 3.4 s and 32 scans, zero-filled to 64k datapoints (0.15 Hz per point) and processed without apodization.

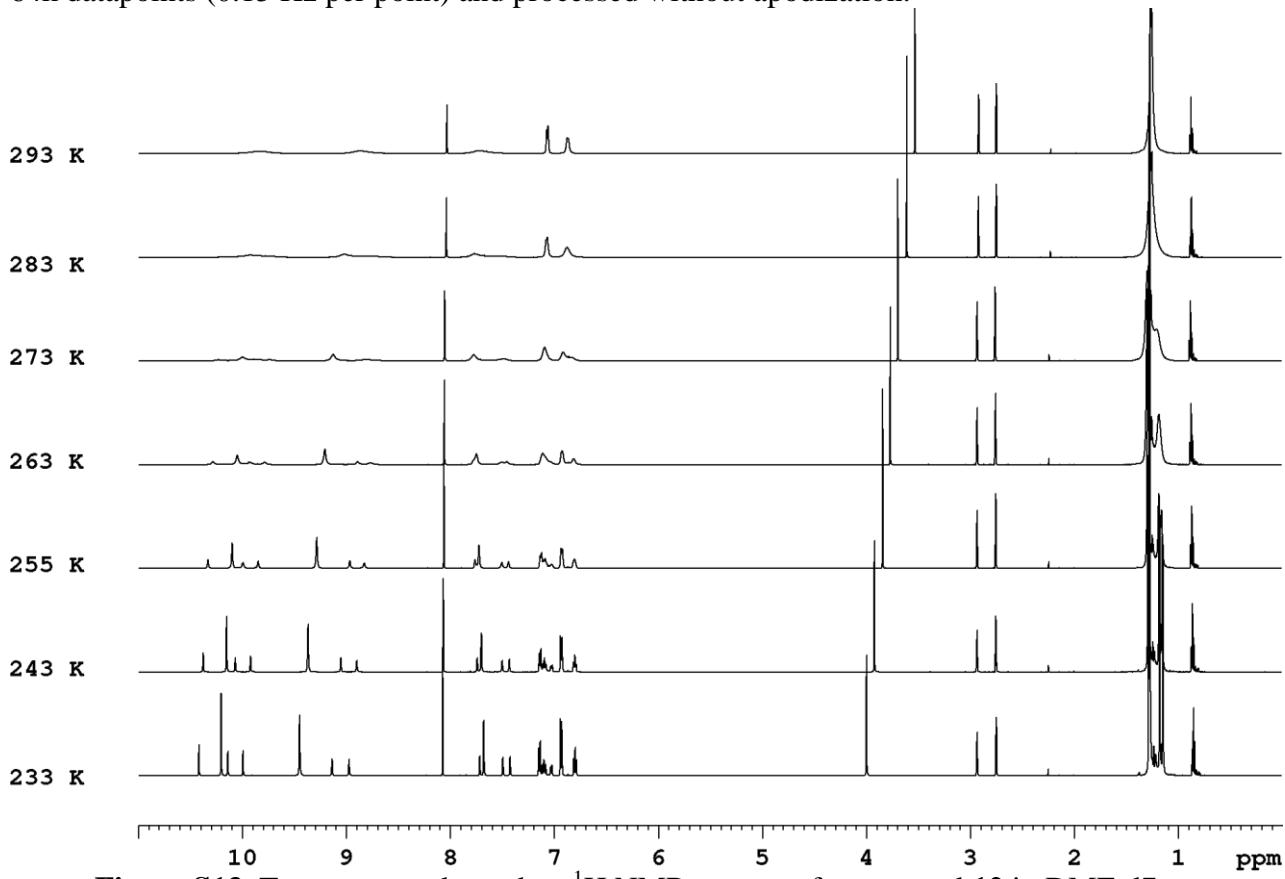


Figure S13. Temperature-dependent ¹H NMR spectra of compound **12** in DMF-d7.

¹H ROESY spectra (roesyph.2) were recorded on a BBO probe in steps of 5 K between 233 and 258 K. The spectra were acquired using a spectral width of 3.0 kHz, 2048 x 256 complex time domain datapoints, mixing times in the range of 0.01 to 0.3 s and 8 scans in about 75 min. The spectra were zero-filled to 4096 x 4096 datapoints and processed with a shifted square sine bell apodization in both dimensions. Populations and exchange rates were obtained from diagonal- and crosspeak integrals using EXSYCalc (MestreLab Research S.L.).

In the ¹H ROESY spectra of **12** the intensity of following peaks were calculated by volume integration in order to obtain the rate constants of *asym* to *sym* exchange:

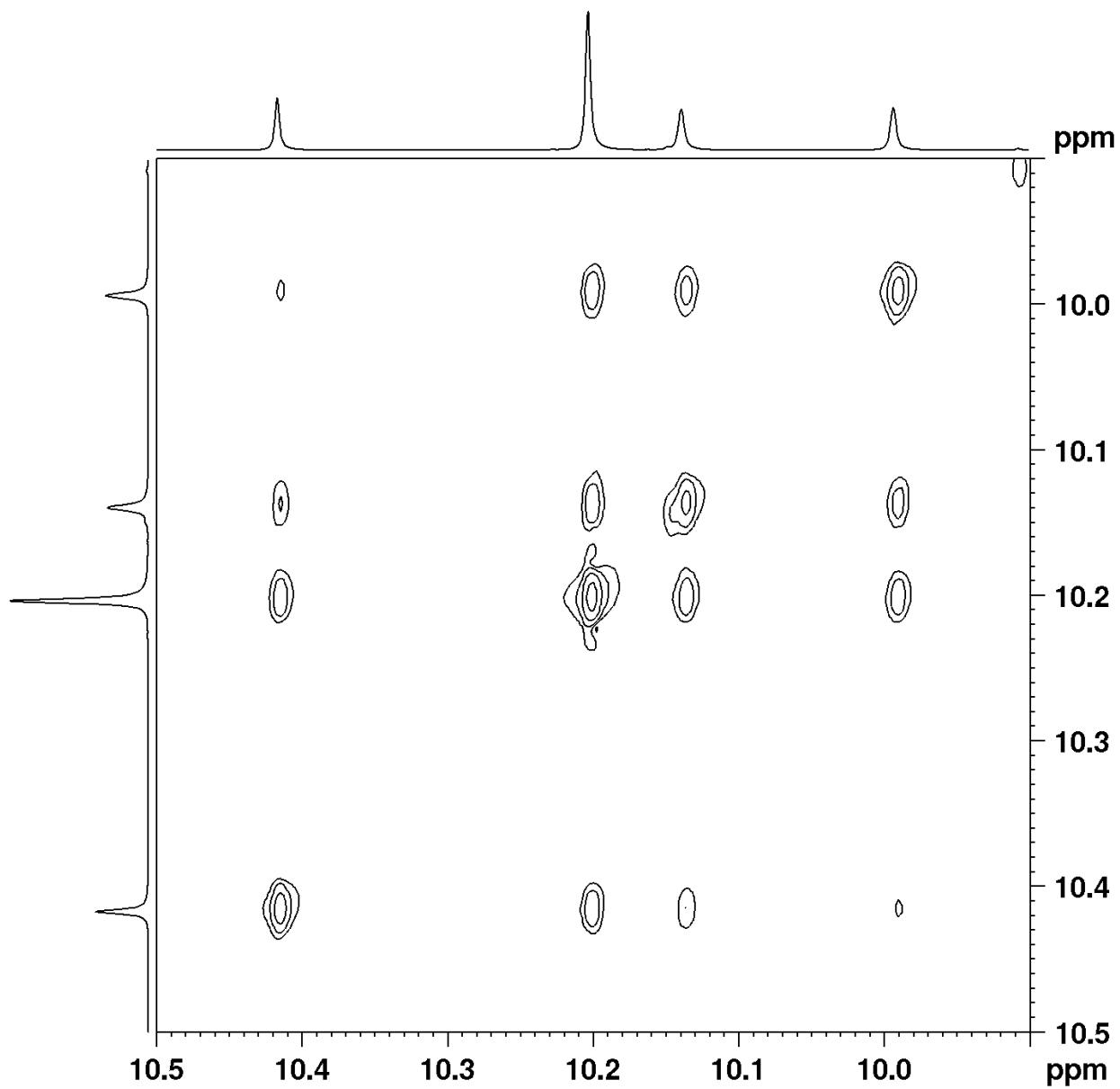


Figure S14. ^1H ROESY spectrum of compound **12** in DMF-d7 at 233K using mixing time of 0.3 s (region of Ar-H-6 protons).

In the ^1H ROESY spectra of **12** the intensity of following peaks were calculated by volume integration:

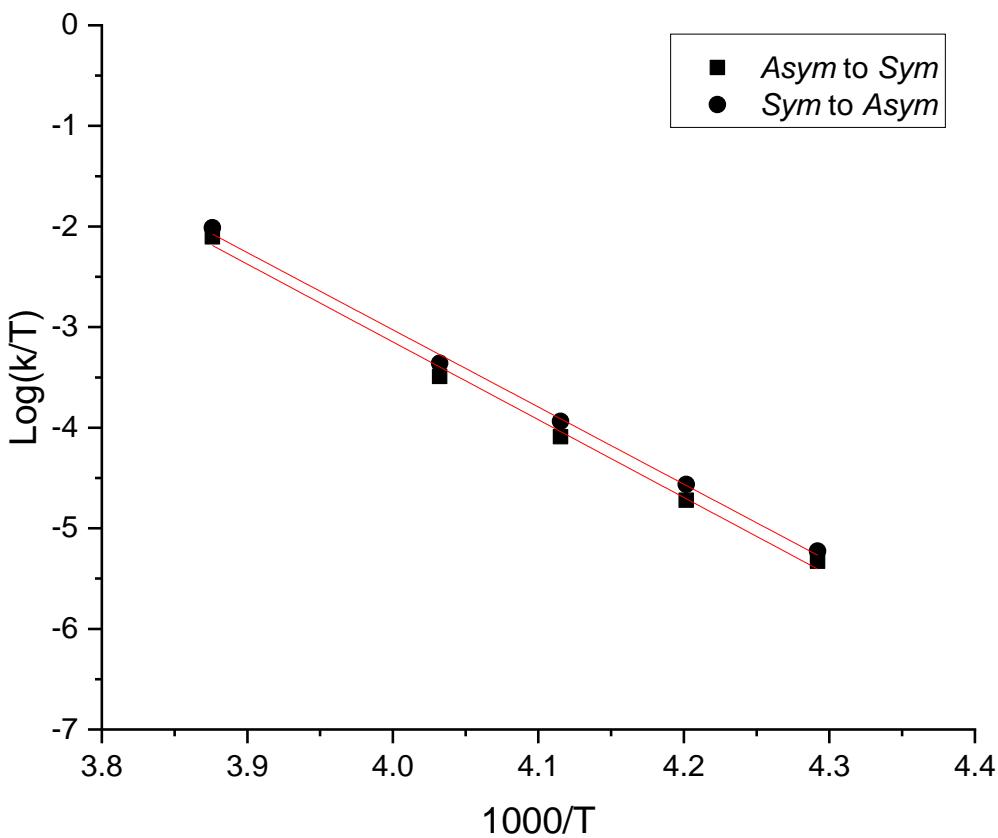
	Asym	Sym	Asym	Asym
Asym	I ₁₁	I ₁₂	I ₁₃	I ₁₄
Sym	I ₂₁	I ₂₂	I ₂₃	I ₂₄
Asym	I ₃₁	I ₃₂	I ₃₃	I ₃₄
Asym	I ₄₁	I ₄₂	I ₄₃	I ₄₄

It can be transformed into:

	Sym	Asym
Sym	I ₂₂	I ₂₁ + I ₂₃ + I ₂₄
Asym	I ₁₂ + I ₃₂ + I ₄₂	I ₁₁ + I ₁₃ + I ₁₄ + I ₃₁ + I ₃₃ + I ₃₄ + I ₄₁ + I ₄₃ + I ₄₄

Table S13. Rate constants of compound **12** calculated from 2D integrals

T, K	Asym to Sym	Sym to Asym
233	1.131	1.251
238	2.118	2.479
243	4.071	4.736
248	7.558	8.621
258	31.445	34.470

**Figure S15.** Eyring plot of rate constants of compound **12**

Errors analysis: Usually the presented errors in activation parameters are the statistical errors based on scattering of the data points around the Eyring straight line only. The errors in this analysis are due to inaccuracies in both the calculated rate constants, k , and the measured temperatures, T and are computed according to the error propagation equations of Binsch [1] and Heinzer and Oth [2]. The absolute error in temperature is assumed to be not more than ± 0.5 K. The relative errors in k are estimated to be not more than $\pm 10\%$ at all temperatures according the precision of the volume integration of peaks. The errors analysis was performed using self-made computer program using the cited equations.

Table S14. Experimental thermodynamic parameters of exchange processes in compound **12** in DMF-d7

Exchange	$\Delta H^\neq(298K)$	$\Delta S^\neq(298K)$	$\Delta G^\neq(298K)$	R^2
Asym to Sym	15.3 ± 0.9	7.6 ± 3.6	13.0 ± 0.1	0.998
Sym to Asym	14.9 ± 0.8	6.4 ± 3.2	13.0 ± 0.1	0.999

ΔG^\neq and ΔH^\neq in kcal mol⁻¹ and ΔS^\neq in cal mol⁻¹ K⁻¹

Table S15. Experimental Thermodynamic parameters of compound **12** in DMF-d7

Conformer	ΔH^0 (298K)	ΔS^0 (298K)	ΔG^0 (298K)
<i>Asym</i>	0.00	0.00	0.00
<i>Sym</i>	0.3 ± 0.03	1.5 ± 0.2	-0.2 ± 0.0

$$\Delta H^0 = H^0(\text{Sym}) - H^0(\text{Asym})$$

$$\Delta S^0 = S^0(\text{Sym}) - S^0(\text{Asym})$$

$$\Delta G^0 = G^0(\text{Sym}) - G^0(\text{Asym})$$

ΔG^0 and ΔH^0 in kcal mol⁻¹ and ΔS^0 in cal mol⁻¹ K⁻¹

Compound 13

¹H and ¹³C spectra were recorded on a Bruker II+ 600 spectrometer (BBO probe) at 600.13 for ¹H NMR and 150.92 MHz for ¹³C NMR with TMS as internal standard for chemical shifts (δ , ppm). The spectra were recorded in steps of 10 K between 273 and 323 K (0.05M in 600 μ L DMF-d7). Temperature calibration was done with B-VT 3000 unit (it was checked and calibrated with methanol and ethylene glycol reference samples). ¹H NMR spectra were acquired using a spectral width of 10 kHz, an acquisition time of 3.4 s and 32 scans, zero-filled to 64k datapoints (0.15 Hz per point) and processed without apodization.

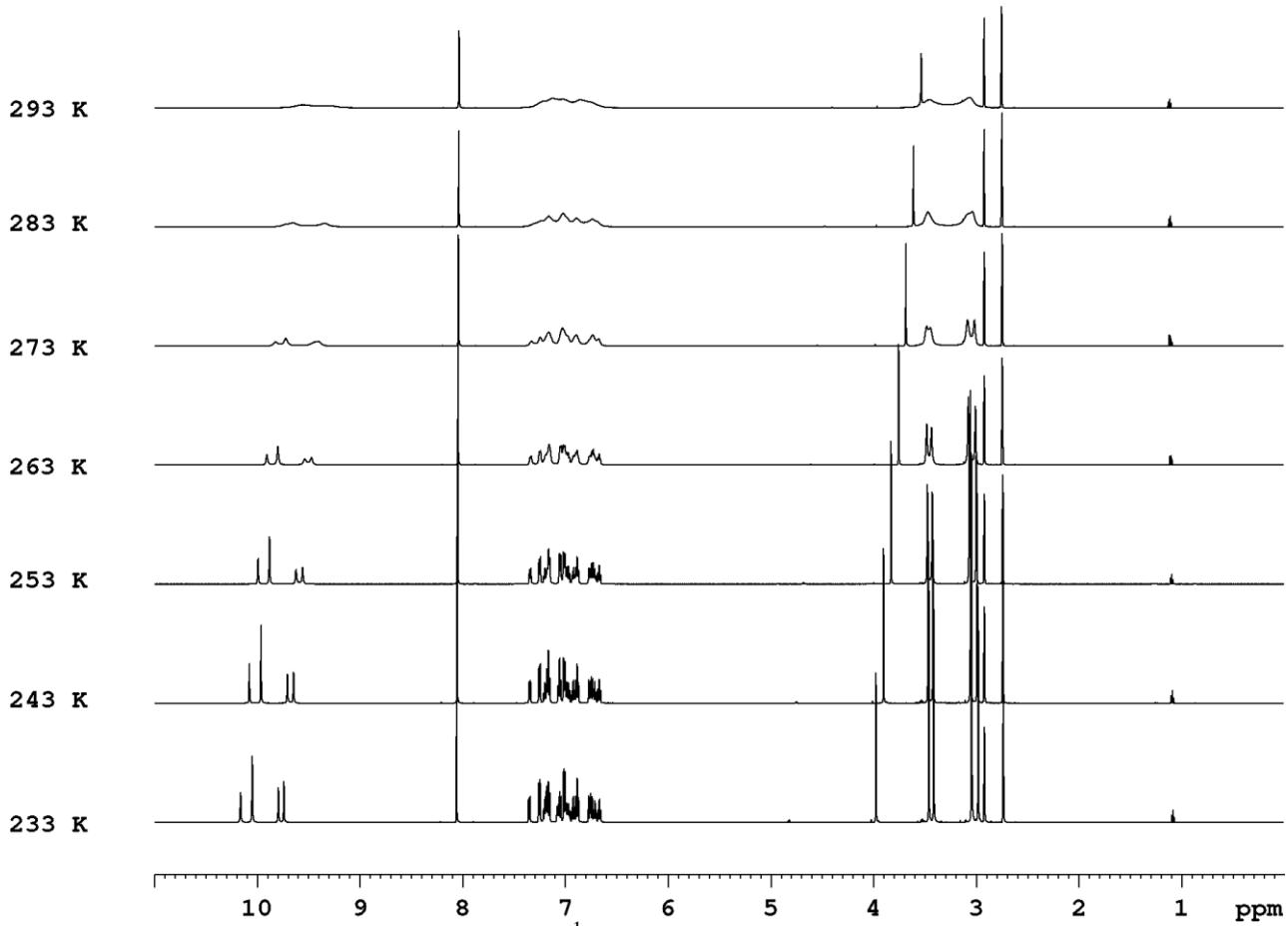


Figure S16. Temperature-dependent ¹H NMR spectra of compound **13** in DMF-d7.

¹H ROESY spectra (roesyph.2) were recorded on a BBO probe in steps of 5 K between 223 and 253 K. The spectra were acquired using a spectral width of 3.0 kHz, 2048 x 256 complex time domain datapoints, mixing times in the range of 0.03 to 0.3 s and 8 scans in about 75 min. The spectra were zero-filled to 4096 x 4096 datapoints and processed with a shifted square sine bell apodization in both dimensions. Populations and exchange rates were obtained from diagonal- and crosspeak integrals using EXSYCalc (MestreLab Research S.L.).

In the ¹H ROESY spectra of **13** the intensity of following peaks were calculated by volume integration in order to obtain the rate constants of *asym* to *sym* exchange:

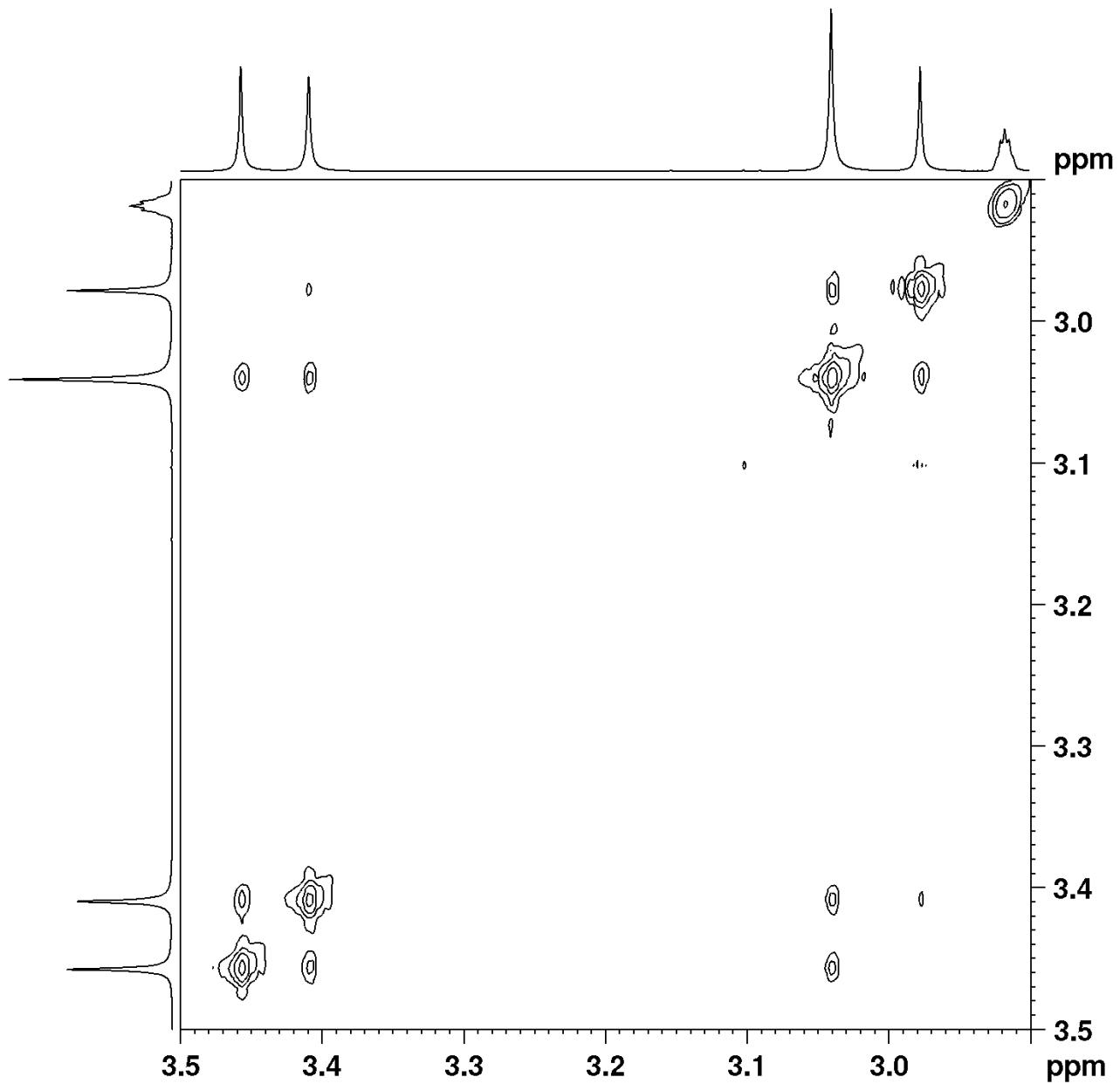


Figure S17. ^1H ROESY spectrum of compound **13** in DMF-d_7 at 233K using mixing time of 0.3 s (region of $\text{N}-\text{CH}_3$ protons).

In the ^1H ROESY spectra of **13** the intensity of following peaks were calculated by volume integration:

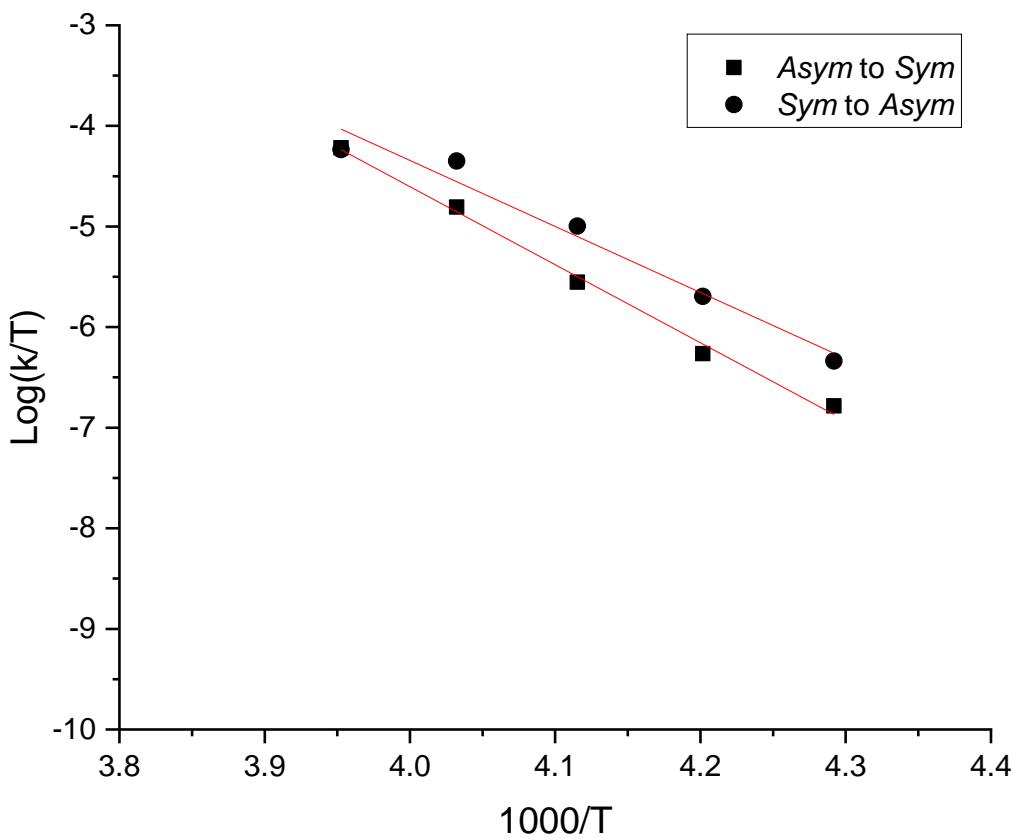
	Asym	Asym	Sym	Asym
Asym	I ₁₁	I ₁₂	I ₁₃	I ₁₄
Asym	I ₂₁	I ₂₂	I ₂₃	I ₂₄
Sym	I ₃₁	I ₃₂	I ₃₃	I ₃₄
Asym	I ₄₁	I ₄₂	I ₄₃	I ₄₄

It can be transformed into:

	Sym	Asym
Sym	I ₃₃	I ₃₁ + I ₃₂ + I ₃₄
Asym	I ₁₃ + I ₂₃ + I ₄₃	I ₁₁ + I ₁₂ + I ₁₄ + I ₂₁ + I ₂₂ + I ₂₄ + I ₄₁ + I ₄₂ + I ₄₄

Table S16. Rate constants of compound **13** calculated from 2D integrals

T, K	Asym to Sym	Sym to Asym
233	0.264	0.412
238	0.453	0.801
243	0.941	1.645
248	2.026	3.202
253	3.726	3.659

**Figure S18.** Eyring plot of rate constants of compound **13**

Errors analysis: Usually the presented errors in activation parameters are the statistical errors based on scattering of the data points around the Eyring straight line only. The errors in this analysis are due to inaccuracies in both the calculated rate constants, k , and the measured temperatures, T and are computed according to the error propagation equations of Binsch [1] and Heinzer and Oth [2]. The absolute error in temperature is assumed to be not more than ± 0.5 K. The relative errors in k are estimated to be not more than $\pm 10\%$ at all temperatures according the precision of the volume integration of peaks. The errors analysis was performed using self-made computer program using the cited equations.

Table S17. Experimental thermodynamic parameters of exchange processes in compound **13** in DMF-d7

Exchange	$\Delta H^\neq(298K)$	$\Delta S^\neq(298K)$	$\Delta G^\neq(298K)$	R^2
Asym to Sym	15.4 ± 1.1	5.3 ± 6.1	13.8 ± 0.1	0.998
Sym to Asym	13.0 ± 1.5	-3.7 ± 4.8	14.1 ± 0.1	0.984

ΔG^\neq and ΔH^\neq in kcal mol⁻¹ and ΔS^\neq in cal mol⁻¹ K⁻¹

Table S18. Experimental Thermodynamic parameters of compound **13** in DMF-d7

Conformer	ΔH^0 (298K)	ΔS^0 (298K)	ΔG^0 (298K)
<i>Asym</i>	0.00	0.00	0.00
<i>Sym</i>	0.4 ± 0.02	2.8 ± 0.1	-0.4 ± 0.0

$$\Delta H^0 = H^0(\text{Sym}) - H^0(\text{Asym})$$

$$\Delta S^0 = S^0(\text{Sym}) - S^0(\text{Asym})$$

$$\Delta G^0 = G^0(\text{Sym}) - G^0(\text{Asym})$$

ΔG^0 and ΔH^0 in kcal mol⁻¹ and ΔS^0 in cal mol⁻¹ K⁻¹

Compound 14

¹H and ¹³C spectra were recorded on a Bruker II+ 600 spectrometer (BBO probe) at 600.13 for ¹H NMR and 150.92 MHz for ¹³C NMR with TMS as internal standard for chemical shifts (δ , ppm). The spectra were recorded in steps of 10 K between 273 and 323 K (0.05M in 600 μ L DMF-d7). Temperature calibration was done with B-VT 3000 unit (it was checked and calibrated with methanol and ethylene glycol reference samples). ¹H NMR spectra were acquired using a spectral width of 10 kHz, an acquisition time of 3.4 s and 32 scans, zero-filled to 64k datapoints (0.15 Hz per point) and processed without apodization.

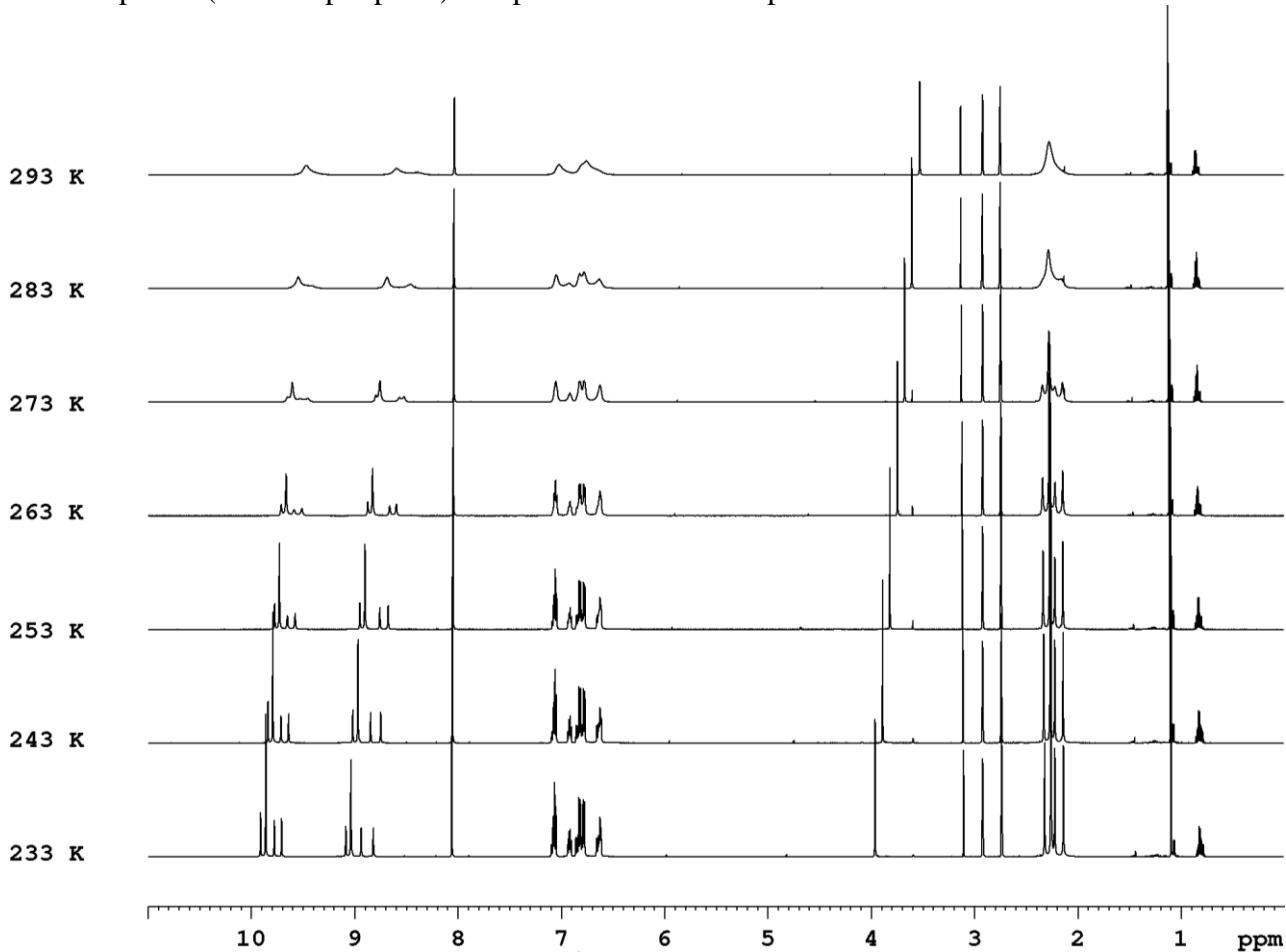


Figure S19. Temperature-dependent ¹H NMR spectra of compound **14** in DMF-d7.

¹H ROESY spectra (roesyph.2) were recorded on a BBO probe in steps of 5 K between 233 and 253 K. The spectra were acquired using a spectral width of 3.0 kHz, 2048 x 256 complex time domain datapoints, mixing times in the range of 0.03 to 0.3 s and 8 scans in about 75 min. The spectra were zero-filled to 4096 x 4096 datapoints and processed with a shifted square sine bell apodization in both dimensions. Populations and exchange rates were obtained from diagonal- and crosspeak integrals using EXSYCalc (MestreLab Research S.L.).

In the ¹H ROESY spectra of **14** the intensity of following peaks were calculated by volume integration in order to obtain the rate constants of *asym* to *sym* exchange:

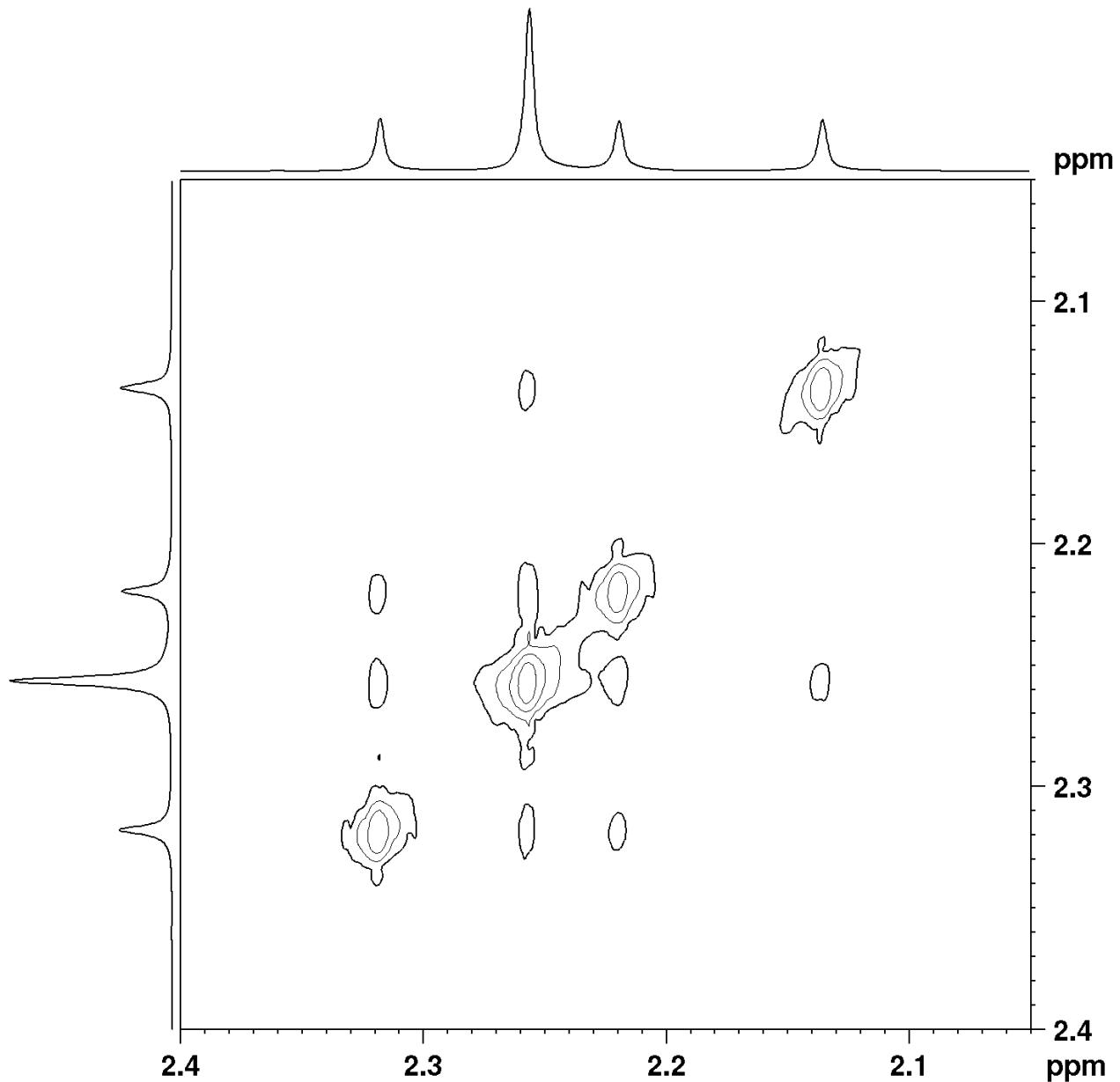


Figure S20. ^1H ROESY spectrum of compound **14** in DMF-d_7 at 233K using mixing time of 0.3 s (region of Ar- CH_3 protons).

In the ^1H ROESY spectra of **14** the intensity of following peaks were calculated by volume integration:

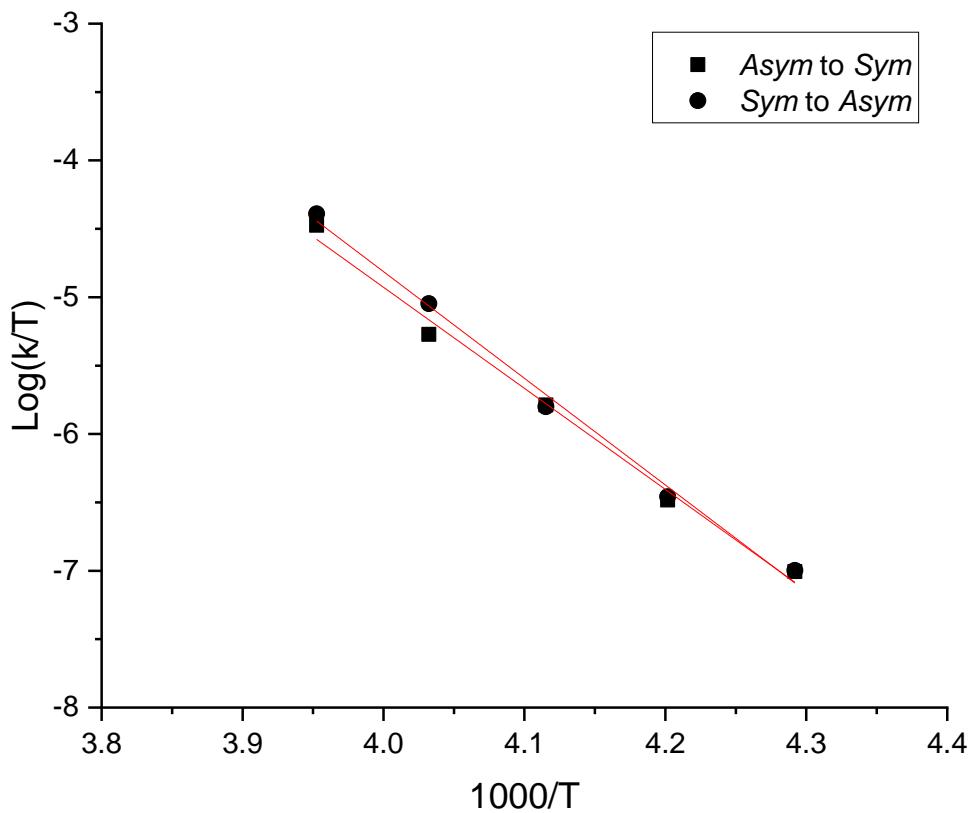
	Asym	Sym	Asym	Asym
Asym	I ₁₁	I ₁₂	I ₁₃	I ₁₄
Sym	I ₂₁	I ₂₂	I ₂₃	I ₂₄
Asym	I ₃₁	I ₃₂	I ₃₃	I ₃₄
Asym	I ₄₁	I ₄₂	I ₄₃	I ₄₄

It can be transformed into:

	Sym	Asym
Sym	I ₂₂	I ₂₁ + I ₂₃ + I ₂₄
Asym	I ₁₂ + I ₃₂ + I ₄₂	I ₁₁ + I ₁₃ + I ₁₄ + I ₃₁ + I ₃₃ + I ₃₄ + I ₄₁ + I ₄₃ + I ₄₄

Table S19. Rate constants of compound **14** calculated from 2D integrals

T, K	Asym to Sym	Sym to Asym
233	0.211	0.213
238	0.364	0.373
243	0.745	0.735
248	1.273	1.595
253	2.885	3.134

**Figure S21.** Eyring plot of rate constants of compound **14**

Errors analysis: Usually the presented errors in activation parameters are the statistical errors based on scattering of the data points around the Eyring straight line only. The errors in this analysis are due to inaccuracies in both the calculated rate constants, k , and the measured temperatures, T and are computed according to the error propagation equations of Binsch [1] and Heinzer and Oth [2]. The absolute error in temperature is assumed to be not more than ± 0.5 K. The relative errors in k are estimated to be not more than $\pm 10\%$ at all temperatures according the precision of the volume integration of peaks. The errors analysis was performed using self-made computer program using the cited equations.

Table S20. Experimental thermodynamic parameters of exchange processes in compound **14** in DMF-d7

Exchange	$\Delta H^\neq(298K)$	$\Delta S^\neq(298K)$	$\Delta G^\neq(298K)$	R^2
Asym to Sym	14.7 ± 1.2	1.7 ± 3.7	14.2 ± 0.1	0.996
Sym to Asym	15.5 ± 1.1	5.2 ± 5.3	13.9 ± 0.1	0.997

ΔG^\neq and ΔH^\neq in kcal mol⁻¹ and ΔS^\neq in cal mol⁻¹ K⁻¹

Table S21. Experimental Thermodynamic parameters of compound **14** in DMF-d7

Conformer	ΔH^0 (298K)	ΔS^0 (298K)	ΔG^0 (298K)
<i>Asym</i>	0.00	0.00	0.00
<i>Sym</i>	0.2 ± 0.02	0.6 ± 0.1	0.0 ± 0.0

$$\Delta H^0 = H^0(\text{Sym}) - H^0(\text{Asym})$$

$$\Delta S^0 = S^0(\text{Sym}) - S^0(\text{Asym})$$

$$\Delta G^0 = G^0(\text{Sym}) - G^0(\text{Asym})$$

ΔG^0 and ΔH^0 in kcal mol⁻¹ and ΔS^0 in cal mol⁻¹ K⁻¹

^{15}N spectra of compound **11** in DMF-d_7 at 243K

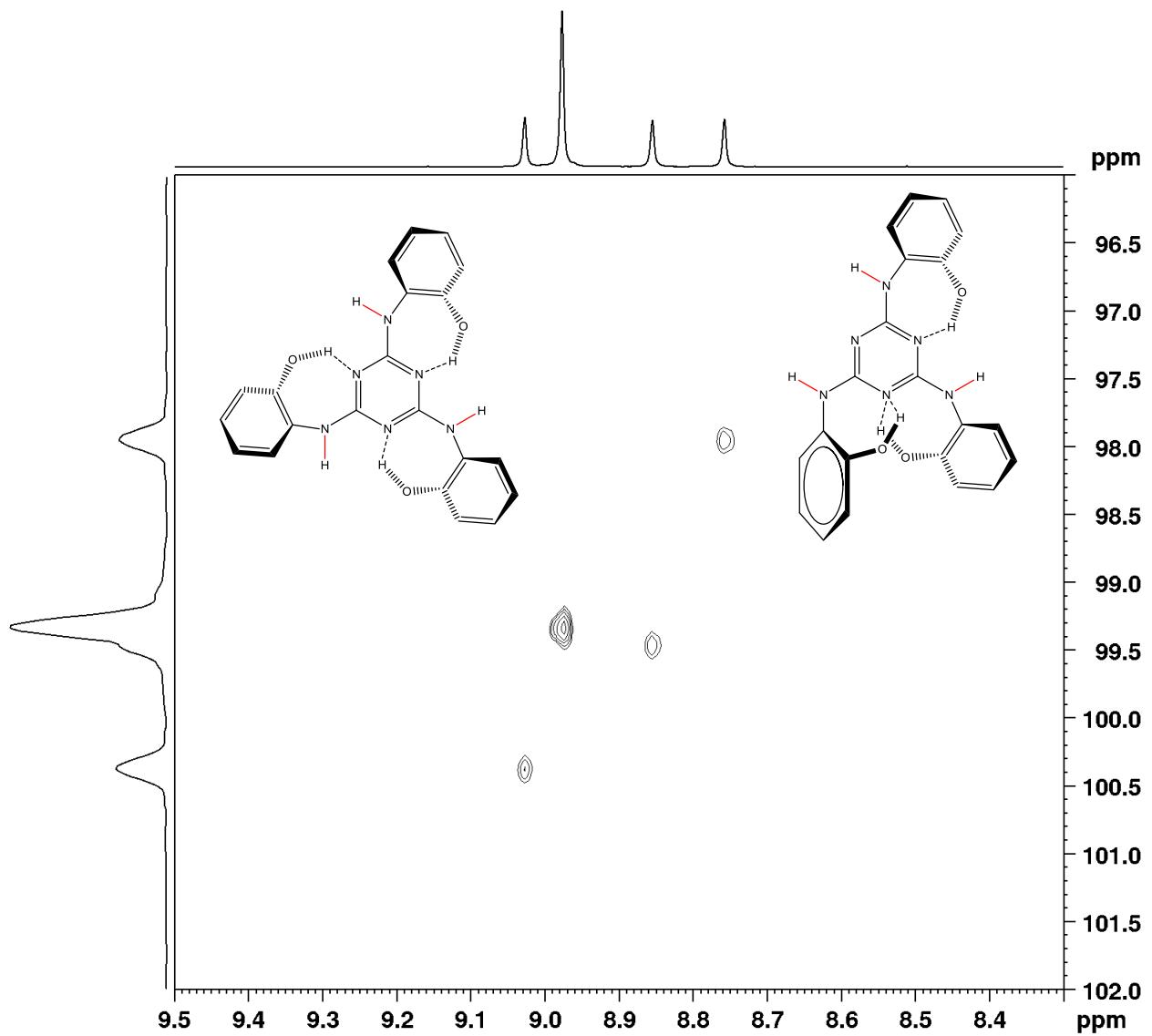


Figure S22. $^1\text{H}, ^{15}\text{N}$ -HSQC spectrum of compound **11** in DMF-d_7 at 243K. The symmetric conformer has only one ^{15}N signal and only one proton signal for NH group. In asymmetric conformer there are 3 signals for NH group either in ^{15}N spectrum or in proton spectrum due to different environment.

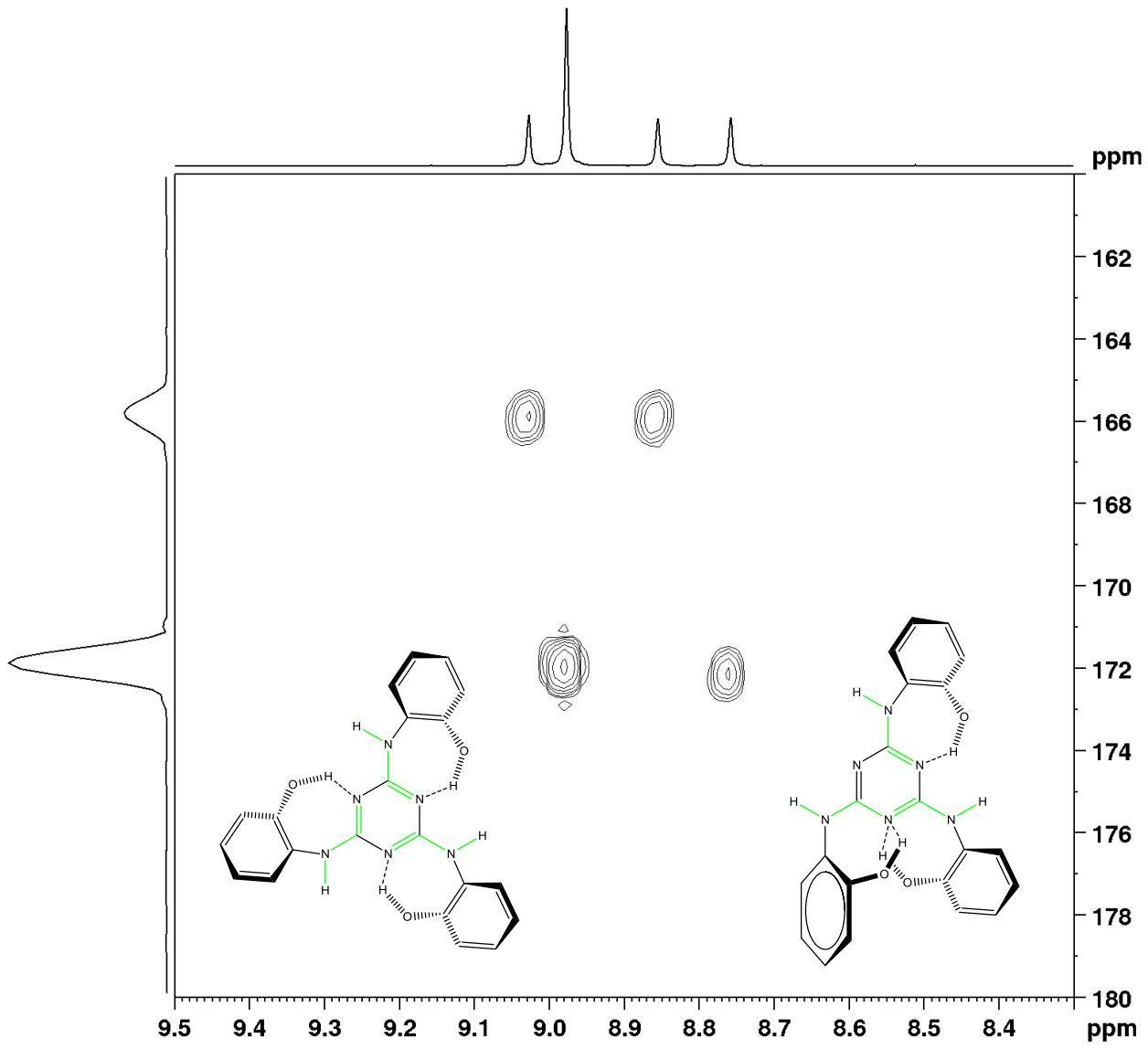


Figure S23. $^1\text{H}, ^{15}\text{N}$ -HMBC spectrum of compound **11** in DMF-d_7 at 243K. The symmetric conformer has only one ^{15}N signal for the 3 nitrogen atoms of 1,3,5-triazine. In asymmetric conformer the two NH protons correlate with one nitrogen atom of 1,3,5-triazine (166 ppm). The third NH proton correlate with a nitrogen atom of 1,3,5-triazine with similar environment and has ^{15}N chemical shift close to that of the symmetric conformer (172 ppm).

DFT calculations

All calculations were performed by means of quantum chemical calculations at the density functional theory (DFT) level using Gaussian09 program package [1].

Geometry optimization

The geometries of all compounds have been fully optimized using B3LYP [2] functional with 6-31+G(d,p) basis set [3] or using M06-2X [4,5] functional with TZVP [6] basis set. All ground state structures were optimized without restrictions and using an ultrafine grid in the computation of two-electron integrals and their derivatives. Solvent effect was included implicitly to the optimizations via the SMD [7] model with the built in parameters for solvents (DMF or CH₃CN). The nature of all critical points was confirmed by means of the vibrational analysis. The thermal corrections to Gibbs free energy to 298.15 K have been calculated for all minima from unscaled vibrational frequencies obtained at the same level.

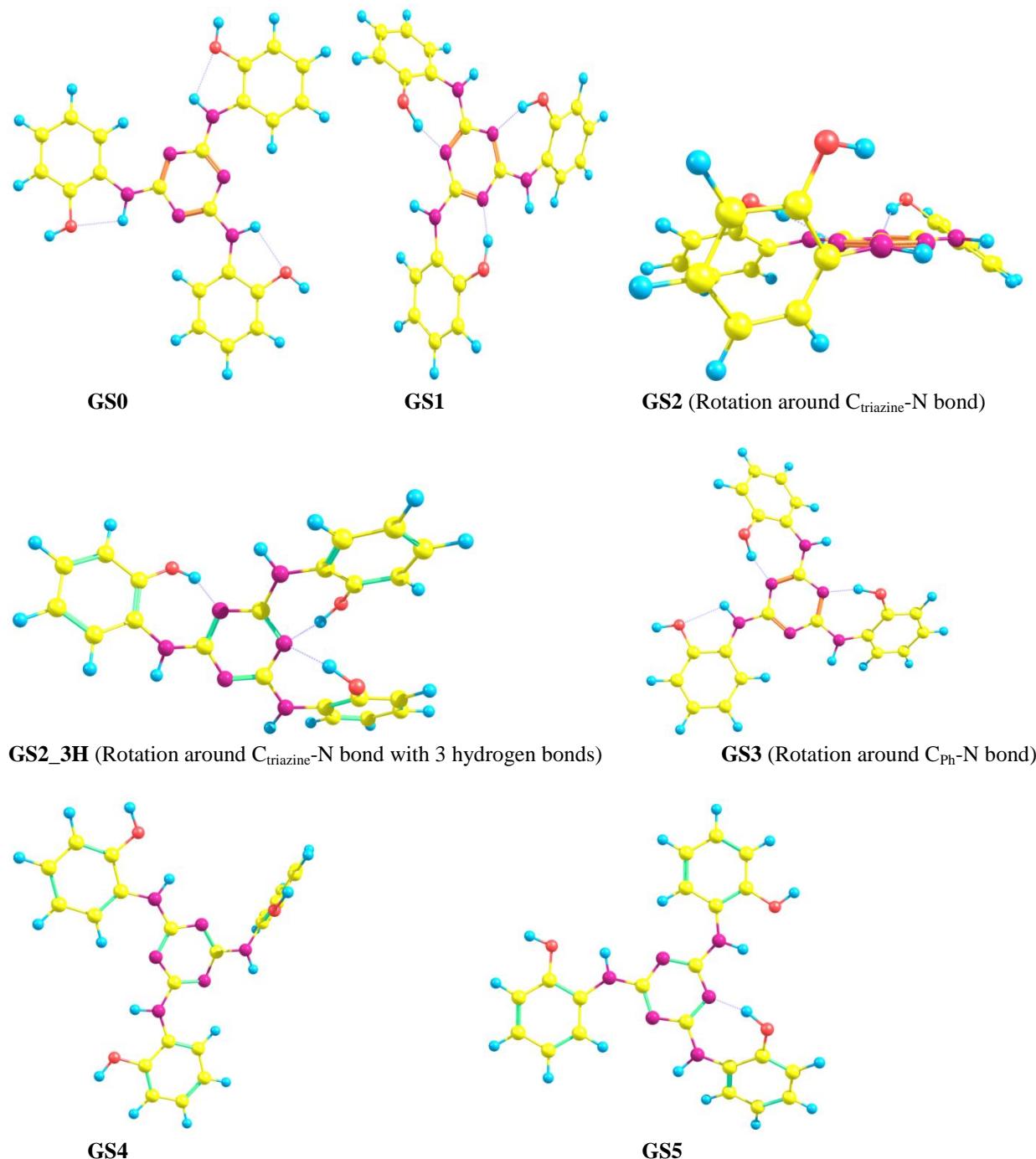
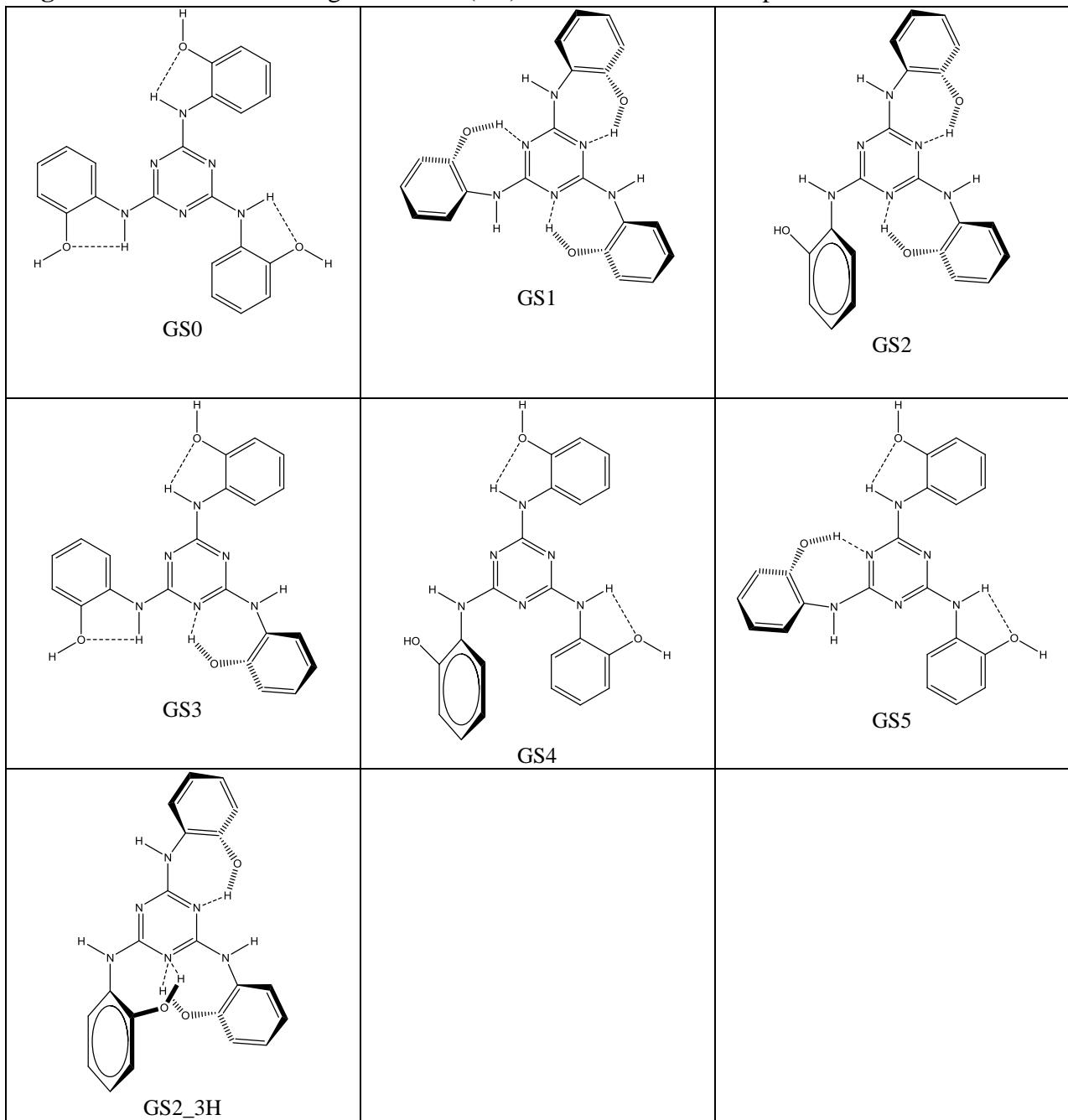


Figure S24. DFT calculated ground state (GS) conformations of compound **11**.



Off: no hydrogen bond

O-bond: N-H...O hydrogen bond

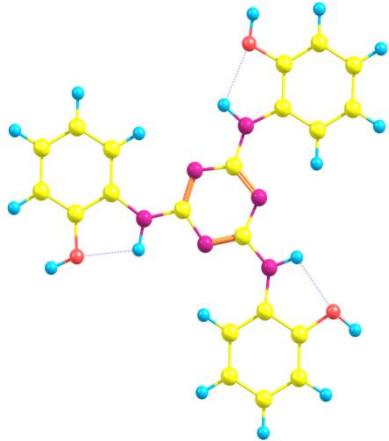
N-bond: O-H...N hydrogen bond

Conformer	First subst.	Second subst.	Third subst.
GS0	O-bond	O-bond	O-bond
GS1	N-bond	N-bond	N-bond
GS2	Off	N-bond	N-bond
GS2_3H	N-bond	N-bond	N-bond
GS3	N-bond	N-bond	O-bond
GS4	Off	O-bond	O-bond
GS5	N-bond	O-bond	O-bond

Table S22. Theoretical thermodynamic parameters of studied GS structures

Comp.	Structure	Method	ΔH^\ddagger (298 K) kcal mol ⁻¹	ΔS^\ddagger (298 K) cal K ⁻¹ mol ⁻¹	ΔG^\ddagger (298 K) kcal mol ⁻¹
11	Sym GS GS1	SMD(DMF)//M062X/TZVP	0.0	0.0	0.0
	GS2	SMD(DMF)//M062X/TZVP	0.2	1.9	-0.4
	GS2_3H	SMD(DMF)//M062X/TZVP	-1.2	-2.3	-0.5
	GS3	SMD(DMF)//M062X/TZVP	1.1	-3.7	2.2
	GS5	SMD(DMF)//M062X/TZVP	3.4	6.1	1.6
	GS0	SMD(DMF)//M062X/TZVP	3.8	-5.6	5.5
	GS4	SMD(DMF)//M062X/TZVP	6.4	9.7	3.6
11	Sym GS GS1	SMD(DMF)//B3LYP/6-31+G(d,p)	0.0	0.0	0.0
	GS2	SMD(DMF)//B3LYP/6-31+G(d,p)	2.1	1.9	1.5
	GS2_3H	SMD(DMF)//B3LYP/6-31+G(d,p)	1.2	-1.4	1.6
	GS3	SMD(DMF)//B3LYP/6-31+G(d,p)	1.6	2.5	0.9
	GS5	SMD(DMF)//B3LYP/6-31+G(d,p)	3.5	2.8	2.6
	GS0	SMD(DMF)//B3LYP/6-31+G(d,p)	4.9	2.4	4.2
	GS4	SMD(DMF)//B3LYP/6-31+G(d,p)	6.8	6.2	4.9

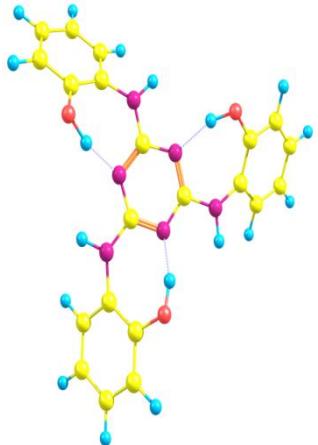
Cartesian coordinates of the
SMD(DMF)//M062X/TZVP optimized GS geometries
for **11-14** and SMD(DMF)//B3LYP/6-31+G(d,p)
optimized geometries for **4-6**:



11-GS0

C	1.01053800	-0.79742700	-0.03077300
N	2.13687900	-1.55728400	-0.01401300
N	-0.18797300	-1.35910800	-0.04027800
C	2.31085500	-2.94977100	-0.02920000
N	1.25597800	0.53165900	-0.02192100
C	-1.21199000	-0.47922900	-0.04627900
C	3.64546700	-3.38624500	0.03792400
C	1.30183700	-3.90522300	-0.10674700
C	0.17433900	1.28801200	-0.02575500
N	-2.43124500	-1.07037000	-0.03772400
N	-1.09750900	0.84141900	-0.04179500
C	3.95282400	-4.73504300	0.02619200
C	1.61499600	-5.26239400	-0.11757300
H	0.27533200	-3.59079100	-0.15988100
N	0.28285400	2.63777400	-0.00656900
C	-3.72118000	-0.52067500	-0.01821600
C	2.93338600	-5.68125800	-0.04890500
H	0.81063600	-5.98445500	-0.17693800
C	1.40780400	3.46914900	0.02008800
C	-4.03581800	0.83351400	-0.04706300
C	-4.77198700	-1.44877600	0.05656000
C	2.73141400	3.05679700	0.13468600
C	1.13531000	4.84343500	-0.06339200
C	-5.36686900	1.24896700	-0.00287200
H	-3.24114000	1.55772900	-0.09716700
C	-6.08623900	-1.03457100	0.10400200
C	3.76187100	3.99311300	0.15405200
H	2.95455600	2.00479500	0.20764800
C	2.16306500	5.77021200	-0.04494300
C	-6.39353700	0.31963200	0.07427800
H	-5.58566700	2.30894800	-0.02404200
C	3.48586300	5.34733700	0.06590300
H	4.78429300	3.64650900	0.24068400
H	-2.39425700	-2.08286800	-0.02725500
H	-0.61177900	3.11230300	-0.04371000
H	2.99423100	-1.01774300	0.00329500
O	-4.41820700	-2.76325400	0.09437700

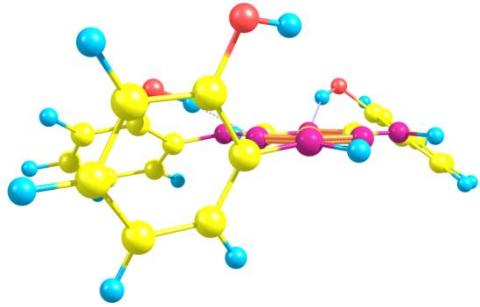
H	-5.20163200	-3.32236100	0.17085500
O	4.60371200	-2.40401000	0.11011100
H	5.49186800	-2.79727000	0.14811900
O	-0.18785100	5.17545200	-0.16564500
H	-0.30103400	6.13462700	-0.23572400
H	3.18012100	-6.73519700	-0.05353300
H	4.99313000	-5.03668600	0.08052200
H	4.28254300	6.07914300	0.07914500
H	1.91569100	6.82493700	-0.11588000
H	-7.42933900	0.63377100	0.11113800
H	-6.86337200	-1.78684800	0.16627300



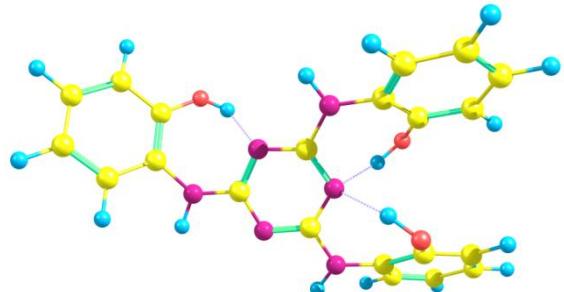
11-GS1

C	-0.20581300	1.28968500	0.07791100
N	-0.37462900	2.62469300	0.09252000
N	-1.27509900	0.49746100	0.07373900
C	-1.57052800	3.35828100	-0.11936900
N	1.07002100	0.85924800	0.07479200
C	-1.01050600	-0.82272000	0.07756500
C	-1.50448100	4.44999700	-0.98449100
C	-2.76683000	3.09478200	0.55938300
C	1.22084600	-0.46324300	0.07826900
N	-2.08337200	-1.63492300	0.09229800
N	0.21006400	-1.35310200	0.07433900
C	-2.60046900	5.27286800	-1.18127000
C	-3.86954800	3.91524000	0.34050200
N	2.46080900	-0.98591900	0.09367100
C	-2.12370300	-3.03701900	-0.12091700
C	-3.78975100	5.00332600	-0.51267800
H	-4.78357300	3.68661600	0.87509200
C	3.69495700	-0.31969300	-0.12012300
C	-1.29990400	-3.94304800	0.55846500
C	-3.10401100	-3.52311900	-0.98535000
C	4.06827000	0.84585900	0.56009700
C	4.60468700	-0.92420900	-0.98713700
C	-1.46296000	-5.30791300	0.34045200
C	-3.27307600	-4.88338600	-1.18060100
C	5.33102500	1.38815600	0.34026900
C	5.86633700	-0.38923100	-1.18455200
C	-2.44710600	-5.78037500	-0.51185600
H	-0.80977300	-5.98699000	0.87494000
C	6.23085100	0.77385700	-0.51489400

H	5.59333200	2.29236400	0.87607600	C	5.29147700	-1.58381200	0.56210700
H	-2.97005600	-1.15477000	-0.01292600	H	5.24630700	-1.30849600	-1.57905200
H	2.48778200	-1.99343400	-0.01461800	C	-6.80620300	0.60209300	0.37518700
H	0.48338300	3.15320900	-0.01729200	H	-6.01122400	1.95255600	-1.10502300
H	-4.65627100	5.63579700	-0.65934400	H	0.93201300	-3.54346000	0.35374200
H	-2.52537600	6.11767100	-1.85364100	H	-3.32291700	-2.51838100	0.15999300
H	7.21262400	1.20610500	-0.66220100	H	-0.87188100	2.42504200	-0.14793000
H	6.55872200	-0.87768300	-1.85791100	H	4.44935500	4.43403300	0.68946500
H	-2.56473800	-6.84678600	-0.65785100	H	2.31861000	5.16851800	1.74605300
H	-4.04392300	-5.23903100	-1.85195200	H	-7.74702400	1.12965600	0.46960900
O	3.26162200	1.45248800	1.47800600	H	-7.30217100	-0.91144900	1.82493800
H	2.33915800	1.43742900	1.12406800	H	6.33543300	-1.30969800	0.65165800
O	-2.88906000	2.09040600	1.47446000	H	5.03718800	-1.94747700	2.66864300
H	-2.41211500	1.30120300	1.11899600	O	-3.75536800	0.86717700	-1.59303100
O	-0.36836000	-3.54754300	1.47352900	H	-2.84388200	0.79014500	-1.21456600
H	0.07822900	-2.74106900	1.11761000	O	2.44330700	1.00448000	-1.42343400
H	-3.73954500	-2.80948900	-1.49735100	H	1.87599900	0.27969300	-1.06489700
H	-0.56950800	4.64590500	-1.49705800	O	2.79598100	-1.91624800	-2.05289000
H	4.30373300	-1.83063200	-1.50014700	H	1.91071600	-2.31090700	-2.02416600
				H	2.63322800	-2.54231000	2.43696400
				H	0.24688000	3.87877400	1.33691800
				H	-5.13847600	-2.08475000	1.58560700



11-GS2

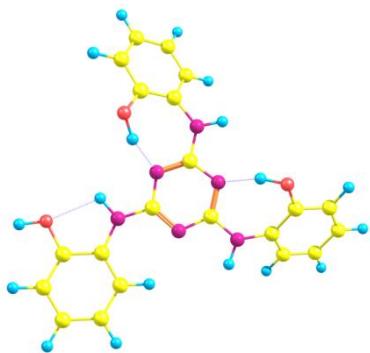


11-GS2_3H

C	-0.35211300	0.50399800	-0.09402800
N	-0.06181300	1.81725600	-0.19075600
N	0.64608500	-0.37461700	0.00609700
C	1.18410000	2.44875900	0.05904700
N	-1.65423900	0.18245800	-0.11581600
C	0.26288600	-1.65999100	0.09465000
C	1.18217700	3.57452900	0.88122100
C	2.38060600	2.04718300	-0.54721500
C	-1.91492400	-1.12504300	-0.01482800
N	1.23603000	-2.59469800	0.17224400
N	-0.99568400	-2.09023400	0.10047000
C	2.34348200	4.29434500	1.10834300
C	3.54788800	2.76161600	-0.29581900
N	-3.20323600	-1.53042900	-0.03091300
C	2.61501500	-2.27043100	0.32182100
C	3.53285800	3.88421200	0.51586400
H	4.46045700	2.42399900	-0.77232300
C	-4.37210600	-0.74087800	0.11436600
C	3.35452900	-1.93331600	-0.81263800
C	3.22578600	-2.27730700	1.56940400
C	-4.62915200	0.40180200	-0.65405700
C	-5.34702400	-1.19505700	1.00239600
C	4.69255300	-1.57785500	-0.68807000
C	4.56548900	-1.94048500	1.69470900
C	-5.84054800	1.06959600	-0.50105200
C	-6.55844300	-0.53677700	1.13357700

C	0.39845300	0.52964700	0.12836300
N	0.10205400	1.82525900	0.33976300
N	-0.61236100	-0.31817600	-0.08358700
C	-1.16032100	2.43588000	0.10738200
N	1.68782500	0.17544300	0.15611100
C	-0.26272400	-1.60290600	-0.27120400
C	-1.19462500	3.57199100	-0.69848000
C	-2.34531600	1.97986600	0.69863700
C	1.92121700	-1.12409300	-0.07665000
N	-1.26088400	-2.48979400	-0.46336600
N	0.98564800	-2.05735000	-0.29572800
C	-2.38179500	4.24881200	-0.92551900
C	-3.53821700	2.64876900	0.44466600
N	3.19899600	-1.55417500	-0.08561700
C	-2.63866900	-2.26206000	-0.19849200
C	-3.55955900	3.78182500	-0.35250100
H	-4.44128400	2.26684500	0.90553800
C	4.38400000	-0.77537200	-0.11415600
C	-3.36428000	-1.21761100	-0.78619600
C	-3.29906800	-3.16328200	0.63464800
C	4.64642300	0.25616200	0.79597100
C	5.36467700	-1.13129300	-1.03960700
C	-4.71954500	-1.08134100	-0.50373900

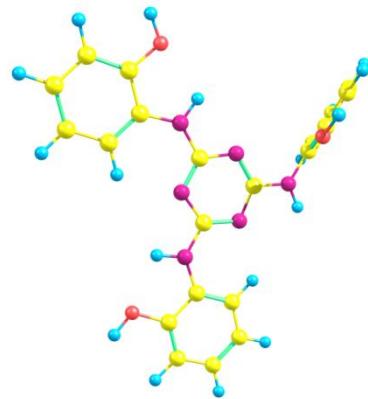
C	-4.65464900	-3.03680800	0.89094000
C	5.86970500	0.91746200	0.74462200
C	6.58748500	-0.48209000	-1.07079900
C	-5.36706800	-1.98828600	0.31970500
H	-5.25258300	-0.25803500	-0.96396100
C	6.84076600	0.54804100	-0.17173600
H	6.04424000	1.71444400	1.45722600
H	-0.96681400	-3.45949900	-0.47375600
H	3.30572600	-2.52020600	-0.37220300
H	0.90118500	2.44842300	0.36589000
H	-4.49579700	4.29606500	-0.52974500
H	-2.38634800	5.13189600	-1.55127300
H	7.79048500	1.06777200	-0.18709200
H	7.33592500	-0.77893200	-1.79408800
H	-6.42503400	-1.87259600	0.51905300
H	-5.14864000	-3.75039200	1.53764600
O	3.76577500	0.61223700	1.77604000
H	2.86146200	0.61161600	1.37923900
O	-2.38206300	0.92251800	1.56330300
H	-1.81391300	0.20999200	1.20277200
O	-2.80973200	-0.33806700	-1.67290000
H	-1.92641500	-0.07903800	-1.33598500
H	-2.72731300	-3.97039300	1.07799500
H	-0.26866000	3.91682400	-1.14386300
H	5.15165600	-1.93661300	-1.73308800



11-GS3

C	0.45523500	1.16304700	0.08544600
N	0.77501700	2.47292200	0.12776500
N	-0.82102700	0.80382400	0.01997500
C	-0.06919500	3.58506900	-0.12059300
N	1.49033000	0.30399900	0.12581600
C	-1.04740500	-0.53088400	0.00991000
C	0.42358800	4.59111700	-0.95137900
C	-1.31498900	3.75773200	0.49607800
C	1.15084300	-0.98494400	0.10114100
N	-2.35263900	-0.86678400	-0.03954600
N	-0.10410700	-1.45978100	0.04230500
C	-0.29724800	5.75250400	-1.17291600
C	-2.04236800	4.91878400	0.25116600
N	2.12637500	-1.91618000	0.14392700
C	-2.98290000	-2.12063100	-0.06706700
C	-1.53765300	5.91676600	-0.56606700
H	-3.00422900	5.02493100	0.73805200
C	3.52178400	-1.73673100	-0.03190500

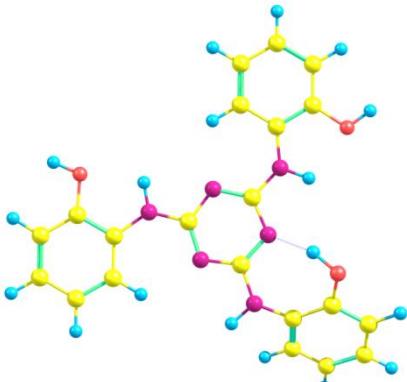
C	-4.38840000	-2.08011200	-0.09076900
C	-2.34904100	-3.35971500	-0.07909700
C	4.27035100	-0.77878000	0.66437700
C	4.18037600	-2.63297500	-0.87388400
C	-5.13081900	-3.24600100	-0.12387300
C	-3.10274100	-4.52989200	-0.11132300
C	5.64951600	-0.72743200	0.48354400
C	5.55534400	-2.58879000	-1.03123700
C	-4.48685600	-4.47869500	-0.13381200
H	-6.21271600	-3.17752400	-0.14117600
C	6.29388800	-1.62974700	-0.34657500
H	6.20299100	0.02630700	1.03044500
H	-2.98274000	-0.07328800	-0.06200700
H	1.79263200	-2.86392000	0.01354100
H	1.76898300	2.66026700	0.06041500
H	-2.11437000	6.81781500	-0.73303700
H	0.10778200	6.52246700	-1.81678400
H	7.36924100	-1.58007100	-0.46291100
H	6.04493400	-3.29825000	-1.68579700
H	-5.07260000	-5.38872500	-0.15931400
H	-2.59114100	-5.48388200	-0.11984300
O	3.70979100	0.08385500	1.55992400
H	2.84651300	0.38819100	1.18000200
O	-1.83130100	2.85156600	1.37533600
H	-1.64272000	1.94785600	1.01562700
O	-4.95461200	-0.83661900	-0.07967400
H	-5.91887700	-0.90135200	-0.11041000
H	-1.27300300	-3.40786600	-0.06364500
H	1.39215200	4.44749300	-1.41660900
H	3.59064700	-3.37501100	-1.39992500



11-GS4

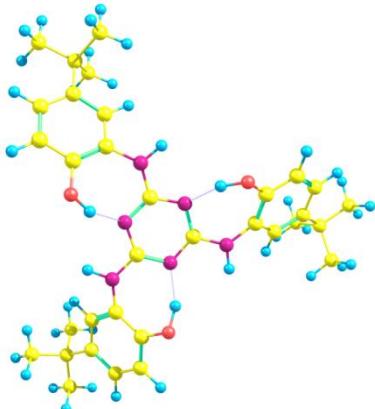
C	0.29728200	-1.44932700	-0.12061300
N	0.68597100	-2.74357700	-0.15240200
N	1.22430900	-0.50051900	-0.14806500
C	2.03423000	-3.17619800	-0.19719300
N	-1.03421200	-1.24602500	-0.07289700
C	0.73744400	0.75316100	-0.10186800
C	2.87056100	-2.97115300	0.90477200
C	2.52216000	-3.84213900	-1.31356700
C	-1.38997500	0.02895300	-0.04100100
N	1.69222400	1.71799600	-0.11874100
N	-0.54553800	1.07985900	-0.04570100
C	4.19096500	-3.40291800	0.85877300

C	3.83430800	-4.29562500	-1.35165600	C	-2.66966300	3.16892500	0.56214100
H	1.85669100	-3.99684000	-2.15459100	C	1.36245900	-0.33359300	0.13344600
N	-2.70037900	0.37865100	0.00211800	N	-1.94429200	-1.52242300	0.12141500
C	1.59583500	3.11440100	-0.09183000	N	0.36538200	-1.24006200	0.09287200
C	4.66746200	-4.06546000	-0.26429800	C	-2.47227500	5.34013700	-1.18329300
C	-3.86395800	-0.39993900	0.01811200	C	-3.77723700	3.96795200	0.29352600
C	0.42040300	3.86105800	-0.10722900	N	2.60489500	-0.86637100	0.11556300
C	2.82451500	3.79950900	-0.05554000	C	-2.04877600	-2.92111100	0.07957000
C	-3.92529700	-1.79058800	0.05658800	C	-3.68278500	5.05347900	-0.56194600
C	-5.07034400	0.32465500	0.00230300	H	-4.70808700	3.72574400	0.79206100
C	0.47286100	5.25269600	-0.08105700	C	3.84437400	-0.20328200	0.14705700
H	-0.52962400	3.35396800	-0.13707800	C	-3.31207100	-3.42223000	-0.27654400
C	2.87050800	5.18055100	-0.03189400	C	-1.03685700	-3.82106100	0.39976400
C	-5.15832300	-2.43821200	0.07285200	C	4.89756100	-0.80001500	-0.55878800
H	-3.01190100	-2.36150900	0.07116700	C	4.09032500	0.95220900	0.88108000
C	-6.29085100	-0.32370500	0.01945200	C	-3.54566300	-4.78462900	-0.32821800
C	1.68873400	5.91498400	-0.04436000	C	-1.27496600	-5.19103700	0.34005200
C	-6.33862600	-1.71388200	0.05533100	C	6.16382900	-0.23653900	-0.54134300
H	2.63638100	1.35385700	-0.14452000	C	5.35704300	1.52373400	0.88483200
H	-2.85446700	1.37938300	0.00956800	C	-2.52247900	-5.67498200	-0.02114900
H	-0.04865200	-3.42879600	-0.26949200	H	-4.53179100	-5.13736900	-0.60874800
O	3.94835900	3.02040900	-0.04585300	C	6.39285900	0.93032000	0.17680400
H	4.74077500	3.57394900	-0.03385400	H	6.96121600	-0.71845300	-1.09573800
O	2.33790500	-2.36030100	1.99697000	H	-2.82395000	-1.02278900	0.06454100
H	3.00411200	-2.28095700	2.69367600	H	2.63271800	-1.86265800	-0.06388700
O	-4.95240400	1.68658200	-0.03049500	H	0.59910500	3.26783000	0.08277000
H	-5.82463300	2.10350600	-0.02836500	H	-4.55395100	5.66904300	-0.74797500
H	5.69579900	-4.40445000	-0.28371800	H	-2.38454200	6.18239500	-1.85746300
H	4.83101600	-3.23173100	1.71717400	H	7.38280900	1.36874600	0.18151900
H	-7.29667300	-2.21772200	0.06845300	H	5.53204300	2.42638800	1.45605600
H	-7.19828900	0.26955000	0.00548100	H	-2.70844100	-6.74054200	-0.06598600
H	1.72870000	6.99663700	-0.02482800	H	-0.47438300	-5.87609300	0.58844500
H	3.83693000	5.67147000	-0.00408900	O	4.60193400	-1.94626000	-1.23931100
H	-5.18224800	-3.52027800	0.10193500	H	5.39313700	-2.29543100	-1.67240500
H	-0.45348600	5.81302900	-0.09252500	O	-2.80855500	2.16437800	1.47457700
H	4.20269400	-4.81621200	-2.22602100	H	-2.29224500	1.38597700	1.13634000
				O	-4.27167600	-2.49132300	-0.55845800
				H	-5.12035800	-2.92194100	-0.72904300
				H	-0.06724600	-3.44948900	0.68913200
				H	-0.42034700	4.74749200	-1.41506700
				H	3.28696800	1.39995000	1.44652800



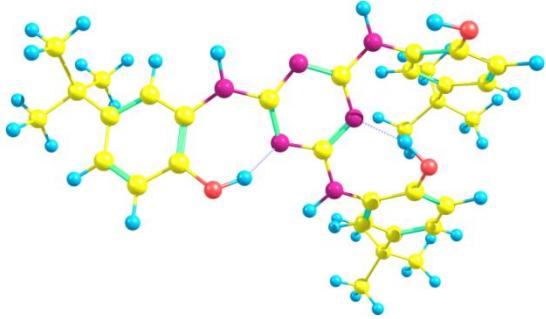
11-GS5

C	-0.06504500	1.39458100	0.17455700
N	-0.25503800	2.73548000	0.19795000
N	-1.13017300	0.59621200	0.16539700
C	-1.45040900	3.44833600	-0.06957100
N	1.21036600	0.98553800	0.17396500
C	-0.85197100	-0.72567800	0.12775900
C	-1.37063100	4.53752300	-0.93735300



12-GS1

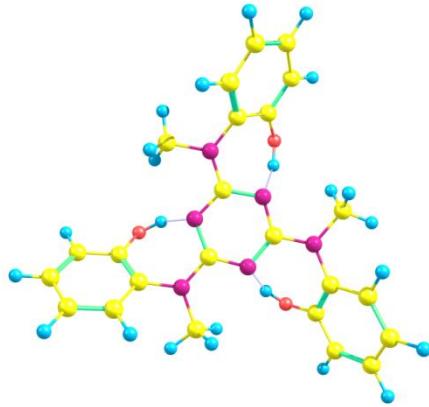
C	1.07563600	0.74020800	-0.84417100	H	0.14313000	-5.51053500	2.77960000
N	2.15691000	1.54108200	-0.85732200	H	-1.56770400	-8.73346200	2.17401100
N	1.24182200	-0.58059100	-0.84383200	H	-2.86264100	-7.57728400	1.85291100
C	3.51476600	1.18087000	-0.65396600	H	-2.08826300	-8.43970200	0.51236900
N	-0.11690600	1.36598100	-0.83854300	C	6.37928200	2.69266300	1.38195500
C	0.10383400	-1.30035500	-0.84978100	C	6.27792300	4.14122100	0.88563000
C	4.26007200	1.97323300	0.21363400	C	5.75503400	2.59457200	2.78054500
C	4.14471700	0.13962500	-1.34647700	C	7.85757300	2.31844600	1.48461800
C	-1.17743000	0.56178600	-0.84588200	H	6.71256800	4.24124200	-0.11200200
N	0.25664500	-2.63732500	-0.86697900	H	5.24052200	4.47855900	0.84182000
N	-1.12292900	-0.78372600	-0.84486900	H	6.81979400	4.80613800	1.56303500
C	5.62335300	1.77398900	0.42224900	H	5.80546600	1.57004100	3.15744000
C	5.49684900	-0.08066500	-1.12900900	H	6.29531100	3.24179200	3.47607800
N	-2.41182900	1.09706000	-0.86323600	H	4.70854600	2.90581600	2.77595700
C	-0.73325500	-3.63339900	-0.66023700	H	8.35336600	3.00045000	2.17857800
C	6.22957500	0.72550400	-0.26919200	H	7.99156400	1.30168600	1.86110700
H	5.97266000	-0.89133200	-1.66783400	H	8.36217800	2.39813500	0.51899700
C	-2.78058000	2.45213500	-0.65599900	C	-5.52740000	4.16914000	1.37981000
C	-1.95306600	-3.65769900	-1.34802500	C	-6.72994600	3.35745200	0.87936400
C	-0.41668900	-4.67424400	0.20721900	C	-5.13199200	3.67425300	2.77761600
C	-2.19055200	3.52135900	-1.34115100	C	-5.94344800	5.63602200	1.48566200
C	-3.84309200	2.69758400	0.20844200	H	-7.03166600	3.68542400	-0.11844300
C	-2.81920200	-4.71835800	-1.12709100	H	-6.50311700	2.29043000	0.83424300
C	-1.27127200	-5.75416000	0.42021400	H	-7.57834000	3.49295500	1.55498300
C	-2.67710600	4.80144600	-1.12017200	H	-4.27253200	4.23171100	3.15811200
C	-4.35226900	3.97711400	0.42139700	H	-5.96459500	3.81380300	3.47177900
C	-2.48454700	-5.75527000	-0.26738300	H	-4.87484300	2.61322200	2.77015500
H	-3.76066100	-4.72582100	-1.66332900	H	-6.78282600	5.72249300	2.17886700
C	-3.74492700	5.02917600	-0.26347100	H	-5.13057100	6.25980400	1.86470800
H	-2.21050800	5.62110500	-1.65346100	H	-6.26354100	6.03557100	0.52056200
H	1.21513300	-2.94674200	-0.75448800				
H	-3.16018700	0.42143400	-0.75743500				
H	1.94714100	2.52637500	-0.74430300				
H	7.28417200	0.51934100	-0.14595400				
H	-4.09369400	6.04504200	-0.13672900				
H	-3.18993600	-6.56535200	-0.14114300				
O	-1.19277300	3.35342700	-2.25944200				
H	-0.56401800	2.68421800	-1.89617300				
O	3.49898000	-0.63378600	-2.26942200				
H	2.60595900	-0.84521600	-1.90611200				
O	-2.30290100	-2.71197600	-2.27020100				
H	-2.03939800	-1.83147600	-1.90924900				
H	0.53848100	-4.62440800	0.71939200				
H	3.74070600	2.77543400	0.72699400				
H	-4.28033400	1.84486000	0.71681200				
C	-0.85370400	-6.86479300	1.38352600				
C	0.45865500	-7.49509400	0.89811500				
C	-0.64058800	-6.27070100	2.78243600				
C	-1.91148400	-7.96380300	1.47975000				
H	0.33845600	-7.92116000	-0.10099300				
H	1.26744600	-6.76272400	0.86200000				
H	0.76074400	-8.29624400	1.57740300				
H	-1.56032800	-5.81216100	3.15399600				
H	-0.34438800	-7.05768200	3.48070900				



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C	0.33827600	0.35768200	0.57362800
N	0.07282800	1.58826800	1.04984000
N	-0.66577200	-0.33249200	0.02416900
C	-1.10789600	2.33814300	0.79119400
N	1.59077700	-0.09615400	0.69263500
C	-0.34864900	-1.55986700	-0.42427900
C	-0.96134300	3.62155700	0.27748700
C	-2.38994000	1.85571500	1.08328300
C	1.79850900	-1.31992100	0.18649900
N	-1.34069000	-2.29308000	-0.97046100
N	0.86681700	-2.09604900	-0.38248700

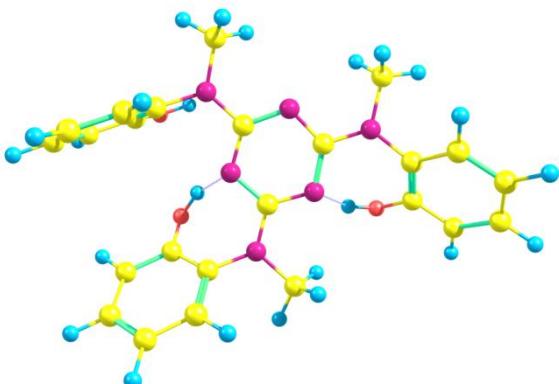
C	-2.05217900	4.45549900	0.03466800	H	6.49022500	-1.11866500	-2.77444700
C	-3.48348100	2.66660800	0.82164300	H	7.20882500	0.44538500	-2.36210500
N	3.04095100	-1.83961100	0.25110500	H	8.20562900	-0.82930500	-3.08150100
C	-2.73262100	-2.02335200	-0.86330100	C	7.98305900	-2.66997200	-1.06173900
C	-3.32071300	3.94921600	0.31522400	H	8.24224000	-3.07089700	-0.07878300
H	-4.47049000	2.27724600	1.04173100	H	7.09602000	-3.19475200	-1.42175200
C	4.25365400	-1.17304800	0.56476000	H	8.80524700	-2.88856800	-1.74788600
C	-3.30485100	-0.81279400	-1.27522300	C	-5.33411500	-4.40463800	1.66041600
C	-3.55464000	-3.03794300	-0.38521300	H	-4.28660400	-4.71053100	1.69111300
C	4.42505200	-0.39550000	1.71668300	H	-5.45962200	-3.54674100	2.32550400
C	5.33839400	-1.39135800	-0.27913100	H	-5.93674400	-5.22951500	2.04895700
C	-4.67713400	-0.65091000	-1.16390300	C	-5.57777300	-5.28314700	-0.66892400
C	-4.93893900	-2.89643100	-0.29476000	H	-6.17801900	-6.11949800	-0.30188700
C	5.67416900	0.15085700	1.97089900	H	-5.88582700	-5.06510700	-1.69443700
C	6.60284700	-0.86452200	-0.02156100	H	-4.53338900	-5.60064800	-0.68595500
C	-5.48533000	-1.67671300	-0.69183400	C	-7.26956700	-3.71757300	0.26108300
H	-5.10518400	0.29444500	-1.47590300	H	-7.47710700	-2.86752700	0.91516500
C	6.74952400	-0.08514100	1.12524000	H	-7.64909500	-3.48577100	-0.73672300
H	5.79371100	0.75316600	2.86357800	H	-7.82760400	-4.57599600	0.64076100
H	-1.09037400	-3.25397400	-1.17308900				
H	3.14395800	-2.71809700	-0.24310100				
H	0.88639300	2.12158300	1.33462300				
H	-4.20463100	4.54713700	0.13895300				
H	7.70558600	0.35400800	1.37590000				
H	-6.55183400	-1.50551100	-0.63641200				
O	3.42815800	-0.19858900	2.63105100				
H	2.59407600	-0.03351300	2.12949200				
O	-2.61131700	0.63554900	1.66215400				
H	-2.03595800	-0.02084100	1.21742600				
O	-2.57590000	0.20471900	-1.82904800				
H	-1.75570200	0.31194500	-1.30329800				
H	-3.07877200	-3.96392200	-0.08101700				
H	0.04618800	3.96361700	0.06708300				
H	5.17022300	-2.00446500	-1.15827800				
C	-1.81523600	5.85588600	-0.53018500	C	0.92257400	-0.92628600	0.09703600
C	-5.78005400	-4.05840200	0.23330500	N	1.87274400	-1.88839700	0.09037100
C	7.75065800	-1.15484200	-0.98851900	N	1.32580900	0.35301200	0.09930000
C	-0.92575300	6.65083900	0.43509800	C	3.24974700	-1.59562100	-0.15609000
H	0.04633000	6.17312200	0.57163300	N	-0.35575800	-1.32484100	0.10131300
H	-0.75412300	7.65576200	0.04122600	C	0.34156700	1.26071900	0.09889100
H	-1.40177500	6.74423100	1.41426200	C	3.88880000	-2.23368100	-1.21734500
C	-3.12367300	6.62104800	-0.72500500	C	3.99355100	-0.75190600	0.67681500
H	-3.78646700	6.11455400	-1.43036500	C	-1.26215500	-0.33594700	0.10139800
H	-3.65889400	6.75176100	0.21834300	N	0.69991700	2.56463500	0.09184600
H	-2.90375300	7.61278400	-1.12571400	N	-0.96797400	0.97033000	0.10494600
C	-1.11043400	5.74355500	-1.88894500	C	5.24476100	-2.05618100	-1.44390100
H	-0.14133600	5.24892500	-1.79868100	C	5.35168300	-0.57001700	0.44092100
H	-1.71964700	5.17558700	-2.59632400	N	-2.57066900	-0.67704700	0.09830200
H	-0.94246300	6.74008700	-2.30514500	C	-0.24222300	3.61039100	-0.15620300
C	9.05187600	-0.48604600	-0.54628300	C	5.97984000	-1.22551700	-0.60611100
H	9.83914500	-0.72086000	-1.26572300	H	5.90054800	0.08826700	1.10336000
H	8.95222200	0.60096800	-0.50231200	C	-3.00811800	-2.01436200	-0.15314900
H	9.37689600	-0.84280400	0.43376400	C	-1.34440700	3.83451000	0.67673600
C	7.38673500	-0.63255400	-2.38489700	C	-0.00956600	4.48036700	-1.21958700



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C	0.92257400	-0.92628600	0.09703600
N	1.87274400	-1.88839700	0.09037100
N	1.32580900	0.35301200	0.09930000
C	3.24974700	-1.59562100	-0.15609000
N	-0.35575800	-1.32484100	0.10131300
C	0.34156700	1.26071900	0.09889100
C	3.88880000	-2.23368100	-1.21734500
C	3.99355100	-0.75190600	0.67681500
C	-1.26215500	-0.33594700	0.10139800
N	0.69991700	2.56463500	0.09184600
N	-0.96797400	0.97033000	0.10494600
C	5.24476100	-2.05618100	-1.44390100
C	5.35168300	-0.57001700	0.44092100
N	-2.57066900	-0.67704700	0.09830200
C	-0.24222300	3.61039100	-0.15620300
C	5.97984000	-1.22551700	-0.60611100
H	5.90054800	0.08826700	1.10336000
C	-3.00811800	-2.01436200	-0.15314900
C	-1.34440700	3.83451000	0.67673600
C	-0.00956600	4.48036700	-1.21958700

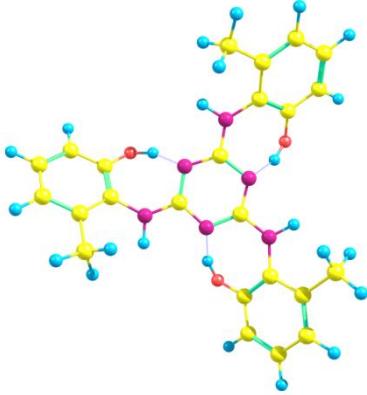
C	-2.64697400	-3.08559300	0.67202400	C	-1.30039800	2.43440000	0.01493800
C	-3.88509000	-2.24158700	-1.21200200	N	1.59055200	0.26054300	0.19826200
C	-2.18059600	4.91973100	0.43920100	C	-0.36901600	-1.51275300	-0.22723600
C	-0.84097600	5.56572300	-1.44794700	C	-1.41420400	3.43060100	-0.95254500
C	-3.17169900	-4.35057900	0.43144100	C	-2.45237800	1.99859300	0.68147900
C	-4.41223600	-3.50252200	-1.44334800	C	1.82301600	-1.04482400	-0.03814700
C	-1.92724100	5.78919500	-0.60978900	N	-1.38081200	-2.39598200	-0.39138300
H	-3.02463400	5.06770000	1.10186700	N	0.88197700	-1.97145000	-0.25174100
C	-4.05844900	-4.55959600	-0.61279100	C	-2.64254800	4.00146800	-1.24754100
H	-2.87446200	-5.15918500	1.08811700	C	-3.68333800	2.56908000	0.37657000
H	7.03999900	-1.08021000	-0.77196100	N	3.11185800	-1.45684500	-0.05050800
H	5.72231800	-2.56377200	-2.27207700	C	-2.73423600	-2.04131100	-0.09146500
H	-4.46504900	-5.54880000	-0.78222200	C	-3.78069000	3.57239800	-0.57459900
H	-5.09433400	-3.65672600	-2.26951000	H	-4.55604100	2.21081800	0.90936200
H	-2.58294500	6.63456200	-0.77696300	C	4.21316300	-0.54652400	-0.09647700
H	-0.64063800	6.23112700	-2.27781400	C	-3.41578000	-1.02848500	-0.77861200
O	-1.81507000	-2.92444300	1.74402500	C	-3.41057900	-2.76656100	0.88765800
H	-1.06718600	-2.36532300	1.44308300	C	4.44184500	0.40670700	0.90338700
O	3.43479000	-0.12063000	1.75239600	C	5.13699800	-0.67248100	-1.13286500
H	2.57744000	0.24970900	1.45308800	C	-4.74873300	-0.76799400	-0.47988600
O	-1.61141400	3.03672200	1.75360900	C	-4.74142100	-2.50757500	1.17671700
H	-1.50198500	2.10855000	1.45590400	C	5.58073300	1.20326900	0.85125500
H	0.84056900	4.30012900	-1.86657400	C	6.27499300	0.11763400	-1.17570100
H	3.30902700	-2.88121600	-1.86417100	C	-5.41450000	-1.50729000	0.48488000
H	-4.15753400	-1.41162800	-1.85290900	H	-5.24715600	0.02295200	-1.02740400
C	-3.57719900	0.38743400	0.04475900	C	6.50052300	1.05497900	-0.17425100
H	-3.40858300	1.10014600	0.84955300	H	5.72898500	1.93116200	1.63969900
H	-3.54924600	0.91664300	-0.90928600	H	-4.74552000	4.01156100	-0.79554500
H	-4.55498000	-0.06509800	0.18203400	H	-2.70858800	4.77582400	-2.00098200
C	2.12427700	2.90519700	0.02633000	H	7.38686000	1.67671400	-0.19537800
H	2.66506500	2.39927900	0.82352300	H	6.98022000	0.00036000	-1.98842500
H	2.55967800	2.62087300	-0.93321500	H	-6.45421300	-1.29600000	0.70144200
H	2.22214900	3.97768900	0.16742600	H	-5.24747400	-3.08376700	1.94062600
C	1.45587100	-3.29242600	0.02891700	O	3.59352400	0.56247500	1.96206700
H	0.74877900	-3.50583600	0.82787800	H	2.68127700	0.55123200	1.59261100
H	0.99043100	-3.52977400	-0.92928000	O	-2.41417800	1.04137000	1.65747700
H	2.33619500	-3.91282100	0.17011700	H	-1.85307800	0.30958100	1.32782200



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C	0.30705100	0.62542600	0.14703800
N	0.00170600	1.92953000	0.32644800
N	-0.70922500	-0.22234000	-0.06435400

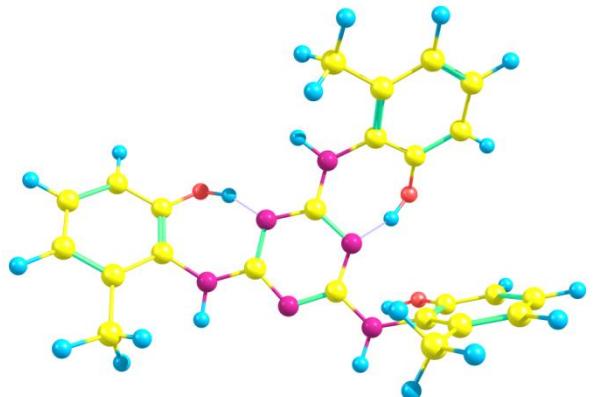
C	-1.30039800	2.43440000	0.01493800
N	1.59055200	0.26054300	0.19826200
C	-0.36901600	-1.51275300	-0.22723600
C	-1.41420400	3.43060100	-0.95254500
C	-2.45237800	1.99859300	0.68147900
C	1.82301600	-1.04482400	-0.03814700
N	-1.38081200	-2.39598200	-0.39138300
N	0.88197700	-1.97145000	-0.25174100
C	-2.64254800	4.00146800	-1.24754100
C	-3.68333800	2.56908000	0.37657000
N	3.11185800	-1.45684500	-0.05050800
C	-2.73423600	-2.04131100	-0.09146500
C	-3.78069000	3.57239800	-0.57459900
H	-4.55604100	2.21081800	0.90936200
C	4.21316300	-0.54652400	-0.09647700
C	-3.41578000	-1.02848500	-0.77861200
C	-3.41057900	-2.76656100	0.88765800
C	4.44184500	0.40670700	0.90338700
C	5.13699800	-0.67248100	-1.13286500
C	-4.74873300	-0.76799400	-0.47988600
C	-4.74142100	-2.50757500	1.17671700
C	5.58073300	1.20326900	0.85125500
C	6.27499300	0.11763400	-1.17570100
C	-5.41450000	-1.50729000	0.48488000
H	-5.24715600	0.02295200	-1.02740400
C	6.50052300	1.05497900	-0.17425100
H	5.72898500	1.93116200	1.63969900
H	-4.74552000	4.01156100	-0.79554500
H	-2.70858800	4.77582400	-2.00098200
H	7.38686000	1.67671400	-0.19537800
H	6.98022000	0.00036000	-1.98842500
H	-6.45421300	-1.29600000	0.70144200
H	-5.24747400	-3.08376700	1.94062600
O	3.59352400	0.56247500	1.96206700
H	2.68127700	0.55123200	1.59261100
O	-2.41417800	1.04137000	1.65747700
H	-1.85307800	0.30958100	1.32782200
O	-2.82459300	-0.28936900	-1.76586300
H	-1.94476600	-0.01309300	-1.43269000
H	-2.87886500	-3.54410700	1.42287300
H	-0.52157700	3.75871700	-1.47175000
H	4.95664900	-1.40720900	-1.90822100
C	3.39394800	-2.86830100	-0.32570900
H	2.77291900	-3.49374500	0.31094700
H	3.19635200	-3.12132600	-1.36889200
H	4.43938000	-3.05555300	-0.09727800
C	1.09104000	2.89364100	0.49813400
H	1.73295400	2.58367800	1.32074300
H	1.69247600	2.98416300	-0.40818100
H	0.65393900	3.85734800	0.74373500
C	-1.05947900	-3.81893100	-0.51658100
H	-0.30171000	-3.95356500	-1.28489600
H	-0.68679300	-4.23111500	0.42304400
H	-1.96271700	-4.34562200	-0.81244500



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C	-0.76199800	-1.05918700	-0.22682200
N	-1.51090600	-2.17672900	-0.24429900
N	-1.36532900	0.12763800	-0.22406900
C	-2.91289600	-2.29111700	-0.05546000
N	0.57182300	-1.24654200	-0.22358500
C	-0.53630300	1.18917400	-0.22687900
C	-3.36913700	-3.24915200	0.86256500
C	-3.82902700	-1.54787200	-0.80879300
C	1.29790100	-0.13061700	-0.22639200
N	-1.12994300	2.39646800	-0.24392300
N	0.79305300	1.11825300	-0.22496300
C	-4.73796800	-3.44851900	1.00216400
C	-5.19333200	-1.75432400	-0.63947100
N	2.64027900	-0.21991800	-0.24333700
C	-0.52782200	3.66761100	-0.05514100
C	-5.64616800	-2.70963600	0.25402000
H	-5.87887100	-1.16203300	-1.23285800
C	3.44063700	-1.37653600	-0.05475500
C	0.57337400	4.08907700	-0.80921500
C	-1.12885700	4.54197900	0.86313300
C	3.25585000	-2.54062900	-0.80950700
C	4.49804500	-1.29319900	0.86372100
C	1.07721900	5.37363900	-0.64003800
C	-0.61697600	5.82709900	1.00223700
C	4.11716100	-3.61877000	-0.64120400
C	5.35579100	-2.37863800	1.00210600
C	0.47691700	6.24367400	0.25364700
H	1.93271000	5.67102200	-1.23383800
C	5.17077600	-3.53379200	0.25250300
H	3.94734500	-4.50799800	-1.23561800
H	-2.13961100	2.36174900	-0.16410000
H	3.11499700	0.67226100	-0.16626200
H	-0.97591400	-3.03382800	-0.16612300
H	-6.70994300	-2.87247200	0.37534700
H	-5.09039300	-4.18905700	1.71000900
H	5.84401700	-4.37347900	0.37296100
H	6.17300000	-2.31410700	1.71036600
H	0.86814500	7.24624300	0.37460300
H	-1.08172100	6.50290300	1.71001100
O	2.27448800	-2.64423000	-1.75459600

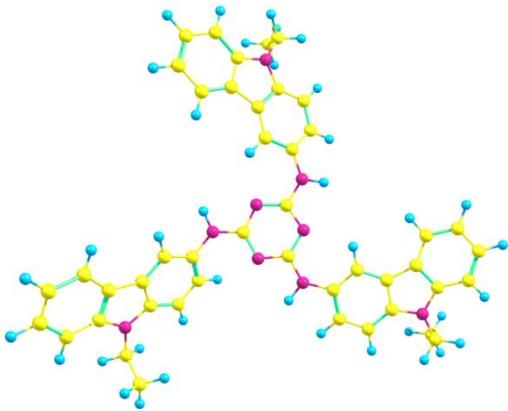
H	1.44961800	-2.26269700	-1.37193100
O	-3.42856500	-0.64542400	-1.75338300
H	-2.68570300	-0.12179200	-1.37007800
O	1.15341700	3.29148500	-1.75493200
H	1.23504600	2.38592200	-1.37359700
C	4.70152800	-0.04444800	1.67368400
H	4.99259300	0.79991000	1.04174500
H	3.78728700	0.24039800	2.19887100
H	5.49035400	-0.19693000	2.40858200
C	-2.31362900	4.09423400	1.67107800
H	-3.18811100	3.92037800	1.03699400
H	-2.10303400	3.16205500	2.19978000
H	-2.57973100	4.85538100	2.40277300
C	-2.38885400	-4.05116500	1.67056700
H	-1.80179500	-4.72255300	1.03690000
H	-1.68623100	-3.40245600	2.19820800
H	-2.91501000	-4.66097400	2.40328400



14-GS2_3H

C	-0.30052800	0.60256800	-0.25800000
N	0.00524900	1.88118100	-0.54511200
N	0.70445100	-0.22253400	0.04916600
C	1.25934000	2.50310300	-0.29098500
N	-1.58685400	0.23983000	-0.31142600
C	0.35230400	-1.49044300	0.32290000
C	1.27148200	3.65945000	0.50166900
C	2.45060400	2.01619200	-0.84227700
C	-1.82495500	-1.03893000	0.01602700
N	1.34799200	-2.35227600	0.61442100
N	-0.89565700	-1.94744900	0.34289900
C	2.48070100	4.31028500	0.72227300
C	3.64998500	2.67156200	-0.59057900
N	-3.10127800	-1.47194200	0.01136100
C	2.73238700	-2.13440500	0.37351200
C	3.66287500	3.82165600	0.18040200
H	4.55658900	2.26653400	-1.02320700
C	-4.28642800	-0.69744000	-0.08455400
C	3.42057000	-1.04835700	0.92913700
C	3.42028500	-3.07916200	-0.40200600
C	-4.50177100	0.20566000	-1.13214800
C	-5.29470000	-0.92634100	0.86418700
C	4.78157700	-0.89480500	0.69230600

C	4.78627400	-2.91627600	-0.60661100	C	-1.03963800	-0.36442000	-0.31806400
C	-5.71284600	0.88131000	-1.22734300	C	-0.43992300	3.86808900	-0.04880400
C	-6.50334500	-0.25039700	0.73876700	C	1.88840100	4.50948900	0.28162400
C	5.46458200	-1.83218400	-0.06397300	C	1.02809400	-1.27439000	-0.17287800
H	5.28394700	-0.03914100	1.12673800	N	-2.39484400	-0.43861700	-0.45083100
C	-6.71471400	0.64568700	-0.30169900	N	-0.30697900	-1.47981200	-0.30870500
H	-5.84872600	1.57730000	-2.04588000	C	-0.77749900	5.22946800	-0.00281300
H	1.05186200	-3.31560600	0.71718800	H	-1.19949700	3.11347200	-0.19333900
H	-3.21080300	-2.42438600	0.33900400	C	1.56499000	5.86039800	0.33011900
H	-0.79296100	2.49291000	-0.67114900	H	2.92829600	4.21049300	0.38769300
H	4.59846400	4.33396200	0.36758400	N	1.76299900	-2.42274600	-0.16492200
H	2.49111400	5.20418000	1.33422700	C	-3.22559800	-1.58878800	-0.51546300
H	-7.65939100	1.16853900	-0.38537100	C	0.21869700	6.22136300	0.18975800
H	-7.28176300	-0.42790800	1.47099800	C	-2.03702900	5.93391800	-0.11938600
H	6.52669800	-1.71315100	-0.23879600	H	2.34517500	6.60161700	0.47002000
H	5.31762300	-3.64641700	-1.20514200	C	3.14887600	-2.66805500	-0.04123900
O	-3.56874300	0.41929700	-2.10774400	C	-2.90326300	-2.69627700	-1.33125400
H	-2.69048000	0.49886500	-1.66653300	C	-4.42584200	-1.56865500	0.20112700
O	2.48225900	0.92506100	-1.66752000	N	-0.37423100	7.47924900	0.21254200
H	1.92701900	0.22406700	-1.26800800	C	-3.36363900	5.52391300	-0.31682800
O	2.80966000	-0.13415100	1.74310500	C	-1.73760300	7.32120600	0.00886400
H	1.95117400	0.10849300	1.33458800	C	3.52978700	-4.03421500	-0.07316900
C	-5.06898200	-1.89522400	1.98969500	C	4.12650400	-1.67763600	0.10266000
H	-4.96474100	-2.91985800	1.62113600	C	-3.75128600	-3.79823200	-1.42262300
H	-4.15869500	-1.65358800	2.54282200	H	-1.98037200	-2.68848300	-1.89750000
H	-5.91057200	-1.87394600	2.68026500	C	-5.29749900	-2.66017600	0.10649900
C	2.68649600	-4.24812300	-0.99553900	C	0.33378200	8.75398500	0.30623300
H	2.30389100	-4.91609100	-0.21841000	C	-4.36745800	6.48933400	-0.38977600
H	1.83254900	-3.91742800	-1.59092900	H	-3.60458600	4.46852500	-0.41372900
H	3.35153000	-4.82629000	-1.63503200	C	-2.74465100	8.29406700	-0.06835500
C	-0.00528900	4.18081100	1.09688900	C	4.85664800	-4.43352200	0.03649900
H	-0.69676900	4.52291400	0.32162600	H	2.75750600	-4.79082800	-0.18802500
H	-0.51737800	3.40677400	1.67264700	C	5.46956600	-2.06946600	0.21401600
H	0.20169000	5.02276900	1.75546400	C	-4.95268500	-3.77656900	-0.70307100

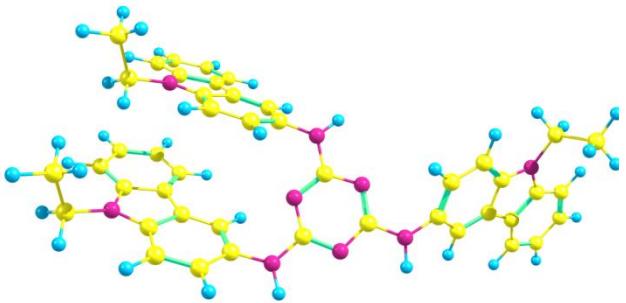


4-GS1

C	0.76881100	0.97357400	-0.06964900
N	1.38973000	2.17932100	0.06334000
N	-0.55797500	0.89939200	-0.20066300
C	0.90365400	3.50558000	0.09472600
N	1.62133500	-0.08408400	-0.05312200

C	-1.03963800	-0.36442000	-0.31806400
C	-0.43992300	3.86808900	-0.04880400
C	1.88840100	4.50948900	0.28162400
C	1.02809400	-1.27439000	-0.17287800
N	-2.39484400	-0.43861700	-0.45083100
N	-0.30697900	-1.47981200	-0.30870500
C	-0.77749900	5.22946800	-0.00281300
H	-1.19949700	3.11347200	-0.19333900
C	1.56499000	5.86039800	0.33011900
H	2.92829600	4.21049300	0.38769300
N	1.76299900	-2.42274600	-0.16492200
C	-3.22559800	-1.58878800	-0.51546300
C	0.21869700	6.22136300	0.18975800
C	-2.03702900	5.93391800	-0.11938600
H	2.34517500	6.60161700	0.47002000
C	3.14887600	-2.66805500	-0.04123900
C	-2.90326300	-2.69627700	-1.33125400
C	-4.42584200	-1.56865500	0.20112700
N	-0.37423100	7.47924900	0.21254200
C	-3.36363900	5.52391300	-0.31682800
C	-1.73760300	7.32120600	0.00886400
C	3.52978700	-4.03421500	-0.07316900
C	4.12650400	-1.67763600	0.10266000
C	-3.75128600	-3.79823200	-1.42262300
H	-1.98037200	-2.68848300	-1.89750000
C	-5.29749900	-2.66017600	0.10649900
C	0.33378200	8.75398500	0.30623300
C	-4.36745800	6.48933400	-0.38977600
H	-3.60458600	4.46852500	-0.41372900
C	-2.74465100	8.29406700	-0.06835500
C	4.85664800	-4.43352200	0.03649900
H	2.75750600	-4.79082800	-0.18802500
C	5.46956600	-2.06946600	0.21401600
C	-4.95268500	-3.77656900	-0.70307100
H	-3.47894700	-4.64153600	-2.04900800
C	-6.58326400	-2.96332400	0.69838500
C	0.77061100	9.30861300	-1.05034100
H	-0.32448300	9.46363200	0.81547500
H	1.20100000	8.60592800	0.95623600
C	-4.05537000	7.85897800	-0.26675900
H	-5.39921800	6.18663200	-0.54438900
H	-2.51932700	9.35221700	0.01935000
C	5.83346300	-3.44059300	0.18561900
H	5.11181200	-5.48776800	0.00415000
C	6.70105200	-1.32408200	0.36985300
N	-5.96783400	-4.72350700	-0.63940400
C	-6.95324000	-4.25191300	0.21718200
H	-0.09199600	9.48711600	-1.70098300
H	1.29373700	10.26100300	-0.90827200
H	1.45153800	8.61820600	-1.55928200
H	-4.85231300	8.59507800	-0.33025100
N	7.21129200	-3.56037700	0.33235900
C	7.75087400	-2.28587200	0.42871900
C	-5.95060600	-6.03754100	-1.27868200

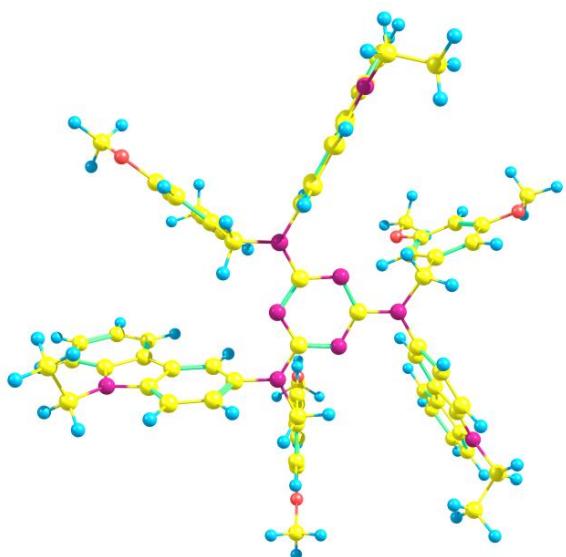
C	-8.15606300	-4.85749300	0.60718400	C	0.77559200	-0.24871200	0.49473800
C	7.97042500	-4.80712800	0.26889300	N	3.78798100	-2.08916300	0.45407900
C	9.08999800	-1.89528000	0.57219200	N	2.10916300	-0.46115200	0.51693800
C	-5.28156700	-7.11809400	-0.42828900	C	-4.14644700	-2.70177300	-0.46190500
H	-6.98574900	-6.31200200	-1.50070600	H	-2.32687800	-1.53736700	-0.60201500
H	-5.43806100	-5.93415900	-2.23944300	C	-3.90954900	-5.03581400	0.24590400
C	-8.98614600	-4.15216300	1.47914500	H	-1.89505200	-5.63329300	0.66780900
H	-8.43692100	-5.84295800	0.24957300	N	0.40543200	1.05791600	0.60034800
C	8.38210700	-5.19655000	-1.15152400	C	4.92480000	-1.23811300	0.48053000
H	7.35718100	-5.59337500	0.71866900	C	-4.71695000	-3.96732000	-0.16345700
H	8.85279800	-4.69200900	0.90491800	C	-5.24436800	-1.84074400	-0.84920800
C	9.36306800	-0.53008800	0.66349700	H	-4.32622600	-6.00901300	0.48432800
H	9.89270000	-2.62495800	0.60952700	C	-0.89652300	1.62646400	0.59699600
H	-4.23646700	-6.86647700	-0.21918900	C	5.01764700	-0.14993900	1.37687700
H	-5.30168000	-8.07379200	-0.96407300	C	5.99879100	-1.55245700	-0.35714900
H	-5.80362300	-7.25042500	0.52525600	N	-6.09227500	-3.91618500	-0.36206500
C	-8.63507900	-2.87416300	1.96002600	C	-5.33013700	-0.50170500	-1.25728100
H	-9.92345500	-4.60188400	1.79557000	C	-6.42720600	-2.63068400	-0.76310400
H	9.01897700	-4.42862100	-1.60319400	C	-1.94674000	1.08039500	1.36823400
H	8.94528100	-6.13632700	-1.12816000	C	-1.09362600	2.80592800	-0.12650400
H	7.50542900	-5.34025000	-1.79194800	C	6.15733700	0.64997800	1.42851500
C	8.33438000	0.43299500	0.61102100	H	4.18917000	0.06333300	2.04091200
H	10.39364400	-0.20386600	0.77504800	C	7.16009700	-0.77167000	-0.30304000
C	-7.43594400	-2.27571500	1.57385600	C	-7.03233800	-5.00206300	-0.09326100
H	-9.30532500	-2.35417300	2.63855400	C	-6.58056800	0.03363100	-1.56569100
C	7.00360300	0.04209700	0.46484700	H	-4.43500000	0.11008100	-1.32880700
H	8.58358500	1.48781900	0.68402100	C	-7.68602500	-2.09305500	-1.06775700
H	-7.16482100	-1.29131000	1.94625400	C	-3.20232600	1.68254600	1.40933500
H	6.21139000	0.78506400	0.42322500	H	-1.77033300	0.17997600	1.94359200
H	3.85031600	-0.63341200	0.12618300	C	-2.34365900	3.43550600	-0.07972500
H	-4.67334900	-0.71184800	0.82254400	C	7.22862300	0.33878600	0.58149300
H	-2.86843000	0.44344400	-0.29528300	H	6.20561800	1.48056700	2.12529600
H	1.19081900	-3.25301100	-0.26499100	C	8.42452600	-0.81489000	-1.00655000
H	2.39398300	2.09151400	0.16388300	C	-7.54129800	-5.02270900	1.34859900



4-GS2

C	0.31115200	-2.44688900	0.28186200	C	-8.06897000	-4.09521600	1.59498000
N	-0.54504700	-3.49959100	0.14765100	H	-8.23848400	-5.85761100	1.48194200
N	1.61434700	-2.78987900	0.31812800	H	-6.71641200	-5.15072800	2.05749400
C	-1.95503100	-3.56238000	0.04940000	H	-8.70791100	-0.32035300	-1.71187200
N	-0.17044500	-1.19497700	0.37198200	N	-4.53878600	3.64712800	0.55303800
C	2.46557100	-1.75058500	0.43120700	C	-4.23258600	4.73558000	-0.25280300
C	-2.76209300	-2.49813200	-0.36437200	C	8.93289800	2.10308600	1.22684600
C	-2.53969700	-4.81785400	0.34937400	C	10.49463700	0.52074700	-0.98343400
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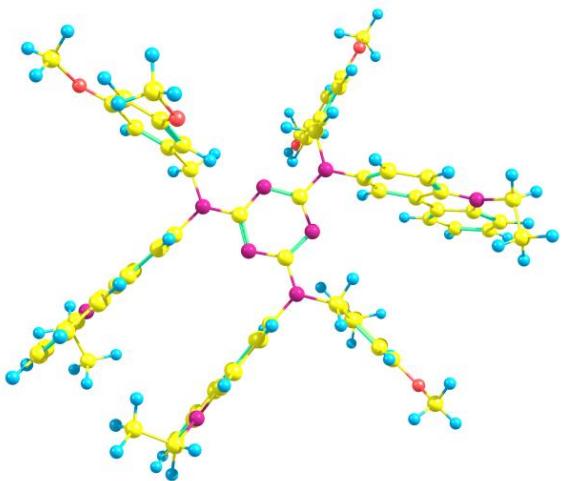
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H	9.60413600	2.69352200	0.59666300	C	-1.01921500	0.77988500	-1.52413400
H	8.07044500	2.73751000	1.45083400	N	-1.30203700	-0.53721100	-1.49779300
C	11.00434300	-0.33427600	-1.96114800	N	2.49986500	0.88906300	-1.57972000
H	11.08930800	1.34512400	-0.60291100	N	-0.44787500	-2.69780400	-1.48815700
C	-5.84713100	4.10154700	2.63400700	N	-2.07998700	1.64791200	-1.53443700
H	-5.95249200	2.35580200	1.35061200	C	2.79636200	3.04575500	-0.43515200
H	-6.60614300	3.81341200	0.62227600	C	3.30885100	4.28270200	-2.94827900
C	-4.48928200	6.77186900	-1.48703800	C	3.08104800	4.41568700	-0.50242200
H	-6.07679400	5.88874400	-0.31621700	C	2.75866800	2.30520500	-1.61578700
H	8.96911700	1.11342500	3.16761300	C	3.01691600	2.92319700	-2.85727500
H	9.96633200	2.57710100	3.06373100	C	3.34212400	5.02644100	-1.76083400
H	10.52194500	1.07293600	2.30469200	C	3.19012000	5.46179900	0.49241400
C	10.24921400	-1.41382100	-2.46330400	C	3.53829200	7.87986700	1.84408200
H	12.00800300	-0.16332000	-2.34108500	C	3.04994200	5.49380600	1.88722700
H	-5.72214500	5.18644200	2.55227700	C	3.51207700	6.65549900	-0.21339600
H	-6.81567500	3.90435000	3.10715700	C	3.68439900	7.87482700	0.45633700
H	-5.06169300	3.71061400	3.28942400	C	3.22540700	6.70456700	2.55688000
C	-3.15172600	6.68571600	-1.92436900	N	3.61635800	6.37341600	-1.56992200
H	-5.10178900	7.61061100	-1.80682800	C	-4.05631200	0.82341600	-0.32376900
C	8.96021700	-1.65852100	-1.99030200	C	-5.47272300	0.66986300	-2.78928100
H	10.67822800	-2.06023400	-3.22365500	C	-5.38733600	0.38778100	-0.34697000
C	-2.34187000	5.62295200	-1.52463200	C	-3.43728600	1.16704200	-1.52477600
H	-2.75028300	7.45635200	-2.57627800	C	-4.14584600	1.09297400	-2.74235300
H	8.37915300	-2.49186000	-2.37651900	C	-6.09105800	0.31825100	-1.58170500
H	-1.31008600	5.55809800	-1.85991400	C	-6.31294500	-0.04566900	0.67836300
H	-0.27923500	3.22739500	-0.71003600	C	-8.53403100	-0.95703600	2.10356500
H	5.92726200	-2.39618300	-1.03861700	C	-6.22175800	-0.19162800	2.06996100
H	3.96461400	-3.06060500	0.22654900	C	-7.53237900	-0.35730000	0.01313500
H	1.17880400	1.71023100	0.54634600	C	-8.65122700	-0.81938200	0.71991400
H	-0.07634000	-4.39761000	0.17330400	C	-7.33467400	-0.64713800	2.77643300
N	-7.38757700	-0.11830200	-1.34794900				
C	1.29326100	-3.96271100	-0.29427600				
C	2.06553600	-5.17221700	-2.75387200				
C	2.34111700	-4.89174300	-0.32568100				
C	0.64753500	-3.63288500	-1.48512000				
C	1.03198600	-4.23921200	-2.69944200				
C	2.71878400	-5.49623800	-1.55710100				
C	3.21581400	-5.44321300	0.68766700				
C	5.17466300	-6.85463900	2.08972000				
C	3.34017100	-5.25224500	2.07122600				
C	4.08160500	-6.35425100	0.01889100				
C	5.07065600	-7.06391000	0.71401500				
C	4.32044700	-5.96024900	2.76618700				
N	3.75831400	-6.38771700	-1.33212400				
C	3.66284600	0.00083700	-1.69643800				
C	-1.79970400	-3.25875700	-1.57809700				
C	-1.89463700	3.09780800	-1.66869100				
C	4.46705000	-7.14666900	-2.36092800				
C	5.65103100	-6.39092000	-2.96519900				
C	-8.39588000	-0.38415100	-2.37236000				
C	-8.34037200	-1.80902100	-2.92432100				
C	3.86391100	7.35193600	-2.62721400				
C	2.58791800	8.00192200	-3.16328100				



5-GS1

C	1.21839800	0.40390200	-1.54758400
N	1.05614000	-0.93199600	-1.52484100
C	-0.22558800	-1.34520100	-1.50230000

H	2.59594800	2.56471000	0.51694200	C	6.68625500	-0.34596900	0.59062600
H	3.49685800	4.74116000	-3.91370800	H	6.37712900	-0.08938800	-1.52237600
H	2.98024300	2.32202200	-3.76135200	C	4.71048500	-0.37953400	1.96178900
H	3.66735600	8.81333200	2.38523700	H	2.83070500	-0.17223200	0.94626100
H	2.80712200	4.58828400	2.43691900	C	6.10802700	-0.44761100	1.86293800
H	3.92102400	8.78849500	-0.07959700	H	6.72122100	-0.57033900	2.74428200
H	3.11843700	6.74541000	3.63710700	C	-2.17364600	3.89650000	-0.40494500
H	-3.50600500	0.88249800	0.60985400	C	-2.81160500	5.13577400	-0.51646300
H	-5.99893700	0.61271500	-3.73655800	C	-1.76172900	3.43721900	0.85011300
H	-3.63865000	1.36701500	-3.66313600	C	-3.02594600	5.91585300	0.62683600
H	-9.38815900	-1.31340000	2.67305400	H	-3.14818800	5.50540500	-1.48090100
H	-5.29687400	0.04592300	2.58889200	C	-1.99078800	4.22229600	1.98554700
H	-9.57951000	-1.06643200	0.21474800	H	-1.27158700	2.47623200	0.96460500
H	-7.27893000	-0.76690200	3.85464400	C	-2.62167900	5.47158100	1.89285400
H	0.99431400	-3.49244500	0.63700200	H	-2.79638000	6.07081100	2.77486900
H	2.35116500	-5.62176500	-3.69922200	O	-3.65705400	7.11665100	0.41516600
H	0.51153000	-3.96353900	-3.61230000	O	-1.55853800	3.68587200	3.17386400
H	5.93421900	-7.39330100	2.64988200	O	4.03731100	-0.46324800	3.15611500
H	2.68298000	-4.56135800	2.59263300	O	8.04096000	-0.39412400	0.37180000
H	5.73872300	-7.75206200	0.20598000	O	-2.26542500	-3.07743100	3.28909900
H	4.43010900	-5.82151000	3.83797900	O	-4.73222100	-6.39921400	0.89285500
H	4.29351300	0.36790400	-2.51224300	C	-5.10136900	-7.04283900	-0.33402100
H	3.29630500	-0.98617800	-1.98369900	H	-4.22933400	-7.49383300	-0.82006800
H	-1.78201100	-4.06675700	-2.31608400	H	-5.80748300	-7.82553400	-0.05285200
H	-2.45981400	-2.47984700	-1.96551200	H	-5.58770500	-6.33881700	-1.01795200
H	-2.55197700	3.45384800	-2.46810900	C	-2.81779100	-3.53198500	4.53133100
H	-0.86570400	3.27118900	-1.98863100	H	-3.90761700	-3.42101300	4.54190400
H	3.74371600	-7.40912200	-3.13814300	H	-2.54654900	-4.57578500	4.72427200
H	4.80132800	-8.08583700	-1.91123500	H	-2.37864200	-2.89300300	5.29889500
H	6.13593300	-7.01324800	-3.72570600	C	4.78969200	-0.61238200	4.36707200
H	6.39523600	-6.14514700	-2.20036600	H	4.04988700	-0.64940500	5.16817700
H	5.32449200	-5.46107300	-3.44266800	H	5.36816700	-1.54264800	4.36130400
H	-8.25318800	0.34382000	-3.17601200	H	5.45668900	0.24224000	4.52498000
H	-9.37692000	-0.18145900	-1.93341500	C	8.91894700	-0.55853100	1.49305700
H	-9.12074400	-1.94106100	-3.68220100	H	8.82418300	0.27771400	2.19441700
H	-8.50579200	-2.54682400	-2.13217600	H	8.72516200	-1.50450500	2.01045100
H	-7.37203400	-2.01459800	-3.39263400	H	9.92695100	-0.57139100	1.07592500
H	4.54115400	8.11094700	-2.22540000	C	-3.91976900	7.96848100	1.53787000
H	4.40222600	6.84344900	-3.43203400	H	-4.41862600	8.84767500	1.12752700
H	2.84297700	8.72136800	-3.94947800	H	-4.58055800	7.47648200	2.25998400
H	2.05381900	8.53703300	-2.37108800	H	-2.98875500	8.27193500	2.02913000
H	1.91299800	7.25346600	-3.59169500	C	-1.77656100	4.41936000	4.38605200
C	-2.36698000	-3.79546500	-0.27186400	H	-1.36608800	3.79660200	5.18232000
C	-3.26551000	-4.87661600	-0.33446600	H	-1.25088300	5.38031200	4.36666700
C	-2.05519600	-3.21451500	0.95384800	H	-2.84572600	4.58084300	4.56258600
C	-3.84517000	-5.35197200	0.84340300				
H	-3.49237600	-5.32712500	-1.29356100				
C	-2.64132700	-3.71142800	2.13085800				
H	-1.36019000	-2.38473100	1.02360000				
C	-3.53929900	-4.77717600	2.08883000				
H	-4.00457200	-5.18199700	2.97930200				
C	4.50326700	-0.11849600	-0.43476000				
C	5.89521600	-0.17648900	-0.55274400				
C	3.90792500	-0.22041400	0.82671500				

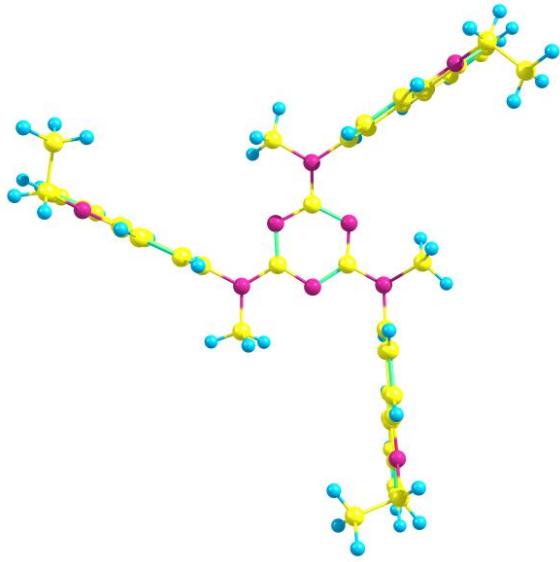


5-GS2

C	0.58248200	1.61234100	0.09388900	C	1.21595600	-2.04836400	-1.52321600
N	0.82529400	0.41663400	-0.47254300	C	2.04503500	-2.25101800	-2.64330400
C	-0.21245500	-0.11275000	-1.14086800	C	3.56318700	-3.52446100	-1.30508100
N	-0.59261100	2.26844600	0.04634500	C	3.37953200	-4.00238700	0.93653200
C	-1.55807300	1.64376600	-0.65523300	C	5.05895200	-5.53225800	2.55484600
N	-1.41540300	0.46948700	-1.29698600	C	3.06017100	-4.16411800	2.29100300
N	1.60707800	2.17808700	0.80166800	C	4.54851800	-4.61669000	0.40377500
N	-0.02667200	-1.34719100	-1.71084500	C	5.39787000	-5.38587500	1.20924300
N	-2.78866000	2.24421700	-0.71864900	C	3.90476400	-4.92923700	3.09597300
C	3.72666000	1.43608000	-0.20581200	N	4.63799100	-4.32746300	-0.95246700
C	4.50240000	0.36392000	2.31904900	C	1.49567700	3.50298200	1.41894300
C	4.96002300	0.79226600	-0.06137400	C	-1.19832800	-2.17615800	-2.09195900
C	2.88236000	1.52307300	0.90021100	C	-3.15045500	3.34445700	0.19083500
C	3.26855200	0.98887400	2.14575400	C	5.74646300	-4.67229400	-1.83845600
C	5.34944000	0.27766000	1.20741700	C	6.80176600	-3.56982600	-1.90560900
C	6.04809500	0.50505800	-0.97102500	C	-7.38309600	-0.38527400	-4.79323200
C	8.43567900	-0.33201000	-2.14891400	C	-6.63138900	-1.51105600	-5.50304400
C	6.25315700	0.73510300	-2.33796700	C	7.31390800	-0.97411600	2.18473700
C	7.05215700	-0.15296800	-0.20487000	C	6.89404100	-2.43943600	2.27867900
C	8.25402300	-0.57524600	-0.78722000	H	3.41680500	1.84424200	-1.16185200
C	7.44831800	0.31353600	-2.92152800	H	4.78391700	-0.04855200	3.28223000
N	6.62243600	-0.26451300	1.11141800	H	2.58145500	1.06429300	2.98358800
C	-4.76855200	0.78324700	-0.76741600	H	9.35616700	-0.65808100	-2.62544700
C	-5.02368700	1.26967700	-3.56252100	H	5.48904000	1.23137100	-2.93032200
C	-5.80354700	0.18924100	-1.49614500	H	9.01336700	-1.08939900	-0.20731700
C	-3.86571300	1.61150000	-1.43424400	H	7.62118200	0.48011000	-3.98094300
C	-4.00370600	1.85707900	-2.81519800	H	-4.65383300	0.57899400	0.29005700
C	-5.92612700	0.43350400	-2.89164900	H	-5.10448400	1.45428800	-4.62870900
C	-6.86216800	-0.72952800	-1.14231300	H	-3.28296700	2.50621100	-3.30367300
C	-9.03006700	-2.48482000	-1.15470300	H	-9.86836000	-3.17621300	-1.14261100
C	-7.25423400	-1.33786600	0.05777800	H	-6.71536900	-1.13184900	0.97699900
C	-7.57631200	-1.00107800	-2.34348100	H	-9.19821200	-2.10725700	-3.27874500
C	-8.66205500	-1.88665100	-2.36134400	H	-8.65436000	-2.69788000	0.96525900
C	-8.33924700	-2.21446900	0.04487300	H	0.92407300	-2.40309600	0.58231100
N	-7.01784100	-0.26851600	-3.38410200	H	3.85949400	-3.12892300	-3.42306500
C	1.56396600	-2.56910400	-0.27683900	H	1.74783500	-1.82323700	-3.59640900
C	3.22822000	-2.98473800	-2.55258900	H	5.70598500	-6.11902500	3.20120100
C	2.74468000	-3.30689800	-0.16123800	H	2.16873800	-3.69848800	2.70266400
				H	6.29677200	-5.84313500	0.80898700
				H	3.67446900	-5.06207700	4.14920000
				H	1.87850600	3.44325100	2.44199300
				H	0.43632500	3.75811300	1.47786200
				H	-0.83327000	-2.93745600	-2.78422700
				H	-1.91419600	-1.54662800	-2.62024600
				H	-3.80668200	4.02661000	-0.35550900
				H	-2.23755000	3.88484100	0.44440300
				H	5.33055800	-4.87158200	-2.83087600
				H	6.18253900	-5.60951300	-1.48326000
				H	7.59804900	-3.85125500	-2.60359400
				H	7.24964900	-3.40022200	-0.92248700
				H	6.36134600	-2.62842000	-2.24813200
				H	-7.18213200	0.57697600	-5.27251500
				H	-8.46332400	-0.54646300	-4.84665800
				H	-6.93734800	-1.56177800	-6.55384900

H	-6.84578800	-2.47744000	-5.03438400
H	-5.55021200	-1.34007000	-5.46671100
H	8.38889000	-0.88622000	2.00680500
H	7.10388600	-0.44894900	3.12156500
H	7.41285700	-2.92848900	3.11049500
H	7.14099900	-2.97371600	1.35725600
H	5.81635400	-2.52747700	2.44647700
C	-1.83465700	-2.81215800	-0.86928000
C	-1.32188000	-4.01783500	-0.35692300
C	-2.84604200	-2.13669600	-0.19172300
C	-1.81071500	-4.50005800	0.85892300
H	-0.53475400	-4.53355000	-0.89122800
C	-3.32939700	-2.63567700	1.02761700
H	-3.23767300	-1.20515000	-0.575557500
C	-2.81926700	-3.81920600	1.56330700
H	-3.16127100	-4.22623400	2.50705900
C	2.24854800	4.57695900	0.65324200
C	2.99319500	5.53053700	1.35108600
C	2.18610800	4.62366800	-0.74295600
C	3.66841500	6.53601600	0.64709300
H	3.06609400	5.50121500	2.43432000
C	2.86991700	5.62856500	-1.43343500
H	1.62616500	3.88445500	-1.30565700
C	3.61882500	6.59981700	-0.75177700
H	4.14786700	7.37193300	-1.29088800
C	-3.84858200	2.85276800	1.44915900
C	-5.12752300	3.31649100	1.76026100
C	-3.23883500	1.88748000	2.26067000
C	-5.79701300	2.81230900	2.88396800
H	-5.62582500	4.04808200	1.13118900
C	-3.92156900	1.38539000	3.37130000
H	-2.25216500	1.50089800	2.03049700
C	-5.20796100	1.84035500	3.70166400
H	-5.73089500	1.44571300	4.56044500
O	-7.05187400	3.32312900	3.10301300
O	-3.25860700	0.42486200	4.09363400
O	2.75610900	5.58886100	-2.80145800
O	4.37496800	7.42531100	1.41799600
O	-4.28968400	-1.86770300	1.63112300
O	-1.35174700	-5.64467600	1.46771700
C	-0.20406100	-6.29921400	0.90658000
H	0.65517200	-5.61966500	0.86681600
H	0.01784000	-7.12965400	1.57880100
H	-0.41924700	-6.68892500	-0.09485200
C	-4.85439200	-2.31718300	2.86765400
H	-5.37026500	-3.27579200	2.73691700
H	-4.08579600	-2.41095200	3.64204400
H	-5.57388300	-1.55134300	3.15919900
C	3.42945100	6.58653800	-3.58129900
H	3.19462600	6.35344900	-4.62105300
H	3.06268500	7.59089800	-3.34012800
H	4.51423400	6.53897800	-3.43196600
C	5.11752600	8.46641800	0.76819200
H	5.88529300	8.04958500	0.10633100

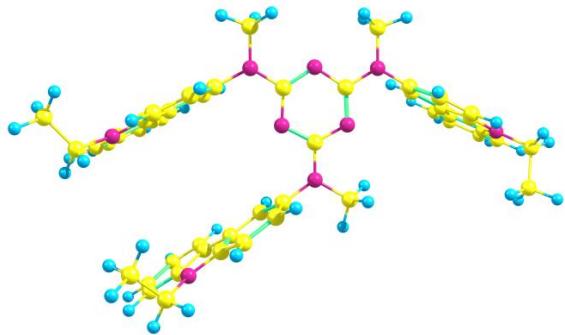
H	4.45466700	9.12957200	0.20063100
H	5.59560000	9.02991600	1.57093400
C	-7.81301000	2.83167000	4.21519200
H	-8.76106500	3.37067200	4.18236800
H	-7.99988000	1.75571800	4.12067500
H	-7.30598400	3.04107600	5.16410500
C	-3.81045600	-0.00186100	5.34710000
H	-3.09617100	-0.72043000	5.75194300
H	-3.91081100	0.84472200	6.03625800
H	-4.78113800	-0.49075700	5.21536900



6-GS1

C	-0.88587400	0.96750900	-0.26920600
N	-1.80418000	1.97989800	-0.23868500
N	-1.35270500	-0.29970500	-0.27481200
C	-1.36633800	3.37780400	-0.31575500
C	-3.20676200	1.71821400	-0.42964400
N	0.41243900	1.31942600	-0.27926700
C	-0.39881100	-1.24846000	-0.27838000
H	-2.22387600	4.01517800	-0.09655400
H	-0.98315400	3.63221600	-1.31246800
H	-0.58303800	3.57795400	0.41820700
C	-4.05409900	1.63774900	0.67395200
C	-3.72109600	1.60675900	-1.73855600
C	1.27669200	0.28159700	-0.28378900
N	-0.81588100	-2.54997700	-0.25570800
N	0.93191900	-1.01886600	-0.29099600
C	-5.42439300	1.43299300	0.46455400
H	-3.64998800	1.72901000	1.67818000
C	-5.07991400	1.40396300	-1.97171900
H	-3.03766400	1.67587700	-2.58008500
N	2.61245200	0.57168400	-0.27122100
C	-2.24608400	-2.86967500	-0.32297700
C	0.11234900	-3.63370600	-0.44446000
C	-5.93048900	1.32063500	-0.86063100
C	-6.56074800	1.29728100	1.35111800

H	-5.45621000	1.31305700	-2.98552600	C	4.84485600	6.64291000	-1.96804400
C	3.60441800	-0.50533100	-0.35836400	C	5.04901200	6.29670000	3.28131700
C	3.08446100	1.91898600	-0.45532100	H	4.25667100	4.28873600	3.37215600
H	-2.36608000	-3.93413800	-0.11768500	C	5.31879600	7.29300900	1.06144800
H	-2.66810800	-2.65136800	-1.31238200	C	4.63624200	-6.91425200	-2.35541200
H	-2.80474500	-2.30282600	0.42475600	H	3.41747900	-8.59821000	-1.73460500
C	0.60889800	-4.32242100	0.66074200	H	2.59244300	-7.48165800	-2.80933700
C	0.46436200	-4.02769000	-1.75254800	C	3.72541500	-8.34963000	2.44836200
N	-7.30618200	1.14147700	-0.81365500	H	3.05864000	-7.59280300	4.36169900
C	-6.71259400	1.31886400	2.74497700	H	4.25038600	-8.91211300	0.42847400
C	-7.69998700	1.10808200	0.51839100	C	3.62119200	7.48721400	-2.32588200
H	4.58812100	-0.07827500	-0.15904700	H	5.69897400	7.28552400	-1.73629800
H	3.61649000	-0.96981200	-1.35280400	H	5.14111900	6.01819900	-2.81555300
H	3.40075900	-1.28016400	0.38362300	C	5.42755100	7.37086500	2.45038700
C	3.45776900	2.68027100	0.65074700	H	5.14619800	6.39277300	4.35897200
C	3.22365900	2.43488300	-1.76105100	H	5.60882900	8.13043500	0.43501000
C	1.47090000	-5.40751900	0.45380900	H	5.35597200	-6.98786300	-1.53329600
H	0.32833700	-4.01538500	1.66429300	H	5.05247000	-7.44001800	-3.22204200
C	1.32046600	-5.10282400	-1.98332300	H	4.51988900	-5.85803600	-2.62035400
H	0.06068800	-3.47382500	-2.59530000	H	4.33318800	-9.13184500	2.89514800
C	-8.17620000	0.91586300	-1.96643300	H	3.33074200	8.13577500	-1.49259900
C	-7.98546100	1.14984700	3.28934900	H	3.85119100	8.12222200	-3.18877500
H	-5.85034600	1.46439900	3.39035600	H	2.76637300	6.85419800	-2.58638500
C	-8.97987300	0.93259000	1.06297700	H	5.81071600	8.28314500	2.89959800
C	3.96296400	3.97132900	0.44738500				
H	3.35232300	2.27296400	1.65229400				
C	3.72266300	3.71603400	-1.98809600				
H	2.92777900	1.81759200	-2.60446100				
C	1.81987300	-5.79373800	-0.87055900				
C	2.15777500	-6.32098600	1.34263200				
H	1.58572300	-5.38679500	-2.99661200				
C	-8.30460700	-0.55862300	-2.35060100				
H	-9.15749200	1.33707000	-1.73016700				
H	-7.77798300	1.49610400	-2.80349400				
C	-9.10379000	0.95834400	2.45255900				
H	-8.11895100	1.16332500	4.36730400				
H	-9.84950700	0.77971100	0.43189400				
C	4.09502800	4.48159500	-0.87443200				
C	4.43015700	5.01242000	1.33814200				
H	3.81425700	4.09868200	-2.99944000				
N	2.66360700	-6.89461700	-0.82082400				
C	2.21727800	-6.45869600	2.73689400				
C	2.89039700	-7.21543400	0.51186800				
H	-8.72830200	-1.14615900	-1.52928400				
H	-8.96697700	-0.65720800	-3.21789700				
H	-7.33090700	-0.98466400	-2.61466600				
H	-10.08617900	0.82513200	2.89754400				
N	4.62733300	5.76263200	-0.82157100				
C	4.55006200	5.11612000	2.73141900				
C	4.82057200	6.10371500	0.51135900				
C	3.29383600	-7.53776100	-1.97205700				
C	3.00146700	-7.47430100	3.28341200				
H	1.66064500	-5.78304400	3.38098900				
C	3.68325500	-8.23422100	1.05840400				



6-GS2

C	-1.08974100	0.14202900	-0.96327300
N	-0.86692700	-1.20006000	-0.81685600
N	-0.01325900	0.95213700	-1.01867400
C	-1.99131300	-2.14192000	-0.83520100
C	0.45067300	-1.75652800	-0.98087000
N	-2.37367200	0.54381000	-1.02594400
C	-0.30378400	2.26269600	-1.12994800
H	-1.62371500	-3.11599600	-0.50932600
H	-2.42349400	-2.24574600	-1.83917700
H	-2.77710000	-1.81650200	-0.15103200
C	1.22313900	-2.05812800	0.13903000
C	0.92047200	-2.05467000	-2.27723800
C	-2.54103300	1.87742700	-1.13651800
N	0.74006700	3.14282300	-1.20369800
N	-1.54641300	2.78523100	-1.18483800
C	2.47842500	-2.65409100	-0.04208600
H	0.85193700	-1.82900400	1.13389400

C	2.16374500	-2.64966900	-2.48236800	H	-7.26139400	-0.32958200	-2.72998800
H	0.29640200	-1.80994500	-3.13204100	C	-7.26781700	0.09635600	1.72401300
N	-3.81939500	2.35104200	-1.21689500	N	5.97378500	1.69644500	0.14577800
C	0.48958700	4.58597900	-1.28049900	C	5.89712200	1.72222500	1.53278300
C	2.08517500	2.72951700	-0.89958000	H	6.62872700	-2.53228700	-2.15592600
C	2.93946500	-2.95251800	-1.35492500	H	6.51383500	-3.23459900	-3.78107700
C	3.51859600	-3.08714300	0.86673200	H	5.35482500	-1.99219200	-3.27049800
H	2.51041500	-2.86564600	-3.48779000	H	6.74922700	-4.49886900	2.48360000
C	-4.07548200	3.79310800	-1.29260900	N	-8.31094800	-0.79665700	-0.11465100
C	-4.94935900	1.49278500	-0.97378600	C	-8.34824500	-0.71302600	1.27177700
H	1.42592400	5.08005200	-1.54408000	C	7.18437400	1.46008000	-0.63847600
H	0.13541800	4.99102400	-0.32337700	C	6.89574000	1.46743300	2.48302000
H	-0.25325600	4.80811600	-2.04891400	C	-9.21192100	-1.59204400	-0.94677400
C	2.99746400	2.51368700	-1.95164800	C	-9.25819000	-1.28376200	2.17260100
C	2.49457500	2.61439900	0.42910900	C	7.99612200	2.72940500	-0.89963700
N	4.18776300	-3.55486000	-1.27793100	H	7.78905800	0.72177000	-0.10416800
C	3.65918800	-3.06705700	2.26177500	H	6.88231700	0.99777500	-1.58227400
C	4.55848000	-3.62890400	0.05903200	C	6.54617500	1.55110200	3.83133200
H	-5.12738600	3.93815800	-1.54246200	H	7.90938600	1.21630100	2.18739900
H	-3.86709800	4.29605100	-0.33948700	C	-8.73710600	-3.03102500	-1.15150000
H	-3.46331600	4.25478300	-2.07029700	H	-9.31364700	-1.08130700	-1.90856200
C	-5.62582600	0.91022400	-2.06433800	H	-10.19895700	-1.57782600	-0.47604000
C	-5.40428500	1.29707200	0.33013600	C	-9.07527800	-1.02625900	3.53173600
C	4.32545800	2.16827600	-1.70428200	H	-10.07825800	-1.90780300	1.83194000
H	2.65221800	2.62102400	-2.97587300	H	7.40938400	3.46597800	-1.45868700
C	3.82264600	2.26466300	0.70253900	H	8.88589900	2.48279900	-1.48977600
C	5.00875800	-3.96581400	-2.41566900	H	8.32576100	3.18857500	0.03829200
C	4.82482400	-3.57850300	2.83162500	C	5.23656200	1.88215900	4.23449600
H	2.87151000	-2.65723000	2.88846300	H	7.30379800	1.35865500	4.58619800
C	5.73280400	-4.14041100	0.62890000	H	-8.65460300	-3.55991500	-0.19612800
C	-6.75758100	0.11759500	-1.87928400	H	-9.45534100	-3.57031400	-1.77927700
H	-5.24931000	1.08279100	-3.06837200	H	-7.76161700	-3.05884900	-1.64836800
C	-6.53923300	0.50376900	0.54121700	C	-8.01257900	-0.22344400	3.99368800
C	4.73126200	2.03871600	-0.36952500	H	-9.76828900	-1.45784100	4.24890100
H	5.01504000	2.00918900	-2.52691000	C	4.24586600	2.13852400	3.28680000
C	4.57139100	2.06207400	1.92505500	H	5.00013200	1.93921600	5.29320900
C	5.93000200	-2.86054300	-2.93252400	C	-7.10646600	0.33979100	3.09547000
H	5.59225800	-4.83789300	-2.10685100	H	-7.89975300	-0.04478400	5.05922700
H	4.33429700	-4.30313900	-3.20782300	H	3.23664000	2.39533100	3.59775600
C	5.84785000	-4.10820200	2.01910700	H	-6.28639500	0.95744800	3.45205100
H	4.94897900	-3.56816700	3.91073000	H	-4.87985200	1.75395900	1.16475100
H	6.53092400	-4.54669900	0.01568900	H	1.78750500	2.79143700	1.23474800
C	-7.21337700	-0.07871100	-0.56879800				

Transition structure calculations

The geometries of all compounds have been fully optimized and the corresponding transition states were localized using B3LYP [2] functional with 6-31+G(d,p) basis set [3] or using M06-2X [4,5] functional with TZVP [6] basis set. All ground state structures were optimized without restrictions and using an ultrafine grid in the computation of two-electron integrals and their derivatives. Solvent effect was included implicitly to the optimizations via the SMD [7] model with the built in parameters for solvents (DMF or CH₃CN). The nature of all critical points was confirmed by means of the vibrational analysis.

The ΔH , ΔS and ΔG values were calculated at T = 298.15 K at the same level of theory including zero-point energy in the particular solvent environment (represented by relative permittivity) and vibrational, rotational and translational thermal energy corrections.

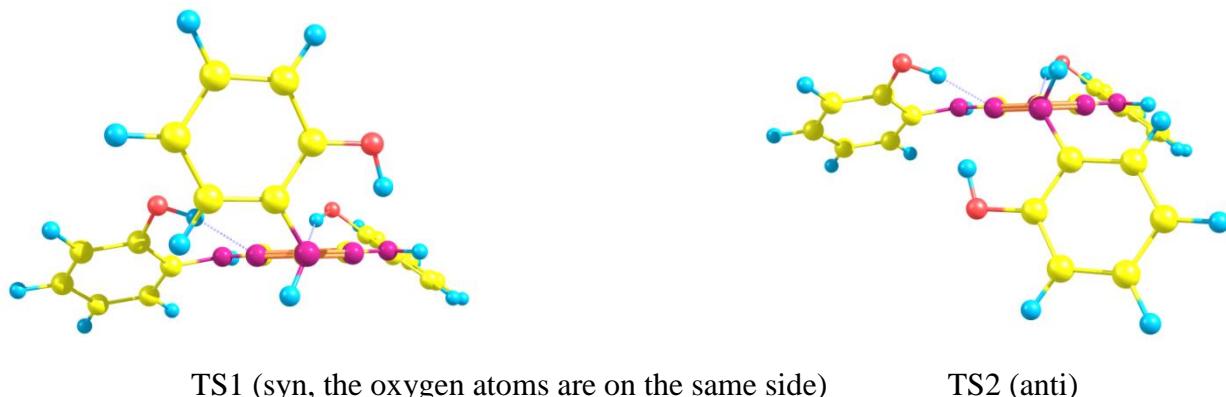


Figure S25. The transition states (TS) structures of **11** regarding rotation around triazine-N bond.

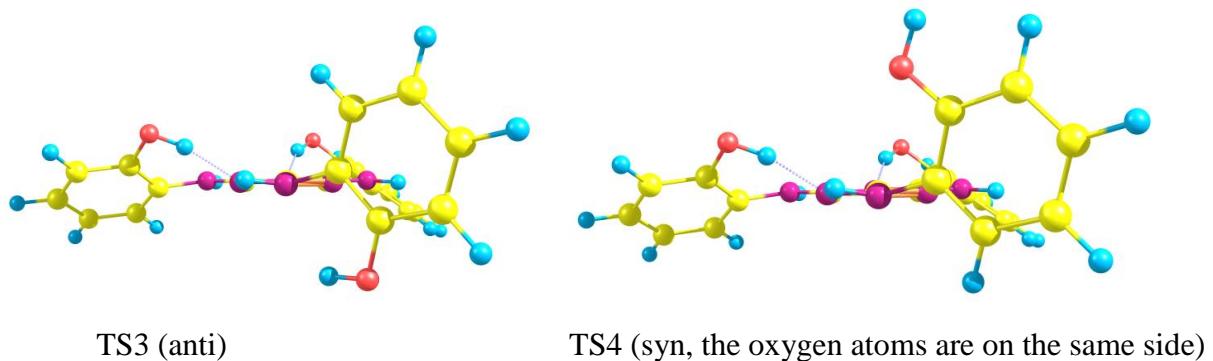
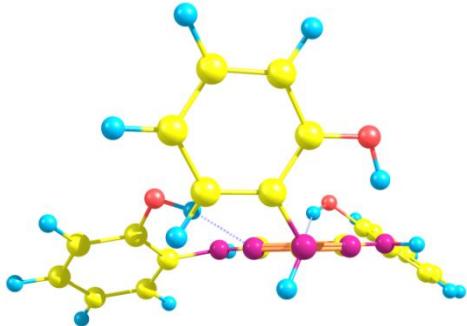


Figure S26. The transition states (TS) structures of **11** regarding rotation around N-Ph bond.

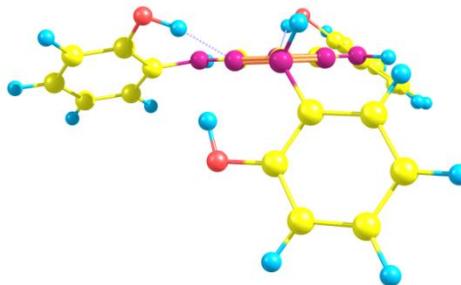
Cartesian coordinates of the
SMD(DMF)//M062X/TZVP optimized TS geometries
for **11-14** and SMD(DMF)//B3LYP/6-31+G(d,p)
optimized geometries for **4-6**:



11-TS1 (syn)

C	0.15184100	0.83222000	-0.22414300
N	-0.13655300	2.06788800	0.21320300
N	-0.82459800	0.07515100	-0.74304400
C	-1.34359100	2.79386900	0.03851700
N	1.42575600	0.43017000	-0.09448800
C	-0.45152800	-1.14837500	-1.11787700
C	-1.23872900	4.11669300	-0.38896200
C	-2.60324500	2.27558100	0.36240700
C	1.68320700	-0.80250900	-0.52104700
N	-1.46729800	-2.01652200	-1.62502400
N	0.75781600	-1.64679300	-1.04307000
C	-2.36014800	4.92167800	-0.49702600
C	-3.72721700	3.08527200	0.23152400
N	2.93221900	-1.28764900	-0.44009700
C	-2.49534200	-2.28063500	-0.66538100
C	-3.61123500	4.40158000	-0.18379700
H	-4.69021900	2.65885500	0.48500000
C	4.12823600	-0.58446200	-0.14517000
C	-2.20865200	-3.18858600	0.35874700
C	-3.75309000	-1.69512800	-0.72875400
C	4.27137100	0.25677000	0.96444800
C	5.23033800	-0.82788100	-0.96434300
C	-3.16655900	-3.48116700	1.31910600
C	-4.72024700	-2.00025500	0.22062900
C	5.50402100	0.85349700	1.21241400
C	6.45836500	-0.24710500	-0.69807800
C	-4.41891600	-2.88530500	1.24906500
H	-2.91999600	-4.18459700	2.10500400
C	6.59458500	0.59839100	0.39787900
H	5.58659400	1.50402500	2.07459000
H	-1.87287000	-1.59609100	-2.45864400
H	3.05305700	-2.19517000	-0.87529700
H	0.66887400	2.61633100	0.49350100
H	-4.49724200	5.01834400	-0.26689400
H	-2.25640300	5.94781000	-0.82510800
H	7.54789800	1.06323800	0.61583500
H	7.30234600	-0.45301700	-1.34355400
H	-5.16296800	-3.12102100	1.99967900

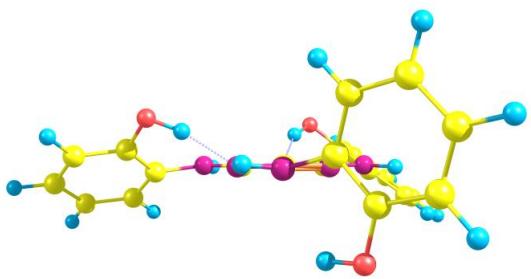
H	-5.69818200	-1.54002100	0.16183800
O	3.26345100	0.47713700	1.85796800
H	2.42757100	0.59707900	1.35033900
O	-2.77753900	1.01615700	0.86015300
H	-2.21400600	0.40101900	0.33756900
O	-0.99153400	-3.79951500	0.44178800
H	-0.47004300	-3.61030400	-0.35584300
H	-3.96178700	-0.99348400	-1.52905000
H	-0.25551800	4.50572600	-0.62758000
H	5.10571200	-1.48950700	-1.81395400



11-TS2 (anti)

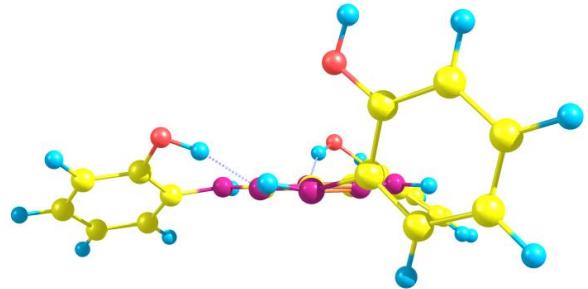
C	-0.15075700	-1.10985400	-0.31475400
N	-0.47990600	-2.37462600	-0.00954200
N	-1.12063400	-0.24358900	-0.65062200
C	-1.77228900	-2.91233800	0.23001700
N	1.15116100	-0.79585600	-0.26809100
C	-0.70221300	0.98424000	-0.94957200
C	-1.91957100	-3.73550600	1.34594000
C	-2.85732500	-2.73287800	-0.63680200
C	1.44789400	0.46609100	-0.57265500
N	-1.73337700	1.90257000	-1.31822300
N	0.53863700	1.40649200	-0.92018500
C	-3.11853600	-4.37638000	1.60706900
C	-4.06469200	-3.36565600	-0.35557400
N	2.72830700	0.87027000	-0.55042800
C	-1.79143800	3.06890900	-0.49570000
C	-4.19677400	-4.19084500	0.74858900
H	-4.88911800	-3.20720400	-1.04009100
C	3.85913400	0.18254900	-0.04016100
C	-2.36835300	2.93225000	0.77049900
C	-1.34410600	4.31559000	-0.91179300
C	4.17264800	-1.13933600	-0.37855400
C	4.73829300	0.90750500	0.76405900
C	-2.46386100	4.02693900	1.61719200
C	-1.45679000	5.41861800	-0.07442900
C	5.34153000	-1.71056800	0.11540500
C	5.90931200	0.33815300	1.23393500
C	-2.00640800	5.26782900	1.19330200
H	-2.91196000	3.89443300	2.59440100
C	6.21175700	-0.97935500	0.90647700
H	5.55772700	-2.73625300	-0.15766800
H	-1.61651900	2.15997600	-2.29578700
H	2.85078400	1.86570600	-0.69857900

H	0.29306900	-2.93819900	0.32711600
H	-5.14175200	-4.68292700	0.94161700
H	-3.20879000	-5.01524200	2.47598700
H	7.12196400	-1.43910200	1.27040100
H	6.57981100	0.92013900	1.85285700
H	-2.08805000	6.12027200	1.85614300
H	-1.10825600	6.38733000	-0.40879300
O	3.40625000	-1.88550900	-1.22680200
H	2.46071300	-1.73100800	-0.99827300
O	-2.77271100	-2.00110100	-1.78541900
H	-2.26033600	-1.18142600	-1.58376200
O	-2.84142400	1.72556400	1.20000400
H	-2.88282900	1.10648600	0.45225600
H	-0.90551200	4.40990200	-1.89879500
H	-1.06881700	-3.86999700	2.00411700
H	4.48691700	1.93291200	1.00929400



11-TS3 (anti)

H	-5.74901500	-2.52165100	1.77315200
C	0.59806900	6.26756500	0.40921100
H	2.09771900	5.65474400	-1.01316300
H	-1.10622400	-3.00553100	-0.09189700
H	-2.07304000	2.44025900	0.03183100
H	3.12919300	0.59850600	-0.08180400
H	5.80011000	-4.42965100	0.65537700
H	6.24202100	-2.24197900	1.75968400
H	1.00550700	7.26302000	0.53351200
H	-1.02780100	6.56520300	1.78983300
H	-6.85147100	-2.03948200	-0.39600600
H	-5.48051200	-1.57859400	-2.41348100
O	1.30844600	3.29401300	-1.56693500
H	1.32765600	2.37550200	-1.19849300
O	2.13821000	-2.85671600	-1.43564800
H	1.34610500	-2.38147500	-1.07624700
O	-3.21577900	-2.59224000	2.18774600
H	-2.24990400	-2.54630700	2.12126300
H	-2.99966000	-1.61590700	-2.23820600
H	4.69497800	-0.35077100	1.37834200
H	-1.92498300	4.28083400	1.48348500

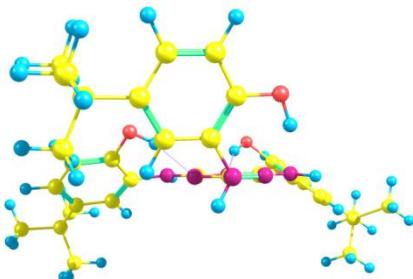


11-TS4 (syn)

C	1.28601800	-0.15027500	-0.11957200
N	2.62765300	-0.27866100	-0.16236300
N	0.52658600	-1.24165400	-0.07842800
C	3.40441200	-1.44171500	0.07315700
N	0.81519800	1.10836500	-0.13621200
C	-0.80271000	-1.01309000	-0.06400900
C	4.51657400	-1.30929900	0.90424100
C	3.16325400	-2.67005200	-0.55538600
C	-0.51533500	1.21224600	-0.10116600
N	-1.58380900	-2.11307700	-0.03793900
N	-1.37451600	0.18359300	-0.06033900
C	5.38187900	-2.36950200	1.11523800
C	4.02639800	-3.73662300	-0.32090100
N	-1.07040100	2.44241300	-0.11375800
C	-3.00275700	-2.08160900	-0.15722300
C	5.13461700	-3.59036900	0.49690800
H	3.81449100	-4.67646100	-0.81625600
C	-0.43345500	3.69497800	0.07262300
C	-3.77673800	-2.33167400	0.97638900
C	-3.62074100	-1.81076600	-1.37192900
C	0.70317700	4.09434200	-0.64216500
C	-1.04038000	4.59961300	0.94387500
C	-5.16472300	-2.32024600	0.88378600
C	-5.00350900	-1.79023800	-1.46544900
C	1.21526700	5.37421500	-0.45088900
C	-0.53685700	5.87852400	1.11237800
C	-5.77032000	-2.04895300	-0.33227700

C	-1.26269700	0.24320700	0.00375200
N	-2.57487400	0.52846700	0.13360100
N	-0.88415100	-1.01854500	-0.17453200
C	-3.68177700	-0.31949000	-0.12589300
N	-0.42321100	1.29014200	0.08064600
C	0.44974300	-1.21075700	-0.26391300
C	-4.73686700	0.21290200	-0.86651600
C	-3.80026900	-1.61298000	0.39876400
C	0.87145700	0.98286900	-0.03319500
N	0.84575500	-2.48368700	-0.44277700
N	1.36576300	-0.25035700	-0.20545300
C	-5.89378100	-0.51479800	-1.08880000
C	-4.95787300	-2.34549300	0.15231700
N	1.78132300	1.97838000	0.03540000
C	2.20801200	-2.89303900	-0.40572100
C	-6.00418500	-1.80208400	-0.57459000
H	-5.02111900	-3.34486500	0.56553600
C	1.55991100	3.37722200	-0.03070900
C	2.76147800	-3.30730100	0.80698800
C	2.98514900	-2.88578300	-1.55450700
C	0.62361800	4.04845700	0.76658300
C	2.39325000	4.11862500	-0.86838700

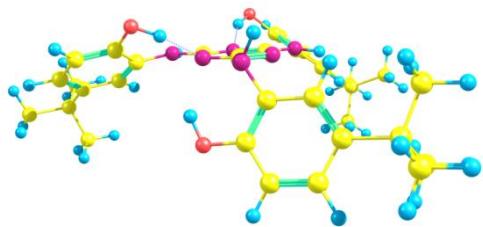
C	4.08821800	-3.72041700	0.85616500	C	4.54603800	-0.94253800	-0.36433400
C	4.31231000	-3.29030000	-1.50801900	C	-1.63476600	-4.03508400	0.14896900
C	0.53138700	5.43516700	0.69043300	C	-3.20903100	-2.40583700	-0.67297700
C	2.30929600	5.49973800	-0.92257700	C	4.67752400	-0.06029700	0.71527200
C	4.85649100	-3.70914500	-0.29922900	C	5.64573600	-1.15105300	-1.18931800
H	4.50550600	-4.04607000	1.80244400	C	-2.54740800	-4.39955200	1.13022100
C	1.37253600	6.16151000	-0.13637400	C	-4.13974400	-2.75678700	0.30053300
H	-0.20407700	5.92770400	1.31498900	C	5.88392100	0.59561100	0.91878900
H	0.12563900	-3.19071400	-0.35485000	C	6.85195500	-0.50603700	-0.96242700
H	2.72844400	1.68067100	-0.16655300	C	-3.77730700	-3.76455600	1.20154200
H	-2.78408600	1.52003700	0.15236600	H	-2.28280800	-5.18566500	1.82715400
H	-6.90091300	-2.38481700	-0.74394100	C	6.99340900	0.38543600	0.10142000
H	-6.70197100	-0.07852300	-1.66144700	H	5.93400400	1.27311400	1.76350800
H	1.29223200	7.24075800	-0.17050300	H	-1.45922200	-2.23465600	-2.53433100
H	2.97093600	6.05371900	-1.57592000	H	3.53879100	-2.61932200	-1.03873100
H	5.88927000	-4.03164100	-0.25094500	H	0.91960800	2.08150100	0.32526500
H	4.91424500	-3.28258900	-2.40725500	H	-2.35058900	5.13836200	-0.90871400
O	-0.17779800	3.40119000	1.66065100	H	7.67711800	-0.70837200	-1.63090800
H	-0.48241100	2.56086800	1.23090500	H	-4.46903700	-4.06752100	1.97883300
O	-2.84240100	-2.17547500	1.19031600	O	3.67800500	0.14662800	1.62335900
H	-1.96073400	-1.93659800	0.80481300	H	2.82724000	0.20439300	1.12795800
O	1.95562300	-3.28365200	1.90277700	O	-2.34315000	0.24561400	0.92531000
H	2.44195400	-3.59199600	2.68002700	H	-1.79555000	-0.33871400	0.35603000
H	2.53340700	-2.55780800	-2.48303700	O	-0.42890400	-4.67301400	0.09088500
H	-4.63536800	1.21786500	-1.26009400	H	0.05001600	-4.37839000	-0.70178300
H	3.11895500	3.58803700	-1.47410200	H	-3.41901100	-1.62496700	-1.39394200



12-TS1 (syn)

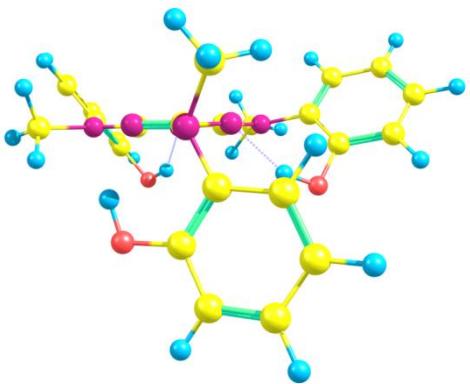
C	0.49481700	0.25973900	-0.36716300	C	-5.63484900	3.32407700	1.69098000
N	0.14532200	1.47976900	0.06827200	H	-5.76299500	6.14902600	-0.69109800
N	-0.45012600	-0.55498800	-0.85659800	H	-4.11676600	6.28822400	-0.06825600
C	-1.12383200	2.10603400	-0.03959700	H	-4.39807900	5.68847200	-1.71203800
N	1.79263300	-0.06896800	-0.26719800	C	8.29614200	1.12673000	0.39819400
C	-0.01662100	-1.75755300	-1.23643700	C	8.04344200	2.63950400	0.34502100
C	-1.17264700	3.41464100	-0.50331100	C	8.78683200	0.74645700	1.80179100
C	-2.31204900	1.50367300	0.39240300	C	9.39278800	0.78243000	-0.60906600
C	2.10646300	-1.29350700	-0.68030900	H	7.68358200	2.93916300	-0.64232200
N	-0.99139600	-2.67223000	-1.74316700	H	7.30520000	2.94930000	1.08695300
N	1.21823500	-2.19145700	-1.17673900	H	8.97212500	3.17854500	0.54841500
C	-2.36627800	4.12159400	-0.54144700	H	8.96894200	-0.32873400	1.87169800
C	-3.50053600	2.21661800	0.34068300	H	9.72239600	1.26667500	2.02204400
N	3.38057600	-1.71161600	-0.61608300	H	8.06034500	1.02101500	2.56889500
C	-1.96642800	-3.02707300	-0.75155100	H	10.29904600	1.33688600	-0.35665000
C	-3.55749200	3.53202800	-0.11875700	H	9.63629700	-0.28231700	-0.59267700
H	-4.39228900	1.70927200	0.69128900	H	9.10576000	1.05529300	-1.62718100

C	-5.50004200	-2.07025200	0.42386400	H	2.90613900	1.73131200	-1.37372900
C	-5.61370400	-1.41446400	1.80724200	H	0.24756500	-2.93374300	-0.01072500
C	-5.69225500	-0.98825200	-0.63903000	H	-3.29511600	-4.77245000	2.27255700
C	-6.61463100	-3.11299700	0.26763200	H	6.60746400	0.88483800	1.23243300
H	-5.53665200	-2.15200900	2.60850800	H	-0.97247700	6.34477400	-1.45317800
H	-4.82563600	-0.67095500	1.95030400	O	3.38221600	-2.06254000	-1.63562800
H	-6.57999600	-0.91254400	1.90367300	H	2.44157100	-1.86945800	-1.41801200
H	-5.66496700	-1.40468900	-1.64888300	O	-2.80797800	-2.08226500	-2.17958200
H	-6.66562800	-0.51321300	-0.49850600	H	-2.27440000	-1.26408400	-2.03768200
H	-4.92572800	-0.21234200	-0.56642700	O	-2.72481700	1.86678200	0.56747700
H	-7.59213200	-2.63162500	0.35473800	H	-2.80472300	1.19449500	-0.12954900
H	-6.55823100	-3.59831400	-0.70986100	H	-0.83393300	4.27738600	-2.76904800
H	-6.55010900	-3.88534900	1.03661600	H	-1.15049300	-3.71842800	1.73267700



12-TS2 (anti)

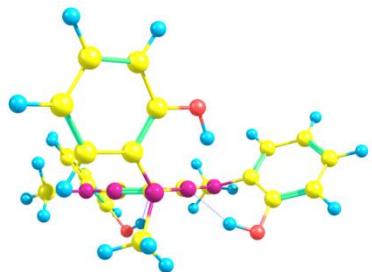
C	-0.15800500	-1.14377100	-0.77536200	H	-1.54190900	5.59502900	3.02003700
N	-0.51372200	-2.37536600	-0.38084200	H	-1.47925800	8.75598900	1.11301200
N	-1.11064100	-0.28292700	-1.17127900	H	-0.33698700	7.77406400	0.19181200
C	-1.81809300	-2.86746600	-0.10979100	H	-1.94532800	8.12082500	-0.46668500
N	1.15062900	-0.85490000	-0.75261500	C	7.49711400	-1.76278900	0.96492600
C	-0.66705600	0.91136800	-1.55754100	C	7.09925900	-2.92932700	1.87944300
C	-1.99351100	-3.60815700	1.05974900	C	8.31922400	-2.30264100	-0.21315800
C	-2.89914800	-2.73184700	-0.98137000	C	8.37078400	-0.79633000	1.76373000
C	1.47292100	0.37561600	-1.14684700	H	6.50376600	-2.57498400	2.72439800
N	-1.68074500	1.82322300	-1.98544900	H	6.51736700	-3.68021400	1.34172700
N	0.58276400	1.30797900	-1.56053300	H	7.99545900	-3.41555600	2.27289700
C	-3.20445100	-4.20117100	1.35692800	H	8.61049000	-1.49306500	-0.88684300
C	-4.12232600	-3.31957800	-0.66041400	H	9.22829600	-2.78284300	0.15743000
N	2.76166300	0.75192800	-1.15539700	H	7.75858600	-3.04167000	-0.78855900
C	-1.70126300	3.05144800	-1.25726600	H	9.25637400	-1.32535400	2.12190900
C	-4.30093800	-4.06762800	0.49547100	H	8.70718100	0.04374400	1.15187200
H	-4.92528500	-3.17503800	-1.37142100	H	7.84248300	-0.39993800	2.63381300
C	3.87770400	0.07540900	-0.59899400	C	-5.63076000	-4.72988100	0.85077100
C	-2.24838600	3.03008500	0.02970800	C	-6.13024500	-4.17153800	2.19025700
C	-1.25218800	4.25651100	-1.76878400	C	-6.70166800	-4.47835300	-0.20978800
C	4.16753100	-1.27266500	-0.84358300	C	-5.42066800	-6.24458900	0.98167300
C	4.77752800	0.82208800	0.15318900	H	-5.42265700	-4.37061200	2.99716500
C	-2.30945400	4.18664900	0.78619700	H	-6.28350300	-3.09140600	2.12786100
C	-1.33210200	5.42422500	-1.01490300	H	-7.08291100	-4.63735300	2.45460700
C	5.32375000	-1.83042600	-0.31612200	H	-6.40702000	-4.87742900	-1.18307100
C	5.93966100	0.25826600	0.65776500	H	-7.62722900	-4.97468100	0.08920000
C	-1.85036400	5.40620000	0.27928700	H	-6.91500100	-3.41304400	-0.32371400
H	-2.73853900	4.11857600	1.77923400	H	-6.36703700	-6.73060900	1.23177400
C	6.23516900	-1.08635300	0.43156200	H	-5.05625900	-6.66871000	0.04282100
H	5.50084500	-2.87860600	-0.52814700	H	-4.70156400	-6.48377500	1.76721400
H	-1.57503300	1.99844000	-2.98212300				



13-TS1 (syn)

C	-0.12941100	0.89320300	0.11252800
N	0.11697000	2.15045600	-0.30369400
N	0.89948200	0.16836800	0.59635400
C	1.35375100	2.81492500	-0.03103300
N	-1.37928100	0.42921900	0.00665400
C	0.59005000	-1.06241000	0.97330300
C	1.31572000	4.02777700	0.65387200
C	2.58345400	2.33091800	-0.49203100
C	-1.57809200	-0.81838500	0.44800900
N	1.65968400	-1.88851500	1.44714200
N	-0.60477400	-1.61363900	0.94992400
C	2.47153500	4.76165700	0.86841600
C	3.74129100	3.06722800	-0.26657000
N	-2.82124700	-1.33216700	0.38652100
C	2.58261100	-2.18835000	0.39421600
C	3.68873500	4.28130100	0.39923800
H	4.67813200	2.66765200	-0.63552000
C	-3.96931500	-0.52727600	0.10652400
C	2.18162200	-3.14332900	-0.55116300
C	3.83573500	-1.59832700	0.27068800
C	-4.11260400	0.17945200	-1.09242100
C	-5.01203000	-0.51531400	1.03081000
C	3.01856900	-3.48062300	-1.60503200
C	4.67939800	-1.94448400	-0.77838800
C	-5.28817600	0.87845500	-1.34423200
C	-6.18507600	0.17515600	0.77143100
C	4.26473700	-2.87893300	-1.71868500
H	2.68325100	-4.22262800	-2.31946000
C	-6.32463900	0.86965100	-0.42500600
H	-5.37089300	1.41586600	-2.28105200
H	4.59864900	4.84606300	0.55924700
H	2.41962700	5.70282400	1.40038900
H	-7.23721100	1.41147000	-0.63995100
H	-6.98468000	0.17026600	1.50091800
H	4.91411500	-3.14949800	-2.54201200
H	5.65268700	-1.47795200	-0.86141100
O	-3.14805700	0.17370500	-2.05979700
H	-2.28582600	0.30266200	-1.61501700
O	2.68994100	1.16543300	-1.19935600
H	2.18446100	0.48110100	-0.71254800
O	0.97160200	-3.76548700	-0.46237100

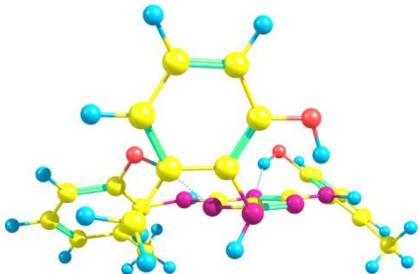
H	0.51019300	-3.48355200	0.34621900
H	4.15516400	-0.86235700	0.99800300
H	0.36194400	4.39527500	1.01303400
H	-4.89474200	-1.06253500	1.95848600
C	-0.99963300	2.96058500	-0.79996300
H	-1.52125100	2.42596000	-1.59144900
H	-1.70662200	3.19353300	-0.00200800
H	-0.59407400	3.88088400	-1.20968700
C	-3.05154000	-2.69715800	0.87257300
H	-2.31726300	-3.36866600	0.43351000
H	-2.97822900	-2.75120500	1.95967400
H	-4.04534000	-3.00268200	0.55811200
C	2.24586500	-1.35266200	2.67999000
H	1.46415200	-1.30285900	3.43794800
H	3.01972500	-2.03847500	3.02155200
H	2.67497900	-0.35475200	2.55245400



13-TS2 (anti)

C	-0.03464400	-1.12611700	0.29706500
N	0.12439900	-2.43753700	0.03266400
N	1.06668000	-0.39642200	0.58618600
C	1.40812600	-3.01758200	-0.21912800
N	-1.26976100	-0.62173400	0.26594500
C	0.83983400	0.88501400	0.82885400
C	1.60393000	-3.68854100	-1.42512000
C	2.44029500	-3.00099800	0.72586900
C	-1.37072600	0.69346900	0.50348400
N	1.99590400	1.65725900	1.17099300
N	-0.32572300	1.49583800	0.79223800
C	2.79230400	-4.35074400	-1.68797800
C	3.63377000	-3.66086500	0.45328100
N	-2.59358300	1.25794300	0.45396900
C	2.26744700	2.68571300	0.21753900
C	3.80933300	-4.34172800	-0.74039600
H	4.41396100	-3.63090300	1.20413600
C	-3.72623800	0.57472300	-0.08858100
C	2.80474900	2.28244000	-1.01329400
C	2.06334500	4.04010200	0.45434800
C	-4.21650500	-0.61445600	0.46158000
C	-4.40521500	1.15986100	-1.15540900
C	3.09900600	3.21921000	-1.99253300
C	2.37340300	4.98164400	-0.52077800
C	-5.37078100	-1.18999800	-0.05816600
C	-5.55959100	0.58702000	-1.66482000
C	2.88027000	4.56829900	-1.74592700

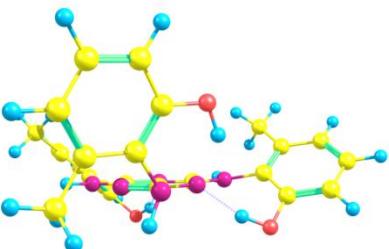
H	3.51319400	2.87728300	-2.93324700	N	-2.91964500	-1.22616900	0.25045000
C	-6.04678500	-0.59019100	-1.10844900	C	2.40731100	-2.45290300	0.52837100
H	-5.72736600	-2.10998900	0.38877600	C	3.88753700	4.10156100	0.11086900
H	4.74210100	-4.85680800	-0.93314100	H	4.84113900	2.32240500	-0.65759400
H	2.92213000	-4.86842400	-2.62960700	C	-4.08481100	-0.48997400	-0.08662500
H	-6.94862800	-1.04669500	-1.49670900	C	2.02738500	-3.46898100	-0.35337900
H	-6.07359300	1.05816200	-2.49262900	C	3.68025400	-1.88056600	0.43966200
H	3.11764000	5.29594200	-2.51199500	C	-4.16909900	0.27723600	-1.25332000
H	2.21142800	6.03337600	-0.32204000	C	-5.20061600	-0.62266600	0.75359400
O	-3.62327900	-1.21879400	1.53438700	C	2.89325200	-3.90281400	-1.34714700
H	-2.65796500	-1.21854400	1.37691100	C	4.54371100	-2.33436600	-0.55635000
O	2.30791000	-2.38617500	1.94000600	C	-5.35912800	0.92089800	-1.57294700
H	1.93507000	-1.49429300	1.77317800	C	-6.38361200	0.01816300	0.40474000
O	3.05312500	0.96703600	-1.27868900	C	4.15115200	-3.32787600	-1.44465100
H	2.93123900	0.43783400	-0.47201200	H	2.57184000	-4.68793200	-2.02018200
H	1.65998600	4.36195800	1.40608500	C	-6.46529200	0.78296600	-0.75271000
H	0.80520800	-3.69290100	-2.15708100	H	-5.39482400	1.51191700	-2.47968000
H	-4.01933800	2.07860400	-1.58035300	H	1.89858300	-1.61498200	2.30608300
C	1.95348300	2.07066600	2.57696700	H	-3.06777600	-2.13444400	0.67512900
H	2.87925500	2.59304000	2.81377000	H	-0.50543000	2.59886500	-0.70810800
H	1.10176800	2.71807200	2.80505500	H	4.81302000	4.65160600	0.22792100
H	1.89043900	1.17566500	3.19632400	H	2.65765400	5.69957100	0.85213600
C	-2.71888000	2.70131400	0.68229000	H	-7.39217400	1.28001100	-1.01087500
H	-2.19408200	2.97290700	1.59480900	H	-7.24595200	-0.08324700	1.05257200
H	-2.30540700	3.27432900	-0.14916500	H	4.83230300	-3.66100600	-2.21804800
H	-3.77400600	2.93321400	0.79655600	H	5.53084600	-1.89489600	-0.63559700
C	-1.06048500	-3.22956800	-0.31191200	O	-3.12771500	0.37955900	-2.13295500
H	-1.82576800	-3.09852000	0.45041100	H	-2.30628700	0.52996900	-1.61410100
H	-1.46915000	-2.93320300	-1.27948400	O	2.79745600	0.85601700	-1.10445200
H	-0.77224600	-4.27620900	-0.34086300	H	2.22339100	0.25678200	-0.57843400



14-TS1 (syn)

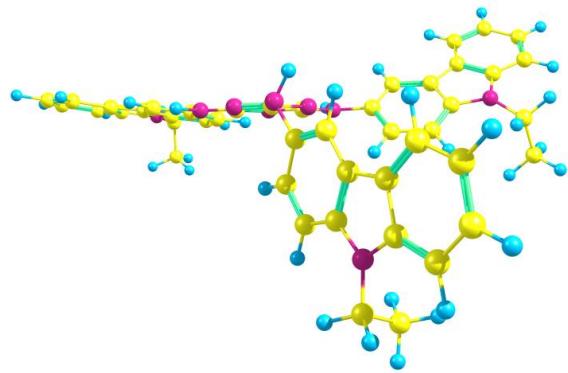
C	-0.07810800	0.80956700	0.05962500
N	0.26742500	2.02880900	-0.38291400
N	0.86677900	0.03064600	0.60350800
C	1.50954500	2.68848400	-0.18191300
N	-1.35969000	0.44253500	-0.09351200
C	0.45481500	-1.17653000	0.98708600
C	1.48112400	3.99530100	0.32624600
C	2.72770200	2.10030600	-0.54238600
C	-1.65835100	-0.77743600	0.34653700
N	1.44077400	-2.06425900	1.51668900
N	-0.76761800	-1.64111900	0.89733200
C	2.67846900	4.68954300	0.46098400
C	3.91339000	2.80679900	-0.37859500

N	-2.91964500	-1.22616900	0.25045000
C	2.40731100	-2.45290300	0.52837100
C	3.88753700	4.10156100	0.11086900
H	4.84113900	2.32240500	-0.65759400
C	-4.08481100	-0.48997400	-0.08662500
C	2.02738500	-3.46898100	-0.35337900
C	3.68025400	-1.88056600	0.43966200
C	-4.16909900	0.27723600	-1.25332000
C	-5.20061600	-0.62266600	0.75359400
C	2.89325200	-3.90281400	-1.34714700
C	4.54371100	-2.33436600	-0.55635000
C	-5.35912800	0.92089800	-1.57294700
C	-6.38361200	0.01816300	0.40474000
C	4.15115200	-3.32787600	-1.44465100
H	2.57184000	-4.68793200	-2.02018200
C	-6.46529200	0.78296600	-0.75271000
H	-5.39482400	1.51191700	-2.47968000
H	1.89858300	-1.61498200	2.30608300
H	-3.06777600	-2.13444400	0.67512900
H	-0.50543000	2.59886500	-0.70810800
H	4.81302000	4.65160600	0.22792100
H	2.65765400	5.69957100	0.85213600
H	-7.39217400	1.28001100	-1.01087500
H	-7.24595200	-0.08324700	1.05257200
H	4.83230300	-3.66100600	-2.21804800
H	5.53084600	-1.89489600	-0.63559700
O	-3.12771500	0.37955900	-2.13295500
H	-2.30628700	0.52996900	-1.61410100
O	2.79745600	0.85601700	-1.10445200
H	2.22339100	0.25678200	-0.57843400
O	0.79868700	-4.05409100	-0.26063800
H	0.33802100	-3.72153300	0.52797800
C	4.11670400	-0.81174300	1.40385100
H	4.25463700	-1.22366300	2.40797300
H	5.06499600	-0.38103300	1.08426800
H	3.38131900	-0.00786300	1.47755900
C	0.17428300	4.63037500	0.70706600
H	-0.46247000	4.78855600	-0.16823400
H	-0.38181000	4.00183700	1.40595700
H	0.34707600	5.59898800	1.17337800
C	-5.11059500	-1.45261500	2.00232400
H	-4.94745800	-2.50892500	1.76935100
H	-4.28213200	-1.12634400	2.63491200
H	-6.03426600	-1.37599300	2.57353800



14-TS2 (anti)

C	-0.44222400	-1.10939600	-0.45018200
N	-0.99338200	-2.31396800	-0.23542600
N	-1.24370100	-0.05976500	-0.69685700
C	-2.36283300	-2.62000100	-0.01284800
N	0.89545700	-1.04052800	-0.41317300
C	-0.61357400	1.09401500	-0.90889600
C	-2.67472400	-3.42684700	1.09206000
C	-3.37107500	-2.21451300	-0.89477400
C	1.41066600	0.17050000	-0.61755000
N	-1.46753200	2.20630700	-1.18078300
N	0.68378400	1.28402300	-0.87080500
C	-3.99425900	-3.81910900	1.28610700
C	-4.68534600	-2.60755700	-0.66991900
N	2.74309200	0.33492900	-0.58521000
C	-1.35090500	3.27849700	-0.24122700
C	-4.99434600	-3.41612700	0.41001300
H	-5.44537600	-2.27516200	-1.36604600
C	3.72713400	-0.59270500	-0.15609100
C	-1.98738500	3.10238000	0.99066600
C	-0.68770100	4.47476600	-0.52622600
C	3.80642700	-1.88834200	-0.67806900
C	4.68942700	-0.14067100	0.75964300
C	-1.93386800	4.09079900	1.96262300
C	-0.65725300	5.46772200	0.45146800
C	4.83493900	-2.73345400	-0.27792100
C	5.71772200	-0.99876300	1.13141400
C	-1.26390800	5.27322500	1.68635600
H	-2.43035100	3.92534500	2.91072700
C	5.79386100	-2.28630000	0.61441900
H	4.86916700	-3.73254700	-0.69431900
H	-1.31212500	2.52577600	-2.13353700
H	3.04226300	1.29909500	-0.67376500
H	-0.32681700	-3.03807700	0.00844800
H	-6.01883400	-3.72570000	0.57533900
H	-4.23580700	-4.44240800	2.13854800
H	6.59828800	-2.94577600	0.91561100
H	6.46169400	-0.65064300	1.83775800
H	-1.22070800	6.05156700	2.43830000
H	-0.14502100	6.39856200	0.23912100
O	2.92949600	-2.34741800	-1.62149100
H	2.02346000	-2.08440800	-1.34698200
O	-3.10578000	-1.47456800	-2.01270700
H	-2.48710700	-0.75274200	-1.75490000
O	-2.67104000	1.95242400	1.26582600
H	-2.76328300	1.42658500	0.45362300
C	-0.03496600	4.68220800	-1.86340800
H	0.67702500	3.88421800	-2.08352000
H	-0.77613500	4.69162900	-2.66782600
H	0.49453700	5.63364800	-1.88426600
C	4.60750400	1.25175900	1.31723300
H	4.77033000	2.00492800	0.54063600
H	3.62710500	1.44418800	1.75835900
H	5.36688700	1.39530700	2.08415100
C	-1.59514500	-3.86615900	2.04011300

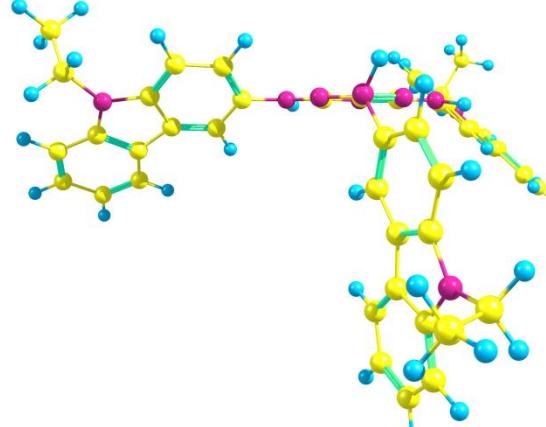


4-TS1 (syn)

C	0.05360000	-1.43656100	-1.34860400
N	-0.88363000	-2.35843300	-1.91616200
N	1.32183100	-1.81748800	-1.34645800
C	-1.88835400	-2.89552000	-1.06143000
N	-0.42779700	-0.27465800	-0.89147600
C	2.18894700	-0.89922000	-0.82024700
C	-3.18409000	-3.09127900	-1.54883800
C	-1.56263700	-3.30236700	0.25342700
C	0.50861200	0.55987000	-0.39497700
N	3.48464100	-1.30194300	-0.82719800
N	1.83181300	0.29212000	-0.33655200
C	-4.14185700	-3.70168000	-0.72647400
H	-3.43985000	-2.77346800	-2.55705900
C	-2.50740300	-3.89630200	1.08908300
H	-0.55321600	-3.15498700	0.62559600
N	0.14085300	1.77471300	0.08461700
C	4.68230900	-0.68191700	-0.39783400
C	-3.79897200	-4.10326200	0.59198000
C	-5.53571700	-4.04718200	-0.90912000
H	-2.23113300	-4.18981700	2.09677500
C	-1.15650800	2.35830800	0.12229600
C	4.72784800	0.51781500	0.34895000
C	5.87222000	-1.34406500	-0.73190300
N	-4.90676700	-4.68800200	1.20244500
C	-6.43782500	-3.90819700	-1.97391800
C	-5.96797100	-4.64398300	0.31139900
C	-2.27150200	1.64533000	0.61445600
C	-1.28731100	3.69160600	-0.27335800
C	5.94434300	1.06525100	0.75811300
H	3.80663700	1.01842700	0.60843200
C	7.09580100	-0.80700600	-0.32370300
C	-4.96735000	-5.15324000	2.58589200
C	-7.74940400	-4.35466400	-1.81440000
H	-6.11838000	-3.45687200	-2.90969800
C	-7.28790000	-5.08988200	0.47491700
C	-3.53021600	2.23713300	0.69005900
H	-2.14476100	0.62149600	0.94491600

C	-2.54139000	4.30792600	-0.18585600
C	7.12901300	0.40593800	0.41738900
H	5.95104000	1.98492500	1.33416500
C	8.47286000	-1.22275300	-0.49152900
C	-5.35215000	-4.05733600	3.58093300
H	-5.68462800	-5.97781000	2.62987700
H	-3.98939700	-5.57333200	2.83939700
C	-8.16471000	-4.93801600	-0.59959000
H	-8.45941100	-4.25168100	-2.63009200
H	-7.62426300	-5.53612800	1.40541400
C	-3.66331200	3.57099100	0.28308600
H	-4.37407700	1.67181700	1.07185000
C	-3.02426100	5.63567200	-0.50034100
N	8.44938600	0.74730900	0.68648900
C	9.27200800	-0.23781700	0.15710800
H	-6.34275000	-3.64857700	3.35495300
H	-5.37725500	-4.47142500	4.59525900
H	-4.62725000	-3.23659700	3.56580000
H	-9.19213300	-5.27621000	-0.49440700
N	-4.79195400	4.37937500	0.25074300
C	-4.41763000	5.63632200	-0.20592100
C	8.88503400	1.88462600	1.49387600
C	10.67001300	-0.34120000	0.18938500
C	-6.12221700	4.00569300	0.72697500
C	-5.20139200	6.78347700	-0.39284600
C	8.95701900	1.57609200	2.98995300
H	9.86304800	2.20236300	1.12152600
H	8.19233700	2.71019000	1.30616400
C	11.25583400	-1.43883600	-0.44210500
H	11.28222200	0.40260400	0.68936900
C	-6.33460000	4.28313800	2.21569500
H	-6.26607100	2.94313200	0.51102200
H	-6.85547700	4.55228900	0.12715500
C	-4.57249800	7.92651200	-0.88763300
H	-6.26162600	6.79045700	-0.16127700
H	7.97789200	1.27906200	3.38029500
H	9.28525500	2.46823000	3.53509700
H	9.67018200	0.77029600	3.19351700
C	10.47760100	-2.41857100	-1.09174700
H	12.33777200	-1.53964800	-0.42951700
H	-6.21855000	5.34874700	2.43999200
H	-7.34732500	3.98163500	2.50600000
H	-5.62241800	3.72041200	2.82843300
C	-3.19529200	7.93881500	-1.18913700
H	-5.15983800	8.82773700	-1.04154900
C	9.08693800	-2.31553300	-1.11945700
H	10.96751200	-3.26050300	-1.57244500
C	-2.41682700	6.79768900	-0.99742400
H	-2.73869300	8.84698500	-1.57217900
H	8.48694400	-3.07169000	-1.61892000
H	-1.35485000	6.80808400	-1.22818300
H	-0.42260900	4.23689400	-0.64219400
H	5.83813800	-2.26883900	-1.30288600
H	3.60835100	-2.21434600	-1.25170700

H	0.91770200	2.38646600	0.30837400
H	-1.29991300	-1.95217700	-2.75189100

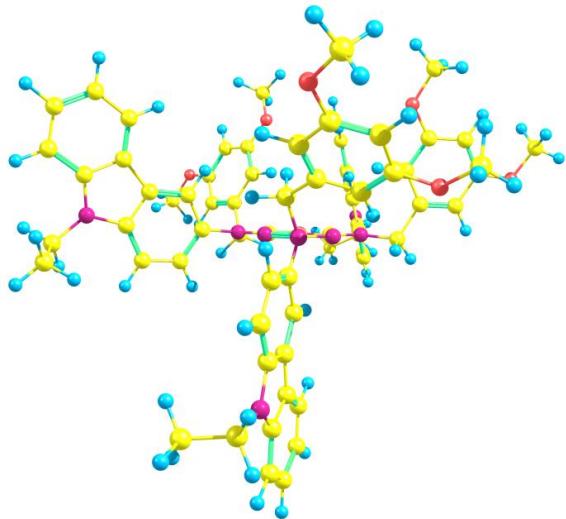


4-TS2 (anti)

C	-0.53773900	0.95643900	-2.15274000
N	-1.31903800	2.03326100	-2.68044300
N	0.78376600	1.09580300	-2.15659300
C	-1.27638700	3.28930500	-2.01505300
N	-1.22135300	-0.10263500	-1.71856000
C	1.46669700	0.03214800	-1.64869300
C	-1.20903200	3.37446600	-0.62090400
C	-1.37949900	4.46986400	-2.78755800
C	-0.44794300	-1.10435000	-1.23717100
N	2.81746300	0.16840000	-1.64593100
N	0.89814200	-1.08111400	-1.17574100
C	-1.23857000	4.63858700	-0.01321700
H	-1.14164500	2.47763900	-0.01194300
C	-1.42021300	5.73210500	-2.19859100
H	-1.43183200	4.38541600	-3.87033500
N	-1.03742600	-2.22922000	-0.76111500
C	3.80403100	-0.73570700	-1.16484400
C	-1.34283400	5.81365400	-0.80355300
C	-1.18929800	5.07739400	1.36560500
H	-1.50454800	6.61895300	-2.81849000
C	-2.42453400	-2.53957400	-0.68207700
C	3.75866900	-2.11319900	-1.47335500
C	4.87376400	-0.20999100	-0.43566500
N	-1.34031000	6.93354300	0.02586000
C	-1.08864500	4.40788400	2.59385000
C	-1.26629500	6.50078900	1.34048300
C	-3.27787200	-2.37668900	-1.79512200
C	-2.90900300	-3.08877800	0.50719700
C	4.75620300	-2.98333400	-1.03951900
H	2.93737500	-2.50016700	-2.06410500
C	5.89448800	-1.06763100	-0.00835600
C	-1.51749600	8.31557300	-0.41164100
C	-1.07152700	5.15255100	3.77303100
H	-1.02661100	3.32316800	2.62534500
C	-1.25409200	7.25129000	2.52550300

C	-4.62356900	-2.72972300	-1.73069700
H	-2.87651700	-1.97676700	-2.71873800
C	-4.25491900	-3.46756300	0.58334700
C	5.82387700	-2.45725800	-0.30071300
H	4.70175400	-4.03796800	-1.28895800
C	7.11563400	-0.86719100	0.74241000
C	-2.98343300	8.74066400	-0.51003000
H	-0.97914500	8.95913000	0.29013200
H	-1.02272200	8.42374900	-1.38134100
C	-1.15492100	6.55973200	3.73315200
H	-0.99541000	4.64688600	4.73145600
H	-1.32247400	8.33444900	2.51121400
C	-5.11147500	-3.27302400	-0.53493800
H	-5.26219800	-2.59765900	-2.59792600
C	-5.06842200	-4.05457900	1.62674400
N	6.92578600	-3.10056400	0.24846200
C	7.72439500	-2.14848600	0.86866600
H	-3.48357300	8.66368200	0.46123800
H	-3.04439400	9.78275800	-0.84360000
H	-3.52780500	8.12013400	-1.22972800
H	-1.14390800	7.12114900	4.66358900
N	-6.39424700	-3.69563500	-0.21201100
C	-6.37972300	-4.18620500	1.08722100
C	7.25254500	-4.51669300	0.09205700
C	8.94199800	-2.31287000	1.54393800
C	-7.53407400	-3.74009000	-1.12591400
C	-7.42680100	-4.73402400	1.84140100
C	8.06724700	-4.81631300	-1.16683100
H	7.79837600	-4.83230500	0.98559100
H	6.31289300	-5.07636700	0.08259400
C	9.53651700	-1.17852200	2.09763000
H	9.41315900	-3.28620900	1.63581200
C	-7.62402000	-5.04304000	-1.92117600
H	-7.45298800	-2.88385000	-1.80145800
H	-8.44067500	-3.59008300	-0.53290900
C	-7.14428400	-5.14052600	3.14589900
H	-8.42517700	-4.84328100	1.43006600
H	7.51908000	-4.52966900	-2.07051000
H	8.27855400	-5.89013200	-1.22221500
H	9.02242200	-4.28074600	-1.15650100
C	8.94297200	0.09531000	1.98452300
H	10.48044300	-1.28189000	2.62600600
H	-7.73131400	-5.90601000	-1.25558200
H	-8.49701700	-5.01170500	-2.58274800
H	-6.73260000	-5.19126900	-2.53982500
C	-5.85220100	-5.01151300	3.69516800
H	-7.94003000	-5.56818400	3.74984900
C	7.73367500	0.25683900	1.30895900
H	9.43460100	0.95686800	2.42723800
C	-4.81154600	-4.46949400	2.94137000
H	-5.66810700	-5.33919900	4.71435200
H	7.27705800	1.23911300	1.22063500
H	-3.81541800	-4.37130000	3.36475700
H	-2.24353400	-3.21976900	1.35625500

H	4.90827300	0.85254600	-0.20970600
H	3.13986800	1.09789100	-1.88983200
H	-0.40251100	-2.87126800	-0.30027500
H	-1.13524100	2.14002600	-3.67568200

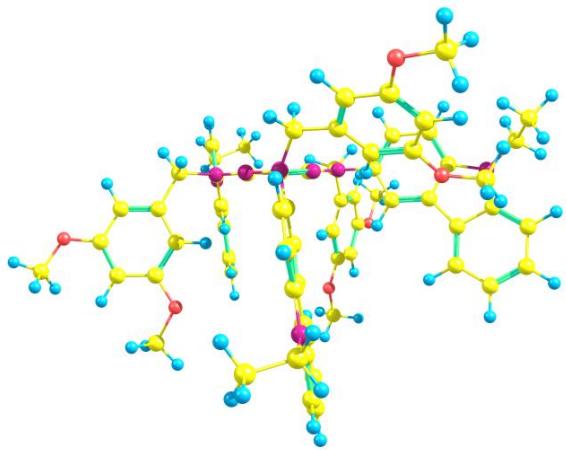


5-TS1 (syn)

C	1.31582900	-0.73860500	0.30329200
N	1.16588500	0.58287700	0.31640900
C	-0.04651900	1.00731700	0.76306300
N	0.41367400	-1.64699500	0.66010000
C	-0.77116300	-1.12600000	1.08246700
N	-1.03469300	0.18846700	1.15849800
N	2.57009700	-1.24096600	-0.17034900
N	-0.25907300	2.35210000	0.81735700
N	-1.75352200	-1.99719000	1.44755500
C	3.46893400	-1.11812700	2.10385800
C	6.10833200	-1.19200100	1.06966100
C	4.57183600	-1.08590000	2.96569300
C	3.67255700	-1.17903900	0.71463300
C	5.00144000	-1.21372800	0.21939900
C	5.89269500	-1.12948900	2.44815900
C	4.70050500	-1.01449200	4.40700400
C	5.63380900	-0.87994300	7.03618000
C	3.77795500	-0.94718700	5.46065100
C	6.09811900	-1.01919700	4.68911800
C	6.57352800	-0.94750400	6.00687100
C	4.24883500	-0.88039300	6.77213300
N	6.80684700	-1.10777100	3.50123100
C	-3.95571400	-1.13493100	0.78416200
C	-4.74065700	-1.08795800	3.52095900
C	-5.23768900	-0.70232500	1.14235100
C	-3.07181100	-1.52607800	1.78917900
C	-3.46523300	-1.50386000	3.14239800
C	-5.62666400	-0.68781000	2.51146800
C	-6.37548700	-0.22410200	0.38590300
C	-8.86010100	0.75131700	-0.42973400
C	-6.61304800	-0.01159600	-0.97965600

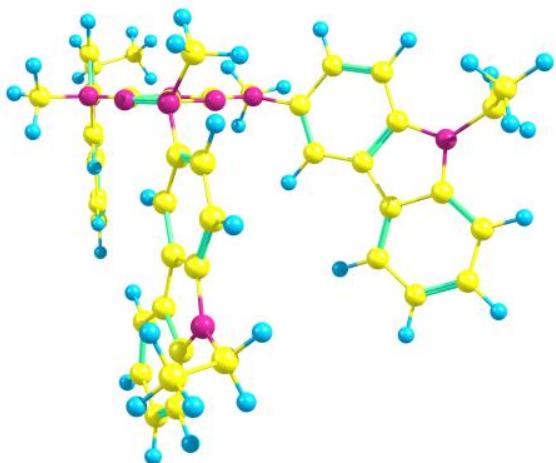
C	-7.39900500	0.05560500	1.33460000	H	4.57962500	7.77055600	-1.16665600
C	-8.64849000	0.54919400	0.93468700	H	6.57597200	6.78024700	-0.04553700
C	-7.85656500	0.47593000	-1.38083000	H	6.19072300	5.85189000	-1.50747500
N	-6.93779700	-0.24449800	2.61083400	H	5.75578900	5.21309500	0.09256000
C	0.80777400	3.56859100	-1.03095700	H	-7.34367400	-0.78478300	4.57236600
C	2.51135000	4.87527800	0.84004400	H	-8.73083100	-0.22208400	3.65485800
C	1.75344800	4.50293000	-1.47126100	H	-8.06077700	1.46988100	5.36282100
C	0.72578700	3.28514200	0.33144000	H	-7.83946100	2.14149500	3.73571500
C	1.56831000	3.93720700	1.25470100	H	-6.43402900	1.57219600	4.66212700
C	2.59771600	5.15674400	-0.53032100	H	8.69715000	-1.55670700	4.23058500
C	2.11381200	5.01881700	-2.77482500	H	8.53198000	-1.64682400	2.48499100
C	3.27970700	6.38391700	-4.91251900	H	9.89871700	0.33628700	3.13477300
C	1.65469600	4.77335500	-4.07681100	H	8.56629100	0.96534300	4.12304800
C	3.15957800	5.96019000	-2.55905400	H	8.39790500	0.87391500	2.35662500
C	3.75340000	6.64748300	-3.62678100	C	-2.48480100	3.46353300	0.41397100
C	2.24161700	5.45783200	-5.14075500	C	-2.99902200	4.75812900	0.60220800
N	3.42901000	6.04426400	-1.19822700	C	-2.93100400	2.67776100	-0.64735700
C	2.77775500	-1.08166500	-1.61300800	C	-3.96718500	5.24386600	-0.28164900
C	-1.47704900	2.92282900	1.41597600	H	-2.63769000	5.36068300	1.42695700
C	-1.52897000	-3.45026500	1.51118900	C	-3.90307500	3.18182400	-1.52636200
C	4.48604100	6.84813300	-0.58657500	H	-2.54843500	1.67502800	-0.80604700
C	5.83083200	6.12452800	-0.50979600	C	-4.42827900	4.46321200	-1.35347500
C	-7.67333400	-0.02766300	3.85543500	H	-5.17703100	4.87712700	-2.01776400
C	-7.48688900	1.37530400	4.43414300	C	3.26858600	-2.33299400	-2.33007200
C	8.25950900	-1.05388300	3.36324200	C	3.94512300	-2.18189100	-3.54536900
C	8.80807900	0.36835500	3.23727400	C	3.00926100	-3.61130300	-1.83177100
H	2.46625900	-1.09763200	2.51806800	C	4.35012300	-3.31367800	-4.26166000
H	7.10899800	-1.21818100	0.64980900	H	4.16384500	-1.19530900	-3.94443000
H	5.18383600	-1.26307200	-0.84682000	C	3.42688600	-4.73508700	-2.55564600
H	5.98051800	-0.82322200	8.06458800	H	2.49248300	-3.74685100	-0.88801100
H	2.71018900	-0.94497800	5.25715700	C	4.09983800	-4.60621000	-3.77821000
H	7.63661500	-0.94034100	6.22597700	H	4.42127600	-5.47779800	-4.33010500
H	3.54527000	-0.82570900	7.59802300	C	-2.17597100	-4.23909100	0.38413200
H	-3.64507900	-1.15680600	-0.25548100	C	-2.87229400	-5.41196100	0.68908700
H	-5.02384400	-1.07033700	4.56828800	C	-2.04322800	-3.83494800	-0.94881200
H	-2.75482300	-1.81280100	3.90375400	C	-3.42594800	-6.18248600	-0.34190300
H	-9.82095200	1.13308100	-0.76421300	H	-2.99262500	-5.73838000	1.71800800
H	-5.83856200	-0.22062200	-1.71244800	C	-2.60681000	-4.61013100	-1.96770900
H	-9.42860300	0.77114300	1.65577900	H	-1.50919700	-2.92838000	-1.21315400
H	-8.05567100	0.64743000	-2.43470700	C	-3.30413300	-5.79344700	-1.68199400
H	0.15405100	3.06206800	-1.73437300	H	-3.73887100	-6.38670600	-2.47375100
H	3.15802100	5.36066700	1.56359900	O	-4.08824200	-7.31705200	0.05594700
H	1.48174100	3.69429600	2.30985000	O	-2.42677900	-4.13339300	-3.24299000
H	3.72513700	6.90404700	-5.75623700	O	3.13257500	-5.94901600	-1.98416000
H	0.85531500	4.05845600	-4.25274800	O	5.00342200	-3.06565900	-5.44384700
H	4.55641800	7.35983200	-3.46715300	O	-4.28681600	2.33329100	-2.53328700
H	1.89850400	5.27699500	-6.15541200	O	-4.53248000	6.49169900	-0.18926600
H	3.45880000	-0.24650300	-1.82844300	C	-4.12574500	7.35202800	0.88343600
H	1.81179200	-0.80442900	-2.04692700	H	-3.05654100	7.58202100	0.82067700
H	-1.16853600	3.72921000	2.08703800	H	-4.70379300	8.26875000	0.75806600
H	-1.94162800	2.14504600	2.02409100	H	-4.35552400	6.90400600	1.85633200
H	-1.91717200	-3.80723400	2.46927200	C	-5.29085700	2.77304000	-3.45706500
H	-0.45131500	-3.61941000	1.50942700	H	-6.22925300	3.00221600	-2.94124500
H	4.14836100	7.13690900	0.41270900	H	-4.95020100	3.65057100	-4.01795800

H	-5.44397600	1.93927900	-4.14366800	C	0.71436900	1.15408300	-1.36724500
C	3.51635900	-7.14847300	-2.66883200	N	0.65117600	2.34106400	-0.70792300
H	3.17762100	-7.96874200	-2.03421600	N	-0.43076300	0.67830500	-1.92892600
H	3.02809400	-7.21757800	-3.64715400	C	1.85552900	2.90513000	-0.08688700
H	4.60389200	-7.20433800	-2.78875400	C	-0.61063100	2.96875800	-0.41138900
C	5.45428500	-4.17410900	-6.23342500	N	1.90522400	0.53580200	-1.43106200
H	6.18245700	-4.78035000	-5.68356100	C	-0.29141300	-0.47584000	-2.57184600
H	4.61302700	-4.79854900	-6.55366800	H	1.63241700	3.92694200	0.22126900
H	5.93423600	-3.73346100	-7.10848800	H	2.68484600	2.92237800	-0.79724400
C	-4.68170400	-8.15778100	-0.94238200	H	2.16058100	2.32888200	0.79531900
H	-5.13931500	-8.98318100	-0.39511000	C	-1.40876300	2.47613900	0.62055300
H	-5.45300200	-7.61951100	-1.50403000	C	-0.99688100	4.11384900	-1.13601300
H	-3.92346900	-8.54995400	-1.62894200	C	1.91787400	-0.62580500	-2.11091300
C	-2.95141600	-4.88540000	-4.34485600	N	-1.46017900	-1.00971500	-3.20888900
H	-2.67843500	-4.32296900	-5.23899000	N	0.82831800	-1.18250500	-2.70839200
H	-2.50313600	-5.88398300	-4.38996000	C	-2.61226400	3.12803700	0.91484800
H	-4.04219600	-4.96698800	-4.28376000	H	-1.10062800	1.59556500	1.17682900



5-TS2 (anti)

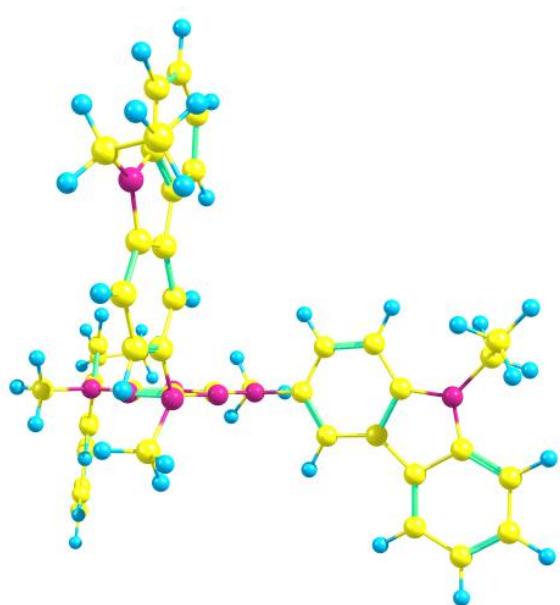
C	0.69079600	1.15823000	-1.92501000
N	0.97907100	-0.09424900	-1.58065600



6-TS1 (syn)

C	0.71436900	1.15408300	-1.36724500
N	0.65117600	2.34106400	-0.70792300
N	-0.43076300	0.67830500	-1.92892600
C	1.85552900	2.90513000	-0.08688700
C	-0.61063100	2.96875800	-0.41138900
N	1.90522400	0.53580200	-1.43106200
C	-0.29141300	-0.47584000	-2.57184600
H	1.63241700	3.92694200	0.22126900
H	2.68484600	2.92237800	-0.79724400
H	2.16058100	2.32888200	0.79531900
C	-1.40876300	2.47613900	0.62055300
C	-0.99688100	4.11384900	-1.13601300
C	1.91787400	-0.62580500	-2.11091300
N	-1.46017900	-1.00971500	-3.20888900
N	0.82831800	-1.18250500	-2.70839200
C	-2.61226400	3.12803700	0.91484800
H	-1.10062800	1.59556500	1.17682900
C	-2.18602100	4.78466300	-0.85418700
H	-0.35199400	4.47458000	-1.93210500
N	3.08910500	-1.30183300	-2.21896200
C	-1.97726700	-0.14869400	-4.27867800
C	-2.39157200	-1.66996700	-2.36500100
C	-2.99218600	4.28503700	0.17743200
C	-3.66231600	2.89464900	1.88351100
H	-2.47029800	5.66175000	-1.42638600
C	3.15257500	-2.57242700	-2.95436300
C	4.29464800	-0.81660600	-1.59826500
H	-2.53028000	-0.74885500	-5.00616400
H	-1.13162400	0.30239000	-4.80189100
H	-2.63133700	0.65443400	-3.90994700
C	-3.76389800	-1.73644600	-2.71661800
C	-1.96236400	-2.30549800	-1.18724100
N	-4.20161400	4.76175500	0.66301200
C	-3.866663100	1.92942700	2.87990700
C	-4.62740500	3.92191200	1.68489900
H	4.19099900	-2.90314400	-2.96454600
H	2.54205300	-3.34348300	-2.47262600
H	2.81142800	-2.44980600	-3.98637300
C	5.18862600	-0.02841800	-2.35058000
C	4.59138700	-1.17574200	-0.28449000
C	-4.69632700	-2.41887800	-1.93250500
H	-4.11832900	-1.25297700	-3.61858000
C	-2.88937200	-2.98641700	-0.38933900
C	-4.95497900	5.88917100	0.11683400
C	-5.02229600	1.99504600	3.65778200
H	-3.13556000	1.14168400	3.04116200
C	-5.79186800	3.98810900	2.46254700
C	6.38961200	0.42421300	-1.80731800
H	4.92919100	0.23073900	-3.37290700
C	5.79122000	-0.72906000	0.28354400
C	-4.25857500	-3.03988200	-0.76085700
H	-5.73691100	-2.45022000	-2.23993900
C	-2.77460000	-3.72498100	0.85203700
C	-5.92021200	5.48982900	-0.99978000

H	-5.49683600	6.35880800	0.94270900
H	-4.23327800	6.62592700	-0.24657800
C	-5.97192500	3.01535400	3.44659900
H	-5.19537100	1.25368200	4.43261100
H	-6.53422800	4.76464200	2.30858600
C	6.68654500	0.06715800	-0.48517400
H	7.06474300	1.03489000	-2.39778800
C	6.40473400	-0.89758300	1.58386200
N	-4.97441000	-3.75389700	0.19939400
C	-4.08510500	-4.18792300	1.17006400
H	-6.66502600	4.77157600	-0.64122200
H	-6.44972100	6.37741300	-1.36388400
H	-5.38475900	5.04173800	-1.84343900
H	-6.86717600	3.04590000	4.06176000
N	7.80420600	0.36927500	0.27905200
C	7.64143700	-0.19390400	1.53868000
C	-6.39326300	-4.09079900	0.12476500
C	-4.32605300	-4.95338600	2.32064100
C	8.91508500	1.22314800	-0.13738200
C	8.49439400	-0.14593600	2.65002500
C	-6.67306100	-5.38806600	-0.63576500
H	-6.77428100	-4.15853300	1.14788900
H	-6.91060900	-3.25126400	-0.34910600
C	-3.24173400	-5.24271200	3.14992700
H	-5.32027900	-5.31574400	2.56241400
C	8.68819000	2.70477600	0.16456500
H	9.06801600	1.06996200	-1.20937400
H	9.81737700	0.86316600	0.36508100
C	8.09542300	-0.82054600	3.80437700
H	9.43361400	0.39713800	2.62104900
H	-6.31937000	-5.32457000	-1.67031000
H	-7.75191700	-5.57966100	-0.65547000
H	-6.18393800	-6.24163100	-0.15445600
C	-1.94133900	-4.78796200	2.84998300
H	-3.40619200	-5.83453500	4.04647000
H	8.55665500	2.87415300	1.23846000
H	9.55548200	3.28560800	-0.16886600
H	7.80289400	3.08356800	-0.35700500
C	6.87607100	-1.52571600	3.86219400
H	8.74034900	-0.79832100	4.67869400
C	-1.70309400	-4.02994200	1.70329100
H	-1.11997700	-5.03297600	3.51736700
C	6.02726400	-1.56767300	2.75643600
H	6.59706300	-2.03919400	4.77788200
H	-0.70007100	-3.68129400	1.47115900
H	5.08678000	-2.11034100	2.80180500
H	3.89693800	-1.78735500	0.28437600
H	-0.91831000	-2.28144700	-0.89263300



6-TS2 (anti)

C	0.47777600	-0.68592200	-0.23358600
N	0.51789200	-1.78660000	0.55954300
N	-0.67798600	-0.43801000	-0.91593100
C	1.72757700	-2.09261600	1.33325800
C	-0.63788000	-2.62490400	0.74950000
N	1.58039000	0.07722900	-0.29878100
C	-0.64073800	0.65074100	-1.67299900
H	1.57043800	-3.04133900	1.84627500
H	1.93252500	-1.31601400	2.07855000
H	2.59851000	-2.18471300	0.67794600
C	-0.81551700	-3.75184800	-0.05097800
C	-1.54363100	-2.32803200	1.78809200
C	1.49338300	1.15161900	-1.10656300
N	-1.82426200	0.93942900	-2.42981800
N	0.38743200	1.48627300	-1.82125800
C	-1.91794300	-4.58281900	0.18631300
H	-0.10893300	-3.97315300	-0.84572600
C	-2.64656300	-3.14076200	2.04305800
H	-1.37576300	-1.44386000	2.39602000
N	2.57348200	1.96508400	-1.22363600
C	-1.62402100	0.81645000	-3.87821100
C	-2.64198100	1.99354000	-1.94722800
C	-2.82624800	-4.27378500	1.23796800
C	-2.40386300	-5.79781000	-0.43234700
H	-3.33810300	-2.89356300	2.84177100
C	2.52763700	3.13888200	-2.10663900
C	3.79727900	1.69747900	-0.51339600
H	-2.57432700	0.59076400	-4.36951200
H	-0.95044000	-0.02222100	-4.06663000
H	-1.19493900	1.72093600	-4.33326700
C	-3.47695600	2.72286600	-2.83147600
C	-2.67414700	2.30072500	-0.57616000
N	-3.81555000	-5.24509700	1.29036900
C	-1.95581800	-6.59055100	-1.49862000
C	-3.58290300	-6.16544200	0.27568100

H	3.48456800	3.65469900	-2.02976800	H	8.13694200	-0.82513700	3.32584600
H	2.36585000	2.84793300	-3.14953500	H	8.07654100	0.36455800	4.64052100
H	1.73140500	3.82755300	-1.80813400	H	6.59487200	-0.05631900	3.76001900
C	3.95371100	2.16981400	0.80543400	C	9.05648400	-0.98766200	-1.96510400
C	4.83544400	1.02682800	-1.15804400	H	10.88065000	-1.28249900	-0.84402600
C	-4.33495400	3.72749500	-2.37919100	C	-3.28799300	3.58534600	2.48516100
H	-3.46616200	2.50384500	-3.89202600	H	-3.39083400	4.11582200	4.56971200
C	-3.52311200	3.31237400	-0.11224400	C	7.76283700	-0.46670700	-1.96695500
C	-4.96175200	-5.24746500	2.19778700	H	9.43731100	-1.49308700	-2.84798900
C	-2.68298300	-7.72824700	-1.84748300	H	-2.54057000	2.80956400	2.63002900
H	-1.05605100	-6.32055300	-2.04512100	H	7.12994600	-0.56137100	-2.84533700
C	-4.31837600	-7.30606600	-0.07554500	H	4.70619400	0.67195400	-2.17663000
C	5.13935900	1.97214400	1.51041600	H	-2.05421900	1.75681700	0.12917200
H	3.12791300	2.69243900	1.27900000				
C	6.03808000	0.82055500	-0.47018100				
C	-4.35282700	4.02758300	-1.01551100				
H	-4.96288000	4.25769400	-3.08832300				
C	-3.78481300	3.86065600	1.20329500				
C	-6.17212400	-4.49148300	1.64885300				
H	-5.22147000	-6.29011700	2.40191100				
H	-4.63613500	-4.81258300	3.14692400				
C	-3.85159800	-8.07734900	-1.14045800				
H	-2.34943700	-8.35152200	-2.67226200				
H	-5.22253000	-7.58463200	0.45638100				
C	6.18344000	1.29710500	0.86322300				
H	5.24015300	2.33525500	2.52799900				
C	7.28925800	0.18081600	-0.81686600				
N	-5.08462400	4.98651600	-0.31610600				
C	-4.76246100	4.88350400	1.02804600				
H	-6.52330300	-4.93468400	0.71105000				
H	-6.99241200	-4.53309900	2.37421000				
H	-5.93141000	-3.43895100	1.46596200				
H	-4.40510600	-8.96620600	-1.43101200				
N	7.45559700	0.98954800	1.32443700				
C	8.13101700	0.30016300	0.32489700				
C	-6.10563400	5.85944300	-0.88809300				
C	-5.24892000	5.61876400	2.11910300				
C	7.96118200	1.24588600	2.67203200				
C	9.43003500	-0.22649400	0.33146200				
C	-7.49998300	5.23114900	-0.91488900				
H	-6.11581600	6.78666500	-0.30774700				
H	-5.78742600	6.12474900	-1.90069500				
C	-4.73773400	5.32389800	3.38355700				
H	-6.00026100	6.39171700	1.99177100				
C	7.67206700	0.11036200	3.65435400				
H	7.51361200	2.17966000	3.02358800				
H	9.03794400	1.42154400	2.59498700				
C	9.87690200	-0.86662800	-0.82504200				
H	10.07144000	-0.14526400	1.20309500				
H	-7.50982900	4.31558500	-1.51575900				
H	-8.21465300	5.93570000	-1.35518000				
H	-7.84225100	4.98543000	0.09601900				
C	-3.76629900	4.31934400	3.57087400				
H	-5.10031200	5.88175700	4.24286700				

Table S23. Theoretical thermodynamic parameters of restricted rotation around triazine-N bond

Comp.	Process	Via	Method	ΔH^\ddagger (298 K) kcal mol ⁻¹	ΔS^\ddagger (298 K) cal K ⁻¹ mol ⁻¹	ΔG^\ddagger (298 K) kcal mol ⁻¹	$\Delta G_{\text{eff}}^\ddagger$ (298 K) kcal mol ⁻¹
11	GS1->GS2	Anti-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	15.5	-2.6	15.9	
		Syn-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	15.4	-3.0	16.3	
		Anti-TS	SMD(DMF)//M062X/TZVP	14.6	-1.4	15.0	14.4
		Syn-TS	SMD(DMF)//M062X/TZVP	13.4	-4.3	14.7	
		<i>Exp. S to A</i>		13.1 ± 1.3	2.2 ± 4.4		12.4 ± 0.1
11	GS2->GS1	Anti-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	13.4	-4.5	14.8	
		Syn-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	13.3	-4.9	14.8	
		Anti-TS	SMD(DMF)//M062X/TZVP	14.4	-3.4	15.4	14.8
		Syn-TS	SMD(DMF)//M062X/TZVP	13.2	-6.2	15.1	
		<i>Exp. A to S</i>		12.9 ± 1.2	0.8 ± 4.2		12.7 ± 0.1
12	GS1->GS2	Anti-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	14.3	-2.0	14.8	
		Syn-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	14.7	-3.2	15.6	14.7
		Anti-TS	SMD(DMF)//M062X/TZVP	13.7	-5.5	15.3	
		Syn-TS	SMD(DMF)//M062X/TZVP	11.2	-10.5	14.3	14.2
		<i>Exp. S to A</i>		14.9 ± 0.8	6.4 ± 3.2		13.0 ± 0.1
12	GS2->GS1	Anti-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	13.2	-6.4	15.1	
		Syn-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	13.7	-7.6	15.9	15.0
		Anti-TS	SMD(DMF)//M062X/TZVP	15.1	-3.2	16.0	
		Syn-TS	SMD(DMF)//M062X/TZVP	12.5	-8.2	15.0	14.6
		<i>Exp. A to S</i>		15.3 ± 0.9	7.6 ± 3.6		13.0 ± 0.1
13	GS1->GS2	Anti-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	12.2	-4.9	13.7	
		Syn-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	12.1	-6.6	14.1	13.5
		Anti-TS	SMD(DMF)//M062X/TZVP	13.6	-7.4	15.8	
		Syn-TS	SMD(DMF)//M062X/TZVP	12.2	-6.9	14.3	14.2
		<i>Exp. S to A</i>		13.0 ± 1.5	-3.7 ± 4.8		14.1 ± 0.1
13	GS2->GS1	Anti-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	12.8	-4.7	14.2	
		Syn-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	12.7	-6.4	14.6	13.9
		Anti-TS	SMD(DMF)//M062X/TZVP	15.8	-1.8	16.3	
		Syn-TS	SMD(DMF)//M062X/TZVP	14.4	-1.4	14.8	14.7
		<i>Exp. A to S</i>		15.4 ± 1.1	5.3 ± 6.1		13.8 ± 0.1
14	GS1->GS2	Anti-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	15.7	-5.7	17.4	
		Syn-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	15.4	-6.4	17.3	16.9
		Anti-TS	SMD(DMF)//M062X/TZVP	14.4	-1.9	14.9	
		Syn-TS	SMD(DMF)//M062X/TZVP	12.1	-4.6	13.5	13.5
		<i>Exp. S to A</i>		15.5 ± 1.1	5.2 ± 5.3		13.9 ± 0.1
14	GS2->GS1	Anti-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	14.2	-6.5	16.1	
		Syn-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	13.9	-7.2	16.0	15.7
		Anti-TS	SMD(DMF)//M062X/TZVP	15.8	-0.3	15.9	
		Syn-TS	SMD(DMF)//M062X/TZVP	13.6	-3.0	14.5	14.4
		<i>Exp. A to S</i>		14.7 ± 1.2	1.7 ± 3.7		14.2 ± 0.1
4	GS1->GS2	Anti-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	11.2	-7.5	13.5	
		Syn-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	11.4	-7.6	13.7	13.2
		Anti-TS	SMD(DMF)//M062X/TZVP	11.0	-6.9	13.0	
		Syn-TS	SMD(DMF)//M062X/TZVP	11.0	-7.2	12.8	12.5
		<i>Exp. S to A</i>		14.4 ± 0.8	1.8 ± 3.0		13.9 ± 0.1
4	GS2->GS1	Anti-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	10.8	-4.0	12.0	
		Syn-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	11.0	-4.1	12.2	11.7
		Anti-TS	SMD(DMF)//M062X/TZVP	16.1	3.6	15.0	
		Syn-TS	SMD(DMF)//M062X/TZVP	15.8	3.2	14.9	14.5
		<i>Exp. A to S</i>		15.6 ± 0.7	6.6 ± 3.1		13.6 ± 0.1
5	GS1->GS2	Anti-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	14.1	-11.2	17.5	
		Syn-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	11.6	-8.2	14.1	
		Anti-TS	SMD(DMF)//M062X/TZVP				
		Syn-TS	SMD(DMF)//M062X/TZVP				
		<i>Exp. S to A</i>		14.8 ± 1.0	1.7 ± 3.7		14.3 ± 0.1
5	GS2->GS1	Anti-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	12.9	-11.2	16.3	
		Syn-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	10.4	-8.2	12.9	
		Anti-TS	SMD(DMF)//M062X/TZVP				
		Syn-TS	SMD(DMF)//M062X/TZVP				
		<i>Exp. A to S</i>		16.5 ± 1.0	6.1 ± 4.4		14.7 ± 0.1
6	GS1->GS2	Anti-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	10.5	-3.9	11.7	
		Syn-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	10.5	-3.2	11.4	11.1
		Anti-TS	SMD(DMF)//M062X/TZVP				
		Syn-TS	SMD(DMF)//M062X/TZVP				
		<i>Exp. S to A</i>		14.6 ± 0.9	9.8 ± 4.2		11.7 ± 0.1
6	GS2->GS1	Anti-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	9.9	-6.0	11.1	
		Syn-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	9.9	-5.2	11.4	11.1
		Anti-TS	SMD(DMF)//M062X/TZVP				
		Syn-TS	SMD(DMF)//M062X/TZVP				
		<i>Exp. A to S</i>		15.3 ± 1.0	9.6 ± 4.1		12.5 ± 0.1

Table S24. Theoretical thermodynamic parameters of restricted rotation around N-Ph bond

Comp.	Process	Via	Method	ΔH^\ddagger (298 K) kcal mol ⁻¹	ΔS^\ddagger (298 K) cal K ⁻¹ mol ⁻¹	ΔG^\ddagger (298 K) kcal mol ⁻¹	$\Delta G_{\text{eff}}^\ddagger$ (298 K) kcal mol ⁻¹
11	GS1->GS3	Anti-TS	B3LYP/6-31+G(d,p)	3.1	4.6	1.8	1.8
		Syn-TS	B3LYP/6-31+G(d,p)	4.5	-2.3	5.2	
		Anti-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	1.6	-2.3	2.3	2.0
		Syn-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	1.9	-1.8	2.4	
11	GS3->GS1	Anti-TS	B3LYP/6-31+G(d,p)	1.2	1.8	0.7	0.7
		Syn-TS	B3LYP/6-31+G(d,p)	2.6	-5.1	4.1	
		Anti-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	0.1	-4.9	1.4	1.1
		Syn-TS	SMD(DMF)//B3LYP/6-31+G(d,p)	0.3	-4.4	1.6	

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