Supporting Information

Bis-(1,2,4-triazin-3-yl) ligand structure driven selectivity reversal between Am^{3+} and Cm^{3+}: Solvent extraction and DFT studies

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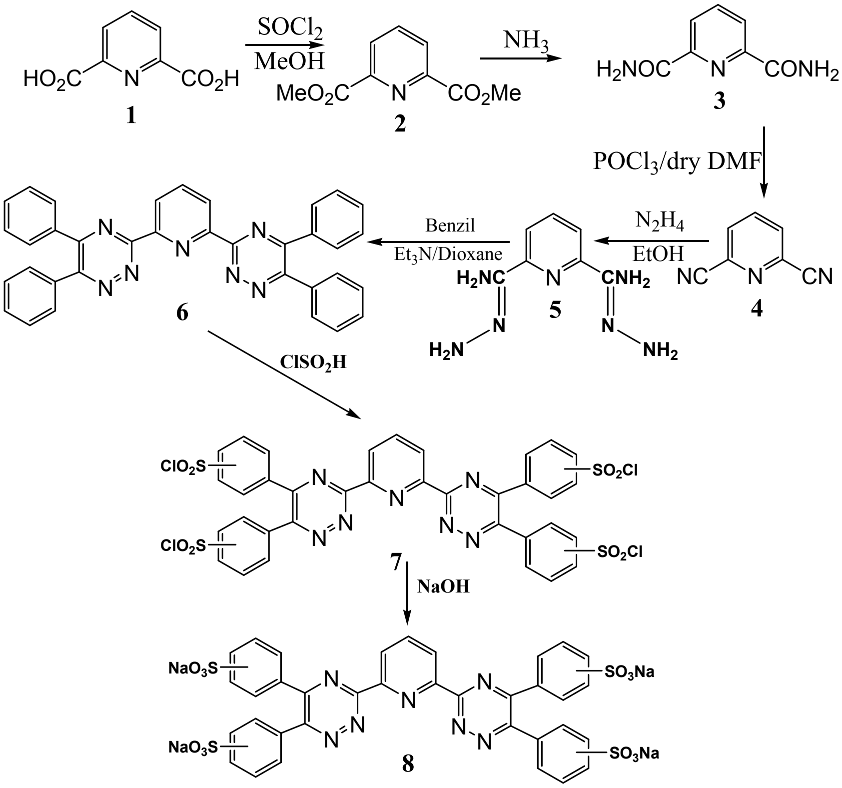
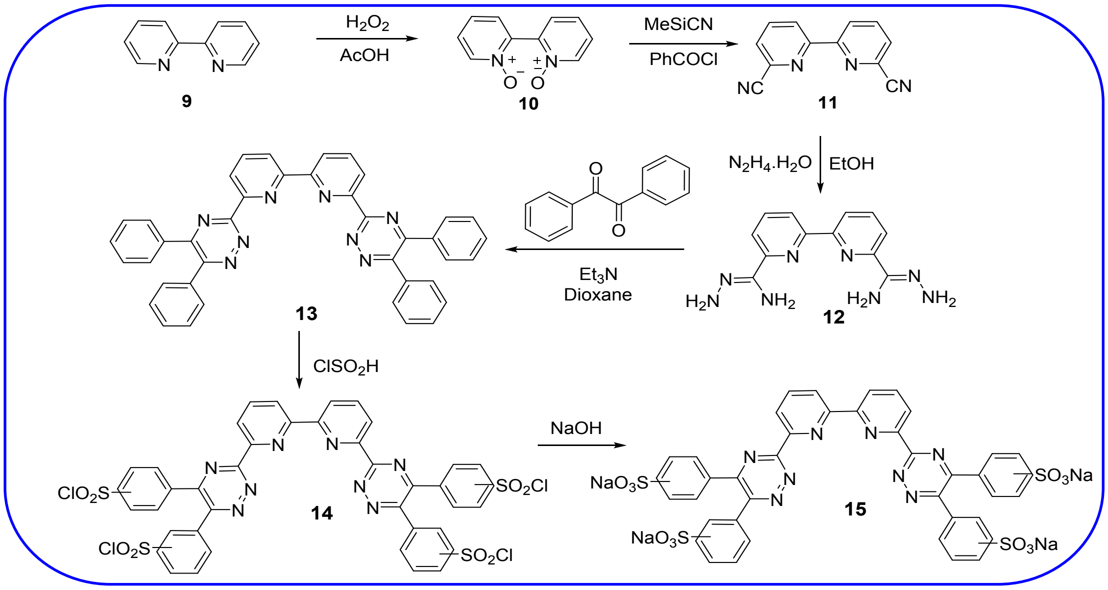
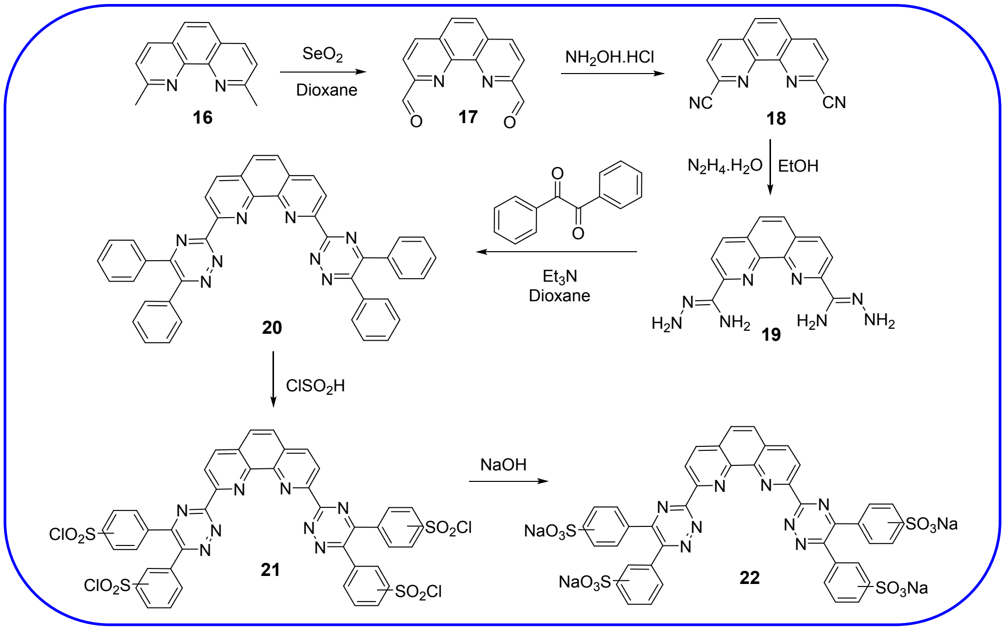


Scheme 1 - Synthesis of SO$_3$PhBTP (8)



Scheme 2. Synthesis of SO_3PhBTBP (15)



Scheme 3 - Synthesis of SO_3PhBTPhen (22)

Synthesis of dimethyl pyridine-2,6-dicarboxylate (2)

A suspension of pyridine-2,6-dicarboxylic acid (30 mmol) in methanol was slowly added to methanolic Thionyl chloride (75 mmol) at O^0c (ice bath), and the resulting mixture was stirred and refluxed for 14 hrs. The reaction mixture was cooled and quenched with ice-cold water and extracted with chloroform (3 x 50 ml). The organic phases were washed with saturated $NaHCO_3$ and dried with $MgSO_4$. The solvent was concentrated under reduced pressure to yield pure pyridine-2,6-dicarboxylate(2) as a white solid. Yield - 88%; mp 120-122°C. ^{1}H NMR: ($CDCl_3$, 400MHz) δ: 4.03 (s,6H), 8.04-8.08 (t,1H), 8.32-8.34 (d, 2H) ppm.^{13}C NMR: ($CDCl_3$, 400 MHz) δ: 53.17, 128.03, 138.40, 148.16, 165.00 ppm.

Synthesis of pyridine-2,6-dicarboxamide (3)

In a dry round bottom flask, dimethyl pyridine-2,6-dicarboxylate (5.1 mmol) was dissolved in an ammonia solution (1.8ml). The solution temperature was brought up to ~40° C and stirred vigorously for 1 hour. The reacting reaction progress was monitored by TLC analysis. The reaction mass was cooled in an ice bath for 2-3 hours, and the resulting solid was filtered, washed with deionised water followed by vacuum dry obtained white solid of pyridine-2,6-dicarboxamide (3). Yield – 91%; mp 325-330°C. ^{1}H NMR (DMSO-d_6, 400MHz) δ:7.71 (s, 2H) 8.12–8.20 (m, 3H)8.91 (s, 2H) ppm. ^{13}C NMR (DMSO-d_6, 400MHz): 124.72, 139.70, 149.4, 165.97ppm.

Synthesis of pyridine-2,6-dicarbonitrile (4)

To a stirred solution of Pyridine-2,6-dicarboxamide (3mmol) in 15 ml of dry DMF at 0^{o}C and Phosphorus oxychloride (18 mmol) was added over 5 min dropwise. The reaction mixture was vigorously stirred overnight at room temperature and poured into ice water. The aqueous layer was extracted with DCM (30ml x 3), and the combined organic layer was washed with water (30ml x 3) then dried with anhydrous Na_2SO_4; the solvent was removed by rotavapor. The product pyridine-2,6-dicarbonitrile(4) was obtained with 64% yield as a white power; mp 120-123°C.^{1}H NMR ($CDCl_3$, 400 MHz) δ: 7.94-7.96(d, 2H) 8.08-8.12 (t, 1H) ppm. ^{13}C NMR ($CDCl_3$, 400MHz): 115.47, 131.18, 135.31, 138.95 ppm.

Synthesis of pyridine-2,6-dicarbohydrazonamide (5)

Hydrazine hydrate (10 mL, 75 %) was added to the pyridine-2,6-dicarbonitrile (3.9 mmol) dissolved in ethanol (10ml). The resulting solution was stirred at room temperature for 14-15 days. The crude mixture was poured into ice water (100 ml), and the resulting solid was filtered. The solid residue was dried to give pyridine-2,6-dicarbohydrazonamide as a pale white powder with 45% yield; mp 245°C. ^{1}H NMR (DMSO–d_6, 400 MHz) δ: 5.32 (s, 4H), 6.12 (s, 4H), 7.64-7.68 (dd, 1H), 7.81-7.83 (d, 2H) ppm. ^{13}C NMR (DMSO–d_6, 400 MHz) δ: 118.5, 136.4, 144.2, 150.6 ppm.

Synthesis of 2,6-bis(5,6-diphenyl-1,2,4-triazin-3-yl)pyridine (6)

A solution of benzil (1.5.7 mmol), Triethylamine (4.6 mL) and pyridine-2,6-dicarbohydrazonamide (2.6 mmol) in 1,4-dioxane (50 mL) was refluxed for 3 days. The reaction mixture was then cooled to room temperature and the solid was filtered and washed with ether. The residue was purified using column chromatography to provide 2,6-bis(5,6-diphenyl-1,2,4-triazin-3-yl) pyridine as yellow solid. Yield – 88 %; mp 309-310°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 7.37-7.49(m, 12H), 7.66-7.68 (m, 4H), 7.79-7.81 (m, 4H), 8.19-8.23 (t, 1H), 8.91-8.93 (d, 2H)ppm. ^{13}C NMR ($CDCl_3$, 400 MHz) δ: 125.61, 128.54, 128.72,129.58, 129.87, 130.15, 130.89, 135.36, 135.65, 138.39, 153.56, 156.27, 156.53, 160.51ppm.

Synthesisof 3,3',3'',3'''-(pyridine-2,6-diylbis(1,2,4-triazine-3,5,6-triyl))tetrabenzenesulfonyl chloride (7)

2,6-Bis(5-phenyl-1,2,4-triazin-3-yl)pyridine (0.923 mmol) was dissolved in chlorosulfonic acid (10 mL) in a 50 mL round-bottom flask. The reaction mixture was stirred at 170^{o}C for 3 hours. After cooling to room temperature, the reaction mass was slowly poured into the ice. The solid precipitate was filtered off and washed twice using deionised water to give yellow-green powder in 97% yield; mp above 300^{o}C. ^{1}H NMR (DMSO-d_6, 400 MHz) δ: 7.33-7.36 (m, 8H), 7.61-7.73 (m, 4H), 8.19-8.22 (m, 4H), 8.40-8.43 (t, 1H), 8.72-8.74 (d, 2H)ppm. ^{13}CNMR (DMSO-d_6, 400MHz) δ: 126.22, 126.38, 126.90, 127.36, 128.36, 130.50, 130.70, 135.33,135.49, 139.52, 148.80, 148.88, 153.86, 156.31, 156.72, 160.82 ppm.

Synthesis of sodium 3,3',3'',3'''-(pyridine-2,6-diylbis(1,2,4-triazine-3,5,6-triyl)) tetra benzenesulfonate (SO_3PhBTP) (8) - L_I

A mixture of 3,3',3'',3'''-(pyridine-2,6-diylbis(1,2,4-triazine-3,5,6-triyl))tetrabenzene (0.320 mmol) and NaOH (2.56 mmol) in methanol (30 mL) was stirred and refluxed for 4 h. After cooling to room temperature, the reaction mass was filtered and the resulting solution was neutralized with 2M HCl to 7-8 pH. The product separated was washed with cold methanol followed by acetone and dried in vacuum to give sodium 3,3',3'',3'''-(pyridine-2,6-diylbis(1,2,4-triazine-3,5,6-triyl)) tetra benzenesulfonate (8) as greenish black solid with 70% yield; mp above 300 °C.^{1}H NMR (DMSO-d_6, 400 MHz) δ: 7.25-7.34 (m, 8H), 7.60-7.75 (m, 4H), 8.26-8.29 (m, 4H), 8.43-8.47 (t, 1H), 8.75-8.77 (d, 2H), ppm. ^{13}C NMR (DMSO-d_6) δ: 126.93, 127.36, 128.18, 130.28, 130.50, 135.18, 135.35, 149.34, 156.36, 156.87 ppm.

Synthesis of bipyridine N- oxide (10)

Hydrogen peroxide (25.24 mmol) was added to the 2,2'-bipyridine(6.40 mmol) dissolved in acetic acid (20 mL). The resulting solution was stirred at 75^{o}C for 8 h. After the completion of the reaction, the reaction mass was allowed to cool to room temperature and stirring was continued overnight. The solution was diluted with acetone (100 mL) and the precipitated solid was filtered. The solid was allowed to dry in air to afford the title compound (10) as a white solid (0.799 gm, 67 %), mp: 295℃.^{1}H NMR: (D_2O, 400MHz) δ: 7.66–7.69(m, 4H), 7.75–7.79(m, 2H), 8.38–8.40 (m, 2H) ppm.^{13}C NMR:(D_2O,400MHz) δ: 128.4, 128.8, 131.4, 139.7, 141.7 ppm.

Synthesis of 2,2'-Bipyridine-6,6'-dicarbonitrile (11)

A solution of 2,2'-Bipyridine-1,1'-dioxide (2.66 mmol) in DCM (10 mL) and 7.98 mmol of trimethylsilyl cyanide, 7.98 mmol of benzoyl chloride was stirred at room temperature for 3 days. After 3 days, the reaction mixture was refluxed for 24h and the reaction mass was stirred vigorously with 10ml of 10% KOH solution. The precipitate was filtered off and rinsed with water and ether to yield 0.2 g (41%) of off-white powder. (0.225 gm, 41%),mp: 245-250℃. ^{1}H NMR: ($CDCl_3$, 400MHz) δ:7.77-7.79 (dd,2H), 8.00-8.04 (dd,2H), 8.71-8.73 (dd, 2H) ppm. ^{13}CNMR:($CDCl_3$, 400MHz) δ:117.0, 124.7, 129.1, 133.4, 138.4, 155.4 ppm.

Synthesis of 1,10-phenanthroline-2,9-dicarbaldehyde (17)

Selenium dioxide (30.57 mmol) was reflux in dioxane (150 mL) and water (3 mL). A solution of 2, 9-dimethyl-1, 10-phenanthroline (3 gm, 14.42 mmol) in dioxane was added dropwise and heated under reflux for 3 hr. The reaction mass was filtered while hot and the filtrate was cool to 0^{o}C. The precipitated solid was filtered and washed with dioxane (30 mL), and triturated with chloroform. The filtrate was evaporated to afford dialdehyde 1,10-Phenanthroline-2,9-dicarbaldehyde (17)as a light yellow solid (43%), mp: 241℃.^{1}H NMR: (DMSO–d_6, 400MHz) δ: 8.27 (s, 2H), 8.41 (s, 2H) 8.77 (dd, 2H), 10.34 (d, 2H) ppm. ^{13}C NMR: (DMSO–d_6, 400MHz) δ: 120.5,131, 138.8, 194 ppm.

Synthesis of 1,10-Phenanthroline-2,9- dicarbonitrile (18)

1,10-Phenanthroline-2,9-dicarbaldehyde (21.18 mmol), hydroxylamine hydrochloride (46.59 mmol, 2.2 eq) and triethylamine (139.83 mmol, 6.6 eq) was added in dry acetonitrile (350 mL). The mixture was heated under reflux for 3 h. *p*-toluenesulfonyl chloride (69.91 mmol, 3.3 eq) and DBU (63.54 mmol, 3 eq) was added after cooling the reaction mixture and heated under reflux for 24 h. The mixture was filtered while still hot and the solid residue was washed with hot acetonitrile (15mL). The filtrate was evaporated and the obtained brown semi-solid was triturated with methanol. The undissolved solids are filtered and washed with methanol and ether to afford 1,10-Phenanthroline-2,9- dicarbonitrile (18) as an off-white solid (1.70 gm, 35%).^{1}H NMR: (DMSO–d_6, 400MHz) δ: 8.28 (s, 2H), 8.42-8.44 (d, 2H), 8.84-8.86 (d, 2H) ppm. ^{13}C NMR: (DMSO–d_6, 400MHz) δ: 118.1, 128.0, 129.7, 131.0, 133.3, 139.1, 145.3 ppm.

General Synthesis of 2,2'-Bipyridine-6,6'-dicarbohydrazonamide (12) &1,10-phenanthroline-2,9-bis(carbohydrazonamide) (19)

Hydrazine hydrate (8 mL, 75 %) was added to the respective carbonitrile (2.43 mmol) dissolved in ethanol (20mL). The resulting solution was stirred at room temperature for 14-15 days. The crude reaction mixture was poured into ice water (100 mL), and the resulting solid was filtered. The solid product was dried to give title compound.

2,2'-Bipyridine-6,6'-dicarbohydrazonamide (12)

Pale-yellow powder (0.565 gm, 87%).^{1}H NMR: (DMSO–d_6, 400MHz) δ:5.59 (s, 4H), 6.13(s, 4H), 7.89-7.94 (t, 2H), 7.97-8.01 (dd, 2H), 8.63-8.91 (dd, 2H) ppm.

1,10-phenanthroline-2,9-bis(carbo hydrazonamide) (19)

Yellow powder (0.512 gm, 69%), mp above 300 °C.^{1}H NMR: (DMSO–d_6, 400MHz) δ: 5.64 (s, 4H), 6.13 (s, 4H), 7.94 (s, 2H), 8.28-8.30 (d, 2H), 8.37-8.39 (d, 2H) ppm. ^{13}C NMR: (DMSO–d_6, 400MHz) δ: 119.4, 128.6, 136.5, 143.8, 143.9, 151.7 ppm.

General Synthesis of Compound 6,6'-Bis(5,6-diphenyl-1,2,4-triazin-3-yl)-2,2'-bipyridine (13) & 9-Bis(5,6-diphenyl-1,2,4-triazin-3-yl)-1,10-phenanthroline (20)

The solution of respective dicarbohydrazonamide (1.69 mmol), benzil (16.28 mmol, 2.2 eq) and triethylamine (15 mL) in 1,4-dioxane (100 mL) was refluxed for 3 days. The reaction mixture was then cooled to room temperature and the solid was filtered and washed with DCM. The solid product was purified using column chromatography.

6,6'-Bis(5,6-diphenyl-1,2,4-triazin-3-yl)-2,2'-bipyridine (13)

Yellow solid (78% yield), mp: above 300 °C.^{1}H NMR: ($CDCl_3$, 400MHz) δ: 7.40–7.49 (m, 12H), 7.67–7.69 (m, 4H), 7.76–7.78 (m, 4H), 8.12-8.16 (t,2H), 8.74-8.76 (dd, 2H), 9.01-9.03 (dd, 2H) ppm. ^{13}C NMR:($CDCl_3$, 400MHz): δ: 123.4, 124.5, 128.6, 128.7, 129.6, 129.8, 130.0, 130.8, 135.3, 135.7,138.1, 152.2, 156.0, 156.2, 156.3, 160.7 ppm.

9-Bis(5,6-diphenyl-1,2,4-triazin-3-yl)-1,10-phenanthroline (20)

Yellow solid (47% Yield), mp: above 290ºC.^{1}H NMR: ($CDCl_3$, 400MHz) δ: 7.35–7.44 (m, 12H), 7.74 (s, 4H), 7.93 (d, 4H), 7.98 (s, 2H), 8.51-8.53 (d, 2H), 9.02-9.03 (d, 2H) ppm.^{13}C NMR:($CDCl_3$, 400MHz): δ: 123.4, 127.7, 128.6, 128.7, 129.0, 129.6, 130.0, 130.4, 130.8, 135.4, 135.5, 137.4, 146.6, 153.0, 156.3, 156.5, 160.8 ppm.

General Synthesis of 3,3',3'',3'''-[3-(2,2'-Bipyridine-6,6'-diyl)-1,2,4-triazine-5,5,6,6-tetrayl]tetrabenzenesulfonyl chloride (14) &3,3',3'',3'''-[3-(1,10-Phenanthroline-2,9-diyl)-1,2,4- triazine-5,5,6,6-tetrayl] tetra benzenesulfonyl Chloride (21)

The respective bipyridine / phenanthroline (0.467 mmol) was added to chlorosulfonic acid (10 mL) and stirred at 170℃ for 5 h. After cooling to room temperature, the reaction mass was slowly poured into the ice. The solid precipitate was filtered off and washed using water to afford the title compound.

3,3',3'',3'''-[3-(2,2'-Bipyridine-6,6'-diyl)-1,2,4-triazine-5,5,6,6-tetrayl] tetrabenzenesulfonyl chloride (14)

Brown powder. (90% Yield), mp: above 300 ºC.^{1}H NMR: (DMSO–d_6, 400MHz) δ: 7.28–7.37 (m, 8H), 7.61–7.75 (m, 4H), 8.22 (t, 2H), 8.33–8.37 (m, 4H), 8.64-8.66(d, 2H), 8.86-8.88 (d, 2H) ppm.

3,3',3'',3'''-[3-(1,10-Phenanthroline-2,9-diyl)-1,2,4- triazine-5,5,6,6-tetrayl] tetra benzenesulfonyl Chloride (21)

Brown solid (85% Yield), mp: above 300 ºC.^{1}H NMR (DMSO–d_6, 400MHz) δ:7.39 (m, 6H), 7.68–7.69 (m, 6H), 8.16–8.38 (m, 4H), 8.38 (s, 2H), 8.95-8.97 (d, 2H), 9.05-9.06 (d, 2H) ppm.

General Synthesis of Tetrasodium 3,3',3'',3'''-[3-(2,2'-bipyridine-6,6'-diyl)-1,2,4-Triazine -5,5,6,6- tetrayl] tetra benzenesulfonate, SO_3PhBTBP (15) &Compound sodium 3,3',3'',3'''-((1,10-phenanthroline-2,9-diyl) bis (1,2,4-triazine- 3,5,6-triyl)) tetra benzene sulfonate, SO_3PhBTPhen (22)

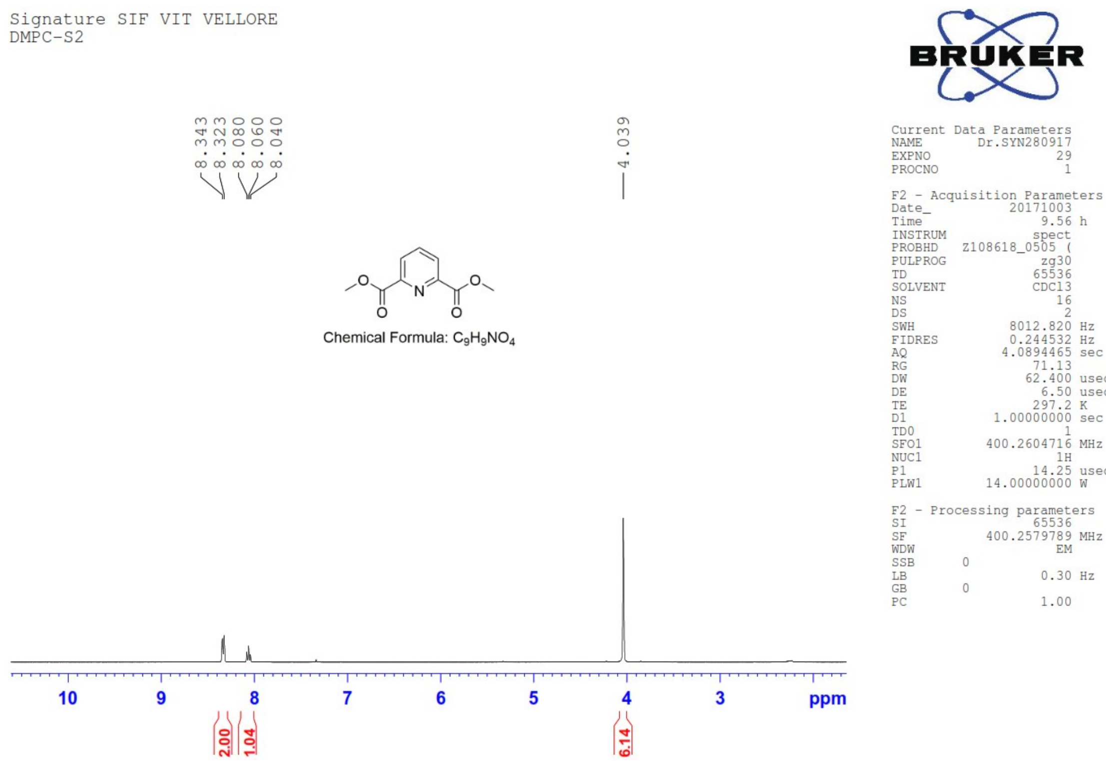
The respective tetrabenzene sulfonyl chloride (0.987 mmol) and NaOH (5.92 mmol, 6 eq) was added in MeOH (100 mL) and reflux for 4 h. The solution was allowed to cool to room temperature and neutralized by 2M HCl. The filtrate was diluted with acetone and the precipitated solid was filtered and washed with methanol and acetone. The solid was dried to afford the title compound.

Tetrasodium 3,3',3'',3'''-[3-(2,2'-bipyridine-6,6'-diyl)-1,2,4-Triazine -5,5,6,6-tetrayl]tetra benzenesulfonate, SO_3PhBTBP (15)

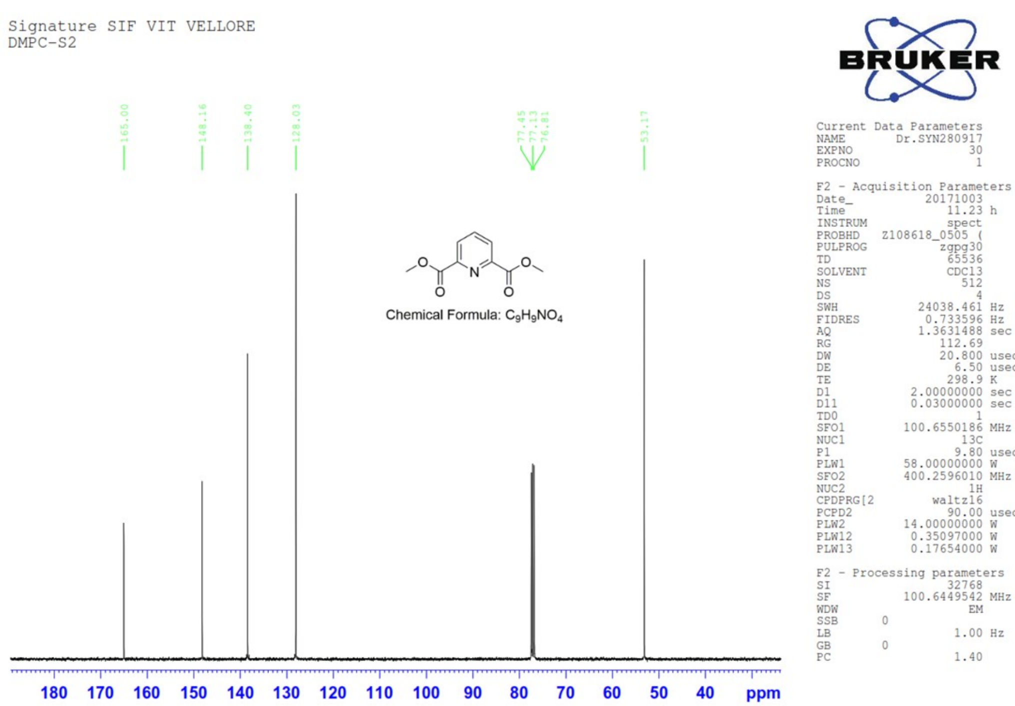
Brown solid (50% Yield), mp: above 300 °C. ^{1}H NMR: (DMSO–d_6, 400MHz) δ: 7.35–7.38 (m, 6H), 7.63–7.77 (m, 6H), 8.20 (t, 2H), 8.32–8.38 (m, 4H), 8.64-8.67 (d, 2H), 8.86-8.88 (d, 2H) ppm. ^{13}C NMR: (DMSO–d_6, 400MHz) δ: 131.0, 131.6,132.2, 133.0,133.1, 133.2, 134.3, 135.2, 135.3,140.0, 140.2, 144.3, 153.7,153.8, 154.0, 157.4, 160.4, 160.9, 161, 165.4 ppm.

Sodium 3,3',3'',3'''-((1,10-phenanthroline-2,9-diyl) bis (1,2,4-triazine- 3,5,6-triyl)) tetra benzene sulfonate, SO_3PhBTPhen (22)

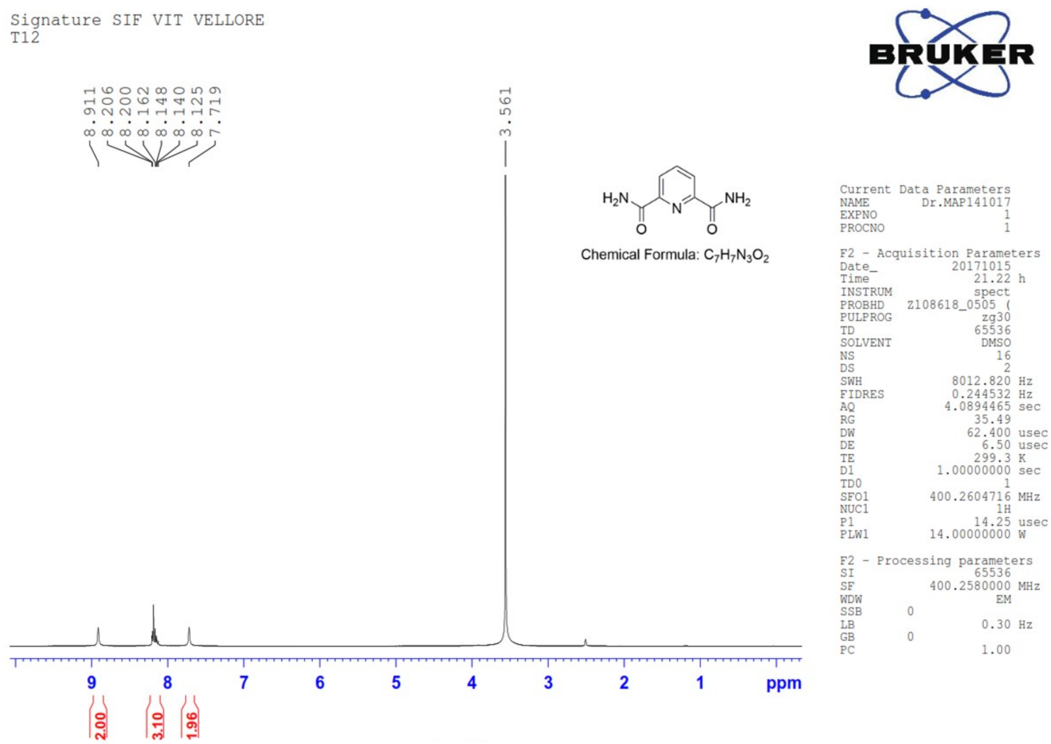
Brown solid (66% Yield), mp: above 300 °C. ^{1}H NMR (DMSO–d_6, 400MHz) δ:7.37 (m, 6H),7.71–7.78 (m, 6H), 8.32–8.38 (m, 6H) 8.99 (m, 4H) ppm.



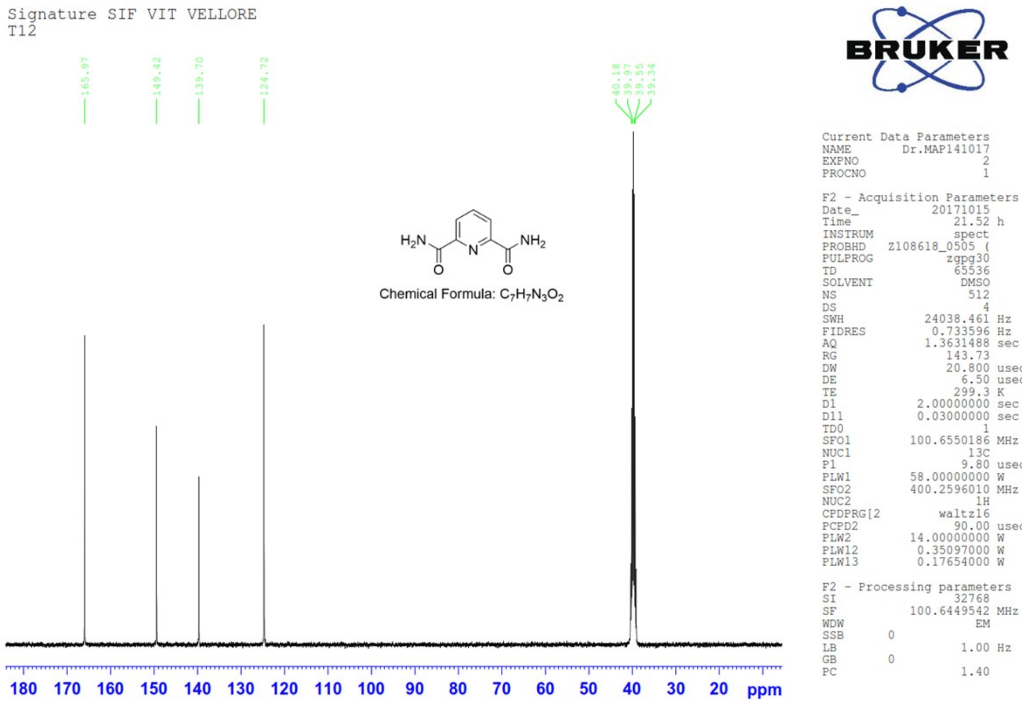
[1]H NMR spectrum of dimethyl pyridine-2,6-dicarboxylate (2)



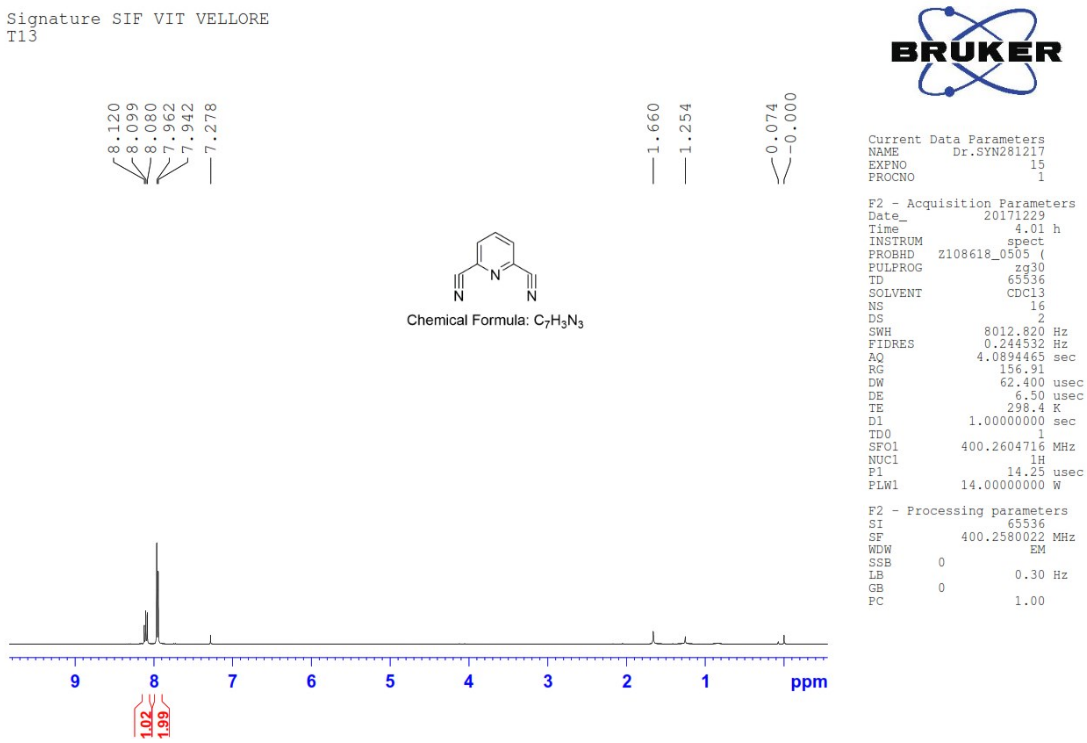
[13]C NMR spectrum of dimethyl pyridine-2,6-dicarboxylate (2)



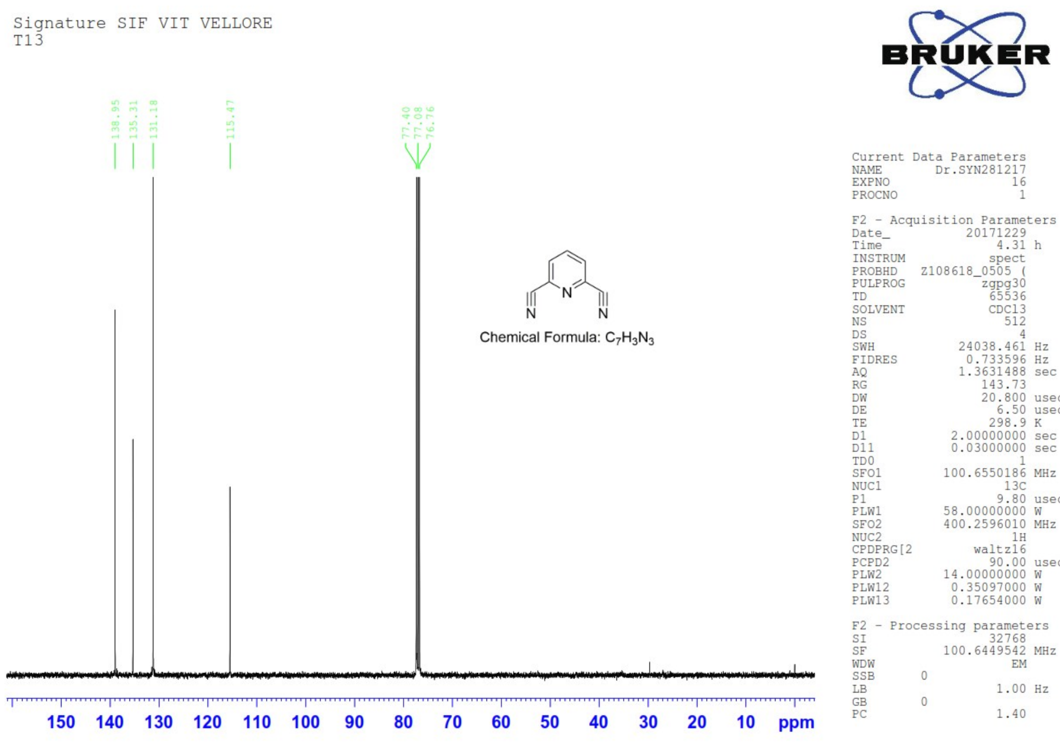
^{1}H NMR spectrum of pyridine-2,6-dicarboxamide (3)



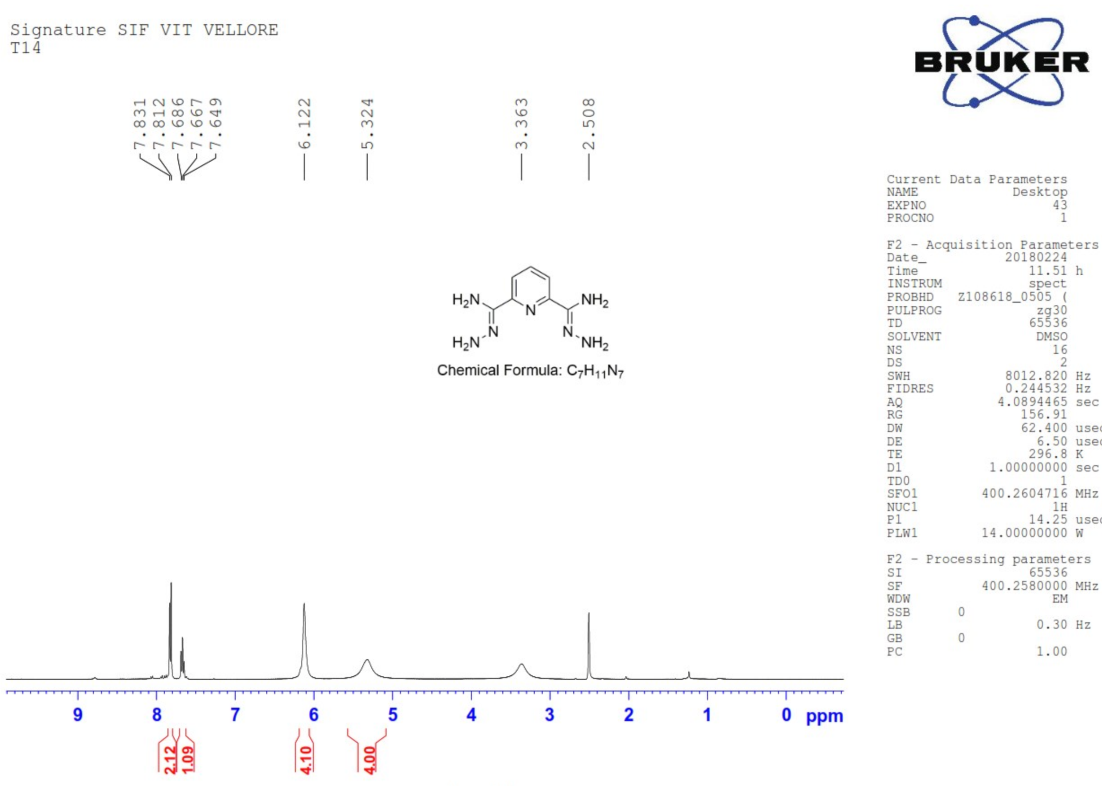
^{13}C NMR spectrum of pyridine-2,6-dicarboxamide (3)



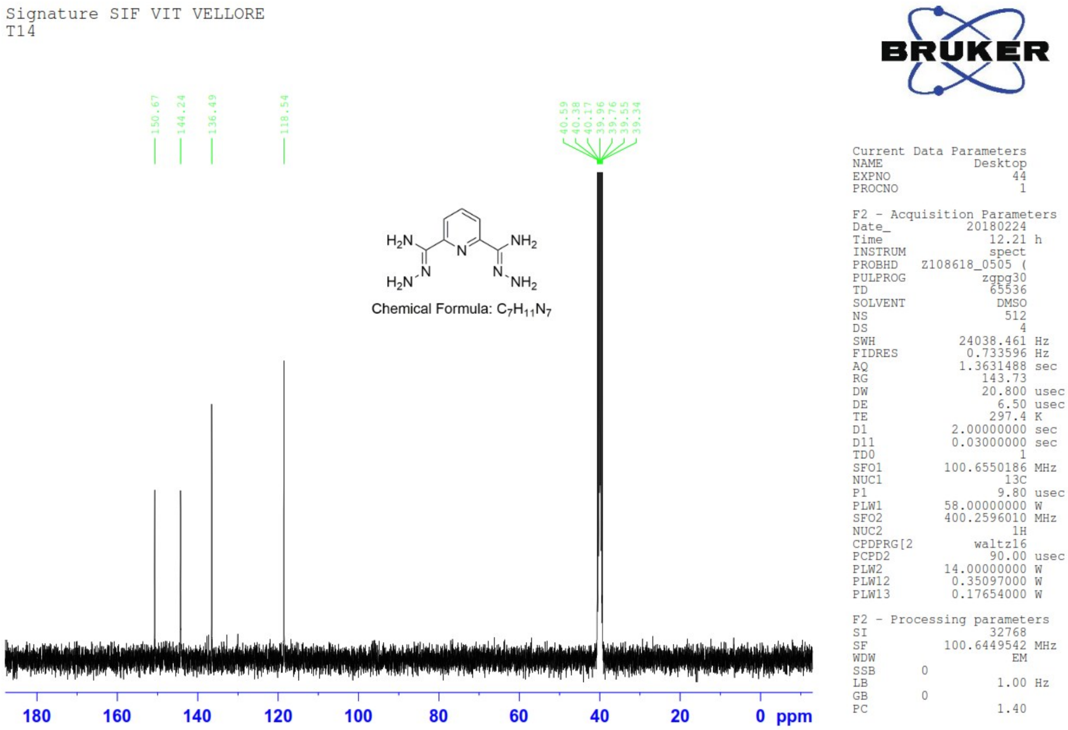
^{1}H NMR spectrum of pyridine-2,6-dicarbonitrile (4)



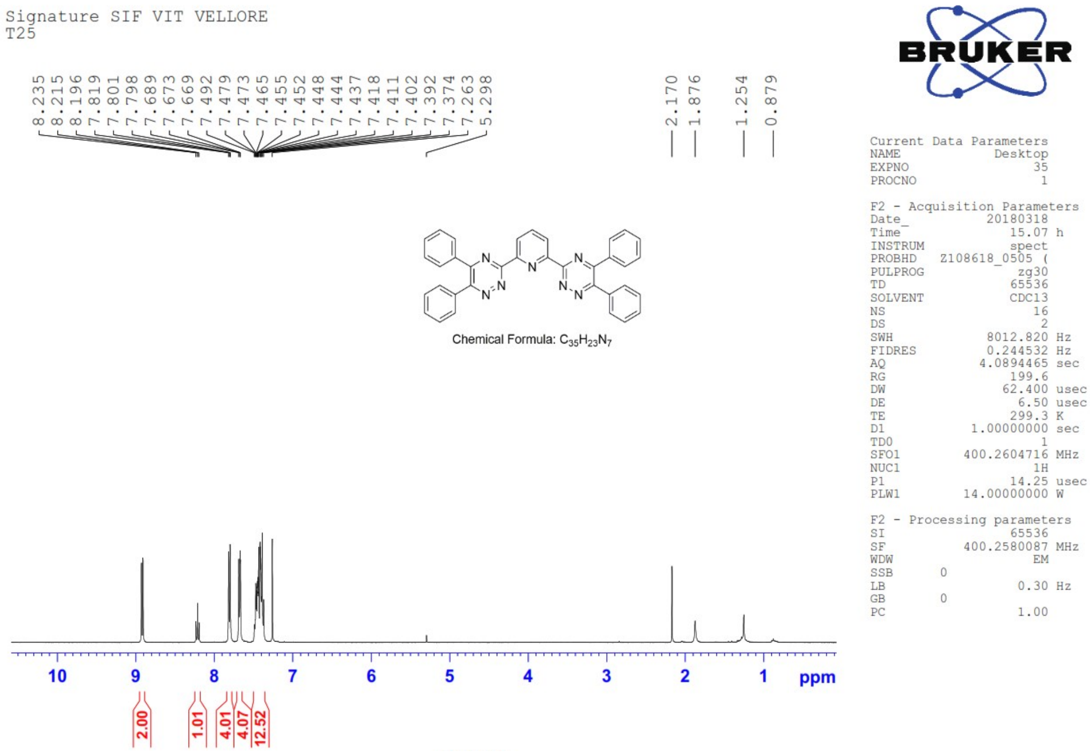
^{13}C NMR spectrum of pyridine-2,6-dicarbonitrile (4)



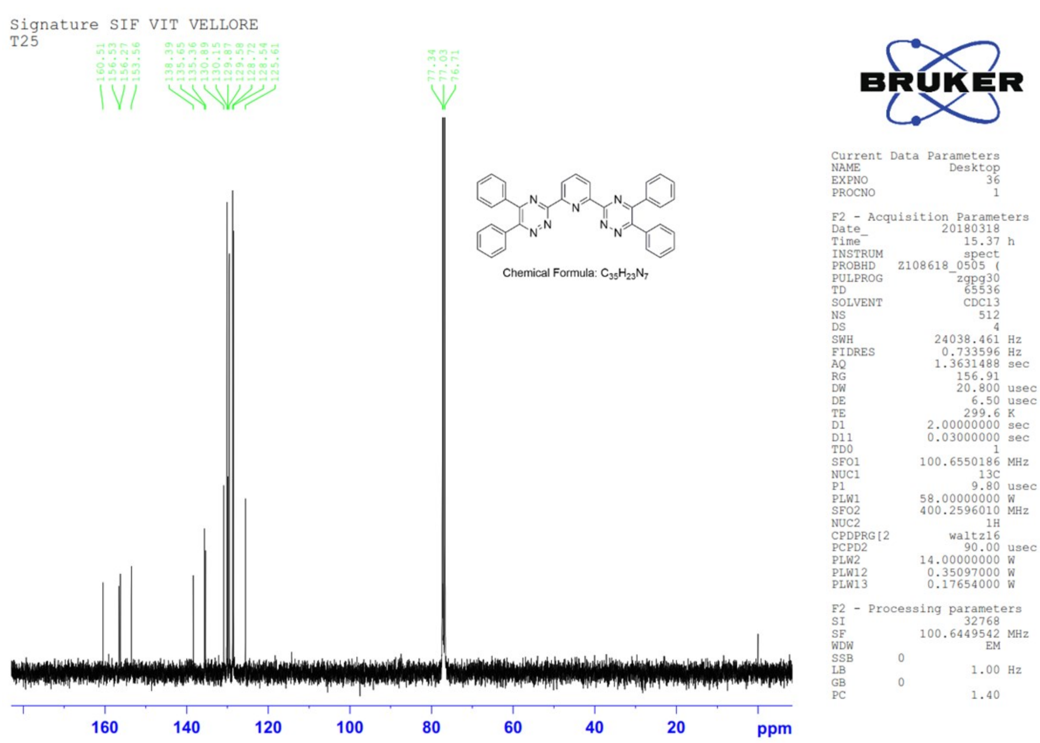
^{1}H NMR spectrum of pyridine-2,6-dicarbohydrazonamide (5)



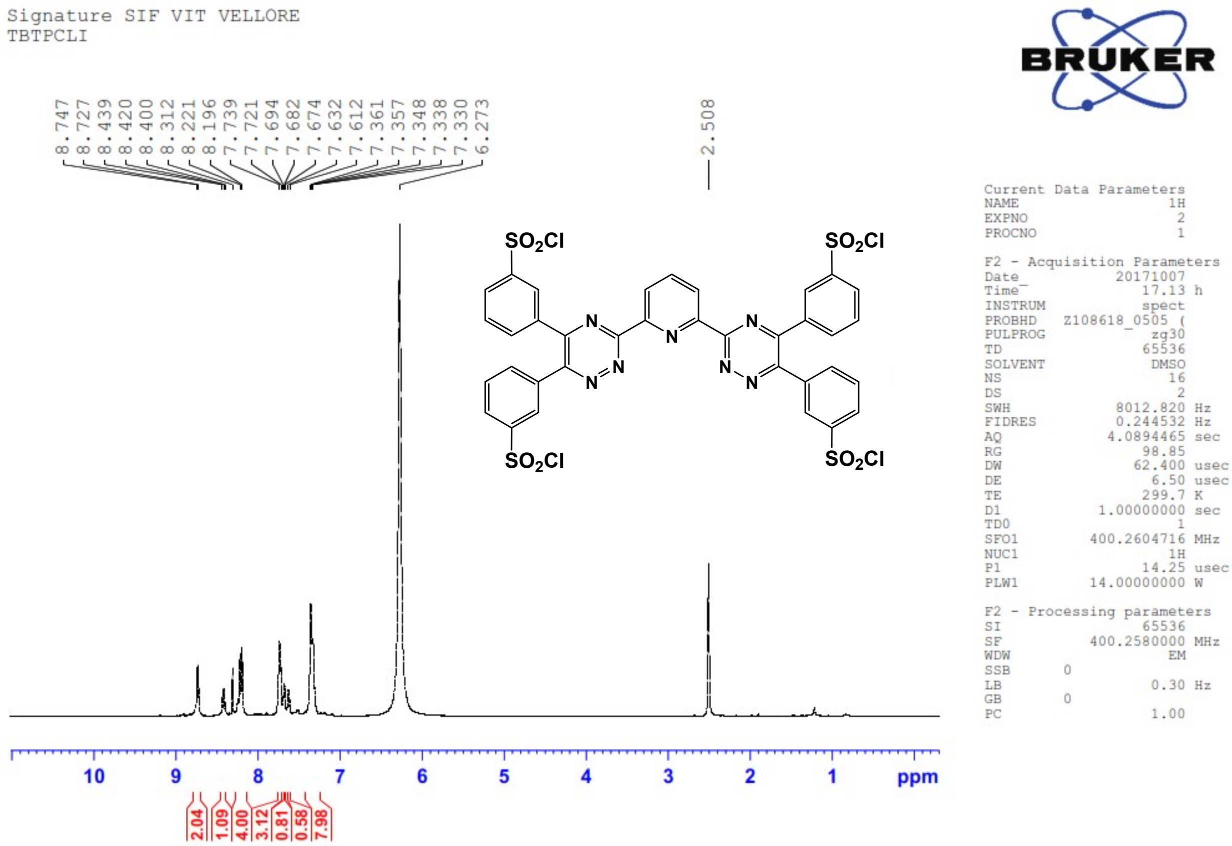
^{13}C NMR spectrum of pyridine-2,6-dicarbohydrazonamide (5)



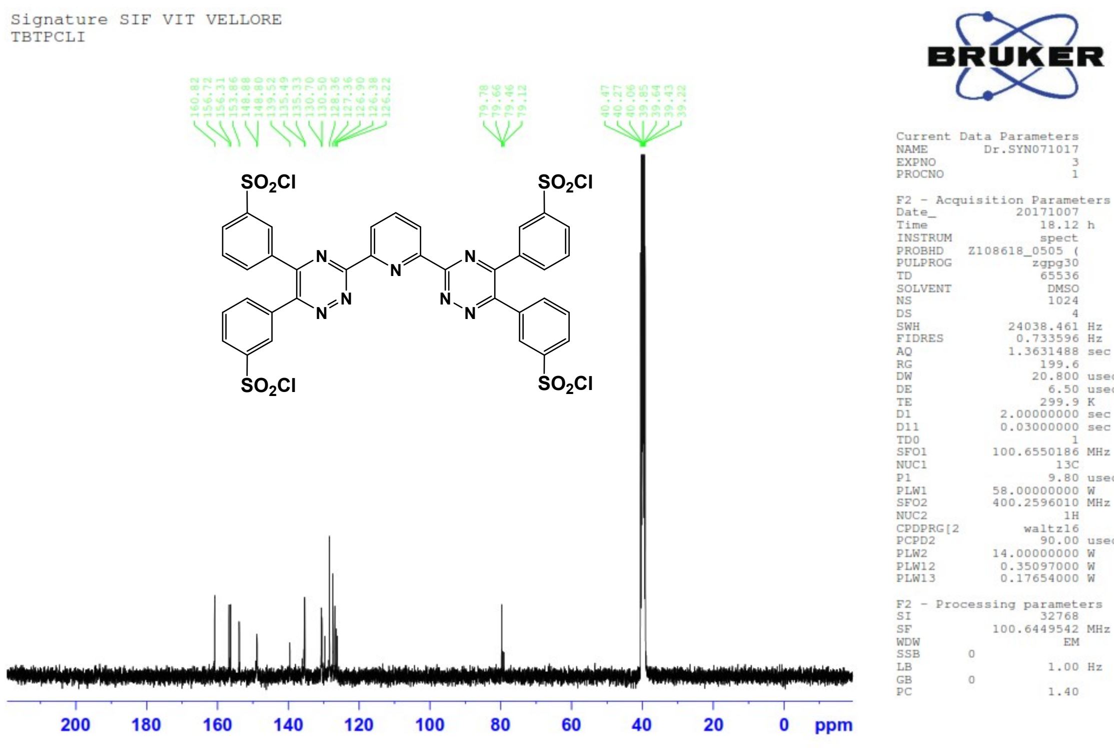
[1]H NMR spectrum of Synthesis of 2,6-bis(5,6-diphenyl-1,2,4-triazin-3-yl) pyridine (6)



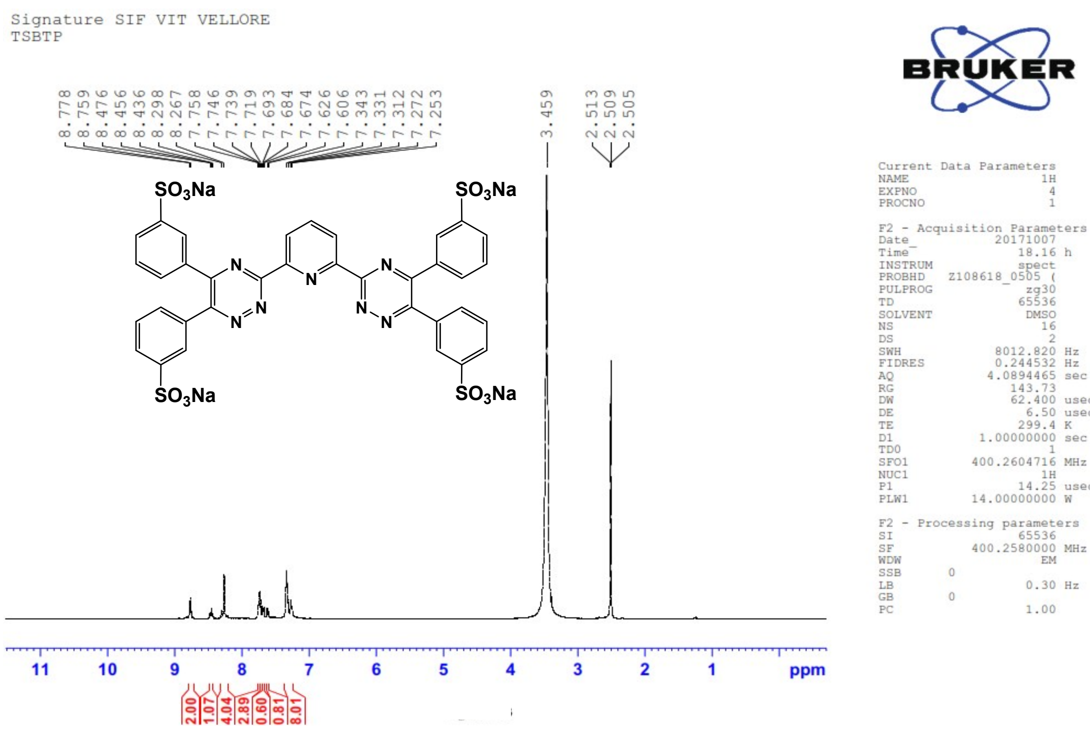
[13]C NMR spectrum of Synthesis of 2,6-bis(5,6-diphenyl-1,2,4-triazin-3-yl) pyridine (6)



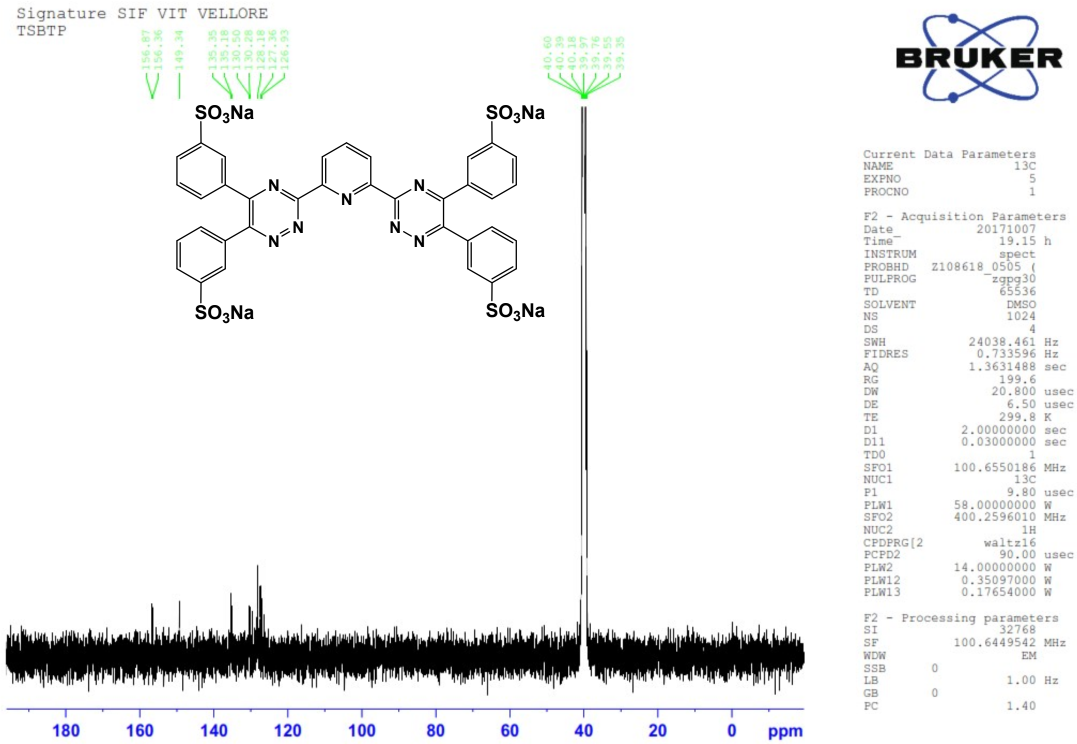
^{1}H-NMR spectrum of of 3,3',3'',3'''-(pyridine-2,6-diylbis(1,2,4-triazine-3,5,6-triyl))tetrabenzenesulfonyl chloride (7)



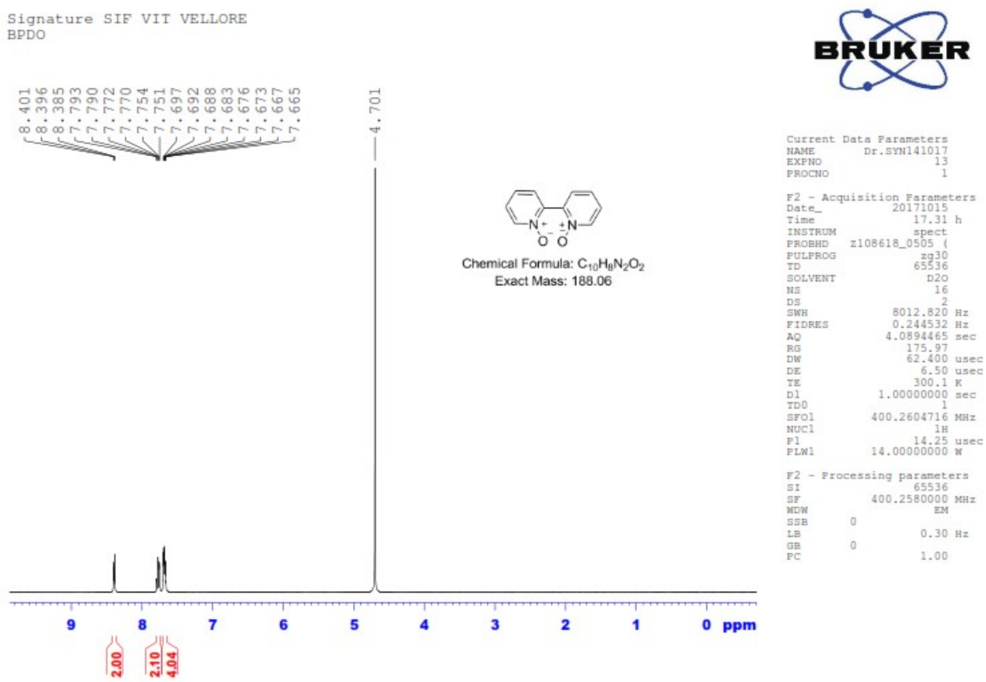
[13]C-NMR spectrum of of 3,3',3'',3'''-(pyridine-2,6-diylbis(1,2,4-triazine-3,5,6-triyl))tetrabenzenesulfonyl chloride (7)



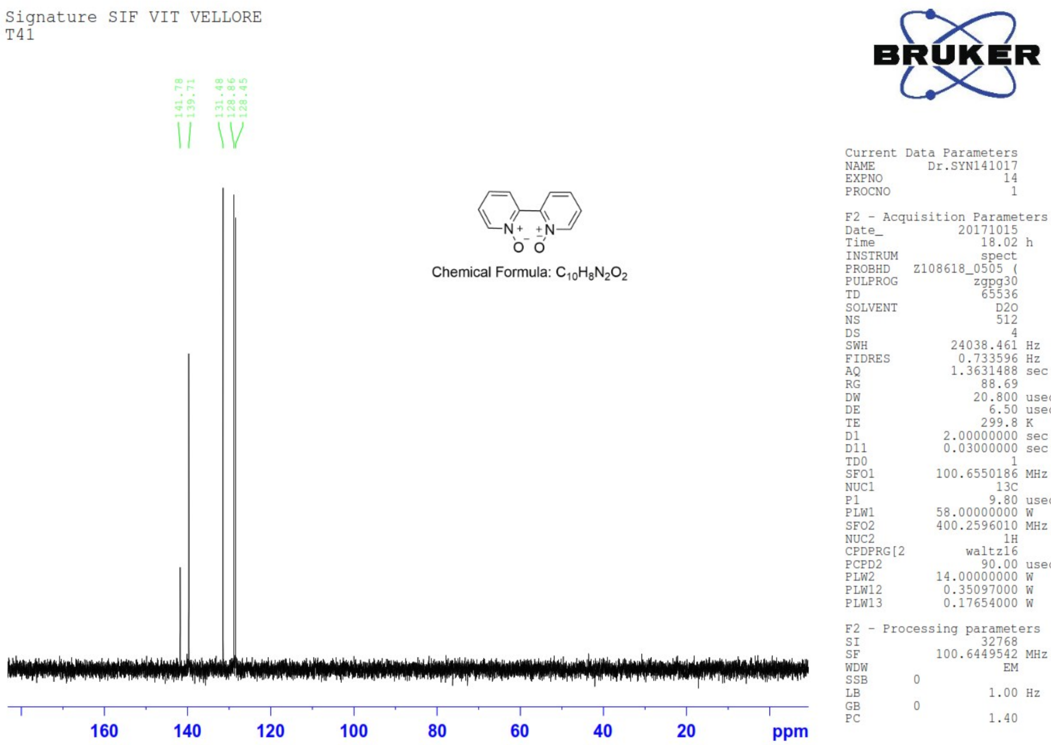
[1]H-NMR spectrum of sodium 3,3',3'',3'''-(pyridine-2,6-diylbis(1,2,4-triazine-3,5,6-triyl))tetra benzenesulfonate, SO_3PhBTP (8)



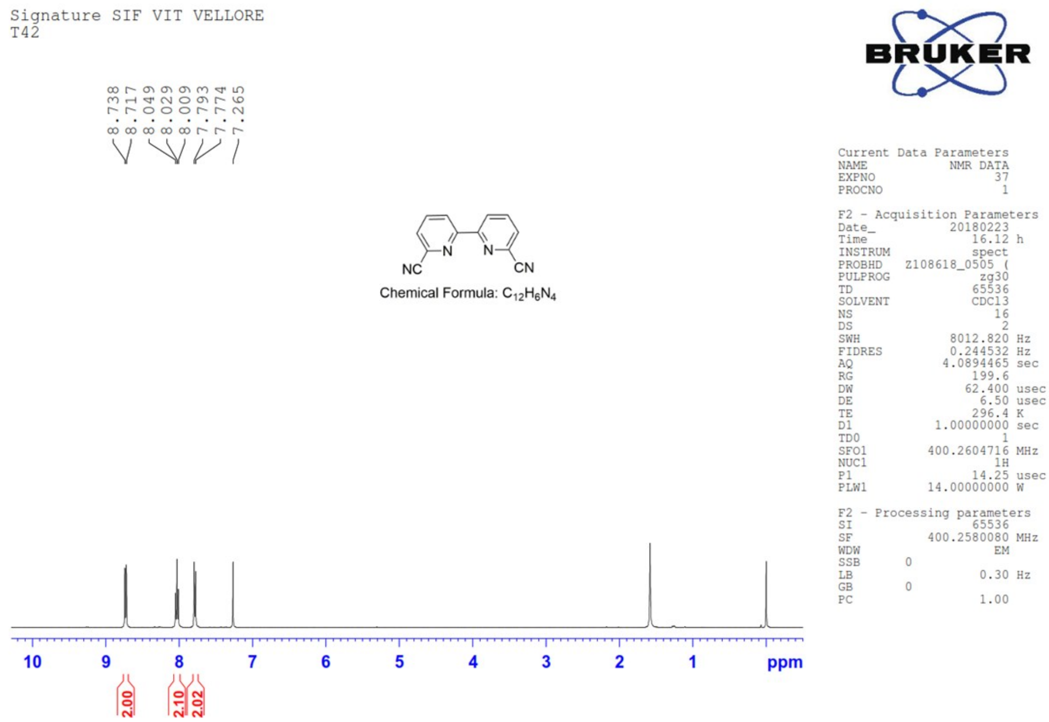
^{13}C-NMR spectrum of sodium 3,3',3'',3'''-(pyridine-2,6-diylbis(1,2,4-triazine-3,5,6-triyl))tetra benzenesulfonate, SO_3PhBTP (8)



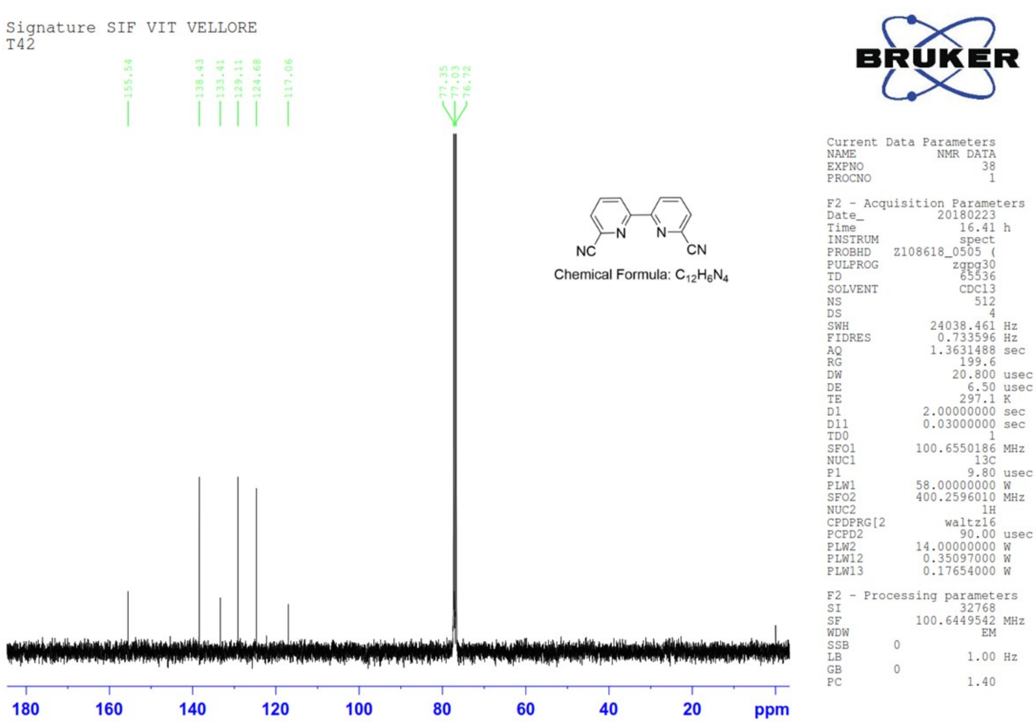
[1]H-NMR spectrum of bipyridine N- oxide (10)



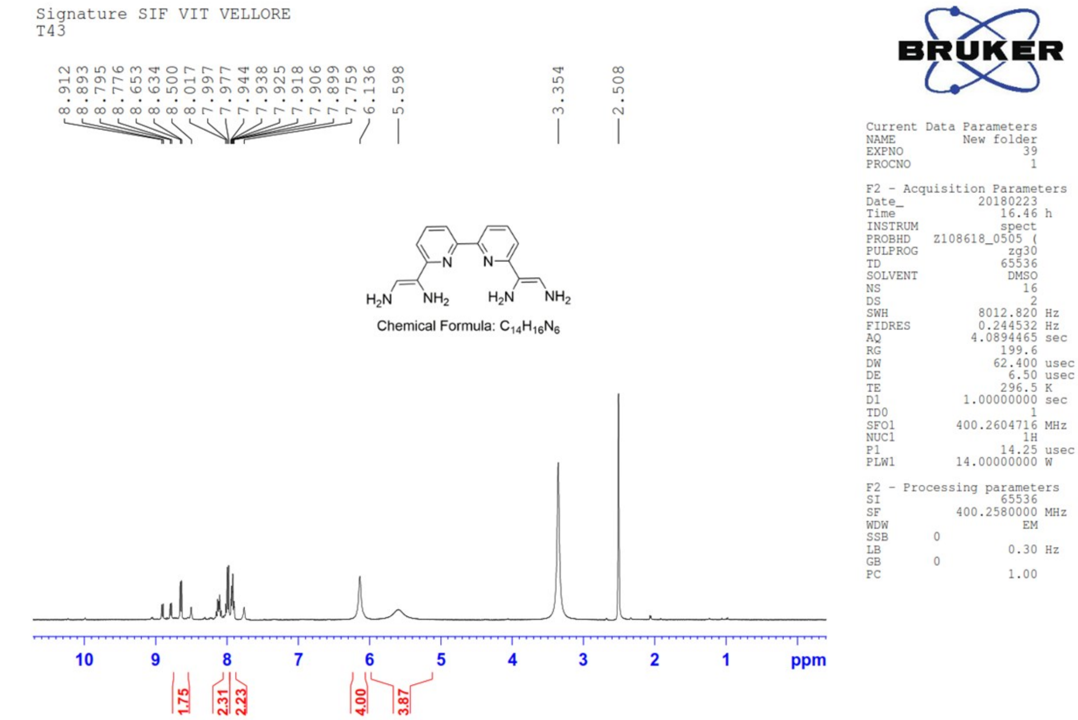
^{13}C-NMR spectrum of bipyridine N- oxide (10)



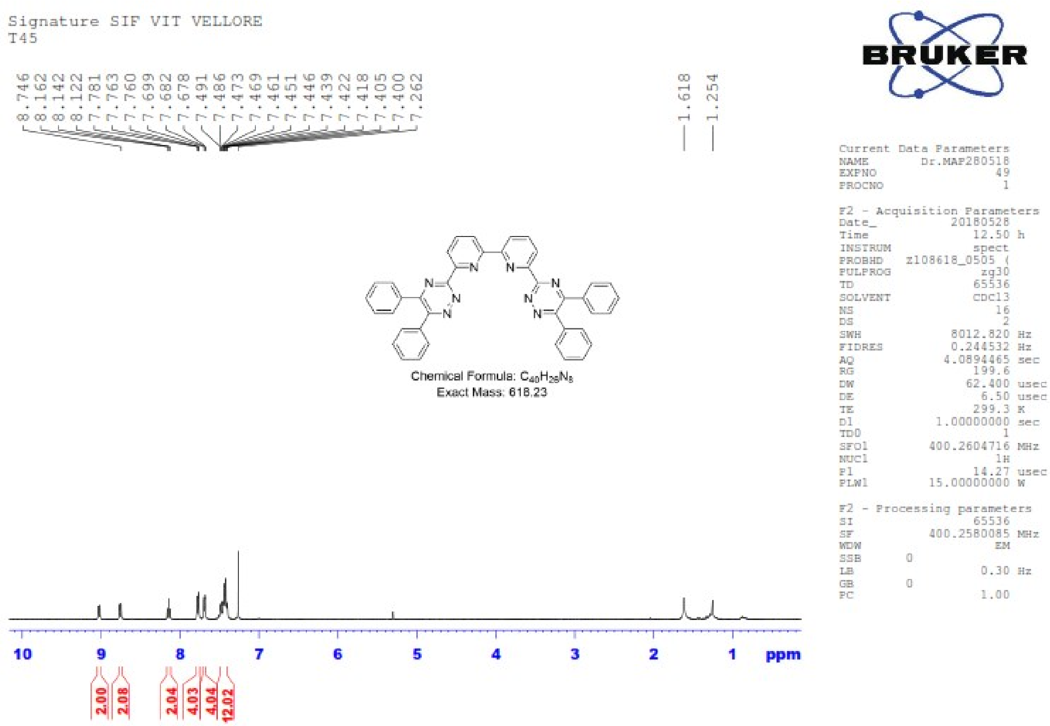
^{1}H-NMR spectrum of [2,2′-Bipyridine-6,6′-dicarbonitrile (11)



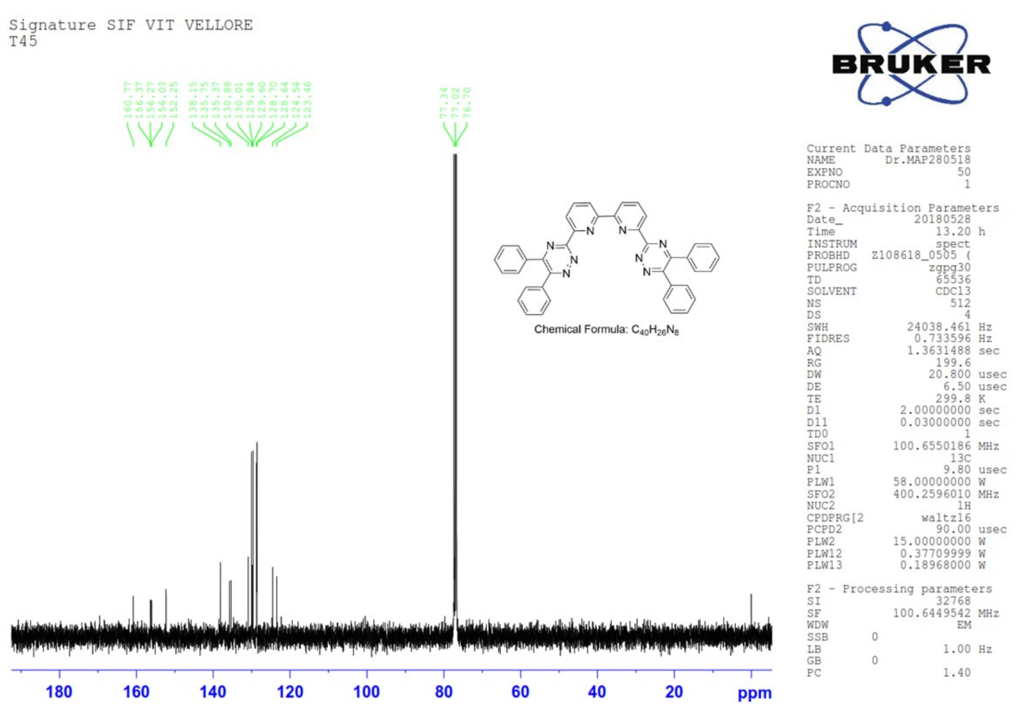
^{13}C-NMR spectrum of [2,2′-Bipyridine-6,6′-dicarbonitrile (11)



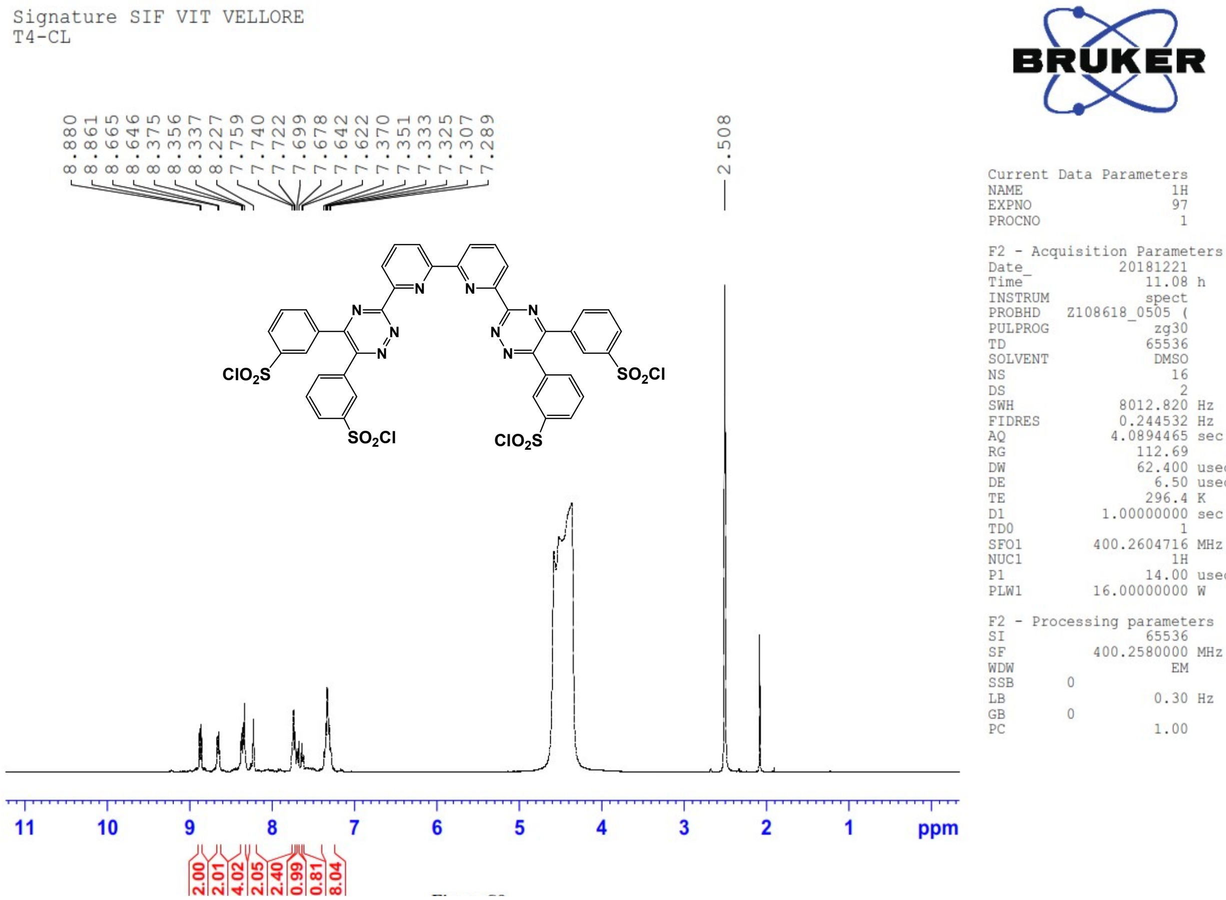
[1]H-NMR spectrum of 2,2'-Bipyridine-6,6'-dicarbohydrazonamide (12)



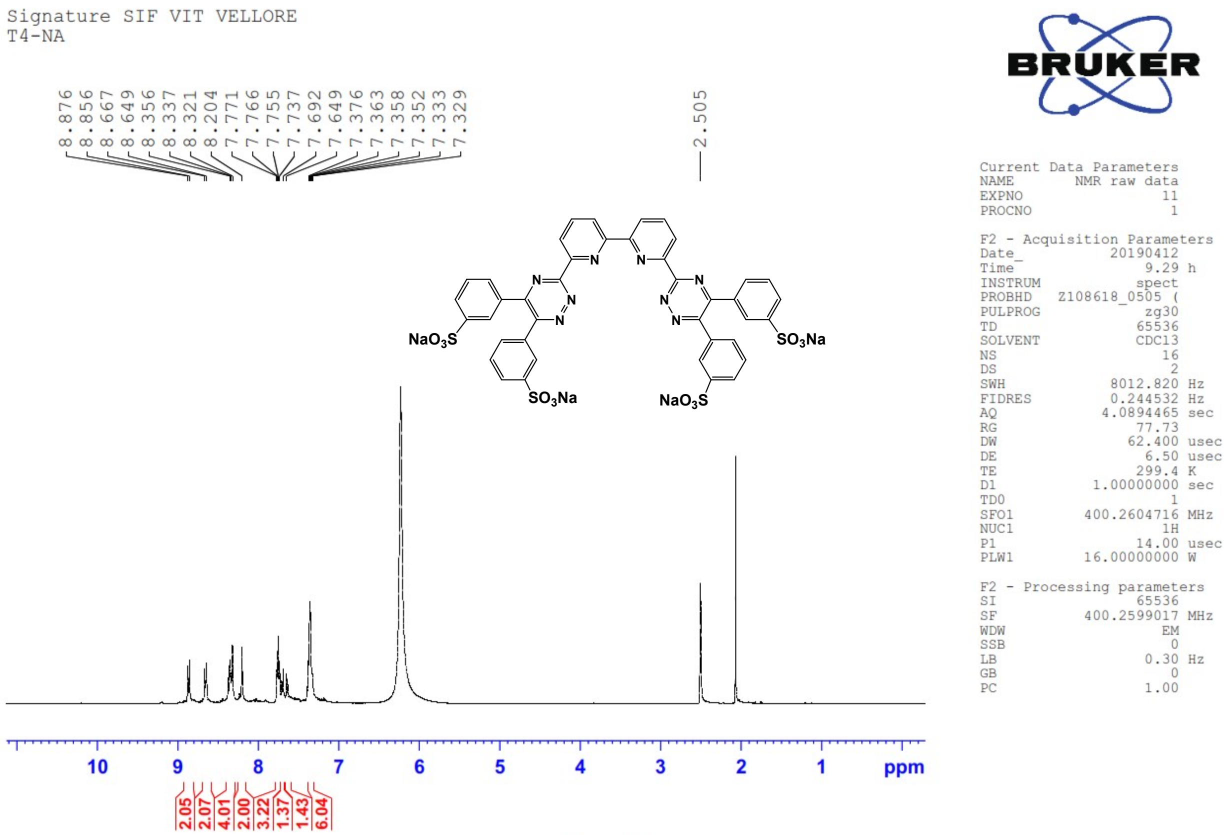
^{1}H-NMR spectrum of 6,6'-Bis(5,6-diphenyl-1,2,4-triazin-3-yl)-2,2'-bipyridine (13)



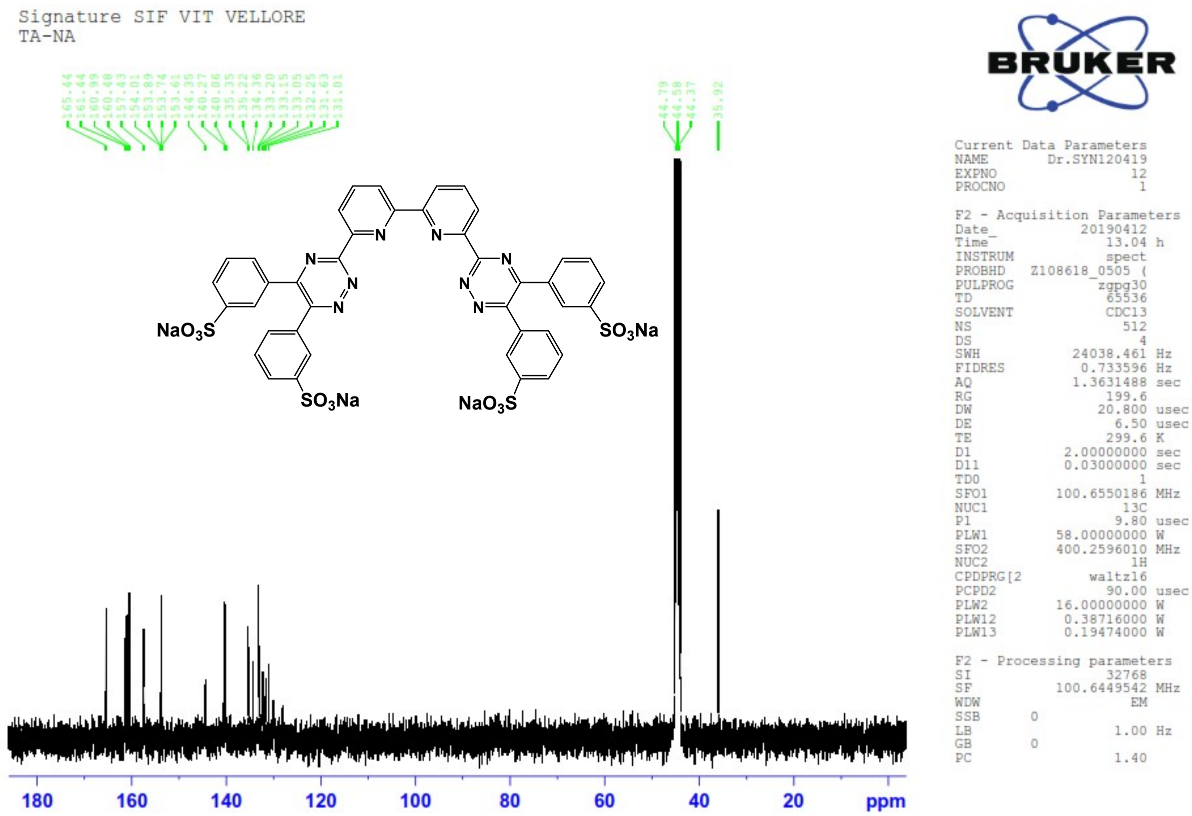
^{13}C-NMR spectrum of 6,6'-Bis(5,6-diphenyl-1,2,4-triazin-3-yl)-2,2'-bipyridine (13)



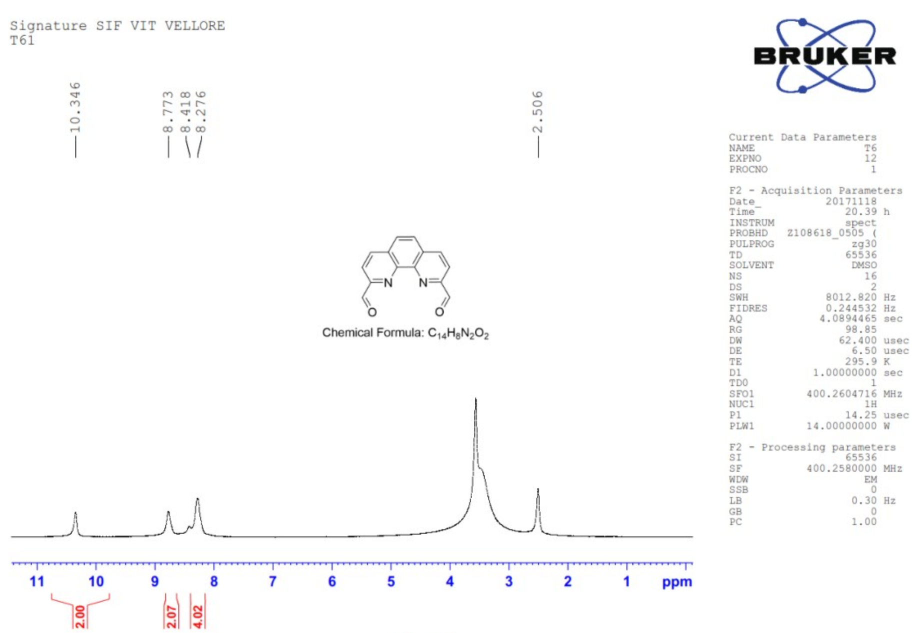
^{1}H-NMR spectrum of 3,3′,3′′,3′′′-[3-(2,2′-Bipyridine-6,6′-diyl)-1,2,4-triazine-5,5,6,6-tetrayl]tetrabenzene sulfonyl chloride (14)



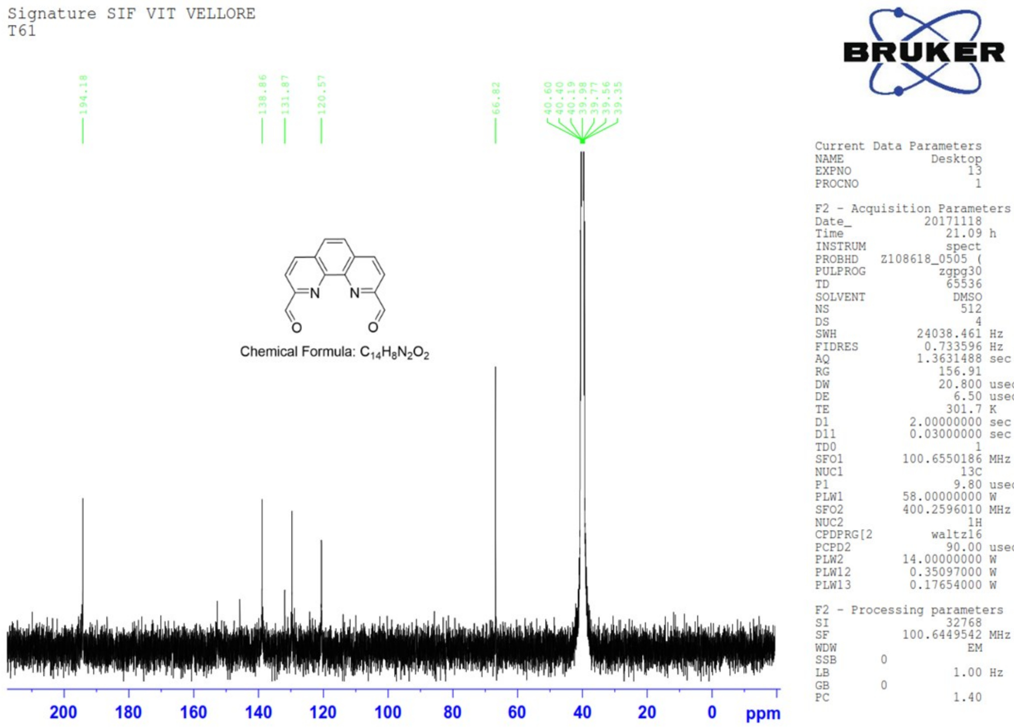
[1]H-NMR spectrum of Tetrasodium 3,3′,3′′,3′′′-[3-(2,2′-bipyridine-6,6′-diyl)-1,2,4-Triazine -5,5,6,6- tetrayl] tetra benzenesulfonate (15)



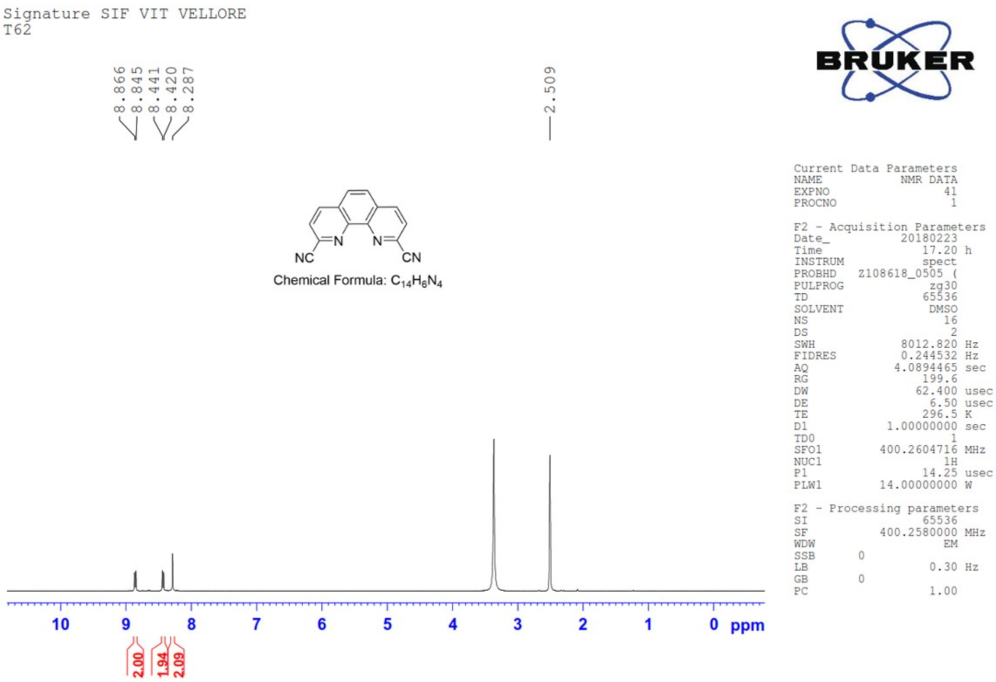
[13]C-NMR spectrum of Tetrasodium 3,3′,3′′,3′′′-[3-(2,2′-bipyridine-6,6′-diyl)-1,2,4-Triazine -5,5,6,6- tetrayl] tetra benzenesulfonate (15)



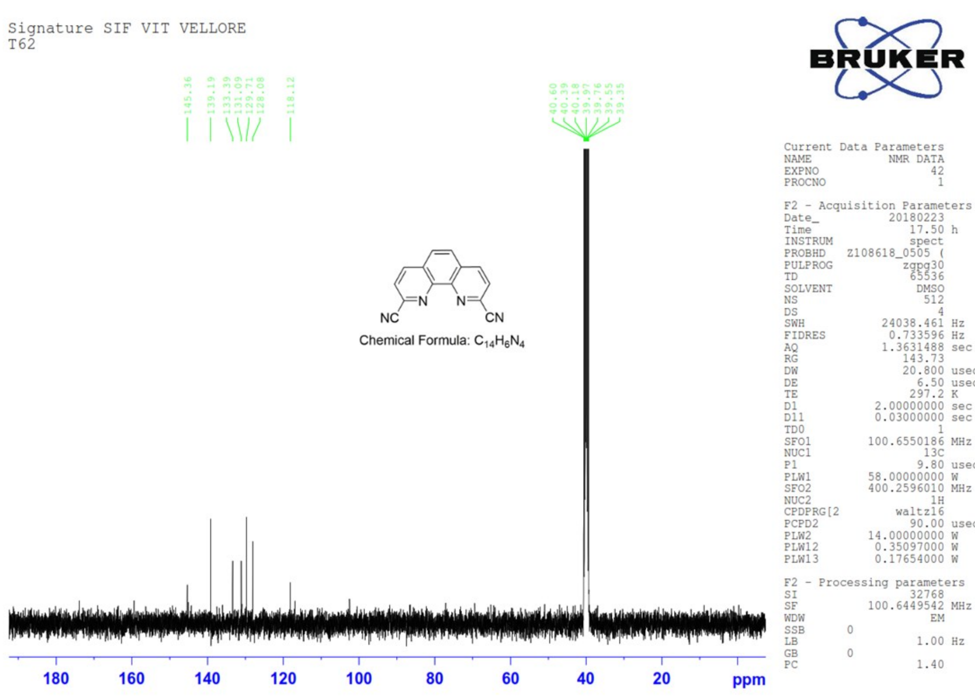
[1]H-NMR spectrum of 1,10-phenanthroline-2,9-dicarbaldehyde (17)



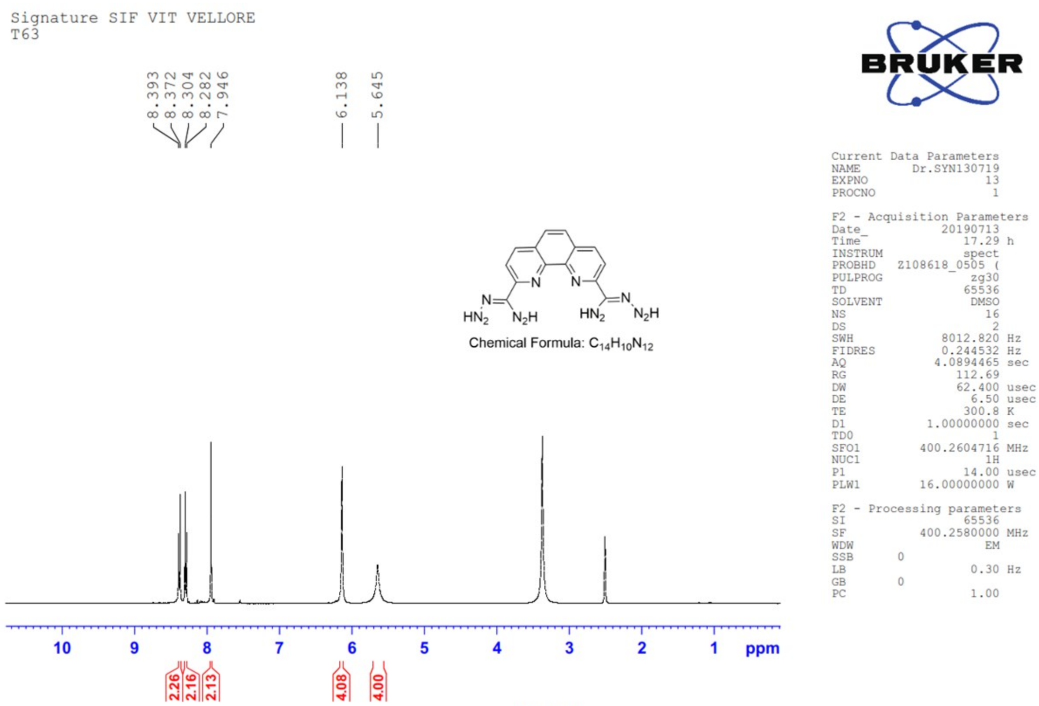
^{13}C-NMR spectrum of 1,10-phenanthroline-2,9-dicarbaldehyde (17)



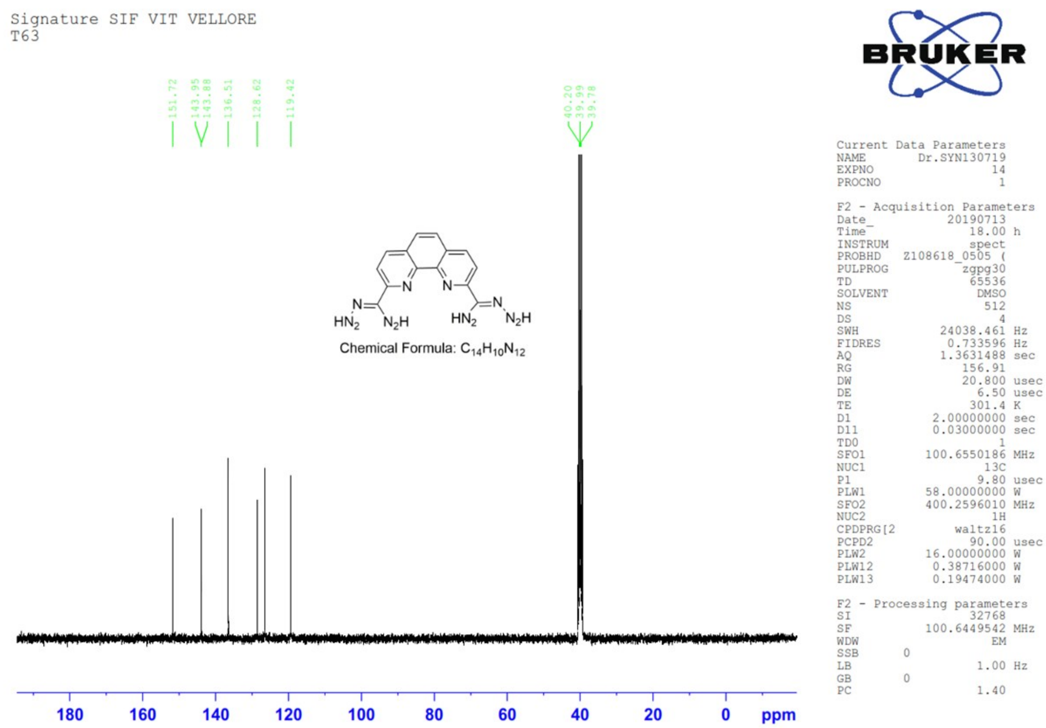
^{1}H-NMR spectrum of 1,10-Phenanthroline-2,9- dicarbonitrile (18)



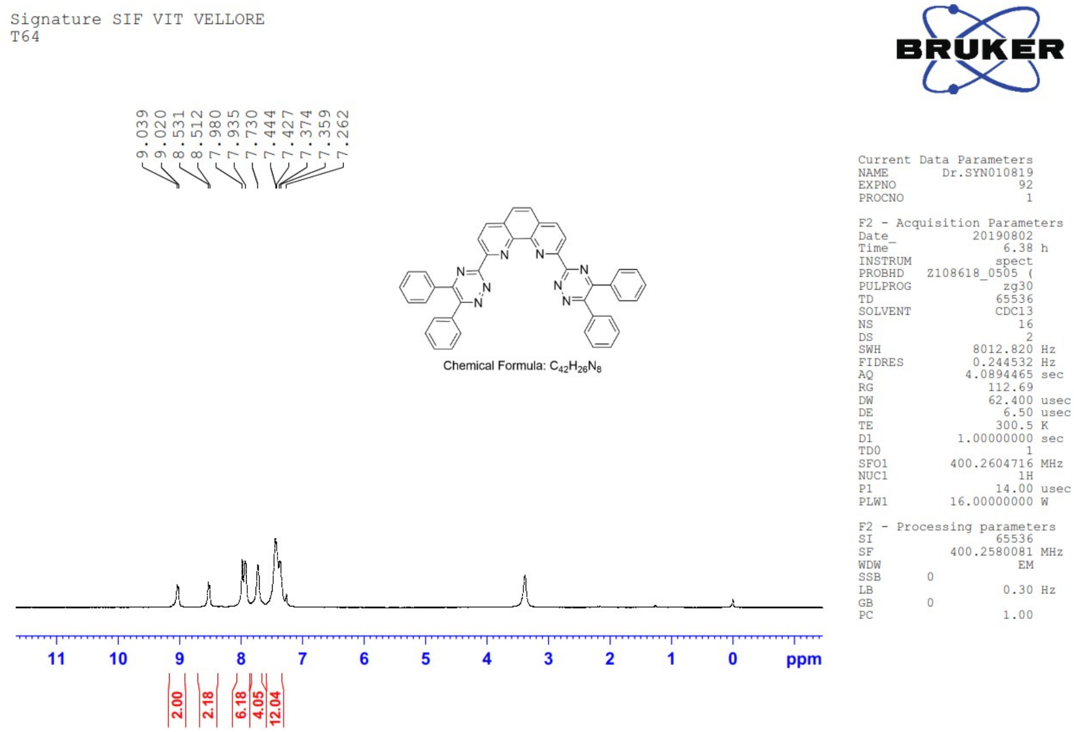
^{13}C-NMR spectrum of 1,10-Phenanthroline-2,9-dicarbonitrile (18)



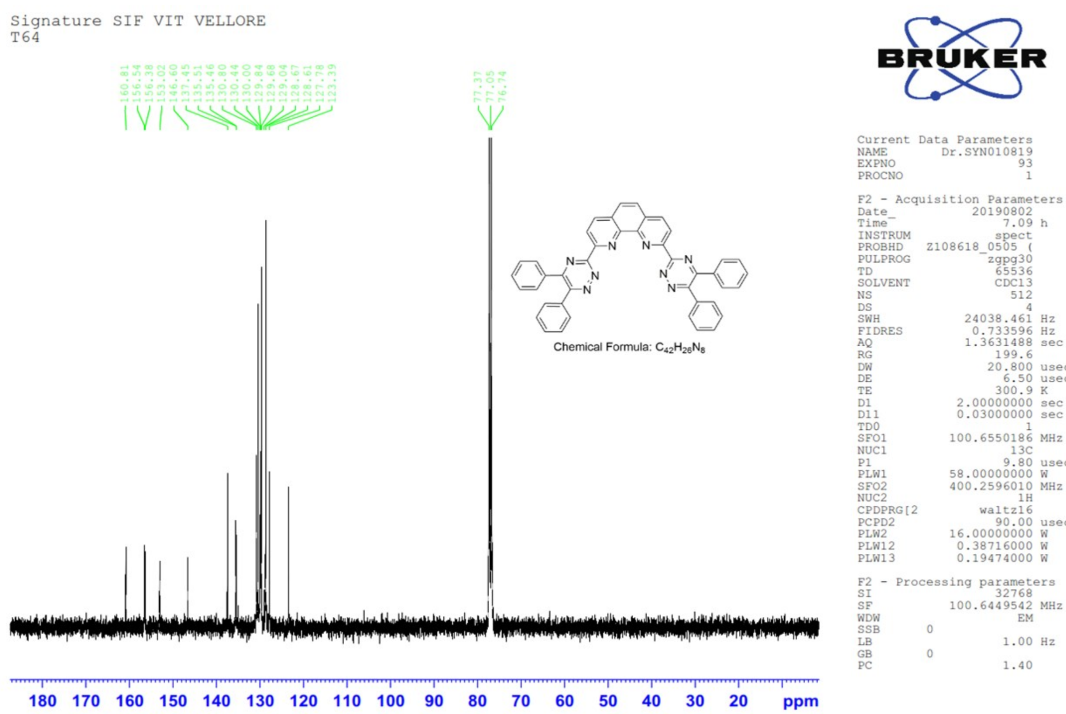
^{1}H-NMR spectrum of1,10-phenanthroline-2,9-bis(carbohydrazonamide) (19)



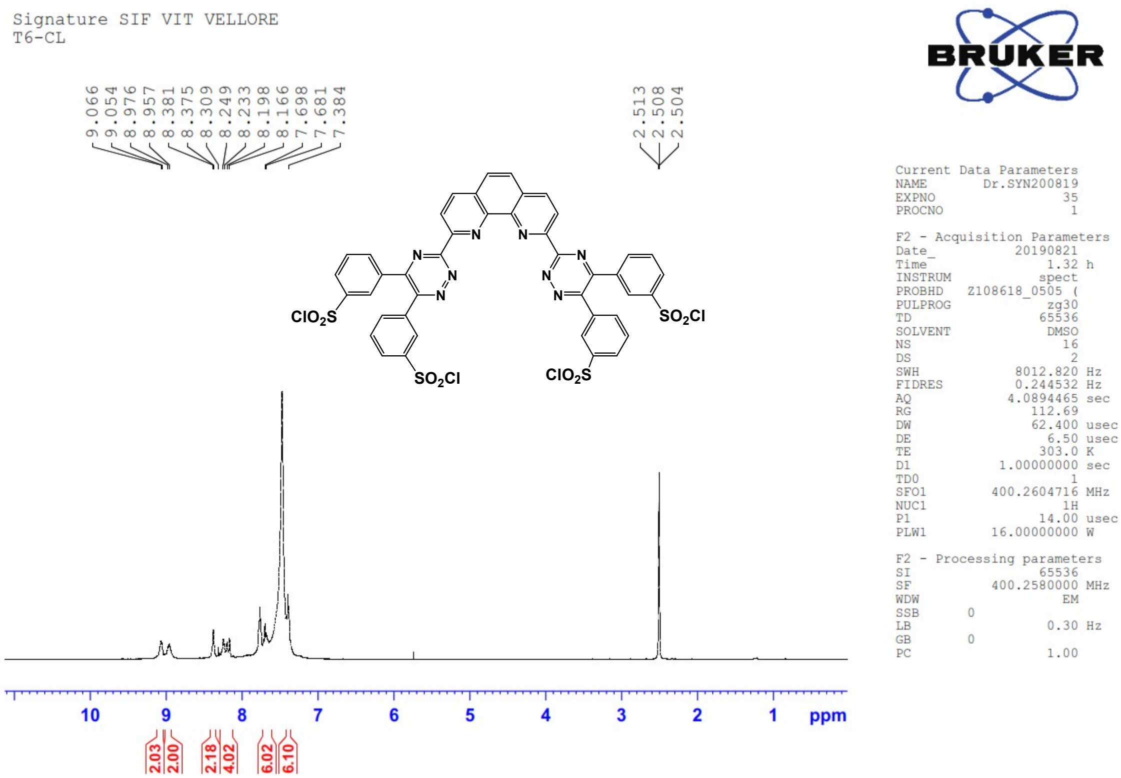
^{13}C-NMR spectrum of1,10-phenanthroline-2,9-bis(carbohydrazonamide) (19)



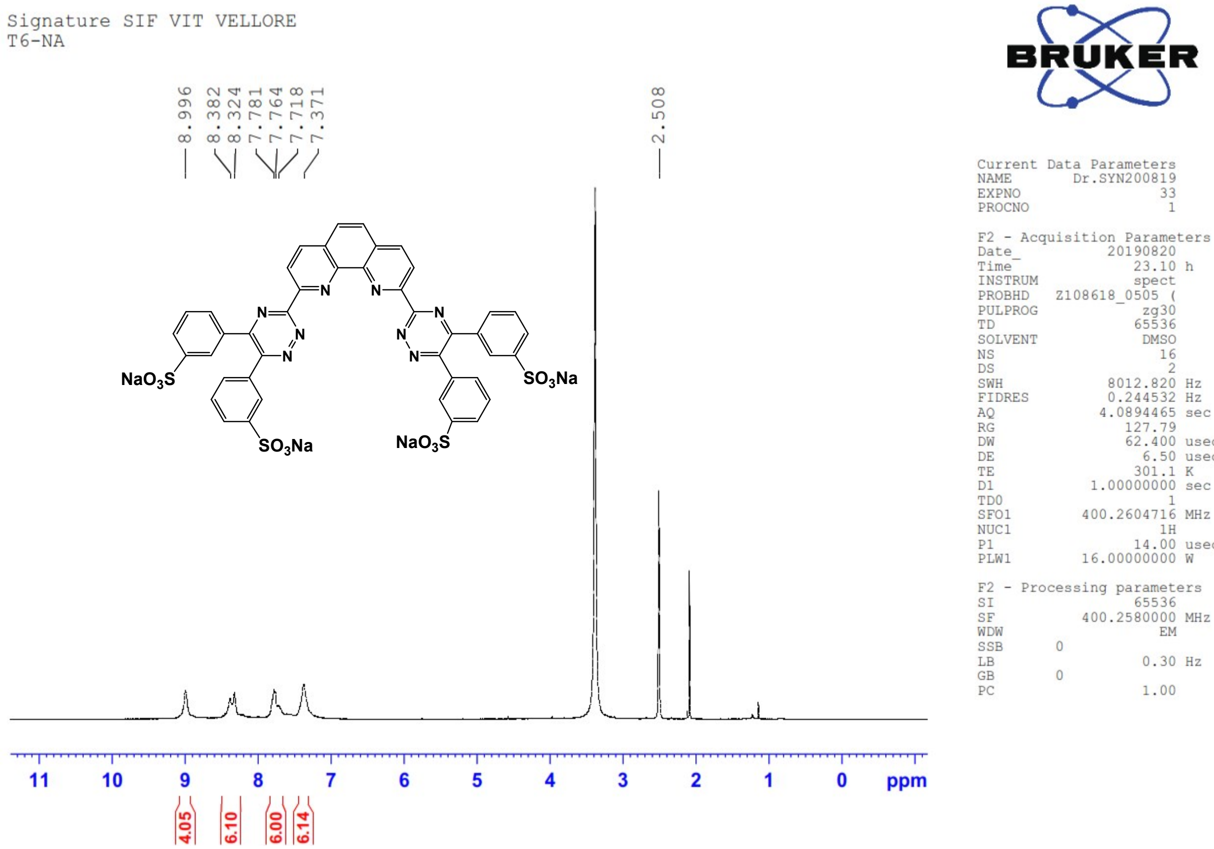
^{1}H-NMR spectrum of 9-Bis(5,6-diphenyl-1,2,4-triazin-3-yl)-1,10-phenanthroline (20)



^{13}C-NMR spectrum of 9-Bis(5,6-diphenyl-1,2,4-triazin-3-yl)-1,10-phenanthroline (20)



-2,9-diyl)-1,2,4- triazine-5,5,6,6-tetrayl]tetra benzenesulfonyl Chloride (21)

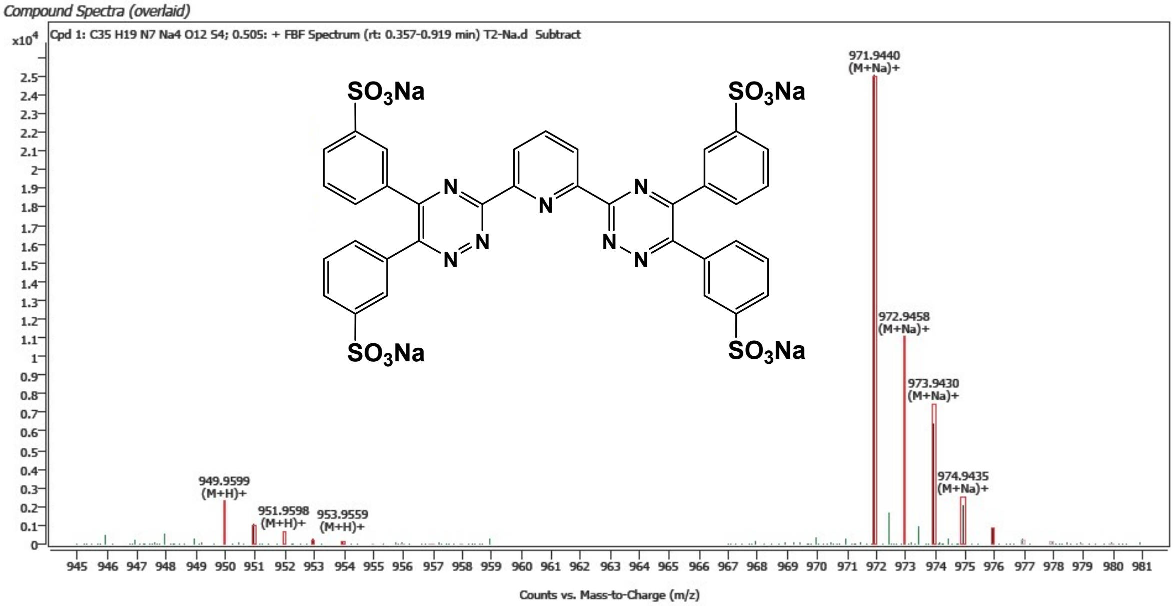


^{1}H-NMR spectrum of Sodium 3,3',3'',3'''-((1,10-phenanthroline-2,9-diyl) bis (1,2,4-triazine- 3,5,6-triyl)) tetra benzene sulfonate, SO_3PhBTPhen (22)

Compound Details

Cpd. 1: C35 H19 N7 Na4 O12 S4

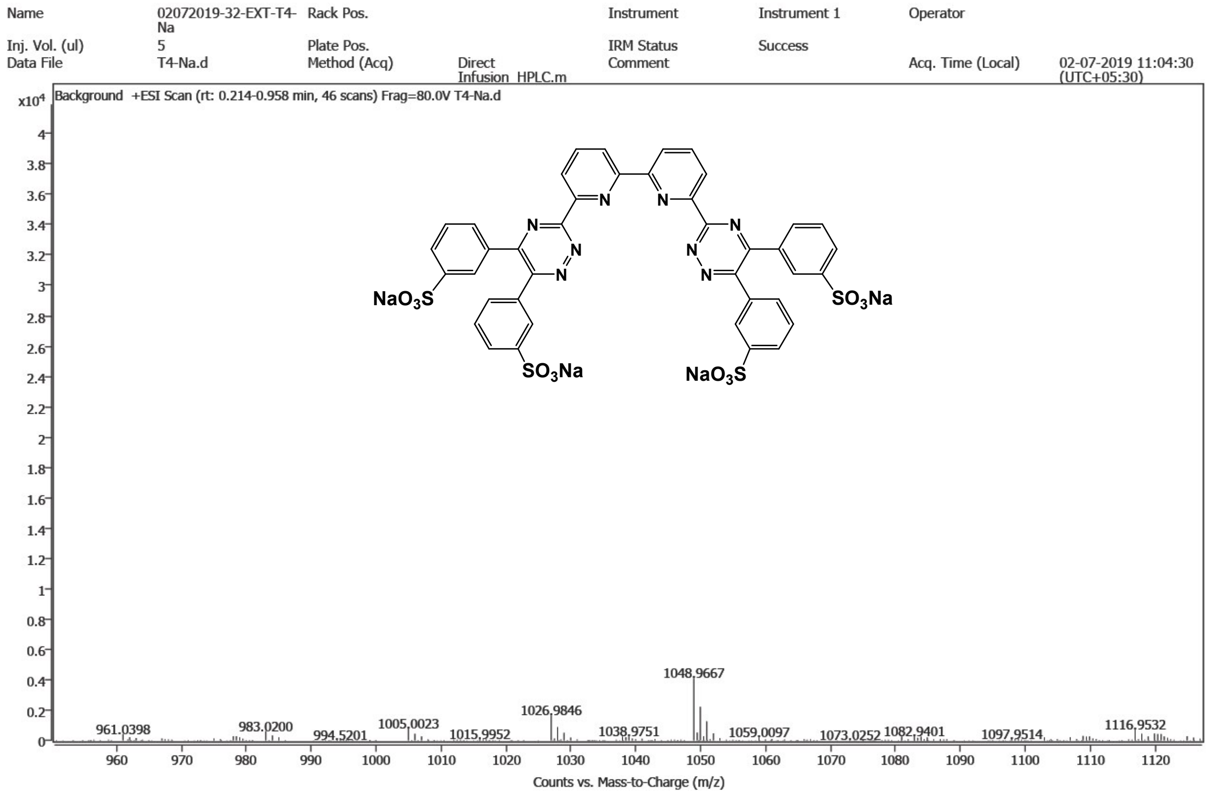
Compound Spectra (overlaid)



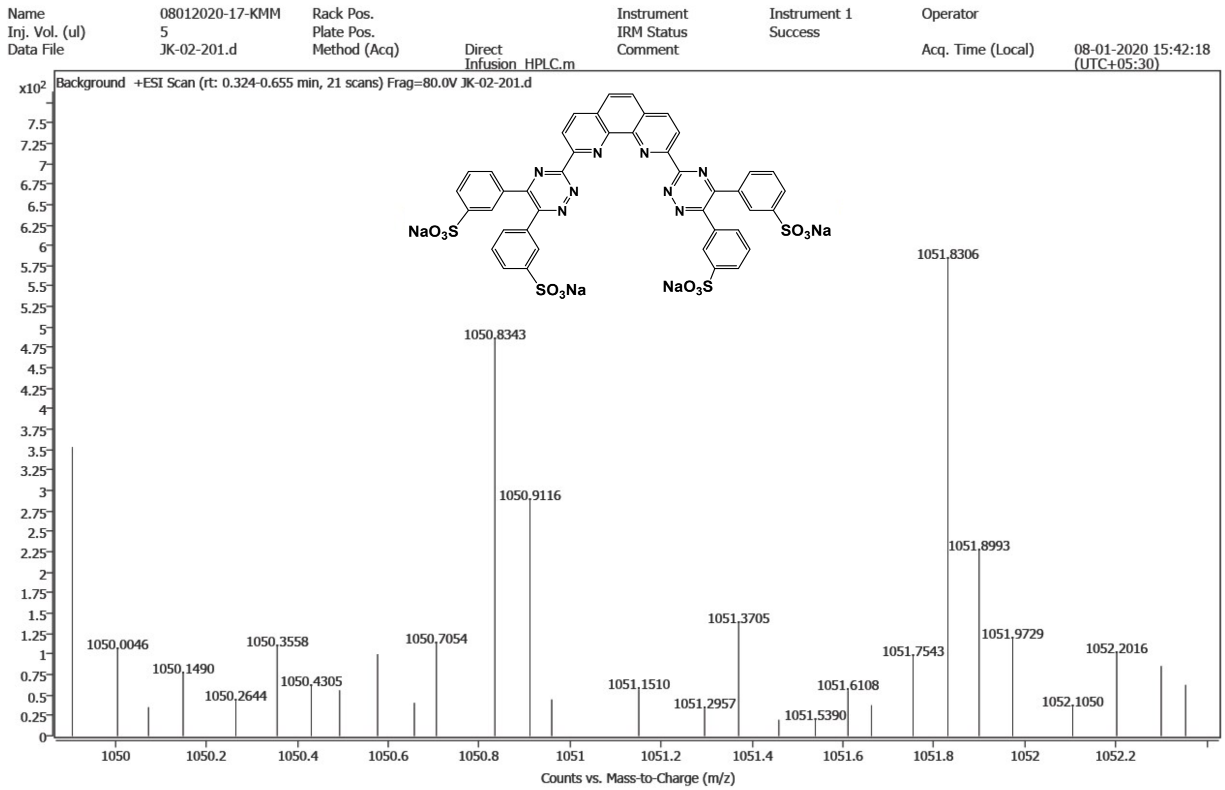
Compound ID Table

Cpd	Formula	Mass (Tgt)	Calc. Mass	Mass	Species	Diff(Tgt.ppm)	mDa
1	C35 H19 N7 Na4 O12 S4	948.9565	948.9543	949.9599 971.9440	(M+H)+ (M+Na)+	-2.40	-2.27

ESI-MS spectra of sodium 3,3',3'',3'''-(pyridine-2,6-diylbis(1,2,4-triazine-3,5,6-triyl))tetra benzenesulfonate, SO_3PhBTP (8)



ESI-MS Spectra Tetrasodium 3,3′,3′′,3′′′-[3-(2,2′-bipyridine-6,6′-diyl)-1,2,4-Triazine -5,5,6,6- tetrayl] tetra benzenesulfonate, SO_3PhBTBP (15)



ESI-MS spectra of Sodium 3,3',3'',3'''-((1,10-phenanthroline-2,9-diyl) bis (1,2,4-triazine- 3,5,6-triyl)) tetra benzene sulfonate, SO_3PhBTPhen (22)

Computational Methodology

Geometries of the free BTP, BTBP, BTPhen and TMDGA and their Am^{3+} and Cm^{3+} complexes of the type $ML(H2O)_6$ (for BTP), $ML(H2O)_5$ (for BTBP and BTPhen) and ML_3 (for TMDGA) were optimized using def-SV(P) basis sets[1] for all the atoms as implemented in the TURBOMOLE-7.2 suits of program [2, 3]. In the cases of Am^{3+} and Cm^{3+}, 60 electron effective core potential (ECP) along with the corresponding def-SV(P) basis sets for the valence electrons are used for the optimization of the geometries of the complexes [4-7]. All the geometry optimizations were carried out employing the GGA functional BP86 which is composed of the Becke 1988 exchange functional[8] along with the Perdew 86 correlation functional[9]. The single point energies of the free ligands and the complexes were calculated using the hybrid functional B3LYP, which is a combination of Becke's three parameter Hartree Fock exchange (B3) and the correlation functional of Lee, Yang and Parr (LYP)[10]. The basis sets of the valence triple zeta quality, viz. def-TZVP [11] as implemented in TURBOMOLE-7.2 package were used for the calculations of single point energies.

Table S1: Cartesian coordinates of the free BTP, BTBP, BTPhen and TMDGA and their Am^{3+} and Cm^{3+} complexes

BTP

N	3.8038380	-5.2698290	-4.4355443
C	4.4777405	-6.4210324	-4.5945152
N	4.4789109	-4.1216614	-4.4334828
C	5.8772313	-6.4298698	-4.7418818
H	3.8730070	-7.3446457	-4.5950417
C	5.8227489	-4.1612940	-4.5920987
H	6.4475220	-7.3716719	-4.8597424
N	6.5623040	-5.2875059	-4.7395675
C	6.5625765	-2.8582389	-4.5920154
C	7.9780028	-2.8637281	-4.6088988
N	5.8384904	-1.7283151	-4.5735638
C	8.6482562	-1.6338775	-4.5807980
H	8.5154477	-3.8229519	-4.6386562
C	6.4848306	-0.5521075	-4.5595764
C	7.8968801	-0.4518329	-4.5499555
H	9.7501405	-1.5965301	-4.5835398
C	5.6595195	0.6987006	-4.5647946
H	8.3690841	0.5413787	-4.5250208
N	6.3253767	1.8743334	-4.4569433
N	4.3178700	0.5670019	-4.6888686
C	5.5674399	2.9695074	-4.4781417
N	3.5696150	1.6686420	-4.7117865
C	4.1701577	2.8658128	-4.6090353
H	6.0762197	3.9491689	-4.3907644
H	3.5073943	3.7483012	-4.6344056

BTBP

C	-1.4016901	-3.0589486	2.6765058
C	-0.0066295	-2.9731477	2.5985812
C	0.5709562	-1.6895208	2.4587539
C	-1.4966816	-0.6403231	2.4569175
C	-2.1617968	-1.8838950	2.6090989
H	-1.8978148	-4.0366604	2.7940421

H	0.6400898	-3.8613591	2.6472166
H	-3.2577213	-1.9449758	2.6856008
C	-2.2584506	0.6561954	2.3671943
C	-3.6733163	0.6817352	2.2717581
C	-4.3287607	1.9179587	2.2018004
H	-4.2644518	-0.2455719	2.2415092
C	-2.1622873	2.9719168	2.3053720
C	-3.5690634	3.0935823	2.2204530
H	-5.4280054	1.9620364	2.1283532
H	-4.0289308	4.0911769	2.1671432
C	-1.3219869	4.2138305	2.3125496
C	-1.2096021	6.4850740	2.2432434
C	0.1904554	6.3659833	2.3156430
C	2.0635015	-1.5646841	2.3873072
C	4.1027687	-2.5730397	2.4116178
C	4.6779007	-1.2959099	2.2789297
N	-1.5344299	1.7885312	2.3788677
N	-0.1566311	-0.5644132	2.3888918
N	0.0217494	4.0680476	2.3875578
N	0.7815887	5.1619505	2.3883360
N	-1.9788802	5.3979123	2.2414432
N	2.7794547	-2.7134256	2.4665422
N	2.5875911	-0.3241071	2.2503936
N	3.9120265	-0.1951702	2.1968297
H	-1.7114861	7.4707540	2.1867008
H	0.8633466	7.2412523	2.3176662
H	4.7207436	-3.4900286	2.4723683
H	5.7693769	-1.1356264	2.2332767

BTPhen

C	-1.4124325	-3.0133683	2.4007953
C	-0.0263227	-2.9640130	2.3925893
C	0.6080852	-1.6864583	2.4154739
C	-1.4174743	-0.5712969	2.4134380
C	-2.1599509	-1.8053651	2.4220239
H	-1.9434402	-3.9806820	2.3955466
H	0.5915106	-3.8737097	2.3778686
C	-2.1602588	0.6978678	2.4077842
C	-3.5988319	0.6556426	2.4567394
C	-4.2849610	1.8994986	2.4729603
C	-2.1407400	3.0092016	2.3514672
C	-3.5635604	3.0831290	2.4233430
H	-5.3872427	1.9115045	2.5202965
H	-4.0530479	4.0678242	2.4299025
C	-1.3540053	4.2801604	2.2578486
C	-1.3362414	6.5527124	2.1488289

C	0.0652891	6.4850755	2.0491265
C	2.1037675	-1.6220689	2.4536391
C	4.0992956	-2.7150037	2.4464604
C	4.7271113	-1.4614620	2.5609263
N	-1.4711018	1.8552475	2.3517097
N	-0.0698043	-0.5372676	2.4167656
N	-0.0051733	4.1844552	2.1768771
N	0.7066099	5.3042184	2.0703602
N	-2.0587996	5.4385605	2.2541509
N	2.7710149	-2.8009188	2.3925727
N	2.6803613	-0.4008024	2.5596511
N	4.0081110	-0.3270669	2.6138940
H	-1.8779175	7.5186721	2.1436024
H	0.6998535	7.3834064	1.9536000
H	4.6784430	-3.6577298	2.3988737
H	5.8239735	-1.3466590	2.6123947
C	-4.2907847	-0.6037541	2.4815296
C	-3.5966627	-1.7914559	2.4556891
H	-5.3935487	-0.6001253	2.5155199
H	-4.1341724	-2.7548756	2.4662778

$Am(BTP)(H2O)_6^{3+}$

N	3.6972025	-5.0967255	-4.2746882
C	4.2500318	-6.3074280	-4.1832373
N	4.4642775	-4.0240757	-4.4828288
C	5.6581327	-6.4513946	-4.3465710
H	3.5736478	-7.1581137	-3.9934854
C	5.8055558	-4.1831354	-4.5755845
H	6.1457327	-7.4441609	-4.3234518
N	6.4226726	-5.3803227	-4.5335887
C	6.6216561	-2.9498144	-4.6926481
C	8.0256101	-3.0308417	-4.7986916
N	5.9500131	-1.7704985	-4.6354773
C	8.7699398	-1.8410428	-4.8301723
H	8.5078854	-4.0200031	-4.8439882
C	6.6817268	-0.6272261	-4.6244305
C	8.0898536	-0.6184969	-4.7234342
H	9.8684432	-1.8676107	-4.9176296
C	5.9382535	0.6460562	-4.4407253
H	8.6242875	0.3441821	-4.7056368
N	6.6333542	1.7928220	-4.3043793
N	4.5910148	0.5666709	-4.3927207
C	5.9331504	2.8973620	-4.0623097
N	3.8900212	1.6726843	-4.1339347
C	4.5153720	2.8367153	-3.9462535

H	6.4825201	3.8515704	-3.9573589
H	3.8891266	3.7159007	-3.7186727
Am	3.3260107	-1.7107900	-4.9228020
O	3.8506640	-0.5106472	-7.0280604
H	3.8619636	-1.1765149	-7.7618735
O	1.0941303	-2.1290498	-6.2947416
H	0.6255891	-2.7776365	-5.7063107
O	1.6848561	-3.4430305	-4.1035841
H	1.1727457	-3.4017490	-3.2624655
O	3.3643100	-3.0576641	-7.1589757
H	2.3814355	-3.0734085	-7.3282989
O	3.4368653	-1.5660299	-2.4018666
H	2.8451222	-0.9547870	-1.9042018
O	1.8739559	0.0983098	-4.2717009
H	0.9299415	0.3245627	-4.4295481
H	2.4254702	0.9755805	-4.1479011
H	0.4210979	-1.6021683	-6.7880227
H	3.9549316	0.3910207	-7.4082488
H	3.7735651	-3.8479368	-7.5800689
H	2.2189116	-4.3277965	-4.0993997
H	4.0760206	-1.9344547	-1.7496066

Cm(BTP)(H2O)$_6^{3+}$

N	3.5373379	-5.0728698	-4.0425419
C	4.0753248	-6.2926617	-4.0355122
N	4.3072293	-4.0090127	-4.3004105
C	5.4611311	-6.4566219	-4.3233943
H	3.4043415	-7.1371721	-3.8038885
C	5.6339163	-4.1883126	-4.4958212
H	5.9275178	-7.4584518	-4.3711032
N	6.2335234	-5.3948263	-4.5322377
C	6.4685409	-2.9650806	-4.6368935
C	7.8648128	-3.0730260	-4.8095820
N	5.8278758	-1.7723681	-4.5458169
C	8.6293729	-1.8978320	-4.8773988
H	8.3254040	-4.0710680	-4.8765437
C	6.5755790	-0.6411410	-4.6037062
C	7.9776237	-0.6598952	-4.7654527
H	9.7228881	-1.9465638	-5.0074373
C	5.8592417	0.6544899	-4.4563143
H	8.5301812	0.2919573	-4.7957029
N	6.5800931	1.7932583	-4.4120019
N	4.5113032	0.6114428	-4.3585350
C	5.9089772	2.9255125	-4.2238518
N	3.8382555	1.7460266	-4.1422534

C	4.4943051	2.9041398	-4.0584972
H	6.4801431	3.8723306	-4.1976169
H	3.8949042	3.8104661	-3.8679810
Cm	3.2056915	-1.6493192	-4.5140305
O	3.6678600	-1.1008623	-6.8129282
H	3.7729113	-1.7448723	-7.6418209
O	1.3186499	-2.3845408	-5.8989835
H	0.6883353	-2.9624765	-5.4026569
O	1.6395655	-3.3369176	-3.5118728
H	1.0948830	-3.3448629	-2.6918550
O	3.9649361	-2.7231080	-8.7607791
H	3.2569445	-2.9096716	-9.4202356
O	3.6519149	-1.3444672	-2.0637555
H	3.0690420	-0.7991817	-1.4847513
O	1.7899009	0.1845719	-3.9195724
H	0.8242181	0.3739527	-3.9392168
H	2.3288481	1.0696682	-3.9510918
H	0.9196954	-2.1255625	-6.7605452
H	3.8293797	-0.1889090	-7.1413947
H	4.8133416	-2.7560690	-9.2604556
H	2.1157147	-4.2444725	-3.5983447
H	4.3254128	-1.7567371	-1.4747912

Am(BTBP)(H2O)$_5$$^{3+}$

C	-1.4490250	-3.0579593	2.0451217
C	-0.0481589	-2.9980374	2.0780423
C	0.5626762	-1.7421908	2.2534408
C	-1.4944947	-0.6426029	2.3784684
C	-2.1765408	-1.8728982	2.2082390
H	-1.9688324	-4.0189651	1.9002694
H	0.5780549	-3.8977235	1.9775451
H	-3.2747158	-1.9121137	2.1829308
C	-2.2364575	0.6395185	2.5519172
C	-3.6282578	0.6627972	2.8171835
C	-4.2977949	1.8865615	2.9332544
H	-4.1935729	-0.2707778	2.9470660
C	-2.1920164	2.9744861	2.4928445
C	-3.5711639	3.0724804	2.7491865
H	-5.3777065	1.9155665	3.1508553
H	-4.0473405	4.0641404	2.7929712
C	-1.4059425	4.1969988	2.2096535
C	-1.3078032	6.4410660	1.7977257
C	0.0620646	6.2776851	1.4418075
C	2.0395446	-1.6605202	2.3699546
C	4.0699174	-2.7026656	2.4907409

C	4.6557540	-1.4419341	2.7973492
N	-1.5254967	1.7897606	2.4276285
N	-0.1368564	-0.5812020	2.3774957
N	-0.0849777	4.0317678	1.9708320
N	0.6339206	5.0788808	1.5592814
N	-2.0334250	5.3894513	2.1601957
N	2.7594441	-2.7989068	2.2968449
N	2.5784801	-0.4395802	2.5853481
N	3.8902826	-0.3510280	2.8215323
Am	1.0875454	1.7545501	2.5118701
O	0.5819398	1.0134444	4.8032496
H	0.8097349	1.7741765	5.3999189
O	1.5400547	3.3879437	4.5733456
H	2.5264661	3.2672855	4.6224034
O	3.4194779	2.1294927	3.2821346
H	3.8149952	2.7679957	2.6387187
O	2.4847463	3.3308426	1.0471870
H	3.1076446	3.3396858	0.2859241
O	0.8394273	1.1071838	0.1141231
H	1.1746239	1.6526568	-0.6338785
H	0.2787843	0.3997229	-0.2785570
H	2.0114300	4.2434157	1.1023844
H	3.9426524	1.2346331	3.2103760
H	1.3195395	4.2819327	4.9224311
H	0.2992257	0.2381774	5.3368877
H	-1.7979962	7.4324126	1.7762800
H	0.6939059	7.1047309	1.0763727
H	4.6790362	-3.6225523	2.4141581
H	5.7286655	-1.3093965	3.0162845

Cm(BTBP)(H2O)$_5$$^{3+}$

C	-1.5223152	-2.9730440	2.6606147
C	-0.1427494	-2.9035647	2.9078065
C	0.4981867	-1.6583925	2.7709616
C	-1.5046086	-0.5760347	2.2279432
C	-2.2073283	-1.8019629	2.3114697
H	-2.0611370	-3.9307138	2.7470236
H	0.4446246	-3.7896314	3.1933699
H	-3.2916680	-1.8458285	2.1356949
C	-2.2084666	0.7175665	1.9801142
C	-3.5643979	0.7819821	1.5787064
C	-4.2033815	2.0260896	1.4922983
H	-4.1265563	-0.1303287	1.3324917
C	-2.1422687	3.0447019	2.2194587
C	-3.4926863	3.1823307	1.8529979

H	-5.2563077	2.0913025	1.1732979
H	-3.9633804	4.1775161	1.8637212
C	-1.3702646	4.2185372	2.6996111
C	-1.2920464	6.3939382	3.3830827
C	0.0540831	6.1792600	3.7944068
C	1.9714986	-1.5676962	2.9417289
C	3.9748787	-2.5625938	3.3938891
C	4.6203430	-1.3562423	2.9987007
N	-1.4988574	1.8466788	2.2361269
N	-0.1645179	-0.5154521	2.4458566
N	-0.0724418	4.0088263	3.0110269
N	0.6298062	4.9962813	3.5703296
N	-1.9964114	5.4041318	2.8423257
N	2.6516319	-2.6663338	3.3289725
N	2.5536475	-0.3841633	2.6493705
N	3.8887467	-0.3001370	2.6400238
Cm	1.0817908	1.7554968	2.2627064
O	0.8131362	1.3323711	4.6858847
H	1.3831491	1.9033973	5.2541306
O	2.4942136	3.2083492	3.6635519
H	3.4663121	3.3390969	3.7243966
O	3.3841973	1.7505543	1.1049008
H	3.9503713	2.4898223	0.7866783
O	0.8145204	3.3052999	0.3278580
H	0.8182614	2.7551268	-0.4958680
O	1.2531599	0.7827919	-0.1231255
H	0.9136218	0.0080449	-0.6273303
H	2.2454732	0.8154228	-0.2057775
H	0.8109830	4.2564804	0.0772959
H	3.9599990	1.0952616	1.6435760
H	2.0200478	4.1227859	3.7804306
H	0.1518669	0.8826047	5.2593927
H	-1.7809849	7.3793481	3.4980901
H	0.6680035	6.9554149	4.2814647
H	4.5505574	-3.4402112	3.7423925
H	5.7171237	-1.2440924	2.9632702

Am(BTPhen)(H2O)$_5$$^{3+}$

C	-1.5088973	-2.9784465	2.5703906
C	-0.1371334	-2.9319075	2.8014870
C	0.5233096	-1.6789172	2.7408640
C	-1.4694996	-0.5472601	2.3283813
C	-2.2186410	-1.7741041	2.3163905
H	-2.0466106	-3.9408594	2.5883445
H	0.4474367	-3.8403541	3.0119101

C	-2.1762906	0.7134339	2.1702482
C	-3.5953431	0.6991533	1.9419161
C	-4.2548800	1.9517465	1.8259879
C	-2.1431895	3.0411431	2.2687389
C	-3.5315025	3.1282418	2.0033262
H	-5.3389886	1.9870573	1.6288947
H	-4.0127491	4.1175900	1.9682340
C	-1.3745504	4.2551575	2.6215411
C	-1.3035878	6.4810771	3.1278939
C	0.0406283	6.3028945	3.5595505
C	1.9950541	-1.6108378	2.8924018
C	3.9978800	-2.6320593	3.2941771
C	4.6453207	-1.4034426	2.9822780
N	-1.4708153	1.8685894	2.3058905
N	-0.1220022	-0.5135317	2.5126293
N	-0.0680672	4.0802142	2.9292980
N	0.6207040	5.1084291	3.4219054
N	-2.0048413	5.4450220	2.6787832
N	2.6748602	-2.7295088	3.2185082
N	2.5805894	-0.4147950	2.6516192
N	3.9122200	-0.3342188	2.6672620
Am	1.1398348	1.7974650	2.3502990
O	0.8895643	1.3668174	4.7692869
H	1.4277514	2.0258791	5.2737730
O	2.4133205	3.3125352	3.8713643
H	3.3880592	3.4342521	3.9132189
O	3.4245205	1.8882270	1.4797233
H	3.9948007	2.6041057	1.1224859
O	0.9579912	3.2478582	0.3367976
H	0.9973599	2.6017663	-0.4180538
O	1.1380522	0.7145501	-0.1740671
H	0.4618395	0.1305300	-0.5907801
H	2.0100770	0.4102441	-0.5195567
H	1.0400685	4.1651008	-0.0073428
H	3.9996657	1.1465142	1.9051370
H	1.9626662	4.2430871	3.8420960
H	0.3472031	0.8382117	5.3968914
H	-1.7955300	7.4711856	3.1580053
H	0.6490080	7.1120027	3.9971821
H	4.5717470	-3.5310611	3.5865867
H	5.7416495	-1.2831530	2.9751815
C	-4.2974004	-0.5554750	1.8713148
C	-3.6361519	-1.7474306	2.0668050
H	-5.3830702	-0.5454660	1.6829737
H	-4.1879636	-2.7009004	2.0412281

$Cm(BTPhen)(H2O)_5^{3+}$

C	-1.5217959	-2.9720642	2.5485817
C	-0.1565884	-2.9224733	2.8200405
C	0.5042563	-1.6695057	2.7730005
C	-1.4828666	-0.5434614	2.3004856
C	-2.2291714	-1.7705282	2.2734608
H	-2.0570745	-3.9360492	2.5553256
H	0.4218327	-3.8294273	3.0528815
C	-2.1886549	0.7177176	2.1365897
C	-3.6060972	0.7061879	1.9055063
C	-4.2650410	1.9622612	1.8197169
C	-2.1539335	3.0439670	2.2890397
C	-3.5443925	3.1351508	2.0354022
H	-5.3487672	2.0025108	1.6211907
H	-4.0307151	4.1226247	2.0365697
C	-1.3775982	4.2451839	2.6793065
C	-1.2932018	6.4501467	3.2602003
C	0.0651048	6.2614255	3.6413036
C	1.9740482	-1.5943987	2.9611393
C	3.9687563	-2.6024071	3.4187637
C	4.6209661	-1.3874197	3.0653933
N	-1.4832096	1.8703681	2.2851024
N	-0.1404132	-0.5085625	2.5199384
N	-0.0687908	4.0555524	2.9634638
N	0.6409830	5.0708698	3.4570022
N	-2.0076892	5.4326490	2.7880363
N	2.6464194	-2.7047681	3.3280496
N	2.5621242	-0.4043621	2.7010676
N	3.8961770	-0.3232780	2.7133302
Cm	1.1012864	1.7653331	2.2924543
O	0.8587419	1.4096441	4.7234751
H	1.4090187	2.0106700	5.2798383
O	2.5015184	3.2864611	3.6292665
H	3.4731986	3.4188159	3.6919940
O	3.4050934	1.7150867	1.1553392
H	3.9749753	2.4471894	0.8277012
O	0.8609038	3.2730970	0.3215074
H	0.8516341	2.7098486	-0.4928050
O	1.2610254	0.7348021	-0.0703026
H	0.8966201	-0.0404018	-0.5560446
H	2.2513365	0.7411903	-0.1665244
H	0.8475441	4.2199557	0.0559966
H	3.9759559	1.0682921	1.7087237
H	2.0277032	4.2063574	3.6996001
H	0.2418941	0.9168008	5.3108619
H	-1.7849926	7.4371780	3.3448385

H	0.6879085	7.0616252	4.0750696
H	4.5386093	-3.4895147	3.7523672
H	5.7181474	-1.2750298	3.0524204
C	-4.3041411	-0.5494491	1.8094783
C	-3.6424187	-1.7428028	1.9981497
H	-5.3880322	-0.5401794	1.6111160
H	-4.1927209	-2.6965273	1.9549922

$Am(TMDGA)_3^{3+}$

H	13.0542181	-17.0351639	10.4872245
C	12.6278268	-17.0150343	9.4544630
H	11.7016631	-17.6379979	9.4547026
O	12.3221096	-15.6801197	9.0716013
C	13.6457295	-17.5494252	8.4402853
C	11.3602828	-15.0547202	9.9139308
O	14.0724500	-16.7601189	7.5501656
H	10.4218300	-15.6592218	9.9414977
H	11.7531993	-14.9805412	10.9562866
C	11.0890271	-13.6627238	9.3268071
O	11.6787949	-13.3394097	8.2593984
H	9.8292923	-13.5476457	4.7002423
C	10.8085994	-14.0532376	4.5146410
H	10.9861428	-14.0595950	3.4121466
O	11.8542799	-13.3612996	5.1806996
C	10.7923571	-15.4821307	5.0731651
C	11.9787794	-12.0002804	4.7945480
O	11.6022905	-15.7734731	5.9976742
H	12.1562672	-11.9217145	3.6940479
H	11.0395526	-11.4437978	5.0305392
C	13.1682142	-11.4231995	5.5738443
O	13.8116984	-12.1933866	6.3408325
H	17.2704091	-13.9293120	5.0228405
C	16.6863824	-14.7975970	5.4147616
H	17.3982953	-15.6415753	5.5796993
O	16.0457482	-14.4449606	6.6348940
C	15.5814256	-15.1979007	4.4277335
C	16.9514467	-14.0300726	7.6495379
O	14.3806389	-15.0976488	4.8001980
H	17.6468736	-14.8639313	7.9123508
H	17.5684549	-13.1711782	7.2908636
C	16.1077739	-13.6231392	8.8633765
O	14.8536636	-13.7652260	8.7916801
Am	13.4229583	-14.5016549	6.9854500
N	15.9391012	-15.6425868	3.2104737
N	16.7257962	-13.1325480	9.9490605

N	14.0450477	-18.8273760	8.5349596
N	10.2375039	-12.8443171	9.9689118
N	9.9205466	-16.3670007	4.5617131
N	13.4851221	-10.1277525	5.4116875
C	8.9629855	-16.0626894	3.4911290
H	9.2686197	-16.5602751	2.5436521
H	7.9609274	-16.4472781	3.7783239
H	8.8691966	-14.9751276	3.3122337
C	9.9016449	-17.7549630	5.0367619
H	10.7091305	-17.8996977	5.7772738
H	8.9167929	-17.9831375	5.5005324
H	10.0539769	-18.4439535	4.1773833
C	12.8006348	-9.2138465	4.4893548
H	12.5123831	-8.2881953	5.0329105
H	13.4810077	-8.9297323	3.6556288
H	11.8841162	-9.6612432	4.0621355
C	14.6191092	-9.5440650	6.1372504
H	14.2786727	-8.6451102	6.6952923
H	15.0249478	-10.2903738	6.8441859
H	15.4102095	-9.2344173	5.4190684
C	14.9220404	-16.0926348	2.2537547
H	14.9410699	-15.4478691	1.3478338
H	15.1385332	-17.1390360	1.9460109
H	13.9258647	-16.0438341	2.7299515
C	17.3292004	-15.7770741	2.7575722
H	17.4034109	-15.4186696	1.7089806
H	18.0251891	-15.1716439	3.3685920
H	17.6514154	-16.8424203	2.7838219
C	15.9483554	-12.6854852	11.1109352
H	16.1745542	-13.3292418	11.9891701
H	16.2263940	-11.6384804	11.3602743
H	14.8701206	-12.7382247	10.8738968
C	18.1797757	-12.9617668	10.0644733
H	18.5100645	-13.3313876	11.0584153
H	18.7276528	-13.5339648	9.2924484
H	18.4537985	-11.8860706	9.9842598
C	14.9815364	-19.3909925	7.5555485
H	15.9282357	-19.6834243	8.0610157
H	14.5336257	-20.2981038	7.0948149
H	15.1899555	-18.6391851	6.7728570
C	13.5624012	-19.7658606	9.5564958
H	14.4197376	-20.3644743	9.9299714
H	13.1157625	-19.2424244	10.4230939
H	12.8116161	-20.4651941	9.1241901
C	9.4986456	-13.1993641	11.1858791
H	9.6804755	-12.4317066	11.9691952

H	8.4067006	-13.2279185	10.9739038
H	9.8044249	-14.1828276	11.5883707
C	9.9531335	-11.5060176	9.4397593
H	10.1465734	-10.7465793	10.2279636
H	10.6039091	-11.3117799	8.5678914
H	8.8846775	-11.4358098	9.1376965

$Cm(TMDGA)_3^{3+}$

H	13.0775751	-17.0391816	10.4417058
C	12.6620806	-17.0303103	9.4042458
H	11.7550541	-17.6808803	9.3946285
O	12.3233390	-15.7040561	9.0213779
C	13.7077692	-17.5342510	8.4020015
C	11.3763980	-15.0870196	9.8844859
O	14.1331832	-16.7322293	7.5247785
H	10.4290333	-15.6778642	9.9054928
H	11.7778967	-15.0423968	10.9253458
C	11.1224223	-13.6764591	9.3351629
O	11.7114386	-13.3350494	8.2719420
H	9.7941259	-13.5172640	4.7146346
C	10.7606051	-14.0437647	4.5213629
H	10.9228090	-14.0663685	3.4169684
O	11.8296539	-13.3600761	5.1622157
C	10.7269621	-15.4652060	5.0984037
C	11.9771208	-12.0107608	4.7378538
O	11.5408219	-15.7550675	6.0194677
H	12.1360070	-11.9672840	3.6328066
H	11.0533834	-11.4300654	4.9749493
C	13.1925753	-11.4375087	5.4801314
O	13.8393019	-12.2036035	6.2475944
H	17.2526127	-13.8930344	5.0602447
C	16.6725888	-14.7622610	5.4556325
H	17.3904852	-15.5962409	5.6432207
O	16.0093304	-14.4023110	6.6608108
C	15.5881862	-15.1907247	4.4578169
C	16.8956748	-14.0013063	7.6977810
O	14.3803402	-15.1077171	4.8153107
H	17.5975475	-14.8336604	7.9475655
H	17.5064115	-13.1260611	7.3696387
C	16.0318455	-13.6372498	8.9120226
O	14.7824867	-13.8019270	8.8282792
Cm	13.3959845	-14.4877077	6.9519188
N	15.9640238	-15.6385552	3.2483371
N	16.6347362	-13.1561485	10.0113555
N	14.1274191	-18.8062804	8.4992061

N	10.2871723	-12.8615118	10.0005638
N	9.8382854	-16.3425629	4.6041925
N	13.5239496	-10.1501790	5.2862609
C	8.8833548	-16.0381169	3.5311259
H	9.1867149	-16.5413279	2.5858396
H	7.8793891	-16.4163125	3.8196345
H	8.7945591	-14.9506963	3.3483437
C	9.8020615	-17.7243513	5.0963465
H	10.5971047	-17.8652218	5.8508647
H	8.8086043	-17.9383666	5.5479860
H	9.9622638	-18.4260990	4.2486873
C	12.8298840	-9.2404614	4.3669583
H	12.5269065	-8.3203998	4.9124723
H	13.5109963	-8.9446997	3.5381485
H	11.9229509	-9.6986244	3.9310910
C	14.6778217	-9.5676284	5.9809450
H	14.3574424	-8.6566464	6.5314165
H	15.0893944	-10.3071860	6.6915584
H	15.4579448	-9.2775441	5.2430251
C	14.9626371	-16.1065113	2.2832163
H	14.9888883	-15.4700961	1.3716381
H	15.1921567	-17.1537652	1.9883107
H	13.9599035	-16.0615959	2.7455784
C	17.3584867	-15.7487706	2.8025853
H	17.4475488	-15.3251013	1.7793560
H	18.0511480	-15.1916272	3.4607480
H	17.6723035	-16.8159180	2.7652999
C	15.8420715	-12.7408493	11.1743406
H	16.0810478	-13.3872870	12.0471765
H	16.0913953	-11.6893603	11.4354426
H	14.7666363	-12.8187866	10.9317821
C	18.0841085	-12.9547515	10.1354189
H	18.4121968	-13.3032918	11.1374439
H	18.6491753	-13.5301949	9.3781570
H	18.3401939	-11.8756583	10.0411532
C	15.0843458	-19.3525674	7.5301708
H	16.0226484	-19.6482074	8.0491205
H	14.6497916	-20.2544784	7.0465622
H	15.3040387	-18.5883534	6.7627100
C	13.6288497	-19.7549877	9.5040394
H	14.4639743	-20.4148245	9.8179187
H	13.2541007	-19.2390852	10.4091850
H	12.8205053	-20.3944553	9.0824270
C	9.5502210	-13.2342064	11.2136922
H	9.7609822	-12.4971135	12.0188257
H	8.4562686	-13.2247747	11.0112699

H	9.8306158	-14.2387244	11.5808503
C	10.0230250	-11.5048607	9.5078774
H	10.2440821	-10.7687768	10.3109244
H	10.6640038	-11.3025090	8.6306400
H	8.9516187	-11.4063079	9.2250710

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