Supporting Information

Ligand structure and diluent nature in defining improved Am^{3+} and Cm^{3+} separation using diglycolamides: A combined solvent extraction and DFT studies

A.S. Kanekar, A. Bhattacharyya* and P.K. Mohapatra*

Radiochemistry Division, Bhabha Atomic Research Centre, Trombay, Mumbai-400085, India

Email: arun12@barc.gov.in (AB); mpatra@barc.gov.in (PKM)

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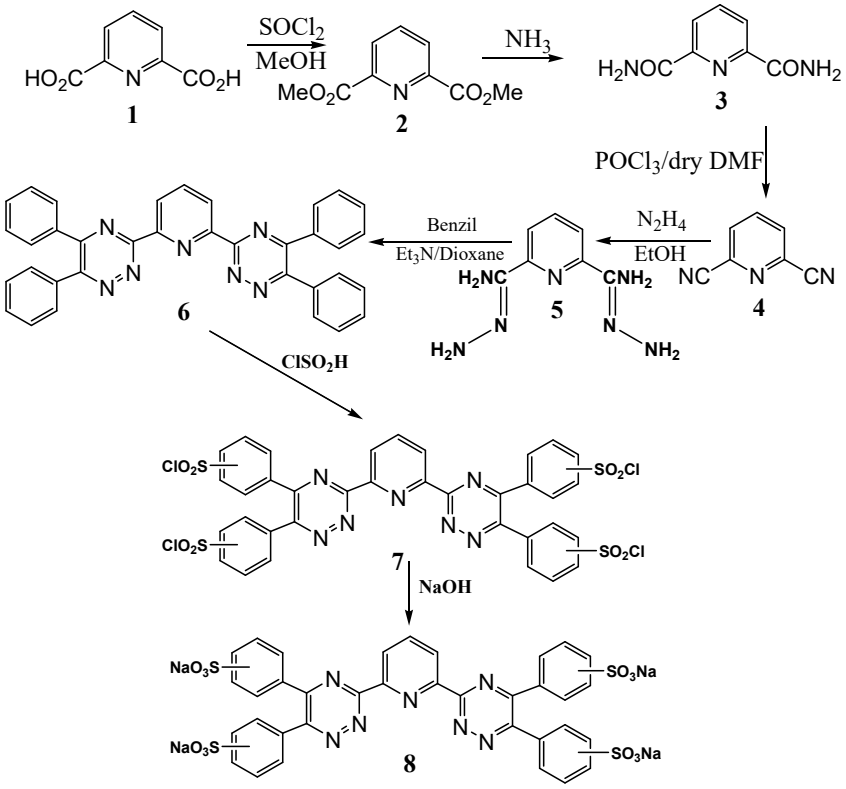
Synthesis of SO_3PhBTP



Scheme 1 - Synthesis of SO_3PhBTP

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 0^0c (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 (Fig. S1).^{13}C NMR: ($CDCl_3$, 400 MHz) δ: 53.17, 128.03, 138.40, 148.16, 165.00 ppm (Fig. S2).

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 (Fig. S3). ^{13}C NMR (DMSO-d_6, 400MHz): 124.72, 139.70, 149.4, 165.97ppm (Fig. S4).

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 (Fig. S5). ^{13}C NMR ($CDCl_3$, 400MHz): 115.47, 131.18, 135.31, 138.95 ppm (Fig. S6).

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 (Fig. S7). ^{13}C NMR (DMSO–d_6, 400 MHz) δ: 118.5, 136.4, 144.2, 150.6 ppm (Fig. S8).

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 (Fig. S9). ^{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 (Fig. S10).

Synthesis of 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 (Fig. S11). ^{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 (Fig. S12).

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

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 (Fig. S13). ^{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 (Fig. S14).

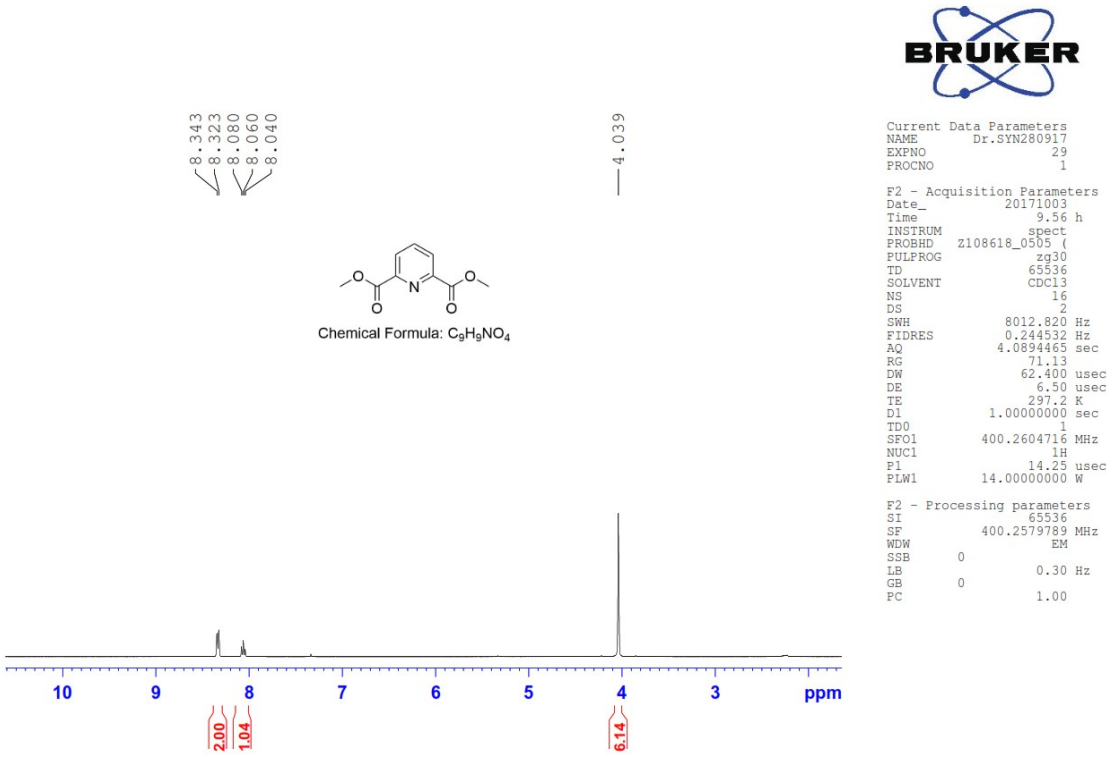


Fig. S1: ^{1}H-NMR spectrum of dimethyl pyridine-2,6-dicarboxylate (2)

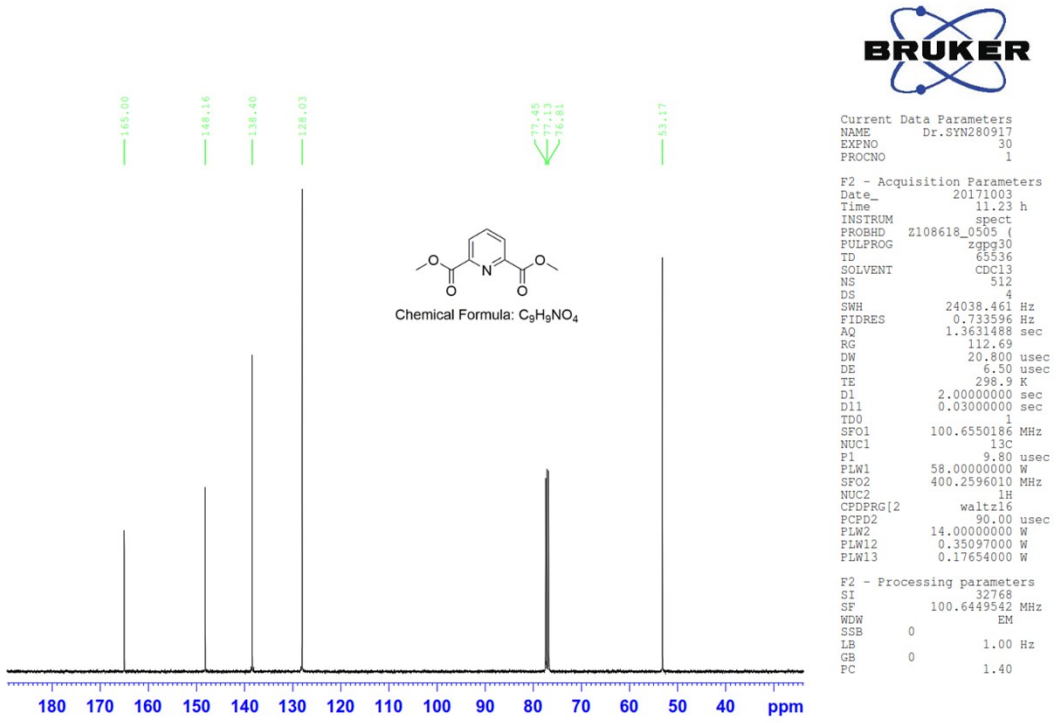


Fig. S2: ^{13}C-NMR spectrum of dimethyl pyridine-2,6-dicarboxylate (2)

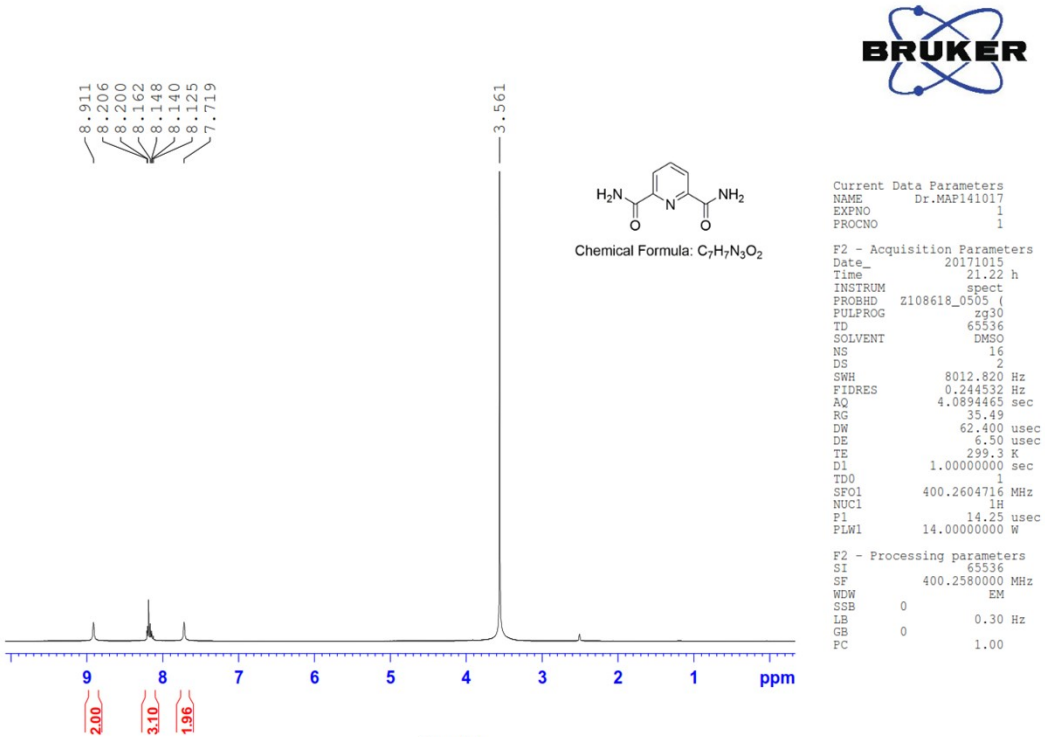


Fig. S3: ^{1}H-NMR spectrum of pyridine-2,6-dicarboxamide (3)

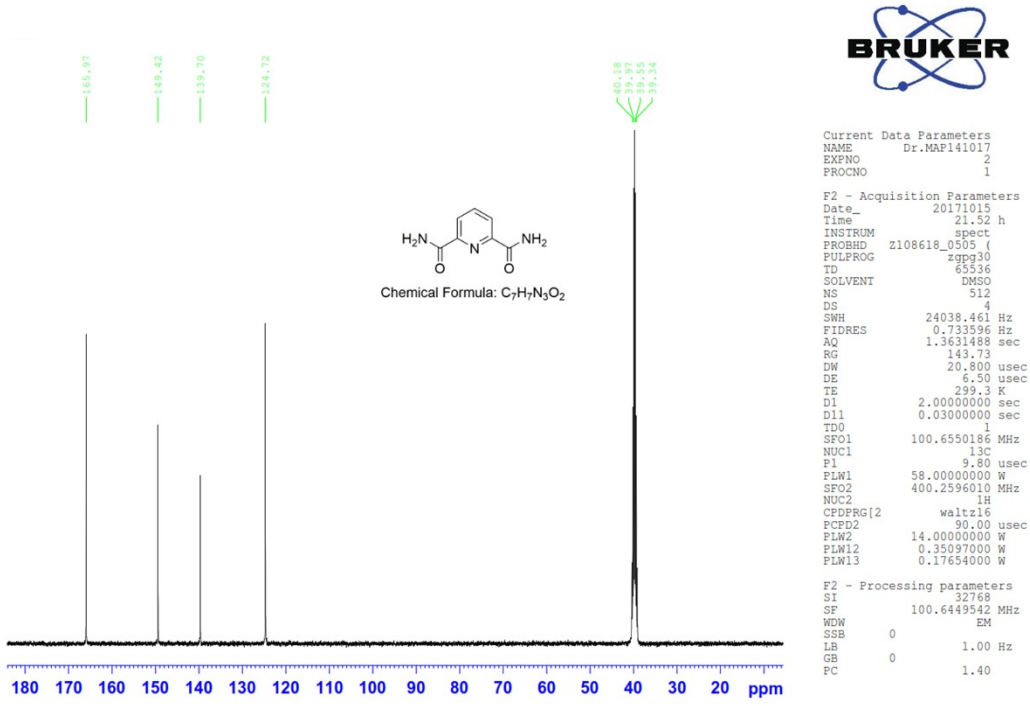


Fig. S4: ^{13}C-NMR spectrum of pyridine-2,6-dicarboxamide (3)

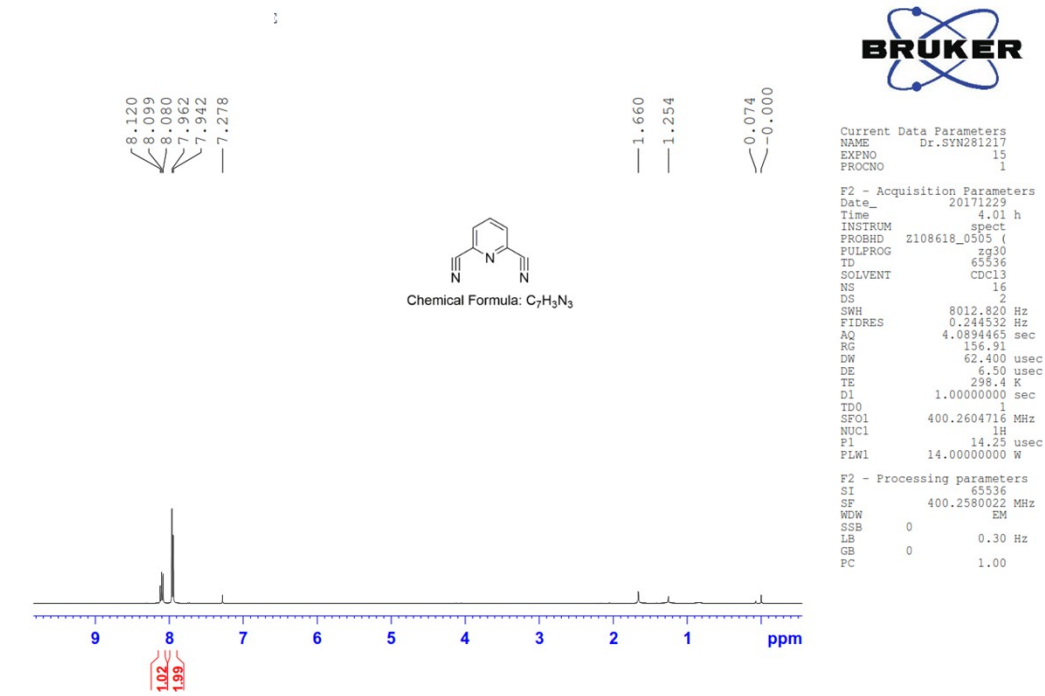


Fig. S5: ^{1}H-NMR spectrum of pyridine-2,6-dicarbonitrile (4)

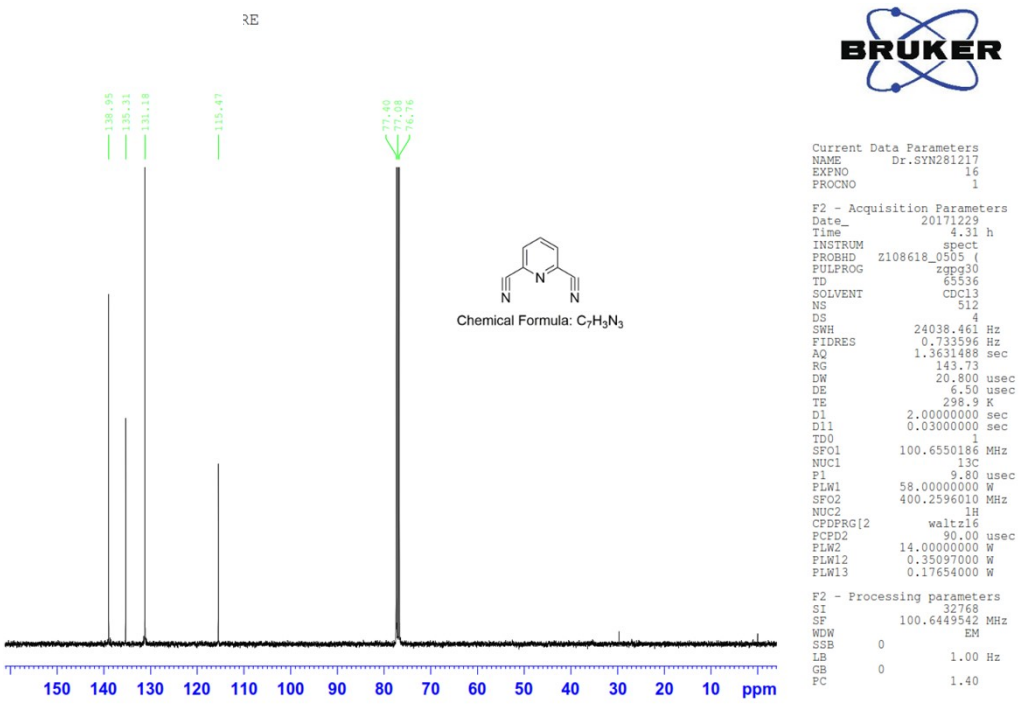


Fig. S6: ^{13}C-NMR spectrum of pyridine-2,6-dicarbonitrile (4)

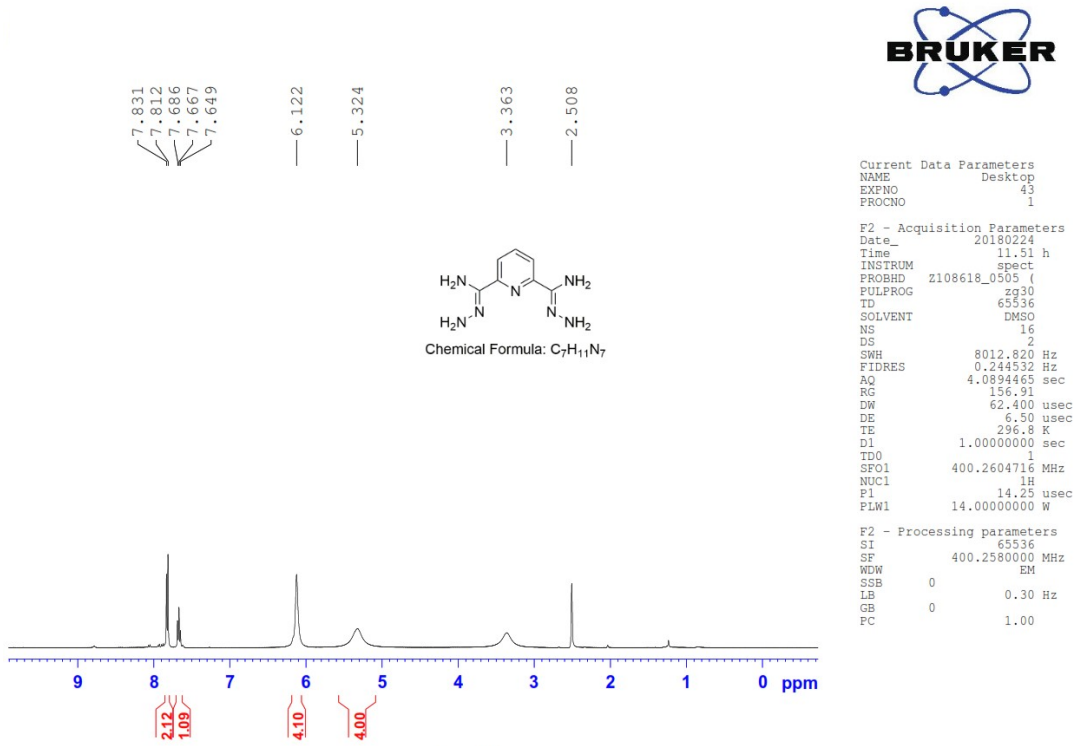


Fig. S7: ^{1}H-NMR spectrum of pyridine-2,6-dicarbohydrazonamide (5)

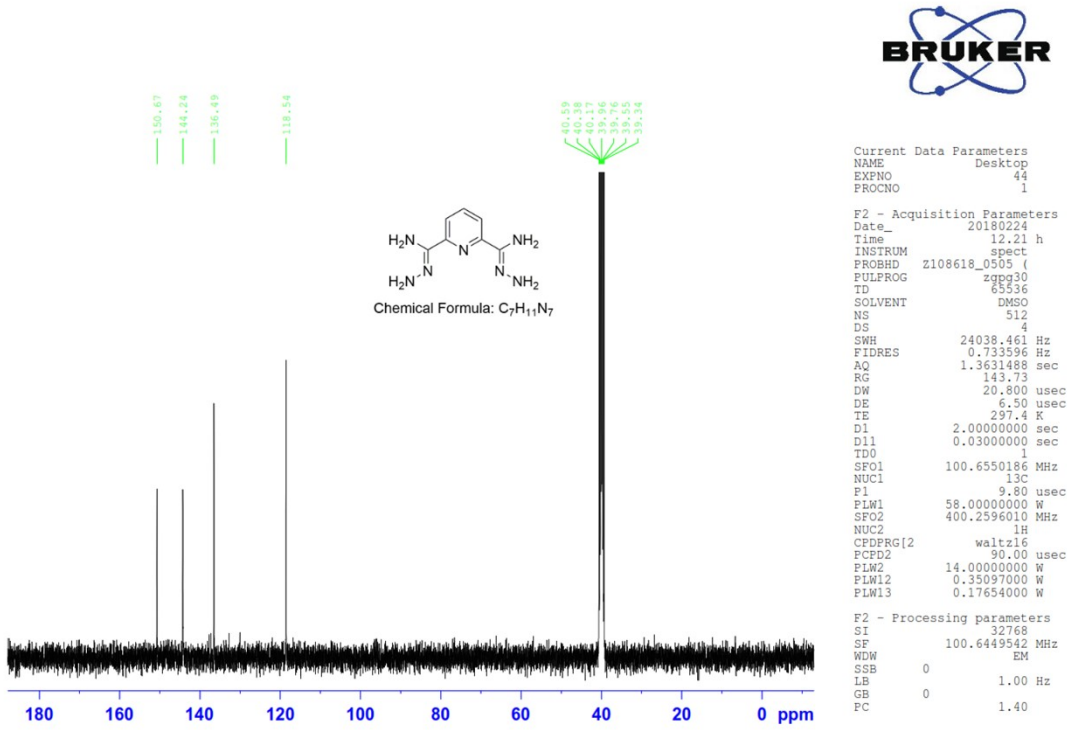


Fig. S8: ^{13}C-NMR spectrum of pyridine-2,6-dicarbohydrazonamide (5)

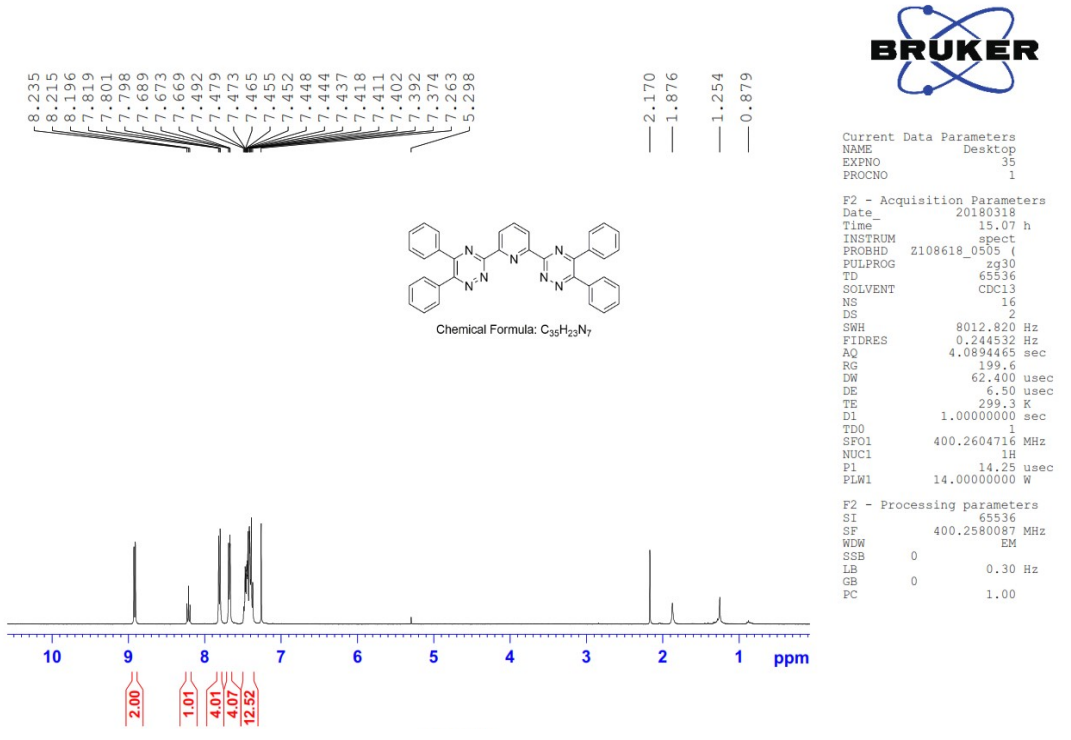


Fig. S9: ^{1}H-NMR spectrum of 2,6-bis(5,6-diphenyl-1,2,4-triazin-3-yl) pyridine (6)

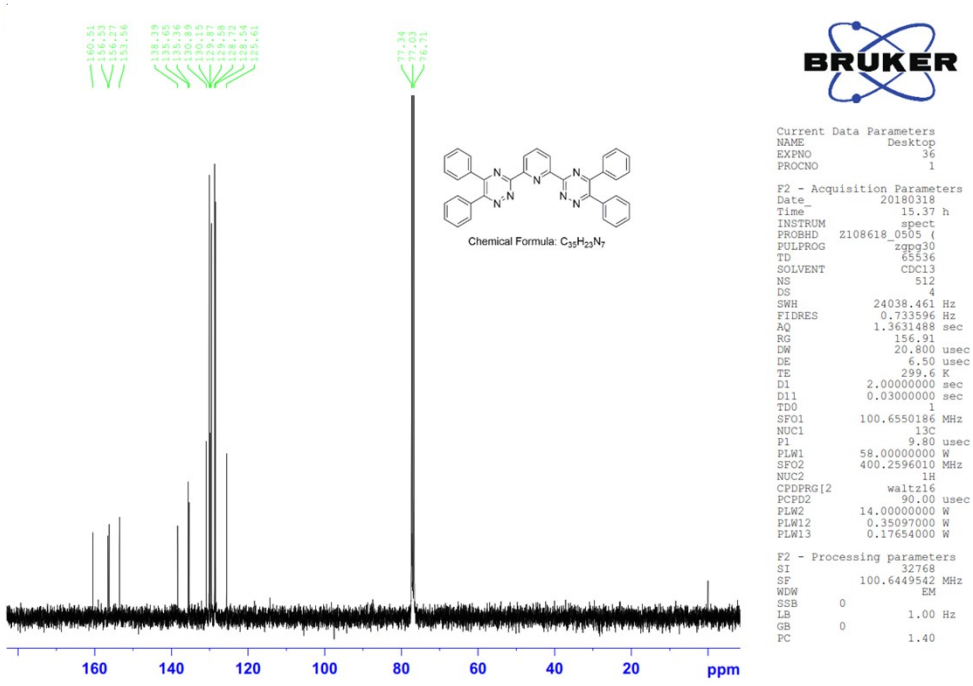


Fig. S10: ^{13}C-NMR spectrum of 2,6-bis(5,6-diphenyl-1,2,4-triazin-3-yl) pyridine (6)

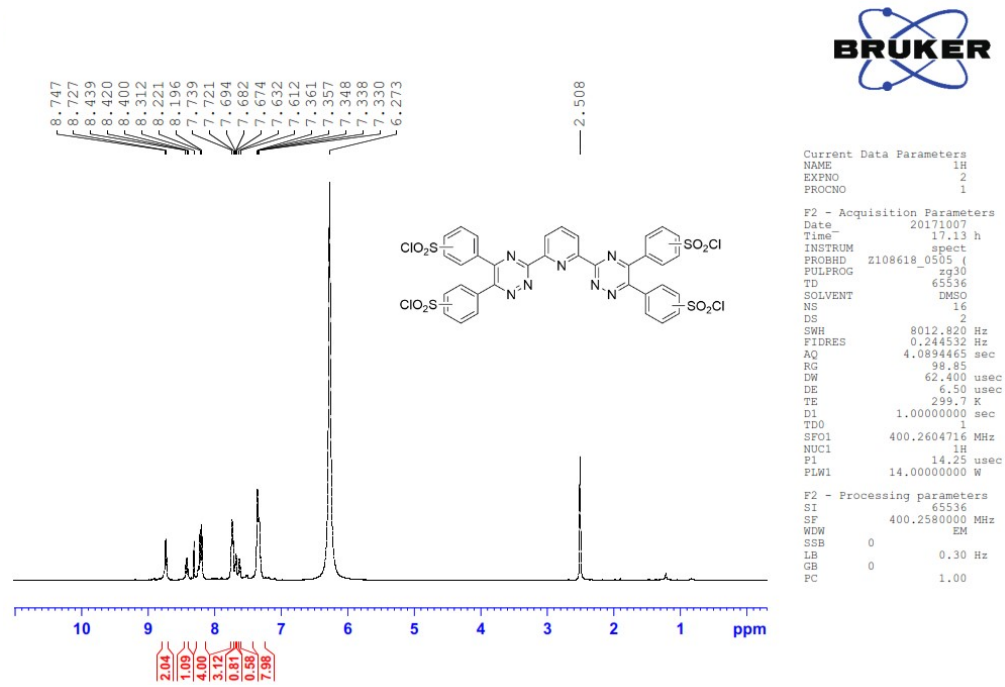


Fig. S11: ^{1}H-NMR spectrum of 3,3',3",3"'-(pyridine-2,6-diylbis(1,2,4-triazine-3,5,6-triyl))tetrabenzenesulfonyl chloride (7)

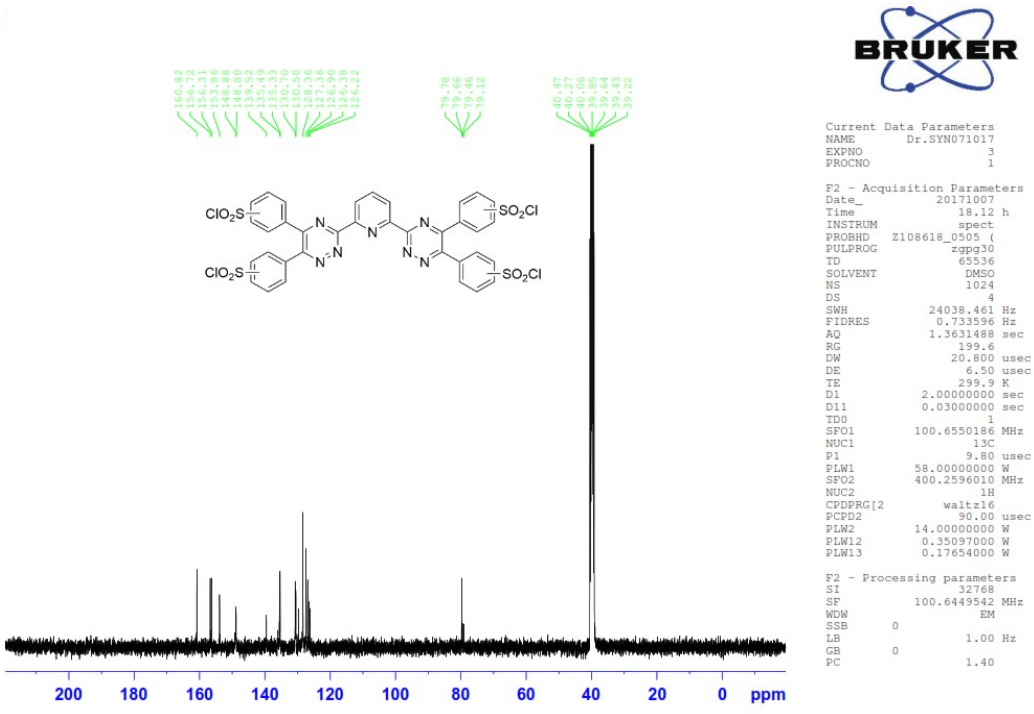


Fig. S12: ^{13}C-NMR spectrum of 3,3',3",3'"-(pyridine-2,6-diylbis(1,2,4-triazine-3,5,6-triyl))tetrabenzenesulfonyl chloride (7)

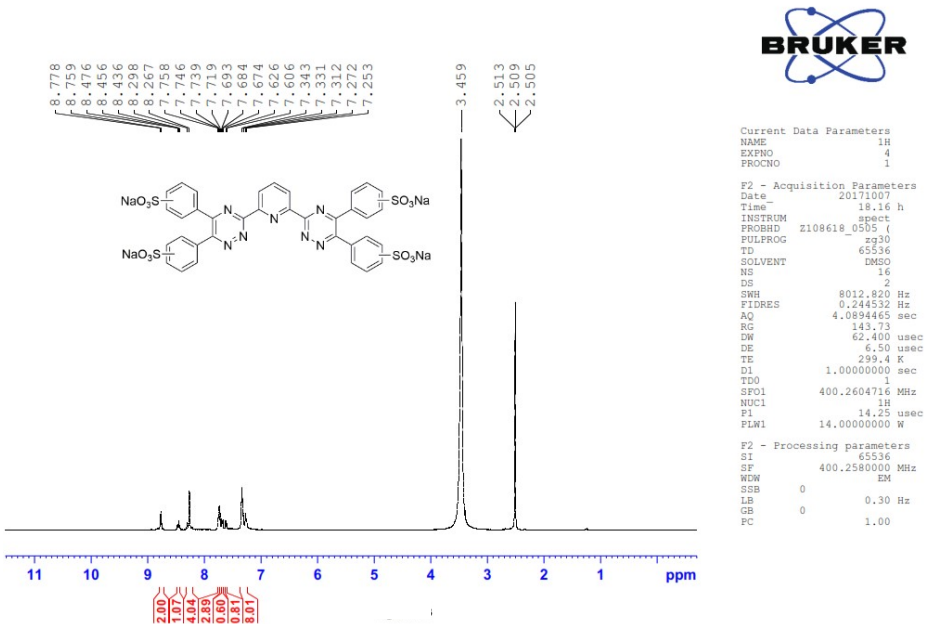


Fig. S13: ^{1}H-NMR spectrum of 3,3',3",3'"-(pyridine-2,6-diylbis(1,2,4-triazine-3,5,6-triyl))tetra benzenesulfonate (8)

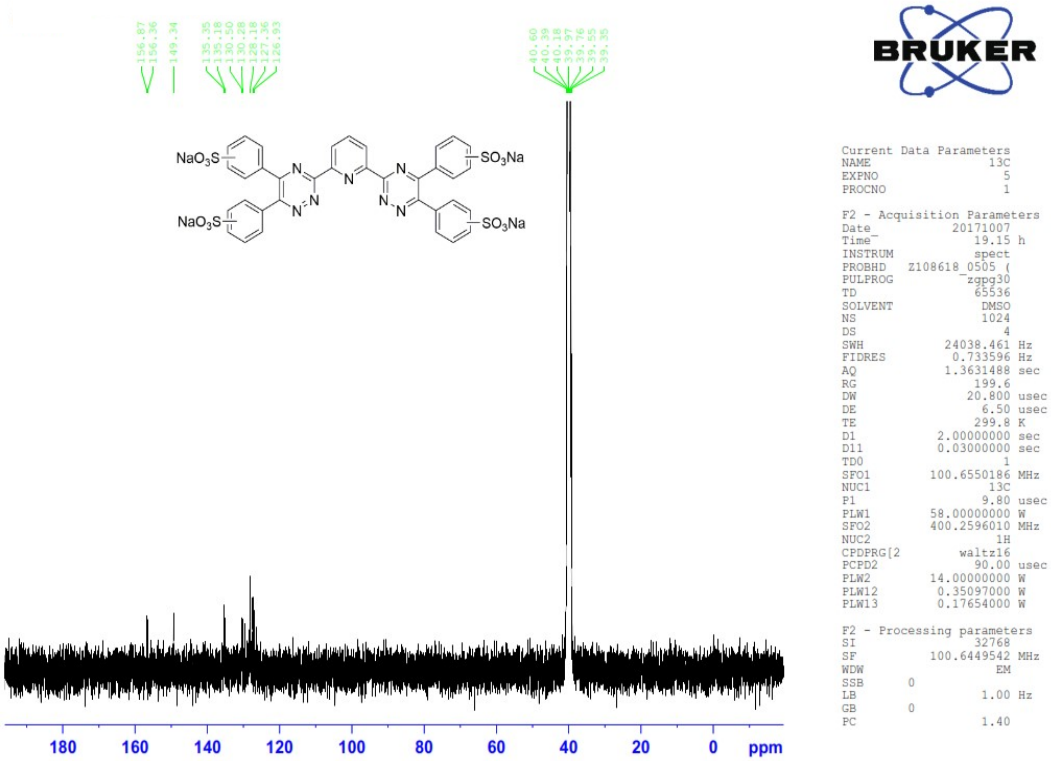


Fig. S14: ^{13}C-NMR spectrum of 3,3',3",3'"-(pyridine-2,6-diylbis(1,2,4-triazine-3,5,6-triyl))tetra benzenesulfonate (8)

Liq-Liq Extraction studies

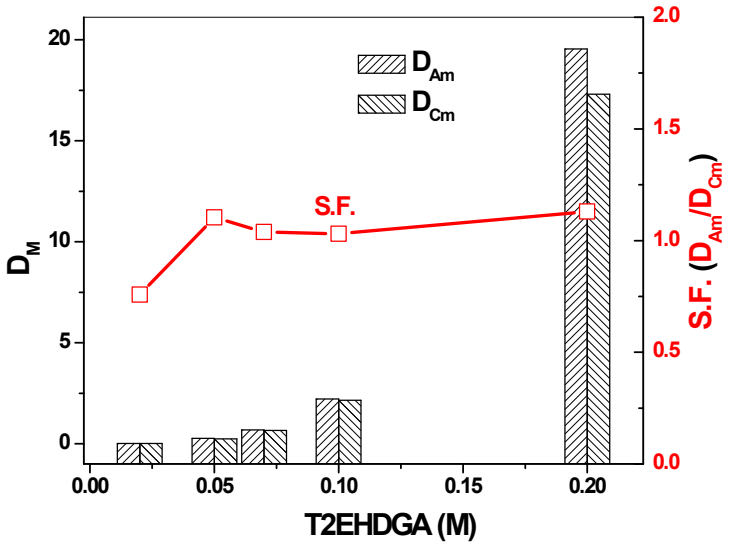


Fig. S15: Effect of T2EHDGA concentration on the extraction behaviour of Am^{3+} and Cm^{3+} in absence of SO_3PhBTP in the aqueous phase; Org. Phase: T2EHDGA in n-dodecane; Aq. Phase : 1.5 M HNO_3

The extraction equilibrium for both Am^{3+} and Cm^{3+} by both the DGA derivatives in absence of SO3PhBTP in the aqueous phase is considered as:

$$M^{3+}{}_{aq} + 3NO_3{}^{-}{}_{aq} + 3L_{org} = ML_3(NO_3)_{3org} \quad \text{..... (1)}$$

where M = Am or Cm and L is TODGA or T2EHDGA, the subsripts 'aq' and 'org' represent the species in the aqueous and organic phases, respectively. The species in the aqueous phase are represented without any subscript henceforth for simplicity. The two phase binary extraction constant (K_{ex}) is defined as:

$$K_{ex} = \frac{[ML_3(NO_3)_3]_{org}}{[M^{3+}][NO_3{}^{-}]^3[L]_{org}^3} \quad \text{---------- (2)}$$

While the distribution ratio is defined as:

$$D_0 = \frac{[M^{3+}]_{org}}{[M^{3+}]} \quad \text{---------- (3)}$$

which can be modified by taking into consideration the aqueous complexation by nitrate as follows:

$$D_0 = \frac{[ML_3(NO_3)_3]_{org}}{[M^{3+}]\left(1 + \Sigma\beta_n^{NO_3}[NO_3]^n\right)} \quad \text{---------- (4)}$$

From eqns. (2) and (4),

$$K_{ex} = \frac{D_0\left\{1 + \Sigma\beta_n^{NO_3}[NO_3]^n\right\}}{[NO_3^-]^3[L]_{org}^3} \quad \text{----------(5)}$$

where $\beta_n^{NO3}{}_1$ is the overall formation constant of the metal ions with nitrate.

In the presence of SO_3PhBTP (S) in the aqueous phase, the extraction equilibria can be considered as follows,

$$MS_2^{3+}{}_{aq} + 3NO_3^-{}_{aq} + 3L_{org} = ML_3(NO_3)_{3org} + 2S_{aq} \quad \text{…….. (6)}$$

$$K_{ex} = \frac{[ML_3(NO_3)_3]_{org}[S]^2}{\left[MS_2^{3+}\right][NO_3^-]^3[L]_{org}^3} \quad \text{---------- (7)}$$

$$D = \frac{[ML_3(NO_3)_3]_{org}}{[M^{3+}]\left(1 + \Sigma\beta_n^{NO_3}[NO_3]^n + \Sigma\beta_n^S[S]^n\right)} \quad \text{---------- (8)}$$

Where β_n^S values are the formation constants of the metal complexes of SO3PhBTP for different metal to ligand stoichiometries. However, in the present case, SO3PhBTP variation experiments showed the presence of 1:2 complex (Fig. 4b and S16) and the log β_2^S values of 6.15±0.09 and 6.45±0.15 were used for Am^{3+} and Cm^{3+}. In presence of such a strongly complexing ligand (7 mM) which formed 1:2 complex in the aqueous phase nitrate complexation can easily be neglected and the equation 8 can be written as

$$D = \frac{[ML_3(NO_3)_3]_{org}}{[M^{3+}]\left(1 + \Sigma\beta_2^S[S]^2\right)} \quad \text{---------- (9)}$$

As in the present case metal ions are in the tracer quantity (<10^{-6} M), they are solely presnt as the 1:2 complex with SO_3PhBTP (MS_2^{3+}) and therefore, equation 9 further simplies to

$$D = \frac{[ML_3(NO_3)_3]_{org}}{[MS_2^{3+}]} \quad \text{---------- (10)}$$

Combining equation (7) and (10) we can get

$$K_{ex} = D\frac{[S]^2}{[NO_3^-]^3[L]_{org}^3} \quad \text{---------- (11)}$$

$$logK_{ex} = logD + 2\log[S] - 3\log[NO_3^-] - 3log[L]_{org} \text{ ------ (12)}$$

These calculated $logK_{ex}$ values are plotted against

The temperature variation experiments were carried out in a wide range of temperature (15-55 ^oC).

The thermodynamic parameters were calculated from the van't Hoff plots as well as the Gibbs – Helmholtz equation as follows. Free energy change (ΔG_{ex}) for the extraction equilibria can be expressed as

$$\Delta G = -2.303\ RT\ K_{ex} \quad \text{..... (12)}$$

and

$$\Delta G = \Delta H - T\Delta S \quad \text{.....(13)}$$

From eqn (10) and (11),

$$logK_{ex} = -(\Delta H/2.303R)(1000/T) + (\Delta S/2.303R) \quad \text{.....(14)}$$

where R (8.314 $JK^{-1}mol^{-1}$) is the universal gas constant. ΔH (in $kJ.mol^{-1}$) and ΔS (in $J.K^{-1}.mol^{-1}$) were therefore calculated from the slope ($-\Delta H / 2.303\ R$) and intercept ($\Delta S / 2.303\ R$) of the plot of $logK_{ex}$ vs 1000/T (Fig 6). The ΔH and ΔS values calculated from the plots, along with the ΔG values are given in Table 3.

Comparing distribution ratio values in absence (equation (3)) and presence of SO_3PhBTP (equation ((9)), we can write,

$$\frac{D_0}{D} = \{1 + \beta_2^s[S]^2\} \quad \text{---------- (15)}$$

$$\log\left(\frac{D_0}{D} - 1\right) = log\beta_2^s + 2log[S] \quad \text{---------- (16)}$$

$log\beta_2^s$ values were, therefore, determined from the intercept of the plot of $\log\left(\frac{D_0}{D} - 1\right)$ vs $log[S]$ as shown in Fig. S1.

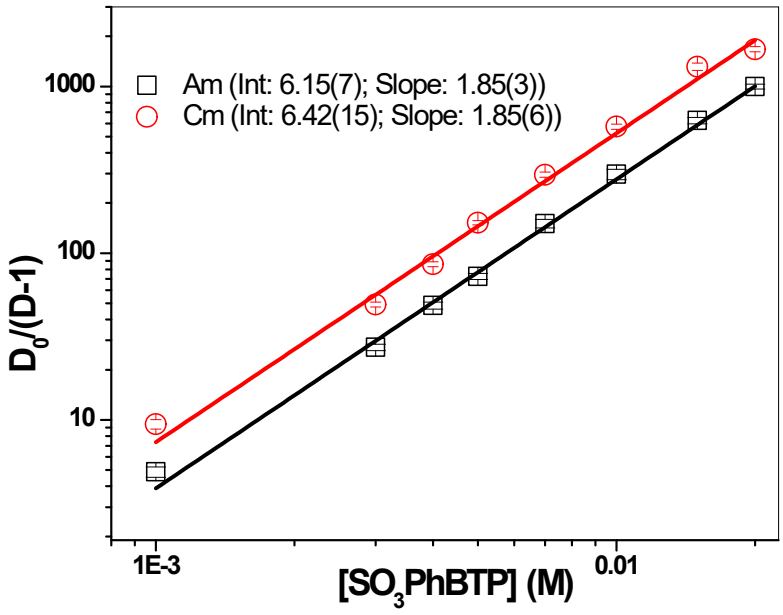


Fig. S16: Plot of $\log\left(\frac{D_0}{D}-1\right)$ vs $log[SO3PhBTP]$ used to determine the $log\beta_2^s$ values for the Am^{3+}/Cm^{3+} complexes of SO_3PhBTP; Org. Phase 0.2 M TODGA or T2EHDGA in n-dodecane; Aq. Phase: 1.5 M HNO_3 containing varying concentration of SO_3PhBTP

Computational studies:

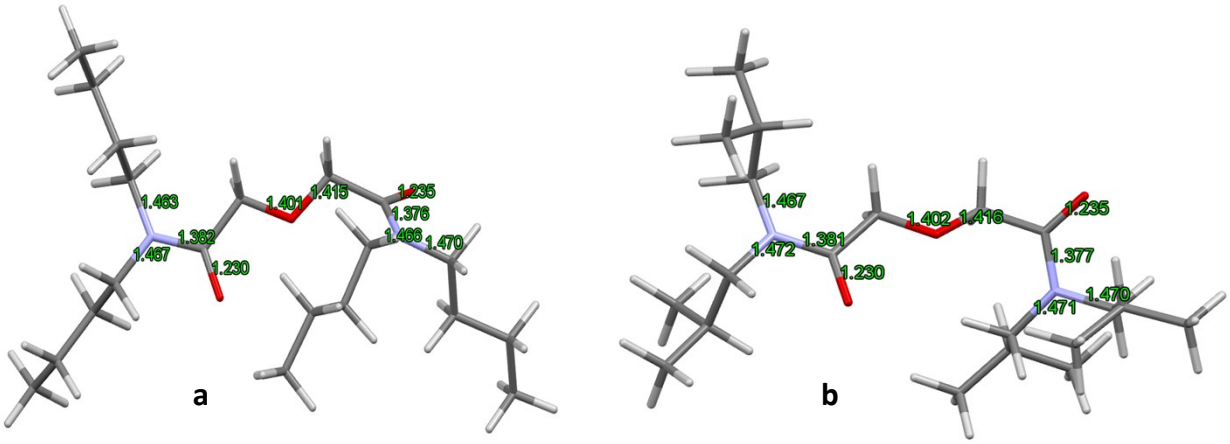


Fig. S17: Optimized structures (a) TBDGA and (b) TiBDGA showing different bond length in Å

Table S1: Cartesian coordinates of the optimized structures of the free ligands (TBDGA and TiBDGA) and their Am^{3+}/Cm^{3+} complexes

TBDGA

C	-3.8346370	-2.8084149	-3.3900037
C	-3.1563725	-3.9170095	-2.5624190
H	-3.8986115	-4.7179387	-2.2944512
H	-2.4028917	-4.3751421	-3.2462887
O	-2.5456062	-3.3842443	-1.4022189
C	-1.7869452	-4.3256372	-0.6948124
H	-2.4163440	-5.2007197	-0.3797951
H	-0.9668594	-4.7412126	-1.3401388
C	-1.1778982	-3.6304912	0.5436441
N	-0.4078870	-4.4220260	1.3746194
N	-4.7259025	-1.9707912	-2.7600108
O	-1.3712847	-2.4353459	0.7582325
O	-3.5777415	-2.7130364	-4.5940333
C	0.2159192	-3.7849991	2.5401649
H	0.1440959	-4.4834748	3.4053082
H	-0.3887600	-2.8856040	2.7784499
C	-0.2010902	-5.8595879	1.1949712
H	-0.2526527	-6.1125911	0.1146910
H	0.8440447	-6.0934270	1.5018173
C	1.6806533	-3.3769671	2.3054719
H	2.2851627	-4.2760518	2.0344877
H	1.7202092	-2.6928547	1.4272027
C	2.3094306	-2.6887257	3.5277216
H	2.2110017	-3.3534823	4.4190124
H	1.7247700	-1.7697100	3.7683772
C	3.7852814	-2.3209062	3.3263740
H	4.2019758	-1.8070103	4.2206144
H	4.4066374	-3.2262093	3.1393798
H	3.9178674	-1.6402113	2.4552357
C	-1.1776691	-6.7485813	1.9892122
H	-2.2218956	-6.5204062	1.6714418
H	-1.1196923	-6.4807523	3.0700035
C	-0.8960563	-8.2496153	1.8160843
H	0.1581096	-8.4625113	2.1137266
H	-0.9640299	-8.5146371	0.7342089
C	-1.8454437	-9.1447916	2.6232209
H	-2.9064066	-8.9835462	2.3261389
H	-1.6140653	-10.2220750	2.4712449
H	-1.7694353	-8.9349226	3.7141688
C	-5.3158349	-0.9070778	-3.5857002

H	-6.2621505	-0.5906192	-3.0936980
H	-5.5727459	-1.3498445	-4.5730257
C	-4.4000974	0.3088915	-3.8104353
H	-3.4580789	-0.0480634	-4.2825310
H	-4.1203625	0.7547019	-2.8282125
C	-5.0509742	1.3792401	-4.7012641
H	-5.3160358	0.9250687	-5.6852154
H	-6.0171222	1.7056803	-4.2466373
C	-4.1562537	2.6048417	-4.9287790
H	-3.1942711	2.3173447	-5.4102247
H	-4.6507108	3.3556322	-5.5847092
H	-3.9082146	3.1091880	-3.9672086
C	-5.1611350	-2.0939554	-1.3650845
H	-6.2737224	-1.9993165	-1.3520268
H	-4.9296374	-3.1183532	-1.0106800
C	-4.5362355	-1.0802767	-0.3925685
H	-3.4319630	-1.2044453	-0.4245305
H	-4.7717122	-0.0431924	-0.7284637
C	-5.0298390	-1.2722565	1.0496066
H	-4.8213836	-2.3218338	1.3655550
H	-6.1396938	-1.1519494	1.0909669
C	-4.3643445	-0.3100289	2.0421447
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H	-4.5595730	0.7525140	1.7697921

TiBDGA

O	-1.4994429	1.3586253	1.5661596
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N	-2.0911704	3.2448253	2.7203021
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C	-0.7510797	6.6225803	4.0558528
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C	3.0103526	4.2920424	-2.8031757
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Am(TBDGA)33+

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H	2.9737734	-4.1776185	-2.8282826
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H	2.8304758	-7.1680770	-3.7495239
C	2.6790585	-8.3222894	-1.9103709
H	3.8763777	-6.5780246	-2.4361125
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H	3.6631908	6.8035221	-2.3159512
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Cm(TBDGA)33+

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C	3.4876897	0.5055186	-5.8585107
H	-4.2125815	-2.4133391	3.6937157
H	-0.3866203	-5.6535227	3.2861788
H	-5.9035252	1.1501765	-1.1863788
H	-3.4196249	0.9641736	-5.5504634
H	5.1673467	2.4778958	3.1604531
H	4.2398864	-2.4216763	3.6838456
H	1.8870201	-5.7030240	-1.2002086
H	0.7850546	-3.4313345	-5.5520078
H	-4.7442997	3.2828111	3.1181527

H	-0.0082672	4.8096521	3.7769290
H	4.0426642	4.4798901	-1.1071549
H	2.5895606	2.4559022	-5.5019003
H	-2.9078920	-3.1152231	0.1976331
H	-3.6719819	-1.9611305	1.3569913
H	-2.6274701	-5.0613837	3.3526890
H	-3.4678042	-4.2160007	2.0471893
H	-3.3261527	-3.2460975	4.9971878
C	-6.0633167	-3.6970719	5.3708024
H	-4.7683725	-5.3036983	4.6796267
H	-5.6645770	-4.4852670	3.3781646
H	-1.0215585	-3.6346608	4.7174782
H	0.0448326	-2.6028013	3.7129080
H	0.7020137	-4.6111668	2.3289292
H	0.9392122	-5.1234459	5.3820141
H	2.0422637	-4.1050969	4.4279949
C	2.2335244	-6.2441542	4.0403020
H	-4.3350360	-0.5836996	-0.5690045
H	-3.5030647	-1.7147905	-1.7027583
H	-5.0948075	-0.6597748	-2.8036701
H	-5.1958076	0.4943709	-4.1392689
H	-5.9867744	2.3058699	-2.5410940
H	-7.6851861	0.8243725	-3.7067124
C	-8.5947606	1.5573490	-1.8696358
H	-7.6152456	-0.3291128	-2.3531050
H	-2.3583154	2.5259107	-3.0832723
H	-4.0037053	2.7060909	-3.7724656
H	-1.7695219	0.8561396	-4.8727995
C	-1.7016301	2.3085912	-7.2876177
H	-1.4169673	3.3218646	-5.3777279
H	-3.0715944	3.4305560	-6.0248343
H	4.1446845	-0.9905932	0.1608604
H	3.5123671	-2.2125994	1.3291650
H	5.7566246	0.2512413	3.2405221
H	5.3972231	-0.9241758	1.9706969
H	4.5732624	-1.2150277	4.9527609
C	6.3244909	-3.3648579	5.3200453
H	7.0640725	-1.4679846	4.5518924
H	6.7442690	-2.6837540	3.2926362
H	3.7525646	0.9581074	4.6553924
H	2.3079702	1.3705587	3.6789747
H	3.6951555	2.9185613	2.2525852
H	4.1380230	3.3902616	5.2895413
H	2.6783776	3.8577890	4.3863482
C	4.4421018	5.0582680	3.9282512
H	2.6156207	-3.4722560	-0.5796709

H	3.2019431	-2.2067115	-1.7240944
H	3.0425308	-4.1125586	-2.8264957
H	2.0698107	-4.7601887	-4.1534830
H	0.8732806	-6.3196939	-2.5309895
H	2.9471991	-7.1052226	-3.7580038
C	2.7881084	-8.2620319	-1.9210036
H	3.9688113	-6.5020444	-2.4313926
H	-1.0758563	-3.2736236	-3.0691372
H	-0.4341429	-4.7977989	-3.7611582
H	0.0584809	-1.9450724	-4.8758634
C	-1.2560217	-2.6121916	-7.2740124
H	-2.2584934	-2.8827934	-5.3563247
H	-1.5227854	-4.3641779	-6.0129367
H	-1.1710317	4.1313121	0.2246190
H	0.1955584	4.1319643	1.4041769
H	-3.0750452	4.8636532	3.2948951
H	-1.8533058	5.1498195	2.0500925
H	-1.2393952	4.4689962	5.0198655
C	-0.2095817	7.0274943	5.4919386
H	-2.2214296	6.7820005	4.6996593
H	-0.9949315	7.1407687	3.4618648
H	-2.7708419	2.7297053	4.6490509
H	-2.4130515	1.2912532	3.6419322
H	-4.3968255	1.8091748	2.1725104
H	-5.1117066	1.8748934	5.1939716
H	-4.7944360	0.3995698	4.2517635
C	-6.6798429	1.3869193	3.7683016
H	1.7473954	4.0047848	-0.4935712
H	0.3682891	3.9397612	-1.6557476
H	2.1027993	4.7394308	-2.7425941
H	3.1510224	4.2294103	-4.0722528
H	5.0859523	3.9203722	-2.4403179
H	4.7772147	6.1325046	-3.6293337
C	5.8277404	6.5357145	-1.7652661
H	3.7250787	6.7059520	-2.3132697
H	3.3962567	0.7447180	-3.0394460
H	4.3938477	2.0635403	-3.7325185
H	1.6543031	1.0939262	-4.8198378
C	2.8465099	0.2750856	-7.2325234
H	3.5978310	-0.4693844	-5.3262533
H	4.5228652	0.8970178	-5.9935286
H	-6.9326610	-4.3649918	5.5488067
H	-5.5542060	-3.5457617	6.3486349
H	-6.4609604	-2.7122627	5.0377675
H	3.0336069	-6.3928887	4.7967243
H	1.6143587	-7.1685319	4.0285168

H	2.7232853	-6.1553353	3.0438687
H	-9.6101831	1.1883713	-2.1271507
H	-8.4804249	1.4796534	-0.7649074
H	-8.5535995	2.6356674	-2.1403850
H	-1.4015815	3.1902498	-7.8935262
H	-0.8175001	1.6360263	-7.2110568
H	-2.4887484	1.7675024	-7.8579676
H	-7.2740690	0.7920953	4.4945491
H	-7.1254066	2.4057989	3.7329964
H	-6.8160897	0.9258097	2.7635987
H	-0.3342397	8.1135295	5.6887015
H	-0.3907621	6.4921135	6.4503529
H	0.8524580	6.8596743	5.2041340
H	6.0667728	7.5868261	-2.0329397
H	5.6666631	6.4991629	-0.6643449
H	6.7248890	5.9203498	-1.9983034
H	3.4495854	-0.4318398	-7.8415715
H	1.8210401	-0.1489761	-7.1402441
H	2.7686917	1.2240553	-7.8076773
H	-2.1724642	-2.7986323	-7.8736896
H	-1.1229802	-1.5097585	-7.1946184
H	-0.3949111	-3.0151210	-7.8518395
H	3.5850071	-8.9803585	-2.2084966
H	2.8387595	-8.1302224	-0.8169412
H	1.8103455	-8.7355937	-2.1625078
H	7.3390077	-3.7900484	5.4738760
H	5.9768398	-2.9693903	6.3001274
H	5.6505991	-4.2029767	5.0329571
H	4.2152726	5.8337133	4.6909910
H	5.5491266	4.9625582	3.8732659
H	4.0885463	5.4403254	2.9437856

Am(TiBDGA)33+

C	-5.4374153	-4.1518796	3.9399317
C	-4.1492209	-3.3110334	3.8700965
C	-3.1357253	-4.0440202	2.9564690
N	-1.8432973	-3.3539475	2.7320335
C	-1.6672412	-2.4399705	1.7633310
C	-2.8226758	-2.1723811	0.7917860
O	-2.4272722	-1.0995030	-0.0489693
C	-3.3686785	-0.8030912	-1.0691137
C	-2.8186227	0.3906450	-1.8564811
N	-3.5977265	0.9807401	-2.7780945
C	-4.9830368	0.5534465	-3.0869301
C	-6.1023689	1.4670299	-2.5318403

C	-7.4544079	0.9930681	-3.0967145
C	-0.7067194	-3.6988696	3.6153967
C	0.2487924	-4.7786591	3.0535462
C	1.3547996	-5.0381372	4.0919090
O	-0.5817580	-1.8137750	1.5964672
Am	-0.0072669	-0.0660369	0.0065341
O	-0.0015671	-1.9677753	-1.5612187
C	0.9207253	-2.7917589	-1.8197820
N	0.7744314	-3.8076853	-2.6874356
C	1.8495146	-4.7934070	-2.9551906
C	1.9121556	-6.0133707	-2.0023226
C	3.1403008	-6.8626340	-2.3800755
O	-1.2932483	1.2530526	1.6229384
C	-1.2864862	2.4946896	1.8530865
N	-1.9849521	3.0586530	2.8531624
C	-1.9400034	4.5115374	3.1435293
C	-0.8011198	4.9864807	4.0794443
C	-0.8793436	6.5195453	4.2011250
O	0.2847053	2.5575888	0.0663683
C	1.0481316	3.2662215	-0.8998244
C	1.7906398	2.2244320	-1.7428284
N	2.7110414	2.6400133	-2.6278547
C	3.0778789	4.0676066	-2.7899802
C	4.1861524	4.6023442	-1.8490972
C	4.3580387	6.1106640	-2.1087124
O	1.4995472	1.0044887	-1.5761445
O	-1.6403885	0.7794049	-1.6076860
O	2.1129702	-1.5945469	-0.1431297
C	3.2945828	-1.3432636	0.6080944
C	2.9560234	-0.2470059	1.6257558
N	3.8902771	0.1470171	2.5058757
C	5.2514564	-0.4325697	2.5860789
C	5.5042691	-1.3710509	3.7902910
C	6.9975109	-1.7438831	3.8232249
C	-0.4646417	3.4034112	0.9300628
C	2.2746991	-2.6105083	-1.1245105
O	1.7994892	0.2636679	1.5880442
C	-3.0722613	2.1452878	-3.5257416
C	-2.1751180	1.8181117	-4.7416815
C	-1.7072121	3.1461030	-5.3650242
C	3.5533417	1.2166770	3.4727772
C	3.6473793	2.6605383	2.9248608
C	3.2817833	3.6351264	4.0589040
C	-0.5101237	-3.9534664	-3.4082385
C	-0.6552448	-3.0810880	-4.6771203
C	-2.0657741	-3.2951261	-5.2547911

C	-2.8397271	2.1988574	3.7028707
C	-4.2469949	1.9101423	3.1283976
C	-4.9970070	0.9924392	4.1101780
C	3.3933522	1.6347094	-3.4747260
C	2.6313321	1.2257384	-4.7567893
C	3.4176199	0.0999581	-5.4524400
H	-4.4011114	-2.3346267	3.3881855
H	2.0651530	-5.6302702	-0.9636482
H	0.1713740	4.7283985	3.5934785
H	3.8355116	4.4721501	-0.7958679
H	-3.0215356	-3.0892161	0.1827597
H	-3.7614520	-1.9148330	1.3353570
H	-2.8944631	-5.0324484	3.3987018
H	-3.6043075	-4.2634354	1.9730278
H	-5.2474186	-5.1389898	4.4188238
H	-5.8702271	-4.3418531	2.9324665
H	-1.1385835	-4.0431625	4.5769952
H	-0.1404794	-2.7652513	3.8138413
H	0.7202703	-4.3492362	2.1377832
H	0.9346478	-5.4805678	5.0229441
H	1.8883765	-4.1035457	4.3738967
H	-4.3577975	-0.5622430	-0.6178736
H	-3.5014187	-1.6837168	-1.7451459
H	-5.1329740	-0.4894699	-2.7370269
H	-5.0616303	0.5171218	-4.1933961
H	-5.9181445	2.4964011	-2.9192035
H	-7.4635996	1.0016376	-4.2086212
H	-7.6959574	-0.0408299	-2.7603389
H	-2.5055363	2.7729660	-2.8068815
H	-3.9530985	2.7339162	-3.8592506
H	-1.2805766	1.2776706	-4.3540513
H	-1.1759696	3.7884188	-4.6266864
H	-2.5661055	3.7316671	-5.7643213
H	4.1189086	-1.0080229	-0.0680499
H	3.6297110	-2.2741384	1.1215586
H	5.9588260	0.4219817	2.6357879
H	5.4795396	-0.9658053	1.6391119
H	5.2802829	-0.7956011	4.7187687
H	7.6475157	-0.8438808	3.8880822
H	7.2942204	-2.3162673	2.9148247
H	4.2433585	1.0982078	4.3343862
H	2.5232403	1.0252945	3.8393729
H	2.8780591	2.7527803	2.1215948
H	4.0261725	3.5887173	4.8859747
H	2.2829075	3.4098684	4.4945941
H	2.6147189	-3.5560946	-0.6432547

H	3.0501128	-2.3096963	-1.8716315
H	2.8273414	-4.2657169	-2.9570994
H	1.7006891	-5.1494793	-3.9956634
H	3.0426772	-7.2751375	-3.4095680
H	4.0852617	-6.2762627	-2.3379250
H	-1.3212391	-3.7059241	-2.6924945
H	-0.6115133	-5.0254511	-3.6749984
H	-0.5664190	-2.0163479	-4.3570946
H	-2.8603309	-3.0577200	-4.5114617
H	-2.2151351	-4.3492346	-5.5813827
H	-1.1475463	4.0567768	0.3328450
H	0.2181330	4.0638579	1.5122807
H	-2.9179973	4.7743562	3.5965176
H	-1.8958337	5.0692939	2.1835390
H	-1.8313966	6.8360598	4.6834820
H	-0.8177953	7.0235028	3.2110369
H	-2.9310117	2.7046093	4.6857683
H	-2.2982804	1.2432863	3.8627663
H	-4.1006594	1.3547033	2.1712869
H	-5.1743215	1.5037293	5.0833009
H	-4.4305363	0.0575043	4.3207665
H	1.7598807	3.9612326	-0.3974214
H	0.3767719	3.8777147	-1.5525998
H	2.1609315	4.6859156	-2.6828215
H	3.4018429	4.1925136	-3.8436843
H	4.7142162	6.3017537	-3.1458260
H	3.4076762	6.6719141	-1.9684229
H	3.5686813	0.7375605	-2.8449416
H	4.3829793	2.0568355	-3.7446825
H	1.6442524	0.8166685	-4.4368989
H	3.5659414	-0.7773439	-4.7831589
H	4.4225311	0.4498127	-5.7797777
H	-0.0475835	6.9055676	4.8282348
H	-5.9912808	0.7067625	3.7040440
H	5.1105522	6.5442161	-1.4160313
H	2.8818799	-0.2535960	-6.3594825
H	-1.0136719	2.9608882	-6.2128564
H	-8.2759137	1.6564350	-2.7517554
H	-6.2108685	-3.6340503	4.5462658
H	2.1073448	-5.7551414	3.6982984
H	3.2678923	4.6838772	3.6909639
H	7.2209238	-2.3805270	4.7054959
H	3.2482062	-7.7244824	-1.6876132
H	-2.2296870	-2.6502291	-6.1446621
C	5.5224257	3.8549529	-1.9921814
H	5.4365500	2.7764188	-1.7329652

H	5.9243021	3.9346551	-3.0278986
H	6.2845916	4.2962196	-1.3141040
C	2.3836870	2.4031946	-5.7146808
H	3.3397659	2.8688470	-6.0457282
H	1.8600515	2.0544240	-6.6312042
H	1.7491447	3.1955602	-5.2591132
C	0.4260592	-3.3612410	-5.7337968
H	0.3956830	-4.4199060	-6.0788143
H	0.2682766	-2.7240035	-6.6308875
H	1.4512116	-3.1466828	-5.3588836
C	0.6262120	-6.8560810	-2.0044350
H	0.4106160	-7.2649334	-3.0176841
H	0.7339660	-7.7254653	-1.3204390
H	-0.2618687	-6.2786529	-1.6649370
C	4.6051501	-2.6156995	3.7765894
H	3.5239789	-2.3516770	3.7405098
H	4.8412923	-3.2762853	2.9099179
H	4.7627287	-3.2214070	4.6946057
C	5.0194493	3.0013077	2.3207369
H	5.0352330	4.0531357	1.9601261
H	5.8337994	2.9071040	3.0745692
H	5.2735848	2.3528918	1.4527246
C	-0.8240942	4.3123553	5.4615212
H	-1.7752978	4.5223963	6.0015449
H	-0.6939095	3.2094793	5.3991953
H	0.0007509	4.7057160	6.0943536
C	-5.0596585	3.1803774	2.8289172
H	-6.0647639	2.9150010	2.4349107
H	-5.2234943	3.7872565	3.7484446
H	-4.5716907	3.8288482	2.0674319
C	-0.4578733	-6.0871840	2.6618869
H	0.2790654	-6.8241931	2.2749021
H	-0.9566709	-6.5613645	3.5374476
H	-1.2210951	-5.9377270	1.8664850
C	-3.5992371	-3.0086709	5.2735465
H	-3.3193657	-3.9431641	5.8111014
H	-2.7095337	-2.3412057	5.2474100
H	-4.3735943	-2.5010908	5.8884256
C	-6.1232704	1.5372277	-0.9972206
H	-6.3965297	0.5522618	-0.5508285
H	-5.1450857	1.8627625	-0.5744723
H	-6.8862523	2.2680180	-0.6525732
C	-2.8630454	0.9276822	-5.7896501
H	-3.7817198	1.4081551	-6.1960971
H	-2.1833547	0.7492531	-6.6511676
H	-3.1414199	-0.0697496	-5.3828899

Cm(TiBDGA)33+

C	-5.4341146	-4.1870600	3.9380298
C	-4.1313271	-3.3692022	3.8642442
C	-3.1460142	-4.1028261	2.9208424
N	-1.8461551	-3.4302732	2.6858389
C	-1.6717848	-2.5014894	1.7315826
C	-2.8394881	-2.1949621	0.7862663
O	-2.4402642	-1.1107115	-0.0413867
C	-3.4053692	-0.7723320	-1.0282119
C	-2.8607347	0.4339658	-1.8008762
N	-3.6417847	1.0281416	-2.7179106
C	-5.0249222	0.5978102	-3.0317016
C	-6.1482796	1.5029998	-2.4711309
C	-7.4976210	1.0278290	-3.0414069
C	-0.6995122	-3.8075419	3.5431249
C	0.2323635	-4.8868550	2.9426576
C	1.3622465	-5.1708672	3.9484209
O	-0.5806310	-1.8881117	1.5567460
Cm	-0.0371467	-0.0845814	0.0188655
O	0.0332359	-1.9220031	-1.5873423
C	0.9543016	-2.7564209	-1.8195325
N	0.8285578	-3.7569885	-2.7067394
C	1.9000379	-4.7538365	-2.9474554
C	1.9112498	-5.9888033	-2.0117894
C	3.1312296	-6.8576944	-2.3711641
O	-1.2630181	1.2348400	1.6469152
C	-1.2645904	2.4821142	1.8504162
N	-1.9465288	3.0574515	2.8541282
C	-1.9194604	4.5178952	3.1090693
C	-0.7680471	5.0335241	4.0069894
C	-0.8691607	6.5676181	4.0938233
O	0.2727120	2.5223645	0.0347246
C	1.0343653	3.2152648	-0.9435419
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C	4.3031848	6.0774650	-2.2291703
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O	2.0906346	-1.6064345	-0.0717073
C	3.2561753	-1.3555414	0.7036614
C	2.9194020	-0.2122132	1.6702397
N	3.8465080	0.1948983	2.5530645

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C	6.8618279	-1.7351521	4.0192773
C	-0.4754712	3.3784814	0.8879354
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O	1.7772926	0.3217089	1.5895997
C	-3.1186820	2.2003119	-3.4553747
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C	-1.9026128	-3.2013214	-5.3830580
C	-2.7642928	2.2034037	3.7457412
C	-4.1823895	1.8794021	3.2188554
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C	4.4329323	-2.5023916	3.9930086
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