A novel highly selective ligand for separation of actinides and lanthanides in the nuclear fuel cycle. Experimental verification of the theoretical prediction.

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Electronic Supplementary Information (ESI)

Synthetic protocols.

2-Bromo-4,*N*-diethylaniline.

To a solution of 4,*N*-diethylaniline (10.62 g, 0.071 mol) in glacial acetic acid (40 mL), bromine (11.4 g, 0.071 mol) in glacial acetic acid (15 mL) was added dropwise. The solution was stirred for 1 h at room temperature and adjusted to pH 11 - 12 with 20% KOH. After cooling, the mixture was extracted with dichloromethane (3 × 80 mL); the organic extracts were dried over potassium carbonate and evaporated. The residue was distilled in oil-pump vacuum collecting the main fraction (108 - 110 °C, 3 mm Hg) to yield 12.85 g (79 %) of compound **5** as a yellowish oily liquid which becomes dark when left to stand in air.

^{1}H NMR ($CDCl_3$): 7.27 (s, 1H), 7.01 (d, 1H), 6.58 (d, 1H), 4.06 (br. s, 1H), 3.19 (m, 2H), 2.54 (m, 2H), 1.31 (m, 3H), 1.21 (m, 3H).

^{13}C NMR ($CDCl_3$): 143.06 133.69, 131.77, 127.81, 111.31, 109.55, 38.63, 27.59, 15.85, 14.76.

MS (ESI): *m/z* 228.03 (calcd. for $[C_{10}H_{14}BrN + H]^+$ 228.03).

$C_{10}H_{14}BrN$. Calculated: C, 52.65; H, 6.19; Br, 35.03; N, 6.14

Found: C, 52.63; H, 6.25; Br, 34.99; N, 6.23

2-Bromo-4-hexyl-*N*-ethylaniline (1).

To a solution of 4-hexyl-*N*-ethylaniline (25 g, 0.122 mol) in glacial acetic acid (100 mL), bromine (19.5 g, 0.122 mol) in glacial acetic acid (40 mL) was added dropwise with stirring. The resulting dark-brown solution was stirred for 1 h at room temperature and adjusted to pH 11-12 with 20% KOH. After

cooling, the mixture was extracted with dichloromethane (3 x 100 ml); the organic extracts were dried over potassium carbonate and evaporated. The residue was distilled in oil-pump vacuum collecting the main fraction to yield 26.3 g (76 %) of compound **1** as a yellowish oily liquid which becomes dark in air.

^{1}H NMR ($CDCl_3$): 7.30 (s, 1H), 7.04 (d, 1H), 6.61 (d, 1H), 4.10 (br. s, 1H), 3.17 (m, 2H), 2.54 (t, 2H), 1.59 (m, 2H), 1.38 (m, 8H), 0.87 (t, 3H).

^{13}C NMR ($CDCl_3$): 143.09, 132.31, 132.11, 128.25, 111.23, 109.56, 38.59, 34.63, 31.69, 31.51, 28.83, 22.55, 14.72, 13.96.

MS (ESI): *m/z* 284.10 (calcd. for $[C_{14}H_{22}BrN + H]^+$ 284.10).

$C_{14}H_{22}BrN$. Calculated: C, 59.16; H, 7.80; Br, 28.11; N, 4.93. Found: C, 58.51; H, 7.48; Br, 29.77; N, 4.55

2-Bromo-4,*N*-di-*n*-hexylaniline (2)

To a solution of 4,*N*-di-*n*-hexylaniline (12.32 g, 0.047 mol) in glacial acetic acid (80 mL), bromine (7.55 g, 0.047 mol) in glacial acetic acid (20 mL) was added dropwise. The mixture was stirred for 1 h, diluted three-fold with water, and neutralized with 40% aqueous KOH. The resulting mixture was extracted with dichloromethane (3 × 100 mL); the extract was dried over potash and evaporated. The residue was distilled in vacuo (155-164 °C, 0.1 mbar) to yield 12.94 g (80.6%) of compound **2** as a yellowish oily liquid which becomes dark on storage.

^{1}H NMR ($CDCl_3$): 7.31 (s, 1H), 7.17 (m, 1H), 7.05 (d, 1H), 3.23 (m, 2H), 2.50 (m, 2H), 1.73 (m, 2H), 1.57 (m, 4H), 1.34 (m, 14H), 0.89 (m, 6H).

^{13}C NMR ($CDCl_3$): 133.47, 132.59, 132.48, 130.36, 128.45, 128.34, 52.20, 35.29, 31.59, 31.46, 31.00, 28.86, 27.43, 26.66, 26.35, 22.57, 14.08, 14.00.

MS (ESI): *m/z* 340.16 (calcd. for $[C_{18}H_{30}BrN+ H]^+$ 262.25).

$C_{18}H_{30}BrN$. Calculated: C 63.52 %; H 8.88 %; N 4.12 %; Br 23.48 %

Found: C 63.38 %; H 8.62 %; N 4.17 %; Br 24.00 %

N,N´-Diethyl-N,N´-di(2-bromo-4-ethylphenyl)-pyridine-2,6-dicarboxamide (3).

Anhydrous triethylamine (30 mL) and DMAP (0.2 g) were added to a solution of 2-bromo-4,N-diethylaniline (12.85 g, 0.056 mol) in dry dichloromethane (120 mL). The mixture was cooled on ice bath and a solution of pyridine-2,6-dicarboxylic acid dichloride (5.22 g, 0.026 mol) in dry dichloromethane (30 mL) was added dropwise. The cooling bath was removed and the mixture was

stirred for one day at room temperature. Then it was washed twice with 10% HCl, once with 5% KOH, and once with water. The organic phase was dried over potassium carbonate and evaporated. The resulting viscous oil was dissolved in a minimum amount of dichloromethane–petroleum ether 40/70 (1: 1) and chromatographed on a silica gel column (h = 12 cm, d = 10 cm, 300 g). The starting amine was eluted first with the same mixture until it disappeared in the extracts (TLC control). The product was eluted with ethyl acetate (TLC control). The ethyl acetate extracts were evaporated. The resulting product was dried in oil-pump vacuum for 6 h at 90 °C to yield 9.27 g (61.7 %) of compound **3** as a dark heavy oil which slowly crystallizes when left to stand.

^{1}H NMR (DMSO-d6): 7.92-7.02 (m, 8H), 6.80 (d, 1H), 4.06 (m, 2H), 3.38 (m, 2H), 3.20 (s, 2H), 2.61 (dd, 1H), 2.51 (m, 1H), 1.12 (m, 12H), 0.84 (t, 2H).

^{13}C NMR (DMSO-d6): 166.72, 166.56, 164.60, 155.03, 153.60, 152.66, 152.20, 146.02, 145.89, 145.82, 138.76, 138.38, 137.03, 132.68, 132.43, 132.28, 132.20, 132.05, 131.92, 127.79, 123.64, 123.03, 122.71, 62.32, 44.10, 43.81, 27.73, 24.88, 15.55, 15.39, 15.29, 15.16, 14.28, 13.95, 12.79, 12.58.

MS (MALDI-TOF+): m/z 586 (calcd. for $[C_{27}H_{29}Br_2N_3O_2 + H]^+$ 586).

$C_{27}H_{29}Br_2N_3O_2$ Calculated: C, 55.21; H, 4.98; Br, 27.21; N, 7.15

Found: C, 55.21; H, 5.07; Br, 26.35; N, 7.18

The product was used for the synthesis of compound 2 without further purification.

N,N´-Diethyl-N,N´-di(2-bromo-4-n-hexylphenyl)-pyridine-2,6-dicarboxamide (4).

This compound was prepared as described above for N,N´-Diethyl-N,N´-di(2-bromo-4-ethylphenyl)-pyridine-2,6-dicarboxamide starting from 4-n-hexyl-2-bromo-N-ethylaniline (21.36 g, 0.075 mol) and pyridine-2,6-dicarboxylic acid dichloride (6.67 g, 0.033 mol) as a dark heavy oil (16.58 g, 72.4%).

^{1}H NMR (DMSO-d6), 50 °C: 7.92-6.99 (m, 8H), 6.76 (d, 1H), 4.21 (m, 1H), 4.08 (dd, 1H), 3.98 (dd, 1H), 3.52 (m, 1H), 3.33 (ddd, 1H), 3.18 (s, 2H), 2.58 (m, 1H), 1.65-1.55 (br. s, 1H), 1.55-1.37 (br. s, 4H), 1.37-1.00 (m, 20H), 0.93-0.72 (m, 8H).

^{13}C NMR 150 MHz, (DMSO-d6) , 50 °C: 166.91, 152.11, 144.20, 138.45, 138.36, 136.98, 135.90, 135.86, 132.55, 132.48, 132.40, 131.89, 131.25, 127.83, 127.56, 126.72, 125.02, 124.04, 123.17, 123.06, 122.76, 122.46, 43.92, 34.98, 31.34, 30,72, 29.53, 28.68, 22.20, 13.90, 12.20.

MS (MALDI-TOF+): m/z 720 (calcd. for $[C_{35}H_{45}Br_2N_3O_2 + Na]$+ 720).

$C_{35}H_{45}Br_2N_3O_2$ Calculated: C, 60.09 %; H, 6.48 %; Br, 22.84 %; N, 6.01 %.

Found: C, 59.55 %; H, 6.22 %; Br, 22.78 %; N, 6.30 %.

N,N´-Di(*n*-hexyl)-N,N´-di(2-bromo-4-*n*-hexylphenyl)-pyridine-2,6-dicarboxdiamide (5).

This compound was prepared as described above for N,N´-diethyl-N,N´-di(2-bromo-4-n-hexylphenyl)-pyridine-2,6-dicarboxamide, starting from pyridine-2,6-dicarboxylic acid dichloride (3.22 g, 0.016 mol) and 2-bromo-4,*N*-di(n.hexyl)aniline (12.85 g, 0.038 mol). The yield of a dark heavy oil was 10.03 g (78.3%).

^{1}H NMR ($CDCl_3$), 600 MHz: 7.49 (m, 1H), 7.40 (m, 1H), 7.33 (m, 2H), 7.20 (m, 2H), 7.02 (m 1H), 6.92 (m, 1H) 6.77 (m, 1H), 4.24 (m, 1H), 4.14 (m, 1H), 3.34 (m, 1H), 3.27 (m, 1H), 2.51 (m, 4H), 2.14 (broad s, 2H), 1.60 (m, 8H), 1.29 (m, 24H), 0.87 (m, 10H).

^{13}C NMR ($CDCl_3$), 600 MHz: 167.08, 152.24, 144.28, 138.57, 136.31, 132.78, 132.59, 132.06, 131.65, 127.74, 123.32, 123.19, 122.66, 122.55, 49.36, 49.21, 35.13, 31.68, 31.63, 31.58, 30.87, 30.84, 28.90, 27.23, 27.13, 26.70, 26.67, 22.64, 22.55, 14.06.

MS (MALDI-TOF+): *m/z* 832 (calcd. for $[C_{43}H_{61}Br_2N_3O_2 + Na]^+$ 832).

$C_{43}H_{61}Br_2N_3O_2$ Calculated: C 63.62 %; H 7.57 %; N 5.18 %; Br 19.69%

Found: C 63.64 %; H 7.38 %; N 5.06 %; 19.56 %

2,5,9,12-Tetraethylbenzo[f]quinolino[3,4-b][1,7]naphthyridine-6,8(5H,9H)-dione monohydrate (V).

A mixture of **3** (7.40 g, 0.013 mol), potassium acetate (2.50 g, 0.025 mol), tetrabutylammonium bromide (8.13 g, 0.025 mol), and palladium acetate (0.37 g, 13 mol.% of the starting diamide) in anhydrous DMF (370 mL) was stirred in argon atmosphere for 16 h at 110 °C, diluted with water (0.7 L), and extracted with dichloromethane (3 × 100 mL). The organic extracts were washed with water, dried over potassium carbonate, and evaporated. The dry residue was suspended in ethyl acetate (50 mL) and filtered. The filter residue was washed with ethyl acetate (2 x 30 mL) and diethyl ether (2 x 40 mL), dried in oil-pump vacuum for 6 h at 90-100 °C to yield 3.57 g of compound **V** (64%) as a light-yellow powder, m.p. in under Ar sealed capillary 392 °C (with decomposition).

^{1}H NMR (CDCl3): 9.33 (s, 2H), 8.18 (s, 3H), 7.41 (d, 2H), 7.30 (d, 2H), 4.36 (s, 6H), 2.73 (s, 4H), 1.66 (s, 4H), 1.32 (m, 18H), 0.85 (s, 6H).

^{13}C NMR (CDCl3): 158.51, 141.46, 137.46, 135.62, 131.82, 131.24, 132.96, 116.99, 115.21, 38.08, 35.34, 31.73, 31.70, 29.02, 22.58, 14.05, 12.56.

MS (MALDI-TOF+): m/z 426 (calcd. for [$C_{27}H_{27}N_3O_2$ + H]+ 426).

HRMS (ESI): m/z 426.2174 (calcd. for [$C_{27}H_{27}N_3O_2$ + H]+ is 426.2182),

m/z 448.1991 (calcd. for [$C_{27}H_{27}N_3O_2$ + Na]+ is 448.2001),

m/z 873.4093 (calcd. for [($C_{27}H_{27}N_3O_2$)$_2$ + Na]+ is 873.4104).

$C_{27}H_{27}N_3O_2$ Calculated: C, 73.11; H, 6.59; N, 9.47

Found: C, 73.05 %; H, 6.05 %; N, 9.28 %

5,9-Diethyl-2,12-di(n-hexyl)benzo[f]quinolino[3,4-b][1,7]naphthyridine-6,8(5H,9H)-dione monohydrate (VI).

This compound was prepared using the synthesis protocol described above for compound **V** with slight modifications. A mixture of N,N´-diethyl-N,N´-di(2-bromo-4-n-hexylphenyl)-pyridine-2,6-dicarboxamide (**4**) (14.20 g, 0.020 mol), potassium acetate (3.96 g, 0.040 mol), tetrabutylammonium bromide (13.06 g, 0.040 mol), and palladium acetate (0.592 g, 13 mol.% based on the starting diamide) in anhydrous DMF (700 mL) was stirred for 18 h in an inert atmosphere at 110 °C. Then the mixture was cooled, diluted with water (1.5 L), and extracted with dichloromethane (3 × 500 mL). The organic extracts were washed with water three times, dried over potassium carbonate, and evaporated. The dry residue was stirred in ethyl acetate (70 mL) and filtered off. The filter residue was washed with ethyl acetate (2 × 30 mL) and diethyl ether (2 × 40 mL) and dried in oil-pump vacuum for 6 h at 90-100°C to yield compound **VI** (6.5 g, 58 %) as a light-yellow powder, m.p. in under Ar sealed capillary 322 °C (with decomposition).

^{1}H NMR (CDCl3): 9.33 (s, 2H), 8.18 (s, 3H), 7.41 (d, 2H), 7.30 (d, 2H), 4.36 (s, 6H), 2.73 (s, 4H), 1.66 (s, 4H), 1.32 (m, 18H), 0.85 (s, 6H).

^{13}C NMR (CDCl3) 150 MHz: 158.51, 141.46, 137.46, 135.62, 131.82, 131.24, 132.96, 116.99, 115.21, 38.08, 35.34, 31.73, 31.70, 29.02, 22.58, 14.05, 12.56.

MS (MALDI-TOF+): m/z 538 (calcd. for [$C_{35}H_{43}N_3O_2$ + H]+ 538).

HRMS (ESI): m/z 538.3423 (calcd. for [$C_{35}H_{43}N_3O_2$ + H]+ is 538.3434),

m/z 560.3241 (calcd. for [$C_{35}H_{43}N_3O_2$ + Na]+ is 560.3253)

$C_{35}H_{43}N_3O_2$ Calculated: C, 75.64 %; H, 8.16 %; N, 7.56 %.

Found: C, 75.21 %; H, 8.18 %; N, 7.24 %.

This compound is well soluble in polar organic solvents (DMSO, DMFA, CH2Cl2), moderately soluble in benzene and ethyl acetate, but insoluble in acetonitrile, diethyl ether, and aliphatic hydrocarbons.

Complex of 2,5,9,12-tetrahexylbenzo[f]quinolino[3,4-b][1,7]naphthyridine-6,8(5H,9H)-dione with lanthanum nitrate (VIII).

A mixture of compound dilactam (**VII**) (100 mg, 0.150 mmol) and lanthanum nitrate hexahydrate $La(NO_3)_3 \times 6H_2O$ (30.8 mg, 0.071 mmol) was refluxed in acetonitrile (4 mL) for 2 h in argon atmosphere. After cooling, the mixture was filtered and the filter residue was washed with diethyl ether (3 × 5 mL) to yield 96.8 mg (84%) of the 2 : 1 complex $(VII)_2La(NO_3)_3$ as a bright-yellow powder, m.p. in under Ar sealed capillary 295°C (with decomposition).

^{1}H NMR (CDCl3), 600 MHz: 9.75 (s, 2H), 8.63 (s, 4H), 7.61 (s, 4H), 7.43 (s, 4H), 4.33 (s, 8H), 2.91 (s, 8H), 1.68 (m, 16H), 1.27 (m, 54H), 0.82 (m, 28H).

^{13}C NMR (CDCl3), 150 MHz: 162.46, 140.58, 138.61, 133.39, 133.16, 132.52, 127.15, 124.98, 116.62, 116.26, 43.81, 34.87, 31.27, 30.90, 28.49, 26.89, 26.08, 22.14, 21.94, 13.62, 13.45.

MS (MALDI-TOF+): The mass-spectrum displays a fragment ion $[(VII)_2La(NO_3)_2]$+ m/z 1562 , calcd. for $[C_{86}H_{118}N_8O_{10}La]^+$ 1562).

$C_{86}H_{118}LaN_9O_{13}$. Calculated: C 63.57 %; H 7.32 %; N 7.76 %; La 8.55%

Found: C 63.49 %; H 7.12 %; N 7.65 %; La 8.57 %

This compound is well soluble in polar (DMSO, DMFA) and chlorinated ($CHCl_3$, CH_2Cl_2) organic solvents, but is insoluble in diethyl ether, acetonitrile, and hexane.

Quantun chemical calculations details.

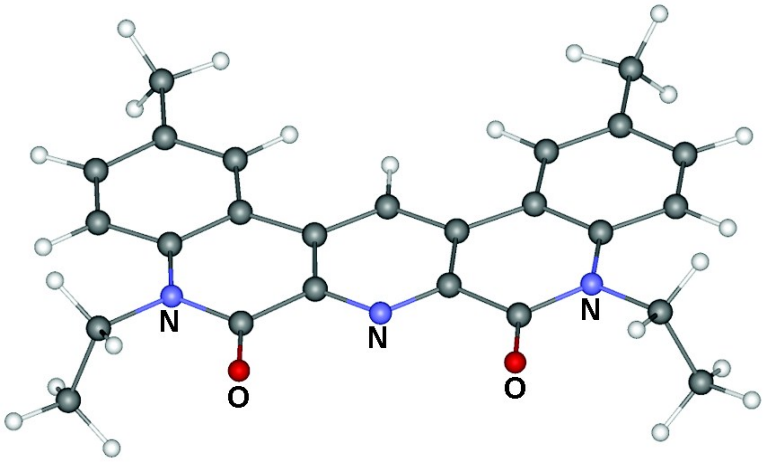
Table 1. Total energies (E in hartree or au), Gibbs energies (G in kcal/mol) and binding energies (E^b and G^b in kcal/mol).

Sructures	E	G	E^b	G^b
IV	-1280.665548	225.5	-	-
IX	-12969.430982	240.0	51.9	34.7

X	-32541.938632	240.2	54.3	36.9
XIII	-14250.110770	482.8	60.9	27.4
XIV	-33822.618809	482.6	63.5	29.2
XV	-14250.123691	481.6	69.0	35.7
XVI	-13969.636783	477.3	172.0	139.4
XVII	-33542.146152	476.8	176.2	144.7

Atomic cartesian coordinates

Dilactam **IV**



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6	-0.24715490	-0.82894240	0.89012698
6	0.53419306	-0.21923380	-0.09814860
6	-0.05426803	0.53860274	-1.11713424
6	-1.46917607	0.65415912	-1.08831851
7	-2.23393053	0.08508580	-0.15680281
6	-2.20934456	1.43841901	-2.12266739
8	-3.41980279	1.58012845	-2.12454973
7	-1.40426551	2.01257658	-3.13258686
6	-0.01216207	1.93569925	-3.16366598
6	-2.14439658	2.75116560	-4.17210659
7	-1.97459144	-2.03516515	2.79213714

1	1.61733958	-0.33790509	-0.07490757
6	0.69795195	1.20074989	-2.17596553
8	-3.79573843	-1.08866454	1.76599951
6	-0.59679926	-2.21047770	2.91768285
6	-2.90707519	-2.66411220	3.74541738
6	0.29884807	-1.62828155	1.98022464
6	0.72867255	2.58436122	-4.17563843
6	2.10264107	1.14028747	-2.25624185
6	1.68129883	-1.84379739	2.14037625
6	-0.05479108	-2.96975634	3.97762267
1	-2.55718890	-3.68668061	3.95214020
6	-3.09054615	-1.84716547	5.02577455
1	-3.86463394	-2.72463739	3.20899931
1	-3.78947357	-2.36745855	5.70009235
1	-2.14023073	-1.69684002	5.56052122
1	-3.51631979	-0.86224121	4.78338980
1	-1.68708236	2.53142393	-5.14854001
1	-3.15746083	2.32479482	-4.15697169
6	-2.21964268	4.25380879	-3.89512472
1	-2.77535794	4.75237319	-4.70538315
1	-2.75422037	4.43397757	-2.95072755
1	-1.22138419	4.71248626	-3.82635304
6	2.11148409	2.49826891	-4.21848815
1	0.21741255	3.17231572	-4.93650562
6	2.83337492	1.76979629	-3.25708748
1	2.65002357	0.57360302	-1.49912573
6	4.33782113	1.68596495	-3.31507295
1	2.64803513	3.01572248	-5.01970267
1	4.67569631	1.23661576	-4.26371414
1	4.79594944	2.68673379	-3.24637621
1	4.73561385	1.07492046	-2.49095540
6	1.31319202	-3.15854233	4.09758221

1	-0.71142620	-3.41240786	4.72521430
6	2.21646402	-2.59960596	3.17684898
1	2.37168175	-1.39837241	1.42002293
6	3.70229224	-2.81373251	3.31913581
1	1.69266118	-3.75353974	4.93397737
1	4.06747620	-2.44358037	4.29154495
1	3.95784629	-3.88494398	3.26068143
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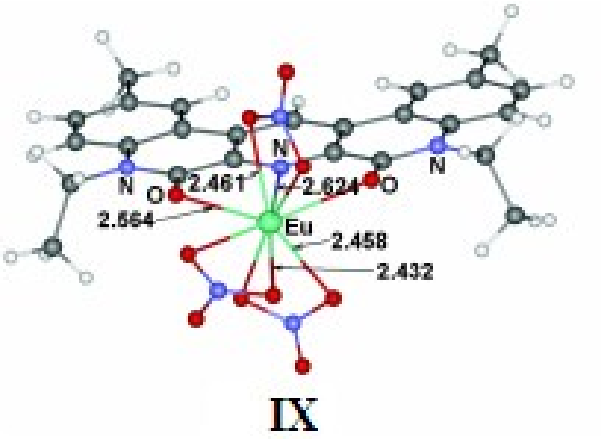
Energy = -1280.66554997

Complex **IX**



IX

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6	1.70627221	-0.36029251	-0.07031387
6	1.10711322	0.37388534	-1.10514697
6	-0.30472210	0.45739870	-1.08988052
7	-1.05812225	-0.11440628	-0.15240210
6	-1.07611263	1.16484220	-2.12827964
8	-2.31277625	1.19280441	-2.10730841
7	-0.34303022	1.77289194	-3.12883486
6	1.05996054	1.76569556	-3.15581158

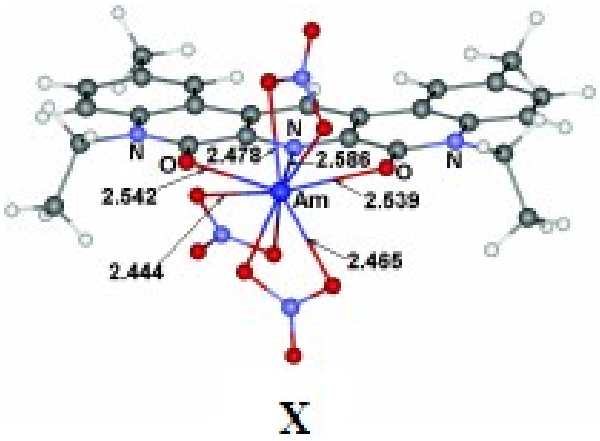
6	-1.13471560	2.47425688	-4.16739223
7	-0.87278185	-2.20766303	2.76428941
1	2.79217603	-0.44758496	-0.03219534
6	1.81392404	1.06260424	-2.17401527
8	-2.64790831	-1.34191844	1.59669886
6	0.51357688	-2.34465292	2.94611179
6	-1.84097775	-2.83721098	3.69398369
63	-3.64408860	0.32684342	-0.09467454
8	-2.69738671	2.57787312	0.31604734
8	-3.23997170	1.40209545	2.07805140
7	-2.77936568	2.51785717	1.60895374
8	-2.43653397	3.43693844	2.32794281
8	-5.03400665	-1.66619100	-0.23486990
8	-3.34229670	-1.57896775	-1.62181928
7	-4.35114105	-2.25581130	-1.16594913
8	-4.63478988	-3.36322935	-1.57885159
8	-5.24043684	1.37828808	-1.58022886
8	-5.85456793	1.14218736	0.50821930
7	-6.17210586	1.53186199	-0.68685532
8	-7.25616799	2.00917579	-0.95173896
6	1.43769343	-1.76700066	2.03075265
6	1.75704505	2.45867842	-4.16491212
6	3.21947728	1.06901578	-2.26417177
6	2.81608815	-1.95802414	2.24715638
6	1.02025146	-3.06432253	4.04558020
1	-1.45579064	-3.83102869	3.96336738
6	-2.12528104	-1.96448931	4.91552059
1	-2.76055774	-2.97592552	3.10888319
1	-2.85633899	-2.47309825	5.56329050
1	-1.21634847	-1.76642998	5.50399561
1	-2.55849170	-1.00236311	4.60168140
1	-0.64634071	2.30625751	-5.13803494

1	-2.10936985	1.96704565	-4.18294641
6	-1.32464009	3.95711262	-3.85181367
1	-1.92760197	4.42335352	-4.64666810
1	-1.86544250	4.07485189	-2.90032007
1	-0.36557681	4.49283516	-3.78111372
6	3.14179507	2.44087628	-4.21619824
1	1.21166682	3.02925268	-4.91488927
6	3.90769507	1.73926202	-3.26761504
1	3.79896232	0.52748153	-1.51261321
6	5.41231893	1.72599796	-3.34562162
1	3.64632446	2.99276773	-5.01468720
1	5.81754456	2.75097140	-3.34773748
1	5.85357411	1.18700750	-2.49429259
1	5.75533421	1.23672975	-4.27236005
6	2.38512495	-3.22681746	4.22314893
1	0.34128614	-3.49538693	4.77952514
6	3.31740527	-2.68061902	3.32267250
1	3.52652881	-1.51771603	1.54344663
6	4.79719226	-2.87289029	3.53050436
1	2.73991584	-3.79163008	5.09017923
1	5.11293459	-2.48175057	4.51151506
1	5.06417706	-3.94226187	3.50347966
1	5.38173431	-2.35724330	2.75443718

$end

Energy = -12969.43098318

Complex **X**



X

6	-1.40469094	-1.37178249	1.80544810
6	-0.46685729	-0.77725385	0.85259564
6	0.92890076	-0.97462594	0.92620941
6	1.70996178	-0.36251299	-0.06769701
6	1.10675051	0.39400584	-1.08741121
6	-0.29974409	0.51214915	-1.05060722
7	-1.05855552	-0.03942412	-0.09564554
6	-1.06507627	1.22711500	-2.07770409
8	-2.30717127	1.26688561	-2.04682923
7	-0.34113947	1.82730257	-3.08735992
6	1.06046213	1.79522065	-3.13377903
6	-1.13585651	2.53095789	-4.12133446
7	-0.86837607	-2.13962389	2.81614963
1	2.79312972	-0.47881568	-0.05111437
6	1.81157878	1.07297106	-2.16358421
8	-2.63403053	-1.19296503	1.69198856
6	0.51521065	-2.32840732	2.96450059
6	-1.83936910	-2.74087124	3.76049308
95	-3.61434131	0.35494216	-0.06628656
8	-2.68644403	2.57643503	0.38517149
8	-3.54279547	1.52634622	2.10180325

7	-2.98141002	2.60441507	1.65863160
8	-2.73760121	3.56252175	2.36008003
8	-4.86363675	-1.72072642	-0.20822053
8	-3.22148084	-1.51918269	-1.63919474
7	-4.19126375	-2.25503465	-1.18765062
8	-4.45096227	-3.35149313	-1.63443254
8	-5.24898313	1.06656642	-1.73735746
8	-5.89294989	1.08882389	0.35720434
7	-6.21520994	1.28081739	-0.89144659
8	-7.32032641	1.63636350	-1.23326042
6	1.43626196	-1.77619567	2.02957064
6	1.75695108	2.47765016	-4.15022620
6	3.21597030	1.05213959	-2.27313840
6	2.81200101	-2.01686014	2.21315087
6	1.02161140	-3.07283314	4.04744577
1	-1.48378587	-3.74946413	4.01531711
6	-2.06896489	-1.87033932	4.99507682
1	-2.77512540	-2.84351865	3.19375987
1	-2.79785801	-2.36339859	5.65719709
1	-1.14041075	-1.70315915	5.56204910
1	-2.48307626	-0.89418380	4.69964033
1	-0.65832388	2.35306153	-5.09558647
1	-2.11584012	2.03389266	-4.12575969
6	-1.30616518	4.01791952	-3.81353709
1	-1.91083040	4.48637909	-4.60580725
1	-1.83601400	4.14823863	-2.85758086
1	-0.34029018	4.54268165	-3.75507948
6	3.14029366	2.43281210	-4.22004022
1	1.21272034	3.06095091	-4.89134778
6	3.90375456	1.71267043	-3.28325580
1	3.79430565	0.49656410	-1.53113126
6	5.40699714	1.67233152	-3.37890494

1	3.64547491	2.97700790	-5.02337294
1	5.83334748	2.68834785	-3.34549450
1	5.84584360	1.09201486	-2.55389851
1	5.73056682	1.21303810	-4.32759897
6	2.38367343	-3.28373868	4.19188836
1	0.34505943	-3.48505705	4.79450428
6	3.31256369	-2.76351217	3.27232880
1	3.52022762	-1.59758418	1.49460603
6	4.78931174	-3.00928939	3.44284253
1	2.73910208	-3.86633345	5.04679156
1	5.13969762	-2.65029750	4.42436540
1	5.01964910	-4.08613674	3.38747942
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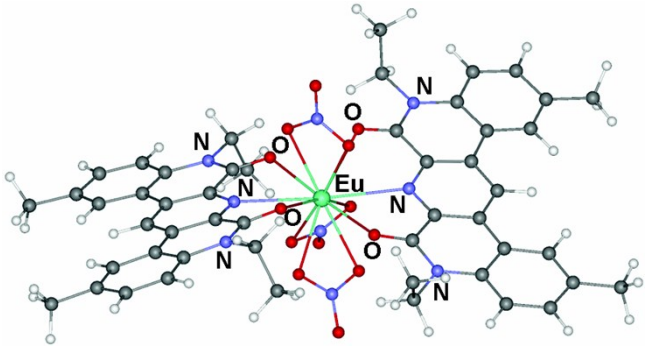
Energy = -32541.93862990

Complex **XIII**



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6	-2.76739289	0.61915837	2.08189218
6	-3.33633043	0.99727028	0.77292496
6	-4.55976720	1.69893781	0.66093528
6	-5.03530300	1.93290410	-0.63472490
6	-4.34023014	1.45258511	-1.75146916
6	-3.13075916	0.75921685	-1.50288801

7	-2.63452744	0.57266485	-0.27930043
6	-2.34598650	0.13728930	-2.59232283
8	-1.37324289	-0.58394945	-2.37709807
7	-2.77620763	0.41447434	-3.88734249
6	-3.96940582	1.08558795	-4.17412661
6	-1.89332302	-0.07388174	-4.96675586
7	-3.45015501	1.07227951	3.20516775
1	-5.96645071	2.48132972	-0.77562103
6	-4.77760012	1.61452212	-3.13104634
8	-1.75656065	-0.07719219	2.17960111
6	-4.65442087	1.78129114	3.13693452
6	-2.83235191	0.72794873	4.50249131
6	-5.23378019	2.11696721	1.88272287
6	-4.40841725	1.23935579	-5.50532044
6	-5.97087661	2.28082334	-3.47025210
6	-6.44107908	2.84113851	1.86692589
6	-5.32768862	2.17152514	4.31253617
1	-2.94381808	1.59240711	5.17330567
6	-3.40166416	-0.55616000	5.10575312
1	-1.76308390	0.59583120	4.28409011
1	-2.91337261	-0.75678194	6.07262864
1	-4.48788884	-0.48880185	5.27228109
1	-3.19896758	-1.40722015	4.43817621
1	-1.91328625	0.66694121	-5.77877123
1	-0.87862427	-0.07226340	-4.54478981
6	-2.26541342	-1.47520278	-5.45017435
1	-1.58340873	-1.77867297	-6.26033166
1	-2.16641833	-2.19486150	-4.62375611
1	-3.29746779	-1.51771857	-5.83188104
6	-5.58870710	1.90507714	-5.79621440
1	-3.82596335	0.82269130	-6.32564827
6	-6.39827798	2.44609576	-4.78204012

1	-6.59233099	2.69023390	-2.67021013
6	-7.67558588	3.17418412	-5.11506924
1	-5.89527992	2.00306462	-6.84194529
1	-8.34738593	2.54331781	-5.72005488
1	-8.21630738	3.47005270	-4.20370612
1	-7.47073703	4.08735692	-5.69854054
6	-6.51540961	2.88361267	4.25261295
1	-4.92277433	1.90793376	5.28844226
6	-7.09906714	3.23989652	3.02424350
1	-6.88349014	3.10752104	0.90399211
6	-8.38698683	4.02185483	2.97583399
1	-7.00736990	3.16904365	5.18729081
1	-9.19065530	3.49852690	3.51963339
1	-8.26723157	5.01326344	3.44363575
1	-8.72247321	4.17555021	1.93937211
6	2.40769907	-0.08268898	2.65262068
6	3.18223889	-0.75944980	1.58823458
6	4.57560046	-0.98495055	1.69871347
6	5.18682619	-1.69557521	0.65833263
6	4.43221938	-2.19207175	-0.41080192
6	3.04593328	-1.90948083	-0.39692440
7	2.45545676	-1.18158233	0.55236774
6	2.12371821	-2.45759021	-1.41240550
8	0.90527487	-2.29574285	-1.34267815
7	2.70653770	-3.19570234	-2.43769978
6	4.08317195	-3.42472586	-2.53223169
6	1.77265686	-3.68628126	-3.47258126
7	3.14417256	0.39489684	3.73497124
1	6.26081911	-1.87771394	0.68966385
6	4.97204252	-2.95822751	-1.52558493
8	1.18337993	0.02992054	2.59881263
6	4.52835097	0.23313736	3.85490194

6	2.37255689	1.11637983	4.77055397
6	5.27309649	-0.46456455	2.86578319
6	4.62149004	-4.13458337	-3.62499474
6	6.34571070	-3.24031532	-1.65085069
6	6.66049015	-0.62351465	3.04765262
6	5.21772331	0.74835951	4.97223202
1	2.71836497	0.77221194	5.75761598
6	2.45364329	2.63597237	4.61575143
1	1.33611890	0.77830939	4.63337370
1	1.86354499	3.11220953	5.41503181
1	3.48873473	3.00350952	4.68696463
1	2.03869567	2.95296678	3.64551173
1	2.08044058	-4.70037290	-3.76776096
1	0.79734925	-3.75348946	-2.97066522
6	1.68138866	-2.72694397	-4.65961906
1	0.94771887	-3.10924268	-5.38689474
1	1.34976026	-1.73731648	-4.30869885
1	2.64969358	-2.60658236	-5.16954327
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1	3.97013420	-4.48520014	-4.42410379
6	6.87723288	-3.95002745	-2.72089988
1	7.03023719	-2.88187395	-0.87825859
6	8.35392494	-4.23233149	-2.83141993
1	6.36048610	-4.94312051	-4.57534048
1	8.77872839	-3.77441187	-3.74015388
1	8.90270110	-3.83522531	-1.96447838
1	8.54834363	-5.31604402	-2.88965971
6	6.58499596	0.57105819	5.11256310
1	4.67930204	1.30290622	5.73891153
6	7.34046094	-0.12286231	4.15103773
1	7.23398074	-1.16175427	2.28921525
6	8.82790228	-0.30352826	4.31643556

1	7.08312110	0.98670089	5.99363472
1	9.34561094	0.66975726	4.34321612
1	9.06285217	-0.82488558	5.25908550
1	9.25369189	-0.89026857	3.48882848
7	0.77925454	1.29791879	-2.37044758
8	1.02517678	1.84019854	-3.44577568
8	-0.16718986	1.71441826	-1.60252851
8	1.42172813	0.26705743	-1.95932061
7	-1.10046667	-2.83469510	0.96008494
8	-1.54367912	-3.91818797	1.32347211
8	-1.68103821	-2.12685212	0.05805126
8	-0.02699883	-2.33386962	1.45744433
7	0.77029539	2.49865473	1.09954073
8	1.12518529	3.58231657	1.56392881
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8	1.60181046	1.71279680	0.50891093

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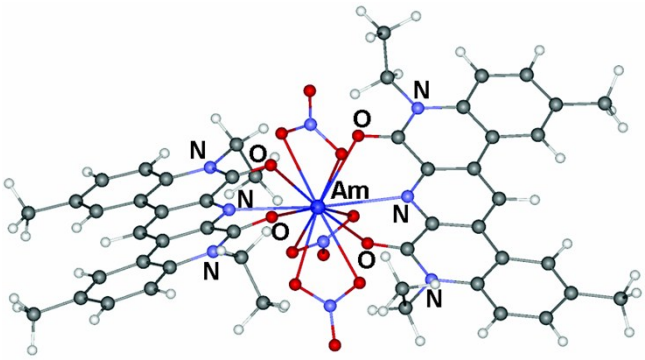
Energy = -14250.11077822

Complex XIV



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6	-5.01068468	1.94386712	-0.63321925
6	-4.31738901	1.46072740	-1.74986521
6	-3.11091582	0.76302198	-1.50237560
7	-2.60975620	0.57917420	-0.27875760
6	-2.33936711	0.12441794	-2.58858631
8	-1.36233740	-0.59290873	-2.36891849
7	-2.78630450	0.36843382	-3.88320358
6	-3.96970491	1.05699888	-4.17044796
6	-1.93141581	-0.16704039	-4.96281504
7	-3.43885253	1.06011670	3.20654640
1	-5.94390098	2.48865756	-0.77311164
6	-4.75870616	1.61673489	-3.12889968
8	-1.72179689	-0.05252485	2.18213416
6	-4.64383105	1.76844055	3.13838489
6	-2.83251010	0.69749389	4.50456069
6	-5.21298482	2.11904939	1.88377465
6	-4.41628647	1.19950974	-5.50021849
6	-5.93882901	2.30579221	-3.46891783
6	-6.41817558	2.84691380	1.86748625
6	-5.32613112	2.14375518	4.31341911
1	-2.95438960	1.55034308	5.18819974
6	-3.40399865	-0.59818680	5.08042697
1	-1.76059621	0.57243523	4.29544563
1	-2.92736324	-0.81179864	6.05027272
1	-4.49251892	-0.53735413	5.23383167
1	-3.18922060	-1.43805092	4.40246924
1	-1.93694421	0.55773759	-5.78935243
1	-0.91323213	-0.19142755	-4.55085311
6	-2.35299249	-1.56571594	-5.41257408
1	-1.69137798	-1.90681236	-6.22464123
1	-2.26594789	-2.27161264	-4.57297940
1	-3.39060366	-1.58397863	-5.78075352

6	-5.58420216	1.88639407	-5.79191313
1	-3.84909405	0.75935814	-6.31891015
6	-6.37263617	2.46135199	-4.77980959
1	-6.54296924	2.74331117	-2.67053642
6	-7.63489125	3.21455729	-5.11441120
1	-5.89676412	1.97597973	-6.83660778
1	-8.32974859	2.58783965	-5.69725423
1	-8.15689360	3.54438193	-4.20381513
1	-7.41379855	4.10888431	-5.72059797
6	-6.51226008	2.85869174	4.25301656
1	-4.93024738	1.86628514	5.28917535
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1	-6.85215611	3.12679306	0.90459942
6	-8.36877080	4.02045851	2.97568630
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1	-9.17671411	3.49732822	3.51324379
1	-8.24652547	5.00851723	3.44991545
1	-8.69945062	4.18187349	1.93886348
6	2.41358276	-0.06386064	2.65270496
6	3.18564796	-0.74356157	1.59534730
6	4.57592471	-0.97512311	1.70769856
6	5.19063129	-1.68795480	0.66739175
6	4.43407861	-2.17897353	-0.40460290
6	3.04984708	-1.89602194	-0.39146612
7	2.45373165	-1.16481514	0.55770466
6	2.13177470	-2.43275258	-1.40503524
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7	2.70203728	-3.15966006	-2.44065459
6	4.07718277	-3.40012938	-2.53372030
6	1.76531988	-3.62130379	-3.48630695
7	3.14136264	0.40086611	3.74476912
1	6.26322698	-1.87563598	0.70224467

6	4.96760875	-2.94450971	-1.52256841
8	1.18857792	0.06617510	2.58507293
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6	2.36346289	1.11407324	4.78044254
6	5.26986999	-0.45973265	2.87862606
6	4.61095829	-4.10967944	-3.62844959
6	6.33942775	-3.23674169	-1.64789107
6	6.65705363	-0.62002424	3.06351923
6	5.21167108	0.74710613	4.98983674
1	2.71299168	0.77313194	5.76705612
6	2.43156284	2.63451391	4.62708251
1	1.32968374	0.76787420	4.64388927
1	1.83253445	3.10596881	5.42248388
1	3.46308415	3.01073646	4.70387564
1	2.02023983	2.94683349	3.65421989
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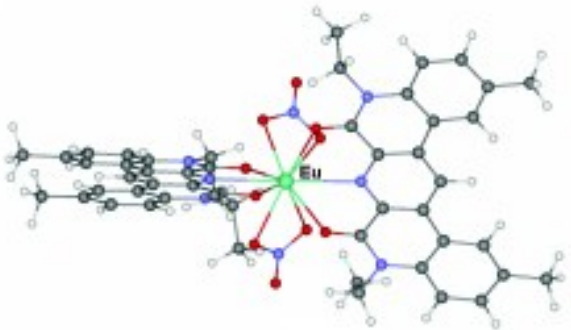
1	0.78647645	-3.67923350	-2.99040916
6	1.69815473	-2.64441069	-4.66069138
1	0.95870476	-3.00118199	-5.39512898
1	1.38872376	-1.65186991	-4.29764815
1	2.67033835	-2.53932853	-5.16647658
6	5.96879090	-4.37452344	-3.71415631
1	3.95762918	-4.45249260	-4.42942077
6	6.86659917	-3.94556669	-2.72057894
1	7.02515396	-2.88708869	-0.87238261
6	8.34100809	-4.24035777	-2.82951611
1	6.34526279	-4.92703471	-4.58024263
1	8.76698073	-3.80133117	-3.74691024
1	8.89450536	-3.83265327	-1.97053193
1	8.52742364	-5.32640823	-2.86948902
6	6.57874742	0.56843140	5.13254914
1	4.67225221	1.30030906	5.75697267

6	7.33500482	-0.12313233	4.16983725
1	7.23150128	-1.15609967	2.30434596
6	8.82233974	-0.30416704	4.33664002
1	7.07573581	0.98124699	6.01556629
1	9.34040867	0.66905823	4.35983821
1	9.05675170	-0.82199073	5.28135886
1	9.24809663	-0.89417313	3.51134539
7	0.75428750	1.32939358	-2.41799143
8	1.03844210	1.84476271	-3.49400890
8	-0.19281318	1.76500297	-1.66952229
8	1.37792169	0.28162451	-1.98175915
7	-1.09872081	-2.81297531	0.98035565
8	-1.60818167	-3.87092461	1.31722008
8	-1.62484563	-2.06991714	0.05004432
8	-0.02552698	-2.34955634	1.50308856
7	0.79994804	2.48353216	1.02598011
8	1.18713611	3.55928744	1.46628979
8	-0.41002842	2.07919980	1.14211254
8	1.60215546	1.66453440	0.42459113

$end

Energy = -33822.61881777

*Complex **XVI***



XVI

63	-0.00013000	-0.00217870	-0.00989286

6	-2.35121308	1.50624952	1.92918440
6	-3.23839057	1.02777526	0.85784436
6	-4.63474201	1.25934237	0.86257602
6	-5.36845205	0.71217074	-0.19970250
6	-4.73204278	-0.02564549	-1.20770871
6	-3.32851583	-0.16714377	-1.10171813
7	-2.61407539	0.34724125	-0.10176947
6	-2.53093260	-0.92218475	-2.07778977
8	-1.29561472	-1.02342570	-1.95745976
7	-3.21766557	-1.51062534	-3.11506617
6	-4.61504891	-1.41111449	-3.25786074
6	-2.40512855	-2.29669194	-4.07357298
7	-2.93612489	2.26097452	2.92243426
1	-6.44829789	0.85387316	-0.23690276
6	-5.39548261	-0.66324801	-2.33377463
8	-1.13720347	1.24025025	1.92934001
6	-4.31983825	2.51102911	2.97693490
6	-2.02251846	2.77987969	3.96656467
6	-5.19257133	2.02937447	1.96260205
6	-5.26999451	-2.05424027	-4.32486725
6	-6.78697002	-0.57718449	-2.53502267
6	-6.56844715	2.31619004	2.05923593
6	-4.87123934	3.24177996	4.04625365
1	-2.34525367	3.79886966	4.22291884
6	-1.94926482	1.86655315	5.18967300
1	-1.03691413	2.84794336	3.48592618
1	-1.26532182	2.30600092	5.93244979
1	-2.93327357	1.73067126	5.66341808
1	-1.56014919	0.87836349	4.90114428
1	-2.78595622	-2.09688739	-5.08542173
1	-1.39060850	-1.88193456	-4.00190025
6	-2.38743233	-3.78778294	-3.73951926

1	-1.78039092	-4.32137234	-4.48735770
1	-1.93280667	-3.95333168	-2.75079970
1	-3.39756764	-4.22397009	-3.73798202
6	-6.64256753	-1.94636202	-4.48567850
1	-4.70695718	-2.65530548	-5.03693434
6	-7.43481553	-1.19919619	-3.59509610
1	-7.38827741	0.00208011	-1.83057887
6	-8.92382957	-1.08974264	-3.79171104
1	-7.11622362	-2.46038071	-5.32693206
1	-9.39483345	-2.08612051	-3.79800082
1	-9.39260959	-0.49593552	-2.99364846
1	-9.15951161	-0.61107780	-4.75630200
6	-6.23148503	3.50195925	4.10374008
1	-4.23574699	3.60715333	4.85128441
6	-7.11411409	3.04701341	3.10714929
1	-7.24070041	1.95218003	1.27889348
6	-8.58799784	3.34603979	3.18565887
1	-6.62301174	4.07335049	4.95021791
1	-9.01699370	2.97146961	4.12915334
1	-8.77146916	4.43252621	3.15219759
1	-9.13744741	2.88274346	2.35332343
6	2.39055236	-0.77493515	2.28150684
6	3.25662910	-0.68894765	1.09562078
6	4.65361038	-0.90946783	1.15290006
6	5.36632837	-0.75463099	-0.04471340
6	4.70940471	-0.39810530	-1.23081371
6	3.30759383	-0.22544245	-1.15333932
7	2.61279747	-0.37029186	-0.02586914
6	2.48979742	0.15809788	-2.31235349
8	1.25651715	0.29752941	-2.21083745
7	3.15559568	0.35991197	-3.49967165
6	4.55055560	0.21443414	-3.62580552

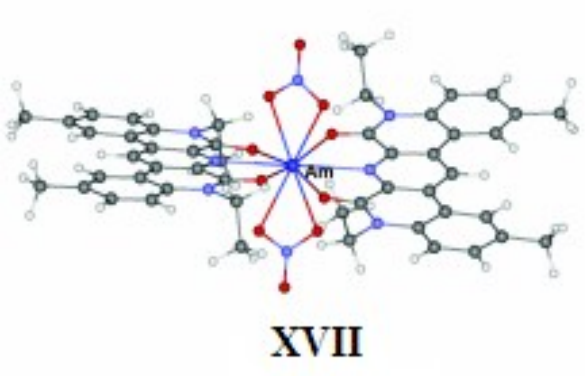
6	2.32314390	0.77883248	-4.65225140
7	2.99570977	-1.15213416	3.46035160
1	6.44581756	-0.90361531	-0.05137779
6	5.35023965	-0.17923037	-2.51772483
8	1.17594063	-0.52052178	2.21384799
6	4.38096664	-1.37354974	3.57093405
6	2.10287641	-1.28507354	4.63480437
6	5.23369006	-1.26497800	2.43796122
6	5.18384880	0.45771375	-4.85902176
6	6.73833155	-0.33081043	-2.70303460
6	6.61195201	-1.50693037	2.60076647
6	4.95381371	-1.70281938	4.81386799
1	2.43275868	-2.15926958	5.21375898
6	2.04992614	-0.01261769	5.47952480
1	1.10874105	-1.50731672	4.22327046
1	1.38056026	-0.17317267	6.33904860
1	3.04207972	0.27103796	5.86209477
1	1.65342461	0.82207111	4.88180378
1	2.68605054	0.24802371	-5.54406731
1	1.31145398	0.41580318	-4.42620789
6	2.30686082	2.29523364	-4.84074682
1	1.68409910	2.54718140	-5.71318343
1	1.87048562	2.78622234	-3.95747375
1	3.31543784	2.70294633	-5.00559941
6	6.55381490	0.29907427	-4.99863395
1	4.60582372	0.78393808	-5.72203709
6	7.36479516	-0.10461575	-3.92235385
1	7.35443624	-0.63899551	-1.85521893
6	8.85060226	-0.27680126	-4.09705156
1	7.01040289	0.49761740	-5.97248180
1	9.31619250	0.65610075	-4.45411373
1	9.33663278	-0.56084690	-3.15240211

1	9.07161213	-1.05811303	-4.84261105
6	6.31567047	-1.93271015	4.93112927
1	4.33404108	-1.77370669	5.70621064
6	7.17872892	-1.84322587	3.82373136
1	7.26880635	-1.42993117	1.73129543
6	8.65484807	-2.10199692	3.97218125
1	6.72416562	-2.18676413	5.91342094
1	9.10228167	-1.42067166	4.71399557
1	8.84089692	-3.13126659	4.32016694
1	9.18545067	-1.96410828	3.01889070
7	0.46178966	2.85475920	-0.37801563
8	0.64716951	4.03822548	-0.59447604
8	-0.60384756	2.24151551	-0.79684547
8	1.29783709	2.12350957	0.27270481
7	-0.45989436	-2.81419035	0.61651402
8	0.59611301	-2.38169811	-0.00387403
8	-0.64570905	-4.00070855	0.81517825
8	-1.28608046	-1.90353275	0.99757841

$end

Energy = -13969.63677029

Complex **XVII**



XVII

95	-0.00001036	0.00131137	-0.00931086

6	-2.32970542	1.53608494	1.90935878
6	-3.21279971	1.04439899	0.84691640
6	-4.60844194	1.27428547	0.84945429
6	-5.34562516	0.70728746	-0.20051213
6	-4.71026770	-0.04705260	-1.19711312
6	-3.30636533	-0.18305229	-1.09617541
7	-2.58583932	0.34946745	-0.10567455
6	-2.51448773	-0.94396355	-2.06554487
8	-1.27499908	-1.03339772	-1.94968386
7	-3.19926255	-1.55076734	-3.09243712
6	-4.59735392	-1.46365190	-3.22752440
6	-2.38492530	-2.34242795	-4.04482910
7	-2.90724281	2.31003660	2.88993091
1	-6.42558633	0.84663389	-0.23672811
6	-5.37606096	-0.70642071	-2.30920758
8	-1.11448034	1.26019326	1.91513534
6	-4.28980195	2.56486395	2.94095403
6	-1.98955679	2.84341118	3.92344625
6	-5.16360536	2.06487084	1.93627410
6	-5.25513427	-2.12754300	-4.28006938
6	-6.76963165	-0.63287650	-2.50217370
6	-6.53903438	2.35584668	2.02869036
6	-4.83854755	3.31725898	3.99646387
1	-2.30920371	3.86735463	4.16319720
6	-1.91714384	1.95066775	5.16169490
1	-1.00464396	2.90137553	3.44014858
1	-1.22787687	2.39904482	5.89413994
1	-2.90027698	1.82933082	5.64112614
1	-1.53509342	0.95525179	4.88921659
1	-2.77602378	-2.16231507	-5.05645077
1	-1.37441825	-1.91582428	-3.98829595
6	-2.34855633	-3.82800125	-3.68831135

1	-1.74142460	-4.36622571	-4.43268282
1	-1.88528863	-3.97389717	-2.70052898
1	-3.35405557	-4.27450312	-3.67305202
6	-6.62929344	-2.03101796	-4.43286722
1	-4.69280830	-2.73587235	-4.98657025
6	-7.42034618	-1.27543646	-3.54800944
1	-7.37021101	-0.04733829	-1.80234060
6	-8.91159861	-1.18051945	-3.73492113
1	-7.10539692	-2.56088466	-5.26282995
1	-9.37721204	-2.17899592	-3.70177767
1	-9.37653133	-0.56155002	-2.95390845
1	-9.15850825	-0.73757790	-4.71359862
6	-6.19821378	3.58062552	4.04996955
1	-4.20143529	3.69738460	4.79340180
6	-7.08232066	3.10753653	3.06295705
1	-7.21263212	1.97879275	1.25577570
6	-8.55578867	3.40950255	3.13779519
1	-6.58817837	4.16930344	4.88523648
1	-8.98752995	3.03658850	4.08080588
1	-8.73696346	4.49626029	3.10298818
1	-9.10434422	2.94625628	2.30485023
6	2.36763628	-0.80533993	2.27283870
6	3.23012695	-0.70436554	1.09116266
6	4.62593849	-0.92654761	1.14595892
6	5.34260159	-0.75050311	-0.04680113
6	4.68767837	-0.37342729	-1.22779096
6	3.28572258	-0.20439299	-1.15338686
7	2.58453660	-0.36818865	-0.02850619
6	2.47487982	0.18889641	-2.30823245
8	1.23762163	0.31803208	-2.20696375
7	3.13958990	0.41059788	-3.49177442
6	4.53496319	0.27505220	-3.61484369

6	2.30676614	0.83991410	-4.64025309
7	2.96463905	-1.20584363	3.44641532
1	6.42188036	-0.89932058	-0.05339359
6	5.33162975	-0.13176839	-2.50905472
8	1.15213990	-0.53855354	2.20703467
6	4.34834837	-1.43498857	3.55547741
6	2.06729509	-1.35548802	4.61565621
6	5.20247562	-1.30718499	2.42543912
6	5.17206296	0.54096019	-4.84149768
6	6.72137964	-0.27364068	-2.69102569
6	6.57981257	-1.55664859	2.58560083
6	4.91794231	-1.78972388	4.79284488
1	2.39333264	-2.24005995	5.18075835
6	2.01601323	-0.09726360	5.48151987
1	1.07372543	-1.56866268	4.19807485
1	1.34126746	-0.26945744	6.33455808
1	3.00757787	0.17431069	5.87416985
1	1.62702979	0.74969375	4.89635531
1	2.67819038	0.32697583	-5.53897244
1	1.29768642	0.46365751	-4.42464375
6	2.27684781	2.35894112	-4.80460338
1	1.65526907	2.61871867	-5.67557694
1	1.83254104	2.83190961	-3.91549129
1	3.28229565	2.77830177	-4.95893473
6	6.54318897	0.39094900	-4.97763340
1	4.59593676	0.87850202	-5.70147688
6	7.35151563	-0.02594244	-3.90414094
1	7.33573828	-0.59113258	-1.84540841
6	8.83856495	-0.18997929	-4.07599376
1	7.00306225	0.60725197	-5.94613351
1	9.30014415	0.74562316	-4.43110871
1	9.32429961	-0.47332145	-3.13096934

1 9.06482345 -0.96922196 -4.82225872

6 6.27880545 -2.02621857 4.90737675

1 4.29652766 -1.87525867 5.68281208

6 7.14346767 -1.91840905 3.80269634

1 7.23829035 -1.46530732 1.71879325

6 8.61810027 -2.18748956 3.94747566

1 6.68532367 -2.30014334 5.88512170

1 9.06304060 -1.54204976 4.72201668

1 8.79930672 -3.23217651 4.24932608

1 9.15431219 -2.00837359 3.00423497

7 0.44822735 2.86152927 -0.39008563

8 0.63146509 4.04601089 -0.58216281

8 -0.61158663 2.24139688 -0.82215302

8 1.28766971 2.11551144 0.25580476

7 -0.44614021 -2.81867890 0.60408168

8 0.60387042 -2.38366044 -0.03048986

8 -0.62911501 -3.99805527 0.82560011

8 -1.27619886 -1.89606172 0.97575834

$end

Energy = -33542.14614990

Determination of solvate numbers

Table 2. The distribution factors D for different solvent

	C(lig) M	0,001	0,002	0,003	0,004	0,005
PhMe	D(Am)	0,3	0,9	1,8	3,1	4,3
	D(Eu)	0,03	0,1	0,21	0,35	0,55
$CHCl_3$	D(Am)	4	16	36	61	94
	D(Eu)	0,5	2	6	9	15
PhCl	D(Am)	5,5	19	39	67	109
	D(Eu)	0,5	2	4	7	9
$C_2H_4Cl_2$	D(Am)	14,4	55	118	225	337
	D(Eu)	2,9	12	30	50	96
CyOH	D(Am)	28,7	87	166	264	377
	D(Eu)	3,1	9	18	29	41
F-3	D(Am)	119,9	226	327	426	522

	D(Eu)	5,8	12	18	24	30
$PhNO_2$	D(Am)	131,8	289	456	631	813
	D(Eu)	7,9	16	25	34	43

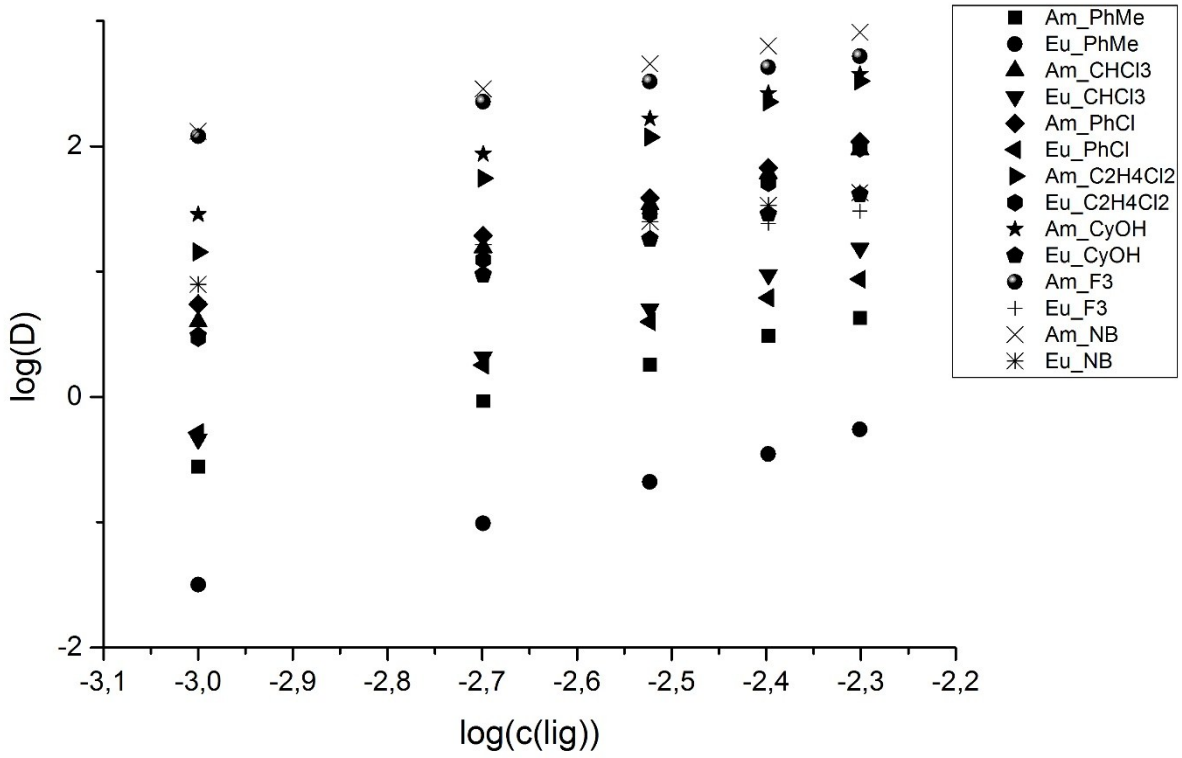


Fig.1. lg(D)/lg [C] plots