Supporting Information

Ciprofloxacin derived task specific ionic liquid as highly selective extractant of thorium *versus* uranium

David Lledó,[a] Guillermo Grindlay,[b] H. Q. Nimal Gunaratne,[c] Abel de Cózar,[d,e] Ana Sirvent,[f] and José M. Sansano.[f]*

[a] Medalchemy, S. L. Ancha de Castelar, 46-48, entlo. A. San Vicente del Raspeig, 03690-Alicante (Spain).
[b] Department of Analytical Chemistry, Nutrition and Food Sciences, University of Alicante, PO Box 99, 03080 Alicante, Spain.
[c] The QUILL Research Centre, School of Chemistry and Chemical Engineering, the Queen's University of Belfast, Stranmillis Road, Belfast, Northern Ireland, BT9 5AG, UK.
[d] Departamento de Química Orgánica I/Kimika Organikoa I Saila, Facultad de Química/Kimika Fakultatea, Universidad del País Vasco/Euskal Herriko Unibertsitatea (UPV/EHU) and Donostia International Physics Center (DIPC), and Centro de Innovación en Química Avanzada (ORFEO-CINQA) P. K, 1072, 20018 San Sebastián-Donostia, Spain
[e] Ikerbasque, Basque Foundation for Science, Plaza Euskadi 5, 48009, Bilbao, Spain
[f] Departamento de Química Orgánica, Centro de Innovación en Química Avanzada (ORFEO-CINQA) and Institute of Orga-nic Synthesis. Universidad de Alicante. Ctra. Alicante-San Vicente s/n, 03080-Alicante, Spain.

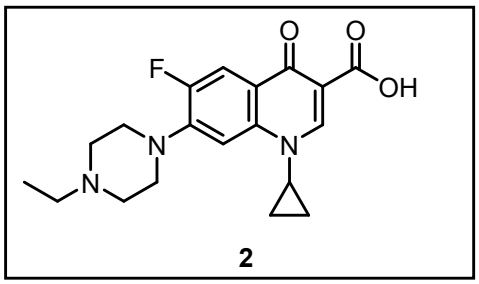
Contents:

1. General Remarks.

Reagents and solvents were purchased from commercial suppliers and used as received. Low-resolution mass spectra (EI) were obtained with an Agilent GC/MS5973N spectrometer at 70 eV; and fragment ions in *m/z* with relative intensities (%) in parentheses. High-resolution mass spectra (HRMS) were also carried out in the electron impact mode (EI) at 70 eV and on a Finnigan MAT95S spectrometer equipped with a time of flight (TOF) analyzer and the samples were ionized by ESI techniques and introduced through an ultra-high pressure liquid chromatography (UPLC) model. NMR spectra were recorded at 300 or 400 MHz for ^{1}H NMR, at 75 or 100 MHz for ^{13}C NMR and at 282 or 376 MHz for ^{19}F NMR with a Bruker AV300 Oxford or a Bruker AV400 spectrometers, respectively, using $CDCl_3$ as solvent, and TMS as internal standard (0.00 ppm). The data are reported as: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet or unresolved, br s = broad signal, coupling constant(s) in Hz, integration. ^{13}C NMR spectra were recorded with ^{1}H-decoupling at 100 MHz and referenced to $CDCl_3$ at 77.16 ppm. ^{19}F NMR spectra were recorded with ^{1}H-decoupling and referenced to CF_3CO_2H at -76.6 ppm. ICP analyses were recorded in a Perkin Elmer, Model: 7300 DV and the microanalyses obtained using a CHNS Micro TruSpec (LECO) at the General Instrumental Service of the University of Alicante.

2. Synthetic procedures and characterization data for compounds 2, 3 and 4

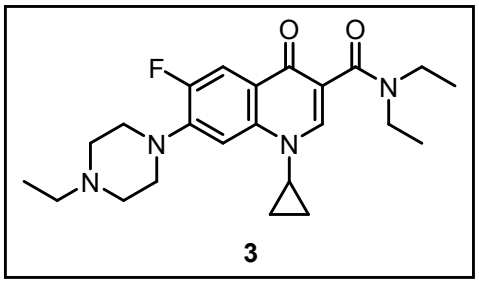
Synthesis of 1-cyclopropyl-7-(4-ethylpiperazin-1-yl)-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid (2): To a solution of ciprofloxacin hydrochloride (3.1 g, 8.0 mmol) and DIPEA (6.7 equiv., 9.3 mL, 6.9 g, 54 mmol) in MeCN:H_2O (1:1, 30 mL/mmol, 240 mL), bromoethane (5.0 equiv., 3.0 mL, 4.4 g, 40 mmol) was added dropwise at 0 ºC. Potassium iodide (10 mol%, 132 mg, 0.8 mmol) was then added at the same temperature. The mixture was stirred at 0 ºC for 1 h and then it was heated to 40 ºC and it was stirred at this temperature for 16 h. The solvent was removed under reduced pressure and the residue was dissolved in DCM (40 mL), washed with a



2

phosphate buffer solution at pH = 6.5 (30 mL) and dried with $MgSO_4$. The solvent was removed under reduced pressure and pure compound **2** was obtained without further purification (2.6 g, 7.4 mmol, 92%) as a white solid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.75 (s, 1H), 7.99 (d, J = 13.1 Hz, 1H), 7.36 (d, J = 7.1 Hz, 1H), 3.58–3.52 (m, 1H), 3.39–3.34 (m, 4H), 2.73–2.65 (m, 4H), 2.52 (q, J = 7.2 Hz, 2H), 1.42–1.32 (m, 2H), 1.22–1.18 (m, 2H), 1.15 (t, J = 7.2 Hz, 3H), *Proton from the carboxylic acid was not observed; ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.2, 167.8, 153.8 (d, J = 252.5 Hz), 147.5, 146.1 (d, J = 10.1 Hz), 139.2, 119.8 (d, J = 8.1 Hz), 112.4 (d, J = 24.2 Hz), 108.2, 104.9, 52.5 (2C), 52.4, 49.9 (2C), 35.4, 12.0, 8.3 (2C); ^{19}F NMR (282 MHz, $CDCl_3$) δ -120.6 (s, 1F); IR (neat) ν_{max} 3420–3395, 1707–1675 cm^{-1}; LRMS (EI) *m/z* 360 (M^++1, 16%), 359 (M^+, 69%), 344 (24), 316 (21), 315 (100), 287 (13), 257 (13), 230 (12), 150 (10), 84 (24), 70 (12), 57 (32), 56 (11), 44 (27), 42 (19); Elemental analysis calcd for $C_{19}H_{22}FN_3O_3$: C, 63.50; H, 6.17; F, 5.29; N, 11.69; O, 13.35. Found: C, 63.3; H, 6.5; N, 11.5.

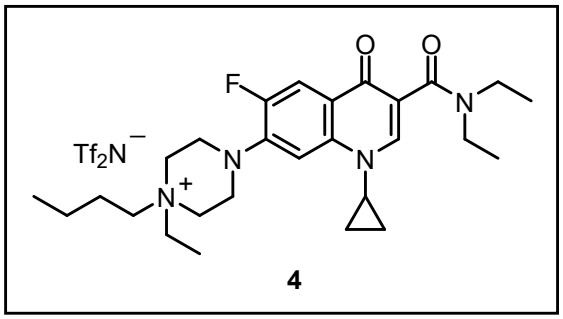
Synthesis of 1-Cyclopropyl-*N*,*N*-diethyl-7-(4-ethylpiperazin-1-yl)-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxamide (3): To a solution of **2** (546 mg, 1.50 mmol) and Et_3N (3.00 equiv, 0.64 mL, 0.45 g, 4.50 mmol) in DCM (5 mL), diethylamine (3.00 equiv., 0.47 mL, 329 mg, 4.50 mmol) and thionyl chloride (1.10 equiv., 0.12 mL, 196 mg, 1.65 mmol) were added dropwise at 0 ºC and the mixture was stirred at this temperature for 30 min. The solvent and the volatile compounds were removed under reduced pressure. The residue was dissolved in $CHCl_3$ (15 mL), washed with a saturated aqueous solution of sodium bicarbonate (3 x 15 mL), then washed again with a saturated aqueous solution of potassium carbonate (2 x 10 mL) and dried with $MgSO_4$. The solvent was removed under reduced pressure and the residue was purified by recrystallization with Et_2O to yield pure compound **3** (590 mg, 1.42 mmol, 95%) as a yellowish solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, J = 13.2Hz, 1H), 7.91 (s, 1H), 7.26 (d, J = 7.1Hz, 1H), 3.55 (q, J = 7.1 Hz, 2H), 3.45–3.25 (m, 7H), 2.81 (br s, 4H), 2.64 (d, J = 7.4Hz, 2H), 1.30–1.20 (m, 8H), 1.14–1.09 (m, 5H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.6, 166.7, 153.8 (d, J = 248.0 Hz), 144.3 (d, J = 11.3 Hz), 142.9, 138.6, 121.8 (d, J = 7.0 Hz), 119.4, 112.7 (d, J = 22.7 Hz), 104.8, 52.4, 49.6 (2C), 43.3 (2C), 39.6 (2C), 34.2, 14.6, 13.1 (2C), 8.3 (2C); ^{19}F NMR (282 MHz, $CDCl_3$) δ -123.7 (s, 1F); LRMS (EI) *m/z* 414 (M^+, 18%), 342 (12), 316 (21),



3

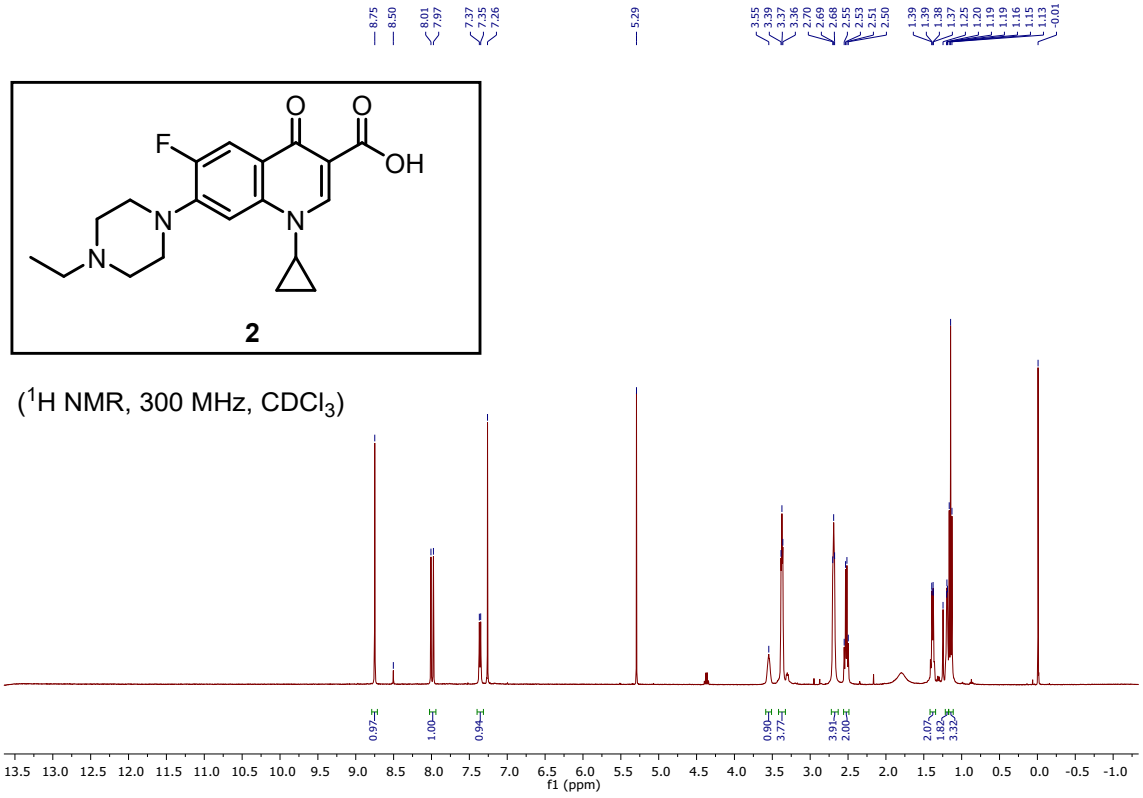
315 (100); Elemental analysis calcd for $C_{23}H_{31}FN_4O_2$: C, 66.64; H, 7.54; F, 4.58; N, 13.52; O, 7.72. Found: C, 68.06; H, 7.84; N, 13.86.

Synthesis of 7-(4-Butyl-4-ethyl-4-((1,1,1-trifluoro-*N*-((trifluoromethyl)sulfonyl)methyl)sulfonamido)-4λ^5-piperazin-1-yl)-1-cyclopropyl-*N*,*N*-diethyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxamide (4): A solution of **3** (207 mg, 0.50 mmol) and iodobutane (2.00 equiv., 0.11 mL, 184 mg, 1.00 mmol) in the minimum amount of MeCN was stirred at 80 ºC for 48 h. The solvent was removed under reduced pressure. The residue was dissolved in $CHCl_3$ (10 mL), an aqueous solution of lithium bistriflamide (1.30 equiv, 1M, 1.3 mL) was added and the mixture was stirred at 25 ºC for 15 h. Then, the aqueous phase was extracted with $CHCl_3$ (3 x 10 mL) and the combined organic fractions were washed with H_2O (2 x 10 mL) and dried with $MgSO_4$. The solvent was removed under reduced pressure and the residue was purified by recrystallization with EtOAc to yield pure compound **4** (330 mg, 0.44 mmol, 89%) as a white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.91 (d, J = 14.3 Hz, 1H), 7.59 (d, J = 7.2 Hz, 1H), 3.91–3.56 (m, 11H), 3.53–3.33 (m, 5H), 2.89–2.57 (m, 2H), 1.79–1.60 (m, 2H), 1.53–1.45 (m, 4H), 1.41–1.34 (m, 3H), 1.26–1.16 (m, 7H), 1.04 (t, J = 7.3 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.6, 167.1, 152.0 (d, J = 247.5 Hz), 141.9 (d, J = 11.0 Hz), 140.9, 138.8, 121.7 (d, J = 6.6 Hz), 120.2 (q, J = 259.0 Hz, 2C), 118.3, 111.6 (d, J = 21.9 Hz), 106.7, 58.4, 57.8 (2C), 52.4, 43.2 (2C), 34.7 (2C), 29.1, 23.4, 19.7, 14.5, 13.6 (2C), 8.2, 7.2 (2C); ^{19}F NMR (282 MHz, $CDCl_3$) δ -77.8 (s, 6F); -125.2 (s, 1F); LRMS (EI) *m/z*: 471 (M^+, 12%), 382 (10), 316 (30), 315 (100). Elemental analysis calcd for $C_{29}H_{40}F_7N_5O_6S_2$: C, 46.33; H, 5.36; F, 17.69; N, 9.32; O, 12.77; S, 8.53. Found: C, 46.8; H, 5.5; N, 9.4; S 8.5.

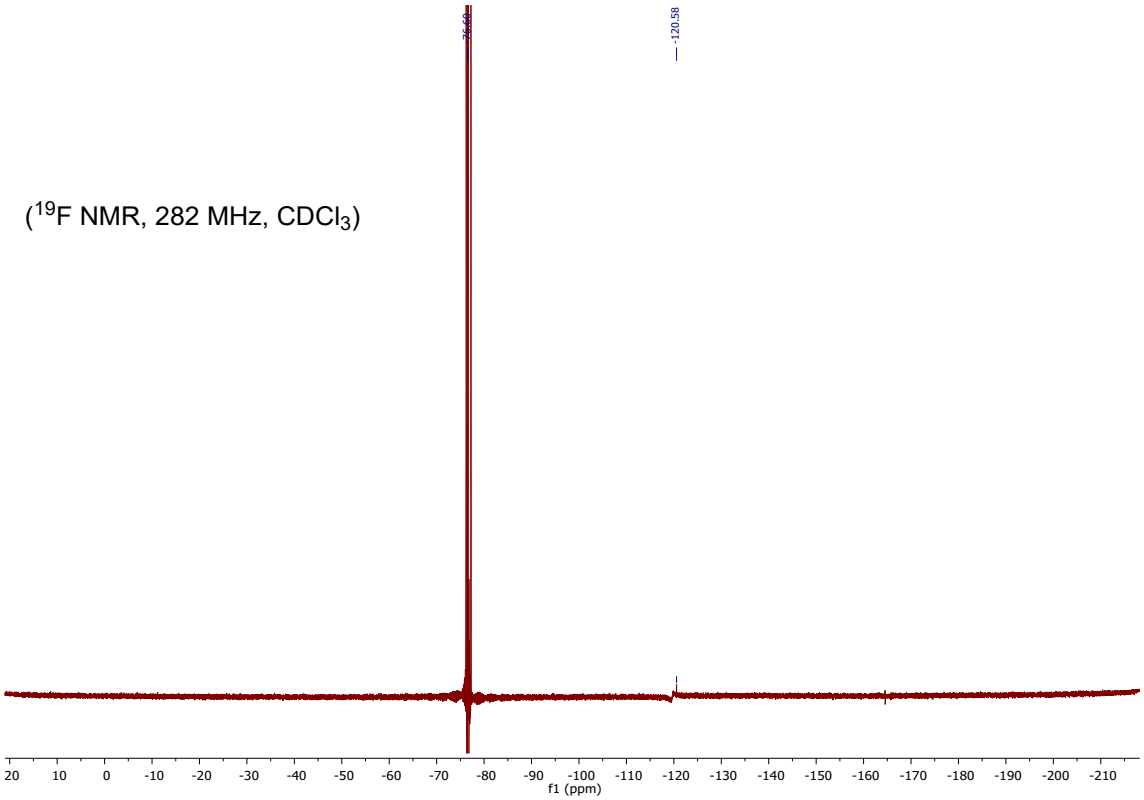


4

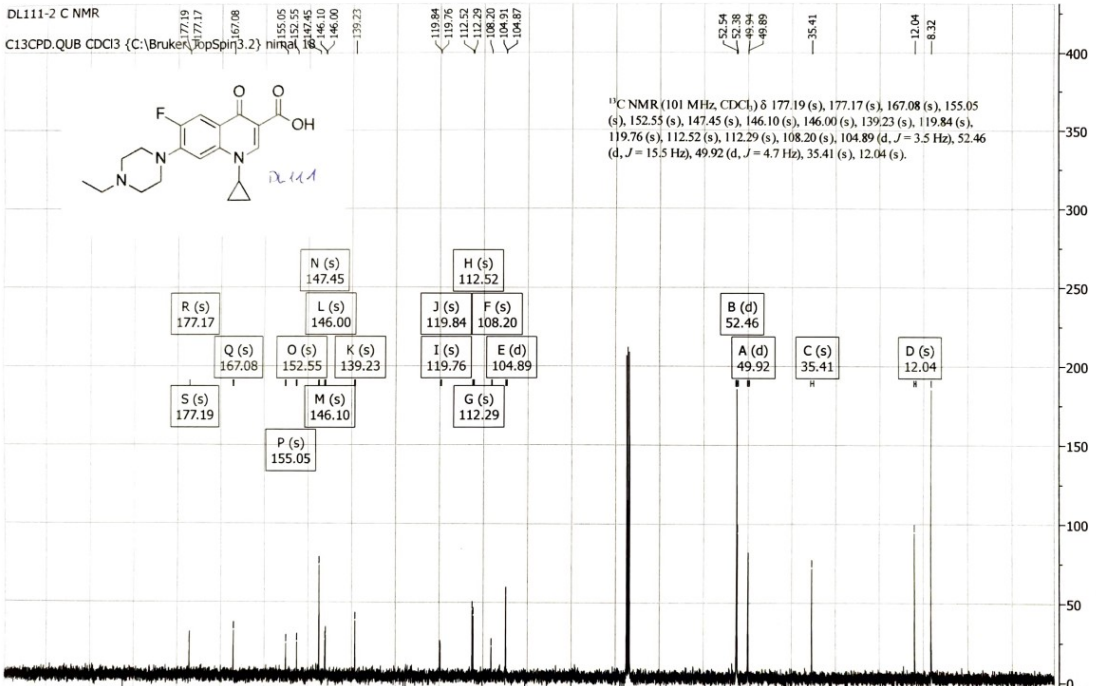
3. ^{1}H-, ^{19}F- and ^{13}C NMR spectra of compounds 2, 3 and 4.

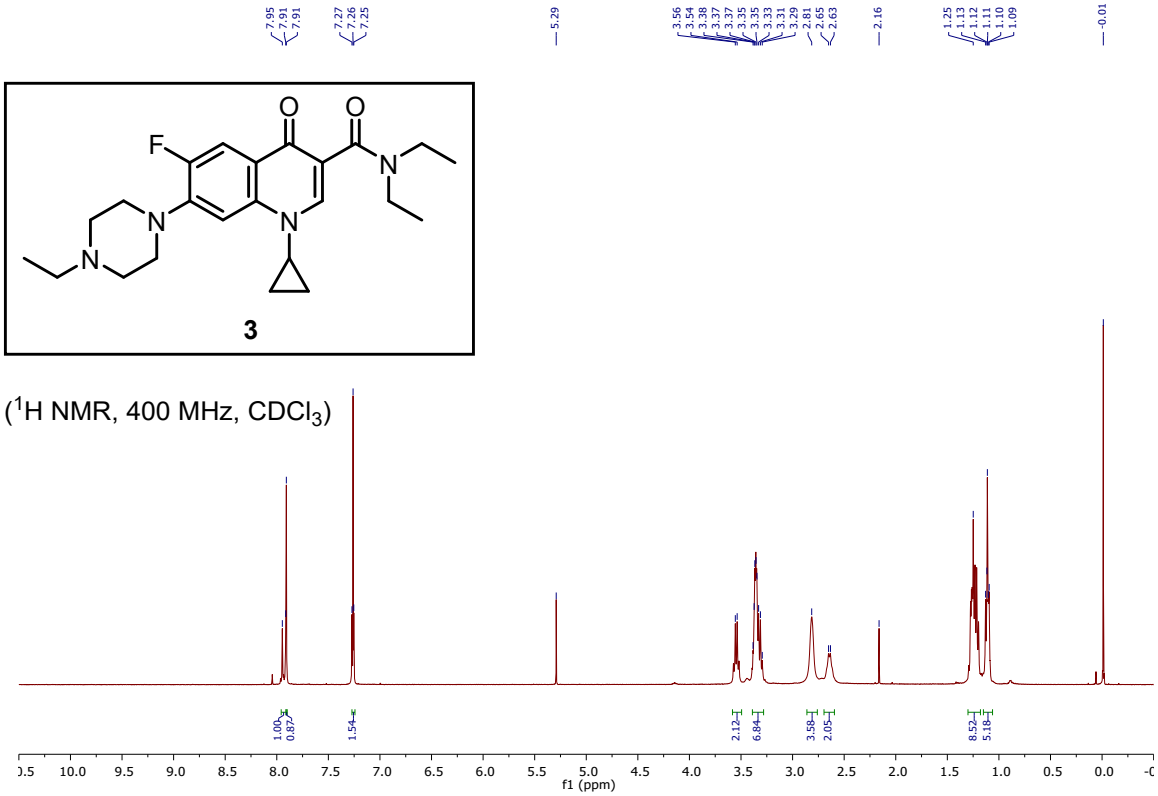


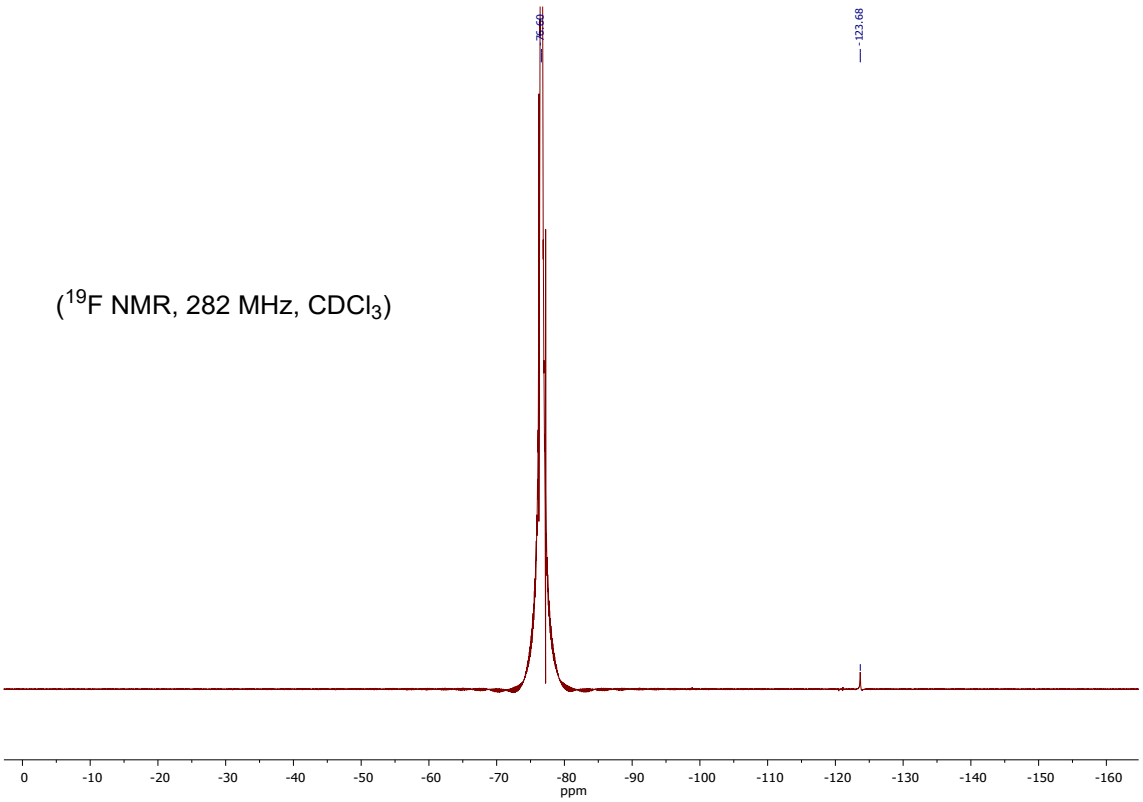
(^{19}F NMR, 282 MHz, $CDCl_3$)

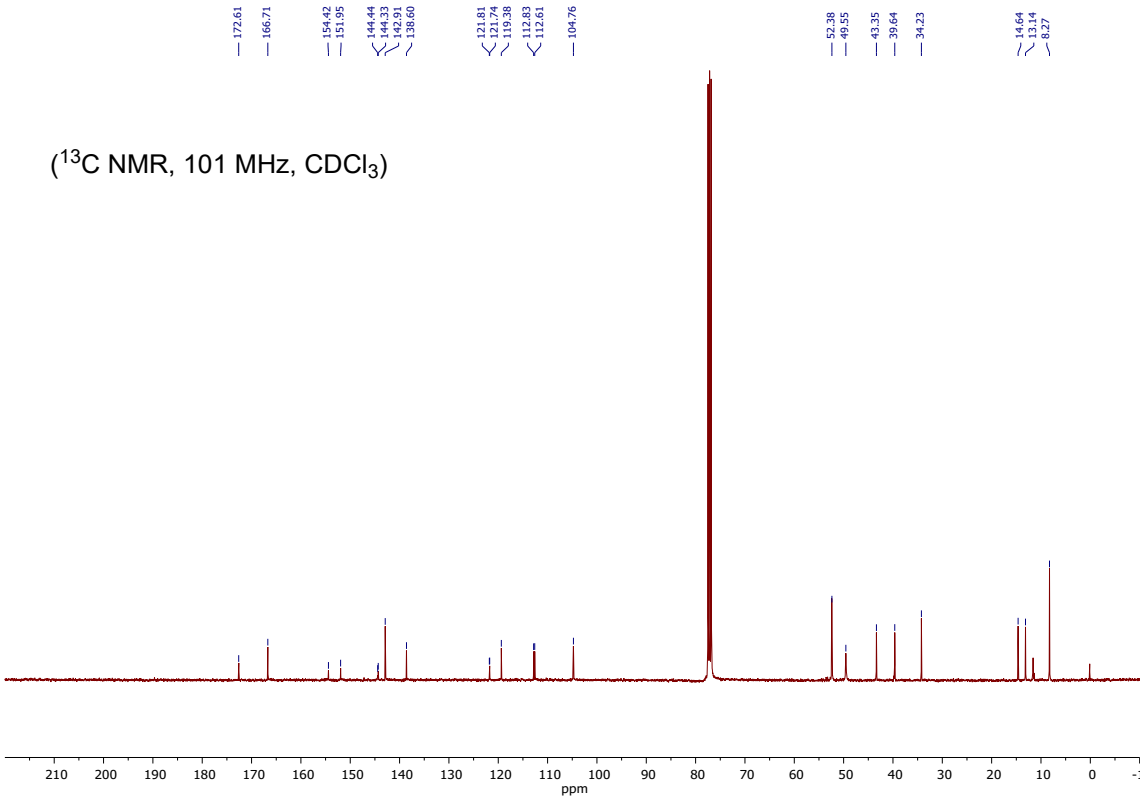


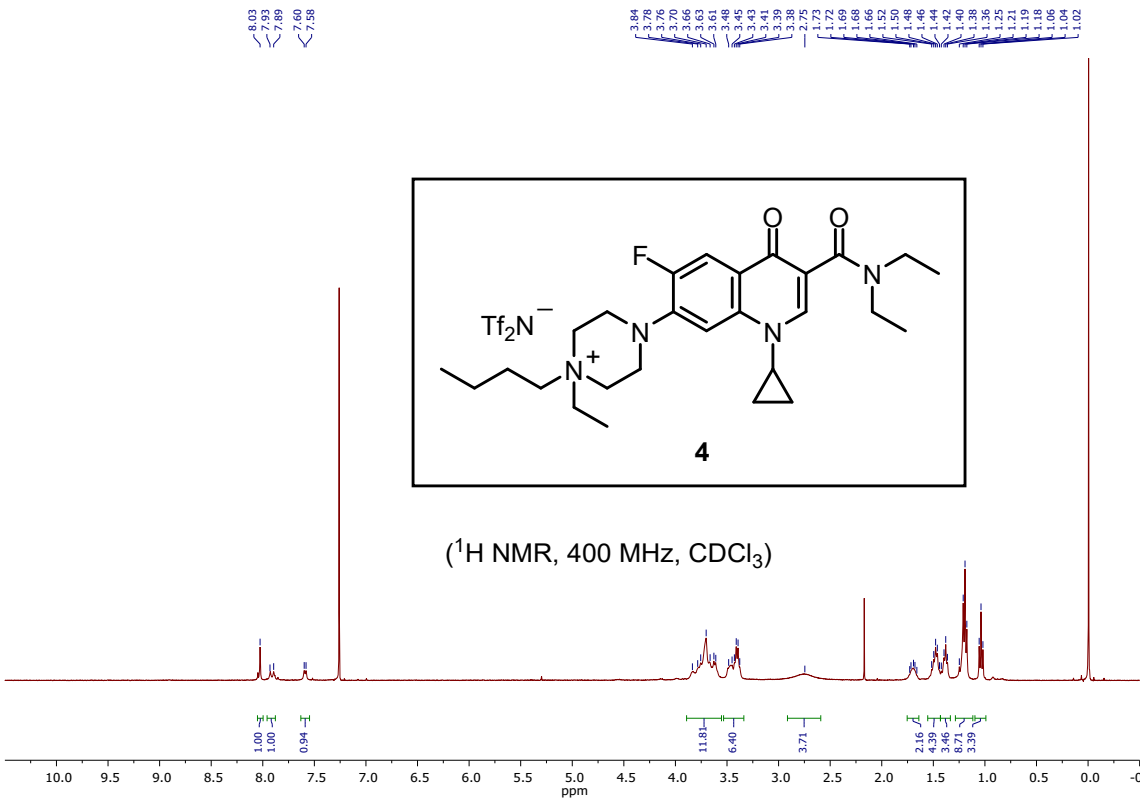
(^{13}C NMR, 101 MHz, $CDCl_3$)



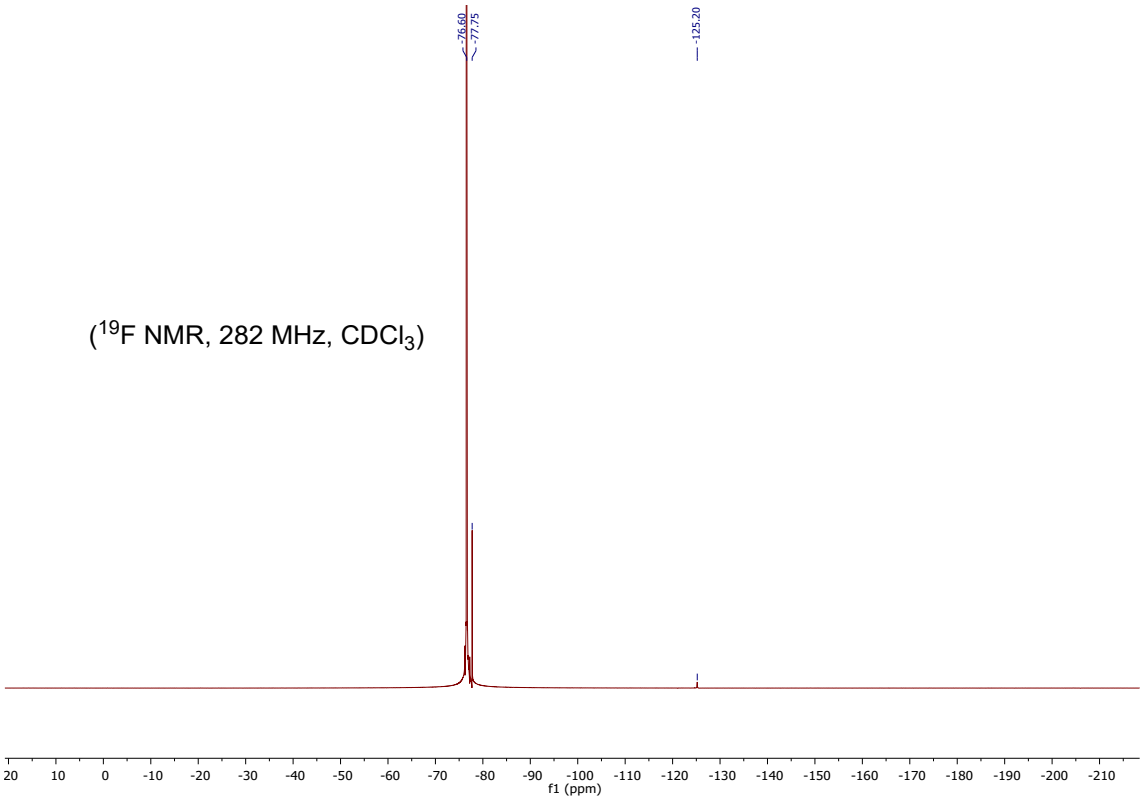

7.95
7.91
7.91
7.27
7.26
7.25
5.29
3.56
3.54
3.38
3.37
3.37
3.35
3.33
3.31
3.29
2.81
2.65
2.63
2.16
1.25
1.13
1.12
1.11
1.10
1.09
-0.01
O
O
F
N
N
N
N
3
(1H NMR, 400 MHz, CDCl3)
1.00
0.87
1.54
2.12
6.84
3.58
2.05
8.52
5.18
f1 (ppm)


-76.60
-123.68
(19F NMR, 282 MHz, CDCl3)
ppm

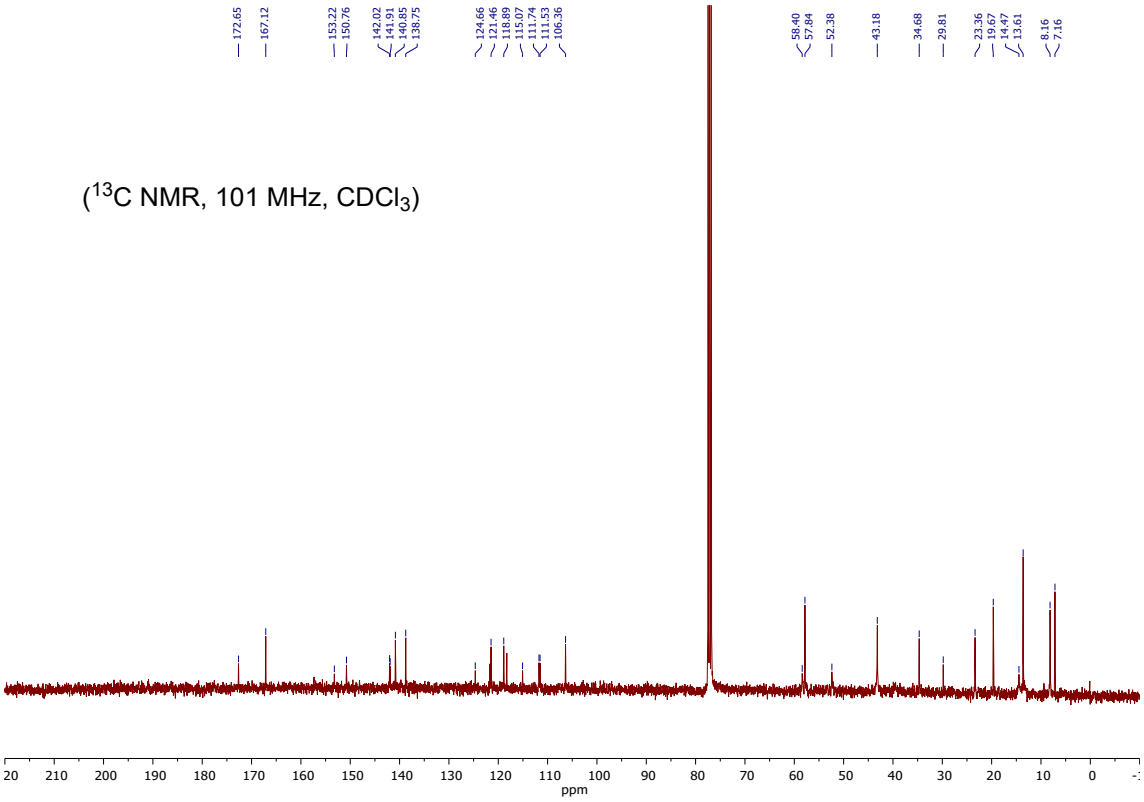

172.61
166.71
154.42
151.95
144.44
144.33
142.91
138.60
121.81
121.74
119.58
112.83
112.61
104.76
52.38
49.55
43.35
39.64
34.23
14.64
13.14
8.27
(^{13}C NMR, 101 MHz, $CDCl_3$)
ppm


8.03
7.93
7.89
7.60
7.58
3.84
3.78
3.76
3.70
3.66
3.63
3.61
3.48
3.45
3.43
3.41
3.39
3.38
2.75
1.73
1.72
1.69
1.68
1.66
1.52
1.50
1.48
1.46
1.44
1.42
1.40
1.38
1.36
1.25
1.21
1.19
1.18
1.06
1.04
1.02
F
O
O
N
N
N
N
Tf_2N^-
4
(^{1}H NMR, 400 MHz, $CDCl_3$)
1.00
1.00
0.94
11.81
6.40
3.71
2.16
4.39
3.46
8.71
3.39
ppm

(^{19}F NMR, 282 MHz, $CDCl_3$)



(^{13}C NMR, 101 MHz, $CDCl_3$)



4. General procedure for the selective extraction of thorium versus uranium.

To extract the analytes (thorium and uranium) from an aqueous sample **A** (5 mL), the pH of this sample is adjusted to 1.0 with HNO_3. Then, the extractant [0.005M solution of compound **4** in [BMIM][NTf_2] (**5**) was added and the solution was stirred using a vortex mixer. The mixture is then allowed to rest and the two phases are separated. Thorium was extracted in the solution **B**, while uranium remains in the aqueous sample **A**. In Figure S1 it is shown a detailed scheme of the selective extraction process of thorium *versus* uranium.

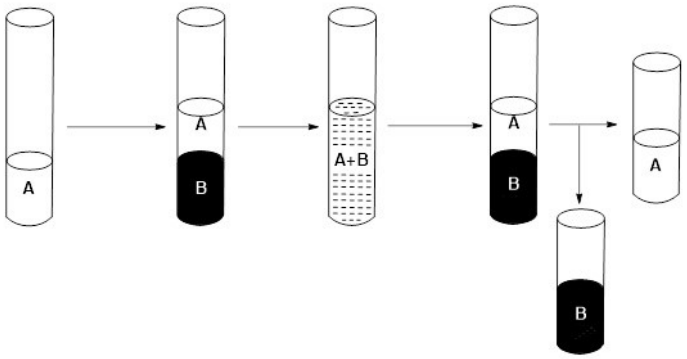


Figure S1. Procedure for the selective extraction process of thorium *versus* uranium in an aqueous sample.

5. General Procedure for the liberation of the extracted metal and recuperation of the extraction system (4 in 5).

To remove the thorium from the solution **B** and recover the extraction system (**4** in **5**), a buffer solution at pH = 6.0 (solution **C**, 5 mL) was added to the solution **B** with the thorium. The mixture was stirred in a vortex mixer for 3 min. The mixture is then allowed to rest and the two phases are separated. Thorium was extracted in aqueous phase, and the extraction system **4**+**5** was recovered. In Figure S2 it is shown a detailed scheme of the recovery of the extraction system. The thorium recovery was higher than 95% and the recovered extraction system could be used in subsequent extraction cycles.

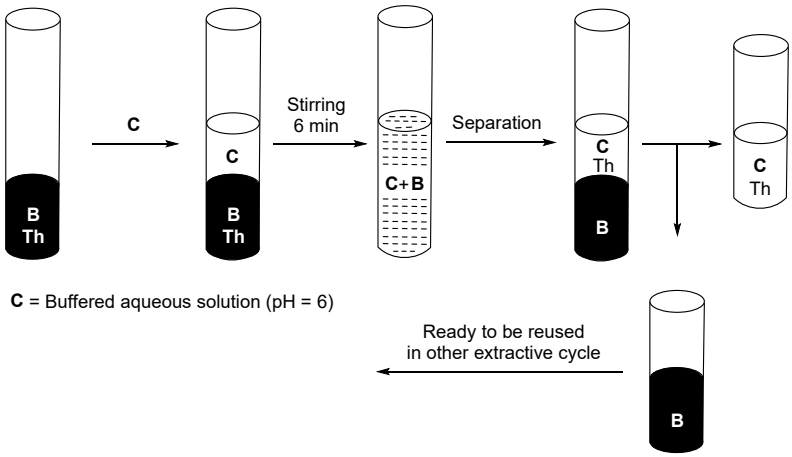


Figure S2. Procedure for the recovery of the extraction system by removing the thorium.

6. Kinetics of the competitive ternary mixture Th/U/Sc.

Kinetics of the extractive system (0.1M solution of **4** in [BMIM][Tf_2N], 1 mL) *versus* an original solution (5 mL) containing 0.1M solution of the ternary thorium(IV), scandium(III) and uranyl nitrates was assessed (Figure S3). The extraction profile of the thorium cation was identical to the plot observed in Figure 7A. However, the scandium(III) and the uranyl cations were slightly extracted at earlier stages of the extractive sequence but finally, after 3-5 min, the complexation of ligand **4** with scandium(III) and uranium(VI) was extremely low. The fragment of the plot recorded between 0-5 min in Figure S3 suggested that the ligand bonded initially to the scandium and uranyl cation were kidnaped by the thorium.

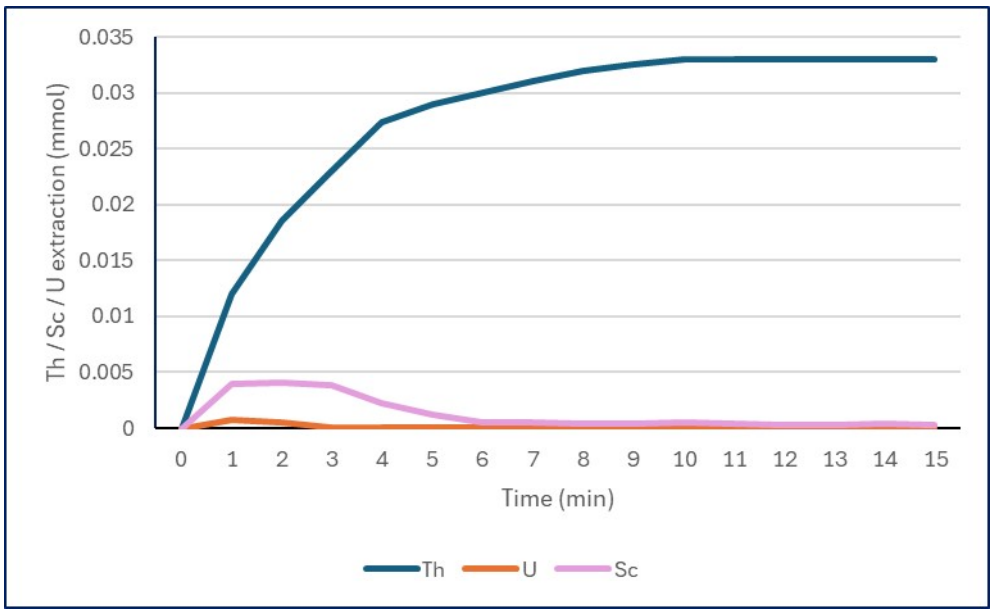


Figure S3. Competitive extraction of 0.1M of each thorium(IV), scandium(III) and uranyl nitrate with 0.1M solution of **4** in [BMIM][Tf_2N].

7. Computational methods and Cartesian coordinates.

Theoretical calculations have been carried out by using the GAUSSIAN 16[1] programs. Optimizations were computed within the DFT framework[2] using the hybrid PBE0[3] functional in combination with 6-31g(d) basis set for C, H, N, Fand O atoms and Stuttgart/Dresden[4] effective core potential SDD for U and Th atoms as implemented in GAUSSIAN 16. Dispersion corrections are included by means of Grimme's GD3 model.[5] All the stationary points were characterized by harmonic vibrational analysis. Local minima showed positive definite Hessians and thermal corrections were not scaled.

Table S1. Total electronic energies[a] (E, in a.u.), zero point correction of the energy[b] (ZPC), thermal corrections to Gibbs free energies[b] (TCGFE, in a.u.), and number of imaginary frequencies (NIMAG) of all stationary points discussed in the main text and in the Supporting Information. $Th{\cdot}2NO_3{\cdot}3$–**4** $Th{\cdot}2NO_3{\cdot}3$–**4'** $Th{\cdot}2NO_3{\cdot}3$–**4''**represent the three most favoured conformations found.

Structure	E	ZPC	TCGFE	NIMAG
4-cation	-1520.381750	0.656588	0.589152	0
H_2O	-76.327227	0.021518	0.003861	0
$UO_2{\cdot}2NO_3{\cdot}$2W-cis	-1340.223883	0.090316	0.044582	0
$UO_2{\cdot}2NO_3{\cdot}$2W-	-1340.226872	0.090008	0.044641	0
$UO_2{\cdot}2NO_3{\cdot}$**4**	-2707.935652	0.698860	0.613308	0
$UO_2{\cdot}NO_3{\cdot}$2W	-1059.966037	0.072381	0.030499	0
$UO_2{\cdot}NO_3{\cdot}$**4**	-2427.702762	0.682204	0.602407	0
$Th{\cdot}2NO_3{\cdot}$6W-cis	-1425.693789	0.185208	0.132230	0
$Th{\cdot}2NO_3{\cdot}$6W-trans	-1425.699156	0.183490	0.128710	0
$Th{\cdot}2NO_3{\cdot}$3–**4**	-5528.913315	2.011762	1.845070	0
$Th{\cdot}2NO_3{\cdot}$3–**4'**	-5528.915127	2.012383	1.847128	0
$Th{\cdot}2NO_3{\cdot}$3–**4''**	-5528.907625	2.011764	1.845309	0

[a]Computed at PBE1PBE(PCM)/6-31G(d)&SDD level. [b]Computed at 298.15 K.

Cartesian coordinates (optimized at the PBE1PBE(PCM)/6-31G(d)&SDD level) of all the stationary points collected in the main text

4-cation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-5.054507	-0.594993	0.402948
2	6	0	-4.563802	0.823263	0.327318
3	6	0	-3.038298	0.924968	0.407906
4	7	0	-2.447517	-0.234314	-0.218664
5	6	0	-3.234710	-0.723053	-1.332795
6	6	0	-4.497902	-1.372470	-0.783136
7	6	0	-1.063625	-0.405700	-0.176166
8	6	0	-0.191854	0.626031	0.150247
9	6	0	1.190085	0.392580	0.248557
10	6	0	1.709459	-0.891242	0.010212
11	6	0	0.825121	-1.930801	-0.308005
12	6	0	-0.518425	-1.691841	-0.380454
13	6	0	3.149800	-1.199695	0.105638
14	6	0	3.977227	-0.055995	0.447252
15	6	0	3.388497	1.147113	0.717094
16	7	0	2.066900	1.417354	0.584435
17	9	0	-1.369741	-2.708485	-0.628732
18	6	0	1.569327	2.732587	0.901908
19	6	0	1.003300	3.588462	-0.197623
20	6	0	2.323724	3.933600	0.419533
21	6	0	5.448281	-0.104591	0.746575
22	7	0	6.287469	-0.717044	-0.128967
23	6	0	7.693619	-0.772274	0.251330
24	6	0	8.483723	0.474880	-0.124920
25	8	0	3.565663	-2.346910	-0.074169
26	6	0	-4.563294	-1.203164	1.712056
27	6	0	-5.166916	-2.543612	2.078599
28	6	0	-6.569059	-0.635178	0.380907
29	6	0	-7.258472	0.161550	-0.727710

30	6	0	-7.736826	1.559800	-0.332600
31	6	0	-8.497085	2.235903	-1.465925
32	8	0	5.861317	0.445040	1.769599
33	6	0	5.920330	-1.066321	-1.498052
34	6	0	5.710793	0.134819	-2.414789
35	1	0	-0.575768	1.623452	0.319408
36	1	0	1.227946	-2.926771	-0.459984
37	1	0	3.996928	1.971556	1.071637
38	1	0	-2.761429	1.874816	-0.079696
39	1	0	-2.698468	0.979531	1.447601
40	1	0	-3.473311	0.090170	-2.035387
41	1	0	-2.682901	-1.474390	-1.894457
42	1	0	-4.929150	1.227737	-0.616988
43	1	0	-5.034157	1.382959	1.138540
44	1	0	-4.278347	-2.378051	-0.424241
45	1	0	-5.275508	-1.434742	-1.545712
46	1	0	-4.784979	-0.459606	2.483464
47	1	0	-3.480896	-1.284524	1.599047
48	1	0	-4.637762	-2.900250	2.967101
49	1	0	-6.226626	-2.483147	2.335264
50	1	0	-5.032528	-3.303106	1.302689
51	1	0	-6.817053	-1.695375	0.305051
52	1	0	-6.895634	-0.285473	1.365845
53	1	0	-8.135192	-0.423666	-1.029250
54	1	0	-6.635368	0.213885	-1.630931
55	1	0	-8.385214	1.473381	0.548943
56	1	0	-6.896338	2.195923	-0.030245
57	1	0	-8.850407	3.226047	-1.163727
58	1	0	-7.862871	2.363269	-2.350713
59	1	0	-9.370427	1.644763	-1.763421
60	1	0	1.099110	2.791798	1.881983
61	1	0	3.210661	3.770477	-0.185513
62	1	0	2.386534	4.782379	1.092822

63	1	0	0.136639	4.201605	0.031786
64	1	0	1.018890	3.173177	-1.201164
65	1	0	6.731421	-1.690478	-1.886667
66	1	0	5.031061	-1.699588	-1.472283
67	1	0	5.444791	-0.204753	-3.422011
68	1	0	4.895624	0.767079	-2.048504
69	1	0	6.611860	0.751247	-2.489521
70	1	0	8.126889	-1.662487	-0.218474
71	1	0	7.729918	-0.912040	1.334358
72	1	0	9.516679	0.391624	0.230971
73	1	0	8.514064	0.624395	-1.209065
74	1	0	8.028607	1.353753	0.340592

H_2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.119418
2	1	0	0.000000	-0.758011	-0.477671
3	1	0	0.000000	0.758011	-0.477671

$UO_2 \cdot 2NO_3 \cdot 2W$-cis

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	92	0	-0.000031	0.230324	-0.000188
2	8	0	1.313766	2.410186	-0.030727
3	8	0	1.362098	-1.796955	0.005951
4	7	0	2.499456	-1.228560	0.014799
5	8	0	3.536760	-1.827361	0.027590
6	8	0	2.440406	0.050848	0.007457

7	8	0	-2.440281	0.050819	-0.007303
8	8	0	-1.362004	-1.796984	-0.005811
9	8	0	0.005185	0.270899	1.746483
10	8	0	-1.313636	2.410446	0.031426
11	8	0	-0.005297	0.270503	-1.746868
12	1	0	-1.167265	2.931440	0.835805
13	1	0	2.264838	2.212798	-0.001754
14	1	0	-2.264594	2.212581	0.001512
15	1	0	1.166665	2.933567	-0.833406
16	7	0	-2.499374	-1.228629	-0.014371
17	8	0	-3.536669	-1.827383	-0.026676

$UO_2 \cdot 2NO_3 \cdot 2W$-trans

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	92	0	-0.000060	-0.000063	-0.043892
2	8	0	0.000089	-2.509952	-0.012771
3	8	0	2.206918	1.070330	0.014146
4	7	0	2.899901	0.000034	0.057819
5	8	0	4.095462	0.000178	0.130398
6	8	0	2.207138	-1.070336	0.014301
7	8	0	-2.206875	1.070407	0.013814
8	8	0	-2.207071	-1.070285	0.014006
9	8	0	-0.000425	0.000410	1.704402
10	8	0	0.000276	2.510025	-0.013227
11	8	0	0.000288	-0.000296	-1.788359
12	1	0	0.783817	2.911634	0.392521
13	1	0	0.783218	-2.912399	0.392889
14	1	0	-0.782212	2.912522	0.393658

15	1	0	-0.782868	-2.913027	0.392603
16	7	0	-2.899870	0.000141	0.057656
17	8	0	-4.095385	0.000256	0.130547

$UO_2 \cdot 2NO_3 \cdot$**4**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.756245	0.999192	0.809105
2	7	0	4.933743	0.079164	0.059043
3	6	0	5.607222	-0.447852	-1.125815
4	6	0	7.111753	-0.515572	-0.879179
5	7	0	7.433722	-0.880279	0.539675
6	6	0	6.899480	0.212354	1.450475
7	6	0	3.555974	0.286168	-0.033914
8	6	0	2.722181	-0.828352	-0.284790
9	6	0	1.362781	-0.718453	-0.366029
10	6	0	0.759622	0.535458	-0.175158
11	6	0	1.562869	1.660879	0.091606
12	6	0	2.958697	1.526780	0.151692
13	7	0	0.949718	2.894312	0.291653
14	6	0	-0.392754	2.995072	0.251586
15	6	0	-1.236238	1.948634	-0.024595
16	6	0	-0.688851	0.633174	-0.217639
17	8	0	-1.378378	-0.387750	-0.426157
18	92	0	-3.644784	-1.196739	0.016807
19	8	0	-3.226380	-1.661313	1.651837
20	6	0	1.739202	4.055789	0.642867
21	6	0	2.627267	4.681804	-0.395072
22	6	0	1.385373	5.387938	0.054300
23	6	0	-2.712341	2.055197	0.034887
24	8	0	-3.328369	1.131337	0.616417
25	9	0	3.303394	-2.030885	-0.407654

26	6	0	6.766587	-2.217248	0.851673
27	6	0	7.161548	-2.854091	2.168330
28	6	0	8.931085	-1.024532	0.731613
29	6	0	9.797252	0.124123	0.210430
30	6	0	10.397867	-0.065230	-1.187501
31	6	0	11.405168	-1.207127	-1.266167
32	8	0	-4.013300	-3.567080	-0.568242
33	7	0	-2.819578	-3.841782	-0.908062
34	8	0	-2.011122	-2.862717	-0.830777
35	8	0	-5.677465	-0.019145	0.822195
36	7	0	-3.387394	3.080996	-0.492154
37	6	0	-4.848648	3.085304	-0.307123
38	6	0	-5.264133	3.476045	1.101993
39	6	0	-2.825484	4.106992	-1.365699
40	6	0	-2.849253	5.498558	-0.750416
41	8	0	-2.481783	-4.939156	-1.273950
42	8	0	-4.058533	-0.707919	-1.615067
43	1	0	3.575375	2.399537	0.324579
44	1	0	0.735832	-1.587357	-0.542153
45	1	0	-0.776245	3.981608	0.481676
46	1	0	5.449524	0.196484	-2.003657
47	1	0	5.204129	-1.433474	-1.364108
48	1	0	6.138465	1.831030	0.196055
49	1	0	5.171706	1.437392	1.621361
50	1	0	7.586045	0.447555	-1.071190
51	1	0	7.576582	-1.257862	-1.531861
52	1	0	6.562256	-0.279127	2.362694
53	1	0	7.725817	0.877560	1.704830
54	1	0	7.029754	-2.873759	0.016725
55	1	0	5.692537	-2.024864	0.818598
56	1	0	6.528699	-3.737085	2.297639
57	1	0	8.199209	-3.193995	2.188504
58	1	0	6.983151	-2.207906	3.033048

59	1	0	9.062500	-1.149446	1.807965
60	1	0	9.203727	-1.969872	0.252923
61	1	0	10.625181	0.231310	0.921234
62	1	0	9.256891	1.077907	0.265568
63	1	0	9.614183	-0.210833	-1.940732
64	1	0	10.897542	0.871903	-1.458424
65	1	0	11.837527	-1.270435	-2.269146
66	1	0	12.226321	-1.056506	-0.556370
67	1	0	10.954949	-2.183471	-1.050454
68	1	0	2.089992	4.030403	1.672107
69	1	0	2.612480	4.243886	-1.389037
70	1	0	3.594289	5.055798	-0.072422
71	1	0	1.472337	6.252556	0.704175
72	1	0	0.566315	5.440132	-0.657793
73	1	0	-5.252394	3.786497	-1.042776
74	1	0	-5.225301	2.086070	-0.542981
75	1	0	-6.356331	3.485330	1.168424
76	1	0	-4.891002	2.745728	1.823627
77	1	0	-4.892795	4.470785	1.369296
78	1	0	-3.414944	4.099124	-2.290185
79	1	0	-1.813004	3.811747	-1.647974
80	1	0	-2.428161	6.224623	-1.452988
81	1	0	-3.871724	5.813444	-0.519940
82	1	0	-2.274515	5.544862	0.181431
83	7	0	-6.472670	-1.009345	0.733327
84	8	0	-5.931319	-2.084566	0.327523
85	8	0	-7.642472	-0.931298	1.011374

$UO_2 \cdot NO_3 \cdot 2W$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.582316	-2.103923	-0.000805
2	92	0	0.408170	0.012338	-0.000040

3	8	0	1.062847	2.335534	0.001336
4	8	0	0.481243	0.021257	-1.731575
5	8	0	0.480939	0.016103	1.731499
6	8	0	-1.626671	-1.157578	-0.000864
7	8	0	-1.745537	0.980400	0.000896
8	7	0	-2.398442	-0.126463	0.000036
9	8	0	-3.582196	-0.194437	-0.000156
10	1	0	1.162065	2.902483	-0.781473
11	1	0	1.163264	2.900460	0.785464
12	1	0	1.842706	-2.615440	-0.785037
13	1	0	1.845873	-2.616178	0.781873

$UO_2 \cdot NO_3 \cdot$ **4**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.103872	0.201598	-0.968840
2	7	0	-4.253792	-0.665231	-0.180947
3	6	0	-4.941807	-1.595319	0.714907
4	6	0	-6.386293	-1.172131	0.894836
5	7	0	-7.164655	-1.186608	-0.394277
6	6	0	-6.307774	-0.566283	-1.487205
7	6	0	-2.927249	-0.351364	-0.015310
8	6	0	-2.009069	-1.316607	0.489964
9	6	0	-0.681853	-1.052875	0.647031
10	6	0	-0.165016	0.206204	0.286893
11	6	0	-1.047762	1.178960	-0.232679
12	6	0	-2.409960	0.895861	-0.375037
13	7	0	-0.531081	2.416203	-0.602822
14	6	0	0.778493	2.670201	-0.476564
15	6	0	1.688989	1.774157	0.043698
16	6	0	1.236306	0.470578	0.406790
17	8	0	2.031184	-0.433053	0.837465
18	92	0	4.003632	-1.163147	-0.023831

19	6	0	-1.387951	3.409881	-1.223836
20	6	0	-2.416650	4.119301	-0.390130
21	6	0	-1.208454	4.856769	-0.879152
22	6	0	3.139579	2.076261	0.094989
23	8	0	3.950334	1.168036	-0.255968
24	9	0	-2.468262	-2.536767	0.785186
25	6	0	-7.476719	-2.632823	-0.754070
26	6	0	-8.272910	-2.826454	-2.029023
27	6	0	-8.480070	-0.448074	-0.226010
28	6	0	-8.389580	1.009194	0.234851
29	6	0	-8.711753	1.246921	1.715004
30	6	0	-10.173503	0.985251	2.060131
31	7	0	3.610059	3.258400	0.478571
32	6	0	5.062972	3.485132	0.370222
33	6	0	5.506844	3.745417	-1.060595
34	6	0	2.834342	4.307963	1.145900
35	6	0	2.736760	5.591078	0.335480
36	1	0	-3.070001	1.669942	-0.739949
37	1	0	-0.017545	-1.824342	1.020204
38	1	0	1.090781	3.638137	-0.847353
39	1	0	-4.488215	-1.571476	1.709377
40	1	0	-4.859755	-2.626509	0.357599
41	1	0	-5.400269	1.111171	-0.425714
42	1	0	-4.556364	0.525370	-1.860052
43	1	0	-6.430188	-0.157497	1.290134
44	1	0	-6.897824	-1.834062	1.597225
45	1	0	-5.948701	-1.383492	-2.115126
46	1	0	-6.942125	0.081920	-2.093393
47	1	0	-8.013123	-3.046294	0.104383
48	1	0	-6.512166	-3.140206	-0.824542
49	1	0	-8.296454	-3.900248	-2.236263
50	1	0	-9.309283	-2.494395	-1.939468
51	1	0	-7.816917	-2.343220	-2.897935

52	1	0	-8.966486	-0.517146	-1.199347
53	1	0	-9.064617	-1.048064	0.478391
54	1	0	-9.108148	1.578920	-0.365393
55	1	0	-7.413918	1.438083	-0.019640
56	1	0	-8.067804	0.635952	2.361203
57	1	0	-8.467751	2.289558	1.947522
58	1	0	-10.363061	1.193123	3.117257
59	1	0	-10.836573	1.625649	1.467859
60	1	0	-10.468895	-0.055451	1.880275
61	1	0	-1.638048	3.152655	-2.250109
62	1	0	-2.451610	3.879799	0.668849
63	1	0	-3.380003	4.323290	-0.847446
64	1	0	-1.313423	5.570896	-1.689268
65	1	0	-0.467648	5.129077	-0.132317
66	1	0	5.292900	4.339469	1.011266
67	1	0	5.573130	2.611787	0.785245
68	1	0	6.587252	3.916559	-1.080988
69	1	0	5.287206	2.887359	-1.701323
70	1	0	5.013757	4.628999	-1.476758
71	1	0	3.335164	4.506173	2.100302
72	1	0	1.848847	3.911825	1.395708
73	1	0	2.152987	6.331173	0.891061
74	1	0	3.724031	6.023932	0.148823
75	1	0	2.258305	5.432952	-0.637316
76	8	0	4.790223	-1.012317	1.522483
77	8	0	3.279089	-1.292746	-1.602897
78	8	0	3.223803	-3.356089	0.538824
79	8	0	5.154631	-3.258255	-0.396462
80	7	0	4.241554	-4.002144	0.102657
81	8	0	4.327230	-5.191580	0.158682

$Th{\cdot}2NO_3{\cdot}6W$-cis

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	8	0	0.528208	-2.626440	0.522391
2	90	0	0.318155	-0.128399	-0.000256
3	8	0	0.225939	-0.647387	2.478035
4	8	0	-1.557526	-1.329785	-0.987481
5	7	0	-2.411813	-1.118862	-0.045454
6	8	0	-3.547439	-1.444123	-0.103720
7	8	0	-1.888193	-0.516661	0.964504
8	8	0	0.428987	-0.741817	-2.441374
9	8	0	1.715885	1.453348	-1.415067
10	8	0	2.145474	1.093905	1.342090
11	8	0	-1.179963	1.511601	-0.964427
12	7	0	-1.117486	2.361361	-0.001351
13	8	0	-1.748263	3.360851	0.040586
14	8	0	2.632132	-1.106273	-0.380347
15	8	0	-0.285491	2.006408	0.924516
16	1	0	0.542956	-2.928821	1.446515
17	1	0	1.167664	-0.922627	-3.043961
18	1	0	2.242242	2.174764	-1.033851
19	1	0	3.046957	0.835209	1.591069
20	1	0	2.813023	-2.052319	-0.248602
21	1	0	-0.671521	-0.724657	2.849778
22	1	0	1.943925	1.939143	1.779404
23	1	0	1.362868	1.777725	-2.261184
24	1	0	-0.387893	-1.049217	-2.873645
25	1	0	3.384325	-0.726275	-0.862907
26	1	0	0.079799	-3.317361	0.005234
27	1	0	0.788814	-0.256202	3.165201

$Th{\cdot}2NO_3{\cdot}6W$-trans

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	8	0	1.405995	-2.205141	-0.079742
2	90	0	-0.007154	-0.081974	0.013317
3	8	0	0.077847	-1.076072	-2.304373
4	8	0	2.239801	0.182610	1.002288
5	7	0	2.830231	0.556587	-0.080928
6	8	0	3.992311	0.767489	-0.154437
7	8	0	2.020684	0.676515	-1.079654
8	8	0	0.109627	-0.835778	2.394369
9	8	0	0.298046	2.056939	1.276777
10	8	0	-0.412513	1.845100	-1.530385
11	8	0	-2.059887	0.752993	1.010582
12	7	0	-2.863894	0.492397	0.035493
13	8	0	-4.024372	0.722642	0.066386
14	8	0	-1.321026	-2.218509	0.282115
15	8	0	-2.270496	-0.045312	-0.976336
16	1	0	1.435237	-2.784121	-0.858866
17	1	0	-0.662903	-0.929485	2.977273
18	1	0	-0.453031	2.619499	1.530781
19	1	0	-1.181403	1.968894	-2.110130
20	1	0	-0.969295	-3.034112	0.674794
21	1	0	0.763352	-0.783797	-2.930100
22	1	0	0.256170	2.509110	-1.767432
23	1	0	1.054949	2.296016	1.835781
24	1	0	0.890949	-0.733609	2.963777
25	1	0	-2.209159	-2.409719	-0.060910
26	1	0	2.213520	-2.367264	0.434749
27	1	0	-0.706994	-1.304503	-2.830935

$Th{\cdot}2NO_3{\cdot}3$–**4**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	7.368975	-5.629011	-0.295799
2	7	0	6.626125	-4.735782	-1.157074
3	6	0	7.267957	-4.389214	-2.424921
4	6	0	8.737387	-4.760209	-2.386537
5	7	0	8.962761	-6.236631	-2.189975
6	6	0	8.011637	-6.736260	-1.112646
7	6	0	5.632558	-3.946706	-0.621095
8	6	0	4.702907	-3.281992	-1.468391
9	6	0	3.695169	-2.503163	-0.980998
10	6	0	3.527948	-2.358247	0.408310
11	6	0	4.414597	-3.028611	1.275099
12	6	0	5.458393	-3.805681	0.757459
13	7	0	4.225240	-2.904740	2.648356
14	6	0	3.179955	-2.207798	3.125488
15	6	0	2.282633	-1.523321	2.338263
16	6	0	2.431716	-1.570001	0.913049
17	8	0	1.668173	-0.972574	0.106772
18	90	0	-0.608186	-0.251402	0.085286
19	8	0	-2.013385	-1.177808	-1.814036
20	7	0	-1.041043	-1.554759	-2.553244
21	8	0	-1.204715	-2.197566	-3.555559
22	6	0	5.090479	-3.608116	3.574301
23	6	0	6.512706	-3.152117	3.736653
24	6	0	5.521635	-2.923799	4.835870
25	6	0	1.071305	-0.900330	2.922137
26	8	0	-0.024423	-1.078199	2.323105
27	9	0	4.808251	-3.461991	-2.791039
28	6	0	8.662885	-6.949019	-3.501327
29	6	0	8.853073	-8.452440	-3.481235
30	6	0	10.411330	-6.505907	-1.826830
31	6	0	10.944881	-5.792672	-0.581288
32	6	0	11.833246	-4.574386	-0.859792
33	6	0	13.164348	-4.938892	-1.507633

34	8	0	-2.586804	-1.117580	1.106487
35	6	0	-3.341411	-2.073872	0.764989
36	6	0	-4.769579	-1.885479	0.733256
37	6	0	-5.632554	-2.882551	0.236038
38	7	0	-5.083361	-4.089149	-0.182144
39	6	0	-3.758487	-4.291826	-0.098792
40	6	0	-2.863191	-3.372464	0.399774
41	6	0	-5.309668	-0.654628	1.144628
42	6	0	-6.652488	-0.443100	1.057183
43	6	0	-7.550463	-1.433296	0.578908
44	6	0	-7.012593	-2.647842	0.158964
45	7	0	-8.892706	-1.140172	0.449886
46	6	0	-9.725997	-1.912848	-0.445782
47	6	0	-11.083615	-1.221592	-0.598560
48	7	0	-10.978160	0.277142	-0.558037
49	6	0	-10.429266	0.698148	0.798539
50	6	0	-9.654320	-0.432317	1.461765
51	6	0	-10.038813	0.723653	-1.671781
52	6	0	-9.994231	2.215090	-1.936062
53	6	0	-12.338279	0.911817	-0.782452
54	6	0	-13.489808	0.381281	0.072281
55	6	0	-14.359698	-0.691803	-0.585705
56	6	0	-15.545230	-1.070075	0.292621
57	9	0	-7.148596	0.768132	1.358792
58	6	0	-1.404151	-3.631030	0.418129
59	8	0	-0.621773	-2.713252	0.077384
60	6	0	-5.920235	-5.101924	-0.796214
61	6	0	-5.683168	-6.546012	-0.474096
62	6	0	-6.905154	-5.857339	0.050293
63	7	0	-0.895184	-4.817395	0.772811
64	6	0	-1.618752	-5.899272	1.439906
65	6	0	-1.703150	-7.167721	0.604163
66	6	0	0.561974	-4.977182	0.649906

67	6	0	1.029084	-5.099996	-0.792310
68	8	0	1.048102	1.333181	1.363190
69	7	0	0.155806	1.998235	1.970196
70	8	0	-1.045503	1.708954	1.647709
71	8	0	0.136059	1.558501	-1.277875
72	6	0	-0.185261	2.784406	-1.185815
73	6	0	0.790823	3.794312	-0.886518
74	6	0	0.416058	5.150823	-0.769794
75	7	0	-0.912863	5.500160	-0.973066
76	6	0	-1.833961	4.551627	-1.223051
77	6	0	-1.531483	3.218864	-1.353717
78	6	0	1.368166	6.115555	-0.411743
79	6	0	2.691600	5.753829	-0.176379
80	6	0	3.046954	4.388062	-0.346493
81	6	0	2.133945	3.431369	-0.671349
82	6	0	-1.342764	6.875075	-0.811205
83	6	0	-0.900589	7.901393	-1.814106
84	6	0	-2.328105	7.449306	-1.783448
85	6	0	-2.572647	2.165133	-1.482845
86	8	0	-2.554635	1.219780	-0.660818
87	9	0	4.337731	4.049799	-0.205853
88	7	0	3.662972	6.687389	0.127026
89	6	0	3.416847	8.092132	-0.120524
90	6	0	4.704166	8.885812	0.114287
91	7	0	5.937026	8.126220	-0.286425
92	6	0	6.038234	6.862331	0.557323
93	6	0	4.686269	6.464633	1.132311
94	6	0	5.819271	7.765706	-1.763127
95	6	0	7.076958	7.217697	-2.406353
96	6	0	7.173353	8.983080	-0.087481
97	6	0	7.321187	9.649420	1.282164
98	6	0	6.849453	11.105371	1.374837
99	6	0	7.680513	12.066453	0.532056

100	7	0	-3.497720	2.232184	-2.446429
101	6	0	-4.535998	1.195504	-2.474588
102	6	0	-5.705612	1.524406	-1.558155
103	6	0	-3.447865	3.158231	-3.578840
104	6	0	-4.609633	4.138657	-3.622451
105	7	0	1.107649	-0.222766	4.069480
106	6	0	-0.177379	0.161728	4.680151
107	6	0	-0.830438	-1.004945	5.402632
108	6	0	2.311631	0.397961	4.626418
109	6	0	2.635230	-0.065292	6.037212
110	8	0	0.416652	2.837840	2.797647
111	8	0	0.108796	-1.202942	-2.138078
112	1	0	1.060660	7.144273	-0.283654
113	1	0	2.432129	2.395246	-0.781033
114	1	0	-2.853345	4.911584	-1.297660
115	1	0	2.654673	8.520204	0.549740
116	1	0	3.059536	8.214424	-1.148631
117	1	0	4.452431	7.035822	2.041964
118	1	0	4.728614	5.417324	1.422682
119	1	0	4.818250	9.136330	1.168990
120	1	0	4.687113	9.819026	-0.452699
121	1	0	6.417599	6.075671	-0.095100
122	1	0	6.764385	7.036215	1.352387
123	1	0	5.500537	8.683047	-2.266911
124	1	0	5.010198	7.035325	-1.818784
125	1	0	6.806302	6.898898	-3.417254
126	1	0	7.868913	7.963186	-2.503299
127	1	0	7.477494	6.338912	-1.892182
128	1	0	8.010388	8.310673	-0.283072
129	1	0	7.152867	9.728682	-0.888177
130	1	0	8.390437	9.625321	1.523212
131	1	0	6.845340	9.044158	2.064559
132	1	0	5.790495	11.198259	1.104541

133	1	0	6.913508	11.404353	2.427283
134	1	0	7.334181	13.095262	0.667715
135	1	0	8.737211	12.027986	0.819398
136	1	0	7.620019	11.848127	-0.540837
137	1	0	-1.418982	7.169197	0.232954
138	1	0	-0.291639	7.554565	-2.644031
139	1	0	-0.652568	8.891531	-1.443930
140	1	0	-3.086759	8.113325	-1.382406
141	1	0	-2.662821	6.827694	-2.609543
142	1	0	-4.868599	1.105934	-3.512566
143	1	0	-4.070273	0.248792	-2.189243
144	1	0	-6.426459	0.699677	-1.578929
145	1	0	-5.367048	1.650270	-0.526854
146	1	0	-6.218069	2.440992	-1.865596
147	1	0	-3.438966	2.548937	-4.490289
148	1	0	-2.492688	3.684636	-3.551805
149	1	0	-4.484285	4.819035	-4.470404
150	1	0	-5.566346	3.625019	-3.754830
151	1	0	-4.674671	4.736575	-2.706687
152	1	0	6.150902	-4.275524	1.441822
153	1	0	2.990001	-2.028844	-1.656191
154	1	0	3.069357	-2.235650	4.202732
155	1	0	7.228637	-3.308852	-2.589710
156	1	0	6.752141	-4.852737	-3.271784
157	1	0	8.105738	-5.103607	0.330620
158	1	0	6.672790	-6.130277	0.384795
159	1	0	9.230127	-4.243649	-1.563007
160	1	0	9.233701	-4.471492	-3.315876
161	1	0	7.220444	-7.292823	-1.617826
162	1	0	8.558533	-7.422941	-0.465052
163	1	0	9.312558	-6.486499	-4.249434
164	1	0	7.629792	-6.697450	-3.750628
165	1	0	8.470592	-8.840105	-4.429920

166	1	0	9.901794	-8.749053	-3.413102
167	1	0	8.289810	-8.945857	-2.683926
168	1	0	10.475526	-7.588220	-1.711278
169	1	0	10.990981	-6.233898	-2.714455
170	1	0	11.537302	-6.525518	-0.021745
171	1	0	10.125323	-5.523573	0.094441
172	1	0	11.309026	-3.841254	-1.486945
173	1	0	12.022718	-4.071903	0.095420
174	1	0	13.774246	-4.044612	-1.665639
175	1	0	13.734177	-5.625973	-0.872190
176	1	0	13.038777	-5.418226	-2.485994
177	1	0	4.882154	-4.674642	3.614871
178	1	0	6.824061	-2.282658	3.164705
179	1	0	7.274224	-3.915459	3.863933
180	1	0	5.574515	-3.532246	5.732752
181	1	0	5.205467	-1.897999	5.004589
182	1	0	0.034368	0.985148	5.366156
183	1	0	-0.839386	0.544403	3.900186
184	1	0	-1.770312	-0.677998	5.857881
185	1	0	-1.057694	-1.811162	4.699196
186	1	0	-0.184845	-1.399121	6.193750
187	1	0	2.135436	1.480354	4.607016
188	1	0	3.143112	0.214571	3.943656
189	1	0	3.527348	0.454312	6.399919
190	1	0	1.819274	0.156628	6.731898
191	1	0	2.823202	-1.143825	6.085016
192	1	0	-7.666713	-3.426974	-0.208240
193	1	0	-4.644000	0.132566	1.481379
194	1	0	-3.423352	-5.244061	-0.490033
195	1	0	-9.924829	-2.932086	-0.078863
196	1	0	-9.220318	-2.003103	-1.412913
197	1	0	-10.327375	-1.129514	1.980100
198	1	0	-9.000410	-0.007525	2.220230

199	1	0	-11.759454	-1.508993	0.207190
200	1	0	-11.551033	-1.499456	-1.545546
201	1	0	-9.777679	1.554600	0.624978
202	1	0	-11.265000	1.016922	1.422799
203	1	0	-10.364679	0.185896	-2.567065
204	1	0	-9.052182	0.358302	-1.381570
205	1	0	-9.204077	2.384942	-2.673558
206	1	0	-10.920734	2.604231	-2.363068
207	1	0	-9.737357	2.803859	-1.050443
208	1	0	-12.179172	1.975928	-0.598469
209	1	0	-12.558712	0.784956	-1.847488
210	1	0	-14.128341	1.244293	0.295008
211	1	0	-13.136729	0.037218	1.054329
212	1	0	-14.719979	-0.309476	-1.549577
213	1	0	-13.777199	-1.592547	-0.814102
214	1	0	-16.167898	-1.824747	-0.196590
215	1	0	-15.214602	-1.481168	1.253353
216	1	0	-16.175944	-0.198543	0.500920
217	1	0	-6.203612	-4.843852	-1.813809
218	1	0	-4.915413	-6.798841	0.252057
219	1	0	-5.781251	-7.254545	-1.290002
220	1	0	-7.871155	-6.089036	-0.388093
221	1	0	-6.925499	-5.631306	1.112579
222	1	0	-1.090105	-6.107477	2.377608
223	1	0	-2.608735	-5.538278	1.724752
224	1	0	-2.236088	-7.944692	1.160824
225	1	0	-2.224204	-7.003533	-0.345561
226	1	0	-0.707764	-7.555732	0.366563
227	1	0	0.826982	-5.872461	1.218028
228	1	0	1.037260	-4.119467	1.136327
229	1	0	2.115208	-5.235421	-0.813149
230	1	0	0.569434	-5.962504	-1.284737
231	1	0	0.788771	-4.197566	-1.360431

$Th{\cdot}2NO_3{\cdot}3$–**4'**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.720301	5.442818	0.694222
2	7	0	3.615743	5.200093	-0.735378
3	6	0	3.703731	6.424685	-1.507443
4	6	0	4.556608	7.451968	-0.764143
5	7	0	5.701699	6.826127	-0.023043
6	6	0	5.146091	5.863598	1.018908
7	6	0	2.908762	4.130723	-1.257221
8	6	0	2.132364	4.257985	-2.406966
9	6	0	1.440613	3.160399	-2.935174
10	6	0	1.510619	1.904028	-2.299446
11	6	0	2.324687	1.763933	-1.161185
12	6	0	3.013182	2.836627	-0.678902
13	7	0	0.632609	3.303202	-4.056860
14	6	0	-0.133580	2.279189	-4.472488
15	6	0	-0.125855	1.036513	-3.889197
16	6	0	0.711587	0.792923	-2.752092
17	8	0	0.738944	-0.318871	-2.152155
18	90	0	-1.184084	-1.439861	-1.086863
19	8	0	-2.736932	-2.946070	-2.495643
20	7	0	-3.809619	-2.336158	-2.207283
21	8	0	-4.874690	-2.615949	-2.693988
22	6	0	0.509535	4.587623	-4.715874
23	6	0	0.485111	4.635322	-6.213629
24	6	0	1.686619	5.134062	-5.471322
25	6	0	-1.125378	-0.001292	-4.226407
26	7	0	-1.413311	-0.359798	-5.475958
27	6	0	-0.658593	0.044601	-6.660342
28	6	0	-1.462036	0.910130	-7.619142
29	9	0	3.829742	2.666684	0.373992

30	6	0	6.564778	6.073687	-1.029130
31	6	0	7.905719	5.597279	-0.510239
32	6	0	6.544411	7.893547	0.649341
33	6	0	5.787842	8.908540	1.509081
34	6	0	5.455007	10.243470	0.832361
35	6	0	6.687908	11.072622	0.490278
36	8	0	0.755977	-2.320427	0.036871
37	8	0	-0.041581	0.294362	0.430727
38	6	0	1.887398	-2.704582	-0.372292
39	6	0	3.086958	-2.269493	0.295492
40	6	0	4.357206	-2.733480	-0.101845
41	7	0	4.443297	-3.588003	-1.196847
42	6	0	3.333490	-3.953998	-1.858490
43	6	0	2.058948	-3.592882	-1.485099
44	6	0	5.505350	-2.342278	0.598000
45	6	0	5.418868	-1.469520	1.683618
46	6	0	4.134211	-0.945472	1.999434
47	6	0	3.000608	-1.346983	1.355370
48	7	0	6.526503	-1.082198	2.407477
49	6	0	7.840689	-1.451549	1.927621
50	6	0	8.914003	-0.641793	2.632921
51	7	0	8.925441	-0.809579	4.144359
52	6	0	7.620062	-1.429664	4.568930
53	6	0	6.424930	-0.837279	3.847381
54	6	0	9.046627	0.556874	4.804189
55	6	0	10.316409	1.320344	4.484987
56	6	0	10.093560	-1.660730	4.608215
57	6	0	10.111891	-3.115360	4.130601
58	6	0	9.676804	-4.150061	5.175056
59	6	0	10.659127	-4.280661	6.333639
60	9	0	4.049868	-0.015764	2.959323
61	6	0	5.738473	-4.002823	-1.698903
62	6	0	5.917164	-5.399252	-2.211600

63	6	0	6.547594	-4.996734	-0.914272
64	6	0	0.863761	-3.947821	-2.284775
65	7	0	0.688670	-5.149673	-2.840041
66	6	0	1.492347	-6.340932	-2.574965
67	6	0	2.280324	-6.821207	-3.784564
68	8	0	-0.014356	-3.063912	-2.455014
69	8	0	-2.299002	-1.029732	1.031777
70	6	0	-3.360790	-1.559127	1.465041
71	6	0	-4.495431	-0.748362	1.825404
72	6	0	-5.692140	-1.332988	2.286506
73	7	0	-5.757411	-2.717069	2.413376
74	6	0	-4.708346	-3.479737	2.063023
75	6	0	-3.508476	-2.973930	1.621528
76	6	0	-6.797412	-0.528605	2.596916
77	6	0	-6.734031	0.853742	2.443370
78	6	0	-5.529485	1.408644	1.935633
79	6	0	-4.436699	0.646132	1.649509
80	6	0	-6.992968	-3.357420	2.818781
81	6	0	-7.461819	-3.215056	4.238722
82	6	0	-6.938288	-4.530328	3.749946
83	6	0	-2.410627	-3.836256	1.127850
84	7	0	-2.021171	-4.939404	1.771786
85	6	0	-0.993846	-5.766896	1.123789
86	6	0	-1.545660	-6.574262	-0.041338
87	9	0	-5.496511	2.728256	1.693952
88	7	0	-7.825521	1.669158	2.674681
89	6	0	-9.151999	1.096285	2.751649
90	6	0	-10.190087	2.219126	2.809063
91	7	0	-9.795897	3.415574	1.990490
92	6	0	-8.499579	3.990442	2.546076
93	6	0	-7.725421	2.951728	3.345905
94	6	0	-9.598111	2.966865	0.546766
95	6	0	-9.444357	4.080131	-0.469606

96	6	0	-10.886826	4.468327	2.032526
97	6	0	-11.407724	4.855859	3.417144
98	6	0	-12.686039	4.142942	3.862768
99	6	0	-13.184500	4.668665	5.202539
100	8	0	-1.845377	-3.514971	0.051817
101	8	0	-1.608221	1.026025	-0.845311
102	7	0	-0.767270	1.274668	0.088676
103	8	0	-0.674067	2.366501	0.589902
104	8	0	-1.735713	-0.541352	-3.268867
105	8	0	-3.679467	-1.390985	-1.353486
106	6	0	-2.411939	-5.311848	3.131180
107	6	0	-3.217323	-6.600831	3.193195
108	6	0	-2.503393	-1.333803	-5.662066
109	6	0	-3.881583	-0.711090	-5.496814
110	6	0	-0.495570	-5.321475	-3.700660
111	6	0	-0.326678	-4.666390	-5.063063
112	1	0	2.025533	5.222155	-2.883228
113	1	0	2.400379	0.799038	-0.673522
114	1	0	-0.795803	2.513865	-5.297271
115	1	0	2.720984	6.895153	-1.669811
116	1	0	4.127654	6.197670	-2.491430
117	1	0	2.993657	6.206185	1.007210
118	1	0	3.493097	4.543499	1.261112
119	1	0	3.960642	7.991507	-0.028182
120	1	0	4.968651	8.182913	-1.463112
121	1	0	5.803931	4.994223	1.029252
122	1	0	5.193929	6.347406	1.995302
123	1	0	6.701998	6.757226	-1.872319
124	1	0	5.956235	5.229125	-1.358098
125	1	0	8.347156	4.967594	-1.288104
126	1	0	8.604882	6.413704	-0.318129
127	1	0	7.823098	4.982707	0.390604
128	1	0	7.266756	7.338933	1.250582

129	1	0	7.094968	8.390821	-0.155069
130	1	0	6.427632	9.118715	2.374224
131	1	0	4.880812	8.460685	1.935354
132	1	0	4.850000	10.091638	-0.069954
133	1	0	4.820716	10.812035	1.521938
134	1	0	6.397172	12.031004	0.050113
135	1	0	7.281588	11.282084	1.387106
136	1	0	7.344254	10.574751	-0.233429
137	1	0	-0.124631	5.281686	-4.169052
138	1	0	2.580699	4.518300	-5.509522
139	1	0	1.866708	6.203437	-5.417793
140	1	0	-0.188697	5.350857	-6.673365
141	1	0	0.598998	3.704327	-6.762368
142	1	0	-2.379670	-1.753461	-6.664193
143	1	0	-2.364560	-2.138763	-4.934807
144	1	0	-4.646452	-1.485016	-5.610540
145	1	0	-3.992888	-0.277791	-4.499309
146	1	0	-4.062999	0.068824	-6.242677
147	1	0	-0.339092	-0.874531	-7.165473
148	1	0	0.252770	0.549909	-6.334416
149	1	0	-0.843914	1.177710	-8.481527
150	1	0	-2.342645	0.380050	-7.994361
151	1	0	-1.810344	1.833829	-7.143957
152	1	0	6.460304	-2.756162	0.307172
153	1	0	2.035146	-0.930809	1.626963
154	1	0	3.513945	-4.550606	-2.743545
155	1	0	5.544350	-1.337978	4.257460
156	1	0	6.303640	0.229903	4.060384
157	1	0	8.031059	-2.533024	2.007020
158	1	0	7.921179	-1.191697	0.866579
159	1	0	7.684904	-2.497717	4.361356
160	1	0	7.527201	-1.296869	5.649361
161	1	0	8.736080	0.415600	2.431697

162	1	0	9.902045	-0.904033	2.252250
163	1	0	8.962028	0.379379	5.879783
164	1	0	8.168083	1.122937	4.486847
165	1	0	10.202097	2.327309	4.896648
166	1	0	11.203852	0.883780	4.947848
167	1	0	10.492449	1.431414	3.411198
168	1	0	10.981405	-1.129467	4.264339
169	1	0	10.078642	-1.606060	5.701248
170	1	0	11.142931	-3.341888	3.836009
171	1	0	9.528547	-3.229963	3.210582
172	1	0	8.677334	-3.917791	5.565919
173	1	0	9.584564	-5.118173	4.670059
174	1	0	10.320847	-5.041983	7.042584
175	1	0	11.651676	-4.573993	5.973945
176	1	0	10.772896	-3.346187	6.896185
177	1	0	6.262595	-3.198295	-2.209256
178	1	0	6.102220	-5.394669	-0.006899
179	1	0	7.622758	-4.850932	-0.873788
180	1	0	6.542608	-5.524375	-3.089349
181	1	0	5.079053	-6.088351	-2.154364
182	1	0	-0.653368	-6.398254	-3.803905
183	1	0	-1.359732	-4.896199	-3.182898
184	1	0	-1.231090	-4.826525	-5.658227
185	1	0	-0.175974	-3.588954	-4.952513
186	1	0	0.522415	-5.085773	-5.611297
187	1	0	0.799236	-7.127095	-2.253793
188	1	0	2.144425	-6.141786	-1.722110
189	1	0	2.854063	-7.715188	-3.521630
190	1	0	1.615370	-7.087108	-4.611733
191	1	0	2.975645	-6.059825	-4.154939
192	1	0	-7.700524	-0.987493	2.975414
193	1	0	-3.543082	1.100925	1.235826
194	1	0	-4.882723	-4.546709	2.127982

195	1	0	-9.303606	0.477932	3.650792
196	1	0	-9.313262	0.454951	1.878640
197	1	0	-8.105848	2.871686	4.374285
198	1	0	-6.689474	3.275035	3.419563
199	1	0	-10.325845	2.570935	3.831970
200	1	0	-11.156794	1.866509	2.443365
201	1	0	-7.910948	4.326820	1.692332
202	1	0	-8.744504	4.855429	3.163853
203	1	0	-10.468120	2.347991	0.307780
204	1	0	-8.709180	2.333802	0.560012
205	1	0	-9.193911	3.608945	-1.424631
206	1	0	-10.362244	4.651828	-0.621656
207	1	0	-8.630222	4.771744	-0.232796
208	1	0	-10.455665	5.333407	1.525657
209	1	0	-11.700531	4.085664	1.407706
210	1	0	-11.616042	5.931559	3.378067
211	1	0	-10.627130	4.752345	4.183521
212	1	0	-13.456995	4.292170	3.095684
213	1	0	-12.533267	3.059116	3.933248
214	1	0	-14.108403	4.164475	5.500574
215	1	0	-12.444485	4.506071	5.994628
216	1	0	-13.390181	5.743875	5.152758
217	1	0	-7.737830	-3.365421	2.026549
218	1	0	-5.971362	-4.844841	4.133248
219	1	0	-7.633677	-5.341729	3.561688
220	1	0	-8.528421	-3.101186	4.407268
221	1	0	-6.827045	-2.652775	4.917597
222	1	0	-1.487628	-5.420925	3.710554
223	1	0	-2.955499	-4.477588	3.578081
224	1	0	-3.470531	-6.829078	4.233048
225	1	0	-4.147498	-6.533897	2.618155
226	1	0	-2.647944	-7.448276	2.799034
227	1	0	-0.587132	-6.426226	1.894684

228	1	0	-0.189096	-5.104357	0.790823
229	1	0	-0.754504	-7.205672	-0.458244
230	1	0	-2.360874	-7.229749	0.279429
231	1	0	-1.917561	-5.913267	-0.828982

$Th{\cdot}2NO_3{\cdot}3$–**4''**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	9.289006	-1.508884	2.391884
2	7	0	8.075135	-2.139454	1.923833
3	6	0	8.092918	-3.600683	1.868170
4	6	0	9.515383	-4.111123	1.989613
5	7	0	10.166094	-3.725168	3.292329
6	6	0	9.847604	-2.266053	3.583943
7	6	0	7.174064	-1.408881	1.180023
8	6	0	5.854470	-1.893294	0.968647
9	6	0	4.923972	-1.192898	0.260153
10	6	0	5.246420	0.069331	-0.269304
11	6	0	6.540305	0.587105	-0.056598
12	6	0	7.490957	-0.155357	0.653645
13	7	0	6.845945	1.849996	-0.556085
14	6	0	5.905926	2.575416	-1.183704
15	6	0	4.628056	2.128631	-1.427124
16	6	0	4.235961	0.834293	-0.951264
17	8	0	3.070562	0.368329	-1.107769
18	90	0	0.946261	1.394120	-0.466213
19	8	0	-1.415239	1.037420	-1.479016
20	7	0	-1.568380	2.236381	-1.865379
21	8	0	-2.550428	2.614228	-2.448927
22	6	0	8.143383	2.443264	-0.300447
23	6	0	9.353118	1.891734	-0.999190
24	6	0	8.813166	3.235266	-1.381992

25	6	0	3.575733	3.004305	-1.989654
26	8	0	2.452767	3.009216	-1.422935
27	9	0	5.512564	-3.064235	1.519466
28	6	0	9.591511	-4.601071	4.396400
29	6	0	10.152107	-4.350899	5.782071
30	6	0	11.662417	-3.968021	3.226278
31	6	0	12.422050	-3.240628	2.113286
32	6	0	12.796229	-4.105430	0.903757
33	6	0	13.826548	-5.180536	1.230719
34	8	0	0.446926	-0.896720	-0.904124
35	6	0	-0.171017	-1.485957	-1.834078
36	6	0	-1.133417	-2.510586	-1.520319
37	6	0	-1.872497	-3.158262	-2.530023
38	7	0	-1.644471	-2.801243	-3.854139
39	6	0	-0.742803	-1.850174	-4.151627
40	6	0	0.034499	-1.202918	-3.219265
41	6	0	-1.377196	-2.837163	-0.174408
42	6	0	-2.318939	-3.772989	0.133180
43	6	0	-3.049624	-4.475259	-0.862633
44	6	0	-2.817112	-4.137393	-2.194897
45	7	0	-4.018060	-5.387920	-0.510985
46	6	0	-5.144380	-5.656830	-1.376728
47	6	0	-6.305540	-6.199500	-0.536358
48	7	0	-6.359485	-5.576586	0.832601
49	6	0	-5.091568	-5.942229	1.593774
50	6	0	-3.950833	-6.267984	0.635872
51	6	0	-6.462365	-4.067051	0.667094
52	6	0	-6.773734	-3.281995	1.926426
53	6	0	-7.576522	-6.068772	1.594088
54	6	0	-7.794497	-7.581713	1.633389
55	6	0	-8.753507	-8.138946	0.579365
56	6	0	-8.997621	-9.629561	0.776027
57	9	0	-2.610961	-4.013223	1.423395

58	6	0	0.965310	-0.113005	-3.601658
59	8	0	0.988090	0.941142	-2.920629
60	6	0	-2.441788	-3.381651	-4.916708
61	6	0	-1.783005	-3.747862	-6.211911
62	6	0	-2.242053	-4.825892	-5.279580
63	7	0	1.756610	-0.227421	-4.676479
64	6	0	2.054250	-1.468920	-5.392912
65	6	0	1.611427	-1.448645	-6.848123
66	6	0	2.535910	0.953402	-5.066401
67	6	0	1.685001	2.002813	-5.765004
68	8	0	2.706865	1.643627	1.374888
69	7	0	2.531863	0.499297	1.913339
70	8	0	1.589259	-0.187222	1.404660
71	8	0	-0.830380	1.473870	1.185989
72	6	0	-1.616299	2.431258	1.455540
73	6	0	-3.047454	2.284204	1.357675
74	6	0	-3.907562	3.370341	1.628779
75	7	0	-3.363401	4.584089	2.025134
76	6	0	-2.028996	4.731191	2.100186
77	6	0	-1.138531	3.716228	1.857312
78	6	0	-5.291464	3.236107	1.456599
79	6	0	-5.852072	2.031460	1.043969
80	6	0	-4.966258	0.939362	0.841043
81	6	0	-3.613155	1.057570	0.960439
82	6	0	-4.213830	5.734929	2.258053
83	6	0	-5.122658	5.744052	3.454027
84	6	0	-3.918679	6.633890	3.420207
85	6	0	0.325364	3.949752	1.791357
86	8	0	0.922253	3.560703	0.760136
87	9	0	-5.494062	-0.265281	0.533935
88	7	0	-7.223591	1.875394	0.913338
89	6	0	-8.086569	2.941554	1.390173
90	6	0	-9.552985	2.578400	1.158904

91	7	0	-9.818683	1.111656	1.329935
92	6	0	-9.005040	0.349314	0.296169
93	6	0	-7.815267	1.158507	-0.204651
94	6	0	-9.397862	0.713046	2.739542
95	6	0	-9.810935	-0.675896	3.180488
96	6	0	-11.296824	0.812876	1.153730
97	6	0	-11.957934	1.382913	-0.102715
98	6	0	-12.700046	2.713133	0.073002
99	6	0	-13.916744	2.612156	0.986228
100	7	0	0.986335	4.560178	2.775417
101	6	0	2.425356	4.801577	2.582388
102	6	0	2.698605	5.977556	1.658530
103	6	0	0.426789	4.881688	4.087409
104	6	0	0.354255	6.376242	4.361050
105	7	0	3.772713	3.786196	-3.052931
106	6	0	2.666670	4.674238	-3.452164
107	6	0	2.520160	5.880812	-2.539926
108	6	0	4.941179	3.742670	-3.930395
109	6	0	5.770054	5.017327	-3.894339
110	8	0	3.213640	0.100606	2.820780
111	8	0	-0.601559	3.022518	-1.573784
112	1	0	-5.922094	4.096765	1.625545
113	1	0	-2.965265	0.210431	0.766429
114	1	0	-1.692408	5.730619	2.348540
115	1	0	-7.916155	3.891443	0.859518
116	1	0	-7.885268	3.114184	2.452619
117	1	0	-8.115458	1.860114	-0.996087
118	1	0	-7.098036	0.473938	-0.650850
119	1	0	-9.863884	2.838745	0.147064
120	1	0	-10.194631	3.120350	1.856899
121	1	0	-8.671077	-0.570128	0.777878
122	1	0	-9.664057	0.085703	-0.531968
123	1	0	-9.832993	1.466799	3.402037

124	1	0	-8.311375	0.816448	2.757760
125	1	0	-9.351504	-0.852007	4.157559
126	1	0	-10.889720	-0.785964	3.306621
127	1	0	-9.453308	-1.463195	2.510009
128	1	0	-11.362434	-0.276488	1.165342
129	1	0	-11.786163	1.184677	2.059039
130	1	0	-12.685134	0.632303	-0.433846
131	1	0	-11.236635	1.454504	-0.927189
132	1	0	-12.028203	3.499425	0.438205
133	1	0	-13.024274	3.040125	-0.921434
134	1	0	-14.437165	3.572809	1.040443
135	1	0	-14.627667	1.866553	0.613069
136	1	0	-13.652612	2.334295	2.013616
137	1	0	-4.565875	6.188904	1.334648
138	1	0	-5.081016	4.884383	4.116710
139	1	0	-6.107498	6.185346	3.334134
140	1	0	-4.050701	7.699514	3.264472
141	1	0	-3.097555	6.372454	4.082144
142	1	0	2.847773	4.980342	3.574892
143	1	0	2.866604	3.882043	2.188903
144	1	0	3.778521	6.120333	1.552377
145	1	0	2.278859	5.788254	0.667666
146	1	0	2.269981	6.906054	2.048057
147	1	0	1.064279	4.395244	4.834922
148	1	0	-0.556245	4.414853	4.171739
149	1	0	-0.068310	6.549715	5.355529
150	1	0	1.346628	6.836658	4.338564
151	1	0	-0.268427	6.897550	3.625538
152	1	0	8.488319	0.244484	0.771641
153	1	0	3.917677	-1.581964	0.145241
154	1	0	6.219208	3.572821	-1.467112
155	1	0	7.722195	-3.950516	0.900189
156	1	0	7.437235	-4.036419	2.628581

157	1	0	10.041082	-1.384502	1.597541
158	1	0	9.049606	-0.506926	2.763313
159	1	0	10.128170	-3.700353	1.187542
160	1	0	9.543962	-5.200791	1.916852
161	1	0	9.098898	-2.254374	4.377869
162	1	0	10.754040	-1.785844	3.955314
163	1	0	9.773609	-5.633590	4.085735
164	1	0	8.512852	-4.430619	4.384018
165	1	0	9.555394	-4.940461	6.484152
166	1	0	11.188519	-4.677816	5.888918
167	1	0	10.073236	-3.305657	6.094612
168	1	0	12.038089	-3.673525	4.206502
169	1	0	11.779879	-5.052786	3.140200
170	1	0	13.348453	-2.858187	2.556899
171	1	0	11.877777	-2.345497	1.791744
172	1	0	11.905713	-4.573025	0.463525
173	1	0	13.200506	-3.442469	0.130561
174	1	0	14.082302	-5.754777	0.335442
175	1	0	14.749156	-4.734225	1.618297
176	1	0	13.464366	-5.896521	1.978206
177	1	0	8.250146	2.784323	0.726653
178	1	0	9.193800	1.077957	-1.700718
179	1	0	10.278730	1.836559	-0.434361
180	1	0	9.348974	4.128785	-1.078831
181	1	0	8.326034	3.308576	-2.350534
182	1	0	2.872220	4.984343	-4.480121
183	1	0	1.744454	4.086400	-3.451286
184	1	0	1.712972	6.520799	-2.908744
185	1	0	2.261864	5.560291	-1.528153
186	1	0	3.439508	6.473411	-2.504235
187	1	0	4.570017	3.571719	-4.948274
188	1	0	5.540377	2.867824	-3.670655
189	1	0	6.620580	4.924658	-4.576432

190	1	0	5.183513	5.884559	-4.212205
191	1	0	6.153659	5.228938	-2.890324
192	1	0	-3.349852	-4.659610	-2.978525
193	1	0	-0.835916	-2.316178	0.608923
194	1	0	-0.680883	-1.600967	-5.203604
195	1	0	-4.923586	-6.403592	-2.154232
196	1	0	-5.433572	-4.730410	-1.883302
197	1	0	-4.005359	-7.310127	0.294872
198	1	0	-3.003981	-6.162963	1.160770
199	1	0	-6.214058	-7.275488	-0.386024
200	1	0	-7.260615	-6.008406	-1.030241
201	1	0	-4.834960	-5.084897	2.215705
202	1	0	-5.315728	-6.789984	2.242367
203	1	0	-7.237418	-3.907276	-0.088040
204	1	0	-5.504214	-3.747778	0.256099
205	1	0	-6.633178	-2.223575	1.683200
206	1	0	-7.799533	-3.423053	2.275045
207	1	0	-6.092046	-3.501832	2.753203
208	1	0	-7.450178	-5.670650	2.602924
209	1	0	-8.438881	-5.570199	1.139593
210	1	0	-8.212877	-7.803307	2.622294
211	1	0	-6.840847	-8.126564	1.607668
212	1	0	-9.705039	-7.595801	0.647265
213	1	0	-8.375429	-7.965846	-0.435376
214	1	0	-9.698337	-10.011538	0.027994
215	1	0	-8.067109	-10.201547	0.685187
216	1	0	-9.420235	-9.833027	1.766315
217	1	0	-3.449257	-2.973945	-4.951336
218	1	0	-0.709622	-3.608723	-6.307320
219	1	0	-2.344026	-3.556924	-7.120815
220	1	0	-3.123070	-5.406515	-5.535766
221	1	0	-1.472773	-5.372071	-4.741042
222	1	0	3.139563	-1.615750	-5.338172

223	1	0	1.607605	-2.303192	-4.849915
224	1	0	1.869318	-2.399100	-7.325356
225	1	0	0.531890	-1.292700	-6.950693
226	1	0	2.111787	-0.653567	-7.409404
227	1	0	3.336949	0.603229	-5.722602
228	1	0	2.997397	1.364638	-4.164735
229	1	0	2.304104	2.859745	-6.049958
230	1	0	1.230384	1.601749	-6.675713
231	1	0	0.889481	2.358386	-5.104591

8. References

[1] Gaussian 16, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.

[2] Density-Functional Theory of Atoms and Molecules, Parr, R. G.; Yang, W. 1989, Oxford, New York.

[3] Adamo, C.; Barone, V. *J. Chem. Phys.* **1999**, *110*, 6158–6159.

[4] Modern Theoretical Chemistry Vol. 3, Dunning, T. H. Jr.; Hay, P. J. in , Ed. Schaefer III, H. F. 1977, Plenum, New York.

[5] Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. J. *Chem. Phys*. **2010**, *132*, 154104.