

Supporting Information

A Quasi-Relativistic DFT Study of the Actinyl(VI, V) (An= U, Np, Pu) Complexes with a Six-Membered Macrocycle Containing Pyrrole, Pyridine and Furan Subunits

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Table S1. The $\langle S^2 \rangle$ values of the actinyl(VI, V) complexes obtained with the B3LYP/6-31g* method.

	S	S(S+1)	$\langle S^2 \rangle$	$\langle S^2 \rangle - S(S+1)$
UO ₂ L	0	0	0.02	0.02
NpO ₂ L	0.5	0.75	0.77	0.02
PuO ₂ L	1	2	2.04	0.04
UO ₂ L ⁻	0.5	0.75	0.75	0
NpO ₂ L ⁻	1	2	2.00	0
PuO ₂ L ⁻	1.5	3.75	3.81	0.06

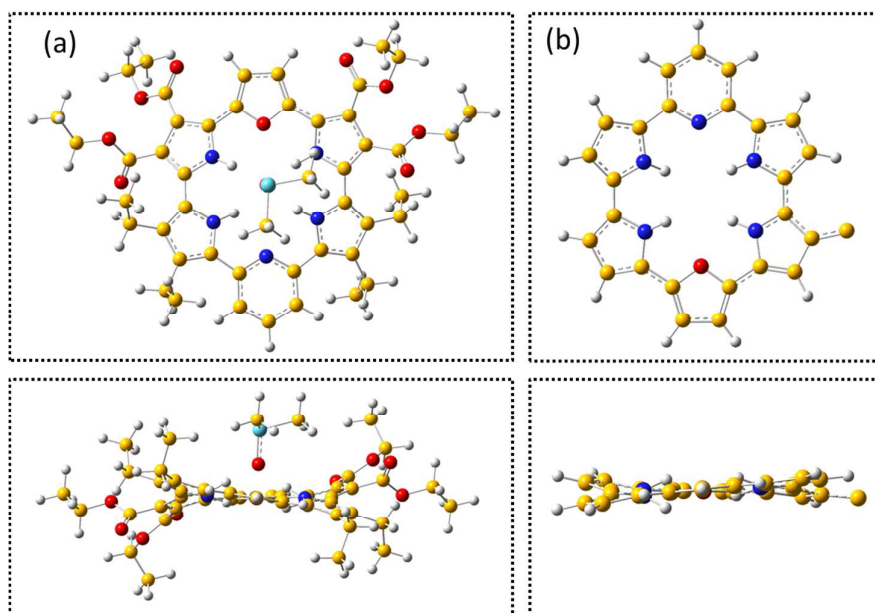
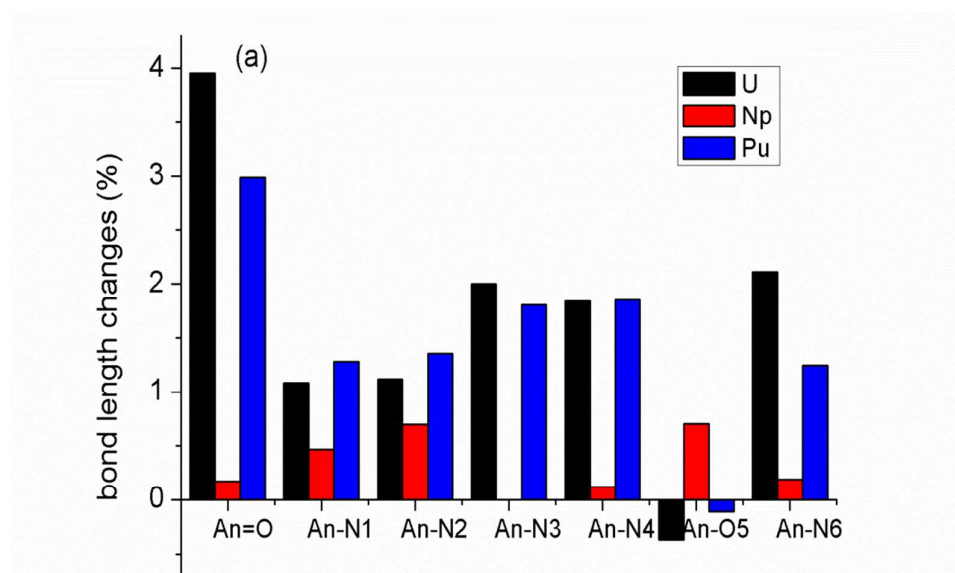


Figure S1. Optimized structures of (a) macrocycle H₄L with one DMSO molecule bound at the cavity site and (b) the unsubstituted analogue of H₄L. Top and side views are provided in the upper and lower panels, respectively. Orange, white, blues, red, and light blue spheres denote C, H, N, O, and S, respectively.



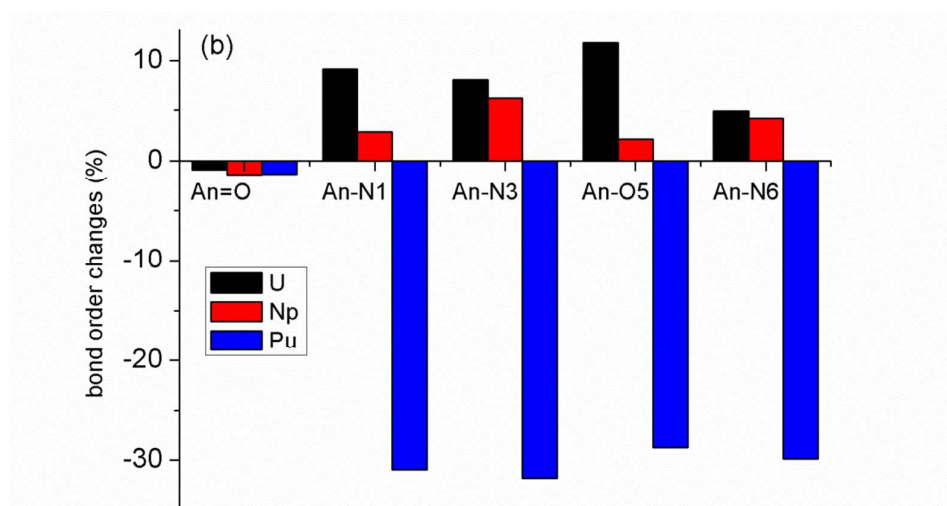


Figure S2. The obtained changes (%) of (a) structural parameters and (b) Mayer bond order values going from the AnO_2L to AnO_2L^- complexes, where An= U, Np and Pu.

Table S2. The Mulliken orbital population and spin densities of actinide in the actinyl(VI, V) complexes.

complexes	Mulliken orbital population				spin density
	5f	6d	7s	7p	An
UO_2L	2.41	1.77	0.09	0.02	0.00
NpO_2L	3.59	1.74	0.09	0.01	1.17
PuO_2L	4.72	1.68	0.10	0.01	2.37
UO_2L^-	2.36	1.75	0.13	0.09	0.00
NpO_2L^-	3.55	1.73	0.11	0.06	1.17
PuO_2L^-	5.02	1.57	0.10	0.09	3.37

Table S3. The Natural orbital population and spin densities of actinide in the free actinyl(VI, V) cations.

actinyls	natural orbital population				spin density
	5f	6d	7s	7p	An
UO ₂ ²⁺	2.54	1.01	0.04	0.03	-
NpO ₂ ²⁺	3.72	0.97	0.04	0.04	1.13
PuO ₂ ²⁺	4.88	0.93	0.03	0.03	2.35
UO ₂ ⁺	2.98	0.90	0.04	0.04	1.08
NpO ₂ ⁺	4.16	0.89	0.04	0.04	2.19
PuO ₂ ⁺	5.29	0.85	0.04	0.04	3.32

Table S4. The natural electron configuration of actinide in the free actinyl(VI, V) cations.

	natural electron configuration							
	alpha				beta			
	5f	6d	7s	7p	5f	6d	7s	7p
UO ₂ ²⁺	-	-	-	-	-	-	-	-
NpO ₂ ²⁺	2.41	0.50	0.02	0.02	1.31	0.47	0.02	0.02
PuO ₂ ²⁺	3.58	0.49	0.02	0.02	1.30	0.44	0.01	0.01
UO ₂ ⁺	2.02	0.46	0.02	0.02	0.96	0.44	0.02	0.02
NpO ₂ ⁺	3.15	0.47	0.02	0.02	1.01	0.42	0.02	0.02
PuO ₂ ⁺	4.28	0.45	0.02	0.02	1.01	0.40	0.02	0.02

Table S5. The natural electron configuration of actinide in the actinyl(VI, V) complexes.

	natural electron configuration							
	alpha				beta			
	5f	6d	7s	7p	5f	6d	7s	7p
UO ₂ L	-	-	-	-	-	-	-	-
NpO ₂ L	2.49	0.73	0.11	0.22	1.40	0.70	0.11	0.21
PuO ₂ L	3.64	0.71	0.12	0.21	1.40	0.66	0.11	0.21
UO ₂ L ⁻	1.28	0.73	0.11	0.21	1.28	0.73	0.11	0.21
NpO ₂ L ⁻	2.47	0.71	0.11	0.22	1.38	0.69	0.11	0.22
PuO ₂ L ⁻	4.28	0.64	0.10	0.21	1.02	0.58	0.10	0.21

Table S6. Charge decomposition analysis ($d > 0.010$) for UO_2L^- .

alpha electrons				beta electrons			
MOs	d	b	d-b	MOs	d	b	d-b
HOMO-12	0.019	0.000	0.019	HOMO-8	0.017	0.001	0.016
HOMO-13	0.033	0.001	0.031	HOMO-11	0.034	0.001	0.033
HOMO-15	0.036	0.000	0.036	HOMO-12	0.039	0.000	0.039
HOMO-16	0.035	0.000	0.035	HOMO-13	0.013	0.000	0.013
HOMO-23	0.019	0.000	0.018	HOMO-14	0.028	0.000	0.028
HOMO-26	0.035	0.000	0.035	HOMO-15	0.029	0.000	0.029
HOMO-27	0.013	0.000	0.013	HOMO-16	0.022	0.000	0.022
-	-	-	-	HOMO-22	0.019	0.000	0.019
-	-	-	-	HOMO-25	0.012	0.000	0.012
-	-	-	-	HOMO-26	0.011	0.000	0.011

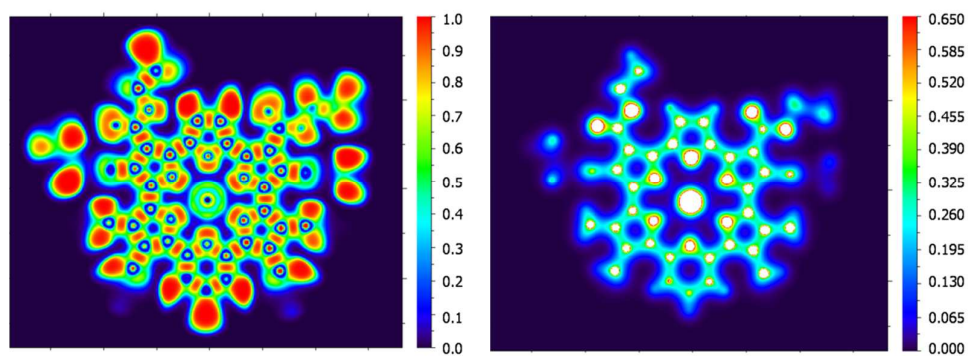
**Figure S3.** Electron localization function (left) and electron density (right) of UO_2L^- .

Table S7. Calculated symmetrical and asymmetrical stretching vibrational frequencies of the actinyl fragments (cm^{-1}) in the actinyl(VI, V) complexes.

	UO_2L	NpO_2L	PuO_2L	UO_2L^-	NpO_2L^-	PuO_2L^-
ν_{symm}	885	885	854	877	867	782
ν_{asymm}	967	979	975	959	966	870

Table S8. Calculated bond lengths and bond angles of the actinyl(VI, V) dichlorides in CH_2Cl_2 .

	UO_2Cl_2	NpO_2Cl_2	PuO_2Cl_2	UO_2Cl_2^-	$\text{NpO}_2\text{Cl}_2^-$	$\text{PuO}_2\text{Cl}_2^-$
U=O	1.758	1.738	1.727	1.826	1.793	1.771
U-Cl	2.534	2.515	2.518	2.699	2.698	2.697
O=U=O	164.7	170.1	173.1	151.3	166.9	172.3
Cl-U-Cl	107.3	105.3	108.1	117.2	122.3	126.6

Table S9. The obtained changes of the Gibbs free energy (kcal/mol), enthalpy (kcal/mol), and entropy (cal/K.mol) for complexing reactions of Equation (2) at $T=298.15$ K in dichloromethane, respectively. The energy data from the B3LYP/6-31g* basis set are presented for reference.

energy	UO_2L	NpO_2L	PuO_2L	UO_2L^-	NpO_2L^-	PuO_2L^-
	Equation (2)			Equation (2)		
ΔS	12.10	13.43	13.91	12.70	11.52	11.45
ΔH	-15.92	-13.74	-11.90	3.12	21.88	15.30
ΔG	-19.53	-17.74	-16.05	-0.66	18.44	11.89

Table S10. The obtained changes of the Gibbs free energy (kcal/mol), enthalpy (kcal/mol), and entropy (cal/K.mol) for complexing reactions (3)-(5) at T= 298.15 K in the gas phase and aqueous solution, respectively. These energy data from the B3LYP/6-31g* basis set are presented for reference.

energy	UO ₂ L	NpO ₂ L	PuO ₂ L	UO ₂ L ⁻	NpO ₂ L ⁻	PuO ₂ L ⁻
Equation (3)			Equation (3)			
ΔS	23.95	25.73	27.21	28.00	25.96	25.63
ΔH	10.75	11.61	12.70	17.80	33.34	25.71
ΔG	3.60	3.94	4.59	9.45	25.60	18.07
Equation (4)			Equation (5)			
ΔS	112.28	112.99	114.20	116.80	113.43	114.57
ΔH	42.63	43.74	41.29	43.42	60.14	50.77
ΔG	9.15	10.05	7.25	8.59	26.32	16.61

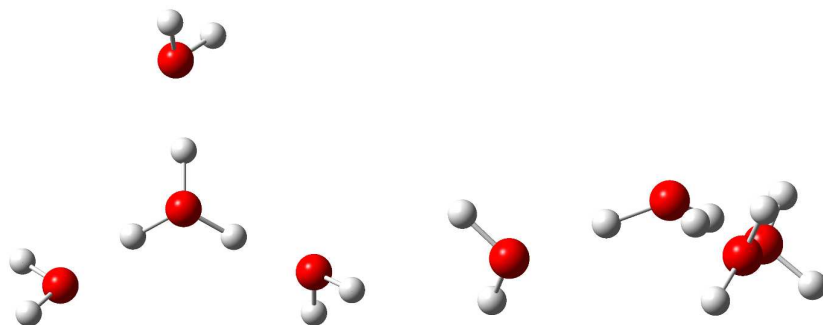


Figure S4. Optimized structure of the H₉O₄⁺ cluster on the right side of equation (3). Snapshots from two different perspectives are provided. H and O atoms are represented by white and red spheres, respectively.

Table S11. The optimized structures of the actinyl(VI, V) complexes in the gas phase.

UO ₂ L (0, 1)			
C	-2.38532000	2.10305000	0.03692000
C	-3.78268700	2.46643200	0.07841800
C	-4.48891700	1.26806300	0.13341200
C	-3.51530100	0.20431700	0.12612800
C	-3.56014000	-1.21927400	0.15079800
C	-4.58817400	-2.22788300	0.15352700
C	-3.93204400	-3.45700900	0.16468300
C	-2.52248000	-3.15910800	0.16309400
C	-1.33539300	-3.99283800	0.17735500
C	-1.38137500	-5.39576900	0.25285500
H	-2.32967500	-5.90964100	0.29880900
C	-0.19386000	-6.11494800	0.27514800
H	-0.21123900	-7.19905000	0.34039500
C	1.01621600	-5.43705000	0.21279100
H	1.94607700	-5.98485100	0.22649700
C	1.01777200	-4.03308200	0.13279000
C	2.23078100	-3.24060100	0.05895200
C	3.62966000	-3.58465300	0.04255400
C	4.32438400	-2.37596500	-0.01477500
C	3.32845600	-1.33680400	-0.03816300
C	3.32665900	0.08926500	-0.08035200
C	4.32797700	1.12746100	-0.12997100
C	3.64765000	2.34427200	-0.14311600
C	2.24564100	2.01495900	-0.09871200
C	1.06728300	2.79448900	-0.08572200
C	0.67267200	4.12940300	-0.11011000
H	1.35479900	4.96233200	-0.15416000
C	-0.72761000	4.15503800	-0.06961700
H	-1.36462300	5.02173900	-0.07598800
C	-1.17854300	2.83813600	-0.01976200
C	-4.46480300	3.77189900	0.09064300
C	-4.29371800	6.12627500	-0.02749500
H	-4.84863500	6.22893100	0.90987000
H	-5.01935000	6.15306300	-0.84600100
C	-3.22803100	7.19592400	-0.17847900
H	-2.51659800	7.16773100	0.65376700
H	-3.69997900	8.18443200	-0.18627000
H	-2.67646300	7.07535400	-1.11683700
C	-5.97739000	1.19097300	0.28106000
C	-8.04383100	1.27273700	-0.90383600
H	-8.39416500	0.62052300	-0.10017200
H	-8.31920400	0.83992100	-1.86877600

C	-8.58480400	2.68558500	-0.74727000
H	-8.19817700	3.33889900	-1.53517800
H	-8.29682400	3.10632300	0.21845600
H	-9.67921200	2.66583200	-0.81425700
C	-6.08384100	-2.05702400	0.15861900
H	-6.53139800	-2.85453600	-0.44798100
H	-6.35692300	-1.12803300	-0.34470500
C	-6.70313300	-2.09439300	1.56990200
H	-6.48124000	-3.04465500	2.06906500
H	-7.79246700	-1.98521100	1.51448100
H	-6.31765400	-1.28089100	2.18886600
C	-4.62068200	-4.79785500	0.12065100
H	-4.17906700	-5.48600700	0.85220100
H	-5.65802700	-4.67140600	0.44640900
C	-4.62384600	-5.44701600	-1.27786600
H	-5.13381500	-4.80050100	-2.00009500
H	-5.14267400	-6.41275700	-1.25889600
H	-3.60738300	-5.61331700	-1.65081400
C	4.26404600	-4.95191400	0.05903600
H	3.79923100	-5.58231500	0.82773300
H	5.30972400	-4.85210900	0.37006300
C	4.23297400	-5.67965800	-1.30073700
H	3.20935100	-5.82401400	-1.66264700
H	4.70978300	-6.66413100	-1.22519300
H	4.76678000	-5.10064900	-2.06110700
C	5.82188400	-2.23560200	-0.05007700
H	6.26655800	-3.03218700	0.55994100
H	6.11717600	-1.30486400	0.43802000
C	6.42568100	-2.30133500	-1.46671900
H	6.19739300	-3.26112700	-1.94255800
H	7.51572200	-2.19320400	-1.42577100
H	6.03611000	-1.50024100	-2.09948900
C	5.81487000	0.99916100	-0.22950000
C	7.84020900	1.01363100	1.00187600
H	8.22295800	1.81773900	0.36658800
H	8.16548900	0.06266000	0.56741600
C	8.28103900	1.16105800	2.44621500
H	7.93899700	2.11359900	2.86356100
H	9.37450100	1.12894400	2.50629200
H	7.87758000	0.35182600	3.06320400
C	4.20888000	3.70225300	-0.21280500
C	6.17913100	5.00296000	-0.40005700
H	5.90352500	5.62000300	0.46108800
H	5.77752800	5.48596500	-1.29624600

C	7.67782900	4.78786200	-0.49499900
H	8.06829200	4.33247200	0.42105900
H	8.18071700	5.75043000	-0.63897300
H	7.92417000	4.13731500	-1.34006700
N	-2.26481500	0.75299200	0.06775200
N	-2.32541000	-1.82606300	0.15085300
N	-0.14791000	-3.33161200	0.12456600
N	2.07626300	-1.90228200	0.00838700
N	2.08994800	0.67099700	-0.06074400
O	-0.07035900	2.01525200	-0.03068500
O	-5.67171700	3.89585500	0.20352700
O	-3.63727200	4.83439000	-0.03673600
O	-6.53563600	1.05519500	1.34774500
O	-6.59194000	1.26032900	-0.91427700
O	6.42055900	0.85876900	-1.26944700
O	6.39362200	1.06360300	0.98504900
O	3.55044700	4.72978000	-0.23701000
O	5.55769100	3.70481600	-0.25975800
O	-0.16673800	-0.71957500	-1.72497200
O	-0.04763500	-0.61594700	1.81291200
U	-0.10768400	-0.68426600	0.04449700

UO ₂ L ⁻ (-1, 2)			
C	-2.42600600	2.09330800	0.03689000
C	-3.82558800	2.45876500	0.08110400
C	-4.53216600	1.24405100	0.14930300
C	-3.55855200	0.19353200	0.14680300
C	-3.58102000	-1.24056500	0.17576500
C	-4.60921900	-2.26676800	0.15679900
C	-3.94469600	-3.48537900	0.17026100
C	-2.52322700	-3.16955200	0.19526700
C	-1.32066200	-4.01378800	0.22180900
C	-1.36174700	-5.41812200	0.33209100
H	-2.30487300	-5.93956700	0.40873400
C	-0.16725200	-6.12685800	0.35495500
H	-0.17967500	-7.21041000	0.44596800
C	1.04402800	-5.45197200	0.26284100
H	1.97300300	-6.00253200	0.27944800
C	1.03760600	-4.04689200	0.15524400
C	2.25947700	-3.23457600	0.05457500
C	3.67367500	-3.58565000	0.02296900
C	4.36573400	-2.38349800	-0.05444400
C	3.36086500	-1.33428500	-0.07168300
C	3.36895100	0.10023400	-0.11976500

C	4.36184900	1.13533900	-0.16332000
C	3.67004100	2.36233900	-0.17593800
C	2.26797300	2.01721500	-0.13866900
C	1.05546400	2.80464300	-0.12186600
C	0.66864100	4.12684800	-0.15563400
H	1.34626200	4.96267700	-0.21311100
C	-0.75155900	4.15015300	-0.10330900
H	-1.38731100	5.01769000	-0.11312400
C	-1.18860500	2.84342300	-0.03809400
C	-4.50838500	3.74787000	0.09635200
C	-4.34246600	6.10258800	-0.00132100
H	-4.90098400	6.20143300	0.93563000
H	-5.07062700	6.14186100	-0.81862000
C	-3.28257400	7.18183900	-0.14112400
H	-2.56727200	7.14124600	0.68718100
H	-3.75644100	8.17036900	-0.13589200
H	-2.73027700	7.07128600	-1.08031400
C	-6.01614300	1.16707700	0.28206000
C	-8.06826500	1.26882500	-0.92325800
H	-8.43108800	0.61002900	-0.12979100
H	-8.34744100	0.85110400	-1.89498800
C	-8.60527500	2.68304400	-0.75051000
H	-8.21235900	3.34374200	-1.52928800
H	-8.30838100	3.09011700	0.21819700
H	-9.70086000	2.67255100	-0.81588900
C	-6.10549400	-2.10047200	0.13249400
H	-6.54422900	-2.89920500	-0.48057300
H	-6.36975200	-1.17040400	-0.37539900
C	-6.75246200	-2.13390900	1.53106900
H	-6.53867800	-3.08375800	2.03573000
H	-7.84172100	-2.02269500	1.45842000
H	-6.37546500	-1.31903600	2.15348900
C	-4.61386900	-4.83368200	0.09783700
H	-4.20001400	-5.51527400	0.85289300
H	-5.67004400	-4.72127700	0.36619500
C	-4.53216900	-5.49080200	-1.29468600
H	-5.01279800	-4.85433900	-2.04578400
H	-5.03435000	-6.46691600	-1.30023100
H	-3.49379900	-5.63970000	-1.60936900
C	4.30176000	-4.95448400	0.03847000
H	3.84719900	-5.57786400	0.81980100
H	5.35609500	-4.86068800	0.32428800
C	4.23340200	-5.69269800	-1.31434700
H	3.19941700	-5.82486600	-1.65009700

H	4.69932900	-6.68420000	-1.24490800
H	4.75683600	-5.12281300	-2.08931200
C	5.86132100	-2.23861900	-0.12634900
H	6.32918400	-3.05471200	0.44036300
H	6.16847900	-1.32213200	0.38272300
C	6.42280200	-2.25014100	-1.56184000
H	6.17397900	-3.19069700	-2.06657000
H	7.51478700	-2.14426600	-1.55319200
H	6.01479300	-1.42419100	-2.14956600
C	5.84596900	1.01772800	-0.23051700
C	7.83865700	1.00285000	1.05063800
H	8.23874000	1.82466700	0.44826200
H	8.18204800	0.06548900	0.59882000
C	8.24945800	1.11107000	2.50876900
H	7.89276400	2.05041800	2.94388800
H	9.34187400	1.07969200	2.59538900
H	7.83147700	0.28499400	3.09326200
C	4.22459600	3.70879000	-0.22973000
C	6.20020100	5.00925500	-0.35798100
H	5.89982700	5.63813600	0.48761100
H	5.82974300	5.49144500	-1.26915300
C	7.70459200	4.80439200	-0.40436400
H	8.06645500	4.35229100	0.52538700
H	8.21075500	5.76771200	-0.53746000
H	7.97888100	4.14729300	-1.23593200
N	-2.30650100	0.76284400	0.07909500
N	-2.35021800	-1.84437300	0.19363100
N	-0.13344400	-3.36183700	0.14526300
N	2.11709800	-1.90766600	-0.00669000
N	2.12547700	0.69152200	-0.10479800
O	-0.07935300	2.03052200	-0.05104600
O	-5.71909700	3.88973800	0.20567700
O	-3.68139400	4.82490800	-0.02258800
O	-6.61049000	1.01946500	1.32960700
O	-6.62467700	1.24911200	-0.92660800
O	6.50102900	0.90550800	-1.24584500
O	6.40038500	1.04969000	1.00658100
O	3.58647500	4.75155600	-0.27865400
O	5.58984400	3.71638700	-0.22887400
O	-0.19372400	-0.72767200	-1.79330400
O	-0.01247900	-0.57977000	1.88022800
U	-0.10533100	-0.65911400	0.04387300

NpO₂L (0, 2)

C	-2.38150600	2.10354400	0.04065000
C	-3.77883800	2.46481600	0.08129700
C	-4.48333000	1.26529500	0.13290200
C	-3.50794300	0.20350700	0.12416400
C	-3.55213500	-1.21910900	0.14509400
C	-4.58183000	-2.22607200	0.14294600
C	-3.92733700	-3.45561900	0.15329200
C	-2.51770700	-3.15912900	0.15632400
C	-1.33327500	-3.99549600	0.17411300
C	-1.38094600	-5.39854000	0.25098500
H	-2.32967400	-5.91181300	0.29459500
C	-0.19384700	-6.11802400	0.27819200
H	-0.21131100	-7.20203900	0.34491800
C	1.01603100	-5.43954600	0.21895700
H	1.94625800	-5.98659300	0.23672200
C	1.01613800	-4.03553800	0.13700700
C	2.22674400	-3.24016600	0.06551700
C	3.62589100	-3.58248600	0.05335900
C	4.31887200	-2.37330000	-0.00327300
C	3.32097300	-1.33602600	-0.03118400
C	3.31955000	0.08886600	-0.07505100
C	4.32238400	1.12495900	-0.12839700
C	3.64394500	2.34284300	-0.14065600
C	2.24214500	2.01559000	-0.09245900
C	1.06603400	2.79764600	-0.07855200
C	0.67301800	4.13309000	-0.10176700
H	1.35546200	4.96574500	-0.14478000
C	-0.72731600	4.15870900	-0.06169100
H	-1.36466400	5.02512500	-0.06758300
C	-1.17672000	2.84121200	-0.01333800
C	-4.46252500	3.76934100	0.09593500
C	-4.29512900	6.12406500	-0.01927700
H	-4.84957400	6.22479800	0.91858400
H	-5.02140600	6.15074700	-0.83722300
C	-3.23126000	7.19560900	-0.16976200
H	-2.51926600	7.16767700	0.66201000
H	-3.70480300	8.18336800	-0.17624000
H	-2.68002800	7.07687200	-1.10854800
C	-5.97186200	1.18723600	0.27935300
C	-8.03758000	1.27223000	-0.90670900
H	-8.38821700	0.61753800	-0.10519100
H	-8.31220900	0.84210300	-1.87307800
C	-8.57940100	2.68434000	-0.74639800
H	-8.19257500	3.34016800	-1.53211800

H	-8.29228200	3.10241100	0.22073000
H	-9.67375600	2.66418400	-0.81422100
C	-6.07745900	-2.05449500	0.14401100
H	-6.52302500	-2.84930100	-0.46763400
H	-6.34899700	-1.12354200	-0.35624300
C	-6.70145900	-2.09842800	1.55300600
H	-6.48190900	-3.05134100	2.04814000
H	-7.79054500	-1.98817500	1.49460800
H	-6.31740800	-1.28834100	2.17727700
C	-4.61690700	-4.79582400	0.10397300
H	-4.18022700	-5.48524100	0.83728600
H	-5.65594200	-4.66864500	0.42394400
C	-4.61295700	-5.44360800	-1.29516300
H	-5.11817500	-4.79579500	-2.01957700
H	-5.13301500	-6.40876600	-1.28003100
H	-3.59462100	-5.61079500	-1.66253600
C	4.26189200	-4.94895700	0.07367300
H	3.79668300	-5.57849400	0.84284300
H	5.30694400	-4.84701400	0.38616300
C	4.23419400	-5.67964200	-1.28461800
H	3.21141100	-5.82641900	-1.64787400
H	4.71243200	-6.66320800	-1.20617600
H	4.76831100	-5.10142300	-2.04536300
C	5.81652500	-2.23193700	-0.03092500
H	6.25757400	-3.02276100	0.58926300
H	6.10852900	-1.29697300	0.45077200
C	6.42952400	-2.31072300	-1.44287500
H	6.20712600	-3.27613700	-1.91000500
H	7.51900800	-2.19907700	-1.39620700
H	6.04162600	-1.51743500	-2.08635700
C	5.80859300	0.99540500	-0.23493300
C	7.84101700	1.02176700	0.98438200
H	8.21940400	1.81946700	0.33851600
H	8.16443800	0.06658100	0.55782400
C	8.29042500	1.18429700	2.42445100
H	7.95020200	2.14085800	2.83404500
H	9.38425000	1.15350500	2.47833000
H	7.89125000	0.38118300	3.05213800
C	4.20640200	3.69998100	-0.21488400
C	6.17593900	4.99850200	-0.42179700
H	5.91013800	5.61514200	0.44271700
H	5.76523900	5.48271200	-1.31321000
C	7.67337400	4.78237800	-0.53308600
H	8.07367800	4.32686300	0.37864300

H	8.17525500	5.74462000	-0.68269200
H	7.91005300	4.13157900	-1.38071800
N	-2.25775100	0.75359700	0.06874100
N	-2.31758600	-1.82691000	0.14687800
N	-0.14763700	-3.33438700	0.12433500
N	2.06894800	-1.90272200	0.01305000
N	2.08317100	0.67183600	-0.05328100
O	-0.07009300	2.01901600	-0.02423100
O	-0.05248900	-0.62335800	1.79431400
O	-0.16234500	-0.71853100	-1.70157100
O	-5.66956300	3.89161200	0.20975500
O	-3.63667900	4.83328800	-0.03055200
O	-6.53104300	1.04863200	1.34517300
O	-6.58573500	1.26035500	-0.91626000
O	6.40856300	0.84650000	-1.27701600
O	6.39440600	1.07059500	0.97573500
O	3.54952500	4.72866600	-0.23162700
O	5.55480900	3.70086600	-0.27605000
Np	-0.10744700	-0.68161600	0.04670300

NpO ₂ L ⁻ (-1, 3)			
C	-2.40119000	2.10929900	0.05586300
C	-3.78767300	2.46495900	0.11904700
C	-4.49354700	1.24257600	0.14997400
C	-3.52545800	0.20308000	0.10081200
C	-3.55445100	-1.23663800	0.07488900
C	-4.57267300	-2.23531500	-0.01444200
C	-3.91290600	-3.47304400	-0.01220200
C	-2.51747800	-3.17887500	0.07170200
C	-1.33744400	-4.00953900	0.13022300
C	-1.38484900	-5.41590700	0.21182100
H	-2.33393900	-5.93087800	0.22621100
C	-0.19655800	-6.12932400	0.29035200
H	-0.21478400	-7.21431800	0.36341800
C	1.01482000	-5.45276000	0.27555500
H	1.94415400	-5.99878900	0.33198700
C	1.01836900	-4.04486300	0.18486000
C	2.22436800	-3.25212000	0.14948300
C	3.61077600	-3.58339000	0.22327100
C	4.30652700	-2.36353000	0.16422900
C	3.31632400	-1.34259000	0.04302800
C	3.32521600	0.09826700	-0.04597100
C	4.31532900	1.11308800	-0.14272300

C	3.63138000	2.35278400	-0.16044100
C	2.24350400	2.02509500	-0.08095200
C	1.05728300	2.81060000	-0.06811700
C	0.66867100	4.13762600	-0.09138500
H	1.35157200	4.96953400	-0.13723500
C	-0.74212800	4.16317500	-0.04588700
H	-1.37880300	5.02976400	-0.05364600
C	-1.18742500	2.85359500	0.00628400
C	-4.46898700	3.75206900	0.20269100
C	-4.31380700	6.10958500	0.17570500
H	-4.83578600	6.17351500	1.13643500
H	-5.07358500	6.17446300	-0.61063500
C	-3.26390800	7.19828900	0.03262200
H	-2.51741500	7.13362600	0.83137200
H	-3.74081600	8.18373700	0.08927700
H	-2.74722000	7.12257100	-0.93008400
C	-5.97355700	1.15836000	0.30960400
C	-8.05364400	1.35138700	-0.83698700
H	-8.39851400	0.65286700	-0.07014400
H	-8.35826200	0.98504800	-1.82196100
C	-8.58370200	2.75502800	-0.57798100
H	-8.20916700	3.45548300	-1.33077600
H	-8.26181000	3.11126800	0.40282100
H	-9.68066700	2.74900900	-0.61630100
C	-6.06668000	-2.06591600	-0.10712500
H	-6.46720900	-2.81169300	-0.80809000
H	-6.30790500	-1.09854400	-0.55287900
C	-6.79545200	-2.21464400	1.24284400
H	-6.60464700	-3.20090700	1.68269700
H	-7.88026700	-2.10276300	1.11637600
H	-6.46045500	-1.45157200	1.94919900
C	-4.60114900	-4.80753300	-0.15627700
H	-4.23406100	-5.52296700	0.59164100
H	-5.66562000	-4.68370300	0.07128700
C	-4.47650300	-5.42249300	-1.56462200
H	-4.90667800	-4.74941300	-2.31468300
H	-5.00325000	-6.38405700	-1.62521000
H	-3.42912700	-5.58914200	-1.83794300
C	4.25791600	-4.94044200	0.33756400
H	3.74689400	-5.55149900	1.09360300
H	5.28046500	-4.81604400	0.71464500
C	4.33006100	-5.72429900	-0.98943700
H	3.33334400	-5.89987900	-1.40799600
H	4.81689700	-6.69814200	-0.84638100

H	4.90079000	-5.16411600	-1.73742200
C	5.80228300	-2.21787700	0.26239600
H	6.18230700	-2.93748400	1.00188600
H	6.05203500	-1.23553700	0.67017200
C	6.55492100	-2.43718000	-1.06405500
H	6.37504100	-3.44666800	-1.45026900
H	7.63736900	-2.31647000	-0.92488700
H	6.23278200	-1.71501300	-1.81803900
C	5.79009600	0.97428000	-0.28281700
C	7.86254900	1.14148400	0.85200800
H	8.21983400	1.83862400	0.08740600
H	8.17768900	0.13546200	0.55274800
C	8.37248300	1.50211300	2.23665600
H	8.04418200	2.50716600	2.52198500
H	9.46840300	1.47576500	2.25368200
H	7.99768800	0.79667700	2.98557100
C	4.18748300	3.69212800	-0.29514500
C	6.14012200	4.97350400	-0.68341800
H	5.95629600	5.60394900	0.19387700
H	5.65938700	5.46089700	-1.53874700
C	7.62456800	4.75922100	-0.92427400
H	8.10325900	4.30931300	-0.04799200
H	8.11361000	5.71918700	-1.12768000
H	7.78546600	4.09686500	-1.78095900
N	-2.27391900	0.75840100	0.05015900
N	-2.32414100	-1.83483700	0.11299900
N	-0.14887500	-3.34653500	0.12425300
N	2.06975600	-1.90480100	0.04512500
N	2.08542600	0.68114300	-0.01586700
O	-0.07925200	2.03101400	-0.00794500
O	-0.07808500	-0.63195500	1.81451700
O	-0.14337100	-0.71562600	-1.71175300
O	-5.67400900	3.88844100	0.36559500
O	-3.65003900	4.83669500	0.08353000
O	-6.54665700	0.94043800	1.35685800
O	-6.61135800	1.33146400	-0.87602800
O	6.38266100	0.70485500	-1.30742900
O	6.42595100	1.19239700	0.89756700
O	3.56157000	4.74414400	-0.26912100
O	5.54096900	3.68572400	-0.47844100
Np	-0.10986600	-0.68881100	0.05172900

PuO ₂ L (0, 3)			
C	-2.37827100	2.10649700	0.01182300

C	-3.77550800	2.46724000	0.05999600
C	-4.47837800	1.26749200	0.12939700
C	-3.50155800	0.20733500	0.12297600
C	-3.54429400	-1.21471600	0.16666500
C	-4.57488900	-2.22038300	0.19354100
C	-3.92045200	-3.44996900	0.20997800
C	-2.51103000	-3.15350000	0.18523700
C	-1.32718800	-3.99101800	0.18970500
C	-1.37545500	-5.39495700	0.25144800
H	-2.32442300	-5.90784500	0.29244300
C	-0.18830500	-6.11491400	0.26278400
H	-0.20521100	-7.19955500	0.31914500
C	1.02085800	-5.43567200	0.19831100
H	1.95166700	-5.98208200	0.20253700
C	1.01948400	-4.03090900	0.12715700
C	2.22864000	-3.23476500	0.04311400
C	3.62686200	-3.57825100	0.00170900
C	4.31939700	-2.36848400	-0.05414500
C	3.32104700	-1.33123300	-0.05268400
C	3.31967700	0.09387500	-0.09542300
C	4.32362900	1.12976900	-0.13584000
C	3.64496400	2.34742800	-0.15500400
C	2.24303300	2.01923000	-0.12221900
C	1.06710100	2.80226500	-0.11642600
C	0.67482600	4.13807500	-0.14281300
H	1.35710100	4.97097500	-0.18711700
C	-0.72590100	4.16347900	-0.10353200
H	-1.36311600	5.03007900	-0.10965400
C	-1.17429900	2.84557600	-0.05316800
C	-4.46164400	3.77024300	0.06223800
C	-4.29856500	6.12493800	-0.05112400
H	-4.86881100	6.22260300	0.87753100
H	-5.01149200	6.15092900	-0.88084300
C	-3.23577400	7.19999900	-0.18254600
H	-2.53657500	7.17215500	0.65996900
H	-3.71225400	8.18631300	-0.19411500
H	-2.66972800	7.08549400	-1.11304900
C	-5.96527200	1.19097600	0.29161300
C	-8.04165700	1.23519700	-0.88066100
H	-8.38610800	0.65751600	-0.01981300
H	-8.32730900	0.72088700	-1.80185400
C	-8.57483300	2.65894700	-0.84399800
H	-8.20154700	3.23570600	-1.69577800
H	-8.26619900	3.16481900	0.07349700

H	-9.67038500	2.63966500	-0.88869800
C	-6.07004500	-2.04924400	0.22149900
H	-6.52736000	-2.85729400	-0.36331500
H	-6.35288000	-1.12934000	-0.29243800
C	-6.66221800	-2.06457200	1.64484900
H	-6.42605000	-3.00551700	2.15498000
H	-7.75290900	-1.96034500	1.60976700
H	-6.26715000	-1.23947800	2.24211600
C	-4.61228000	-4.78999400	0.19970000
H	-4.14327900	-5.47463600	0.91718900
H	-5.63629600	-4.66037800	0.56447600
C	-4.66976200	-5.44632200	-1.19434300
H	-5.20873500	-4.80392600	-1.89902100
H	-5.18566100	-6.41282600	-1.15055700
H	-3.66831700	-5.61225000	-1.60616500
C	4.26284100	-4.94472500	-0.00937800
H	3.81737100	-5.58392000	0.76368100
H	5.31537600	-4.84562300	0.27741700
C	4.20212300	-5.65920700	-1.37519200
H	3.17080300	-5.80648500	-1.71331100
H	4.68647400	-6.64142400	-1.32130100
H	4.71371000	-5.06917200	-2.14228700
C	5.81572200	-2.22683700	-0.11567600
H	6.27209200	-3.03883300	0.46456900
H	6.12066600	-1.30911200	0.39019100
C	6.39067900	-2.25586200	-1.54552700
H	6.15323200	-3.20344900	-2.04114400
H	7.48115700	-2.14684200	-1.52433800
H	5.98754200	-1.43937800	-2.14951500
C	5.81182100	1.00327400	-0.21608600
C	7.81760700	0.97509400	1.04736000
H	8.21322100	1.79530400	0.44131300
H	8.14692500	0.03556300	0.59144100
C	8.23602900	1.07970400	2.50206000
H	7.88905400	2.02046700	2.94153200
H	9.32838100	1.04372200	2.57803600
H	7.82183000	0.25381000	3.08914700
C	4.20915400	3.70445900	-0.21463600
C	6.18807300	5.00096100	-0.33472000
H	5.86803600	5.62971300	0.50215600
H	5.83558800	5.47231800	-1.25750100
C	7.68942000	4.78322600	-0.34680100
H	8.02891700	4.33822100	0.59438400
H	8.20139200	5.74323800	-0.47517400

H	7.97932600	4.12238900	-1.16983100
N	-2.25225800	0.75689700	0.04871600
N	-2.30971900	-1.82212300	0.15996500
N	-0.14296600	-3.32915900	0.13610300
N	2.06963300	-1.89738200	0.00821900
N	2.08309100	0.67567800	-0.08560500
O	-0.06825500	2.02422000	-0.06455500
O	-0.04027900	-0.55889600	1.77689300
O	-0.16700000	-0.78622800	-1.69321900
O	-5.67065600	3.89043000	0.15817300
O	-3.63643600	4.83615100	-0.05275600
O	-6.51394900	1.08723100	1.36682000
O	-6.59004400	1.22090800	-0.90068500
O	6.43424300	0.89535800	-1.25004800
O	6.37173000	1.03004400	1.00906900
O	3.55387600	4.73280100	-0.27071300
O	5.55904100	3.70517800	-0.21013300
Pu	-0.10439500	-0.67899600	0.04190900

PuO ₂ L ⁻ (-1, 4)			
C	-2.41279600	2.09918700	0.04009600
C	-3.81509000	2.46595200	0.08265300
C	-4.51880800	1.25594100	0.14749200
C	-3.54056500	0.19932200	0.14385500
C	-3.57468700	-1.23501900	0.17284700
C	-4.60471500	-2.25423100	0.16412200
C	-3.94269200	-3.47697100	0.17796300
C	-2.52319000	-3.16511200	0.19147700
C	-1.32037000	-4.00458900	0.21157500
C	-1.36305900	-5.40845800	0.31729100
H	-2.30740200	-5.92879500	0.38992100
C	-0.16984600	-6.12002800	0.33991900
H	-0.18270600	-7.20378100	0.42822100
C	1.04064900	-5.44282900	0.25164400
H	1.97055600	-5.99245300	0.26916500
C	1.03451300	-4.03820800	0.14621700
C	2.25740800	-3.23265900	0.04963900
C	3.66770600	-3.58156100	0.01552100
C	4.35916400	-2.37516200	-0.05742100
C	3.35407900	-1.33161000	-0.06923700
C	3.35239000	0.10493400	-0.11247200
C	4.35049100	1.14482700	-0.15640800
C	3.66258500	2.36832300	-0.16675600
C	2.25862900	2.02294400	-0.12736900

C	1.05646900	2.80309900	-0.10866900
C	0.66607500	4.13368300	-0.13800600
H	1.34552800	4.96841200	-0.19169800
C	-0.74406300	4.15704000	-0.08836000
H	-1.38093500	5.02388600	-0.09587100
C	-1.18593400	2.84229600	-0.02856100
C	-4.49931100	3.75719000	0.09148900
C	-4.33437200	6.11114000	-0.02158800
H	-4.89449400	6.21651300	0.91361300
H	-5.06085700	6.14333800	-0.84057400
C	-3.27438400	7.18931700	-0.16789700
H	-2.56151400	7.15668800	0.66285800
H	-3.74874900	8.17755700	-0.17274200
H	-2.71948700	7.07072900	-1.10454600
C	-6.00330200	1.17892600	0.27998500
C	-8.05480300	1.26495700	-0.92659200
H	-8.41506500	0.61004800	-0.12884400
H	-8.33163800	0.83945600	-1.89552500
C	-8.59727200	2.67822300	-0.76358400
H	-8.20649900	3.33531400	-1.54655300
H	-8.30308500	3.09260000	0.20287600
H	-9.69271300	2.66316900	-0.82980200
C	-6.10151100	-2.08714900	0.15155400
H	-6.54611400	-2.88778200	-0.45503500
H	-6.37058300	-1.15949200	-0.35828000
C	-6.73909300	-2.11504000	1.55450800
H	-6.52123600	-3.06271300	2.06151700
H	-7.82916600	-2.00447300	1.49015400
H	-6.35725200	-1.29817800	2.17150700
C	-4.61915700	-4.82278500	0.11594700
H	-4.19606100	-5.50782600	0.86266500
H	-5.67018500	-4.70645200	0.40286300
C	-4.56571400	-5.47993000	-1.27796500
H	-5.05386800	-4.83954000	-2.02094700
H	-5.07451600	-6.45285900	-1.27655500
H	-3.53341400	-5.63483600	-1.60941600
C	4.30098300	-4.94881400	0.02415900
H	3.84979400	-5.57905700	0.80207700
H	5.35503100	-4.85280600	0.31110300
C	4.23707500	-5.68227200	-1.33141500
H	3.20334800	-5.82024000	-1.66578500
H	4.71062200	-6.67080100	-1.26754500
H	4.75445100	-5.10511400	-2.10517100
C	5.85532600	-2.23094300	-0.12794300

H	6.32262000	-3.04568100	0.44162100
H	6.16322300	-1.31393100	0.37989100
C	6.42146400	-2.24600100	-1.56147800
H	6.17293000	-3.18717400	-2.06517500
H	7.51384800	-2.14145500	-1.55107200
H	6.01514900	-1.42129900	-2.15229800
C	5.83464100	1.02526900	-0.22812700
C	7.83036500	0.99820500	1.04756800
H	8.23316500	1.82060100	0.44772400
H	8.16735300	0.06094800	0.59101800
C	8.24508700	1.09803600	2.50515700
H	7.89404000	2.03714100	2.94543200
H	9.33754200	1.06102100	2.58893900
H	7.82456900	0.27125000	3.08676100
C	4.22000900	3.71597500	-0.22105300
C	6.19733100	5.01311100	-0.35390900
H	5.90199800	5.64204100	0.49337600
H	5.82374100	5.49612300	-1.26329000
C	7.70079200	4.80383800	-0.40706200
H	8.06559300	4.35076200	0.52101700
H	8.20890800	5.76576400	-0.54255300
H	7.96927600	4.14592400	-1.23982800
N	-2.29556000	0.76397000	0.07907700
N	-2.34506600	-1.84117600	0.18389100
N	-0.13484300	-3.35301100	0.13614200
N	2.11189700	-1.90498000	-0.00551900
N	2.11716000	0.69204900	-0.09456100
O	-0.07757700	2.03175800	-0.04221200
O	-0.02084800	-0.59998300	1.83245700
O	-0.18542300	-0.72782800	-1.74586600
O	-5.70963000	3.89817700	0.19795100
O	-3.67284500	4.83288400	-0.03192800
O	-6.59606200	1.04151500	1.32948600
O	-6.61087200	1.25111000	-0.92911500
O	6.48513300	0.91700800	-1.24657900
O	6.39209900	1.05260200	1.00719900
O	3.58280400	4.75890900	-0.26882700
O	5.58382400	3.72141100	-0.22255900
Pu	-0.10400700	-0.66984300	0.04358200