Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Theoretically Investigating the Ability of Phenanthroline Derivatives to Separate Transuranic Elements and their Bonding Properties

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Supporting information

Table S1. The calculated S^2 of the ground state for the complexes $AnL(NO_3)_3$ complexes at the BP86/6-31G(d)/RECP level of theory.

complex	S^2	S(S+1)
$NpL_{triazol}(NO_3)_3$	6.02	6.00
$PuL_{triazol}(NO_3)_3$	8.80	8.75
$AmL_{triazol}(NO_3)_3$	12.09	12.00
$CmL_{triazol}(NO_3)_3$	15.76	15.75
$NpL_{pyrazol}(NO_3)_3$	6.02	6.00
$PuL_{pyrazol}(NO_3)_3$	8.80	8.75
$AmL_{pyrazol}(NO_3)_3$	12.09	12.00
$CmL_{pyrazol}(NO_3)_3$	15.76	15.75
$NpL_{pyrrol}(NO_3)_3$	6.02	6.00
$PuL_{pyrrol}(NO_3)_3$	8.80	8.75
$AmL_{pyrrol}(NO_3)_3$	12.09	12.00
$CmL_{pyrrol}(NO_3)_3$	15.76	15.75

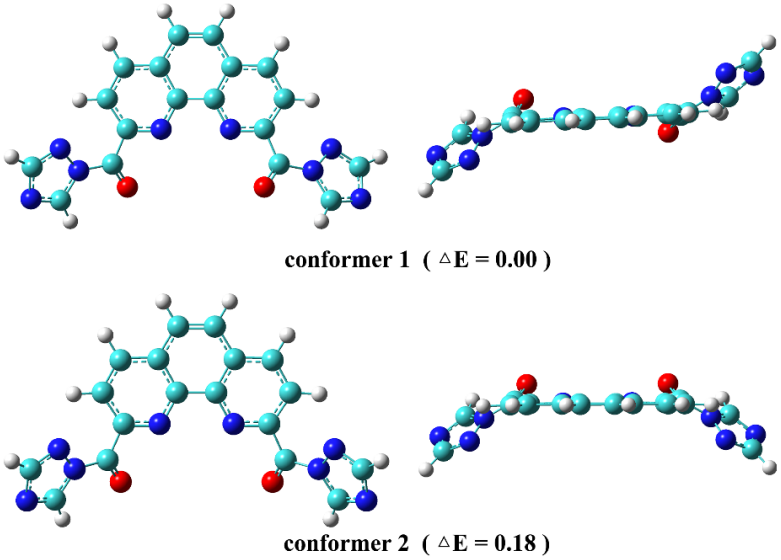

Fig. S1 Optimized structures of the ligand $L_{triazol}$ in different conformers and the relative energies (ΔE, kcal/mol) at BP86/6-31G(d)/RECP level in the gas phase. Light blue, dark blue, red, and white colors denote C, N, O, and H atoms, respectively.

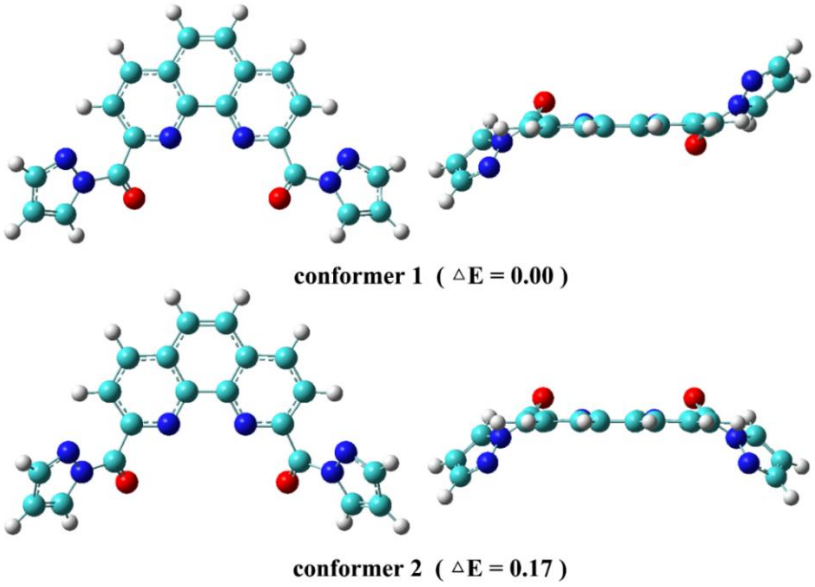

Fig. S2 Optimized structures of the ligand $L_{pyrazol}$ in different conformers and the relative energies (ΔE, kcal/mol) at BP86/6-31G(d)/RECP level in the gas phase. Light blue, dark blue, red, and white colors denote N, O, C, and H atoms, respectively.

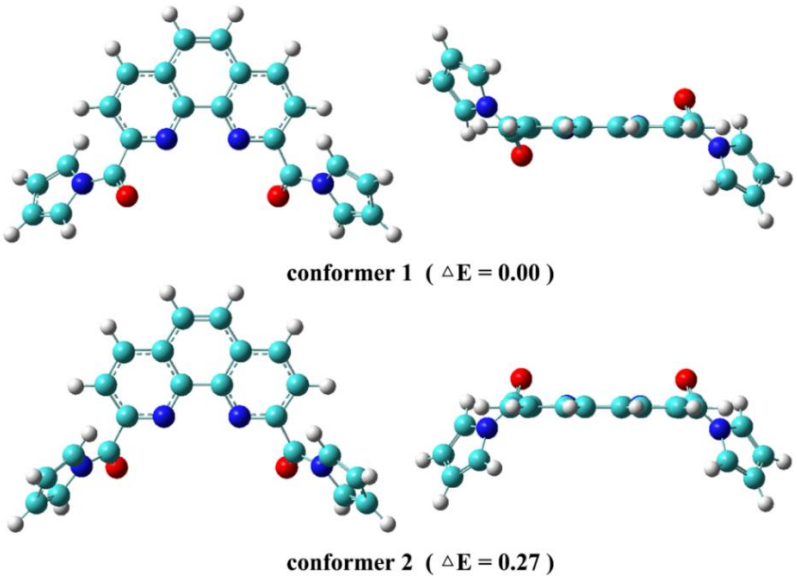

Fig. S3 Optimized structures of the ligand L_{pyrrol} in different conformers and the relative energies (ΔE, kcal/mol) at BP86/6-31G(d)/RECP level in the gas phase. Light blue, dark blue, red, and white colors denote N, O, C, and H atoms, respectively.

Table S2. The relative energies (ΔE, kcal/mol) of conformer 2 compared to conformer 1 of the ligand L (L = $L_{triazol}$, $L_{pyrazol}$ and L_{pyrrol}) at BP86/6-31G(d)/RECP level in the n-dodecane and cyclohexanone phase.

complex	ΔE **(n-dodecane)**	ΔE **(cyclohexanone)**
$L_{triazol}$	0.13	0.08
$L_{pyrazol}$	0.11	0.05
L_{pyrrol}	0.18	0.06

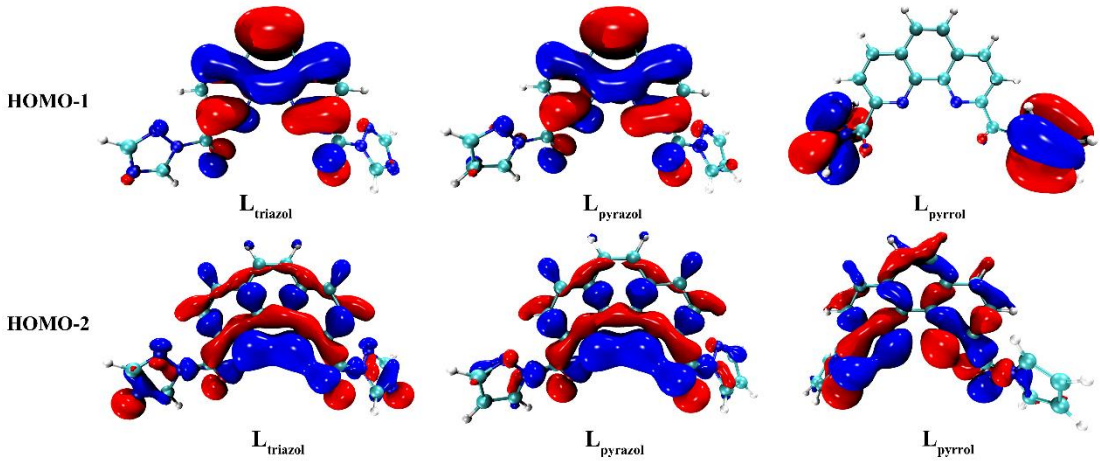

Fig. S4 The diagrams of the frontier MOs of the ligands $L_{triazol}$, $L_{pyrazol}$ and L_{pyrrol} obtained at the BP86/6-31G(d)/RECP level of theory in the gas phase. (The isosurface value is set as 0.02 a.u.)

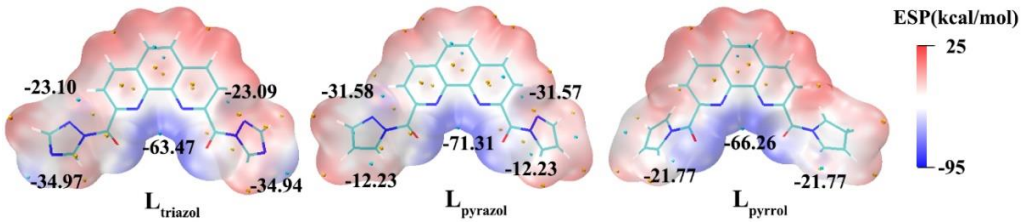

Fig. S5 ESP plots of the optimized ligands $L_{triazol}$, $L_{pyrazol}$ and L_{pyrrol} in the n-dodecane organic phase.

Table S3. Calculated average natural atomic charges on the N and O atoms of ligands $L_{triazol}$, $L_{pyrazol}$ and L_{pyrrol} in the n-dodecane organic phase.

charge	**$L_{triazol}$**	**$L_{pyrazol}$**	**L_{pyrrol}**
Q_N	-0.374	-0.379	-0.381
Q_O	-0.495	-0.511	-0.518

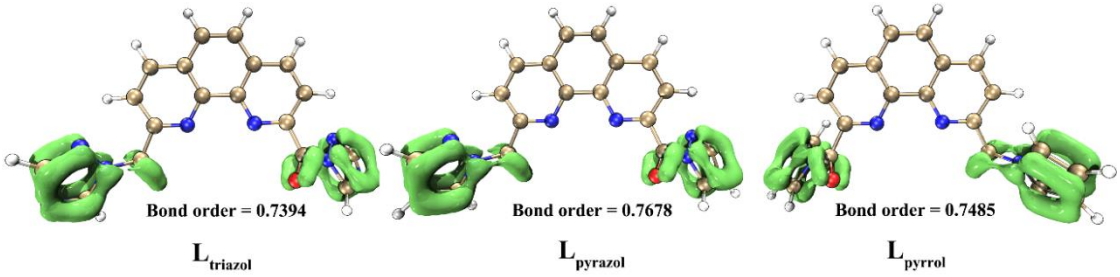

Fig. S6 The 3D-plots of LOL-pi of the five-membered ring and the carbonyl group in the optimized ligands $L_{triazol}$, $L_{pyrazol}$ and L_{pyrrol} in the gas phase. (The isosurface value is set as 0.04 a.u.)

Table S4. Average An-N(L), An-O(L) and An-O(NO_3^-) bond lengths (Å) of the complexes $AnL(NO_3)_3$ at BP86/6-31G(d)/RECP level of theory in the gas phase.

complex	An-N(L)	An-O(L)	An-O(NO_3^-)
$NpL_{triazol}(NO_3)_3$	2.561	2.403	2.450
$PuL_{triazol}$ $(NO_3)_3$	2.589	2.430	2.451
$AmL_{triazol}$ $(NO_3)_3$	2.640	2.487	2.466
$CmL_{triazol}$ $(NO_3)_3$	2.789	2.536	2.474
$NpL_{pyrazol}(NO_3)_3$	2.558	2.396	2.456
$PuL_{pyrazol}$ $(NO_3)_3$	2.588	2.422	2.458
$AmL_{pyrazol}$ $(NO_3)_3$	2.639	2.480	2.472
$CmL_{pyrazol}$ $(NO_3)_3$	2.782	2.521	2.480
$NpL_{pyrrol}(NO_3)_3$	2.583	2.419	2.454
$PuL_{pyrrol}(NO_3)_3$	2.596	2.442	2.455
AmL_{pyrrol} $(NO_3)_3$	2.652	2.516	2.470
CmL_{pyrrol} $(NO_3)_3$	2.775	2.576	2.477

Table S5. The charges of substituents on the amide group in the ligand L before and after coordination with actinide ion.

complex	$q_{monomer}$	$q_{complex}$	Δq
$L_{triazol}$	-0.4042	-0.2607	0.1435
$L_{pyrazol}$	-0.3463	-0.1885	0.1578
L_{pyrrol}	-0.2751	-0.1328	0.1423

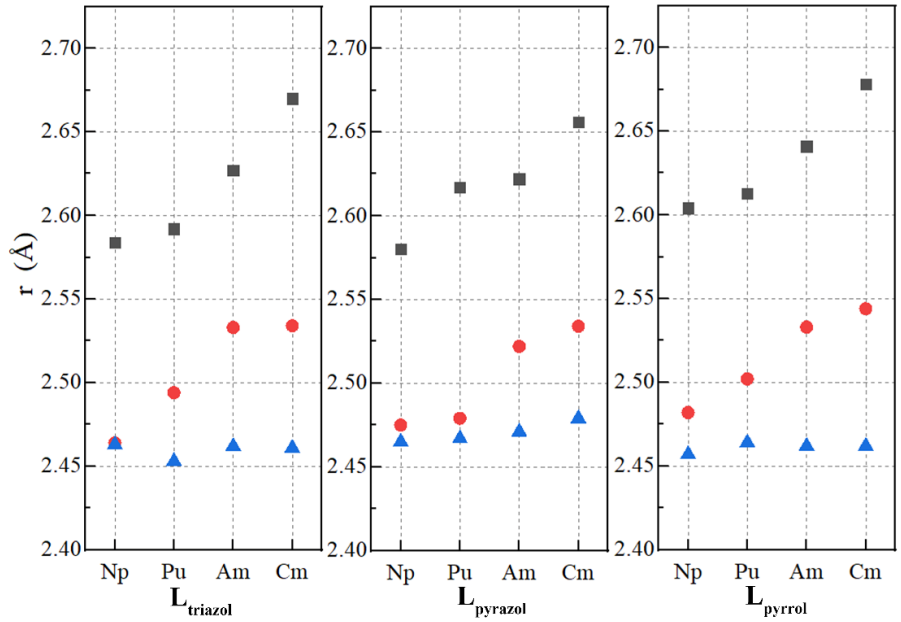

Fig. S7 Average An-N(L), An-O(L) and An-O(NO_3^-) bond lengths (Å) of the complexes $[AnL_2(NO_3)]^{2+}$ at BP86/6-31G(d)/RECP level of theory in the gas phase. Given distances are An-N(L) (■), An-O(L) (●) and An-O(NO_3^-) (▲).

Table S6. Average An-N(L), An-O(L) and An-O(NO_3^-) bond lengths (Å) of the complexes $[AnL_2(NO_3)]^{2+}$ at BP86/6-31G(d)/RECP level of theory in the gas phase.

complex	An-N(L)	An-O(L)	An-O(NO_3^-)
$[Np(L_{triazol})_2(NO_3)]^{2+}$	2.584	2.464	2.463
$[Pu(L_{triazol})_2(NO_3)]^{2+}$	2.592	2.494	2.453
$[Am(L_{triazol})_2(NO_3)]^{2+}$	2.627	2.533	2.462
$[Cm(L_{triazol})_2(NO_3)]^{2+}$	2.670	2.534	2.461
$[Np(L_{pyrazol})_2(NO_3)]^{2+}$	2.580	2.475	2.465
$[Pu(L_{pyrazol})_2(NO_3)]^{2+}$	2.617	2.479	2.467
$[Am(L_{pyrazol})_2(NO_3)]^{2+}$	2.622	2.522	2.471
$[Cm(L_{pyrazol})_2(NO_3)]^{2+}$	2.656	2.534	2.479
$[Np(L_{pyrrol})_2(NO_3)]^{2+}$	2.604	2.482	2.457
$[Pu(L_{pyrrol})_2(NO_3)]^{2+}$	2.613	2.502	2.464
$[Am(L_{pyrrol})_2(NO_3)]^{2+}$	2.641	2.533	2.462
$[Cm(L_{pyrrol})_2(NO_3)]^{2+}$	2.678	2.544	2.462

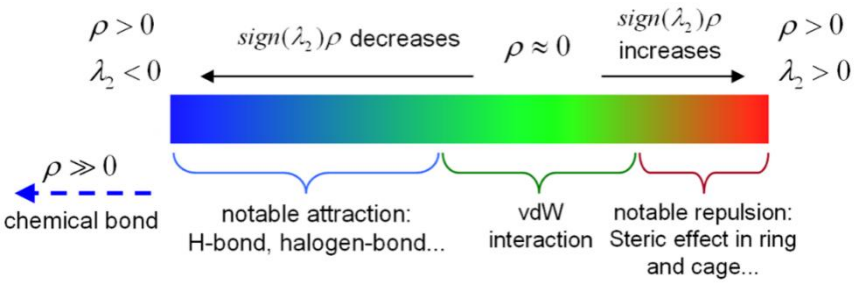

Fig. S8 Standard coloring method and chemical interpretation of $sign(\lambda_2)\rho$ on IRI isosurfaces (a.u.).

Table S7. The second-order stabilization energy ($E_{ij}^{(2)}$, kcal mol^{-1}) between the donor natural bond orbital i (NBO(i)) and acceptor orbital j (NBO(j)) in the complexes $AnL_{pyrazol}(NO_3)_3$ of β spin. T_{fds} is the sum of 5*f*, 6*d* and 7*s*, T_{NO} is the sum of O and N donor atoms on the complexes. [a]

complexes	NBO(i) → NBO(j)	$E_{ij}^{(2)}$	T_{fds}	T_{NO}
$NpL_{pyrazol}(NO_3)_3$	LP(N)→LP*(Np^{3+})	31.96 / 0.49 / 12.83	45.28	117.00
	LP(O)→LP*(Np^{3+})	49.40 / 1.07 / 21.25	71.72	
$PuL_{pyrazol}(NO_3)_3$	LP(N)→LP*(Pu^{3+})	6.52 / 1.29 / 19.57	27.38	92.35
	LP(O)→LP*(Pu^{3+})	27.30 / 1.98 / 35.69	64.97	
$AmL_{pyrazol}(NO_3)_3$	LP(N)→LP*(Am^{3+})	4.62 / 2.21 / 11.83	18.66	45.54
	LP(O)→LP*(Am^{3+})	7.48 / 2.71 / 16.69	26.88	
$CmL_{pyrazol}(NO_3)_3$	LP(N)→LP*(Cm^{3+})	2.22 / 1.98 / 9.95	14.15	33.50
	LP(O)→LP*(Cm^{3+})	4.07 / 1.79 / 13.49	19.35	

[a]... /... /... represents the results of 5*f*, 6*d* and 7*s*, respectively.

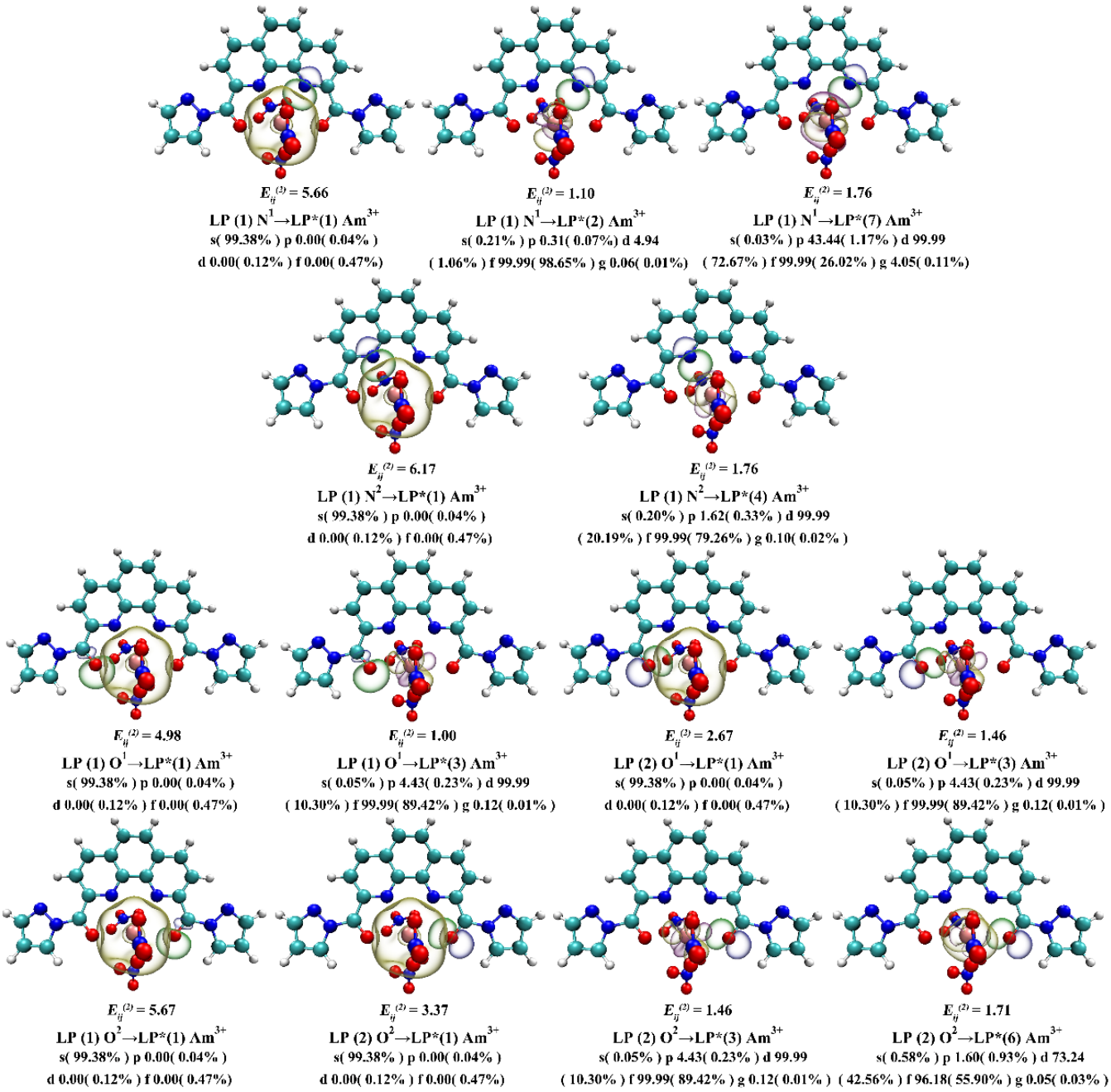

Fig. S9 The interaction between the donor natural bond orbital i (NBO(i)) and acceptor orbital j (NBO(j)) of the β spin in the complexes $AmL_{pyrazol}(NO_3)_3$.

Table S8. Calculated metal-ligand binding energies (ΔG_{BE}, kcal/mol) for the complexes $AnL(NO_3)_3$ in the gas phase, n-dodecane and cyclohexanone organic phases, and water phase at the PBE0/6-311g(d,p)/RECP level of theory.

complex	gas	n-dodecane	cyclohexanone	water
$NpL_{triazol}(NO_3)_3$	-1074.800	-588.086	-157.291	-114.011
$PuL_{triazol}(NO_3)_3$	-1056.782	-573.871	-146.206	-103.107
$AmL_{triazol}(NO_3)_3$	-1062.100	-576.180	-144.473	-100.800
$CmL_{triazol}(NO_3)_3$	-1060.665	-566.886	-128.687	-84.289
$NpL_{pyrazol}(NO_3)_3$	-1089.537	-590.283	-160.076	-116.799
$PuL_{pyrazol}(NO_3)_3$	-1075.349	-577.354	-149.643	-106.493
$AmL_{pyrazol}(NO_3)_3$	-1066.040	-579.889	-147.687	-103.940
$CmL_{pyrazol}(NO_3)_3$	-1064.417	-570.499	-131.936	-87.469
$NpL_{pyrrol}(NO_3)_3$	-1083.081	-584.393	-157.528	-114.909
$PuL_{pyrrol}(NO_3)_3$	-1069.903	-572.485	-147.077	-104.262
$AmL_{pyrrol}(NO_3)_3$	-1060.608	-576.086	-145.652	-102.149
$CmL_{pyrrol}(NO_3)_3$	-1058.838	-566.566	-129.881	-85.709

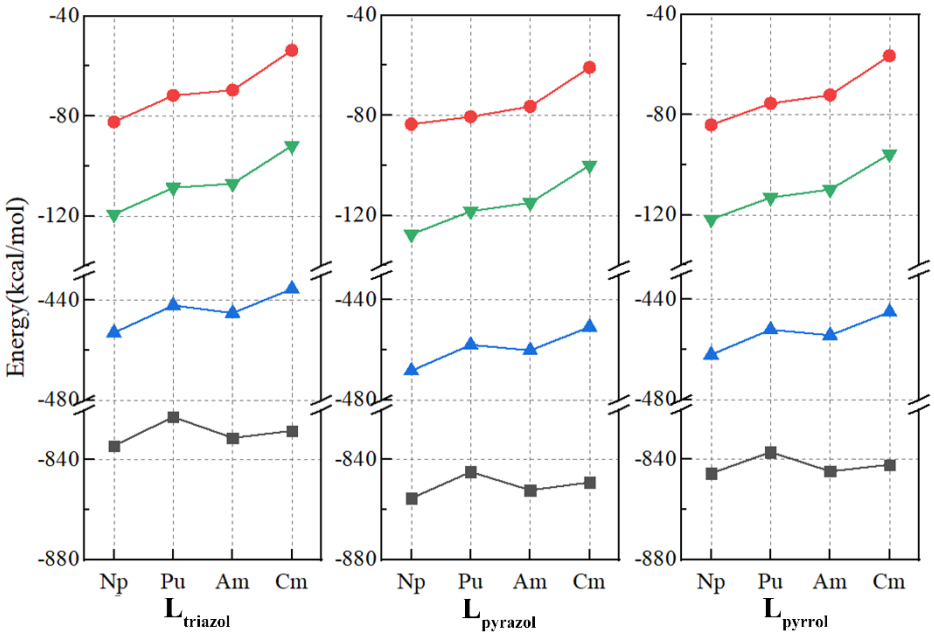

Fig. S10 Metal-ligand binding energy of $[AnL_2(NO_3)]^{2+}$ in the gas (■), n-dodecane (▲), cyclohexanone (▼) and water (●).

Table S9. Calculated metal-ligand binding energies (ΔG_{BE}, kcal/mol) for the complexes $[AnL_2(NO_3)]^{2+}$ in the gas phase, n-dodecane and cyclohexanone organic phases, and water phase at the PBE0/6-311g(d,p)/RECP level of theory.

complex	gas	n-dodecane	cyclohexanone	water
$[Np(L_{triazol})_2(NO_3)]^{2+}$	-834.369	-452.937	-119.325	-82.352
$[Pu(L_{triazol})_2(NO_3)]^{2+}$	-822.857	-442.001	-108.676	-71.787
$[Am(L_{triazol})_2(NO_3)]^{2+}$	-831.261	-445.104	-107.044	-69.600
$[Cm(L_{triazol})_2(NO_3)]^{2+}$	-828.373	-435.421	-91.847	-53.743
$[Np(L_{pyrazol})_2(NO_3)]^{2+}$	-855.445	-468.311	-127.575	-83.535
$[Pu(L_{pyrazol})_2(NO_3)]^{2+}$	-844.915	-457.924	-118.319	-80.566
$[Am(L_{pyrazol})_2(NO_3)]^{2+}$	-852.205	-460.132	-114.936	-76.461
$[Cm(L_{pyrazol})_2(NO_3)]^{2+}$	-849.114	-450.776	-100.015	-60.892
$[Np(L_{pyrrol})_2(NO_3)]^{2+}$	-845.561	-462.023	-121.810	-84.118
$[Pu(L_{pyrrol})_2(NO_3)]^{2+}$	-837.102	-452.004	-113.101	-75.516
$[Am(L_{pyrrol})_2(NO_3)]^{2+}$	-844.777	-454.247	-109.924	-72.188
$[Cm(L_{pyrrol})_2(NO_3)]^{2+}$	-842.153	-445.013	-95.813	-56.590

Table S10. Changes in Gibbs free energies (ΔG, kcal/mol) for the complexes $AnL(NO_3)_3$ in the gas phase at the BP86 functional with 6-31G(d), 6-311G(d,p) basis set, respectively. [a]

complex	6-31G(d)	6-311G(d,p)
$NpL(NO_3)_3$	-560.137 / -562.974 / -558.075	-569.745 / -571.515 / -565.197
$PuL(NO_3)_3$	-554.772 / -557.915 / -552.760	-563.576 / -565.646 / -559.074
$AmL(NO_3)_3$	-546.018 / -549.666 / -544.806	-555.821 / -558.331 / -552.131
$CmL(NO_3)_3$	-537.293 / -541.757 / -536.881	-547.263 / -550.442 / -544.193

[a] …/…/… represents the results of the complexes of $L_{triazol}$, $L_{pyrazol}$ and L_{pyrrol}, respectively.

Table S11. Changes in Gibbs free energies (ΔG, kcal/mol) for the complexes $An(NO_3)_3$ in the n-dodecane, cyclohexanone, and water at the BP86/6-31G(d)/RECP level of theory.

complex	n-dodecane	cyclohexanone	water
$NpL_{triazol}(NO_3)_3$	-310.668	-95.923	-70.434
$PuL_{triazol}(NO_3)_3$	-305.294	-91.798	-67.449
$AmL_{triazol}(NO_3)_3$	-297.642	-86.072	-61.211
$CmL_{triazol}(NO_3)_3$	-288.550	-79.759	-56.184
$NpL_{pyrazol}(NO_3)_3$	-313.754	-98.454	-72.935
$PuL_{pyrazol}(NO_3)_3$	-308.509	-94.706	-70.284
$AmL_{pyrazol}(NO_3)_3$	-301.285	-89.964	-65.055
$CmL_{pyrazol}(NO_3)_3$	-292.974	-83.786	-60.109
$NpL_{pyrrol}(NO_3)_3$	-308.799	-96.303	-70.853
$PuL_{pyrrol}(NO_3)_3$	-304.264	-92.242	-68.085
$AmL_{pyrrol}(NO_3)_3$	-297.567	-87.766	-63.074
$CmL_{pyrrol}(NO_3)_3$	-288.982	-81.714	-58.233

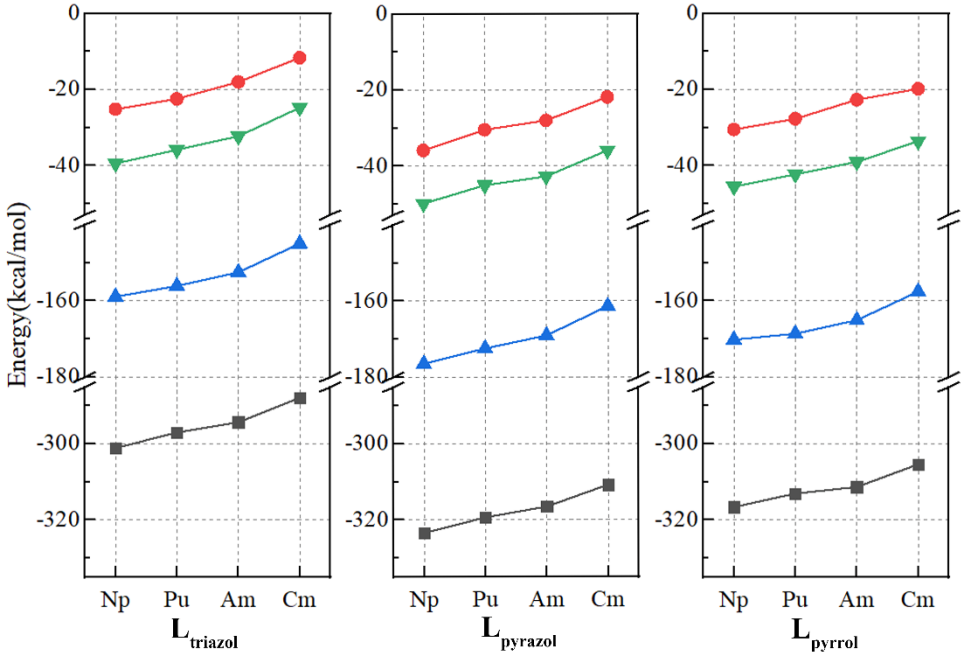

Fig. S11 Changes in Gibbs free energies of $[AnL_2(NO_3)]^{2+}$ in the gas (■), n-dodecane (▲), cyclohexanone (▼) and water (●).

Table S12. Changes in Gibbs free energies (ΔG, kcal/mol) for the complexes $[AnL_2(NO_3)]^{2+}$ in the gas, n-dodecane, cyclohexanone, and water phases at the BP86/6-31G(d)/RECP level of theory.

complex	gas	n-dodecane	cyclohexanone	water
$[Np(L_{triazol})_2(NO_3)]^{2+}$	-301.112	-158.882	-39.447	-25.198
$[Pu(L_{triazol})_2(NO_3)]^{2+}$	-296.992	-156.084	-35.871	-22.480
$[Am(L_{triazol})_2(NO_3)]^{2+}$	-294.321	-152.470	-32.298	-18.042
$[Cm(L_{triazol})_2(NO_3)]^{2+}$	-287.922	-144.928	-24.803	-11.663
$[Np(L_{pyrazol})_2(NO_3)]^{2+}$	-323.423	-176.477	-49.891	-35.910
$[Pu(L_{pyrazol})_2(NO_3)]^{2+}$	-319.361	-172.472	-45.075	-30.473
$[Am(L_{pyrazol})_2(NO_3)]^{2+}$	-316.552	-169.096	-42.797	-28.058
$[Cm(L_{pyrazol})_2(NO_3)]^{2+}$	-310.790	-161.386	-35.992	-21.922
$[Np(L_{pyrrol})_2(NO_3)]^{2+}$	-316.620	-170.195	-45.531	-30.535
$[Pu(L_{pyrrol})_2(NO_3)]^{2+}$	-313.049	-168.638	-42.296	-27.735
$[Am(L_{pyrrol})_2(NO_3)]^{2+}$	-311.330	-165.053	-39.062	-22.690
$[Cm(L_{pyrrol})_2(NO_3)]^{2+}$	-305.378	-157.572	-33.599	-19.825

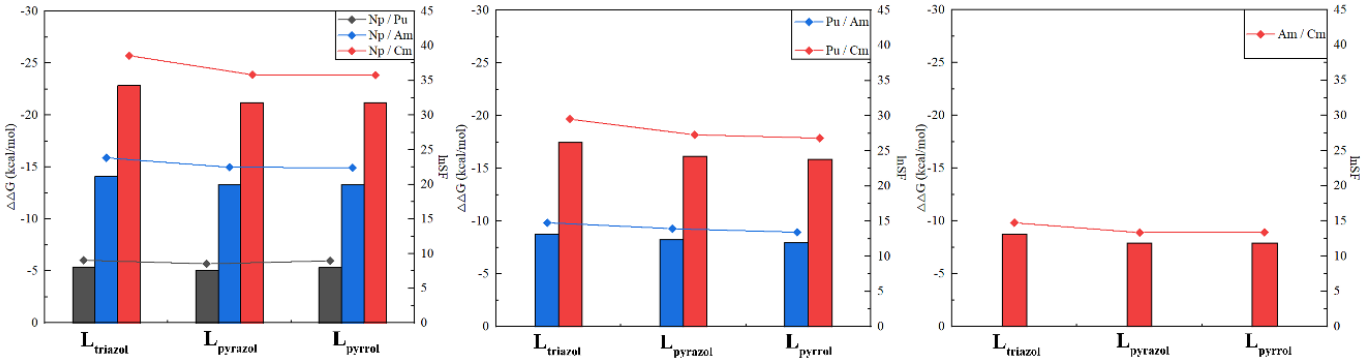

Fig. 12 The differences of ΔG (ΔΔG, kcal/mol) and lnSF of ligands $L_{triazol}$, $L_{pyrazol}$ and L_{pyrrol} in the gas phase. The black, blue, and red bars represent the values of ΔΔG for the separation of actinides from Pu, Am, and Cm, respectively. The lines represent lnSF values respectively.

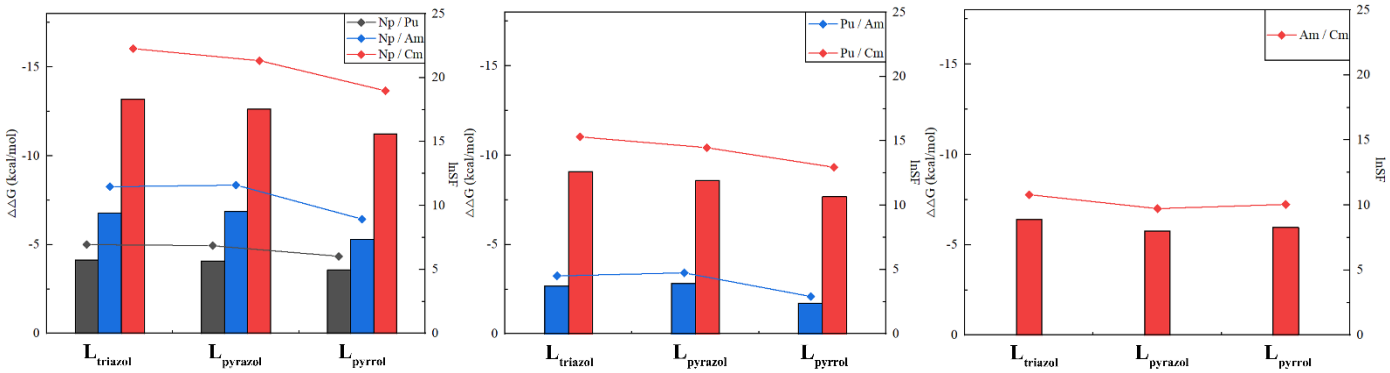

Fig. S13 The differences of ΔG (ΔΔG, kcal/mol) and lnSF of ligands $L_{triazol}$, $L_{pyrazol}$ and L_{pyrrol} in the gas phase. The black, blue, and red bars represent the values of ΔΔG for the separation of actinides from Pu, Am, and Cm, respectively. The lines represent lnSF values respectively.

Table S13. Changes in Gibbs free energies (ΔG, kcal/mol) for the complexes $EuL(NO_3)_3$ (L = $L_{triazol}$, $L_{pyrazol}$ and L_{pyrrol}) in the gas, n-dodecane, cyclohexanone, and water phases at the BP86/6-31G(d)/RECP level of theory.

complex	gas	n-dodecane	cyclohexanone	water
$EuL_{triazol}(NO_3)_3$	-545.018	-297.898	-86.522	-60.729
$EuL_{pyrazol}(NO_3)_3$	-549.106	-302.182	-90.082	-62.966
$EuL_{pyrrol}(NO_3)_3$	-544.949	-298.532	-87.910	-62.631

Table S14. The differences of ΔG (ΔΔG, kcal/mol) with the reactions of the complexes $ML(NO_3)_3$ (M = Np, Pu, Am, Cm, Eu) in the gas phase at the theoretical level of PBE0 and BP86, respectively. [a]

ΔΔG	PBE0	BP86
$\Delta\Delta G_{Np/Pu}$	-2.08 / -0.71 / -0.29	-5.36 / -5.06 / -5.32
$\Delta\Delta G_{Np/Am}$	-5.05 / -3.53 / -2.62	-14.12 / -13.31 / -13.27
$\Delta\Delta G_{Np/Cm}$	-7.16 / -5.69 / -5.61	-22.84 / -21.22 / -21.19
$\Delta\Delta G_{Pu/Am}$	-2.97 / -2.82 / -2.33	-8.75 / -8.25 / -7.95
$\Delta\Delta G_{Pu/Cm}$	-5.07 / -4.98 / -5.32	-17.48 / -16.16 / -15.88
$\Delta\Delta G_{Am/Cm}$	-2.10 / -2.16 / -2.99	-8.73 / -7.91 / -7.93
$\Delta\Delta G_{Np/Eu}$	-3.58 / -3.23 / -3.03	-15.12 / -13.87 / -13.13
$\Delta\Delta G_{Pu/Eu}$	-1.49 / -2.52 / -2.74	-9.75 / -8.81 / -7.81
$\Delta\Delta G_{Eu/Am}$	-1.47 / -0.30 / 0.41	1.00 / 0.56 / 0.14
$\Delta\Delta G_{Eu/Cm}$	-3.58 / -2.46 / -2.58	-7.73 / -7.35 / -8.07

[a] …/…/… represents the results of the complexes of $L_{triazol}$, $L_{pyrazol}$ and L_{pyrrol}, respectively.

Cartesian Coordinates

$NpL_{pyrazol}(NO_3)_3$

C	-3.44290400	2.55413100	0.10686700
C	-2.80355300	3.77529500	-0.03831800
C	-1.38116500	3.84276600	-0.08462700
C	-0.67540900	2.59649100	-0.02227600
C	-2.66155600	1.36644600	0.17882700
C	-0.63921100	5.06101700	-0.17717700
C	0.77555200	2.59622400	-0.01644700
C	1.48451800	3.84092900	-0.08712100
C	0.74550300	5.06007800	-0.17940400
C	2.90701700	3.76849300	-0.05200100
H	3.49438400	4.69167100	-0.11080900
C	3.54486800	2.54424400	0.06355000
C	2.75828300	1.35789300	0.13700300
H	-1.18988800	6.00626100	-0.23870100
H	-4.52846500	2.46891900	0.17621900
H	-3.38872800	4.69978700	-0.09776900
H	1.29722500	6.00451000	-0.24416500
H	4.63142700	2.45443300	0.10093900
N	1.39725400	1.40168700	0.08395900
N	-1.30130000	1.39998200	0.07214700
C	3.22492100	-0.02562300	0.27668600
C	-3.12899300	-0.00600000	0.42174900
O	-2.28562400	-0.93793000	0.55108400
O	2.37237700	-0.96487900	0.36048200
N	4.57391300	-0.40316000	0.32205600
C	5.01230500	-1.71856700	0.42176700
C	6.70942200	-0.27770000	0.33838600
C	6.38957900	-1.66750200	0.43413000
H	4.29842300	-2.53716000	0.46565700
H	7.69433600	0.19183000	0.31676700
H	7.07634400	-2.50964800	0.49981000
N	-4.48100800	-0.36527600	0.53785100
C	-4.92062100	-1.66959300	0.72846300
C	-6.29611200	-1.60804800	0.79291100
H	-4.20741100	-2.48837200	0.78576500
C	-6.61289800	-0.22351400	0.63206800
H	-6.98390500	-2.44047500	0.93144600
H	-7.59563000	0.25108800	0.62311000
N	-5.52660500	0.53444300	0.47724000
N	5.62338400	0.49316100	0.26975600

N	0.03245400	-3.39757800	-1.30192900
O	-0.84554200	-3.06741800	-0.41191200
O	0.90420700	-2.44942800	-1.57331700
O	0.06765200	-4.48724400	-1.84816400
N	-0.63627200	-0.05093500	-2.81411600
O	-1.42352500	-0.77146500	-2.07606400
O	0.42282100	0.39215800	-2.18141800
O	-0.85901200	0.20907000	-3.98502500
N	0.18046200	-1.07305400	2.81787600
O	0.13046800	0.09952900	2.24748300
O	0.13517900	-2.07433300	1.98414400
O	0.26065800	-1.21880800	4.02754800
Np	0.03646600	-0.76781200	-0.06958200

$PuL_{pyrazol}(NO_3)_3$

C	3.34960500	2.64858300	-0.39751000
C	2.68679100	3.85057300	-0.27495000
C	1.28826100	3.87574800	-0.15446300
C	0.61389300	2.62875600	-0.14932200
C	2.59171100	1.46560500	-0.39278400
C	0.54292500	5.09256200	-0.04675200
C	-0.83195600	2.60936800	-0.04545200
C	-1.53264200	3.83886600	0.03834000
C	-0.81217700	5.07491700	0.04430700
C	-2.93364000	3.77712400	0.11157100
H	-3.50885100	4.69640200	0.18227000
C	-3.57330600	2.55773200	0.08680300
C	-2.78722100	1.39405000	0.00567200
H	1.08628200	6.03346200	-0.04409600
H	4.42572300	2.59019400	-0.48885500
H	3.24222200	4.78467700	-0.27741600
H	-1.37442900	6.00153800	0.12039300
H	-4.65075300	2.47263800	0.12199800
N	-1.45766900	1.42717400	-0.04486300
N	1.26486700	1.46341200	-0.26402200
C	-3.29221900	-0.01256900	-0.00466600
C	3.12117800	0.07787000	-0.59007600
O	2.34313500	-0.83843800	-0.81630500
O	-2.49778600	-0.94343000	0.04341900
N	-4.64186100	-0.33233000	-0.06510600
C	-5.11130600	-1.62710000	-0.03123500
C	-6.73998400	-0.15239700	-0.23567700
C	-6.46696800	-1.54491200	-0.13777400
H	-4.42622400	-2.45569700	0.06694700
H	-7.70009400	0.33744200	-0.33704900
H	-7.17316200	-2.36185800	-0.14573800
N	4.47259000	-0.22600200	-0.52945700
C	4.95664800	-1.51341600	-0.60503000
C	6.31032500	-1.41901500	-0.48522800
H	4.27869200	-2.34651700	-0.71546100
C	6.56643000	-0.02740100	-0.33812700
H	7.02529100	-2.22828300	-0.48970400
H	7.52026500	0.46954400	-0.21434100
N	5.46515000	0.68779600	-0.36142800
N	-5.64673400	0.57436200	-0.19302000
N	0.18271900	-3.56912600	1.07724200
O	1.17124600	-2.98523100	0.53738300
O	-0.88579200	-2.86448900	1.14988600

O	0.23432700	-4.69736700	1.49155500
N	0.89906500	0.22426400	2.67437500
O	1.67891400	-0.45643000	1.94010700
O	-0.28635100	0.37689300	2.22002900
O	1.24774100	0.70981700	3.72170700
N	-0.46135500	-1.31422400	-2.73796200
O	-0.54699500	-0.15072700	-2.21765900
O	-0.16400300	-2.24944000	-1.92947400
O	-0.65092400	-1.50638300	-3.91280600
Pu	-0.00115500	-0.86456100	0.09704400

$AmL_{pyrazol}(NO_3)_3$

C	-3.43475800	2.61704700	0.20140600
C	-2.78033900	3.83259700	0.04840700
C	-1.36450400	3.87755400	-0.03564900
C	-0.66988700	2.62436800	0.01714400
C	-2.66135600	1.42765900	0.24979100
C	-0.61941100	5.09829200	-0.15498300
C	0.78642500	2.61319800	-0.02370800
C	1.49188600	3.85797600	-0.12219400
C	0.75722100	5.08819300	-0.19720600
C	2.90944000	3.79623100	-0.13178100
H	3.48973800	4.72269800	-0.20742200
C	3.55659700	2.57207500	-0.03990600
C	2.77291500	1.39033500	0.05288800
H	-1.16930900	6.04480000	-0.20287000
H	-4.52060300	2.54555700	0.27867700
H	-3.35332000	4.76575400	0.00632300
H	1.31655200	6.02667300	-0.28094700
H	4.64407600	2.48594200	-0.03694500
N	1.41985500	1.42186900	0.05337700
N	-1.31276000	1.44069000	0.13708200
C	3.27638800	-0.00972400	0.15398100
C	-3.16587400	0.04051300	0.49461500
O	-2.36229400	-0.87852000	0.74621900
O	2.46615400	-0.95800100	0.24263000
N	4.64304600	-0.34047800	0.14978200
C	5.11663400	-1.64755800	0.19788900
C	6.77464800	-0.16136600	0.12025100
C	6.49069200	-1.56227100	0.17923700
H	4.42315400	-2.48417600	0.23271900
H	7.74742800	0.33256500	0.09083100
H	7.19954700	-2.38822000	0.20169600
N	-4.53162700	-0.28837900	0.46806000
C	-5.01299200	-1.58052900	0.64954900
C	-6.38236300	-1.50235300	0.53154500
H	-4.32483200	-2.40382300	0.82623600
C	-6.65482700	-0.12060300	0.27681700
H	-7.09534900	-2.32145500	0.60837000
H	-7.62126500	0.36196800	0.12069900
N	-5.54789500	0.61885700	0.23379100
N	5.67010800	0.58312100	0.10162600
O	0.44597900	-1.21885100	4.10419200
N	0.00460600	-3.45128700	-1.22011800
O	-0.84453400	-3.09235000	-0.30525000

O	0.88719100	-2.54415900	-1.52777100
O	-0.02015600	-4.55391300	-1.74992900
N	-0.74788600	-0.09107000	-2.73351400
O	-1.53458700	-0.77783400	-1.96679600
O	0.37633600	0.27506100	-2.18086100
O	-1.03394700	0.21057400	-3.88589900
N	0.31341800	-1.08936600	2.89336800
O	0.27169300	0.07645400	2.31496400
O	0.20239900	-2.10332900	2.08704300
Am	0.02036900	-0.82428300	-0.00061500

$CmL_{pyrazol}(NO_3)_3$

C	-3.44870500	2.71013200	0.23864800
C	-2.78174900	3.92683800	0.16334600
C	-1.36802400	3.95902800	0.10048200
C	-0.68122000	2.69909400	0.11030900
C	-2.68137200	1.51807600	0.24404600
C	-0.62013100	5.18532900	0.03010600
C	0.77858800	2.68796700	0.06115100
C	1.48268700	3.93611200	-0.00810300
C	0.75203900	5.17440600	-0.02460900
C	2.89652600	3.87942100	-0.05544700
H	3.47387900	4.80917400	-0.11105900
C	3.54586300	2.65140000	-0.03168400
C	2.75946100	1.47292700	0.04369600
H	-1.17058200	6.13274000	0.02007600
H	-4.53662000	2.64292500	0.28354200
H	-3.34528700	4.86669100	0.15654700
H	1.31485400	6.11298100	-0.07968200
H	4.63282200	2.56543200	-0.06729200
N	1.41360200	1.49676400	0.09042800
N	-1.33469100	1.51695800	0.17344900
C	3.28004400	0.05948800	0.07965300
C	-3.22575200	0.12201100	0.39890500
O	-2.46000100	-0.82144300	0.64302000
O	2.49362400	-0.89463500	0.16671000
N	4.65015700	-0.25136500	0.01154800
C	5.13295200	-1.55751300	-0.01096000
C	6.77757100	-0.05522400	-0.08573200
C	6.50349100	-1.46088700	-0.07469400
H	4.44415300	-2.39895500	0.01404600
H	7.74640000	0.44556500	-0.12926000
H	7.21801300	-2.28139700	-0.11165500
N	-4.59404100	-0.17548600	0.28599200
C	-5.09890800	-1.47145900	0.35468700
C	-6.45896000	-1.36415700	0.17962500
H	-4.42817300	-2.31531900	0.50088600
C	-6.70339600	0.03696200	0.00913600
H	-7.18451200	-2.17563300	0.16466900
H	-7.65619100	0.54271400	-0.15741400
N	-5.58849500	0.76127000	0.06801800
N	5.67052200	0.68154500	-0.03472900
N	-0.17628700	-3.67731200	-0.83848600
O	-1.18239500	-3.06576300	-0.28797900
O	0.89229400	-2.94518200	-1.00005800

O	-0.22368400	-4.85197900	-1.18203900
N	-0.41836800	-0.05111700	-2.77329300
O	-1.39172200	-0.50795700	-2.03985700
O	0.74820800	-0.02750300	-2.19779700
O	-0.59041700	0.34050800	-3.92306300
N	0.42311000	-1.18175000	2.88516500
O	0.14244100	-0.03603900	2.31777400
O	0.48222200	-2.19674000	2.08213000
O	0.61720300	-1.27562800	4.09250000
Cm	-0.02182800	-0.90817000	0.00764400

$EuL_{pyrazol}(NO_3)_3$

C	-3.42305400	2.55318900	0.31134200
C	-2.76669000	3.76861000	0.15479300
C	-1.35585700	3.80691800	0.04152600
C	-0.66208300	2.55249200	0.08029500
C	-2.64908000	1.36538000	0.34021500
C	-0.61618100	5.03224300	-0.10172400
C	0.79565300	2.54395300	-0.00345500
C	1.49245800	3.79104400	-0.13020200
C	0.75459400	5.02437500	-0.18597600
C	2.90620100	3.73923100	-0.19140400
H	3.47747900	4.66852700	-0.29592800
C	3.56379900	2.51782900	-0.11283300
C	2.78549200	1.33845700	0.01708800
H	-1.17104100	5.97641900	-0.13905600
H	-4.50797100	2.48389400	0.40241700
H	-3.33698900	4.70397900	0.12521200
H	1.31145200	5.96209800	-0.29215300
H	4.65142000	2.43943500	-0.13876200
N	1.43930600	1.35738400	0.05831500
N	-1.30704100	1.37209400	0.21626000
C	3.31322400	-0.07054800	0.10938600
C	-3.17178100	-0.03336100	0.56786300
O	-2.38798700	-0.96657900	0.78006900
O	2.53246800	-1.03213000	0.13493700
N	4.68988000	-0.36200800	0.17053700
C	5.19183900	-1.65983900	0.20564000
C	6.81307500	-0.13400000	0.29283400
C	6.56040200	-1.54337300	0.28280200
H	4.51688800	-2.51155300	0.16742900
H	7.77354200	0.38155100	0.34767200
H	7.28674700	-2.35317400	0.32559500
N	-4.54738000	-0.33322300	0.56122000
C	-5.04252700	-1.62586000	0.70204300
C	-6.41238500	-1.52581500	0.62204400
H	-4.36094500	-2.46407800	0.82654400
C	-6.67228800	-0.13089200	0.43026600
H	-7.13453800	-2.33822000	0.68259400
H	-7.63578600	0.36957000	0.31819500
N	-5.55743600	0.59536700	0.38972100
N	5.69542300	0.58580100	0.22628400
N	-0.01883100	-3.57281800	-1.34325200
O	-0.92111000	-3.22561300	-0.48895300
O	0.90311200	-2.69130400	-1.58481300

O	-0.02511700	-4.67163100	-1.89564400
N	-0.86498600	0.00337000	-2.70889500
O	-1.64918200	-0.69349000	-1.95543500
O	0.31361900	0.25710300	-2.22490200
O	-1.20997600	0.42046100	-3.81475000
N	0.41725200	-1.33783900	2.81911400
O	0.32638500	-0.14966200	2.30974900
O	0.28825200	-2.32368300	1.98862100
O	0.61465600	-1.51851600	4.02053200
Eu	0.01264500	-0.96151100	-0.06040400