Supporting Information

Inverse trans influence in low-valent actinide-group 10 metal complexes of phosphinoaryl oxides: a theoretical study *via* tuning metals and donor ligands

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Discussions about reduction properties

1. Effects of reduction on molecular properties.

As shown in Table 2 of the main text, metal-metal distances were optimized in the range of 2.48 and 2.52 Å for **XU-Ni**, and those of **U-Pd** and **U-Pt** are slightly longer. The elongation, in part, originates from larger atomic radius of palladium and platinum than nickel. Among them, optimized bimetallic distances of **XU-Ni** (X = Me_3SiO, F and I) and **U-TM** (TM = Pd and Pt) are comparable to values of their experimentally known analogs.[1] The largest difference is less than 0.06 Å and the mean deviation is 0.003 Å, which confirms that our calculations are reliable. Upon reduction, metal-metal distances of [**XU-TM**]$^-$ are lengthened to 2.63~2.93 Å. Similarly, the reduction leads to the increase of An-Ni distances from neutral molecules **An-Ni** to anions [**An-Ni**]$^-$. The comparison of these metal-metal distances are presented in Figure S14.

Smaller (absolute) values of QTAIM data, δ and E_{int} are found in [**XU-TM**]$^-$ than in **XU-TM** (Table 3), indicating that the reduction weakens the metal-metal bonds. This agrees with the lengthening of U-TM distances. The weakening of U-TM bonds is quantitatively reflected by E_{int} values of -0.51 ~ -0.82 eV for [**XU-TM**]$^-$ and -0.84 ~ -1.08 eV for **XU-TM**. Herein, more negative E_{int} means stronger U-TM bond. Our calculated results are comparable to previous reports. Bond dissociation enthalpies were calculated in the range of -0.22 ~ -0.42 eV for U^{III}-Al/Ga complexes,[2] while much more negative bond disruption enthalpies between -1.56 ~ -1.75 eV were experimentally determined for U^{IV}-MM/TM ones.[3, 4] In the next section, we will explain why **XU-TM** corresponds to a *tetra*valent uranium center and [**XU-TM**]$^-$ to *tri*valent one.

In a recent work, Shi and co-workers have computed three uranium-group 8 transition metal complexes.[5] Oxidation state of +III and zero were attributed to U and Fe/Ru/Os, respectively. Considering uranium oxidation state, they correspond to our anions [**U-Ni/Pd/Pt**]$^-$ (+III will be assigned next section). Comparison finds that

optimized U-TM distances are close to their corresponding experimental values (Table S5). Calculated electron spin densities of uranium in our anions and Shi's complexes are close to theoretically expected value of 3.0 for U(III). A TM→U dative bond was assigned according to calculated QTAIM data (Table S6), where $0 < \rho(r) < 0.1$, $\nabla^2\rho(r) > 0$ and $H(r) < 0$. Moreover, the bond is of single-bond character. Furthermore, the $-G(r)/V(r)$ is an indicator for the extent of bond covalency. Values between 0.5 and 1 were obtained in both series of complexes, suggesting partly covalent character.

2. Reduction Mechanism.

One would question the reason that the reduction lengthens/weakens An-TM bonds. To answer this, we need know where the reduced electron goes. The electron-spin density values of each fragment (S_{Frag}) of **XAn-TM** and [**XAn-TM**]$^-$ are collected in Table S2, together with intuitive curves of S_{An} plotted in Figure S15.

For the uranium-transition metal complexes, S_U is 2.18 (mean value) in molecules and 2.82 in anions, being close to theoretically expected formal values 2.0 of U^{IV} and 3.0 of U^{III}, respectively; and computed average value of S_{TM} is 0.06, agreeing well with zero-valence group 10 metal and nd^{10} electronic configuration. In other words, the reduction mainly occurs around the uranium center, changing its valence from +IV into +III, and the oxidation states of transition metal remain almost unchanged. Therefore, the reducing process may include two stages. Firstly, most of reducing electron enters a non-bonding 5f orbital of uranium, and a small amount disperses into transition metal; secondly, an antibonding orbital would form between two metal centers. These two factors together are assumed to result in the lengthening of U-TM bonds. Relative to **XU-Ni** (X = Me_3SiO, F, Cl, Br and I), there is a 0.17 Å (mean value) elongation upon reduction, and it is 0.18 Å to **U-TM** (TM = Pd and Pt). It is known that the U^{III} radius is 0.15 Å longer than the U^{IV} one. Obviously, the change of uranium oxidation state plays a predominant role in lengthening U-TM bond. Comparatively, only a slight contribution (0.02~0.03 Å) comes from the anti-bonding interaction.

When assuming that the actinide is *tetra*valent in molecules **An-Ni** and *tri*valent in anions [**An-Ni**]$^-$, we find that most S_{An} values are close to their respective formal values (Table S2). However, there are two discrepancies. The first is [**Th-Ni**]$^-$, where S_{Th} was calculated to be 0.17 and much lower than the supposed 1.0 formal value of Th^{III}; nickel and oxide ligands (L) have 0.50 and 0.30 electron distribution, respectively. This indicates that the reduction of **Th-Ni** mainly takes place in nickel and ligand parts but not in thorium, so thorium ought to retain its original +IV valence. The second discrepancy is found for S_{An} values in **An-Ni** (An = Np and Pu), which correspond to 3.37 and 4.63, respectively. They are larger than the supposed 3.0 and 4.0 formal values of ***tetra***valent actinides. Actually, this overestimation has been found in previous studies.[6-8] For example, $[Pu^{IV}(CpX)_3]^+$ (X = H, Me, Cl and $SiMe_3$) was calculated to show 4.71 S_{Pu} (mean value).[7]

The An-TM complexes investigated have various active sites including two metal centers, three phosphinoaryl oxide ligands and axial donor. This will make the reduction exploration complicate. In the work, we give the difference of electron-spin density between reduced anion and its neutral molecule (ΔS_{Frag}) in Table 4. And the corresponding picture is shown in Figure 6. One can observe that the reduction mainly occur in the actinide center with the exception of the thorium complexes. The actinide gains about 60% reduced electron, and the transition metal and the phosphinoaryl oxides (L) have 24% and 15%, respectively. ΔS_X of donor ligands is negligible due to its 0.01 average value. **Th-Ni** is exceptional for its Ni and L parts attain the most reduced electron density over 90%, while there is 17% spin electron distribution over around Th.

In brief, spin density calculations demonstrate that the actinide oxidation state is +IV in molecules and +III in anions, and transition metal remains zero-valent in all the cases; one exceptional case is that a Th^{IV} ion is in both molecule and anion because the one-electron reduction mainly occurs in moieties of nickel and oxide ligands.

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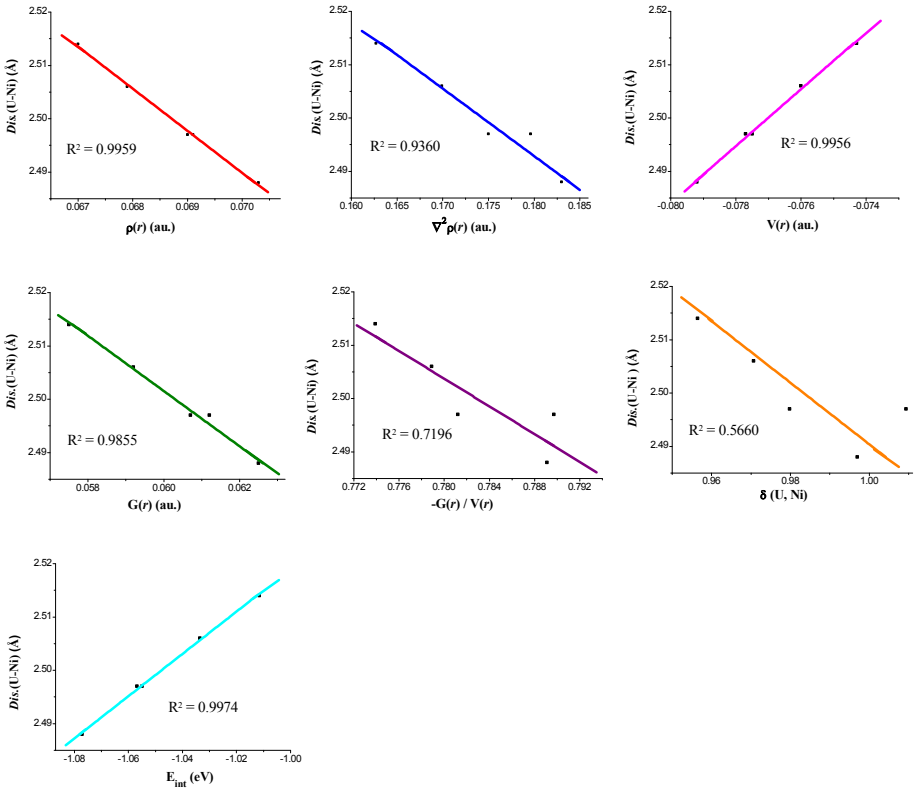

Figure S1. Plots of optimized U-Ni distances (Dis.) of molecular complexes **XU-Ni** (X = Me_3SiO, F, Cl, Br and I) against QTAIM data, delocalization index δ(U, Ni) and interaction energy E_{int}.

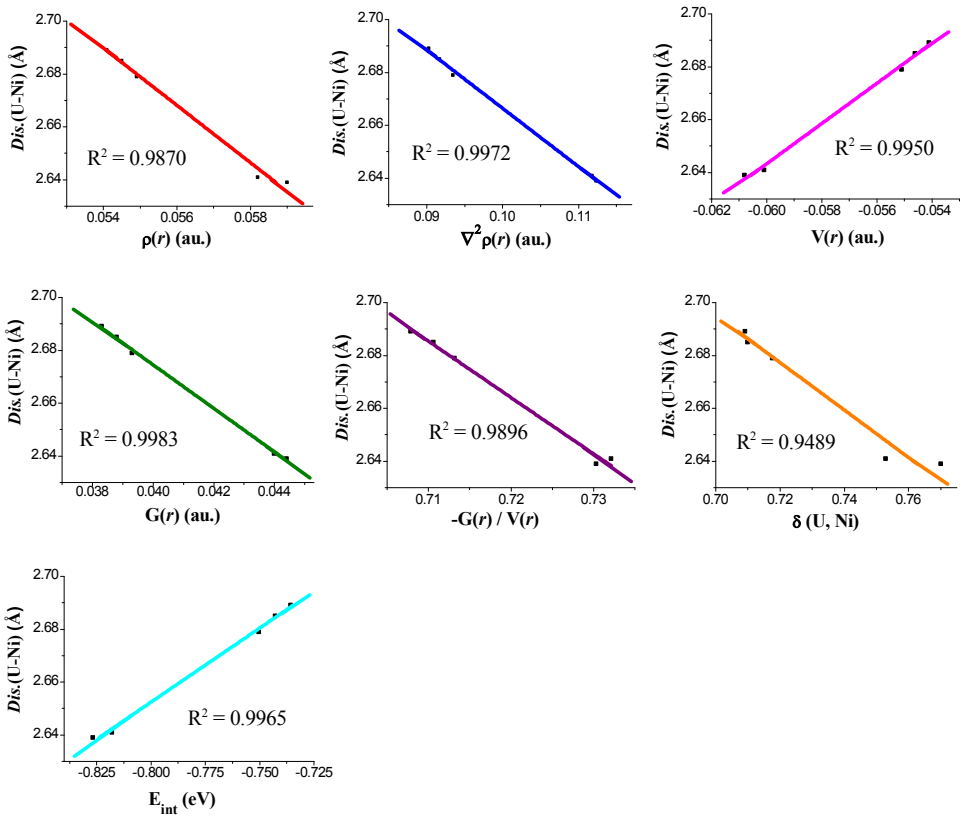

Figure S2. Plots of optimized U-Ni distances (Dis.) of anions [**XU-Ni**]$^-$ (X = Me_3SiO, F, Cl, Br and I) against QTAIM data, delocalization index δ(U, Ni) and interaction energy E_{int}.

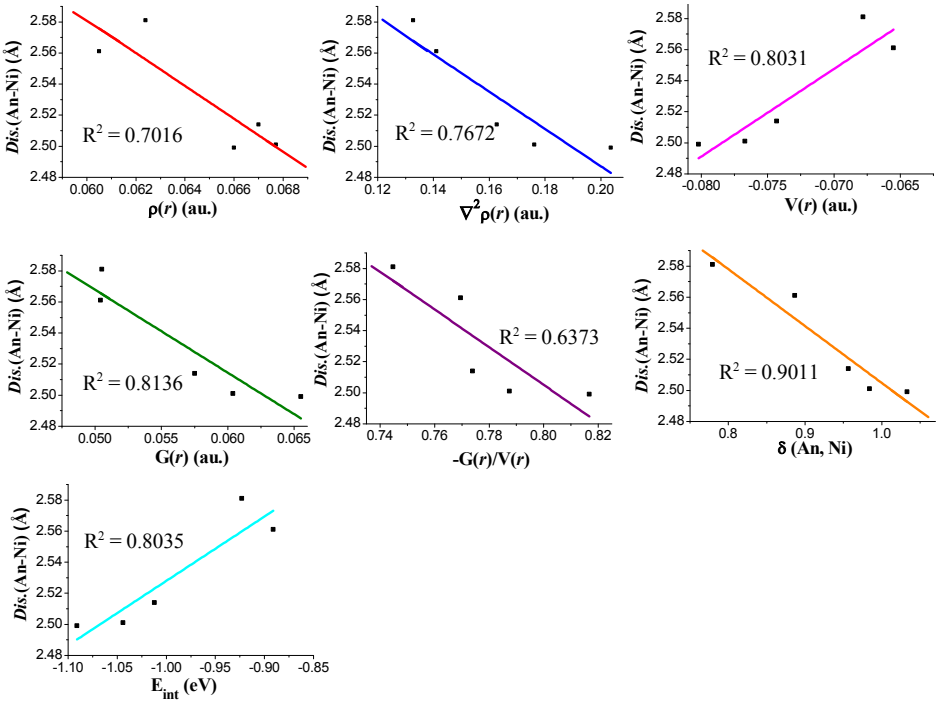

Figure S3. Plots of optimized An-Ni distances (Dis.) of molecules **An-Ni** (An = Th, Pa, U, Np and Pu) against QTAIM data, delocalization index δ(U, Ni) and interaction energy E_{int}.

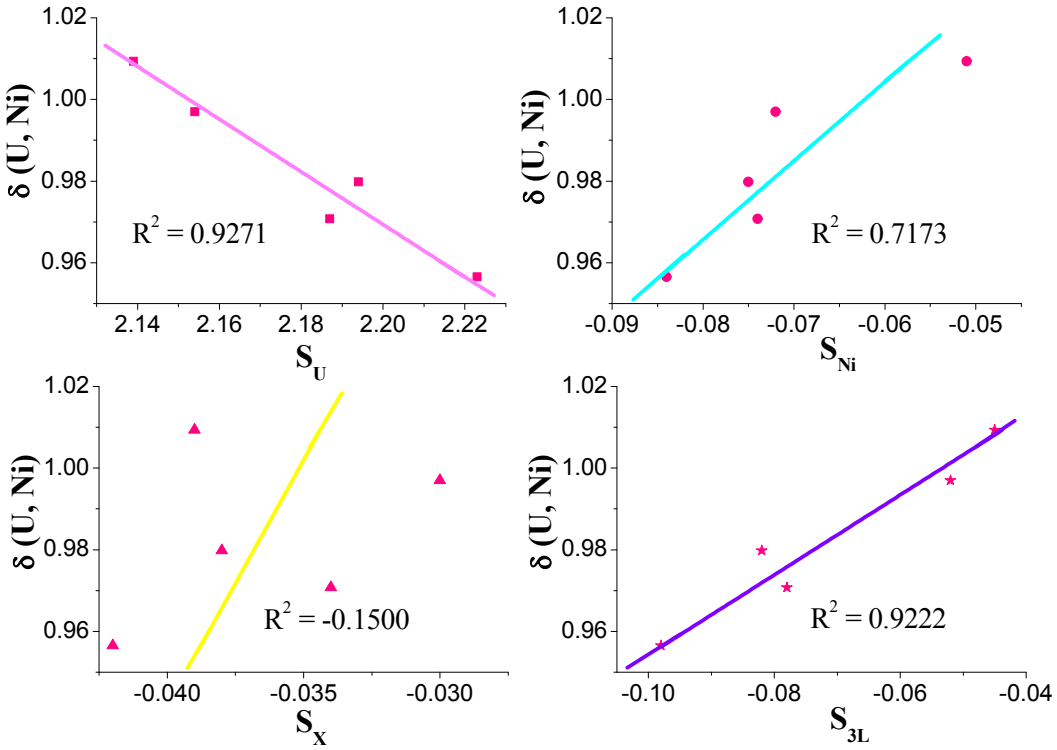

Figure S4. Plots of delocalization index δ(U, Ni) against spin density of each fragment (S_{Frag}) of molecular complexes **XU-Ni** (X = Me_3SiO, F, Cl, Br and I).

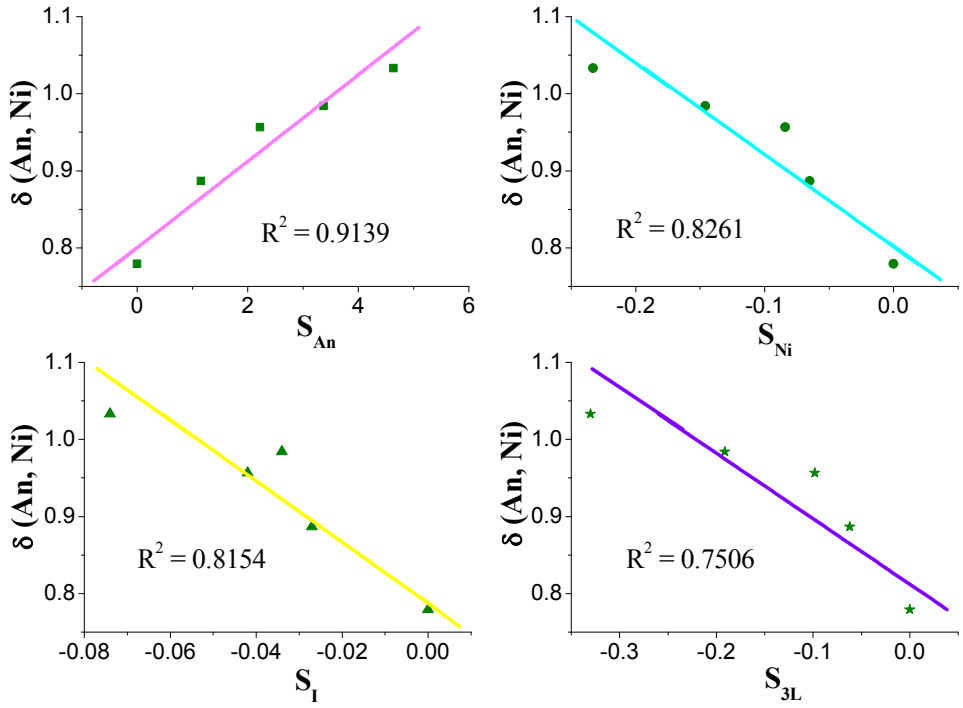

Figure S5. Plots of delocalization index δ(U, Ni) against spin density of each fragment (S_{Frag}) of **An-Ni** (An = Th, Pa, U, Np and Pu).

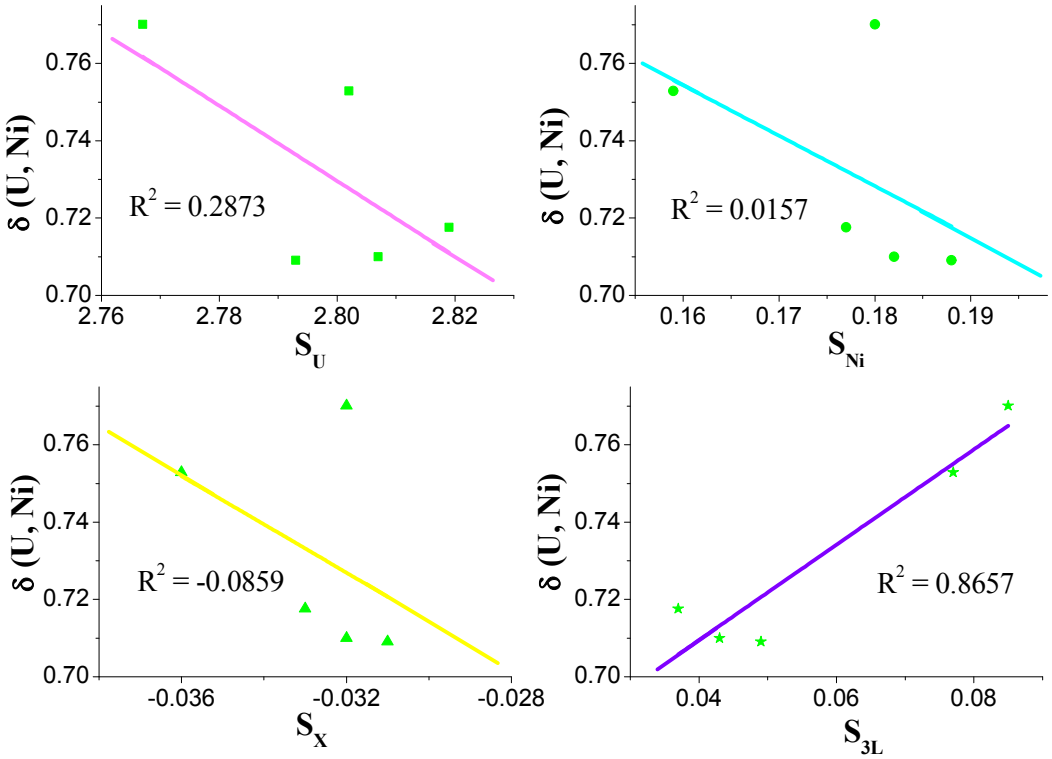

Figure S6. Plots of delocalization index δ(U, Ni) against spin density of each fragment (S_{Frag}) of anions [**XU-Ni**]$^-$ (X = Me_3SiO, F, Cl, Br and I).

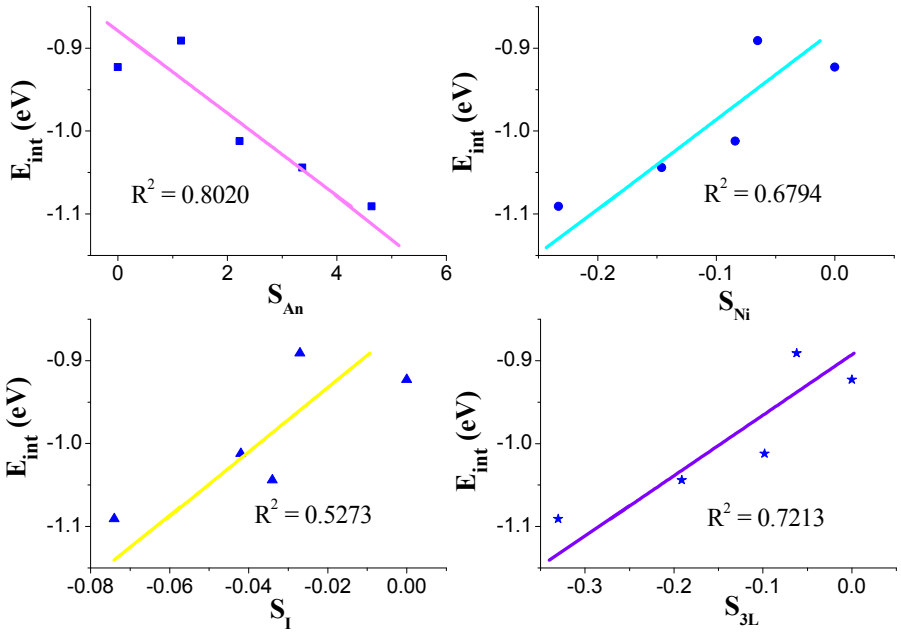

Figure S7. Plots of interaction energy E_{int} against spin density of each fragment (S_{Frag}) of **An-Ni** (An = Th, Pa, U, Np and Pu).

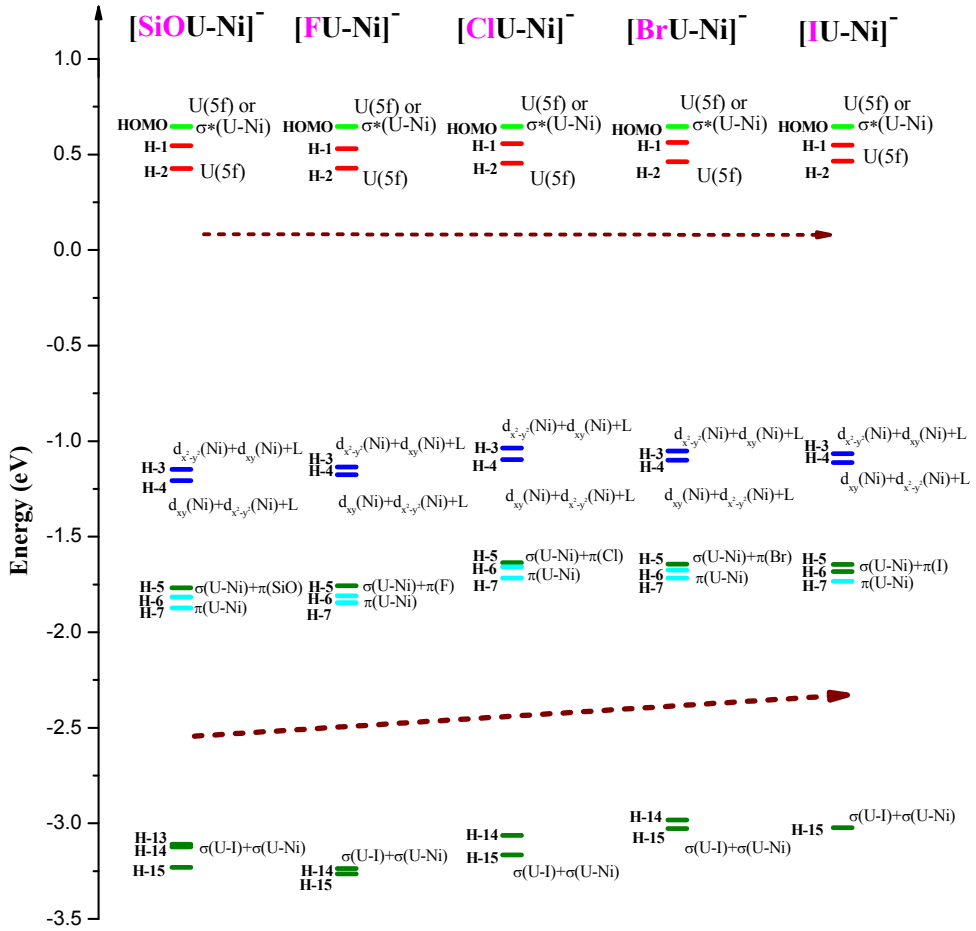

Figure S8. Diagram of occupied orbitals with the metal character for [**U-Ni**]$^{-}$ (X = Me_3SiO, F, Cl, Br and I). Noting that a) the α-spin orbital energy levels are used, b) orbitals with similar character were marked with same color lines, and c) to make identical HOMO energy, overall orbitals of last four complexes are up-shifted by 0.002, 0.14, 0.17 and 0.23 eV, respectively.

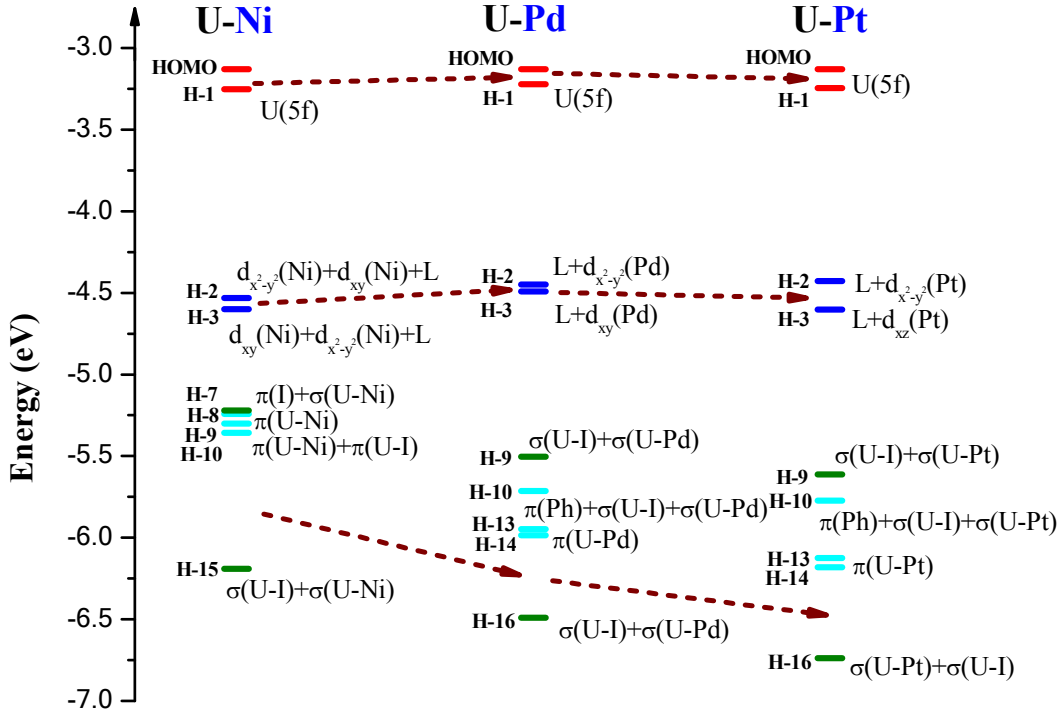

Figure S9. Diagrams of orbitals with the metal character for **U-TM** (TM = Ni, Pd and Pt). Noting that a) the α-spin orbital energy levels are used, b) orbitals with similar character were marked with same color lines, and c) to make identical HOMO energy, overall orbitals of last two complexes are up-shifted by 0.20 and 0.14 eV, respectively.

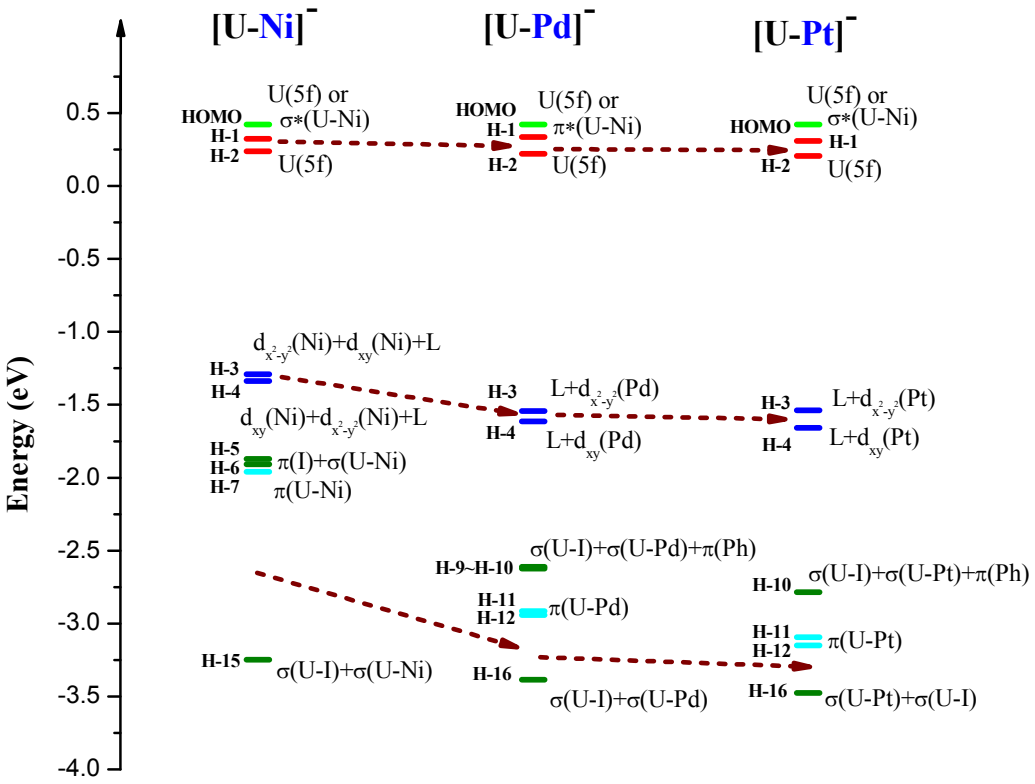

Figure S10. Diagrams of orbitals with the metal character for [**U-TM**]$^-$ (TM = Ni, Pd and Pt). Noting that a) the α-spin orbital energy levels are used, b) orbitals with similar character were marked with same color lines, and c) to make identical HOMO energy, overall orbitals of last two complexes are up-shifted by -0.023 and 0.003 eV, respectively.

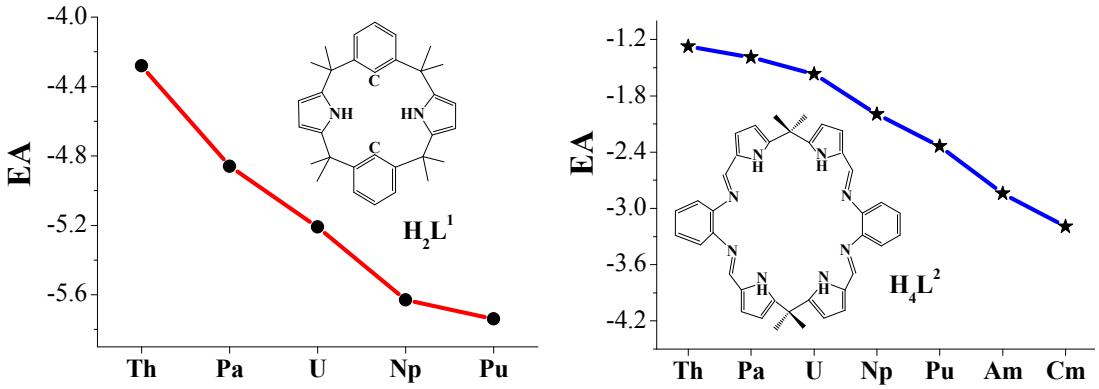

Figure S11. Calculated EA values (eV) of $[An^{IV}(L^1)(BH_4)]^+/[An^{III}(L^1)(BH_4)]$ (left) and $[An^{IV}(L^2)]/[An^{III}(L^2)]^-$ (right), where L^1 is a dianiaon of *trans*-calix[2]pyrrole[2]benzene and L^2 is a tetraanion of polypyrrolic macrocycle.

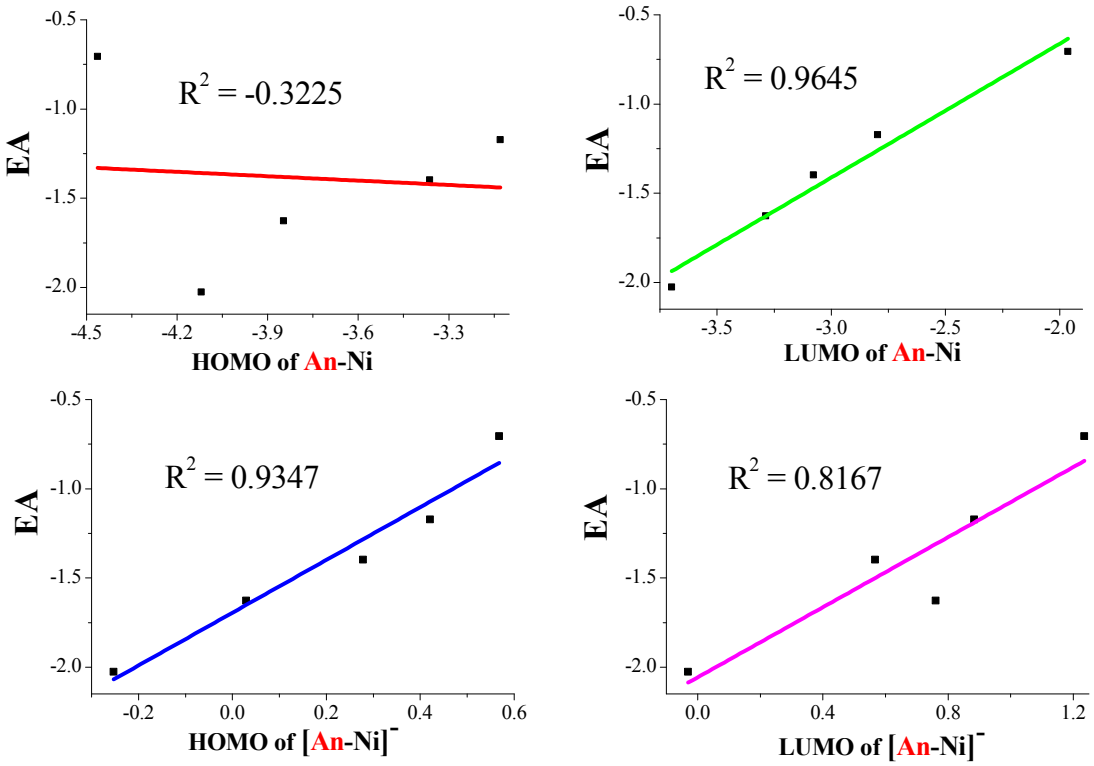

Figure S12. Plots of EA against orbital energies of molecules **An-Ni** and anions [**An-Ni**]$^-$(An = Th, Pa, U, Np and Pu), where unit is eV.

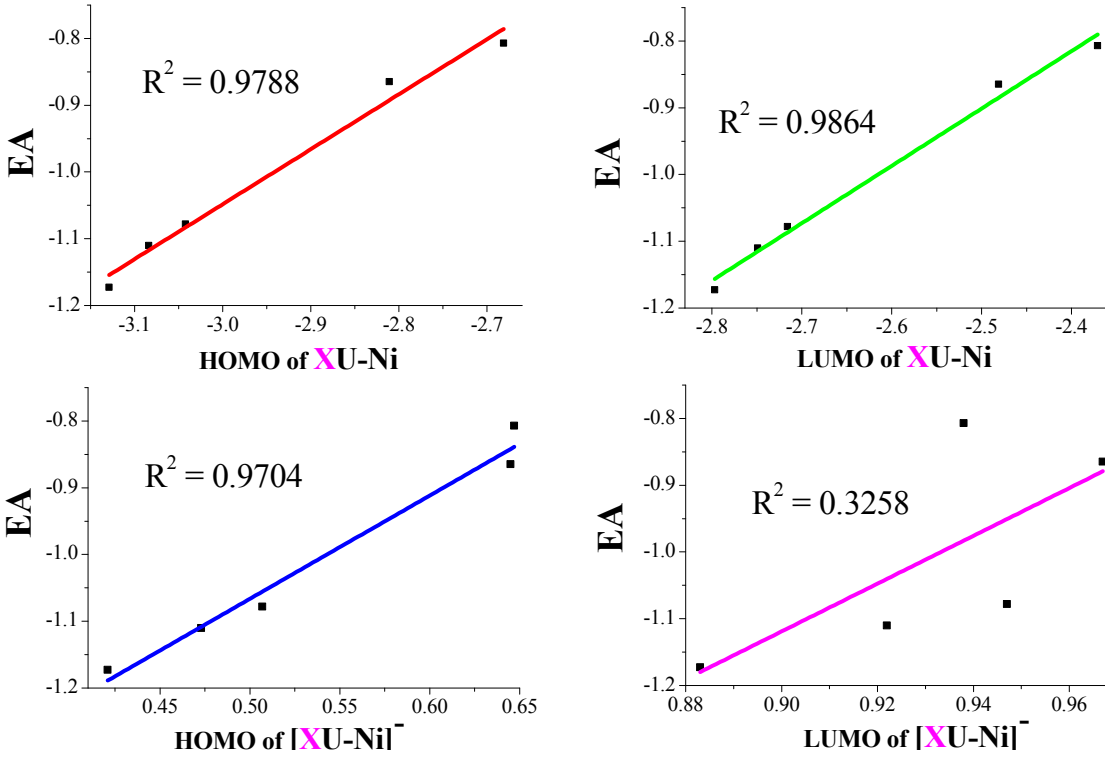

Figure S13. Plots of EA against orbital energies of molecules **XU-Ni** and anions [**XU-Ni**]$^-$ (X = Me_3SiO, F, Cl, Br and I), where the unit is eV.

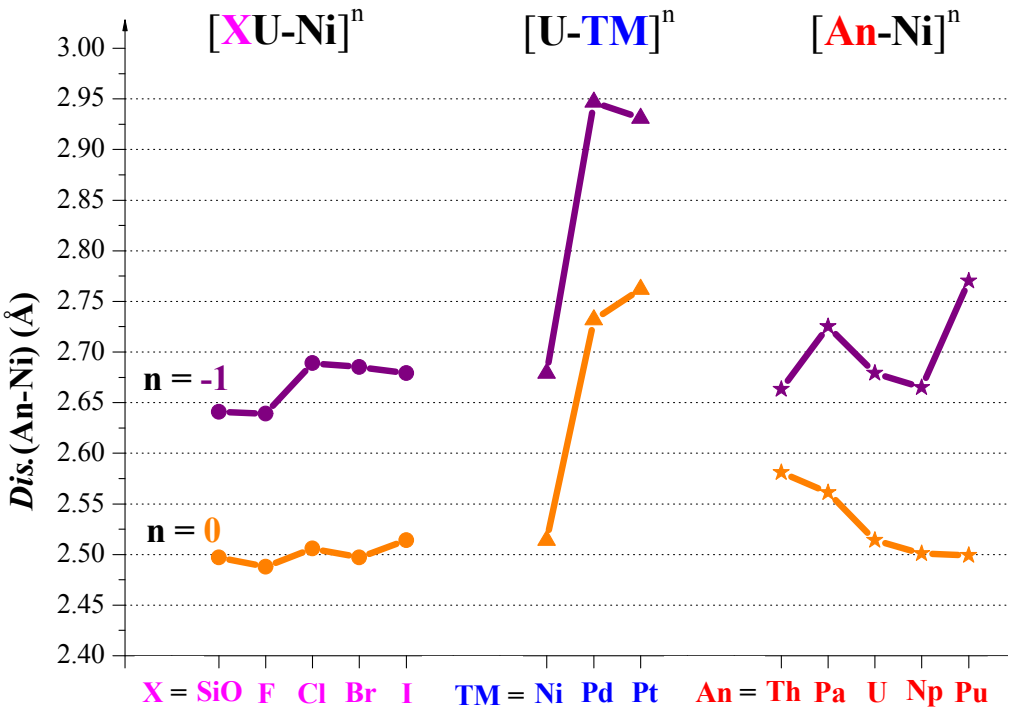

Figure S14. Optimized An-TM distances of heterobimetallic actinide-transitional metal complexes.

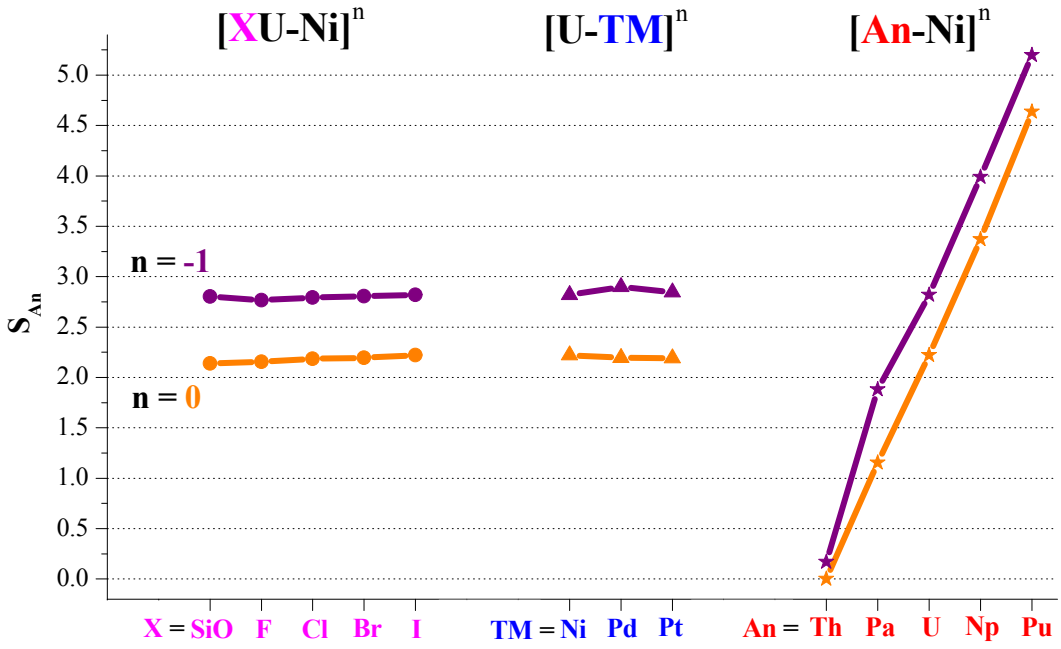

Figure S15. Electron spin density of actinide atom (S_{An}) of heterobimetallic actinide-transitional metal complexes.

Table S1. Optimized bond angles and dihedral angles (º) of heterobimetallic actinide-transitional metal molecules and anions.[a]

Complexes	Aprroaches	X-U-TM	$(X\text{-}U\text{-}O)_{av}$	$(P\text{-}TM\text{-}U)_{av}$	$(O\text{-}U\text{-}TM\text{-}P)_{av}$
SiOU-Ni	Calc.	174.1	92.7	96.2	32.4
FU-Ni	Calc.	175.9	92.0	95.2	34.0
ClU-Ni	Calc.	170.9	92.9	95.7	32.9
BrU-Ni	Calc.	170.6	93.0	96.0	32.8
U-Ni	Calc.	170.5	92.8	96.0	31.5
[**SiOU-Ni**]$^-$	Calc.	173.4	94.1	96.4	30.5
[**FU-Ni**]$^-$	Calc.	175.0	93.8	95.9	30.9
[**ClU-Ni**]$^-$	Calc.	172.3	95.7	95.5	31.6
[**BrU-Ni**]$^-$	Calc.	173.3	95.6	95.6	31.9
[**U-Ni**]$^-$	Calc.	172.1	95.7	96.2	31.2
U-Pd	Calc.	175.7	93.6	91.9	30.9
U-Pt	Calc.	172.8	94.2	92.6	29.0
[**U-Pd**]$^-$	Calc.	174.3	97.7	91.6	29.4
[**U-Pt**]$^-$	Calc.	172.5	96.8	92.3	26.6
Th-Ni	Calc.	175.5	92.8	95.7	29.9
Pa-Ni	Calc.	175.4	92.9	95.1	30.8
Np-Ni	Calc.	179.4	91.7	95.7	31.9
Pu-Ni	Calc.	178.9	92.7	97.3	32.2

Table S2. Calculated NBO charge (Q) and electron-spin density (S) of each fragment of actinide-transitional metal molecules and anions.

Complexes	Q_{An}	Q_{TM}	Q_X	Q_{3L}	S_{An}	S_{TM}	S_X	S_{3L}
SiOU-Ni	1.456	-0.622	-1.012	-0.822	2.139	-0.051	-0.039	-0.045
FU-Ni	1.442	-0.613	-0.417	-0.412	2.154	-0.072	-0.030	-0.052
ClU-Ni	1.245	-0.617	-0.334	-0.293	2.187	-0.074	-0.034	-0.078
BrU-Ni	1.196	-0.628	-0.287	-0.281	2.194	-0.075	-0.038	-0.082
U-Ni	1.179	-0.635	-0.262	-0.282	2.223	-0.084	-0.042	-0.098
[**SiOU-Ni**]$^-$	1.443	-0.951	-1.085	-1.407	2.802	0.159	-0.036	0.077
[**FU-Ni**]$^-$	1.433	-0.973	-0.475	-0.985	2.767	0.180	-0.032	0.085
[**ClU-Ni**]$^-$	1.327	-0.901	-0.476	-0.950	2.793	0.188	-0.031	0.049
[**BrU-Ni**]$^-$	1.222	-0.851	-0.448	-0.922	2.807	0.182	-0.032	0.043
[**U-Ni**]$^-$	1.283	-0.896	-0.454	-0.932	2.819	0.177	-0.033	0.037
U-Pd	1.261	-0.597	-0.277	-0.387	2.196	-0.037	-0.043	-0.115
U-Pt	1.241	-0.745	-0.279	-0.217	2.191	-0.037	-0.044	-0.110
[**U-Pd**]$^-$	1.329	-0.783	-0.477	-1.068	2.900	0.143	-0.031	-0.012
[**U-Pt**]$^-$	1.322	-0.955	-0.475	-0.892	2.847	0.181	-0.031	0.003
Th-Ni	1.348	-0.695	-0.183	-0.469	0.000	0.000	0.000	0.000
Pa-Ni	1.255	-0.614	-0.264	-0.377	1.154	-0.065	-0.027	-0.062
Np-Ni	1.157	-0.600	-0.283	-0.274	3.371	-0.146	-0.034	-0.191
Pu-Ni	0.911	-0.576	-0.128	-0.208	4.637	-0.233	-0.074	-0.330

[**Th-Ni**]$^-$	1.466	-1.224	-0.319	-0.923	0.171	0.499	0.025	0.304
[**Pa-Ni**]$^-$	1.277	-0.643	-0.450	-1.185	1.881	0.089	-0.021	0.050
[**Np-Ni**]$^-$	1.257	-0.776	-0.478	-1.003	3.989	0.069	-0.030	-0.027
[**Pu-Ni**]$^-$	0.980	-0.613	-0.371	-0.997	5.199	-0.068	-0.032	-0.099

Table S3. Electron Affinity (EA in eV) of uranium-nickel complexes calculated at various geometries and different codes, along with cyclic voltammetry data ($E_{1/2}$ in V) of experimental analogues.[a]

	Gaussian		Priroda [d]			
n = 0 → -1	EA [b]	VEA [c]	EA [e]	EA_{ZPVE} [e]	$EA_{G(corr)}$ [e]	$E_{1/2}$ [a]
[**SiOU-Ni**]^n	-0.807	-0.599	-0.940	-1.010	-0.939	-2.50
[**FU-Ni**]^n	-0.865	-0.674	-1.028	-1.098	-0.939	-2.39
[**ClU-Ni**]^n	-1.078	-0.845	-1.168	-1.234	-1.145	
[**BrU-Ni**]^n	-1.110	-0.886	-1.205	-1.265	-1.170	
[**U-Ni**]^n	-1.173	-0.933	-1.296	-1.319	-1.239	-2.20

[a] Experimental CV values from Ref. [1]..

[b] Both molecular complexes and anions were optimized by the Gaussian code, and calculated energy difference corresponds to the adiabatic EA. Herein, we used EA to denote the adiabatic one.

[c] Geometries of anions were not optimized and directly used the optimized geometries of molecular complexes, which corresponds to the vertical EA (denoted as VEA).

[d] With the Priroda code, various EA were calculated at the Gaussian-optimized geometries. In Priroda, we applied all-electron scalar relativistic Hamiltonian, PBE functional and all-electron Gaussian basis sets.

[e] EA is the adiabatic one, and last two were added by zero-point vibrational energy (ZPVE) and free-energy correction [G(corr)], respectively.

Table S4. Calculated QTAIM data (in a.u.) at An-X BCPs for actinide-transitional metal complexes, along with ellipticity (ε), delocalization index (δ) and interaction energy E_{int} (in eV).

Complexes	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$	$V(r)$	$G(r)$	$-G(r)/V(r)$	ε	δ(U, TM)	E_{int}
SiOU-Ni	0.1277	0.4391	-0.0392	-0.1882	0.1490	0.7917	0.0048	0.9794	-2.561
FU-Ni	0.1307	0.4855	-0.0353	-0.1920	0.1567	0.8161	0.0028	0.8926	-2.612
ClU-Ni	0.0687	0.1568	-0.0122	-0.0635	0.0514	0.8094	0.0484	0.7908	-0.864
BrU-Ni	0.0591	0.0992	-0.0123	-0.0493	0.0369	0.7485	0.0590	0.7848	-0.670
U-Ni	0.0489	0.0594	-0.0106	-0.0355	0.0250	0.7042	0.0753	0.7615	-0.484
[**SiOU-Ni**]$^-$	0.1095	0.4044	-0.0243	-0.1498	0.1255	0.8378	0.0384	0.8360	-2.038
[**FU-Ni**]$^-$	0.1223	0.4747	-0.0289	-0.1765	0.1476	0.8363	0.0356	0.8430	-2.402
[**ClU-Ni**]$^-$	0.0583	0.1415	-0.0080	-0.0513	0.0433	0.8441	0.0745	0.6743	-0.698
[**BrU-Ni**]$^-$	0.0492	0.0913	-0.0081	-0.0389	0.0308	0.7918	0.0724	0.6520	-0.530
[**U-Ni**]$^-$	0.0397	0.0564	-0.0067	-0.0272	0.0205	0.7537	0.0819	0.6099	-0.371
U-Pd	0.0486	0.0613	-0.0104	-0.0356	0.0252	0.7079	0.0571	0.7681	-0.484
U-Pt	0.0480	0.0610	-0.0101	-0.0350	0.0249	0.7114	0.0721	0.7612	-0.477
[**U-Pd**]$^-$	0.0399	0.0592	-0.0068	-0.0281	0.0213	0.7580	0.0213	0.6119	-0.382
[**U-Pt**]$^-$	0.0395	0.0583	-0.0066	-0.0275	0.0209	0.7600	0.1148	0.6016	-0.374
Th-Ni	0.0451	0.0568	-0.0091	-0.0320	0.0229	0.7156	0.0125	0.6685	-0.435
Pa-Ni	0.0436	0.0650	-0.0078	-0.0315	0.0237	0.7524	0.0147	0.6875	-0.428
Np-Ni	0.0480	0.0616	-0.0101	-0.0352	0.0251	0.7131	0.0223	0.7466	-0.479
Pu-Ni	0.0483	0.0675	-0.0100	-0.0363	0.0263	0.7245	0.0102	0.7432	-0.494

Table S5. Optimized bond distances, atomic charges and electron spin density of uranium-group 10/8 transition metal complexes, along with available experimental values.

Complexes	OS of U [a]	U-TM	Exptl	Q_U	Q_{TM}	S_U	S_{TM}
U-Ni	IV	2.514	2.534 [b]	1.179	-0.635	2.223	-0.084
U-Pd	IV	2.732	2.690 [b]	1.261	-0.597	2.196	-0.037
U-Pt	IV	2.762	2.708 [b]	1.241	-0.745	2.191	-0.037
[**U-Ni**]$^-$	III	2.679	—	1.283	-0.896	2.819	0.177
[**U-Pd**]$^-$	III	2.947	—	1.329	-0.783	2.900	0.143
[**U-Pt**]$^-$	III	2.931	—	1.322	-0.955	2.847	0.181
U-Fe [c]	III	2.876	2.946	1.026	−0.461	2.773	−0.082
U-Ru [c]	III	3.013	2.989	1.280	−0.610	2.773	−0.065
U-Os [c]	III	3.044	**—**	1.117	−0.420	2.761	−0.052

[a] Oxidation state (OS).

[b] Experimental values from Ref. (J. A. Hlina, J. R. Pankhurst, N. Kaltsoyannis and P. L. Arnold, *J. Am. Chem. Soc.*, 2016, **138**, 3333-3345).

[c] Calculated results of uranium-group 8 TM from Ref. (X.-W. Chi, Q.-Y. Wu, Q. Hao, J.-H. Lan, C.-Z. Wang, Q. Zhang, Z.-F. Chai and W.-Q. Shi, *Organometallics*, 2018, **37**, 3678-3686).

Table S6. QTAIM parameters of uranium-group 10/8 transtion metal complexes.

BCPs	OS of U [a]	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$	$V(r)$	$G(r)$	$-G(r)/V(r)$
U-Ni	IV	0.0670	0.1627	-0.0168	-0.0743	0.0575	0.7739
U-Pd	IV	0.0605	0.1195	-0.0161	-0.0620	0.0459	0.7403
U-Pt	IV	0.0656	0.1267	-0.0178	-0.0672	0.0494	0.7351
[**U-Ni**]$^-$	III	0.0549	0.0935	-0.0159	-0.0551	0.0393	0.7132
[**U-Pd**]$^-$	III	0.0436	0.0719	-0.0099	-0.0377	0.0279	0.7401
[**U-Pt**]$^-$	III	0.0516	0.0881	-0.0119	-0.0457	0.0338	0.7396
U-Fe [b]	III	0.0460	0.0474	−0.0110	−0.0339	0.0229	0.6760
U-Ru [b]	III	0.0476	0.0477	−0.0121	−0.0361	0.0240	0.6650
U-Os [b]	III	0.0512	0.0423	−0.0138	−0.0381	0.0243	0.6380

[a] Oxidation state (OS).

[b] Results from Ref. (X.-W. Chi, Q.-Y. Wu, Q. Hao, J.-H. Lan, C.-Z. Wang, Q. Zhang, Z.-F. Chai and W.-Q. Shi, *Organometallics*, 2018, **37**, 3678-3686).

The full reference of Gaussian code.

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R. P., C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision D.01; Gaussian, Inc., Wallingford CT, 2009.

Cartesian coordinates of optimized complexes

SiOU-Ni

92	0.256300	0.706584	0.209989
28	-0.591338	-1.500308	-0.589213
15	-2.751055	-1.057718	-0.481484
15	0.511123	-1.421992	-2.494010
15	0.230667	-2.713776	1.069153
8	-1.592037	1.611546	-0.589863
8	2.198293	0.169391	-0.700902
8	0.049020	-0.043290	2.251982
6	-2.660671	1.539942	-1.395761
6	2.948925	-0.656474	-1.440835
6	-0.384187	-0.965330	3.124787
6	-3.397547	0.326727	-1.493307
6	2.341297	-1.513806	-2.401793
6	-0.382075	-2.340849	2.761161
6	-4.517960	0.254615	-2.341816
6	3.139694	-2.379232	-3.172947
6	-0.851932	-3.301491	3.676231
6	-4.907261	1.371169	-3.092489
6	4.528863	-2.404661	-2.996865
6	-1.318604	-2.908912	4.937421
6	-4.177103	2.566353	-2.987994
6	5.121812	-1.555413	-2.048345
6	-1.309245	-1.549363	5.289086
6	-3.056640	2.678485	-2.151062
6	4.361235	-0.676959	-1.262344
6	-0.849331	-0.561111	4.405973
1	-4.483680	3.441110	-3.573021
1	6.209332	-1.572757	-1.911714
1	-1.670755	-1.242780	6.277349
1	-5.777849	1.313486	-3.752354
1	5.147764	-3.078093	-3.596922
1	-1.682957	-3.658249	5.646242
1	-5.090266	-0.674781	-2.422483
1	2.678928	-3.041162	-3.913020
1	-0.857059	-4.362535	3.407812
6	4.987846	0.235153	-0.240713
1	4.757570	1.292876	-0.456896
1	4.592476	0.036966	0.771046
1	6.081970	0.113339	-0.216175
6	-2.263682	3.953670	-2.034226

1	-2.230743	4.308585	-0.989840
1	-1.212697	3.800803	-2.337506
1	-2.694282	4.749155	-2.662259
6	-0.843824	0.901833	4.765000
1	0.166055	1.334522	4.660704
1	-1.497401	1.483018	4.090417
1	-1.188098	1.059302	5.799028
6	-3.498425	-0.734520	1.190495
1	-4.595842	-0.655589	1.124755
1	-3.212645	-1.543847	1.880550
1	-3.090242	0.209773	1.580871
6	-3.745598	-2.529535	-1.029594
1	-4.829711	-2.360259	-0.919554
1	-3.519518	-2.769882	-2.079702
1	-3.459075	-3.390189	-0.405393
6	-0.181233	-4.511800	0.826860
1	0.256607	-5.146046	1.615357
1	-1.272578	-4.654353	0.810540
1	0.225989	-4.828696	-0.145862
6	2.069966	-2.815266	1.324464
1	2.319365	-3.572883	2.085083
1	2.561894	-3.055073	0.369082
1	2.433543	-1.833552	1.662617
6	0.219241	-0.057529	-3.728393
1	0.699251	-0.290099	-4.693432
1	-0.864397	0.085092	-3.866502
1	0.646420	0.878925	-3.336931
6	0.026507	-2.905255	-3.505143
1	0.520876	-2.913916	-4.490572
1	0.279725	-3.828644	-2.962513
1	-1.063421	-2.875495	-3.657256
8	0.995736	2.587676	0.684831
14	1.687970	4.047684	1.178475
6	2.406412	3.815641	2.906623
1	2.864604	4.747136	3.280692
1	1.619584	3.512671	3.617471
1	3.180766	3.030579	2.904952
6	3.046803	4.503877	-0.046372
1	2.635951	4.612482	-1.063775
1	3.535368	5.454199	0.228823
1	3.819929	3.718244	-0.077136
6	0.340626	5.367308	1.198039
1	-0.095254	5.496666	0.193559
1	0.739755	6.341912	1.527959

1	-0.471582	5.079448	1.886100

FU-Ni

92	0.014833	-0.023216	-1.266525
9	0.057574	-0.164073	-3.312395
28	-0.003169	-0.028355	1.221352
15	-2.192963	0.016691	1.484318
15	1.071306	-1.956394	1.336799
15	1.103203	1.876526	1.448729
8	-1.919455	-1.073921	-1.218719
8	2.057687	-0.830368	-1.180170
8	-0.089690	2.153643	-1.198480
6	-2.815833	-1.782716	-0.514254
6	3.070479	-1.346622	-0.468123
6	-0.252275	3.289367	-0.499943
6	-3.131369	-1.412279	0.822852
6	2.821220	-1.968744	0.787543
6	0.266965	3.385663	0.820924
6	-4.076374	-2.159181	1.550836
6	3.892296	-2.505510	1.526445
6	0.082321	4.571349	1.556238
6	-4.698836	-3.269983	0.967494
6	5.200155	-2.427048	1.032265
6	-0.609916	5.650721	0.991957
6	-4.375824	-3.633654	-0.349900
6	5.437570	-1.812046	-0.207891
6	-1.115494	5.546075	-0.314085
6	-3.442914	-2.911960	-1.110080
6	4.397123	-1.266185	-0.974872
6	-0.951308	4.381838	-1.079975
1	-4.860165	-4.505318	-0.805055
1	6.461168	-1.751323	-0.595011
1	-1.656152	6.391395	-0.754883
1	-5.432662	-3.849718	1.535110
1	6.031034	-2.845496	1.607817
1	-0.752151	6.571625	1.564969
1	-4.326863	-1.879207	2.578770
1	3.710436	-2.984306	2.493749
1	0.475448	4.656327	2.574146
6	4.638630	-0.597804	-2.302678
1	4.070459	-1.092694	-3.108556
1	4.296696	0.451980	-2.289958
1	5.707719	-0.611134	-2.566074
6	-3.077116	-3.298819	-2.518610

1	-3.271784	-2.473764	-3.224485
1	-1.998957	-3.522325	-2.603898
1	-3.642204	-4.184913	-2.847448
6	-1.499406	4.249608	-2.476670
1	-0.703735	3.993123	-3.196269
1	-2.241798	3.434391	-2.540044
1	-1.983039	5.182842	-2.804442
6	-3.171589	1.480471	0.884171
1	-4.216333	1.418714	1.230309
1	-2.703870	2.409713	1.245567
1	-3.159061	1.491453	-0.216184
6	-2.604073	0.046166	3.296868
1	-3.691463	0.095667	3.472274
1	-2.194765	-0.845731	3.795278
1	-2.136309	0.939642	3.739091
6	1.418273	2.235867	3.244424
1	1.992795	3.166489	3.384141
1	0.466108	2.310389	3.791238
1	1.997466	1.398646	3.663988
6	2.818478	2.035928	0.752595
1	3.277420	2.992075	1.052097
1	3.434679	1.190097	1.094636
1	2.753645	1.992951	-0.344662
6	0.367161	-3.484892	0.538125
1	0.923774	-4.383491	0.851466
1	-0.696953	-3.581612	0.806070
1	0.442337	-3.385581	-0.556032
6	1.133398	-2.498644	3.112803
1	1.659452	-3.460439	3.229058
1	1.632317	-1.733623	3.726782
1	0.099292	-2.619360	3.470940

ClU-Ni

92	-0.017451	-0.050131	1.162820
17	-0.090859	-0.467667	3.730991
28	-0.007406	-0.037981	-1.343350
15	2.172568	-0.050820	-1.680144
15	-1.151994	-1.918998	-1.476608
15	-1.051529	1.903713	-1.535565
8	1.932508	-1.000336	1.074267
8	-2.078874	-0.706600	1.032862
8	0.129860	2.099701	1.138007
6	2.878590	-1.700645	0.423684

6	-3.106454	-1.271019	0.376666
6	0.272024	3.267375	0.481389
6	3.160261	-1.408038	-0.937574
6	-2.884469	-1.923239	-0.866962
6	-0.223143	3.392538	-0.844836
6	4.144521	-2.149992	-1.617541
6	-3.971223	-2.504230	-1.547886
6	-0.048873	4.606422	-1.535733
6	4.839451	-3.169996	-0.955630
6	-5.260047	-2.441952	-1.004616
6	0.603488	5.682057	-0.919516
6	4.556981	-3.443950	0.392490
6	-5.465329	-1.800386	0.227801
6	1.076751	5.548351	0.395384
6	3.585719	-2.725785	1.106822
6	-4.410840	-1.207361	0.937756
6	0.924048	4.355426	1.118672
1	5.106064	-4.238908	0.909667
1	-6.473631	-1.757665	0.654967
1	1.582060	6.392415	0.878146
1	5.603139	-3.746895	-1.485470
1	-6.101714	-2.896806	-1.534922
1	0.737618	6.623967	-1.459367
1	4.372304	-1.934913	-2.666115
1	-3.816272	-3.008731	-2.506532
1	-0.421280	4.717980	-2.558627
6	-4.614195	-0.511507	2.257799
1	-3.943523	-0.920532	3.031519
1	-4.374827	0.564043	2.184738
1	-5.655479	-0.609265	2.601535
6	3.270866	-3.003593	2.552753
1	3.441456	-2.110288	3.177426
1	2.207083	-3.264203	2.690696
1	3.887739	-3.828391	2.941912
6	1.432171	4.194052	2.527312
1	0.617885	3.914541	3.216905
1	2.179082	3.384002	2.594808
1	1.895714	5.124169	2.890641
6	3.154770	1.460425	-1.220589
1	4.205201	1.357647	-1.537907
1	2.702183	2.351666	-1.683451
1	3.119314	1.586653	-0.128051
6	2.532680	-0.169262	-3.499518
1	3.611122	-0.086913	-3.712420

1	2.155224	-1.124006	-3.896087
1	2.009164	0.653387	-4.011214
6	-1.290653	2.307796	-3.334675
1	-1.866272	3.237598	-3.474954
1	-0.316400	2.404580	-3.837192
1	-1.844431	1.478858	-3.802354
6	-2.789237	2.089271	-0.903680
1	-3.216820	3.057906	-1.208979
1	-3.408213	1.260786	-1.281147
1	-2.772582	2.032095	0.194516
6	-0.459566	-3.502709	-0.784832
1	-1.055961	-4.371572	-1.108730
1	0.586973	-3.614617	-1.110479
1	-0.474732	-3.452238	0.315260
6	-1.302425	-2.363228	-3.276674
1	-1.822954	-3.324062	-3.421675
1	-1.845442	-1.571132	-3.814111
1	-0.290146	-2.446782	-3.701348

BrU-Ni

92	-0.023212	-0.104432	0.982645
35	-0.124445	-0.791168	3.680945
28	0.011047	0.110326	-1.504965
15	2.191928	0.122844	-1.838669
15	-1.116943	-1.765513	-1.795691
15	-1.037275	2.056887	-1.564950
8	1.941873	-1.010405	0.836637
8	-2.082103	-0.750972	0.781820
8	0.121242	2.039625	1.133037
6	2.885154	-1.673791	0.142486
6	-3.100004	-1.264168	0.069448
6	0.263441	3.256557	0.572624
6	3.169436	-1.291226	-1.195543
6	-2.858582	-1.817445	-1.217717
6	-0.223524	3.486093	-0.742482
6	4.147821	-1.993754	-1.924178
6	-3.934053	-2.343472	-1.958631
6	-0.053865	4.754086	-1.329855
6	4.834041	-3.061845	-1.332414
6	-5.230763	-2.324045	-1.430771
6	0.586434	5.779997	-0.623130
6	4.549661	-3.423364	-0.005638
6	-5.454771	-1.781713	-0.154661

6	1.054053	5.541465	0.678800
6	3.583723	-2.747443	0.755972
6	-4.411817	-1.245555	0.615408
6	0.906249	4.291904	1.300574
1	5.092695	-4.255131	0.457297
1	-6.469136	-1.773809	0.259902
1	1.550734	6.346310	1.232276
1	5.593091	-3.607874	-1.900264
1	-6.064248	-2.735838	-2.007196
1	0.716095	6.764287	-1.082444
1	4.377898	-1.710900	-2.955972
1	-3.763498	-2.771736	-2.951356
1	-0.421140	4.947097	-2.342418
6	-4.635089	-0.655273	1.982886
1	-3.954241	-1.102603	2.725865
1	-4.424764	0.429041	1.990388
1	-5.673914	-0.805152	2.314965
6	3.266795	-3.121101	2.179681
1	3.433400	-2.270838	2.862735
1	2.203589	-3.393280	2.298544
1	3.885122	-3.968553	2.514553
6	1.410756	4.016853	2.692790
1	0.602969	3.645185	3.345269
1	2.185640	3.230321	2.690923
1	1.840218	4.923981	3.145070
6	3.172986	1.589720	-1.251257
1	4.224336	1.513281	-1.573096
1	2.721622	2.516104	-1.640163
1	3.133925	1.624509	-0.152177
6	2.572693	0.150009	-3.657592
1	3.655059	0.236006	-3.848552
1	2.190476	-0.763299	-4.138449
1	2.066771	1.019259	-4.106390
6	-1.247491	2.605807	-3.328789
1	-1.824587	3.542175	-3.404317
1	-0.263882	2.746141	-3.802046
1	-1.788414	1.816067	-3.872837
6	-2.784329	2.179961	-0.946244
1	-3.210158	3.172516	-1.164034
1	-3.393460	1.389879	-1.412019
1	-2.783564	2.014908	0.141208
6	-0.426592	-3.386848	-1.195998
1	-1.017354	-4.235393	-1.578382
1	0.623526	-3.476084	-1.517282

1	-0.452991	-3.404629	-0.095127
6	-1.228275	-2.087332	-3.623144
1	-1.720443	-3.048585	-3.844191
1	-1.781940	-1.273620	-4.115319
1	-0.205959	-2.113934	-4.030352

U-Ni

92	0.007546	-0.396967	-0.691463
53	0.091562	-2.256865	-3.069524
28	-0.007181	0.807453	1.515689
15	-2.190856	0.972138	1.801190
15	1.155247	-0.756099	2.547080
15	1.038624	2.603858	0.764349
8	-1.958623	-1.129792	-0.204634
8	2.048689	-0.933892	-0.243242
8	-0.083628	1.489242	-1.716956
6	-2.950332	-1.427472	0.656059
6	3.086468	-1.119120	0.591424
6	-0.201502	2.831926	-1.711071
6	-3.228303	-0.541783	1.729693
6	2.880759	-1.070397	1.996415
6	0.261843	3.574094	-0.592037
6	-4.254825	-0.859524	2.639039
6	3.978493	-1.250563	2.859878
6	0.108112	4.973641	-0.582107
6	-4.994565	-2.038505	2.479962
6	5.257722	-1.477662	2.337215
6	-0.490214	5.625955	-1.667893
6	-4.716683	-2.897508	1.404588
6	5.443275	-1.533256	0.946061
6	-0.927301	4.880224	-2.774023
6	-3.702808	-2.617940	0.475472
6	4.378004	-1.357768	0.050588
6	-0.794130	3.484130	-2.824032
1	-5.303499	-3.814367	1.277674
1	6.443963	-1.719187	0.539793
1	-1.387011	5.393313	-3.626372
1	-5.791362	-2.284903	3.187697
1	6.107904	-1.618758	3.010877
1	-0.608790	6.713317	-1.656137
1	-4.482185	-0.189693	3.473906
1	3.839797	-1.216018	3.944949
1	0.455236	5.561178	0.273278

6	4.554618	-1.411570	-1.444190
1	3.875541	-2.151476	-1.899891
1	4.304259	-0.443360	-1.912765
1	5.591115	-1.667199	-1.712872
6	-3.392402	-3.524832	-0.685419
1	-3.476102	-2.988857	-1.645842
1	-2.353600	-3.895552	-0.643747
1	-4.071766	-4.391028	-0.704976
6	-1.259248	2.667529	-4.000862
1	-0.435487	2.066216	-4.421229
1	-2.041063	1.945755	-3.706598
1	-1.664715	3.312492	-4.795645
6	-3.117222	2.144805	0.694497
1	-4.175177	2.219995	0.993534
1	-2.638393	3.136059	0.731155
1	-3.058989	1.778094	-0.341327
6	-2.565019	1.690523	3.473785
1	-3.640148	1.896694	3.602339
1	-2.231163	0.999837	4.262927
1	-2.011162	2.636261	3.578743
6	1.226192	3.834431	2.146233
1	1.819925	4.710684	1.838187
1	0.236932	4.169200	2.493487
1	1.741202	3.337375	2.982904
6	2.799804	2.455958	0.188283
1	3.219267	3.445515	-0.053741
1	3.399432	1.967771	0.972487
1	2.827506	1.818492	-0.707831
6	0.457888	-2.469701	2.747701
1	1.068542	-3.070534	3.441448
1	-0.577478	-2.393784	3.116528
1	0.437874	-2.970109	1.766972
6	1.337188	-0.244361	4.325965
1	1.850016	-1.013602	4.926244
1	1.899385	0.699583	4.389240
1	0.332588	-0.083760	4.746717

[SiOU-Ni]$^{-}$

92	0.790256	0.247306	0.166685
28	-1.687024	-0.464271	-0.411135
15	-2.629697	1.480777	-0.223809
15	-1.192215	-1.259888	-2.366230
15	-1.921264	-1.840243	1.254205

8	0.201007	2.270934	-0.591898
8	1.403465	-1.604562	-0.942692
8	0.300452	-0.154783	2.296707
6	-0.604780	3.040933	-1.322257
6	1.090413	-2.691813	-1.644912
6	-0.624282	-0.361114	3.237467
6	-2.021188	2.861082	-1.287465
6	-0.097753	-2.745630	-2.437348
6	-1.776030	-1.161542	2.968364
6	-2.843733	3.697723	-2.064481
6	-0.388591	-3.911975	-3.169664
6	-2.733946	-1.350514	3.981539
6	-2.291661	4.700100	-2.874591
6	0.464711	-5.023107	-3.127075
6	-2.572993	-0.766711	5.246422
6	-0.897952	4.871917	-2.904826
6	1.629407	-4.966239	-2.343943
6	-1.432965	0.010518	5.505765
6	-0.041951	4.061727	-2.144968
6	1.959526	-3.823181	-1.601929
6	-0.452809	0.224742	4.525803
1	-0.458228	5.654189	-3.536410
1	2.302474	-5.832071	-2.303245
1	-1.297547	0.468258	6.493831
1	-2.941955	5.343707	-3.476367
1	0.225460	-5.925187	-3.699964
1	-3.327931	-0.919982	6.024601
1	-3.930821	3.565878	-2.043455
1	-1.297509	-3.959429	-3.778513
1	-3.623302	-1.957422	3.783166
6	3.200298	-3.749943	-0.750463
1	3.847293	-2.909677	-1.058869
1	2.947117	-3.560715	0.308046
1	3.782129	-4.684459	-0.810338
6	1.455537	4.224073	-2.173371
1	1.857829	4.408631	-1.161919
1	1.949094	3.300590	-2.526199
1	1.755486	5.055842	-2.831994
6	0.770919	1.064774	4.784882
1	1.696415	0.494141	4.592597
1	0.808860	1.936453	4.107286
1	0.791068	1.430564	5.824696
6	-2.626900	2.305585	1.455430
1	-3.249739	3.216472	1.458519

1	-2.989101	1.590530	2.211341
1	-1.590904	2.577189	1.708789
6	-4.469643	1.485432	-0.550825
1	-4.936718	2.472384	-0.376783
1	-4.662494	1.159226	-1.584472
1	-4.923769	0.747687	0.129071
6	-3.575700	-2.713722	1.296818
1	-3.656580	-3.448370	2.119352
1	-4.386941	-1.974109	1.378714
1	-3.690467	-3.238088	0.335158
6	-0.807685	-3.337975	1.370757
1	-1.130066	-4.017687	2.177895
1	-0.814376	-3.861872	0.401780
1	0.220491	-3.000325	1.570009
6	-0.370300	-0.138702	-3.620578
1	-0.280541	-0.628197	-4.605777
1	-0.953754	0.791941	-3.707975
1	0.635965	0.121424	-3.255292
6	-2.674185	-1.782776	-3.379578
1	-2.403699	-2.136468	-4.391798
1	-3.228452	-2.570415	-2.846475
1	-3.332033	-0.904179	-3.469883
8	2.832453	0.836980	0.393139
14	4.434623	1.152659	0.698583
6	4.932329	0.405063	2.365401
1	5.990361	0.605640	2.609867
1	4.306566	0.819936	3.173569
1	4.781857	-0.687656	2.355312
6	5.504261	0.397695	-0.668592
1	5.234319	0.826070	-1.648636
1	6.580774	0.575333	-0.498390
1	5.337781	-0.691360	-0.724786
6	4.710888	3.025269	0.745801
1	4.416591	3.478710	-0.215783
1	5.766172	3.284353	0.942333
1	4.090437	3.484307	1.533962

[FU-Ni]$^{-}$

92	-0.002493	-0.001841	-1.357028
9	0.036935	-0.139361	-3.431349
28	0.005855	-0.052227	1.280980
15	-2.144631	-0.034877	1.572638
15	1.103798	-1.916458	1.444653

15	1.085037	1.827095	1.501450
8	-1.988975	-1.024661	-1.215509
8	2.020525	-0.952102	-1.219647
8	-0.027644	2.211162	-1.211599
6	-2.847175	-1.752529	-0.499266
6	3.042484	-1.399914	-0.491144
6	-0.216779	3.303468	-0.467366
6	-3.114839	-1.437435	0.867844
6	2.838559	-1.946482	0.813241
6	0.268539	3.361628	0.873503
6	-4.035496	-2.218800	1.590026
6	3.945419	-2.415111	1.545952
6	0.052233	4.525667	1.633723
6	-4.685108	-3.306313	0.988319
6	5.242303	-2.346736	1.017847
6	-0.633628	5.622764	1.091685
6	-4.412946	-3.614415	-0.354654
6	5.436391	-1.804231	-0.263036
6	-1.104851	5.557762	-0.229411
6	-3.505664	-2.859415	-1.112031
6	4.362395	-1.327996	-1.028504
6	-0.909680	4.417732	-1.022821
1	-4.915303	-4.465750	-0.831330
1	6.448645	-1.744726	-0.682739
1	-1.642460	6.412140	-0.659716
1	-5.397599	-3.909009	1.561188
1	6.094882	-2.713477	1.599104
1	-0.797291	6.522631	1.693746
1	-4.246171	-1.982634	2.638387
1	3.798360	-2.833949	2.546998
1	0.416499	4.578804	2.664982
6	4.553216	-0.730039	-2.397939
1	3.947474	-1.258976	-3.153590
1	4.213015	0.320693	-2.425170
1	5.612064	-0.761828	-2.703572
6	-3.191600	-3.182497	-2.549475
1	-3.413382	-2.327093	-3.210871
1	-2.115161	-3.390856	-2.684536
1	-3.765063	-4.057697	-2.897097
6	-1.421072	4.323223	-2.436828
1	-0.605661	4.090474	-3.143072
1	-2.152329	3.501870	-2.543097
1	-1.904822	5.262958	-2.750468
6	-3.124768	1.427679	0.938453

1	-4.179922	1.372733	1.257069
1	-2.663126	2.358625	1.303986
1	-3.079039	1.429383	-0.161156
6	-2.700207	0.002279	3.357341
1	-3.798327	0.071363	3.466802
1	-2.330232	-0.891416	3.882672
1	-2.235758	0.885940	3.822233
6	1.515850	2.284020	3.262734
1	2.094414	3.223376	3.335694
1	0.596999	2.366494	3.863415
1	2.116989	1.457773	3.673157
6	2.785039	1.993219	0.739844
1	3.260128	2.948414	1.021457
1	3.408355	1.144763	1.063174
1	2.684052	1.945970	-0.354884
6	0.399633	-3.448774	0.629496
1	0.981715	-4.349712	0.889912
1	-0.650938	-3.569918	0.937846
1	0.423864	-3.309124	-0.462555
6	1.284597	-2.584415	3.182354
1	1.804767	-3.559572	3.215305
1	1.821877	-1.855412	3.808101
1	0.270069	-2.704959	3.593534

[ClU-Ni]$^{-}$

92	0.015285	-0.032295	-1.295872
17	0.099029	-0.379599	-3.949004
28	0.028818	-0.032182	1.393539
15	-2.114613	-0.221970	1.701464
15	1.313079	-1.770665	1.563664
15	0.880472	1.958005	1.542646
8	-1.857423	-1.188443	-1.060405
8	2.123253	-0.662531	-1.059225
8	-0.297981	2.147779	-1.157831
6	-2.653089	-1.999484	-0.357814
6	3.192684	-1.011415	-0.341891
6	-0.619078	3.223388	-0.429894
6	-2.951444	-1.710955	1.006559
6	3.044539	-1.605517	0.947533
6	-0.139427	3.360501	0.906141
6	-3.794776	-2.577136	1.726528
6	4.193467	-1.965555	1.676964
6	-0.505443	4.493567	1.655409

6	-4.336377	-3.719242	1.119239
6	5.475358	-1.740322	1.156518
6	-1.334402	5.482177	1.105211
6	-4.036294	-3.995278	-0.224895
6	5.611794	-1.151422	-0.111688
6	-1.794831	5.341454	-0.213709
6	-3.202965	-3.156948	-0.980373
6	4.494825	-0.780445	-0.874139
6	-1.451841	4.229474	-0.997325
1	-4.457164	-4.887582	-0.705070
1	6.612459	-0.972831	-0.524728
1	-2.442506	6.111975	-0.650211
1	-4.989677	-4.388914	1.688380
1	6.362362	-2.023634	1.732931
1	-1.616740	6.357900	1.698786
1	-4.029588	-2.364262	2.774820
1	4.089882	-2.423200	2.666481
1	-0.146662	4.605264	2.683750
6	4.620638	-0.139385	-2.231579
1	4.059905	-0.705287	-2.994695
1	4.185706	0.876087	-2.235001
1	5.675763	-0.067145	-2.542386
6	-2.861909	-3.442030	-2.419716
1	-3.149745	-2.602438	-3.075028
1	-1.772786	-3.561302	-2.558390
1	-3.363059	-4.357477	-2.774262
6	-1.948459	4.055105	-2.408805
1	-1.110698	3.948334	-3.118993
1	-2.545101	3.131491	-2.511639
1	-2.570532	4.909940	-2.720882
6	-3.235550	1.140226	1.083355
1	-4.278153	0.985334	1.408964
1	-2.859186	2.109312	1.446546
1	-3.198900	1.149438	-0.016313
6	-2.643128	-0.251691	3.494248
1	-3.740147	-0.301251	3.621659
1	-2.171493	-1.105088	4.005777
1	-2.270910	0.673728	3.960904
6	1.262684	2.488515	3.295294
1	1.720156	3.493372	3.349622
1	0.345258	2.467067	3.903269
1	1.965273	1.750013	3.712200
6	2.534368	2.355002	0.760730
1	2.874664	3.366280	1.041977

1	3.276544	1.602743	1.071898
1	2.429820	2.301701	-0.333570
6	0.788161	-3.384625	0.773943
1	1.475047	-4.207245	1.037705
1	-0.237719	-3.623847	1.096885
1	0.781452	-3.258476	-0.320184
6	1.549433	-2.379172	3.315933
1	2.158786	-3.299370	3.375009
1	2.012593	-1.588032	3.925044
1	0.548024	-2.584851	3.725388

[**BrU-Ni**]$^{-}$

92	-0.020151	-0.044944	1.107122
35	-0.117077	-0.492926	3.942170
28	0.029764	0.064214	-1.575050
15	2.185928	0.041738	-1.831240
15	-1.095276	-1.769940	-1.848292
15	-0.996610	1.979816	-1.679782
8	1.919548	-1.091891	0.865485
8	-2.053347	-0.862465	0.802155
8	0.111991	2.148052	1.050436
6	2.778895	-1.814051	0.141506
6	-3.070937	-1.287847	0.051066
6	0.314783	3.295497	0.392964
6	3.096027	-1.429761	-1.194968
6	-2.843641	-1.802080	-1.260886
6	-0.157977	3.452373	-0.943041
6	4.008228	-2.202470	-1.937171
6	-3.939124	-2.243153	-2.027117
6	0.076980	4.665703	-1.615813
6	4.598954	-3.345514	-1.379746
6	-5.243960	-2.180059	-1.519365
6	0.766649	5.713524	-0.988910
6	4.278341	-3.717436	-0.063584
6	-5.457903	-1.672560	-0.226986
6	1.222313	5.550027	0.329092
6	3.377540	-2.973716	0.713144
6	-4.396669	-1.222095	0.571220
6	1.010078	4.357830	1.037248
1	4.737401	-4.611323	0.376870
1	-6.476745	-1.622775	0.177146
1	1.760650	6.367036	0.825411
1	5.305639	-3.942331	-1.965857

1	-6.088476	-2.526758	-2.124026
1	0.944907	6.652786	-1.522758
1	4.258086	-1.915794	-2.964199
1	-3.775849	-2.637910	-3.035482
1	-0.276795	4.797129	-2.643577
6	-4.608628	-0.663537	1.954156
1	-3.968573	-1.173016	2.693835
1	-4.327386	0.403909	2.001516
1	-5.662170	-0.757385	2.264699
6	3.014655	-3.359839	2.123063
1	3.259249	-2.554379	2.836451
1	1.927153	-3.520954	2.227064
1	3.538379	-4.279034	2.432537
6	1.501846	4.159805	2.447417
1	0.674920	3.892232	3.126995
1	2.219292	3.322366	2.507556
1	1.994363	5.069173	2.828906
6	3.205009	1.434304	-1.110245
1	4.263449	1.355545	-1.412391
1	2.784452	2.398000	-1.438565
1	3.138448	1.385525	-0.012995
6	2.762443	0.151647	-3.605710
1	3.863190	0.185945	-3.698975
1	2.369756	-0.700970	-4.180616
1	2.338255	1.074725	-4.030815
6	-1.358405	2.544554	-3.425270
1	-1.915849	3.498086	-3.463626
1	-0.417628	2.643166	-3.988219
1	-1.961711	1.757216	-3.903616
6	-2.710875	2.155505	-0.956822
1	-3.146652	3.142174	-1.188316
1	-3.350612	1.350616	-1.351098
1	-2.643596	2.034709	0.134570
6	-0.440664	-3.373736	-1.139452
1	-1.036249	-4.238096	-1.480481
1	0.613546	-3.493894	-1.436026
1	-0.483465	-3.320550	-0.040390
6	-1.250231	-2.294186	-3.636981
1	-1.781679	-3.255500	-3.759837
1	-1.767860	-1.510065	-4.210251
1	-0.230158	-2.396475	-4.039018

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92	0.081593	-0.633394	-0.651389
53	0.388177	-3.094926	-2.549432
28	-0.113857	1.242811	1.251253
15	-2.265870	1.203484	1.554173
15	1.182039	0.213334	2.657936
15	0.694289	2.833537	0.009177
8	-1.784449	-1.390902	0.240839
8	2.155416	-0.829108	0.078872
8	-0.313231	0.980661	-2.079883
6	-2.660137	-1.530873	1.240459
6	3.181834	-0.521759	0.874328
6	-0.634000	2.245736	-2.375142
6	-3.060461	-0.398996	2.009516
6	2.951537	-0.030112	2.193271
6	-0.231836	3.312822	-1.518957
6	-3.993733	-0.568245	3.049425
6	4.052722	0.275732	3.015472
6	-0.590238	4.631900	-1.855798
6	-4.526535	-1.832753	3.336838
6	5.364276	0.110118	2.548391
6	-1.334614	4.902638	-3.012855
6	-4.124777	-2.941091	2.573661
6	5.579855	-0.368853	1.245161
6	-1.722365	3.843231	-3.849082
6	-3.197330	-2.818973	1.528413
6	4.512779	-0.688303	0.392922
6	-1.387077	2.513864	-3.553212
1	-4.541059	-3.932586	2.791757
1	6.604723	-0.500052	0.875595
1	-2.303769	4.048500	-4.756552
1	-5.253723	-1.953506	4.146799
1	6.213928	0.349812	3.196428
1	-1.607849	5.932893	-3.263834
1	-4.311101	0.294384	3.644673
1	3.889168	0.651411	4.031073
1	-0.289867	5.461692	-1.207353
6	4.719204	-1.191890	-1.011888
1	4.178524	-2.138085	-1.182679
1	4.313028	-0.481587	-1.754470
1	5.789092	-1.345071	-1.228449
6	-2.749043	-3.999864	0.707895
1	-2.902814	-3.824422	-0.370091
1	-1.665690	-4.181551	0.822183

1	-3.287620	-4.915826	1.001502
6	-1.804293	1.362092	-4.430445
1	-0.932124	0.772184	-4.760194
1	-2.451021	0.654287	-3.882212
1	-2.350599	1.715928	-5.319933
6	-3.374258	1.755110	0.152895
1	-4.432706	1.778888	0.463736
1	-3.054228	2.751504	-0.190317
1	-3.258520	1.052211	-0.685480
6	-2.888006	2.360509	2.884925
1	-3.990838	2.382410	2.954583
1	-2.462757	2.073577	3.859090
1	-2.526087	3.370886	2.638051
6	0.841572	4.459005	0.922172
1	1.321318	5.250611	0.318192
1	-0.154399	4.795205	1.248743
1	1.451567	4.273970	1.820088
6	2.441089	2.723674	-0.650518
1	2.739130	3.660155	-1.151998
1	3.126385	2.502721	0.183120
1	2.500694	1.894103	-1.370642
6	0.715444	-1.499255	3.250700
1	1.385728	-1.846813	4.055629
1	-0.328466	-1.483507	3.602848
1	0.780540	-2.198589	2.402464
6	1.310794	1.068126	4.315838
1	1.909389	0.497550	5.049091
1	1.748965	2.069101	4.182232
1	0.287989	1.190148	4.704671

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92	-0.119137	0.082626	0.867602
53	-0.560901	0.584167	3.813090
46	0.132853	-0.236256	-1.834141
15	2.298998	-1.197832	-1.633268
15	-1.800561	-1.590195	-1.963559
15	0.008571	2.113647	-2.133260
8	1.193145	-1.590809	1.071478
8	-2.243441	-0.159960	0.574840
8	1.056433	1.852512	0.618785
6	1.884957	-2.684560	0.683308
6	-3.383109	-0.211707	-0.144873
6	1.697076	2.839661	-0.041737

6	2.499591	-2.704017	-0.597011
6	-3.395069	-0.868817	-1.404270
6	1.342993	3.135124	-1.385431
6	3.204155	-3.854568	-0.999306
6	-4.587574	-0.897165	-2.151778
6	2.040006	4.150857	-2.067732
6	3.301696	-4.960617	-0.145358
6	-5.747642	-0.287939	-1.656624
6	3.062927	4.861691	-1.427115
6	2.696668	-4.920216	1.119965
6	-5.722260	0.347568	-0.405492
6	3.391816	4.563782	-0.095909
6	1.981203	-3.795476	1.560394
6	-4.555071	0.399565	0.372461
6	2.725925	3.557342	0.620858
1	2.777474	-5.784497	1.788502
1	-6.631914	0.819359	-0.017502
1	4.188301	5.125090	0.405365
1	3.852861	-5.850589	-0.463079
1	-6.671418	-0.312370	-2.242064
1	3.598499	5.651426	-1.962246
1	3.683437	-3.890959	-1.982103
1	-4.615901	-1.394353	-3.125933
1	1.785516	4.392116	-3.103975
6	-4.506006	1.082181	1.713924
1	-4.135955	0.401013	2.498227
1	-3.805803	1.936001	1.707110
1	-5.500083	1.454310	2.005731
6	1.315078	-3.742549	2.910207
1	1.640472	-2.861060	3.487357
1	0.218476	-3.654638	2.814399
1	1.535548	-4.648500	3.495508
6	3.073097	3.213064	2.045553
1	2.178324	3.218773	2.689985
1	3.494949	2.194927	2.120916
1	3.811594	3.919514	2.454742
6	3.654091	-0.104466	-0.980125
1	4.623225	-0.629409	-0.984150
1	3.713789	0.809486	-1.591876
1	3.404248	0.190813	0.050099
6	3.008532	-1.688249	-3.277562
1	4.051381	-2.036412	-3.194212
1	2.394313	-2.478462	-3.735040
1	2.983508	-0.805543	-3.935113

6	0.057120	2.552875	-3.935547
1	-0.067837	3.635493	-4.103398
1	1.007882	2.220223	-4.378304
1	-0.765633	2.021154	-4.437780
6	-1.535792	3.006679	-1.603349
1	-1.524399	4.057195	-1.937843
1	-2.410430	2.481811	-2.018766
1	-1.612949	2.983696	-0.504980
6	-1.777945	-3.234908	-1.093860
1	-2.659379	-3.840790	-1.360805
1	-0.852055	-3.768812	-1.358803
1	-1.778394	-3.064919	-0.006336
6	-2.133201	-2.121185	-3.709983
1	-2.990916	-2.810670	-3.776542
1	-2.320883	-1.240900	-4.343050
1	-1.236485	-2.636077	-4.087857

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92	0.127859	0.912200	0.448635
53	0.595115	3.695514	1.542209
78	-0.170396	-1.508908	-0.847358
15	-2.489677	-1.287488	-1.151963
15	1.431781	-0.916878	-2.447580
15	0.507667	-2.699135	1.077885
8	-1.682776	1.497599	-0.543804
8	2.184606	0.803122	-0.154549
8	-0.372724	-0.113267	2.258750
6	-2.599454	1.470688	-1.534499
6	3.281216	0.288793	-0.746865
6	-0.789642	-1.152746	3.011008
6	-3.121112	0.226201	-1.979045
6	3.143374	-0.565698	-1.873544
6	-0.476378	-2.482276	2.618186
6	-4.062826	0.212221	-3.026054
6	4.299415	-1.105517	-2.469543
6	-0.940554	-3.554503	3.404995
6	-4.481310	1.410424	-3.618019
6	5.567715	-0.800233	-1.959862
6	-1.693728	-3.313196	4.560864
6	-3.963293	2.631810	-3.160914
6	5.687174	0.054257	-0.852979
6	-1.983610	-1.993931	4.940863
6	-3.022907	2.692106	-2.120563

6	4.561956	0.613016	-0.227468
6	-1.544839	-0.895934	4.184929
1	-4.294258	3.569057	-3.622019
1	6.680362	0.298789	-0.460181
1	-2.567423	-1.805723	5.848809
1	-5.213345	1.393065	-4.430741
1	6.461924	-1.221132	-2.428802
1	-2.048343	-4.151175	5.168088
1	-4.474929	-0.735808	-3.384256
1	4.215204	-1.766260	-3.337486
1	-0.713537	-4.585857	3.119259
6	4.670492	1.527592	0.964389
1	4.109757	2.463347	0.804195
1	4.235283	1.064227	1.867772
1	5.721675	1.773383	1.179982
6	-2.452461	3.993885	-1.623069
1	-2.614950	4.116956	-0.539220
1	-1.358348	4.037389	-1.765157
1	-2.903996	4.849784	-2.148003
6	-1.856067	0.525858	4.572975
1	-0.937521	1.130553	4.656898
1	-2.479098	1.024051	3.809425
1	-2.392632	0.564983	5.533421
6	-3.540440	-1.368903	0.377706
1	-4.612382	-1.326800	0.123874
1	-3.313539	-2.297268	0.924693
1	-3.288876	-0.518904	1.029289
6	-3.193920	-2.686422	-2.142772
1	-4.294701	-2.646384	-2.186204
1	-2.784279	-2.673271	-3.163628
1	-2.893081	-3.628632	-1.659090
6	0.491394	-4.529920	0.781434
1	0.882027	-5.091615	1.645856
1	-0.531038	-4.868050	0.555013
1	1.128245	-4.737666	-0.092074
6	2.246547	-2.451504	1.684208
1	2.469630	-3.123829	2.528972
1	2.950378	-2.630265	0.856171
1	2.363879	-1.407946	2.013538
6	1.084189	0.535950	-3.554442
1	1.864768	0.642281	-4.325788
1	0.096700	0.403620	-4.023489
1	1.057286	1.452305	-2.944488
6	1.638504	-2.273277	-3.694298

1	2.329261	-1.983756	-4.502944
1	2.009394	-3.184947	-3.202534
1	0.651297	-2.487926	-4.130726

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92	0.245537	-0.759161	0.618012
53	1.119501	-3.249413	2.273393
46	-0.415792	1.489444	-1.168199
15	-2.378612	1.917231	0.034198
15	1.545394	2.647942	-0.634680
15	-0.532487	0.041705	-3.003169
8	-0.903109	0.379668	2.103620
8	2.293999	-0.076900	0.177756
8	-1.070100	-1.853315	-0.770722
6	-1.492698	1.454291	2.641246
6	3.287065	0.487006	-0.518365
6	-1.909150	-2.062325	-1.788568
6	-2.274110	2.329590	1.830845
6	3.156205	1.828161	-0.987319
6	-1.811821	-1.286529	-2.983273
6	-2.882556	3.451635	2.424371
6	4.208947	2.410534	-1.717503
6	-2.711442	-1.536386	-4.037346
6	-2.731022	3.713404	3.793164
6	5.379427	1.688373	-1.987735
6	-3.693689	-2.529905	-3.926613
6	-1.964282	2.841850	4.582017
6	5.499259	0.369213	-1.521245
6	-3.780540	-3.286732	-2.746981
6	-1.337407	1.713099	4.032974
6	4.473761	-0.252286	-0.791773
6	-2.908420	-3.071212	-1.670219
1	-1.844544	3.039077	5.654511
1	6.414214	-0.200076	-1.727649
1	-4.545329	-4.067971	-2.655313
1	-3.212303	4.587982	4.243342
1	6.194635	2.151020	-2.553928
1	-4.383654	-2.717398	-4.755958
1	-3.485517	4.131283	1.813923
1	4.117142	3.438899	-2.082038
1	-2.647187	-0.949214	-4.959102
6	4.587938	-1.672776	-0.303321
1	4.376385	-1.749668	0.776250

1	3.847631	-2.329205	-0.794991
1	5.592708	-2.080059	-0.502399
6	-0.502372	0.774930	4.864706
1	-0.862799	-0.264652	4.784208
1	0.545969	0.753236	4.516626
1	-0.509938	1.071952	5.926330
6	-2.995992	-3.864397	-0.392622
1	-2.023313	-4.313839	-0.130874
1	-3.264723	-3.217870	0.462302
1	-3.751090	-4.663628	-0.471241
6	-3.686939	0.586818	0.063177
1	-4.597714	0.924873	0.586295
1	-3.925693	0.290799	-0.970533
1	-3.271589	-0.290772	0.580418
6	-3.393494	3.324337	-0.650839
1	-4.359955	3.448975	-0.130460
1	-2.819418	4.261884	-0.594766
1	-3.583202	3.104133	-1.712931
6	-0.838576	0.889424	-4.637475
1	-0.821418	0.192106	-5.494221
1	-1.804543	1.416749	-4.610358
1	-0.043719	1.639893	-4.769455
6	0.994869	-0.933991	-3.456453
1	0.855742	-1.492115	-4.398367
1	1.849846	-0.244489	-3.541178
1	1.209141	-1.646720	-2.645143
6	1.782998	3.150155	1.147224
1	2.689207	3.765843	1.280034
1	0.890847	3.698779	1.488215
1	1.875142	2.234888	1.751220
6	1.738221	4.312594	-1.452267
1	2.649011	4.846439	-1.127286
1	1.752592	4.188783	-2.545916
1	0.855021	4.915296	-1.188649

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92	-1.095152	-0.028749	0.300587
53	-4.181797	0.028354	0.781398
78	1.721169	0.051681	-0.500065
15	1.851161	-2.245756	-0.808847
15	1.328909	1.536700	-2.231916
15	2.289268	0.891589	1.592608
8	-1.094072	-1.934184	-0.806296

8	-1.064401	2.014238	-0.529486
8	-0.318464	-0.294730	2.339763
6	-0.699506	-2.704076	-1.828045
6	-0.516093	3.167989	-0.919750
6	0.626949	-0.642074	3.221784
6	0.680683	-3.022027	-1.999451
6	0.621769	3.177131	-1.782110
6	1.959881	-0.158274	3.073605
6	1.072870	-3.833845	-3.080594
6	1.176467	4.409995	-2.176742
6	2.939439	-0.546589	4.006860
6	0.124775	-4.327014	-3.987654
6	0.629751	5.620635	-1.730137
6	2.616619	-1.396775	5.074408
6	-1.231174	-4.008292	-3.810869
6	-0.488670	5.601296	-0.880962
6	1.299230	-1.861049	5.214770
6	-1.666823	-3.204796	-2.746344
6	-1.075548	4.397668	-0.463953
6	0.291968	-1.500577	4.307055
1	-1.977586	-4.389722	-4.518570
1	-0.921833	6.545460	-0.528281
1	1.040847	-2.525210	6.048860
1	0.440458	-4.956212	-4.826524
1	1.070110	6.573028	-2.043331
1	3.386289	-1.692434	5.794901
1	2.130022	-4.080850	-3.223148
1	2.050437	4.428695	-2.836149
1	3.967941	-0.186421	3.901168
6	-2.267385	4.363450	0.456731
1	-3.099784	3.786311	0.020302
1	-2.025155	3.858344	1.409065
1	-2.620935	5.382012	0.686141
6	-3.116394	-2.845204	-2.551902
1	-3.478461	-3.148242	-1.554914
1	-3.271829	-1.752476	-2.596575
1	-3.749811	-3.318742	-3.319703
6	-1.122373	-2.004285	4.432391
1	-1.846622	-1.172410	4.441845
1	-1.402706	-2.633044	3.568318
1	-1.252719	-2.600327	5.350272
6	1.626469	-3.335766	0.687086
1	1.794074	-4.398207	0.439943
1	2.318533	-3.012179	1.480193

1	0.598019	-3.206225	1.055618
6	3.515615	-2.847562	-1.387197
1	3.566157	-3.948243	-1.466407
1	3.761758	-2.391977	-2.358079
1	4.258211	-2.503802	-0.650747
6	4.098694	1.300050	1.758484
1	4.347401	1.732936	2.743796
1	4.704703	0.398629	1.583916
1	4.338634	2.030351	0.970422
6	1.564754	2.519945	2.150599
1	2.018588	2.848510	3.101338
1	1.726422	3.276745	1.367271
1	0.480626	2.396651	2.294179
6	0.194709	1.016916	-3.619415
1	0.160938	1.780043	-4.416308
1	0.538766	0.052715	-4.025468
1	-0.817007	0.879990	-3.208370
6	2.843726	1.979755	-3.221365
1	2.619116	2.655745	-4.065706
1	3.595256	2.441712	-2.563672
1	3.262265	1.039512	-3.611848

Th-Ni

90	0.056595	-0.407876	0.738251
53	0.255115	-1.997425	3.377592
28	-0.134105	0.744977	-1.563222
15	2.016817	1.076314	-1.887855
15	-1.168565	-0.937600	-2.533362
15	-1.318437	2.453673	-0.825119
8	2.081157	-1.056345	0.125365
8	-1.892471	-1.355708	0.262274
8	-0.054516	1.582333	1.693345
6	3.051248	-1.253286	-0.793043
6	-2.973754	-1.530274	-0.525835
6	-0.038735	2.929202	1.596108
6	3.184283	-0.344251	-1.875970
6	-2.843870	-1.390476	-1.933847
6	-0.593745	3.562916	0.452037
6	4.184695	-0.563514	-2.841877
6	-3.973580	-1.570003	-2.755246
6	-0.554567	4.967277	0.356882
6	5.044952	-1.662878	-2.730848
6	-5.215517	-1.879284	-2.186803

6	0.020403	5.730341	1.380837
6	4.914406	-2.541434	-1.644059
6	-5.330125	-2.010331	-0.793462
6	0.553747	5.089991	2.510076
6	3.929170	-2.360427	-0.660383
6	-4.228908	-1.838995	0.060510
6	0.537389	3.692986	2.643813
1	5.596951	-3.393612	-1.550383
1	-6.302868	-2.251370	-0.350292
1	0.997702	5.687616	3.313941
1	5.821791	-1.830410	-3.482584
1	-6.091104	-2.022059	-2.826980
1	0.047035	6.820970	1.302913
1	4.300003	0.126691	-3.683152
1	-3.888827	-1.469361	-3.841922
1	-0.976116	5.472616	-0.517163
6	-4.341520	-1.960023	1.557705
1	-3.628392	-2.700119	1.957486
1	-4.097141	-1.005059	2.056458
1	-5.359970	-2.252104	1.856135
6	3.783748	-3.290697	0.515548
1	3.842552	-2.740755	1.469986
1	2.800019	-3.791736	0.518514
1	4.566106	-4.065049	0.505862
6	1.112258	2.989391	3.845218
1	0.367118	2.326523	4.316235
1	1.959730	2.339273	3.564685
1	1.467113	3.712226	4.595667
6	2.898879	2.297489	-0.794115
1	3.927072	2.477003	-1.147739
1	2.332904	3.241944	-0.767539
1	2.941275	1.897712	0.230818
6	2.271561	1.852949	-3.557922
1	3.322489	2.142756	-3.720465
1	1.960446	1.154687	-4.349742
1	1.645099	2.756056	-3.622919
6	-1.658055	3.579150	-2.265366
1	-2.298808	4.429696	-1.980938
1	-0.712018	3.958336	-2.680802
1	-2.174057	2.996355	-3.044208
6	-3.045170	2.192473	-0.177308
1	-3.569201	3.155009	-0.060637
1	-3.599110	1.536256	-0.867161
1	-2.998734	1.697671	0.805250

6	-0.320701	-2.593003	-2.643942
1	-0.880078	-3.281087	-3.298562
1	0.703396	-2.451612	-3.023773
1	-0.259270	-3.045049	-1.641087
6	-1.416026	-0.554917	-4.334089
1	-1.885122	-1.396064	-4.870218
1	-2.041503	0.343606	-4.446721
1	-0.431526	-0.354887	-4.784275

Pa-Ni

91	-0.047965	-0.216415	0.803083
53	-0.212828	-1.183118	3.707657
28	0.048721	0.433046	-1.673508
15	2.216481	0.139305	-1.961924
15	-1.356254	-1.151325	-2.288189
15	-0.686139	2.486112	-1.333456
8	1.772901	-1.443960	0.437430
8	-2.195145	-0.748329	0.473830
8	0.400603	1.899599	1.299947
6	2.592581	-2.103460	-0.397791
6	-3.270668	-0.861122	-0.321406
6	0.766664	3.137271	0.922413
6	2.941356	-1.517740	-1.645330
6	-3.099441	-1.068763	-1.718989
6	0.353529	3.633216	-0.344424
6	3.787118	-2.213730	-2.528705
6	-4.228742	-1.181950	-2.550832
6	0.758918	4.916271	-0.754543
6	4.281185	-3.477531	-2.179189
6	-5.516133	-1.090026	-2.005377
6	1.562836	5.701247	0.083246
6	3.937023	-4.042715	-0.940350
6	-5.674422	-0.890070	-0.624002
6	1.951491	5.207134	1.338684
6	3.097625	-3.380012	-0.031328
6	-4.574084	-0.771935	0.238914
6	1.566984	3.932733	1.784894
1	4.330518	-5.028333	-0.666947
1	-6.682659	-0.825322	-0.199135
1	2.573533	5.826093	1.995351
1	4.937728	-4.018803	-2.866694
1	-6.393758	-1.180688	-2.652043
1	1.879937	6.697788	-0.237823

1	4.063332	-1.774569	-3.492366
1	-4.109957	-1.341494	-3.627195
1	0.452545	5.308308	-1.729324
6	-4.726030	-0.548794	1.720744
1	-4.161788	-1.299524	2.298837
1	-4.318659	0.432765	2.021953
1	-5.784331	-0.588550	2.022198
6	2.713719	-3.971934	1.298944
1	2.966268	-3.290024	2.128014
1	1.623785	-4.135109	1.369085
1	3.218844	-4.935862	1.466275
6	1.977096	3.386113	3.127125
1	1.096892	3.113040	3.733488
1	2.569309	2.460297	3.021659
1	2.576509	4.119641	3.688216
6	3.385918	1.264179	-1.053933
1	4.425120	1.098733	-1.382057
1	3.093301	2.312260	-1.223836
1	3.314415	1.056941	0.024601
6	2.670425	0.505154	-3.725683
1	3.758815	0.437762	-3.887183
1	2.158595	-0.194072	-4.404174
1	2.341420	1.528531	-3.963827
6	-0.879473	3.330188	-2.976500
1	-1.267291	4.356374	-2.867196
1	0.085959	3.359335	-3.504051
1	-1.591311	2.747046	-3.580891
6	-2.372727	2.748136	-0.593858
1	-2.659794	3.811246	-0.639504
1	-3.108908	2.128622	-1.129530
1	-2.356351	2.431722	0.460669
6	-0.911458	-2.925819	-1.936044
1	-1.599788	-3.611938	-2.456279
1	0.127763	-3.117604	-2.246601
1	-0.993610	-3.115309	-0.853592
6	-1.471724	-1.173450	-4.141283
1	-2.111836	-1.996181	-4.500215
1	-1.871163	-0.215324	-4.507157
1	-0.458496	-1.309485	-4.549391

Np-Ni

93	0.045407	-0.002662	0.799178
53	0.183861	0.012979	3.815086
28	-0.064081	-0.043252	-1.698820
15	2.009375	0.628923	-2.042281
15	-0.552190	-2.192458	-1.846554
15	-1.703427	1.428990	-1.869043
8	2.147581	-0.484435	0.647291
8	-1.497962	-1.522360	0.826613
8	-0.539329	2.065623	0.726741
6	3.232265	-0.848412	-0.059773
6	-2.409066	-2.279680	0.191144
6	-0.831304	3.198270	0.062000
6	3.369225	-0.427826	-1.410020
6	-2.156607	-2.728825	-1.133430
6	-1.402597	3.126733	-1.237129
6	4.496039	-0.828376	-2.151862
6	-3.122965	-3.506951	-1.797877
6	-1.686989	4.316300	-1.933661
6	5.476371	-1.635174	-1.559580
6	-4.323608	-3.836076	-1.154778
6	-1.410984	5.558200	-1.346717
6	5.338502	-2.029434	-0.218704
6	-4.555983	-3.395418	0.158568
6	-0.859546	5.614040	-0.056082
6	4.231578	-1.648836	0.555726
6	-3.617950	-2.618477	0.855357
6	-0.562103	4.451955	0.671942
1	6.112324	-2.651462	0.245125
1	-5.493662	-3.658925	0.660541
1	-0.651580	6.587086	0.402838
1	6.349988	-1.950409	-2.137669
1	-5.075178	-4.439093	-1.672601
1	-1.630277	6.482138	-1.889928
1	4.612626	-0.513885	-3.193718
1	-2.944964	-3.857345	-2.819551
1	-2.123028	4.279822	-2.937079
6	-3.849751	-2.125608	2.259162
1	-3.024063	-2.420468	2.927960
1	-3.884506	-1.022451	2.296128
1	-4.795200	-2.514633	2.667270
6	4.068810	-2.056477	1.995953
1	3.960969	-1.174828	2.649938
1	3.151643	-2.652171	2.145053

1	4.929612	-2.649523	2.340907
6	0.031293	4.487412	2.055553
1	-0.608258	3.954052	2.778680
1	1.008507	3.974984	2.086444
1	0.169510	5.522569	2.403227
6	2.539106	2.327542	-1.504726
1	3.537852	2.570975	-1.902364
1	1.800628	3.070019	-1.845128
1	2.577260	2.355535	-0.405247
6	2.305401	0.721044	-3.873836
1	3.307702	1.115481	-4.108346
1	2.191989	-0.276099	-4.325542
1	1.551594	1.392378	-4.313565
6	-2.107663	1.669011	-3.665850
1	-2.955343	2.359283	-3.806362
1	-1.229003	2.057808	-4.202600
1	-2.376402	0.691283	-4.095005
6	-3.379491	1.027732	-1.171660
1	-4.127163	1.774742	-1.484215
1	-3.681054	0.021519	-1.501912
1	-3.316421	1.024942	-0.072661
6	0.631657	-3.474707	-1.203519
1	0.309599	-4.487352	-1.495667
1	1.643599	-3.270076	-1.587103
1	0.659231	-3.415134	-0.104840
6	-0.660915	-2.671531	-3.638692
1	-0.877934	-3.745468	-3.760365
1	-1.444000	-2.084175	-4.141804
1	0.305142	-2.451336	-4.119086

Pu-Ni

94	-0.061137	-0.000403	-0.830826
53	-0.250045	-0.010881	-3.827563
28	0.085534	-0.038255	1.663645
15	-1.965219	0.661965	2.100734
15	0.550481	-2.190723	1.879190
15	1.756928	1.400192	1.853712
8	-2.173478	-0.462087	-0.610430
8	1.474287	-1.546771	-0.833575
8	0.551643	2.072325	-0.743254
6	-3.242429	-0.797385	0.125827
6	2.373170	-2.310361	-0.198516
6	0.878113	3.186141	-0.070464

6	-3.349286	-0.368418	1.478849
6	2.130074	-2.751957	1.133359
6	1.471912	3.098399	1.220260
6	-4.475567	-0.735403	2.239252
6	3.088489	-3.547540	1.788989
6	1.802673	4.276810	1.914964
6	-5.484840	-1.521807	1.669305
6	4.277007	-3.900329	1.136124
6	1.547636	5.528694	1.340435
6	-5.374871	-1.933095	0.330466
6	4.505936	-3.463905	-0.179104
6	0.969307	5.604356	0.062911
6	-4.272687	-1.583700	-0.463683
6	3.575242	-2.673835	-0.869939
6	0.628561	4.454850	-0.665105
1	-6.169428	-2.541573	-0.115571
1	5.434900	-3.744202	-0.688481
1	0.776558	6.584657	-0.386970
1	-6.358100	-1.808184	2.262490
1	5.021038	-4.517284	1.648403
1	1.805294	6.443098	1.882528
1	-4.570211	-0.408812	3.279453
1	2.913432	-3.894909	2.811941
1	2.261162	4.223285	2.907123
6	3.809023	-2.190224	-2.276372
1	2.976043	-2.474474	-2.940696
1	3.862805	-1.087826	-2.319403
1	4.746712	-2.597161	-2.685483
6	-4.141689	-2.014434	-1.900443
1	-4.008275	-1.145970	-2.566991
1	-3.248680	-2.645842	-2.051818
1	-5.027335	-2.580665	-2.227655
6	0.006365	4.521225	-2.034652
1	0.597760	3.952250	-2.771105
1	-0.999632	4.066314	-2.042221
1	-0.081416	5.562682	-2.380262
6	-2.451347	2.370688	1.554143
1	-3.442550	2.640010	1.953756
1	-1.695031	3.097711	1.888800
1	-2.491589	2.396118	0.454720
6	-2.254550	0.770781	3.931298
1	-3.247586	1.188454	4.165954
1	-2.161867	-0.226414	4.387657
1	-1.484686	1.427702	4.364654

6	2.232679	1.640671	3.631420
1	3.106099	2.304813	3.737801
1	1.385396	2.059098	4.195499
1	2.484704	0.657101	4.057010
6	3.391634	0.950648	1.094266
1	4.169759	1.676575	1.380118
1	3.679164	-0.064223	1.409714
1	3.285855	0.953855	-0.001325
6	-0.682557	-3.426771	1.240168
1	-0.386682	-4.452978	1.511637
1	-1.680956	-3.198549	1.645520
1	-0.729823	-3.348235	0.143278
6	0.681378	-2.691118	3.661852
1	0.882579	-3.769573	3.770633
1	1.482394	-2.120322	4.155397
1	-0.272240	-2.457944	4.160185

[**Th-Ni**]$^{-}$

90	-0.056669	-0.613482	0.613825
53	-0.284601	-3.180040	2.553782
28	0.077618	1.307873	-1.225273
15	2.215108	1.258903	-1.559563
15	-1.213691	0.301904	-2.642028
15	-0.725513	2.850605	0.064194
8	1.819207	-1.408216	-0.272101
8	-2.126501	-0.977110	-0.123873
8	0.254330	0.941045	2.168595
6	2.651983	-1.501327	-1.326656
6	-3.178070	-0.607274	-0.877258
6	0.603821	2.211372	2.456918
6	2.985521	-0.343021	-2.085786
6	-2.971615	0.012043	-2.142840
6	0.223528	3.283139	1.598182
6	3.849691	-0.483008	-3.188843
6	-4.093270	0.398747	-2.900551
6	0.623168	4.591315	1.933470
6	4.378932	-1.733335	-3.537907
6	-5.393621	0.180891	-2.424066
6	1.379998	4.844300	3.085929
6	4.051200	-2.861738	-2.771363
6	-5.580941	-0.438208	-1.178535
6	1.738580	3.778875	3.925151
6	3.193649	-2.772207	-1.664119

6	-4.492639	-0.841371	-0.389290
6	1.361814	2.458974	3.633763
1	4.467295	-3.841642	-3.035051
1	-6.596072	-0.613935	-0.802493
1	2.328806	3.969047	4.829690
1	5.047072	-1.826237	-4.400227
1	-6.257264	0.488089	-3.022814
1	1.686437	5.866706	3.329364
1	4.113588	0.394650	-3.786908
1	-3.952442	0.879330	-3.873784
1	0.344009	5.426891	1.284236
6	-4.671691	-1.497285	0.955599
1	-4.118234	-2.449322	1.015345
1	-4.266566	-0.867079	1.767867
1	-5.736434	-1.688308	1.166012
6	2.826516	-3.975854	-0.835010
1	3.033191	-3.807208	0.235119
1	1.745637	-4.194747	-0.893647
1	3.378616	-4.869396	-1.168754
6	1.747655	1.301724	4.518702
1	0.861771	0.728840	4.840945
1	2.390804	0.581273	3.982749
1	2.289163	1.650131	5.412937
6	3.354193	1.733066	-0.149603
1	4.401394	1.814995	-0.485682
1	3.016236	2.691934	0.273850
1	3.293194	0.970015	0.640904
6	2.877126	2.450823	-2.848434
1	3.979953	2.435082	-2.937542
1	2.418687	2.230448	-3.825029
1	2.552525	3.458458	-2.544640
6	-0.965567	4.526261	-0.742616
1	-1.425755	5.277928	-0.073508
1	0.001242	4.896613	-1.116397
1	-1.621297	4.362414	-1.612354
6	-2.450903	2.659178	0.772547
1	-2.772613	3.571957	1.301641
1	-3.150088	2.431321	-0.047659
1	-2.466942	1.816243	1.480014
6	-0.732742	-1.420720	-3.213884
1	-1.378442	-1.774117	-4.035422
1	0.319937	-1.409486	-3.539573
1	-0.827423	-2.123100	-2.370274
6	-1.407466	1.088292	-4.334981

1	-2.039188	0.494919	-5.022792
1	-1.822251	2.101880	-4.223955
1	-0.395768	1.181652	-4.760314

[Pa-Ni]$^{-}$

91	-0.002347	-0.715125	0.610621
53	-0.007727	-3.321889	2.413982
28	-0.026017	1.323865	-1.196440
15	2.131114	1.590194	-1.376630
15	-1.125451	0.141621	-2.651929
15	-1.092386	2.694049	0.129392
8	2.074844	-1.102553	-0.244764
8	-2.104827	-1.118587	-0.202324
8	0.052497	0.924437	2.183730
6	2.948036	-1.051513	-1.248107
6	-3.120816	-0.860463	-1.019219
6	0.227958	2.200006	2.523154
6	3.168709	0.176017	-1.942132
6	-2.885015	-0.274256	-2.300062
6	-0.259644	3.244979	1.680948
6	4.095081	0.219469	-3.000244
6	-3.970296	-0.004309	-3.153813
6	-0.050281	4.586745	2.049016
6	4.798098	-0.932505	-3.381906
6	-5.282044	-0.301755	-2.757035
6	0.630783	4.907985	3.232388
6	4.574030	-2.138408	-2.695209
6	-5.508251	-0.877350	-1.494619
6	1.099751	3.874156	4.060525
6	3.660715	-2.224815	-1.634452
6	-4.455127	-1.162700	-0.614268
6	0.911842	2.524134	3.731681
1	5.122095	-3.041975	-2.990640
1	-6.533177	-1.112881	-1.180831
1	1.630322	4.119462	4.989111
1	5.516927	-0.891768	-4.206889
1	-6.122254	-0.090395	-3.426380
1	0.791036	5.954917	3.509728
1	4.269882	1.157307	-3.538465
1	-3.796133	0.447955	-4.136269
1	-0.417333	5.394302	1.406657
6	-4.676965	-1.766402	0.748003
1	-4.083324	-2.686992	0.878533

1	-4.341020	-1.081069	1.546844
1	-5.741942	-1.999131	0.913436
6	3.392121	-3.510037	-0.896715
1	3.520433	-3.382965	0.191523
1	2.344860	-3.837294	-1.028996
1	4.056173	-4.318018	-1.245383
6	1.417589	1.402381	4.600480
1	0.597550	0.728517	4.902821
1	2.137121	0.766081	4.054927
1	1.910638	1.790260	5.507015
6	3.073439	2.164983	0.128513
1	4.135011	2.350751	-0.108252
1	2.601716	3.079372	0.522057
1	3.002584	1.383741	0.899636
6	2.604686	2.950301	-2.567448
1	3.694468	3.129388	-2.593275
1	2.249546	2.702140	-3.579579
1	2.098206	3.872769	-2.242432
6	-1.504274	4.307618	-0.719280
1	-2.071168	4.998802	-0.070317
1	-0.579158	4.798050	-1.059457
1	-2.112847	4.068109	-1.605290
6	-2.793180	2.258986	0.772077
1	-3.248201	3.116209	1.297363
1	-3.430506	1.942351	-0.068659
1	-2.704355	1.414926	1.472945
6	-0.453803	-1.509590	-3.222115
1	-1.027075	-1.901383	-4.080183
1	0.607547	-1.390053	-3.492698
1	-0.522824	-2.233048	-2.393967
6	-1.215986	1.003421	-4.306075
1	-1.745208	0.403727	-5.067755
1	-1.716743	1.976466	-4.190679
1	-0.183461	1.182771	-4.643620

[Np-Ni]$^{-}$

93	0.048900	-0.178649	0.880256
53	0.210918	-0.762975	3.939409
28	-0.090771	0.313363	-1.735640
15	2.053411	0.609925	-1.984455
15	-0.997054	-1.599819	-2.230237
15	-1.382705	2.055527	-1.538260
8	2.032110	-1.071998	0.427935

8	-1.819651	-1.352683	0.589755
8	-0.132073	2.024039	1.117851
6	2.960863	-1.495442	-0.425694
6	-2.846532	-1.732926	-0.168367
6	-0.118563	3.255621	0.612434
6	3.179452	-0.810868	-1.659371
6	-2.681832	-1.943589	-1.571356
6	-0.707465	3.525158	-0.659545
6	4.170814	-1.273651	-2.544552
6	-3.787503	-2.330585	-2.351763
6	-0.685385	4.835940	-1.171592
6	4.939946	-2.402915	-2.230648
6	-5.048605	-2.511537	-1.766781
6	-0.084617	5.876435	-0.449108
6	4.718231	-3.072463	-1.014921
6	-5.201380	-2.315485	-0.383735
6	0.495290	5.603238	0.801736
6	3.744247	-2.643967	-0.103010
6	-4.126665	-1.932188	0.430707
6	0.492133	4.312912	1.350099
1	5.318803	-3.955935	-0.763578
1	-6.184789	-2.462523	0.080631
1	0.967217	6.413757	1.371184
1	5.708127	-2.757880	-2.925111
1	-5.904618	-2.808666	-2.381577
1	-0.070080	6.893230	-0.855159
1	4.344561	-0.752762	-3.492132
1	-3.668207	-2.487624	-3.429004
1	-1.135612	5.050550	-2.146670
6	-4.273269	-1.714351	1.913602
1	-3.563619	-2.340061	2.481138
1	-4.033428	-0.672955	2.192441
1	-5.298224	-1.940306	2.250976
6	3.490085	-3.354532	1.200567
1	3.575718	-2.664917	2.057324
1	2.461326	-3.753565	1.246147
1	4.194165	-4.190992	1.342361
6	1.119411	3.996334	2.682090
1	0.393258	3.523635	3.365056
1	1.938632	3.263032	2.574046
1	1.523208	4.904014	3.159821
6	2.898654	1.992739	-1.056263
1	3.955471	2.094082	-1.356225
1	2.354944	2.933162	-1.239621

1	2.848051	1.774486	0.021328
6	2.493835	1.103683	-3.730660
1	3.569263	1.322799	-3.851536
1	2.201833	0.304831	-4.429441
1	1.916521	2.007970	-3.978377
6	-1.877173	2.748869	-3.200774
1	-2.579397	3.596832	-3.114816
1	-0.981793	3.071301	-3.754328
1	-2.362110	1.940481	-3.769932
6	-3.073574	1.893500	-0.761553
1	-3.657996	2.821396	-0.884385
1	-3.603935	1.042804	-1.217525
1	-2.950741	1.686388	0.312497
6	-0.105994	-3.196111	-1.848431
1	-0.631472	-4.063881	-2.282208
1	0.923038	-3.136289	-2.236824
1	-0.054834	-3.316455	-0.755711
6	-1.208782	-1.804659	-4.073970
1	-1.637289	-2.784956	-4.347022
1	-1.849597	-1.001555	-4.469179
1	-0.212755	-1.709905	-4.534033

[Pu-Ni]$^{-}$

94	0.047976	-0.202186	0.893997
53	0.226569	-0.894663	3.922619
28	-0.100055	0.377182	-1.810957
15	2.055742	0.686875	-1.963589
15	-0.987971	-1.556875	-2.279933
15	-1.400500	2.100416	-1.483090
8	2.040649	-1.067629	0.380301
8	-1.813556	-1.377715	0.526464
8	-0.203901	2.001669	1.188392
6	2.972127	-1.462773	-0.482324
6	-2.843208	-1.740807	-0.232556
6	-0.164736	3.242943	0.712326
6	3.189267	-0.738315	-1.694686
6	-2.674745	-1.926416	-1.638888
6	-0.724376	3.545950	-0.566875
6	4.180632	-1.167307	-2.595964
6	-3.776499	-2.302989	-2.428962
6	-0.665337	4.862794	-1.059207
6	4.955085	-2.302758	-2.317903
6	-5.038620	-2.495629	-1.849182

6	-0.060313	5.880432	-0.307925
6	4.735122	-3.012834	-1.125301
6	-5.197405	-2.315409	-0.464804
6	0.487622	5.576726	0.950111
6	3.758359	-2.620319	-0.199912
6	-4.126269	-1.941438	0.359373
6	0.449811	4.278238	1.478163
1	5.341263	-3.900172	-0.903065
1	-6.182495	-2.468471	-0.006386
1	0.962385	6.369584	1.541685
1	5.727530	-2.629128	-3.021643
1	-5.891396	-2.789531	-2.470015
1	-0.018625	6.903001	-0.697179
1	4.354199	-0.614326	-3.525784
1	-3.653994	-2.445395	-3.508043
1	-1.089186	5.101180	-2.040741
6	-4.280901	-1.734855	1.843063
1	-3.569485	-2.357954	2.411312
1	-4.050779	-0.693027	2.129470
1	-5.306166	-1.968753	2.174122
6	3.503167	-3.379458	1.075756
1	3.540240	-2.713907	1.954637
1	2.490492	-3.820938	1.084356
1	4.235432	-4.193016	1.208971
6	1.047713	3.928578	2.815318
1	0.305487	3.444983	3.473111
1	1.864947	3.192621	2.708080
1	1.447527	4.822903	3.320757
6	2.872809	2.011892	-0.934190
1	3.927963	2.153029	-1.224662
1	2.312953	2.954438	-1.041951
1	2.829588	1.707488	0.123032
6	2.523798	1.284081	-3.668099
1	3.604997	1.486706	-3.758534
1	2.227612	0.540349	-4.423982
1	1.970470	2.216336	-3.861495
6	-1.912075	2.832898	-3.123097
1	-2.574581	3.708093	-3.005484
1	-1.022366	3.125356	-3.701916
1	-2.451610	2.054243	-3.684909
6	-3.082098	1.910454	-0.695892
1	-3.671604	2.838011	-0.794798
1	-3.613376	1.066343	-1.162843
1	-2.947554	1.684362	0.372542

6	-0.073423	-3.132304	-1.876287
1	-0.578474	-4.014226	-2.305036
1	0.959602	-3.059653	-2.251744
1	-0.033915	-3.239246	-0.781846
6	-1.180239	-1.766633	-4.124681
1	-1.598140	-2.752549	-4.392348
1	-1.828600	-0.974468	-4.530676
1	-0.182928	-1.668005	-4.581115