

Supplemental Info for:

Actinyl cation-cation interactions in the gas phase: An accurate thermochemical study

Rulin Feng[†], Eric D. Glendening[‡], and Kirk A. Peterson^{1,†}

[†]Department of Chemistry, Washington State University, Pullman, Washington 99164-4630

[‡]Department of Chemistry, Indiana State University, Terre Haute, Indiana 47809

Includes:

Table S1: Bond lengths and harmonic frequencies for the monomers

Table S2. Cartesian coordinate structures for the dimers

Table S3. Harmonic frequencies for the dimers

Table S4. Cartesian coordinate CCI barrier trajectories for the T-shaped dimers

¹ E-mail: kipeters@wsu.edu

Table S1. R/UCCSD(T) equilibrium bond lengths (TZ level, in Å) and harmonic vibrational frequencies (DZ level, in cm⁻¹) for the linear actinyl monomers.

	UO ₂ ²⁺	UO ₂ ⁺	NpO ₂ ²⁺	NpO ₂ ⁺	PuO ₂ ⁺	AmO ₂ ⁺
State	¹ Σ _g ⁺	² Φ _u	² Φ _u	³ H _g	⁴ Φ _u	¹ Σ _g ⁺
<i>r_e</i>	1.6999	1.7601	1.6945	1.7375	1.7192	1.7199
ω ₂ (b ₂)	179.2	142.1	184.1	198.0	227.0	252.1
ω ₁ (a ₁)	1005.5	900.8	968.6	906.5	925.8	839.3
ω ₃ (b ₁)	1095.0	972.0	1076.5	973.9	1017.3	951.4

Table S2. Equilibrium structures (in Å) at the DK3-R/UCCSD(T)/cc-pVTZ-DK3 (aug-cc-pVTZ-DK for O) level of theory for CCI dimers.

$\text{UO}_2^{2+} \cdot \text{UO}_2^+$

O	-1.7100778781	0.0001405678	-2.1710602094
U	0.0000000000	0.0000003176	-2.1705486872
O	0.0000000000	-0.0002740076	0.2752880937
O	1.7100778781	0.0001405678	-2.1710602094
U	0.0000000000	-0.0000288985	2.1812282224
O	0.0000000000	0.0004180793	3.9079489903

$\text{UO}_2^+ \cdot \text{UO}_2^+$

O	0.0206037641	-1.7648701737	-2.1883717282
U	-0.0024492919	0.0000000000	-2.2727297467
O	-0.0063591192	0.0000000000	0.4476557460
O	0.0206037641	1.7648701737	-2.1883717282
U	-0.0001479044	0.0000000000	2.2673753471
O	0.0037910262	0.0000000000	4.0087470629

$\text{UO}_2^{2+} \cdot \text{NpO}_2^+$

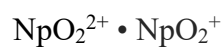
O	0.0003982049	-1.7093095601	-2.1613430146
U	-0.0000621819	0.0000000000	-2.1630223067
O	0.0003053515	0.0000000000	0.3063531486
O	0.0003982049	1.7093095601	-2.1613430146
Np	-0.0000123960	0.0000000000	2.1805568860
O	0.0000070019	0.0000000000	3.8891277060

$\text{NpO}_2^{2+} \cdot \text{UO}_2^+$

O	0.0009616851	-1.6912889384	-2.1619949723
Np	-0.0001224108	0.0000000000	-2.1659508273
O	-0.0001051078	0.0000000000	0.2627921651
O	0.0009616851	1.6912889384	-2.1619949723
U	-0.0000107298	0.0000000000	2.1682001409
O	0.0001550155	0.0000000000	3.8949660937

$\text{NpO}_2^+ \cdot \text{NpO}_2^+$

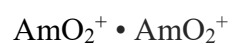
O	0.0075280756	-1.7307665235	-2.2282175145
Np	-0.0009673585	0.0000000000	-2.2592049876
O	-0.0009004532	0.0000000000	0.4656558996
O	0.0075280756	1.7307665235	-2.2282175145
Np	-0.0000346851	0.0000000000	2.2599008674
O	0.0006906468	0.0000000000	3.9804689277



0	0.0000000000	-1.6906357750	-2.1571368971
Np	0.0000000000	0.0000000000	-2.1571368971
0	0.0000000000	0.0000000000	0.2930517870
0	0.0000000000	1.6906357750	-2.1571368971
Np	0.0000000000	0.0000000000	2.1669630719
0	0.0000000000	0.0000000000	3.8756367317



0	0.0059916990	-1.7232985801	-2.2554987003
Pu	-0.0007083442	0.0000000000	-2.2799903234
0	-0.0015571241	0.0000000000	0.5107025089
0	0.0059916990	1.7232985801	-2.2554987003
Pu	-0.0000644542	0.0000000000	2.2809599722
0	0.0013624448	0.0000000000	3.9855033018



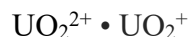
0	0.0000000000	-1.7230141130	-2.3228796793
Am	0.0000000000	0.0000000000	-2.3228796793
0	0.0000000000	0.0000000000	0.5599336079
0	0.0000000000	1.7230141130	-2.3228796793
Am	0.0000000000	0.0000000000	2.3262595153
0	0.0000000000	0.0000000000	4.0344925662

Table S3. R/UCCSD(T) harmonic vibrational frequencies (DZ level) for the T-shaped CCI dimers (cm⁻¹).

UO ₂ ²⁺ • UO ₂ ⁺	UO ₂ ⁺ • UO ₂ ⁺	UO ₂ ²⁺ • NpO ₂ ⁺	NpO ₂ ²⁺ • UO ₂ ⁺	NpO ₂ ⁺ • NpO ₂ ⁺	PuO ₂ ⁺ • PuO ₂ ⁺	AmO ₂ ⁺ • AmO ₂ ⁺
17.5	67.7i ^a	94.9	78.0	64.6i ^a	26.3	19.4
93.1	53.3	98.4	86.8	35.3	46.0	36.1
97.9	63.7	127.2	97.1	90.5	86.4	76.0
115.8	70.0	134.0	114.1	132.7	98.8	93.1
164.3	124.8	180.9	209.2	188.1	237.8	246.5
215.0	162.6	217.0	230.7	211.3	253.0	255.4
228.5	179.0	238.6	244.1	235.6	257.0	261.2
239.2	199.4	257.8	259.6	245.4	260.3	261.5
724.4	824.6	724.8	729.1	818.9	814.8	765.2
983.0	891.0	977.6	972.3	897.6	876.7	820.3
990.6	953.5	992.7	991.0	968.7	962.8	917.3
1073.7	973.7	1075.7	1071.0	976.9	964.8	937.6

^a This imaginary frequency corresponds to a slight bend of the donor molecule in the complex, presumably due to numerical noise.

Table S4. Cartesian coordinate CCI barrier trajectories for the T-shaped dimers. The energies were obtained at the DK3-R/UCCSD(T)/cc-pVTZ-DK3 (aug-cc-pVTZ-DK for O) level in C_{2v} symmetry with linear monomer moieties with fixed bond lengths. The xyz-coordinates are obtained by only varying the donor-acceptor distance (An-O), for each dimer at 20 points along the reaction path. The units for the coordinates and energies are Å and Hartrees, respectively.



Displacement 1:

0	0.0000000000	-1.7101248628	-2.0203657504
0	0.0000000000	1.7101248628	-2.0203657504
U	0.0000000000	0.0000000000	-2.0203657504
0	0.0000000000	0.0000000000	0.1248797039
U	0.0000000000	0.0000000000	2.0309989111
0	0.0000000000	0.0000000000	3.7576583954

Displacement 2:

0	0.0000000000	-1.7101248628	-2.0703657539
0	0.0000000000	1.7101248628	-2.0703657539
U	0.0000000000	0.0000000000	-2.0703657539
0	0.0000000000	0.0000000000	0.1748797074
U	0.0000000000	0.0000000000	2.0809989145
0	0.0000000000	0.0000000000	3.8076583989

Displacement 3:

0	0.0000000000	-1.7101248628	-2.1203657579
0	0.0000000000	1.7101248628	-2.1203657579
U	0.0000000000	0.0000000000	-2.1203657579
0	0.0000000000	0.0000000000	0.2248797109
U	0.0000000000	0.0000000000	2.1309989180
0	0.0000000000	0.0000000000	3.8576584024

Displacement 4:

0	0.0000000000	-1.7101248628	-2.1703657614
0	0.0000000000	1.7101248628	-2.1703657614
U	0.0000000000	0.0000000000	-2.1703657614
0	0.0000000000	0.0000000000	0.2748797149
U	0.0000000000	0.0000000000	2.1809989220
0	0.0000000000	0.0000000000	3.9076584058

Displacement 5:

0	0.0000000000	-1.7101248628	-2.2203657649
0	0.0000000000	1.7101248628	-2.2203657649
U	0.0000000000	0.0000000000	-2.2203657649
0	0.0000000000	0.0000000000	0.3248797184
U	0.0000000000	0.0000000000	2.2309989255
0	0.0000000000	0.0000000000	3.9576584098

Displacement 6:

0	0.0000000000	-1.7101248628	-2.2703657683
0	0.0000000000	1.7101248628	-2.2703657683
U	0.0000000000	0.0000000000	-2.2703657683
0	0.0000000000	0.0000000000	0.3748797219
U	0.0000000000	0.0000000000	2.2809989290
0	0.0000000000	0.0000000000	4.0076584133

Displacement 7:

0	0.0000000000	-1.7101248628	-2.3203657723
0	0.0000000000	1.7101248628	-2.3203657723
U	0.0000000000	0.0000000000	-2.3203657723
0	0.0000000000	0.0000000000	0.4248797253
U	0.0000000000	0.0000000000	2.3309989324
0	0.0000000000	0.0000000000	4.0576584168

Displacement 8:

0	0.0000000000	-1.7101248628	-2.3703657758
0	0.0000000000	1.7101248628	-2.3703657758
U	0.0000000000	0.0000000000	-2.3703657758
0	0.0000000000	0.0000000000	0.4748797288
U	0.0000000000	0.0000000000	2.3809989365
0	0.0000000000	0.0000000000	4.1076584203

Displacement 9:

0	0.0000000000	-1.7101248628	-2.4203657793
0	0.0000000000	1.7101248628	-2.4203657793
U	0.0000000000	0.0000000000	-2.4203657793
0	0.0000000000	0.0000000000	0.5248797328
U	0.0000000000	0.0000000000	2.4309989399
0	0.0000000000	0.0000000000	4.1576584243

Displacement 10:

0	0.0000000000	-1.7101248628	-2.4703657828
0	0.0000000000	1.7101248628	-2.4703657828
U	0.0000000000	0.0000000000	-2.4703657828
0	0.0000000000	0.0000000000	0.5748797363
U	0.0000000000	0.0000000000	2.4809989434
0	0.0000000000	0.0000000000	4.2076584278

Displacement 11:

0	0.0000000000	-1.7101248628	-2.5203657862
0	0.0000000000	1.7101248628	-2.5203657862
U	0.0000000000	0.0000000000	-2.5203657862
0	0.0000000000	0.0000000000	0.6248797398
U	0.0000000000	0.0000000000	2.5309989469
0	0.0000000000	0.0000000000	4.2576584312

Displacement 12:

0	0.0000000000	-1.7101248628	-2.5703657903
0	0.0000000000	1.7101248628	-2.5703657903
U	0.0000000000	0.0000000000	-2.5703657903
0	0.0000000000	0.0000000000	0.6748797433
U	0.0000000000	0.0000000000	2.5809989509
0	0.0000000000	0.0000000000	4.3076584347

Displacement 13:

0	0.0000000000	-1.7101248628	-2.6203657937
0	0.0000000000	1.7101248628	-2.6203657937
U	0.0000000000	0.0000000000	-2.6203657937
0	0.0000000000	0.0000000000	0.7248797473
U	0.0000000000	0.0000000000	2.6309989544
0	0.0000000000	0.0000000000	4.3576584387

Displacement 14:

0	0.0000000000	-1.7101248628	-2.6703657972
0	0.0000000000	1.7101248628	-2.6703657972
U	0.0000000000	0.0000000000	-2.6703657972
0	0.0000000000	0.0000000000	0.7748797507
U	0.0000000000	0.0000000000	2.6809989578
0	0.0000000000	0.0000000000	4.4076584422

Displacement 15:

0	0.0000000000	-1.7101248628	-2.7203658007
0	0.0000000000	1.7101248628	-2.7203658007
U	0.0000000000	0.0000000000	-2.7203658007
0	0.0000000000	0.0000000000	0.8248797542
U	0.0000000000	0.0000000000	2.7309989613
0	0.0000000000	0.0000000000	4.4576584457

Displacement 16:

0	0.0000000000	-1.7101248628	-2.7703658047
0	0.0000000000	1.7101248628	-2.7703658047
U	0.0000000000	0.0000000000	-2.7703658047
0	0.0000000000	0.0000000000	0.8748797577
U	0.0000000000	0.0000000000	2.7809989648
0	0.0000000000	0.0000000000	4.5076584492

Displacement 17:

0	0.0000000000	-1.7101248628	-2.8203658082
0	0.0000000000	1.7101248628	-2.8203658082
U	0.0000000000	0.0000000000	-2.8203658082
0	0.0000000000	0.0000000000	0.9248797617
U	0.0000000000	0.0000000000	2.8309989688
0	0.0000000000	0.0000000000	4.5576584526

Displacement 18:

0	0.0000000000	-1.7101248628	-2.8703658116
0	0.0000000000	1.7101248628	-2.8703658116

U	0.0000000000	0.0000000000	-2.8703658116
O	0.0000000000	0.0000000000	0.9748797652
U	0.0000000000	0.0000000000	2.8809989723
O	0.0000000000	0.0000000000	4.6076584566

Displacement 19:

O	0.0000000000	-1.7101248628	-2.9703658186
O	0.0000000000	1.7101248628	-2.9703658186
U	0.0000000000	0.0000000000	-2.9703658186
O	0.0000000000	0.0000000000	1.0748797721
U	0.0000000000	0.0000000000	2.9809989792
O	0.0000000000	0.0000000000	4.7076584636

Displacement 20:

O	0.0000000000	-1.7101248628	-3.0703658261
O	0.0000000000	1.7101248628	-3.0703658261
U	0.0000000000	0.0000000000	-3.0703658261
O	0.0000000000	0.0000000000	1.1748797796
U	0.0000000000	0.0000000000	3.0809989867
O	0.0000000000	0.0000000000	4.8076584711

Energies

Displacement	1	-56299.6556007711
Displacement	2	-56299.6647542060
Displacement	3	-56299.6690621088
Displacement	4	-56299.6702120890
Displacement	5	-56299.6693935107
Displacement	6	-56299.6674257928
Displacement	7	-56299.6648674097
Displacement	8	-56299.6620854689
Displacement	9	-56299.6593235427
Displacement	10	-56299.6567366320
Displacement	11	-56299.6544164321
Displacement	12	-56299.6524133124
Displacement	13	-56299.6507430407
Displacement	14	-56299.6494073308
Displacement	15	-56299.6483932486
Displacement	16	-56299.6476768902
Displacement	17	-56299.6472364240
Displacement	18	-56299.6470416091
Displacement	19	-56299.6472776277
Displacement	20	-56299.6481733744



Displacement 1:

O	0.0000000000	-1.7532476962	-2.3138150623
O	0.0000000000	1.7532476962	-2.3138150623
U	0.0000000000	0.0000000000	-2.3138150623
O	0.0000000000	0.0000000000	0.4967542399
U	0.0000000000	0.0000000000	2.3186109010
O	0.0000000000	0.0000000000	4.0595264464

Displacement 2:

O	0.0000000000	-1.7532476962	-2.3138150623
O	0.0000000000	1.7532476962	-2.3138150623
U	0.0000000000	0.0000000000	-2.3138150623
O	0.0000000000	0.0000000000	0.4967542399
U	0.0000000000	0.0000000000	2.3186109010
O	0.0000000000	0.0000000000	4.0595264464

Displacement 3:

O	0.0000000000	-1.7532476962	-2.1138150479
O	0.0000000000	1.7532476962	-2.1138150479
U	0.0000000000	0.0000000000	-2.1138150479
O	0.0000000000	0.0000000000	0.2967542254
U	0.0000000000	0.0000000000	2.1186108866
O	0.0000000000	0.0000000000	3.8595264319

Displacement 4:

O	0.0000000000	-1.7532476962	-2.1638150513
O	0.0000000000	1.7532476962	-2.1638150513
U	0.0000000000	0.0000000000	-2.1638150513
O	0.0000000000	0.0000000000	0.3467542289
U	0.0000000000	0.0000000000	2.1686108900
O	0.0000000000	0.0000000000	3.9095264354

Displacement 5:

O	0.0000000000	-1.7532476962	-2.2138150553
O	0.0000000000	1.7532476962	-2.2138150553
U	0.0000000000	0.0000000000	-2.2138150553
O	0.0000000000	0.0000000000	0.3967542329
U	0.0000000000	0.0000000000	2.2186108940
O	0.0000000000	0.0000000000	3.9595264389

Displacement 6:

O	0.0000000000	-1.7532476962	-2.2638150588
O	0.0000000000	1.7532476962	-2.2638150588
U	0.0000000000	0.0000000000	-2.2638150588
O	0.0000000000	0.0000000000	0.4467542364
U	0.0000000000	0.0000000000	2.2686108975
O	0.0000000000	0.0000000000	4.0095264429

Displacement 7:

0	0.0000000000	-1.7532476962	-2.3138150623
0	0.0000000000	1.7532476962	-2.3138150623
U	0.0000000000	0.0000000000	-2.3138150623
0	0.0000000000	0.0000000000	0.4967542399
U	0.0000000000	0.0000000000	2.3186109010
0	0.0000000000	0.0000000000	4.0595264464

Displacement 8:

0	0.0000000000	-1.7532476962	-2.3638150658
0	0.0000000000	1.7532476962	-2.3638150658
U	0.0000000000	0.0000000000	-2.3638150658
0	0.0000000000	0.0000000000	0.5467542433
U	0.0000000000	0.0000000000	2.3686109045
0	0.0000000000	0.0000000000	4.1095264498

Displacement 9:

0	0.0000000000	-1.7532476962	-2.4138150698
0	0.0000000000	1.7532476962	-2.4138150698
U	0.0000000000	0.0000000000	-2.4138150698
0	0.0000000000	0.0000000000	0.5967542473
U	0.0000000000	0.0000000000	2.4186109085
0	0.0000000000	0.0000000000	4.1595264533

Displacement 10:

0	0.0000000000	-1.7532476962	-2.4638150733
0	0.0000000000	1.7532476962	-2.4638150733
U	0.0000000000	0.0000000000	-2.4638150733
0	0.0000000000	0.0000000000	0.6467542508
U	0.0000000000	0.0000000000	2.4686109119
0	0.0000000000	0.0000000000	4.2095264573

Displacement 11:

0	0.0000000000	-1.7532476962	-2.5138150767
0	0.0000000000	1.7532476962	-2.5138150767
U	0.0000000000	0.0000000000	-2.5138150767
0	0.0000000000	0.0000000000	0.6967542543
U	0.0000000000	0.0000000000	2.5186109154
0	0.0000000000	0.0000000000	4.2595264608

Displacement 12:

0	0.0000000000	-1.7532476962	-2.5638150802
0	0.0000000000	1.7532476962	-2.5638150802
U	0.0000000000	0.0000000000	-2.5638150802
0	0.0000000000	0.0000000000	0.7467542578
U	0.0000000000	0.0000000000	2.5686109189
0	0.0000000000	0.0000000000	4.3095264643

Displacement 13:

0	0.0000000000	-1.7532476962	-2.6138150837
---	--------------	---------------	---------------

0	0.0000000000	1.7532476962	-2.6138150837
U	0.0000000000	0.0000000000	-2.6138150837
0	0.0000000000	0.0000000000	0.7967542613
U	0.0000000000	0.0000000000	2.6186109224
0	0.0000000000	0.0000000000	4.3595264677

Displacement 14:

0	0.0000000000	-1.7532476962	-2.6638150877
0	0.0000000000	1.7532476962	-2.6638150877
U	0.0000000000	0.0000000000	-2.6638150877
0	0.0000000000	0.0000000000	0.8467542653
U	0.0000000000	0.0000000000	2.6686109264
0	0.0000000000	0.0000000000	4.4095264712

Displacement 15:

0	0.0000000000	-1.7532476962	-2.7138150912
0	0.0000000000	1.7532476962	-2.7138150912
U	0.0000000000	0.0000000000	-2.7138150912
0	0.0000000000	0.0000000000	0.8967542687
U	0.0000000000	0.0000000000	2.7186109299
0	0.0000000000	0.0000000000	4.4595264752

Displacement 16:

0	0.0000000000	-1.7532476962	-2.7638150947
0	0.0000000000	1.7532476962	-2.7638150947
U	0.0000000000	0.0000000000	-2.7638150947
0	0.0000000000	0.0000000000	0.9467542722
U	0.0000000000	0.0000000000	2.7686109333
0	0.0000000000	0.0000000000	4.5095264787

Displacement 17:

0	0.0000000000	-1.7532476962	-2.8138150981
0	0.0000000000	1.7532476962	-2.8138150981
U	0.0000000000	0.0000000000	-2.8138150981
0	0.0000000000	0.0000000000	0.9967542757
U	0.0000000000	0.0000000000	2.8186109368
0	0.0000000000	0.0000000000	4.5595264822

Displacement 18:

0	0.0000000000	-1.7532476962	-2.8638151021
0	0.0000000000	1.7532476962	-2.8638151021
U	0.0000000000	0.0000000000	-2.8638151021
0	0.0000000000	0.0000000000	1.0467542797
U	0.0000000000	0.0000000000	2.8686109408
0	0.0000000000	0.0000000000	4.6095264857

Displacement 19:

0	0.0000000000	-1.7532476962	-2.9138151056
0	0.0000000000	1.7532476962	-2.9138151056
U	0.0000000000	0.0000000000	-2.9138151056

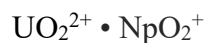
0	0.0000000000	0.0000000000	1.0967542832
U	0.0000000000	0.0000000000	2.9186109443
0	0.0000000000	0.0000000000	4.6595264897

Displacement 20:

0	0.0000000000	-1.7532476962	-2.9638151091
0	0.0000000000	1.7532476962	-2.9638151091
U	0.0000000000	0.0000000000	-2.9638151091
0	0.0000000000	0.0000000000	1.1467542867
U	0.0000000000	0.0000000000	2.9686109478
0	0.0000000000	0.0000000000	4.7095264931

Energies

Displacement	1	-56300.2436644247
Displacement	2	-56300.2387548361
Displacement	3	-56300.2420304604
Displacement	4	-56300.2435242270
Displacement	5	-56300.2439139763
Displacement	6	-56300.2436646676
Displacement	7	-56300.2430856650
Displacement	8	-56300.2423813264
Displacement	9	-56300.2416798229
Displacement	10	-56300.2410581270
Displacement	11	-56300.2405578433
Displacement	12	-56300.2401978353
Displacement	13	-56300.2399816938
Displacement	14	-56300.2399042568
Displacement	15	-56300.2399540473
Displacement	16	-56300.2401182327
Displacement	17	-56300.2403822444
Displacement	18	-56300.2407325154
Displacement	19	-56300.2411559032
Displacement	20	-56300.2421750774



Displacement 1:

0	0.0000000000	-1.7092468530	-2.0130017854
0	0.0000000000	1.7092468530	-2.0130017854
U	0.0000000000	0.0000000000	-2.0130017854
0	0.0000000000	0.0000000000	0.1559755307
Np	0.0000000000	0.0000000000	2.0301796658
0	0.0000000000	0.0000000000	3.7389084485

Displacement 2:

0	0.0000000000	-1.7092468530	-2.0629108276
0	0.0000000000	1.7092468530	-2.0629108276
U	0.0000000000	0.0000000000	-2.0629108276
0	0.0000000000	0.0000000000	0.2060664961
Np	0.0000000000	0.0000000000	2.0802706306
0	0.0000000000	0.0000000000	3.7889994138

Displacement 3:

0	0.0000000000	-1.7092468530	-2.1128198697
0	0.0000000000	1.7092468530	-2.1128198697
U	0.0000000000	0.0000000000	-2.1128198697
0	0.0000000000	0.0000000000	0.2561574609
Np	0.0000000000	0.0000000000	2.1303615960
0	0.0000000000	0.0000000000	3.8390903786

Displacement 4:

0	0.0000000000	-1.7092468530	-2.1627289119
0	0.0000000000	1.7092468530	-2.1627289119
U	0.0000000000	0.0000000000	-2.1627289119
0	0.0000000000	0.0000000000	0.3062484257
Np	0.0000000000	0.0000000000	2.1804525608
0	0.0000000000	0.0000000000	3.8891813440

Displacement 5:

0	0.0000000000	-1.7092468530	-2.2126379540
0	0.0000000000	1.7092468530	-2.2126379540
U	0.0000000000	0.0000000000	-2.2126379540
0	0.0000000000	0.0000000000	0.3563393910
Np	0.0000000000	0.0000000000	2.2305435256
0	0.0000000000	0.0000000000	3.9392723088

Displacement 6:

0	0.0000000000	-1.7092468530	-2.2625469961
0	0.0000000000	1.7092468530	-2.2625469961
U	0.0000000000	0.0000000000	-2.2625469961
0	0.0000000000	0.0000000000	0.4064303559
Np	0.0000000000	0.0000000000	2.2806344910
0	0.0000000000	0.0000000000	3.9893632736

Displacement 7:

0	0.0000000000	-1.7092468530	-2.3124560383
0	0.0000000000	1.7092468530	-2.3124560383
U	0.0000000000	0.0000000000	-2.3124560383
0	0.0000000000	0.0000000000	0.4565213212
Np	0.0000000000	0.0000000000	2.3307254558
0	0.0000000000	0.0000000000	4.0394542389

Displacement 8:

0	0.0000000000	-1.7092468530	-2.3623650804
0	0.0000000000	1.7092468530	-2.3623650804
U	0.0000000000	0.0000000000	-2.3623650804
0	0.0000000000	0.0000000000	0.5066122860
Np	0.0000000000	0.0000000000	2.3808164211
0	0.0000000000	0.0000000000	4.0895452038

Displacement 9:

0	0.0000000000	-1.7092468530	-2.4122741226
0	0.0000000000	1.7092468530	-2.4122741226
U	0.0000000000	0.0000000000	-2.4122741226
0	0.0000000000	0.0000000000	0.5567032508
Np	0.0000000000	0.0000000000	2.4309073859
0	0.0000000000	0.0000000000	4.1396361691

Displacement 10:

0	0.0000000000	-1.7092468530	-2.4621831647
0	0.0000000000	1.7092468530	-2.4621831647
U	0.0000000000	0.0000000000	-2.4621831647
0	0.0000000000	0.0000000000	0.6067942162
Np	0.0000000000	0.0000000000	2.4809983507
0	0.0000000000	0.0000000000	4.1897271339

Displacement 11:

0	0.0000000000	-1.7092468530	-2.5120922069
0	0.0000000000	1.7092468530	-2.5120922069
U	0.0000000000	0.0000000000	-2.5120922069
0	0.0000000000	0.0000000000	0.6568851810
Np	0.0000000000	0.0000000000	2.5310893161
0	0.0000000000	0.0000000000	4.2398180987

Displacement 12:

0	0.0000000000	-1.7092468530	-2.5620012490
0	0.0000000000	1.7092468530	-2.5620012490
U	0.0000000000	0.0000000000	-2.5620012490
0	0.0000000000	0.0000000000	0.7069761463
Np	0.0000000000	0.0000000000	2.5811802809
0	0.0000000000	0.0000000000	4.2899090641

Displacement 13:

0	0.0000000000	-1.7092468530	-2.6119102911
---	--------------	---------------	---------------

0	0.0000000000	1.7092468530	-2.6119102911
U	0.0000000000	0.0000000000	-2.6119102911
0	0.0000000000	0.0000000000	0.7570671111
Np	0.0000000000	0.0000000000	2.6312712462
0	0.0000000000	0.0000000000	4.3400000289

Displacement 14:

0	0.0000000000	-1.7092468530	-2.6618193333
0	0.0000000000	1.7092468530	-2.6618193333
U	0.0000000000	0.0000000000	-2.6618193333
0	0.0000000000	0.0000000000	0.8071580759
Np	0.0000000000	0.0000000000	2.6813622110
0	0.0000000000	0.0000000000	4.3900909942

Displacement 15:

0	0.0000000000	-1.7092468530	-2.7117283754
0	0.0000000000	1.7092468530	-2.7117283754
U	0.0000000000	0.0000000000	-2.7117283754
0	0.0000000000	0.0000000000	0.8572490413
Np	0.0000000000	0.0000000000	2.7314531759
0	0.0000000000	0.0000000000	4.4401819590

Displacement 16:

0	0.0000000000	-1.7092468530	-2.7616374181
0	0.0000000000	1.7092468530	-2.7616374181
U	0.0000000000	0.0000000000	-2.7616374181
0	0.0000000000	0.0000000000	0.9073400061
Np	0.0000000000	0.0000000000	2.7815441412
0	0.0000000000	0.0000000000	4.4902729238

Displacement 17:

0	0.0000000000	-1.7092468530	-2.8115464602
0	0.0000000000	1.7092468530	-2.8115464602
U	0.0000000000	0.0000000000	-2.8115464602
0	0.0000000000	0.0000000000	0.9574309714
Np	0.0000000000	0.0000000000	2.8316351060
0	0.0000000000	0.0000000000	4.5403638892

Displacement 18:

0	0.0000000000	-1.7092468530	-2.8614555024
0	0.0000000000	1.7092468530	-2.8614555024
U	0.0000000000	0.0000000000	-2.8614555024
0	0.0000000000	0.0000000000	1.0075219363
Np	0.0000000000	0.0000000000	2.8817260714
0	0.0000000000	0.0000000000	4.5904548540

Displacement 19:

0	0.0000000000	-1.7092468530	-2.9612735867
0	0.0000000000	1.7092468530	-2.9612735867
U	0.0000000000	0.0000000000	-2.9612735867

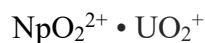
0	0.0000000000	0.0000000000	1.1077038664
Np	0.0000000000	0.0000000000	2.9819080010
0	0.0000000000	0.0000000000	4.6906367842

Displacement 20:

0	0.0000000000	-1.7092468530	-3.0610916709
0	0.0000000000	1.7092468530	-3.0610916709
U	0.0000000000	0.0000000000	-3.0610916709
0	0.0000000000	0.0000000000	1.2078857966
Np	0.0000000000	0.0000000000	3.0820899311
0	0.0000000000	0.0000000000	4.7908187143

Energies

Displacement	1	-57090.0110291016
Displacement	2	-57090.0193383926
Displacement	3	-57090.0232310136
Displacement	4	-57090.0242665146
Displacement	5	-57090.0235384787
Displacement	6	-57090.0217974112
Displacement	7	-57090.0195507982
Displacement	8	-57090.0171359802
Displacement	9	-57090.0147712530
Displacement	10	-57090.0125927527
Displacement	11	-57090.0106816970
Displacement	12	-57090.0090780038
Displacement	13	-57090.0077949968
Displacement	14	-57090.0068285325
Displacement	15	-57090.0061624603
Displacement	16	-57090.0057690007
Displacement	17	-57090.0056345776
Displacement	18	-57090.0057190356
Displacement	19	-57090.0064485984
Displacement	20	-57090.0077544091



Displacement 1:

0	0.0000000000	-1.6912940317	-2.0154432669
0	0.0000000000	1.6912940317	-2.0154432669
Np	0.0000000000	0.0000000000	-2.0154432669
0	0.0000000000	0.0000000000	0.1132998759
U	0.0000000000	0.0000000000	2.0187079931
0	0.0000000000	0.0000000000	3.7454740776

Displacement 2:

0	0.0000000000	-1.6912940317	-2.0655342344
0	0.0000000000	1.6912940317	-2.0655342344
Np	0.0000000000	0.0000000000	-2.0655342344
0	0.0000000000	0.0000000000	0.1632089159
U	0.0000000000	0.0000000000	2.0686170332
0	0.0000000000	0.0000000000	3.7953831171

Displacement 3:

0	0.0000000000	-1.6912940317	-2.1156252018
0	0.0000000000	1.6912940317	-2.1156252018
Np	0.0000000000	0.0000000000	-2.1156252018
0	0.0000000000	0.0000000000	0.2131179554
U	0.0000000000	0.0000000000	2.1185260727
0	0.0000000000	0.0000000000	3.8452921571

Displacement 4:

0	0.0000000000	-1.6912940317	-2.1657161693
0	0.0000000000	1.6912940317	-2.1657161693
Np	0.0000000000	0.0000000000	-2.1657161693
0	0.0000000000	0.0000000000	0.2630269955
U	0.0000000000	0.0000000000	2.1684351122
0	0.0000000000	0.0000000000	3.8952011966

Displacement 5:

0	0.0000000000	-1.6912940317	-2.2158071368
0	0.0000000000	1.6912940317	-2.2158071368
Np	0.0000000000	0.0000000000	-2.2158071368
0	0.0000000000	0.0000000000	0.3129360349
U	0.0000000000	0.0000000000	2.2183441522
0	0.0000000000	0.0000000000	3.9451102361

Displacement 6:

0	0.0000000000	-1.6912940317	-2.2658981047
0	0.0000000000	1.6912940317	-2.2658981047
Np	0.0000000000	0.0000000000	-2.2658981047
0	0.0000000000	0.0000000000	0.3628450744
U	0.0000000000	0.0000000000	2.2682531917
0	0.0000000000	0.0000000000	3.9950192761

Displacement 7:

0	0.0000000000	-1.6912940317	-2.3159890722
0	0.0000000000	1.6912940317	-2.3159890722
Np	0.0000000000	0.0000000000	-2.3159890722
0	0.0000000000	0.0000000000	0.4127541145
U	0.0000000000	0.0000000000	2.3181622317
0	0.0000000000	0.0000000000	4.0449283156

Displacement 8:

0	0.0000000000	-1.6912940317	-2.3660800397
0	0.0000000000	1.6912940317	-2.3660800397
Np	0.0000000000	0.0000000000	-2.3660800397
0	0.0000000000	0.0000000000	0.4626631540
U	0.0000000000	0.0000000000	2.3680712712
0	0.0000000000	0.0000000000	4.0948373557

Displacement 9:

0	0.0000000000	-1.6912940317	-2.4161710071
0	0.0000000000	1.6912940317	-2.4161710071
Np	0.0000000000	0.0000000000	-2.4161710071
0	0.0000000000	0.0000000000	0.5125721940
U	0.0000000000	0.0000000000	2.4179803107
0	0.0000000000	0.0000000000	4.1447463952

Displacement 10:

0	0.0000000000	-1.6912940317	-2.4662619746
0	0.0000000000	1.6912940317	-2.4662619746
Np	0.0000000000	0.0000000000	-2.4662619746
0	0.0000000000	0.0000000000	0.5624812335
U	0.0000000000	0.0000000000	2.4678893507
0	0.0000000000	0.0000000000	4.1946554347

Displacement 11:

0	0.0000000000	-1.6912940317	-2.5163529420
0	0.0000000000	1.6912940317	-2.5163529420
Np	0.0000000000	0.0000000000	-2.5163529420
0	0.0000000000	0.0000000000	0.6123902730
U	0.0000000000	0.0000000000	2.5177983902
0	0.0000000000	0.0000000000	4.2445644747

Displacement 12:

0	0.0000000000	-1.6912940317	-2.5664439095
0	0.0000000000	1.6912940317	-2.5664439095
Np	0.0000000000	0.0000000000	-2.5664439095
0	0.0000000000	0.0000000000	0.6622993130
U	0.0000000000	0.0000000000	2.5677074297
0	0.0000000000	0.0000000000	4.2944735142

Displacement 13:

0	0.0000000000	-1.6912940317	-2.6165348770
0	0.0000000000	1.6912940317	-2.6165348770
Np	0.0000000000	0.0000000000	-2.6165348770
0	0.0000000000	0.0000000000	0.7122083525
U	0.0000000000	0.0000000000	2.6176164697
0	0.0000000000	0.0000000000	4.3443825537

Displacement 14:

0	0.0000000000	-1.6912940317	-2.6666258444
0	0.0000000000	1.6912940317	-2.6666258444
Np	0.0000000000	0.0000000000	-2.6666258444
0	0.0000000000	0.0000000000	0.7621173920
U	0.0000000000	0.0000000000	2.6675255092
0	0.0000000000	0.0000000000	4.3942915937

Displacement 15:

0	0.0000000000	-1.6912940317	-2.7167168119
0	0.0000000000	1.6912940317	-2.7167168119
Np	0.0000000000	0.0000000000	-2.7167168119
0	0.0000000000	0.0000000000	0.8120264320
U	0.0000000000	0.0000000000	2.7174345493
0	0.0000000000	0.0000000000	4.4442006332

Displacement 16:

0	0.0000000000	-1.6912940317	-2.7668077793
0	0.0000000000	1.6912940317	-2.7668077793
Np	0.0000000000	0.0000000000	-2.7668077793
0	0.0000000000	0.0000000000	0.8619354715
U	0.0000000000	0.0000000000	2.7673435888
0	0.0000000000	0.0000000000	4.4941096732

Displacement 17:

0	0.0000000000	-1.6912940317	-2.8168987468
0	0.0000000000	1.6912940317	-2.8168987468
Np	0.0000000000	0.0000000000	-2.8168987468
0	0.0000000000	0.0000000000	0.9118445115
U	0.0000000000	0.0000000000	2.8172526283
0	0.0000000000	0.0000000000	4.5440187127

Displacement 18:

0	0.0000000000	-1.6912940317	-2.8669897142
0	0.0000000000	1.6912940317	-2.8669897142
Np	0.0000000000	0.0000000000	-2.8669897142
0	0.0000000000	0.0000000000	0.9617535510
U	0.0000000000	0.0000000000	2.8671616683
0	0.0000000000	0.0000000000	4.5939277522

Displacement 19:

0	0.0000000000	-1.6912940317	-2.9671716497
0	0.0000000000	1.6912940317	-2.9671716497

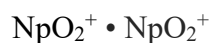
Np	0.0000000000	0.0000000000	-2.9671716497
0	0.0000000000	0.0000000000	1.0615716306
U	0.0000000000	0.0000000000	2.9669797478
0	0.0000000000	0.0000000000	4.6937458317

Displacement 20:

0	0.0000000000	-1.6912940317	-3.0673535846
0	0.0000000000	1.6912940317	-3.0673535846
Np	0.0000000000	0.0000000000	-3.0673535846
0	0.0000000000	0.0000000000	1.1613897101
U	0.0000000000	0.0000000000	3.0667978268
0	0.0000000000	0.0000000000	4.7935639112

Energies

Displacement	1	-57089.9723359804
Displacement	2	-57089.9816387017
Displacement	3	-57089.9860057276
Displacement	4	-57089.9871648436
Displacement	5	-57089.9863300356
Displacement	6	-57089.9843361873
Displacement	7	-57089.9817475325
Displacement	8	-57089.9789407811
Displacement	9	-57089.9761605342
Displacement	10	-57089.9735617822
Displacement	11	-57089.9712356095
Displacement	12	-57089.9692301182
Displacement	13	-57089.9675636116
Displacement	14	-57089.9662345564
Displacement	15	-57089.9652290471
Displacement	16	-57089.9645238997
Displacement	17	-57089.9640934093
Displacement	18	-57089.9639092877
Displacement	19	-57089.9641649732
Displacement	20	-57089.9650784879



Displacement 1:

0	0.0000000000	-1.7307656643	-2.0588036914
0	0.0000000000	1.7307656643	-2.0588036914
Np	0.0000000000	0.0000000000	-2.0588036914
0	0.0000000000	0.0000000000	0.2688219562
Np	0.0000000000	0.0000000000	2.0631937152
0	0.0000000000	0.0000000000	3.7837425295

Displacement 2:

0	0.0000000000	-1.7307656643	-2.1088036949
0	0.0000000000	1.7307656643	-2.1088036949
Np	0.0000000000	0.0000000000	-2.1088036949
0	0.0000000000	0.0000000000	0.3188219597
Np	0.0000000000	0.0000000000	2.1131937192
0	0.0000000000	0.0000000000	3.8337425329

Displacement 3:

0	0.0000000000	-1.7307656643	-2.1588036983
0	0.0000000000	1.7307656643	-2.1588036983
Np	0.0000000000	0.0000000000	-2.1588036983
0	0.0000000000	0.0000000000	0.3688219637
Np	0.0000000000	0.0000000000	2.1631937226
0	0.0000000000	0.0000000000	3.8837425364

Displacement 4:

0	0.0000000000	-1.7307656643	-2.2088037018
0	0.0000000000	1.7307656643	-2.2088037018
Np	0.0000000000	0.0000000000	-2.2088037018
0	0.0000000000	0.0000000000	0.4188219672
Np	0.0000000000	0.0000000000	2.2131937261
0	0.0000000000	0.0000000000	3.9337425399

Displacement 5:

0	0.0000000000	-1.7307656643	-2.2588037058
0	0.0000000000	1.7307656643	-2.2588037058
Np	0.0000000000	0.0000000000	-2.2588037058
0	0.0000000000	0.0000000000	0.4688219707
Np	0.0000000000	0.0000000000	2.2631937296
0	0.0000000000	0.0000000000	3.9837425434

Displacement 6:

0	0.0000000000	-1.7307656643	-2.3088037093
0	0.0000000000	1.7307656643	-2.3088037093
Np	0.0000000000	0.0000000000	-2.3088037093
0	0.0000000000	0.0000000000	0.5188219742
Np	0.0000000000	0.0000000000	2.3131937336
0	0.0000000000	0.0000000000	4.0337425474

Displacement 7:

0	0.0000000000	-1.7307656643	-2.3588037128
0	0.0000000000	1.7307656643	-2.3588037128
Np	0.0000000000	0.0000000000	-2.3588037128
0	0.0000000000	0.0000000000	0.5688219776
Np	0.0000000000	0.0000000000	2.3631937371
0	0.0000000000	0.0000000000	4.0837425508

Displacement 8:

0	0.0000000000	-1.7307656643	-2.4088037163
0	0.0000000000	1.7307656643	-2.4088037163
Np	0.0000000000	0.0000000000	-2.4088037163
0	0.0000000000	0.0000000000	0.6188219816
Np	0.0000000000	0.0000000000	2.4131937406
0	0.0000000000	0.0000000000	4.1337425543

Displacement 9:

0	0.0000000000	-1.7307656643	-2.4588037203
0	0.0000000000	1.7307656643	-2.4588037203
Np	0.0000000000	0.0000000000	-2.4588037203
0	0.0000000000	0.0000000000	0.6688219851
Np	0.0000000000	0.0000000000	2.4631937440
0	0.0000000000	0.0000000000	4.1837425578

Displacement 10:

0	0.0000000000	-1.7307656643	-2.5088037237
0	0.0000000000	1.7307656643	-2.5088037237
Np	0.0000000000	0.0000000000	-2.5088037237
0	0.0000000000	0.0000000000	0.7188219886
Np	0.0000000000	0.0000000000	2.5131937480
0	0.0000000000	0.0000000000	4.2337425618

Displacement 11:

0	0.0000000000	-1.7307656643	-2.5588037272
0	0.0000000000	1.7307656643	-2.5588037272
Np	0.0000000000	0.0000000000	-2.5588037272
0	0.0000000000	0.0000000000	0.7688219921
Np	0.0000000000	0.0000000000	2.5631937515
0	0.0000000000	0.0000000000	4.2837425653

Displacement 12:

0	0.0000000000	-1.7307656643	-2.6088037307
0	0.0000000000	1.7307656643	-2.6088037307
Np	0.0000000000	0.0000000000	-2.6088037307
0	0.0000000000	0.0000000000	0.8188219961
Np	0.0000000000	0.0000000000	2.6131937550
0	0.0000000000	0.0000000000	4.3337425688

Displacement 13:

0	0.0000000000	-1.7307656643	-2.6588037342
0	0.0000000000	1.7307656643	-2.6588037342
Np	0.0000000000	0.0000000000	-2.6588037342
0	0.0000000000	0.0000000000	0.8688219996
Np	0.0000000000	0.0000000000	2.6631937585
0	0.0000000000	0.0000000000	4.3837425722

Displacement 14:

0	0.0000000000	-1.7307656643	-2.7088037382
0	0.0000000000	1.7307656643	-2.7088037382
Np	0.0000000000	0.0000000000	-2.7088037382
0	0.0000000000	0.0000000000	0.9188220030
Np	0.0000000000	0.0000000000	2.7131937619
0	0.0000000000	0.0000000000	4.4337425757

Displacement 15:

0	0.0000000000	-1.7307656643	-2.7588037417
0	0.0000000000	1.7307656643	-2.7588037417
Np	0.0000000000	0.0000000000	-2.7588037417
0	0.0000000000	0.0000000000	0.9688220065
Np	0.0000000000	0.0000000000	2.7631937660
0	0.0000000000	0.0000000000	4.4837425797

Displacement 16:

0	0.0000000000	-1.7307656643	-2.8088037451
0	0.0000000000	1.7307656643	-2.8088037451
Np	0.0000000000	0.0000000000	-2.8088037451
0	0.0000000000	0.0000000000	1.0188220100
Np	0.0000000000	0.0000000000	2.8131937694
0	0.0000000000	0.0000000000	4.5337425832

Displacement 17:

0	0.0000000000	-1.7307656643	-2.8588037486
0	0.0000000000	1.7307656643	-2.8588037486
Np	0.0000000000	0.0000000000	-2.8588037486
0	0.0000000000	0.0000000000	1.0688220140
Np	0.0000000000	0.0000000000	2.8631937729
0	0.0000000000	0.0000000000	4.5837425867

Displacement 18:

0	0.0000000000	-1.7307656643	-2.9088037526
0	0.0000000000	1.7307656643	-2.9088037526
Np	0.0000000000	0.0000000000	-2.9088037526
0	0.0000000000	0.0000000000	1.1188220175
Np	0.0000000000	0.0000000000	2.9131937764
0	0.0000000000	0.0000000000	4.6337425902

Displacement 19:

0	0.0000000000	-1.7307656643	-2.9588037561
0	0.0000000000	1.7307656643	-2.9588037561

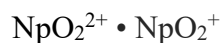
Np	0.0000000000	0.0000000000	-2.9588037561
0	0.0000000000	0.0000000000	1.1688220209
Np	0.0000000000	0.0000000000	2.9631937804
0	0.0000000000	0.0000000000	4.6837425942

Displacement 20:

0	0.0000000000	-1.7307656643	-3.0088037596
0	0.0000000000	1.7307656643	-3.0088037596
Np	0.0000000000	0.0000000000	-3.0088037596
0	0.0000000000	0.0000000000	1.2188220244
Np	0.0000000000	0.0000000000	3.0131937839
0	0.0000000000	0.0000000000	4.7337425976

Energies

Displacement	1	-57880.9443870326
Displacement	2	-57880.9495170633
Displacement	3	-57880.9522631548
Displacement	4	-57880.9534929765
Displacement	5	-57880.9538037362
Displacement	6	-57880.9535996035
Displacement	7	-57880.9531481291
Displacement	8	-57880.9526215519
Displacement	9	-57880.9521256145
Displacement	10	-57880.9517212601
Displacement	11	-57880.9514393108
Displacement	12	-57880.9512911436
Displacement	13	-57880.9512756263
Displacement	14	-57880.9513852386
Displacement	15	-57880.9516079712
Displacement	16	-57880.9519300433
Displacement	17	-57880.9523381088
Displacement	18	-57880.9528185935
Displacement	19	-57880.9533600764
Displacement	20	-57880.9539510404



Displacement 1:

0	0.0000000000	-1.6906359019	-2.0071370373
0	0.0000000000	1.6906359019	-2.0071370373
Np	0.0000000000	0.0000000000	-2.0071370373
0	0.0000000000	0.0000000000	0.1430517978
Np	0.0000000000	0.0000000000	2.0169632121
0	0.0000000000	0.0000000000	3.7256369953

Displacement 2:

0	0.0000000000	-1.6906359019	-2.0571370408
0	0.0000000000	1.6906359019	-2.0571370408
Np	0.0000000000	0.0000000000	-2.0571370408
0	0.0000000000	0.0000000000	0.1930518013
Np	0.0000000000	0.0000000000	2.0669632162
0	0.0000000000	0.0000000000	3.7756369988

Displacement 3:

0	0.0000000000	-1.6906359019	-2.1071370442
0	0.0000000000	1.6906359019	-2.1071370442
Np	0.0000000000	0.0000000000	-2.1071370442
0	0.0000000000	0.0000000000	0.2430518047
Np	0.0000000000	0.0000000000	2.1169632196
0	0.0000000000	0.0000000000	3.8256370028

Displacement 4:

0	0.0000000000	-1.6906359019	-2.1571370477
0	0.0000000000	1.6906359019	-2.1571370477
Np	0.0000000000	0.0000000000	-2.1571370477
0	0.0000000000	0.0000000000	0.2930518082
Np	0.0000000000	0.0000000000	2.1669632231
0	0.0000000000	0.0000000000	3.8756370062

Displacement 5:

0	0.0000000000	-1.6906359019	-2.2071370517
0	0.0000000000	1.6906359019	-2.2071370517
Np	0.0000000000	0.0000000000	-2.2071370517
0	0.0000000000	0.0000000000	0.3430518117
Np	0.0000000000	0.0000000000	2.2169632266
0	0.0000000000	0.0000000000	3.9256370097

Displacement 6:

0	0.0000000000	-1.6906359019	-2.2571370552
0	0.0000000000	1.6906359019	-2.2571370552
Np	0.0000000000	0.0000000000	-2.2571370552
0	0.0000000000	0.0000000000	0.3930518157
Np	0.0000000000	0.0000000000	2.2669632306
0	0.0000000000	0.0000000000	3.9756370132

Displacement 7:			
0	0.0000000000	-1.6906359019	-2.3071370587
0	0.0000000000	1.6906359019	-2.3071370587
Np	0.0000000000	0.0000000000	-2.3071370587
0	0.0000000000	0.0000000000	0.4430518192
Np	0.0000000000	0.0000000000	2.3169632341
0	0.0000000000	0.0000000000	4.0256370172

Displacement 8:			
0	0.0000000000	-1.6906359019	-2.3571370622
0	0.0000000000	1.6906359019	-2.3571370622
Np	0.0000000000	0.0000000000	-2.3571370622
0	0.0000000000	0.0000000000	0.4930518227
Np	0.0000000000	0.0000000000	2.3669632375
0	0.0000000000	0.0000000000	4.0756370207

Displacement 9:			
0	0.0000000000	-1.6906359019	-2.4071370662
0	0.0000000000	1.6906359019	-2.4071370662
Np	0.0000000000	0.0000000000	-2.4071370662
0	0.0000000000	0.0000000000	0.5430518261
Np	0.0000000000	0.0000000000	2.4169632410
0	0.0000000000	0.0000000000	4.1256370242

Displacement 10:			
0	0.0000000000	-1.6906359019	-2.4571370696
0	0.0000000000	1.6906359019	-2.4571370696
Np	0.0000000000	0.0000000000	-2.4571370696
0	0.0000000000	0.0000000000	0.5930518301
Np	0.0000000000	0.0000000000	2.4669632450
0	0.0000000000	0.0000000000	4.1756370276

Displacement 11:			
0	0.0000000000	-1.6906359019	-2.5071370731
0	0.0000000000	1.6906359019	-2.5071370731
Np	0.0000000000	0.0000000000	-2.5071370731
0	0.0000000000	0.0000000000	0.6430518336
Np	0.0000000000	0.0000000000	2.5169632485
0	0.0000000000	0.0000000000	4.2256370311

Displacement 12:			
0	0.0000000000	-1.6906359019	-2.5571370766
0	0.0000000000	1.6906359019	-2.5571370766
Np	0.0000000000	0.0000000000	-2.5571370766
0	0.0000000000	0.0000000000	0.6930518371
Np	0.0000000000	0.0000000000	2.5669632520
0	0.0000000000	0.0000000000	4.2756370351

Displacement 13:			
0	0.0000000000	-1.6906359019	-2.6071370806

0	0.0000000000	1.6906359019	-2.6071370806
Np	0.0000000000	0.0000000000	-2.6071370806
0	0.0000000000	0.0000000000	0.7430518406
Np	0.0000000000	0.0000000000	2.6169632555
0	0.0000000000	0.0000000000	4.3256370386

Displacement 14:

0	0.0000000000	-1.6906359019	-2.6571370841
0	0.0000000000	1.6906359019	-2.6571370841
Np	0.0000000000	0.0000000000	-2.6571370841
0	0.0000000000	0.0000000000	0.7930518446
Np	0.0000000000	0.0000000000	2.6669632589
0	0.0000000000	0.0000000000	4.3756370421

Displacement 15:

0	0.0000000000	-1.6906359019	-2.7071370876
0	0.0000000000	1.6906359019	-2.7071370876
Np	0.0000000000	0.0000000000	-2.7071370876
0	0.0000000000	0.0000000000	0.8430518481
Np	0.0000000000	0.0000000000	2.7169632629
0	0.0000000000	0.0000000000	4.4256370456

Displacement 16:

0	0.0000000000	-1.6906359019	-2.7571370910
0	0.0000000000	1.6906359019	-2.7571370910
Np	0.0000000000	0.0000000000	-2.7571370910
0	0.0000000000	0.0000000000	0.8930518515
Np	0.0000000000	0.0000000000	2.7669632664
0	0.0000000000	0.0000000000	4.4756370496

Displacement 17:

0	0.0000000000	-1.6906359019	-2.8071370945
0	0.0000000000	1.6906359019	-2.8071370945
Np	0.0000000000	0.0000000000	-2.8071370945
0	0.0000000000	0.0000000000	0.9430518550
Np	0.0000000000	0.0000000000	2.8169632699
0	0.0000000000	0.0000000000	4.5256370530

Displacement 18:

0	0.0000000000	-1.6906359019	-2.8571370985
0	0.0000000000	1.6906359019	-2.8571370985
Np	0.0000000000	0.0000000000	-2.8571370985
0	0.0000000000	0.0000000000	0.9930518585
Np	0.0000000000	0.0000000000	2.8669632734
0	0.0000000000	0.0000000000	4.5756370565

Displacement 19:

0	0.0000000000	-1.6906359019	-2.9571371055
0	0.0000000000	1.6906359019	-2.9571371055
Np	0.0000000000	0.0000000000	-2.9571371055

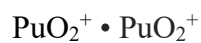
0	0.0000000000	0.0000000000	1.0930518660
Np	0.0000000000	0.0000000000	2.9669632809
0	0.0000000000	0.0000000000	4.6756370635

Displacement 20:

0	0.0000000000	-1.6906359019	-3.0571371130
0	0.0000000000	1.6906359019	-3.0571371130
Np	0.0000000000	0.0000000000	-3.0571371130
0	0.0000000000	0.0000000000	1.1930518729
Np	0.0000000000	0.0000000000	3.0669632878
0	0.0000000000	0.0000000000	4.7756370710

Energies

Displacement	1	-57880.3276101780
Displacement	2	-57880.3361388929
Displacement	3	-57880.3401380362
Displacement	4	-57880.3412125606
Displacement	5	-57880.3404848506
Displacement	6	-57880.3387248293
Displacement	7	-57880.3364509052
Displacement	8	-57880.3340073749
Displacement	9	-57880.3316180626
Displacement	10	-57880.3294205912
Displacement	11	-57880.3274952408
Displacement	12	-57880.3258822860
Displacement	13	-57880.3245936758
Displacement	14	-57880.3236245695
Displacement	15	-57880.3229580053
Displacement	16	-57880.3225703706
Displacement	17	-57880.3224348517
Displacement	18	-57880.3225225356
Displacement	19	-57880.3232588189
Displacement	20	-57880.3245757438



Displacement 1:

0	0.0000000000	-1.7231940539	-2.1322958997
0	0.0000000000	1.7231940539	-2.1322958997
Pu	0.0000000000	0.0000000000	-2.1322958997
0	0.0000000000	0.0000000000	0.3659368301
Pu	0.0000000000	0.0000000000	2.1361008476
0	0.0000000000	0.0000000000	3.8406273401

Displacement 2:

0	0.0000000000	-1.7231940539	-2.1822959032
0	0.0000000000	1.7231940539	-2.1822959032
Pu	0.0000000000	0.0000000000	-2.1822959032
0	0.0000000000	0.0000000000	0.4159368336
Pu	0.0000000000	0.0000000000	2.1861008511
0	0.0000000000	0.0000000000	3.8906273436

Displacement 3:

0	0.0000000000	-1.7231940539	-2.2322959067
0	0.0000000000	1.7231940539	-2.2322959067
Pu	0.0000000000	0.0000000000	-2.2322959067
0	0.0000000000	0.0000000000	0.4659368370
Pu	0.0000000000	0.0000000000	2.2361008546
0	0.0000000000	0.0000000000	3.9406273476

Displacement 4:

0	0.0000000000	-1.7231940539	-2.2822959107
0	0.0000000000	1.7231940539	-2.2822959107
Pu	0.0000000000	0.0000000000	-2.2822959107
0	0.0000000000	0.0000000000	0.5159368411
Pu	0.0000000000	0.0000000000	2.2861008581
0	0.0000000000	0.0000000000	3.9906273510

Displacement 5:

0	0.0000000000	-1.7231940539	-2.3322959141
0	0.0000000000	1.7231940539	-2.3322959141
Pu	0.0000000000	0.0000000000	-2.3322959141
0	0.0000000000	0.0000000000	0.5659368445
Pu	0.0000000000	0.0000000000	2.3361008621
0	0.0000000000	0.0000000000	4.0406273545

Displacement 6:

0	0.0000000000	-1.7231940539	-2.3822959176
0	0.0000000000	1.7231940539	-2.3822959176
Pu	0.0000000000	0.0000000000	-2.3822959176
0	0.0000000000	0.0000000000	0.6159368480
Pu	0.0000000000	0.0000000000	2.3861008655
0	0.0000000000	0.0000000000	4.0906273580

Displacement 7:

0	0.0000000000	-1.7231940539	-2.4322959211
0	0.0000000000	1.7231940539	-2.4322959211
Pu	0.0000000000	0.0000000000	-2.4322959211
0	0.0000000000	0.0000000000	0.6659368515
Pu	0.0000000000	0.0000000000	2.4361008690
0	0.0000000000	0.0000000000	4.1406273615

Displacement 8:

0	0.0000000000	-1.7231940539	-2.4822959251
0	0.0000000000	1.7231940539	-2.4822959251
Pu	0.0000000000	0.0000000000	-2.4822959251
0	0.0000000000	0.0000000000	0.7159368555
Pu	0.0000000000	0.0000000000	2.4861008725
0	0.0000000000	0.0000000000	4.1906273655

Displacement 9:

0	0.0000000000	-1.7231940539	-2.5322959286
0	0.0000000000	1.7231940539	-2.5322959286
Pu	0.0000000000	0.0000000000	-2.5322959286
0	0.0000000000	0.0000000000	0.7659368590
Pu	0.0000000000	0.0000000000	2.5361008760
0	0.0000000000	0.0000000000	4.2406273690

Displacement 10:

0	0.0000000000	-1.7231940539	-2.5822959321
0	0.0000000000	1.7231940539	-2.5822959321
Pu	0.0000000000	0.0000000000	-2.5822959321
0	0.0000000000	0.0000000000	0.8159368624
Pu	0.0000000000	0.0000000000	2.5861008800
0	0.0000000000	0.0000000000	4.2906273724

Displacement 11:

0	0.0000000000	-1.7231940539	-2.6322959355
0	0.0000000000	1.7231940539	-2.6322959355
Pu	0.0000000000	0.0000000000	-2.6322959355
0	0.0000000000	0.0000000000	0.8659368659
Pu	0.0000000000	0.0000000000	2.6361008835
0	0.0000000000	0.0000000000	4.3406273759

Displacement 12:

0	0.0000000000	-1.7231940539	-2.6822959395
0	0.0000000000	1.7231940539	-2.6822959395
Pu	0.0000000000	0.0000000000	-2.6822959395
0	0.0000000000	0.0000000000	0.9159368694
Pu	0.0000000000	0.0000000000	2.6861008869
0	0.0000000000	0.0000000000	4.3906273799

Displacement 13:

0	0.0000000000	-1.7231940539	-2.7322959430
0	0.0000000000	1.7231940539	-2.7322959430
Pu	0.0000000000	0.0000000000	-2.7322959430
0	0.0000000000	0.0000000000	0.9659368734
Pu	0.0000000000	0.0000000000	2.7361008904
0	0.0000000000	0.0000000000	4.4406273834

Displacement 14:

0	0.0000000000	-1.7231940539	-2.7822959465
0	0.0000000000	1.7231940539	-2.7822959465
Pu	0.0000000000	0.0000000000	-2.7822959465
0	0.0000000000	0.0000000000	1.0159368769
Pu	0.0000000000	0.0000000000	2.7861008944
0	0.0000000000	0.0000000000	4.4906273869

Displacement 15:

0	0.0000000000	-1.7231940539	-2.8322959500
0	0.0000000000	1.7231940539	-2.8322959500
Pu	0.0000000000	0.0000000000	-2.8322959500
0	0.0000000000	0.0000000000	1.0659368804
Pu	0.0000000000	0.0000000000	2.8361008979
0	0.0000000000	0.0000000000	4.5406273904

Displacement 16:

0	0.0000000000	-1.7231940539	-2.8822959534
0	0.0000000000	1.7231940539	-2.8822959534
Pu	0.0000000000	0.0000000000	-2.8822959534
0	0.0000000000	0.0000000000	1.1159368838
Pu	0.0000000000	0.0000000000	2.8861009014
0	0.0000000000	0.0000000000	4.5906273938

Displacement 17:

0	0.0000000000	-1.7231940539	-2.9322959575
0	0.0000000000	1.7231940539	-2.9322959575
Pu	0.0000000000	0.0000000000	-2.9322959575
0	0.0000000000	0.0000000000	1.1659368878
Pu	0.0000000000	0.0000000000	2.9361009049
0	0.0000000000	0.0000000000	4.6406273978

Displacement 18:

0	0.0000000000	-1.7231940539	-2.9822959609
0	0.0000000000	1.7231940539	-2.9822959609
Pu	0.0000000000	0.0000000000	-2.9822959609
0	0.0000000000	0.0000000000	1.2159368913
Pu	0.0000000000	0.0000000000	2.9861009089
0	0.0000000000	0.0000000000	4.6906274013

Displacement 19:

0	0.0000000000	-1.7231940539	-3.0822959679
0	0.0000000000	1.7231940539	-3.0822959679

Pu	0.0000000000	0.0000000000	-3.0822959679
0	0.0000000000	0.0000000000	1.3159368983
Pu	0.0000000000	0.0000000000	3.0861009158
0	0.0000000000	0.0000000000	4.7906274083

Displacement 20:

0	0.0000000000	-1.7231940539	-3.1822959754
0	0.0000000000	1.7231940539	-3.1822959754
Pu	0.0000000000	0.0000000000	-3.1822959754
0	0.0000000000	0.0000000000	1.4159369058
Pu	0.0000000000	0.0000000000	3.1861009228
0	0.0000000000	0.0000000000	4.8906274158

Energies

Displacement	1	-59492.6501588305
Displacement	2	-59492.6519564646
Displacement	3	-59492.6527351957
Displacement	4	-59492.6529250664
Displacement	5	-59492.6528117568
Displacement	6	-59492.6525720607
Displacement	7	-59492.6523287035
Displacement	8	-59492.6521461244
Displacement	9	-59492.6520607891
Displacement	10	-59492.6520877853
Displacement	11	-59492.6522291440
Displacement	12	-59492.6524801801
Displacement	13	-59492.6528304053
Displacement	14	-59492.6532682510
Displacement	15	-59492.6537817626
Displacement	16	-59492.6543586147
Displacement	17	-59492.6549878996
Displacement	18	-59492.6556595606
Displacement	19	-59492.6570952472
Displacement	20	-59492.6586099331



Displacement 1:

0	0.0000000000	-1.7230142342	-2.1728802153
0	0.0000000000	1.7230142342	-2.1728802153
Am	0.0000000000	0.0000000000	-2.1728802153
0	0.0000000000	0.0000000000	0.4099332605
Am	0.0000000000	0.0000000000	2.1762592978
0	0.0000000000	0.0000000000	3.8844924705

Displacement 2:

0	0.0000000000	-1.7230142342	-2.2228802188
0	0.0000000000	1.7230142342	-2.2228802188
Am	0.0000000000	0.0000000000	-2.2228802188
0	0.0000000000	0.0000000000	0.4599332640
Am	0.0000000000	0.0000000000	2.2262593013
0	0.0000000000	0.0000000000	3.9344924740

Displacement 3:

0	0.0000000000	-1.7230142342	-2.2728802228
0	0.0000000000	1.7230142342	-2.2728802228
Am	0.0000000000	0.0000000000	-2.2728802228
0	0.0000000000	0.0000000000	0.5099332675
Am	0.0000000000	0.0000000000	2.2762593048
0	0.0000000000	0.0000000000	3.9844924775

Displacement 4:

0	0.0000000000	-1.7230142342	-2.3228802263
0	0.0000000000	1.7230142342	-2.3228802263
Am	0.0000000000	0.0000000000	-2.3228802263
0	0.0000000000	0.0000000000	0.5599332715
Am	0.0000000000	0.0000000000	2.3262593083
0	0.0000000000	0.0000000000	4.0344924815

Displacement 5:

0	0.0000000000	-1.7230142342	-2.3728802298
0	0.0000000000	1.7230142342	-2.3728802298
Am	0.0000000000	0.0000000000	-2.3728802298
0	0.0000000000	0.0000000000	0.6099332750
Am	0.0000000000	0.0000000000	2.3762593117
0	0.0000000000	0.0000000000	4.0844924850

Displacement 6:

0	0.0000000000	-1.7230142342	-2.4228802333
0	0.0000000000	1.7230142342	-2.4228802333
Am	0.0000000000	0.0000000000	-2.4228802333
0	0.0000000000	0.0000000000	0.6599332784
Am	0.0000000000	0.0000000000	2.4262593157
0	0.0000000000	0.0000000000	4.1344924884

Displacement 7:

0	0.0000000000	-1.7230142342	-2.4728802367
0	0.0000000000	1.7230142342	-2.4728802367
Am	0.0000000000	0.0000000000	-2.4728802367
0	0.0000000000	0.0000000000	0.7099332819
Am	0.0000000000	0.0000000000	2.4762593192
0	0.0000000000	0.0000000000	4.1844924919

Displacement 8:

0	0.0000000000	-1.7230142342	-2.5228802407
0	0.0000000000	1.7230142342	-2.5228802407
Am	0.0000000000	0.0000000000	-2.5228802407
0	0.0000000000	0.0000000000	0.7599332859
Am	0.0000000000	0.0000000000	2.5262593227
0	0.0000000000	0.0000000000	4.2344924959

Displacement 9:

0	0.0000000000	-1.7230142342	-2.5728802442
0	0.0000000000	1.7230142342	-2.5728802442
Am	0.0000000000	0.0000000000	-2.5728802442
0	0.0000000000	0.0000000000	0.8099332894
Am	0.0000000000	0.0000000000	2.5762593262
0	0.0000000000	0.0000000000	4.2844924994

Displacement 10:

0	0.0000000000	-1.7230142342	-2.6228802477
0	0.0000000000	1.7230142342	-2.6228802477
Am	0.0000000000	0.0000000000	-2.6228802477
0	0.0000000000	0.0000000000	0.8599332929
Am	0.0000000000	0.0000000000	2.6262593302
0	0.0000000000	0.0000000000	4.3344925029

Displacement 11:

0	0.0000000000	-1.7230142342	-2.6728802512
0	0.0000000000	1.7230142342	-2.6728802512
Am	0.0000000000	0.0000000000	-2.6728802512
0	0.0000000000	0.0000000000	0.9099332964
Am	0.0000000000	0.0000000000	2.6762593337
0	0.0000000000	0.0000000000	4.3844925064

Displacement 12:

0	0.0000000000	-1.7230142342	-2.7228802552
0	0.0000000000	1.7230142342	-2.7228802552
Am	0.0000000000	0.0000000000	-2.7228802552
0	0.0000000000	0.0000000000	0.9599332998
Am	0.0000000000	0.0000000000	2.7262593371
0	0.0000000000	0.0000000000	4.4344925104

Displacement 13:

0	0.0000000000	-1.7230142342	-2.7728802587
---	--------------	---------------	---------------

0	0.0000000000	1.7230142342	-2.7728802587
Am	0.0000000000	0.0000000000	-2.7728802587
0	0.0000000000	0.0000000000	1.0099333038
Am	0.0000000000	0.0000000000	2.7762593406
0	0.0000000000	0.0000000000	4.4844925138

Displacement 14:

0	0.0000000000	-1.7230142342	-2.8228802621
0	0.0000000000	1.7230142342	-2.8228802621
Am	0.0000000000	0.0000000000	-2.8228802621
0	0.0000000000	0.0000000000	1.0599333073
Am	0.0000000000	0.0000000000	2.8262593446
0	0.0000000000	0.0000000000	4.5344925173

Displacement 15:

0	0.0000000000	-1.7230142342	-2.8728802656
0	0.0000000000	1.7230142342	-2.8728802656
Am	0.0000000000	0.0000000000	-2.8728802656
0	0.0000000000	0.0000000000	1.1099333108
Am	0.0000000000	0.0000000000	2.8762593481
0	0.0000000000	0.0000000000	4.5844925208

Displacement 16:

0	0.0000000000	-1.7230142342	-2.9228802691
0	0.0000000000	1.7230142342	-2.9228802691
Am	0.0000000000	0.0000000000	-2.9228802691
0	0.0000000000	0.0000000000	1.1599333143
Am	0.0000000000	0.0000000000	2.9262593516
0	0.0000000000	0.0000000000	4.6344925243

Displacement 17:

0	0.0000000000	-1.7230142342	-2.9728802731
0	0.0000000000	1.7230142342	-2.9728802731
Am	0.0000000000	0.0000000000	-2.9728802731
0	0.0000000000	0.0000000000	1.2099333183
Am	0.0000000000	0.0000000000	2.9762593551
0	0.0000000000	0.0000000000	4.6844925283

Displacement 18:

0	0.0000000000	-1.7230142342	-3.0228802766
0	0.0000000000	1.7230142342	-3.0228802766
Am	0.0000000000	0.0000000000	-3.0228802766
0	0.0000000000	0.0000000000	1.2599333218
Am	0.0000000000	0.0000000000	3.0262593585
0	0.0000000000	0.0000000000	4.7344925318

Displacement 19:

0	0.0000000000	-1.7230142342	-3.1228802835
0	0.0000000000	1.7230142342	-3.1228802835
Am	0.0000000000	0.0000000000	-3.1228802835

0	0.0000000000	0.0000000000	1.3599333287
Am	0.0000000000	0.0000000000	3.1262593660
0	0.0000000000	0.0000000000	4.8344925387

Displacement 20:

0	0.0000000000	-1.7230142342	-3.2228802910
0	0.0000000000	1.7230142342	-3.2228802910
Am	0.0000000000	0.0000000000	-3.2228802910
0	0.0000000000	0.0000000000	1.4599333362
Am	0.0000000000	0.0000000000	3.2262593730
0	0.0000000000	0.0000000000	4.9344925462

Energies

Displacement	1	-61136.0490362629
Displacement	2	-61136.0500360343
Displacement	3	-61136.0504447096
Displacement	4	-61136.0505443236
Displacement	5	-61136.0505154244
Displacement	6	-61136.0504696863
Displacement	7	-61136.0504736150
Displacement	8	-61136.0505613143
Displacement	9	-61136.0507480631
Displacement	10	-61136.0510367685
Displacement	11	-61136.0514229472
Displacement	12	-61136.0518967318
Displacement	13	-61136.0524478599
Displacement	14	-61136.0530650824
Displacement	15	-61136.0537371043
Displacement	16	-61136.0544535636
Displacement	17	-61136.0552056496
Displacement	18	-61136.0559852614
Displacement	19	-61136.0575993876
Displacement	20	-61136.0592492344