Supplementary Information for

Multiconfigurational Actinide Nitrides Assisted by Double Möbius Aromaticity

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Table S1. Energy gaps between different spin states with ANO-RCC basis set with DKH correction and ECP60MDF basis set for U_2N_2.

Method	Basis set	^1A_g	$^3B_{1u}$	^5A_g	$^7B_{1u}$
PBE0	ECP60MDF	114.7	12.7	23.0	0.0
	ANO-RCC	63.4	25.8	20.7	0.0
CASSCF (6,26)	ECP60MDF	0.0	0.2	0.8	1.7
	ANO-RCC	0.0	0.3	0.8	1.8
CASPT2 (6,26)	ECP60MDF	0.0	0.7	2.0	4.2
	ANO-RCC	0.0	0.7	2.1	4.5
CASSCF (6,10)	ECP60MDF	0.0	0.2	0.6	1.3
	ANO-RCC	0.0	0.2	0.7	1.3
CASPT2(6,10)	ECP60MDF	0.0	1.0	2.8	5.5
	ANO-RCC	0.0	1.0	2.9	6.0
MS-CASPT2(6,10)	ECP60MDF	0.0	0.4	0.7	2.2
	ANO-RCC	0.0	0.4	0.8	2.4
CASSCF (6,6)	ECP60MDF	0.0	0.2	0.7	1.4
	ANO-RCC	0.0	0.2	0.7	1.5
CASPT2 (6,6)	ECP60MDF	0.0	1.2	3.1	6.4
	ANO-RCC	0.0	1.1	3.2	6.5
VBSCF (6,6)	ECP60MDF	0.0	0.3	0.8	1.7
VBPT2 (6,6)	ANO-RCC	0.0	0.7	2.4	5.5

Table S2. Computed delocalization energies for each spin multiplicity at VBSCF and VBPT2 level.

Species	Spin	VBSCF				VBPT2			
		$\Delta E_{U\text{-}N}$	ΔE_π	ΔE_σ	ΔE_{total}	$\Delta E_{U\text{-}N}$	ΔE_π	ΔE_σ	ΔE_{total}
U_2N_2	1	2.0	41.9	32.9	77.0	0.8	24.3	20.4	42.4
	3	2.0	42.0	32.9	77.1	0.8	24.4	20.5	42.5
	5	2.0	41.9	33.1	77.1	0.8	24.2	20.8	42.5
	7	2.0	41.9	33.2	77.1	0.8	23.9	21.1	42.3
Pa_2N_2	1	1.9	42.6	33.3	77.9	0.7	24.3	20.5	42.7
	3	1.9	42.6	33.3	77.9	0.7	24.3	20.5	42.7
	5	1.9	42.5	33.3	77.9	0.6	23.9	20.5	42.3
Th_2N_2	1	1.9	40.5	30.2	72.7	0.9	21.6	16.8	36.2
	3	1.9	40.4	30.2	72.7	0.8	21.5	16.8	36.1
Ac_2N_2	1	2.0	30.2	21.6	53.1	1.5	11.5	15.2	25.6
$[U_2N_2]^+$	2	2.2	45.6	35.2	83.6	0.8	26.5	23.7	47.9
	4	2.2	45.7	35.3	83.6	0.8	26.5	24.2	47.8
	6	2.2	45.8	35.4	83.7	0.8	26.7	24.7	48.1
Mol I	2	2.9	49.8	38.3	90.9	1.9	32.5	32.8	60.1
	4	3.0	49.8	38.4	90.9	1.9	32.4	32.8	60.0
Mol II	1	3.7	45.7	34.4	82.7	3.0	28.3	28.2	50.7
	3	3.7	45.7	34.4	82.7	3.0	28.1	28.0	50.4
Mol III	1	1.8	32.4	45.2	80.1	0.8	23.8	28.1	47.4
	3	1.8	32.4	45.2	80.1	0.9	23.8	28.1	47.2
	5	1.8	32.4	45.2	80.1	0.8	23.8	27.8	47.0

Table S3. Major optimal parameter for U2N2 by PBE0/ECP60MDF and CASSCF(CASPT2)/ANO-RCC-DKH.

Method	Spin	U-U	U-N	N-N	θ_{N-U-N}
PBE0	1	3.097	1.979	2.466	77.1
	3	3.120	2.006	2.521	77.9
	5	3.091	2.000	2.540	78.8
	7	3.126	2.013	2.536	78.1
CASSCF(6,10)	1	3.137	2.037	2.599	79.3
	3	3.138	2.037	2.598	79.2
	5	3.140	2.037	2.597	79.2
	7	3.144	2.038	2.595	79.1
CASSCF(6.6)	1	3.131	2.035	2.601	79.4
	3	3.133	2.036	2.600	79.4
	5	3.135	2.036	2.599	79.3
	7	3.139	2.037	2.597	79.2
CASPT2(6,10)	1	3.133	2.035	2.599	79.4
	3	3.136	2.036	2.597	79.3
	5	3.139	2.036	2.596	79.2
	7	3.142	2.037	2.594	79.1
CASPT2(6.6)	1	3.128	2.034	2.601	79.5
	3	3.129	2.034	2.601	79.5
	5	3.134	2.035	2.598	79.3
	7	3.138	2.036	2.596	79.2

Table S4. Computed absolute energies (AE, a.u.) and relative energies (RE, kcal/mol) of all electronic states for singlet U_2N_2 using a (6,10) active space with ANO-RCC-DKH basis set.

State	CASSCF		CASPT2	
	AE	RE	AE	RE
^1A_g	-56008.6780	0.0	-56010.1106	0.0
$^1B_{3u}$	-56008.6611	10.6	-56010.1031	4.7
$^1B_{2u}$	-56008.6629	9.5	-56010.1051	3.5
$^1B_{1g}$	-56008.6758	1.4	-56010.1116	-0.6
$^1B_{1u}$	-56008.6533	15.5	-56010.0986	7.6
$^1B_{2g}$	-56008.6612	10.6	-56010.1032	4.6
$^1B_{3g}$	-56008.6629	9.5	-56010.1049	3.6
^1A_u	-56008.6758	1.4	-56010.1117	-0.7

Table S5. Computed absolute energies (AE, a.u.) and relative energies (RE, kcal/mol) of all electronic states for triplet U_2N_2 using a (6,10) active space with ANO-RCC-DKH basis set.

State	CASSCF		CASPT2	
	AE	RE	AE	RE
^3A_g	-56008.6628	9.3	-56010.0870	13.8
$^3B_{3u}$	-56008.6608	10.6	-56010.1018	4.5
$^3B_{2u}$	-56008.6625	9.5	-56010.1028	3.9
$^3B_{1g}$	-56008.6754	1.4	-56010.1101	-0.7
$^3B_{1u}$	-56008.6777	0.0	-56010.1090	0.0
$^3B_{2g}$	-56008.6607	10.6	-56010.1017	4.5
$^3B_{3g}$	-56008.6625	9.5	-56010.1029	3.8
^3A_u	-56008.6754	1.4	-56010.1100	-0.7

Table S6. Computed absolute energies (AE, a.u.) and relative energies (RE, kcal/mol) of all electronic states for quintet U_2N_2 using a (6,10) active space with ANO-RCC-DKH basis set.

State	CASSCF		CASPT2	
	AE	RE	AE	RE
^5A_g	-56008.6769	0.0	-56010.1059	0.0
$^5B_{3u}$	-56008.6600	10.6	-56010.0986	4.6
$^5B_{2u}$	-56008.6501	16.9	-56010.0863	12.3
$^5B_{1g}$	-56008.6628	8.8	-56010.0935	7.8
$^5B_{1u}$	-56008.6629	8.8	-56010.0873	11.7
$^5B_{2g}$	-56008.6487	17.7	-56010.0852	12.9
$^5B_{3g}$	-56008.6501	16.8	-56010.0863	12.3
^5A_u	-56008.6747	1.4	-56010.1068	-0.6

Table S7. Computed absolute energies (AE, a.u.) and relative energies (RE, kcal/mol) of all electronic states for septet U_2N_2 using a (6,10) active space with ANO-RCC-DKH basis set.

State	CASSCF		CASPT2	
	AE	RE	AE	RE
^7A_g	-56008.6514	15.3	-56010.0900	6.9
$^7B_{3u}$	-56008.6588	10.8	-56010.0944	4.1
$^7B_{2u}$	-56008.6605	9.6	-56010.0950	3.8
$^7B_{1g}$	-56008.6738	1.3	-56010.1025	-1.0
$^7B_{1u}$	-56008.6759	0.0	-56010.1010	0.0
$^7B_{2g}$	-56008.6588	10.7	-56010.0944	4.1
$^7B_{3g}$	-56008.6604	9.7	-56010.0936	4.6
^7A_u	-56008.6737	1.4	-56010.1026	-1.0
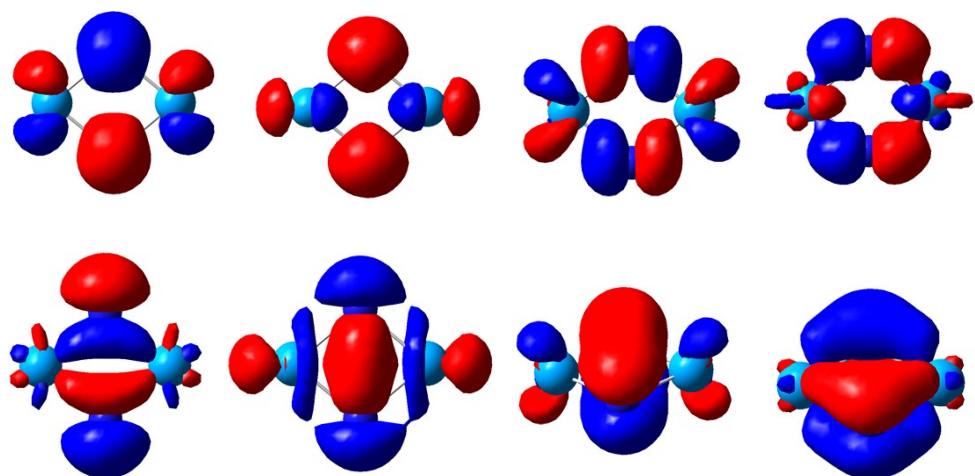
Figure S1. Eight Valence canonical molecular orbitals (CMOs) with the isovalue of 0.05 a.u. for Pa_2N_2.
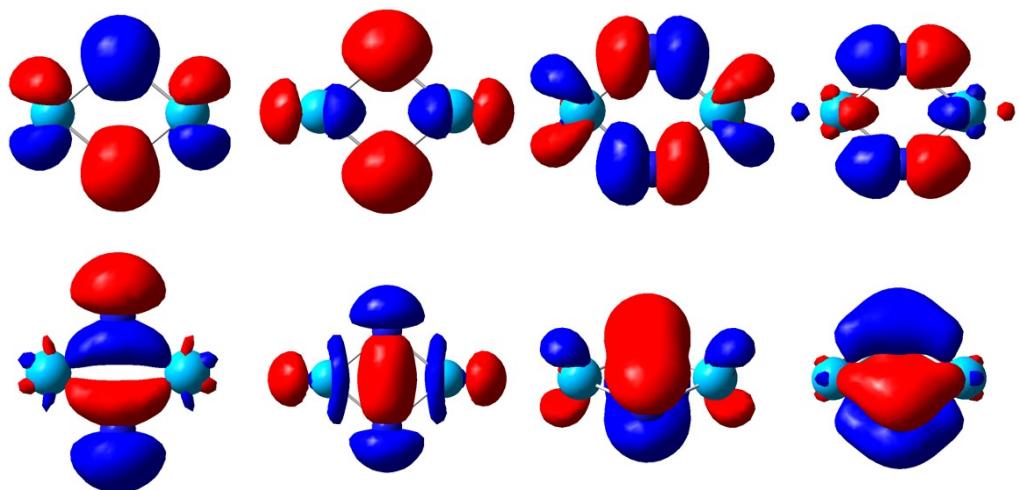
Figure S2. Eight Valence canonical molecular orbitals (CMOs) with the isovalue of 0.05 a.u. for Th_2N_2.
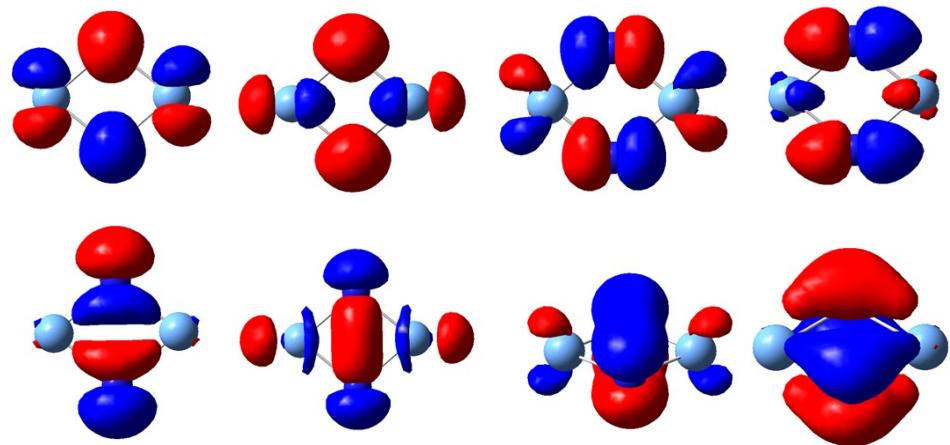
Figure S3. Eight Valence canonical molecular orbitals (CMOs) with the isovalue of 0.05 a.u. for Ac_2N_2.
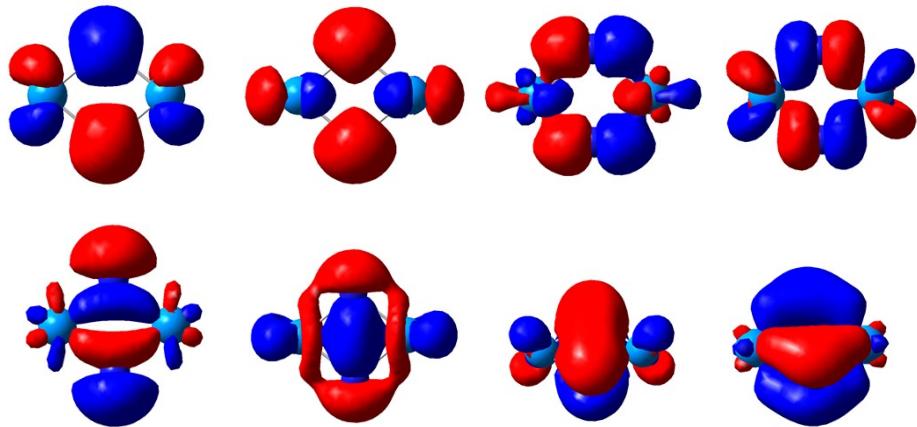
Figure S4. Eight Valence canonical molecular orbitals (CMOs) with the isovalue of 0.05 a.u. for $[U_2N_2]^+$.
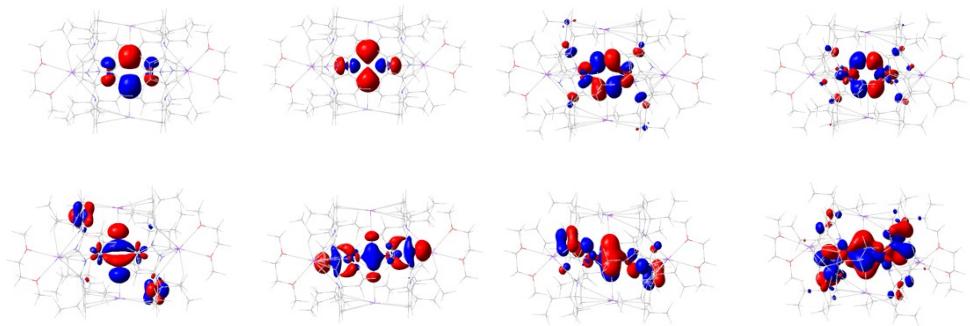
Figure S5. Eight Valence canonical molecular orbitals (CMOs) with the isovalue of 0.04 a.u. for compounds **I**.
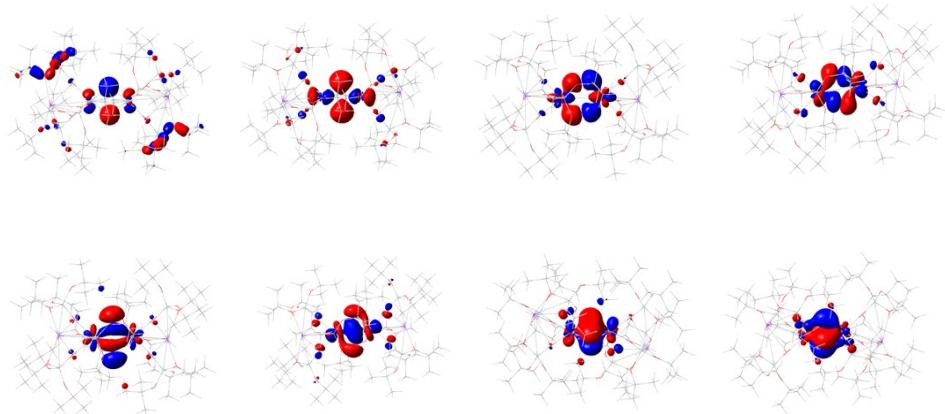
Figure S6. Eight Valence canonical molecular orbitals (CMOs) with the isovalue of 0.04 a.u. for compounds **II**.
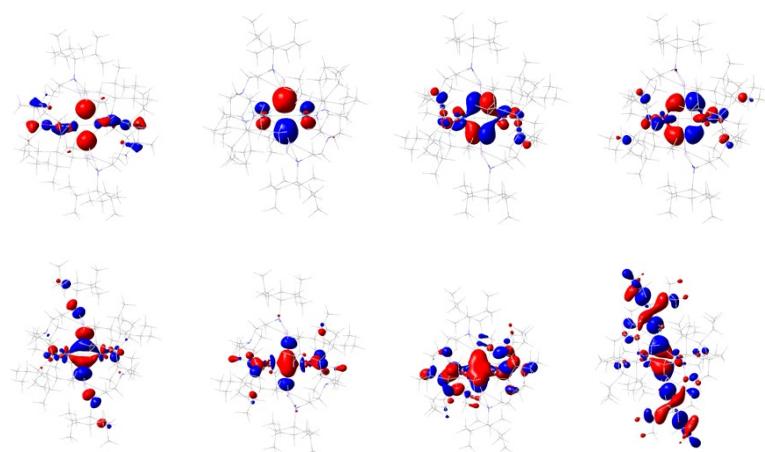
Figure S7. Eight Valence canonical molecular orbitals (CMOs) with the isovalue of 0.04 a.u. for compounds **III**.

N-U-N-U

H$_2$N-U-N-U-NH
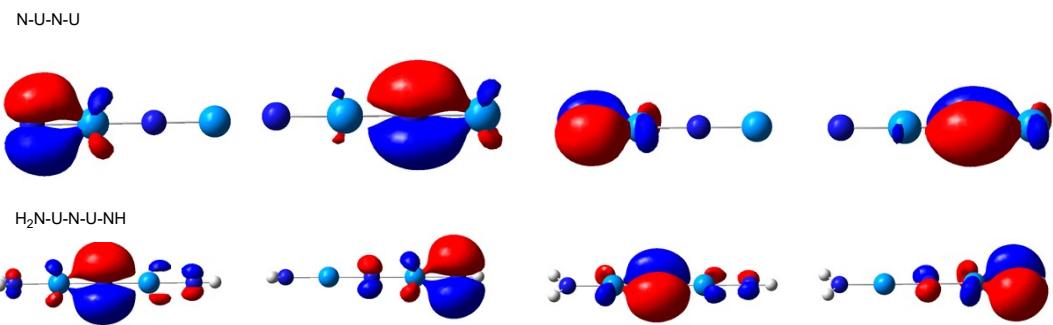
Figure S8. The canonical molecular orbitals (CMOs) with the isovalue of 0.05 a.u. for linear U$_2$N$_2$ and [H$_2$N–An–N–An–NH] relative to the delocalized σ and π orbitals in cyclic U$_2$N$_2$.
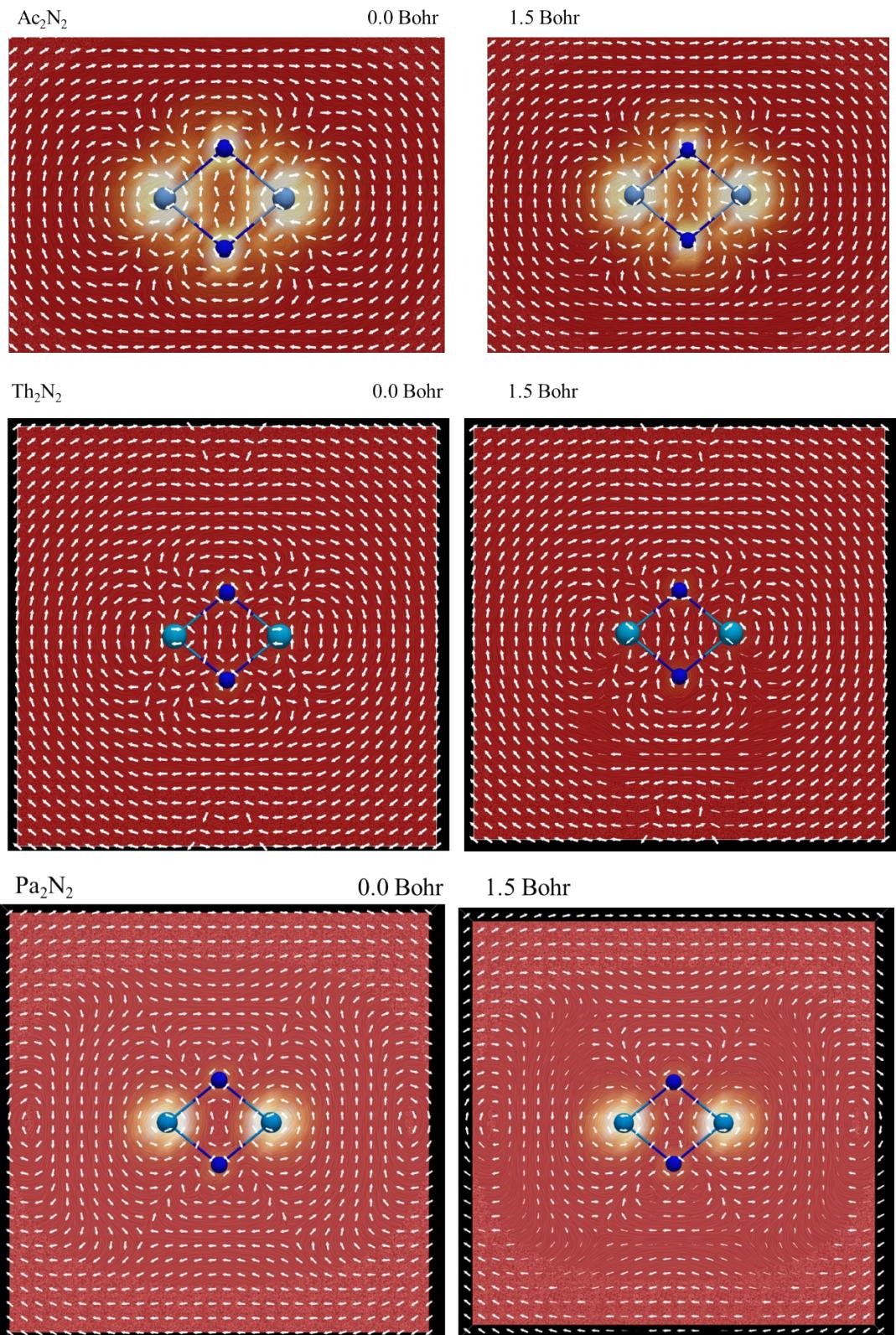
Figure S9. The strength and direction of the induced current for Pa_2N_2, Th_2N_2 and Ac_2N_2 by GIMIC program.
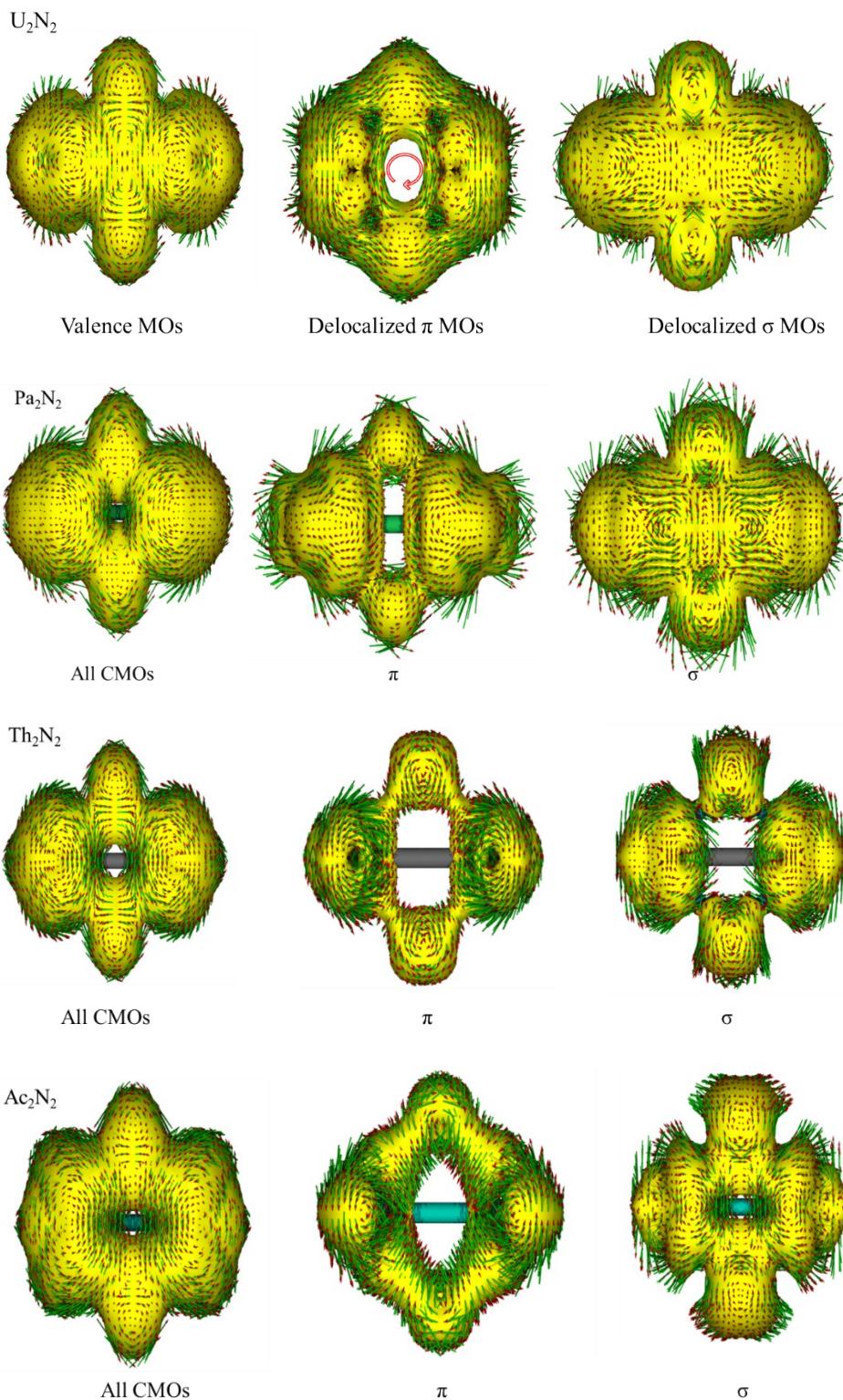
Figure S10. Isosurfaces of AICD (isovalue = 0.03) for Pa_2N_2, Th_2N_2 and Ac_2N_2 generated from all eight CMOs, the two delocalized π MOs, and two delocalized σ MOs.

Optimal geometries for U_2N_2 with CASSCF (6,10)/ANO-RCC

Singlet

U	0.00000000	0.00000000	1.56657001
U	0.00000000	0.00000000	-1.56657001
N	0.00000000	1.29957816	0.00000000
N	0.00000000	-1.29957816	0.00000000

Triplet

U	0.00000000	0.00000000	1.56800149
U	0.00000000	0.00000000	-1.56800149
N	0.00000000	1.29852079	0.00000000
N	0.00000000	-1.29852079	0.00000000

Quintet

U	0.00000000	0.00000000	1.56931707
U	0.00000000	0.00000000	-1.56931707
N	0.00000000	1.29782925	0.00000000
N	0.00000000	-1.29782925	0.00000000

Septet

U	0.00000000	0.00000000	1.57115034
U	0.00000000	0.00000000	-1.57115034
N	0.00000000	1.29722775	0.00000000
N	0.00000000	-1.29722775	0.00000000

Optimal geometries for U_2N_2 with CASSCF (6,6)/ANO-RCC

Singlet

U	0.00000000	0.00000000	1.56409112
U	0.00000000	0.00000000	-1.56409112
N	0.00000000	1.30044046	0.00000000
N	0.00000000	-1.30044046	0.00000000

Triplet

U	0.00000000	0.00000000	1.56441231
U	0.00000000	0.00000000	-1.56441231
N	0.00000000	1.30043270	0.00000000
N	0.00000000	-1.30043270	0.00000000

Quintet

U	0.00000000	0.00000000	1.56681723

U	0.00000000	0.00000000	-1.56681723
N	0.00000000	1.29883034	0.00000000
N	0.00000000	-1.29883034	0.00000000

Septet

U	0.00000000	0.00000000	1.56889426
U	0.00000000	0.00000000	-1.56889426
N	0.00000000	1.29816673	0.00000000
N	0.00000000	-1.29816673	0.00000000

Optimal geometries for U$_2$N$_2$ with PBE0/ECP60MDF

Singlet

U	0.00000000	0.00000000	1.54830500
U	0.00000000	0.00000000	-1.54830500
N	0.00000000	1.23281400	0.00000000
N	0.00000000	-1.23281400	0.00000000

Triplet

U	0.00000000	0.00000000	1.55995600
U	0.00000000	0.00000000	-1.55995600
N	0.00000000	1.26057500	0.00000000
N	0.00000000	-1.26057500	0.00000000

Quintet

U	0.00000000	0.00000000	1.54562700
U	0.00000000	0.00000000	-1.54562700
N	0.00000000	1.26980700	0.00000000
N	0.00000000	-1.26980700	0.00000000

Septet

U	0.00000000	0.00000000	1.56313900
U	0.00000000	0.00000000	-1.56313900
N	0.00000000	1.26815300	0.00000000
N	0.00000000	-1.26815300	0.00000000

Optimal geometries for I with PBE0/ECP60MDF

C	5.48850715	3.88554747	2.95706660
C	2.54594820	3.26923591	4.72656221
C	2.49707949	3.53158908	3.22890253
C	3.30331547	4.31682303	0.40483723
C	4.80123965	2.53648247	2.83099772
C	7.04139821	2.93040385	-0.09240642
C	3.32615394	2.56826674	2.35158921
C	3.28659986	4.19194334	-1.00818859
C	3.24669102	3.01685619	0.90867080
C	-3.81354477	3.91644202	3.00244553
C	-1.38929564	2.55601298	4.33626593
C	-5.19072337	4.18949559	2.41415596
C	-2.70583189	4.54109445	0.32192112
C	-1.51547199	2.91594665	2.86545961
C	5.49409399	3.31723739	-3.17681495
C	2.76264408	1.17034672	2.47849804
C	3.22293328	2.82443265	-1.28393603
C	-2.78243313	4.44112816	-1.09265876
C	-2.94780428	2.85564594	2.27590576
C	8.52211622	1.12269509	-0.35180736
C	1.45138486	0.80782667	2.82179191
C	4.06433601	3.03208107	-3.61756343
C	-2.87783084	3.24712298	0.81704299
C	3.17434686	2.19743406	-2.66261643
C	-3.50907477	1.46589569	2.51916851
C	-2.99410200	3.09250871	-1.36876755
C	-4.56448053	1.17496210	3.37858285
C	8.58505074	-0.32302220	-0.77627916
C	1.44896104	-0.59969066	2.91581467
C	1.71785417	2.28571838	-3.19217288
C	2.76077655	-1.00926599	2.63595495
C	-7.93049188	2.48294222	0.12434197
C	-5.50205377	3.73172317	-3.05980674
C	2.81373797	-2.64080002	5.22439545
C	-2.58540596	3.19160651	-3.82599706
C	3.60434059	0.74084530	-2.69681932
C	4.81987179	-2.38095371	2.92788324
C	-3.29057776	2.42451598	-2.68824813
C	-4.62446863	-0.22891972	3.49193338
C	4.62446863	0.22891972	-3.49193338
C	1.49597680	1.74391581	-4.59544105
C	-1.49597680	-1.74391581	4.59544105
C	3.29057776	-2.42451598	2.68824813

C	-4.81987179	2.38095371	-2.92788324
C	7.93049188	-2.48294222	-0.12434197
C	5.50205377	-3.73172317	3.05980674
C	2.58540596	-3.19160651	3.82599706
C	-2.81373797	2.64080002	-5.22439545
C	-3.60434059	-0.74084530	2.69681932
C	-8.58505074	0.32302220	0.77627916
C	-2.76077655	1.00926599	-2.63595495
C	4.56448053	-1.17496210	-3.37858285
C	-1.71785417	-2.28571838	3.19217288
C	2.99410200	-3.09250871	1.36876755
C	-1.44896104	0.59969066	-2.91581467
C	3.50907477	-1.46589569	-2.51916851
C	-3.17434686	-2.19743406	2.66261643
C	-8.52211622	-1.12269509	0.35180736
C	-4.06433601	-3.03208107	3.61756343
C	2.87783084	-3.24712298	-0.81704299
C	-1.45138486	-0.80782667	-2.82179191
C	2.78243313	-4.44112816	1.09265876
C	2.94780428	-2.85564594	-2.27590576
C	-3.22293328	-2.82443265	1.28393603
C	-5.49409399	-3.31723739	3.17681495
C	-2.76264408	-1.17034672	-2.47849804
C	5.19072337	-4.18949559	-2.41415596
C	2.70583189	-4.54109445	-0.32192112
C	1.51547199	-2.91594665	-2.86545961
C	3.81354477	-3.91644202	-3.00244553
C	1.38929564	-2.55601298	-4.33626593
C	-7.04139821	-2.93040385	0.09240642
C	-3.24669102	-3.01685619	-0.90867080
C	-3.28659986	-4.19194334	1.00818859
C	-3.32615394	-2.56826674	-2.35158921
C	-4.80123965	-2.53648247	-2.83099772
C	-3.30331547	-4.31682303	-0.40483723
C	-2.49707949	-3.53158908	-3.22890253
C	-2.54594820	-3.26923591	-4.72656221
C	-5.48850715	-3.88554747	-2.95706660
H	5.03043815	4.51389273	3.73701659
H	1.85305820	3.93733605	5.26187489
H	6.54898238	3.75766745	3.22888041
H	3.55155557	3.43724437	5.14245713
H	2.82758555	4.56306653	3.02883781
H	5.44524908	4.44808626	2.01244766
H	3.39124125	5.24009207	0.97835729

H	2.25972786	2.23253312	4.95839017
H	1.45174548	3.48859565	2.88344366
H	7.40761909	3.12476076	0.93163078
H	4.84035744	2.00417335	3.79538840
H	-3.24101971	4.85969230	3.00562147
H	5.96805503	3.16230459	-0.13902981
H	3.35986887	5.00148491	-1.73568298
H	-1.94511120	3.25280229	4.98210526
H	-2.60971764	5.45706926	0.90757581
H	7.58076615	3.59156389	-0.79602026
H	-5.72534609	4.95065198	3.00618768
H	-1.12434982	3.93649431	2.69536242
H	-0.33781288	2.57918246	4.66036951
H	5.51957917	4.05549238	-2.36463451
H	5.36351236	1.89632089	2.13602838
H	-3.91357747	3.62897081	4.06006428
H	6.08514206	3.71660346	-4.01785865
H	-5.10906455	4.55313115	1.37915813
H	8.90023554	1.22007991	0.68645278
H	-2.75293944	5.26096896	-1.81121808
H	3.55206765	3.99383570	-3.79578314
H	-1.77855565	1.54441031	4.52240051
H	0.61503286	1.46291781	3.02389114
H	5.99636168	2.41123317	-2.80986450
H	-0.89657921	2.23958076	2.25413108
H	-5.80681208	3.27947178	2.40165954
H	9.19367067	1.71254037	-1.00913413
H	-5.18792195	1.88423720	3.91791179
H	1.41182755	3.34859440	-3.15457205
H	-7.65174839	2.76823811	1.15522788
H	4.07846399	2.52478840	-4.59284250
H	-5.28967055	4.36648875	-2.18511944
H	2.54278987	-1.57523564	5.27812173
H	-2.90162267	4.24630435	-3.79065971
H	9.64373243	-0.65186951	-0.75090570
H	5.02280479	-1.75757977	3.81374356
H	-7.25108301	2.99334868	-0.57218598
H	3.86558530	-2.73410584	5.53768936
H	-5.16993148	4.28129895	-3.95507491
H	-1.80098514	-0.68896691	4.65557480
H	-8.96480151	2.82671671	-0.06937051
H	-1.50597103	3.20513090	-3.60576134
H	5.27324033	-1.83122500	2.09257964
H	1.07813696	1.74739476	-2.47393913

H	0.61359156	-1.22403636	3.20037127
H	8.22684728	-0.42246161	-1.82118178
H	5.31133416	0.78827620	-4.12223921
H	2.06787815	2.30364114	-5.35049592
H	-6.59436827	3.61004527	-3.14271593
H	2.20140933	-3.18155773	5.96324169
H	-0.43504749	-1.80481886	4.88265220
H	-8.22684728	0.42246161	1.82118178
H	6.59436827	-3.61004527	3.14271593
H	8.96480151	-2.82671671	0.06937051
H	-2.20140933	3.18155773	-5.96324169
H	0.43504749	1.80481886	-4.88265220
H	-5.31133416	-0.78827620	4.12223921
H	-2.06787815	-2.30364114	5.35049592
H	-5.27324033	1.83122500	-2.09257964
H	-9.64373243	0.65186951	0.75090570
H	5.16993148	-4.28129895	3.95507491
H	7.25108301	-2.99334868	0.57218598
H	-3.86558530	2.73410584	-5.53768936
H	1.80098514	0.68896691	-4.65557480
H	1.50597103	-3.20513090	3.60576134
H	-0.61359156	1.22403636	-3.20037127
H	-1.07813696	-1.74739476	2.47393913
H	-5.02280479	1.75757977	-3.81374356
H	7.65174839	-2.76823811	-1.15522788
H	2.90162267	-4.24630435	3.79065971
H	5.28967055	-4.36648875	2.18511944
H	-2.54278987	1.57523564	-5.27812173
H	-4.07846399	-2.52478840	4.59284250
H	5.18792195	-1.88423720	-3.91791179
H	-9.19367067	-1.71254037	1.00913413
H	-1.41182755	-3.34859440	3.15457205
H	5.80681208	-3.27947178	-2.40165954
H	-5.99636168	-2.41123317	2.80986450
H	-8.90023554	-1.22007991	-0.68645278
H	-3.55206765	-3.99383570	3.79578314
H	0.89657921	-2.23958076	-2.25413108
H	1.77855565	-1.54441031	-4.52240051
H	2.75293944	-5.26096896	1.81121808
H	-0.61503286	-1.46291781	-3.02389114
H	5.10906455	-4.55313115	-1.37915813
H	-6.08514206	-3.71660346	4.01785865
H	3.91357747	-3.62897081	-4.06006428
H	-7.58076615	-3.59156389	0.79602026

H	-5.51957917	-4.05549238	2.36463451
H	5.72534609	-4.95065198	-3.00618768
H	-5.36351236	-1.89632089	-2.13602838
H	0.33781288	-2.57918246	-4.66036951
H	-5.96805503	-3.16230459	0.13902981
H	1.12434982	-3.93649431	-2.69536242
H	2.60971764	-5.45706926	-0.90757581
H	1.94511120	-3.25280229	-4.98210526
H	-7.40761909	-3.12476076	-0.93163078
H	-3.35986887	-5.00148491	1.73568298
H	3.24101971	-4.85969230	-3.00562147
H	-4.84035744	-2.00417335	-3.79538840
H	-2.25972786	-2.23253312	-4.95839017
H	-1.45174548	-3.48859565	-2.88344366
H	-3.39124125	-5.24009207	-0.97835729
H	-5.44524908	-4.44808626	-2.01244766
H	-6.54898238	-3.75766745	-3.22888041
H	-3.55155557	-3.43724437	-5.14245713
H	-2.82758555	-4.56306653	-3.02883781
H	-1.85305820	-3.93733605	-5.26187489
H	-5.03043815	-4.51389273	-3.73701659
N	3.18435707	2.10989387	-0.11908843
N	3.54647599	0.06225748	2.34605972
N	-3.03658116	2.36291079	-0.20884428
N	0.05401315	1.22915135	-0.07770066
N	-2.92031138	0.29286327	2.08125725
N	2.92031138	-0.29286327	-2.08125725
N	-0.05401315	-1.22915135	0.07770066
N	3.03658116	-2.36291079	0.20884428
N	-3.54647599	-0.06225748	-2.34605972
N	-3.18435707	-2.10989387	0.11908843
O	7.20834533	1.58059444	-0.44005014
O	7.80384277	-1.10301233	0.08695396
O	-7.80384277	1.10301233	-0.08695396
O	-7.20834533	-1.58059444	0.44005014
K	0.25097414	3.86669554	-0.30987416
K	5.17946095	-0.19124731	-0.14243241
K	-5.17946095	0.19124731	0.14243241
K	-0.25097414	-3.86669554	0.30987416
U	1.63149704	-0.06570547	0.19008348
U	-1.63149704	0.06570547	-0.19008348

Optimal geometries for II with PBE0/ECP60MDF

C	-6.34602089	-0.44223745	-4.94511626
C	-4.01688943	-4.49706475	-4.26233011
C	-4.20740667	0.65373837	-4.25440797
C	-5.40642155	-0.15543394	-3.77936345
C	-0.26415735	-0.64585298	-5.32004744
C	-3.16554908	-4.10945697	-3.05777016
C	-7.40809587	-3.05290746	-2.21550741
C	-6.54836324	-4.18141265	-0.15652534
C	-6.12886195	0.60659691	-2.67393740
C	-2.08064589	-3.11787452	-3.46103847
C	-0.33902149	1.86266745	-5.27505795
C	-2.55095027	-5.33896446	-2.40275500
C	-4.80955575	4.61619178	-3.40967554
C	-6.88758369	-2.84092133	-0.79780055
C	0.05635217	0.60317679	-4.51164436
C	4.32393598	-0.09704918	-5.62962380
C	3.94480834	2.38740672	-5.70536055
C	2.88781957	-5.35227930	-2.99816098
C	-0.64855202	0.55587201	-3.15525535
C	-7.93159574	-2.10337402	0.03618239
C	-3.91932299	4.55624449	-2.17501554
C	4.54041462	1.23054149	-4.91042050
C	2.81075179	-2.84969816	-3.00788018
C	-2.56016304	3.96183257	-2.52200218
C	-7.52559825	2.89775544	-0.18139939
C	1.08762824	-4.15960547	-1.73430977
C	2.53797598	-4.10830701	-2.18894556
C	-3.76535673	5.94489940	-1.56259238
C	6.02675439	1.47032052	-4.66489173
C	2.27228848	5.21483287	-3.21303111
C	-6.67179712	3.02974989	1.07525077
C	-3.50162310	-3.76741847	1.58484091
C	2.18416675	3.98729781	-2.31402070
C	6.47780052	-4.49645561	-1.44340902
C	7.31770303	-2.28524084	-2.24076902
C	-7.31770303	2.28524084	2.24076902
C	-6.47780052	4.49645561	1.44340902
C	-1.04606491	-4.13197746	1.31611108
C	1.04606491	4.13197746	-1.31611108
C	6.67179712	-3.02974989	-1.07525077
C	-2.18416675	-3.98729781	2.31402070
C	3.50162310	3.76741847	-1.58484091

C	-2.27228848	-5.21483287	3.21303111
C	-6.02675439	-1.47032052	4.66489173
C	3.76535673	-5.94489940	1.56259238
C	7.52559825	-2.89775544	0.18139939
C	-2.53797598	4.10830701	2.18894556
C	-1.08762824	4.15960547	1.73430977
C	-4.54041462	-1.23054149	4.91042050
C	2.56016304	-3.96183257	2.52200218
C	3.91932299	-4.55624449	2.17501554
C	7.93159574	2.10337402	-0.03618239
C	-2.81075179	2.84969816	3.00788018
C	-2.88781957	5.35227930	2.99816098
C	-3.94480834	-2.38740672	5.70536055
C	0.64855202	-0.55587201	3.15525535
C	-4.32393598	0.09704918	5.62962380
C	6.88758369	2.84092133	0.79780055
C	4.80955575	-4.61619178	3.40967554
C	-0.05635217	-0.60317679	4.51164436
C	2.55095027	5.33896446	2.40275500
C	6.54836324	4.18141265	0.15652534
C	7.40809587	3.05290746	2.21550741
C	0.33902149	-1.86266745	5.27505795
C	6.12886195	-0.60659691	2.67393740
C	2.08064589	3.11787452	3.46103847
C	3.16554908	4.10945697	3.05777016
C	0.26415735	0.64585298	5.32004744
C	5.40642155	0.15543394	3.77936345
C	4.20740667	-0.65373837	4.25440797
C	4.01688943	4.49706475	4.26233011
C	6.34602089	0.44223745	4.94511626
H	-5.81616423	-1.00797528	-5.72574139
H	-6.72486365	0.49243073	-5.38512460
H	-7.20355834	-1.04416656	-4.61190490
H	-3.40431831	-4.97366376	-5.04314594
H	-4.49779234	-3.60264440	-4.68445031
H	-4.80276738	-5.20549825	-3.95895190
H	-3.60476562	0.06502118	-4.96111346
H	-4.52488238	1.58052847	-4.75465478
H	-6.65039407	-3.54192570	-2.84346802
H	0.28712711	-0.62399253	-6.27162688
H	-1.33952728	-0.71392996	-5.53964144
H	-5.74432699	-4.67273397	-0.72122318
H	0.16711422	1.88692942	-6.25196572
H	-6.50354246	1.56834060	-3.05275763

H	-8.30385934	-3.69115286	-2.19380624
H	-1.39325354	-3.57668858	-4.18713655
H	-1.42630349	1.88931289	-5.44655504
H	-7.43099168	-4.83889989	-0.14000679
H	-2.52623671	-2.23216037	-3.93728655
H	-1.89154642	-5.87351752	-3.10303564
H	-3.58649140	0.92910340	-3.39228030
H	-6.98069687	0.03074998	-2.28656991
H	0.03729586	-1.54430668	-4.76378020
H	-3.34293856	-6.02806368	-2.07285892
H	-4.94521574	3.60936644	-3.82930846
H	-4.36779251	5.26227660	-4.18305543
H	-7.67614225	-2.09725025	-2.68548448
H	4.81452096	-0.09648817	-6.61508852
H	-6.20597519	-4.03688010	0.87781695
H	-5.79972259	5.01603849	-3.14466946
H	3.24918362	-0.28171698	-5.76310617
H	2.25015038	-5.42803135	-3.89170493
H	-0.04394208	2.75641683	-4.70813356
H	-5.44394434	0.83634030	-1.84406076
H	4.42847541	2.46417438	-6.69051411
H	-1.49844573	-2.79163155	-2.58652173
H	2.86656851	2.23914220	-5.86064105
H	-1.73121732	0.46181559	-3.30680024
H	-1.95985907	-5.04141984	-1.52539349
H	2.21322751	-2.85529390	-3.93136524
H	-8.87877714	-2.66176964	0.06749041
H	4.74151903	-0.92305338	-5.03352729
H	0.41604105	-4.23897698	-2.60063290
H	3.93857227	-5.32456264	-3.32305920
H	-2.67740298	2.96463711	-2.96745673
H	2.74146736	-6.25486651	-2.38666423
H	-7.02549660	3.39077995	-1.02604736
H	-2.02258612	4.59902947	-3.24012458
H	-7.66710057	1.83691307	-0.43856615
H	4.08564468	3.33817406	-5.17168390
H	-0.28032779	-0.31591013	-2.58535413
H	-8.51697262	3.35244040	-0.03267670
H	3.87310117	-2.79278721	-3.29121925
H	-8.13358375	-1.10713017	-0.38701914
H	6.57649187	1.55818239	-5.61364111
H	-0.44320189	1.47980937	-2.58608339
H	-7.58752543	-1.98538369	1.07703072
H	-3.28440111	6.63219688	-2.27534972

H	1.33728954	5.33449075	-3.78014873
H	-4.75285636	6.35441745	-1.30078018
H	2.54221339	-1.93870380	-2.45359279
H	0.92743187	-5.04172222	-1.09608004
H	3.09866912	5.11200599	-3.93226264
H	-3.75302142	-4.64646419	0.97614270
H	0.80954571	-3.25419734	-1.17187473
H	-1.93655856	3.86282387	-1.62144610
H	5.85812396	-4.59403640	-2.34523433
H	6.66003435	-2.30734218	-3.12341866
H	6.46702214	0.63066160	-4.10264244
H	-3.43083824	-2.91480141	0.89450056
H	6.17658151	2.39862897	-4.09188483
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H	-5.98052653	5.04324505	0.63006698
H	8.28012680	-2.74138810	-2.51569289
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H	-7.45246448	4.96976383	1.63394920
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H	-0.10439255	-4.32411303	1.84663923
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H	-3.09866912	-5.11200599	3.93226264
H	3.75302142	4.64646419	-0.97614270
H	4.75285636	-6.35441745	1.30078018
H	1.93655856	-3.86282387	1.62144610
H	-0.80954571	3.25419734	1.17187473
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H	8.51697262	-3.35244040	0.03267670
H	7.58752543	1.98538369	-1.07703072
H	8.13358375	1.10713017	0.38701914
H	7.66710057	-1.83691307	0.43856615
H	-2.54221339	1.93870380	2.45359279
H	-4.08564468	-3.33817406	5.17168390
H	7.02549660	-3.39077995	1.02604736
H	-3.87310117	2.79278721	3.29121925
H	-2.74146736	6.25486651	2.38666423
H	0.44320189	-1.47980937	2.58608339
H	8.87877714	2.66176964	-0.06749041
H	2.02258612	-4.59902947	3.24012458
H	-3.93857227	5.32456264	3.32305920
H	0.28032779	0.31591013	2.58535413
H	-4.74151903	0.92305338	5.03352729
H	2.67740298	-2.96463711	2.96745673
H	-0.41604105	4.23897698	2.60063290
H	-4.42847541	-2.46417438	6.69051411
H	1.95985907	5.04141984	1.52539349
H	-2.86656851	-2.23914220	5.86064105
H	-2.21322751	2.85529390	3.93136524
H	5.79972259	-5.01603849	3.14466946
H	1.73121732	-0.46181559	3.30680024
H	-2.25015038	5.42803135	3.89170493
H	-4.81452096	0.09648817	6.61508852
H	-3.24918362	0.28171698	5.76310617
H	6.20597519	4.03688010	-0.87781695
H	1.49844573	2.79163155	2.58652173
H	5.44394434	-0.83634030	1.84406076
H	7.67614225	2.09725025	2.68548448
H	0.04394208	-2.75641683	4.70813356
H	4.36779251	-5.26227660	4.18305543
H	4.94521574	-3.60936644	3.82930846
H	3.34293856	6.02806368	2.07285892
H	6.98069687	-0.03074998	2.28656991
H	8.30385934	3.69115286	2.19380624
H	7.43099168	4.83889989	0.14000679
H	-0.03729586	1.54430668	4.76378020
H	1.89154642	5.87351752	3.10303564
H	6.50354246	-1.56834060	3.05275763
H	3.58649140	-0.92910340	3.39228030

H	1.42630349	-1.88931289	5.44655504
H	2.52623671	2.23216037	3.93728655
H	-0.16711422	-1.88692942	6.25196572
H	5.74432699	4.67273397	0.72122318
H	1.39325354	3.57668858	4.18713655
H	6.65039407	3.54192570	2.84346802
H	-0.28712711	0.62399253	6.27162688
H	1.33952728	0.71392996	5.53964144
H	4.52488238	-1.58052847	4.75465478
H	4.80276738	5.20549825	3.95895190
H	3.60476562	-0.06502118	4.96111346
H	4.49779234	3.60264440	4.68445031
H	7.20355834	1.04416656	4.61190490
H	3.40431831	4.97366376	5.04314594
H	6.72486365	-0.49243073	5.38512460
H	5.81616423	1.00797528	5.72574139
N	-0.04891013	-1.18382159	-0.35905239
N	0.04891013	1.18382159	0.35905239
O	-4.94460430	-1.42874902	-3.33090378
O	-4.03342029	-3.54027239	-2.07237041
O	-5.72109897	-2.00474442	-0.78070901
O	1.47348596	0.58616029	-4.33856527
O	-3.31469961	-1.04744851	-1.17081158
O	-4.60380568	3.70326751	-1.25323020
O	1.88026038	2.89148601	-3.18599381
O	3.94773314	1.14491661	-3.61009163
O	-3.09459828	1.69994214	-0.13029029
O	3.36923753	-4.16435529	-1.02243642
O	-5.41653116	2.37587774	0.84549611
O	2.28884649	0.62024265	-1.71987411
O	5.41653116	-2.37587774	-0.84549611
O	-2.28884649	-0.62024265	1.71987411
O	-3.36923753	4.16435529	1.02243642
O	3.09459828	-1.69994214	0.13029029
O	-3.94773314	-1.14491661	3.61009163
O	-1.88026038	-2.89148601	3.18599381
O	4.60380568	-3.70326751	1.25323020
O	3.31469961	1.04744851	1.17081158
O	5.72109897	2.00474442	0.78070901
O	-1.47348596	-0.58616029	4.33856527
O	4.03342029	3.54027239	2.07237041
O	4.94460430	1.42874902	3.33090378
Si	-4.43814244	-1.96484212	-1.85517533
Si	2.35091452	1.32097447	-3.15987434

Si	-4.03874780	2.97851600	0.11282556
Si	4.03874780	-2.97851600	-0.11282556
Si	-2.35091452	-1.32097447	3.15987434
Si	4.43814244	1.96484212	1.85517533
K	-5.01430502	-0.27293858	1.21062445
K	5.01430502	0.27293858	-1.21062445
U	-1.60694058	0.07417576	-0.23643750
U	1.60694058	-0.07417576	0.23643750

Optimal geometries for III with PBE0/ECP60MDF

C	2.27907454	-3.49367048	-5.63079101
C	6.66233183	-0.99589291	-2.68494810
C	2.00323688	-3.55813168	-4.13064479
C	-1.01614276	-5.11930486	-4.85217064
C	3.13989192	-2.90872198	-3.35500493
C	7.68935972	2.65785069	-2.69958609
C	-0.94777529	-3.59576329	-4.92806894
C	6.99071187	-0.30484360	-1.36456613
C	7.03676797	-1.30914358	-0.22010131
C	1.54038386	0.54637111	-4.68377514
C	-2.33268355	-2.96438333	-4.95327506
C	6.20971092	2.53618384	-2.34595416
C	0.30529350	-0.34673984	-4.72408713
C	0.42518888	-4.85507071	-1.47553816
C	3.51295370	0.59044508	-2.40153323
C	2.77210716	1.80995563	-2.97946408
C	5.61245819	3.89717573	-1.99709088
C	3.49931183	-3.32020312	0.15568745
C	-0.11718580	-3.46981295	-1.80665208
C	0.73804311	2.71898806	-3.89505268
C	7.61591966	2.25002097	0.93549219
C	-2.71430380	2.57753497	-5.73699164
C	2.74585019	-5.26840635	1.53706313
C	3.51301493	-3.94959550	1.54120197
C	6.17833288	1.75676700	0.79263134
C	-1.60737425	-3.38459635	-1.49441291
C	-3.40894423	-0.07902012	-3.48267899
C	-2.89927776	3.54943051	-4.57407090
C	5.36535189	-1.44952995	3.14077224
C	-0.10617565	3.19124174	-2.71963404
C	5.19045339	2.76159678	1.37162598
C	4.14303368	-4.41192550	4.78142126
C	-4.14303368	4.41192550	-4.78142126

C	3.93331358	-1.12729607	2.71879896
C	-3.93331358	1.12729607	-2.71879896
C	-5.19045339	-2.76159678	-1.37162598
C	-5.36535189	1.44952995	-3.14077224
C	2.89927776	-3.54943051	4.57407090
C	0.10617565	-3.19124174	2.71963404
C	3.40894423	0.07902012	3.48267899
C	-6.17833288	-1.75676700	-0.79263134
C	-7.61591966	-2.25002097	-0.93549219
C	1.60737425	3.38459635	1.49441291
C	-3.51301493	3.94959550	-1.54120197
C	2.71430380	-2.57753497	5.73699164
C	-2.74585019	5.26840635	-1.53706313
C	-0.73804311	-2.71898806	3.89505268
C	-5.61245819	-3.89717573	1.99709088
C	-3.49931183	3.32020312	-0.15568745
C	0.11718580	3.46981295	1.80665208
C	-2.77210716	-1.80995563	2.97946408
C	-0.42518888	4.85507071	1.47553816
C	-3.51295370	-0.59044508	2.40153323
C	-6.20971092	-2.53618384	2.34595416
C	2.33268355	2.96438333	4.95327506
C	-0.30529350	0.34673984	4.72408713
C	-7.03676797	1.30914358	0.22010131
C	-1.54038386	-0.54637111	4.68377514
C	-7.68935972	-2.65785069	2.69958609
C	-6.99071187	0.30484360	1.36456613
C	0.94777529	3.59576329	4.92806894
C	1.01614276	5.11930486	4.85217064
C	-3.13989192	2.90872198	3.35500493
C	-2.00323688	3.55813168	4.13064479
C	-6.66233183	0.99589291	2.68494810
C	-2.27907454	3.49367048	5.63079101
H	3.27309788	-3.91170060	-5.86721735
H	1.54094998	-4.05673635	-6.22080104
H	7.39857021	-1.78340968	-2.92289129
H	2.27489380	-2.45464113	-6.00096817
H	6.64693600	-0.29393407	-3.53452159
H	4.08670927	-3.46401034	-3.46772807
H	-0.01898869	-5.58683305	-4.87223986
H	5.67462805	-1.48361287	-2.64245072
H	-1.59162053	-5.53628720	-5.69667606
H	1.96121815	-4.62605559	-3.84586482
H	8.10817113	1.70790490	-3.06384196

H	-0.46709944	-3.33900302	-5.89059243
H	7.84720001	3.41030250	-3.49213017
H	7.68328212	-2.17029987	-0.46388744
H	3.32076911	-1.88553980	-3.71332238
H	7.99677635	0.14420276	-1.45694989
H	0.37386034	-0.97215672	-5.63566589
H	1.68310553	1.09477076	-5.63617036
H	2.41773300	-0.09822312	-4.54528739
H	-1.51645379	-5.45589454	-3.92933175
H	-2.93376977	-3.36123416	-5.78998805
H	8.29473273	2.97116968	-1.83427367
H	5.69058073	2.16929066	-3.25287671
H	2.92385939	-2.84218269	-2.27984839
H	4.23251069	0.22631871	-3.15848062
H	6.03595816	-1.71374501	0.00123207
H	-0.00928252	-5.62746968	-2.12913741
H	1.51768646	-4.91058897	-1.58256365
H	3.39834047	2.34517767	-3.72173761
H	3.81505877	-4.02961149	-0.62609487
H	-2.27212077	-1.87471611	-5.07348186
H	7.41873303	-0.86587560	0.71146181
H	-0.58244170	0.29691231	-4.89120339
H	2.73515248	-0.21446490	-2.38299466
H	8.34533038	1.52845992	0.53577696
H	5.67850057	4.59936128	-2.84637686
H	3.18439304	-5.98953143	0.82561243
H	-2.89988404	-3.16079742	-4.03028337
H	-2.56554663	3.11527130	-6.68908793
H	0.05359310	2.50498100	-4.72640414
H	-1.85139632	1.90891138	-5.59393963
H	0.18509682	-5.13604128	-0.43591409
H	4.19331699	-2.46433118	0.08845332
H	1.44943730	3.49624954	-4.23938698
H	2.47561838	-2.98631828	-0.09629709
H	4.56216124	-4.15534567	1.82084688
H	7.76980630	3.20048664	0.39951960
H	6.14872853	4.36371600	-1.15465883
H	-3.60150453	1.93737148	-5.86756327
H	-2.18255608	-4.16373258	-2.01745045
H	0.39772490	-2.73831755	-1.14869244
H	4.55134323	3.82452334	-1.70986490
H	2.60137515	2.53192226	-2.16388313
H	-3.37052503	0.11405167	-4.56434634
H	6.08135326	0.83178577	1.38977217

H	1.70038423	-5.11351231	1.23044693
H	2.73216750	-5.74929099	2.52728300
H	5.78798851	-2.30221310	2.58868034
H	7.87499917	2.43067009	1.99300632
H	-2.38938829	-0.38787928	-3.19431163
H	-2.02481916	-2.41719320	-1.81938405
H	4.26512478	-5.17238102	3.99640820
H	-4.05994247	-0.95592671	-3.33662951
H	-2.02760229	4.23229076	-4.57209938
H	-1.79547102	-3.53317613	-0.41162183
H	6.03187699	-0.58690396	2.97406483
H	-4.09583672	4.94286170	-5.74798487
H	3.96505616	-0.84733566	1.64646762
H	5.13066989	3.68915660	0.78244385
H	-0.46108157	4.21551758	-2.93830518
H	5.06248374	-3.80660707	4.79330835
H	0.56219484	3.32889574	-1.83863177
H	-5.46493294	-3.04628183	-2.40271720
H	5.41675701	-1.68969026	4.21416721
H	4.17601165	2.34332854	1.44114067
H	-5.06248374	3.80660707	-4.79330835
H	-5.41675701	1.68969026	-4.21416721
H	4.09583672	-4.94286170	5.74798487
H	5.46493294	3.04628183	2.40271720
H	-4.17601165	-2.34332854	-1.44114067
H	-5.13066989	-3.68915660	-0.78244385
H	0.46108157	-4.21551758	2.93830518
H	-0.56219484	-3.32889574	1.83863177
H	-6.03187699	0.58690396	-2.97406483
H	-4.26512478	5.17238102	-3.99640820
H	2.02760229	-4.23229076	4.57209938
H	-3.96505616	0.84733566	-1.64646762
H	-7.87499917	-2.43067009	-1.99300632
H	4.05994247	0.95592671	3.33662951
H	1.79547102	3.53317613	0.41162183
H	-5.78798851	2.30221310	-2.58868034
H	-2.73216750	5.74929099	-2.52728300
H	2.38938829	0.38787928	3.19431163
H	2.02481916	2.41719320	1.81938405
H	-6.08135326	-0.83178577	-1.38977217
H	-7.76980630	-3.20048664	-0.39951960
H	-1.70038423	5.11351231	-1.23044693
H	3.37052503	-0.11405167	4.56434634
H	-6.14872853	-4.36371600	1.15465883

H	3.60150453	-1.93737148	5.86756327
H	-4.55134323	-3.82452334	1.70986490
H	-4.56216124	4.15534567	-1.82084688
H	2.18255608	4.16373258	2.01745045
H	-2.60137515	-2.53192226	2.16388313
H	2.56554663	-3.11527130	6.68908793
H	-0.39772490	2.73831755	1.14869244
H	1.85139632	-1.90891138	5.59393963
H	-8.34533038	-1.52845992	-0.53577696
H	-1.44943730	-3.49624954	4.23938698
H	-2.47561838	2.98631828	0.09629709
H	-0.18509682	5.13604128	0.43591409
H	-5.67850057	-4.59936128	2.84637686
H	-4.19331699	2.46433118	-0.08845332
H	-0.05359310	-2.50498100	4.72640414
H	-3.18439304	5.98953143	-0.82561243
H	2.89988404	3.16079742	4.03028337
H	-7.41873303	0.86587560	-0.71146181
H	0.58244170	-0.29691231	4.89120339
H	-2.73515248	0.21446490	2.38299466
H	2.27212077	1.87471611	5.07348186
H	-3.81505877	4.02961149	0.62609487
H	-8.29473273	-2.97116968	1.83427367
H	-3.39834047	-2.34517767	3.72173761
H	0.00928252	5.62746968	2.12913741
H	-1.51768646	4.91058897	1.58256365
H	-6.03595816	1.71374501	-0.00123207
H	-5.69058073	-2.16929066	3.25287671
H	2.93376977	3.36123416	5.78998805
H	1.51645379	5.45589454	3.92933175
H	-4.23251069	-0.22631871	3.15848062
H	-2.92385939	2.84218269	2.27984839
H	-7.84720001	-3.41030250	3.49213017
H	-7.99677635	-0.14420276	1.45694989
H	-1.68310553	-1.09477076	5.63617036
H	-2.41773300	0.09822312	4.54528739
H	-0.37386034	0.97215672	5.63566589
H	-7.68328212	2.17029987	0.46388744
H	-8.10817113	-1.70790490	3.06384196
H	-3.32076911	1.88553980	3.71332238
H	1.59162053	5.53628720	5.69667606
H	0.46709944	3.33900302	5.89059243
H	-5.67462805	1.48361287	2.64245072
H	0.01898869	5.58683305	4.87223986

H	-1.96121815	4.62605559	3.84586482
H	-6.64693600	0.29393407	3.53452159
H	-4.08670927	3.46401034	3.46772807
H	-7.39857021	1.78340968	2.92289129
H	-2.27489380	2.45464113	6.00096817
H	-1.54094998	4.05673635	6.22080104
H	-3.27309788	3.91170060	5.86721735
Li	2.97222100	-0.67557154	-0.47574241
Li	2.70585748	1.58302384	-0.00243449
Li	-2.70585748	-1.58302384	0.00243449
Li	-2.97222100	0.67557154	0.47574241
N	0.16771362	-1.11965378	-3.49615344
N	1.46426257	1.48513462	-3.55369256
N	4.09934281	0.78437751	-1.08661021
N	-1.17293760	2.24733059	-2.42648891
N	1.31763925	0.26117949	-0.04339479
N	1.17293760	-2.24733059	2.42648891
N	-1.31763925	-0.26117949	0.04339479
N	-4.09934281	-0.78437751	1.08661021
N	-1.46426257	-1.48513462	3.55369256
N	-0.16771362	1.11965378	3.49615344
Si	0.26735642	-2.85105170	-3.60760626
Si	5.78614438	1.18070716	-1.01256670
Si	2.80230005	-2.69179721	2.83290091
Si	-2.80230005	2.69179721	-2.83290091
Si	-5.78614438	-1.18070716	1.01256670
Si	-0.26735642	2.85105170	3.60760626
U	-0.14801286	0.31085015	-1.65522429
U	0.14801286	-0.31085015	1.65522429