

Mechanistic and Electronic Structure Insights into Formate Formation in Uranium and Related Actinide Complexes

Ali A Khairbek¹, Maha I. Al-Zaben², Abdullah Yahya Abdullah Alzahrani³, Ralph Puchta⁴ and Renjith Thomas^{5,6}

¹ Centre of Molecular Medicine and Diagnostics (COMManD), Saveetha Dental College and Hospitals, Saveetha Institute of Medical and Technical Sciences, Saveetha University, Chennai 600 077, India

² Department of Chemistry, College of Science, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia

³ Faculty of Science and Arts, Department of Chemistry, King Khalid University, Mohail Asser, Saudi Arabia

⁴ Inorganic Chemistry, Department of Chemistry and Pharmacy, University of Erlangen-Nuremberg, Erlangen, Germany

⁵ Department of Chemistry, St Berchmans College (Autonomous), Mahatma Gandhi University, Changanassery, Kerala, India-686101.

⁶ Centre for Theoretical and Computational Chemistry, St Berchmans College (Autonomous), Changanassery, Kerala, India-686101.

Corresponding Author: **Ali A Khairbek (MRSC, MACS)** alikhairbek@gmail.com

Corresponding Author: **Renjith Thomas (FRSC, MACS)** renjith@sbccollege.ac.in

Table S1. Comparison of spin multiplicities and corresponding electronic energies (in atomic units) for selected actinide complexes. The lowest-energy state for each metal is identified as the ground state, which is used in all reported calculations.

Metal	Charge	Multiplicity	Energy (a.u.)	$\langle S^2 \rangle$	Ground State
Th	+1	1	-864.244831	—	Yes
Th	+1	3	-864.110642	2.008	No
Np	+1	2	-970.256176	1.688	No
Np	+1	4	-970.304564	3.755	Yes
Pu	+1	3	-1009.310269	2.014	Yes
Pu	+1	1	—	—	Failed
U	+1	3	-933.448572	2.010	Yes
U	+1	1	—	—	Failed

All calculations were performed at the same level of theory, and the reported $\langle S^2 \rangle$ values indicate minimal spin contamination for the selected ground states.

Table S2. G_{corr} in the gas phase (in Hartree) of Uranium and Related Actinide Complexes.

G_o	Formic	I	II	TSI
U F	0.010291	-0.011124	0.018243	0.014485
U Cl	0.010291	-0.015009	0.014296	0.011664
U Br	0.010291	-0.01902	0.012995	0.008817
Th F	0.010291	-0.010453	0.016287	0.013632
Np F	0.010291	-0.010414	0.017548	0.013757
Pu F	0.010291	-0.008994	0.017317	0.014982
G_o	III	CH ₂	IV	V

U F	0.017072	0.008022	-0.006866	0.02382
U Cl	0.012268	0.008022	-0.012774	0.018417
U Br	0.010043	0.008022	-0.017124	0.015297
Th F	0.014699	0.008022	-0.007715	0.0228
Np F	0.015265	0.008022	-0.009062	0.022272
Pu F	0.014745	0.008022	-0.007495	0.023938
G_o	TSII	VI	H-X	VII
U F	0.019491	0.021484	-0.006892	0.011662
U Cl	0.012295	0.015582	-0.011009	0.01395
U Br	0.008813	0.011382	-0.012855	0.009006
Th F	0.019386	0.019124	-0.006892	0.011784
Np F	0.020769	0.020067	-0.006892	0.014867
Pu F	0.020272	0.02232	-0.006892	0.011353
G_o	VIII	TSIII	IX	X
U F	0.043564	0.037388	0.040013	0.030286
U Cl	0.040305	0.034498	0.036365	0.030286
U Br	0.038537	0.032622	0.034253	0.030286
Th F	0.042636	0.037954	0.03857	0.03114
Np F	0.043341	0.039521	0.037706	0.030739
Pu F	0.043928	0.040305	0.040378	0.031617

Table S3. (E_o) in the gas phase (in Hartree) of Uranium and Related Actinide Complexes.

E_o	Formic	I	II	TSI
U F	-189.597667400	-743.764088177	-933.448571621	-933.440760627
U Cl	-189.597667400	-1463.732365090	-1653.423772330	-1653.414138650
U Br	-189.597667400	-5650.826681130	-5840.521036110	-5840.509846470
Th F	-189.597667400	-674.557764122	-864.244831506	-864.236537980
Np F	-189.597667400	-780.618739943	-970.304564218	-970.291686182
Pu F	-189.597667400	-819.626453201	-1009.310269250	-1009.299232700
E_o	III	CH₂	IV	V
U F	-933.489100568	-77.253598598	-856.184946129	-1045.870338000
U Cl	-1653.449966570	-77.253598598	-1576.132447890	-1765.822757240
U Br	-5840.545039220	-77.253598598	-5763.222895240	-5952.919201430
Th F	-864.275304960	-77.253598598	-786.972681711	-976.659073784
Np F	-970.333185272	-77.253598598	-893.024795238	-1082.714058970
Pu F	-1009.343193540	-77.253598598	-932.033699333	-1121.722284970
E_o	TSII	VI	H-X	VII
U F	-1045.823047440	-1045.843466610	-100.364712310	-945.428725987
U Cl	-1765.797524850	-1765.814906510	-460.374172589	-1305.406448710
U Br	-5952.892289060	-5952.911987640	-2553.921558420	-3398.953411000
Th F	-976.622048893	-976.639624358	-100.364712310	-876.226419047
Np F	-1082.677320640	-1082.695528220	-100.364712310	-982.278518732
Pu F	-1121.690825780	-1121.705510840	-100.364712310	-1021.292146960
E_o	VIII	TSIII	IX	X
U F	-1135.110806650	-1135.065336290	-1135.082343920	-1034.674537840
U Cl	-1495.089943680	-1495.059502680	-1495.078074650	-1034.674537840
U Br	-3588.637309400	-3588.606289540	-3588.628333500	-1034.674537840
Th F	-1065.902553380	-1065.871939200	-1065.889311020	-965.480183891
Np F	-1171.967598710	-1171.934097590	-1171.948910670	-1071.516401280
Pu F	-1210.974700920	-1210.944276390	-1210.959079930	-1110.551972880

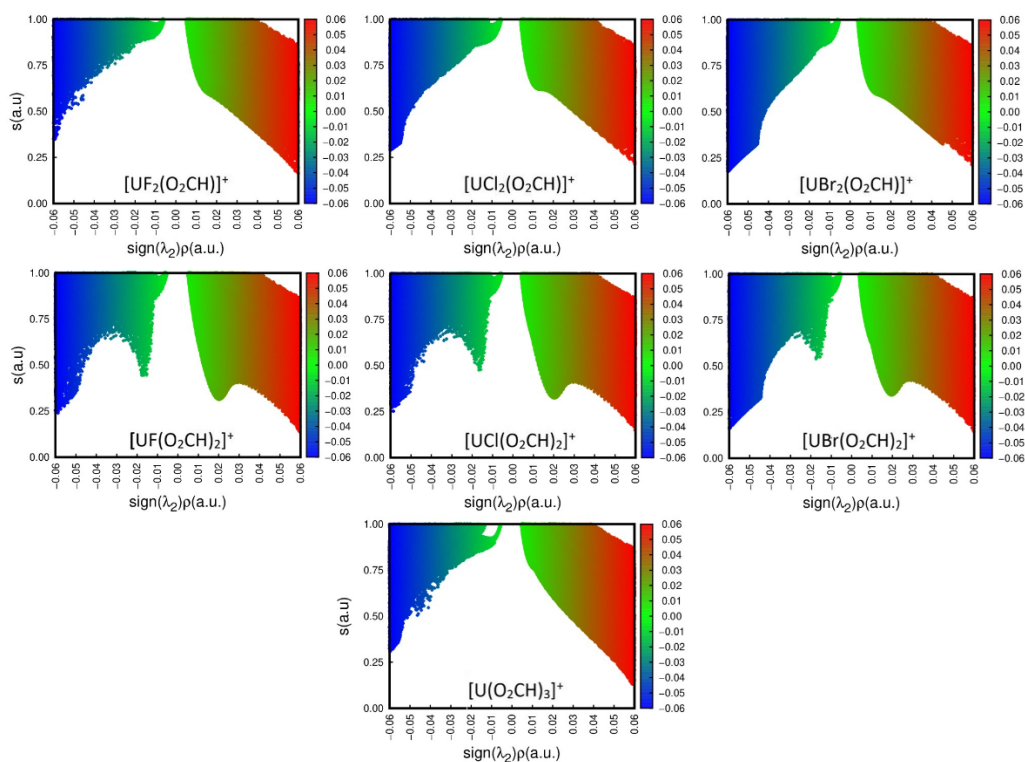


Fig. S1 RDG plots of uranium–halogen systems (F, Cl, Br) Formate Complexes.

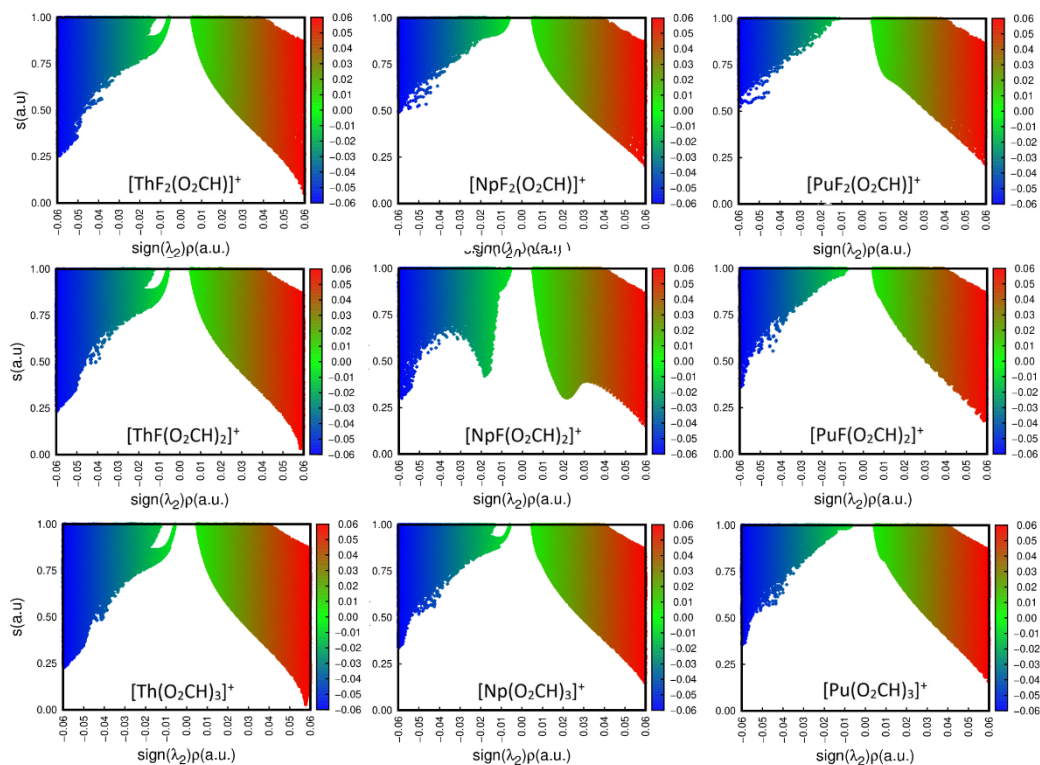
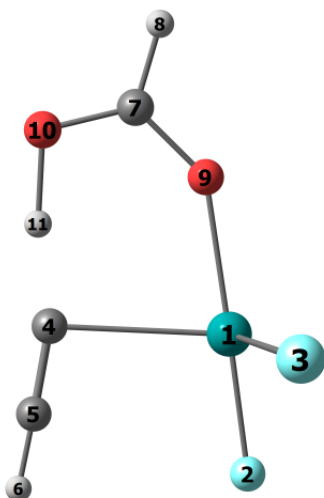
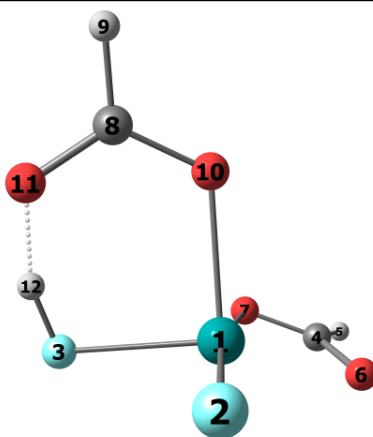


Fig. S2 RDG plots of actinide-substituted systems (Th, Np, and Pu) Formate Complexes.



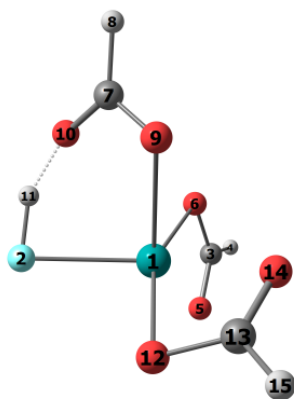
Atom 1(U):	1.40751938	Atom 7(C):	0.48271703
Atom 2(F):	-0.12470745	Atom 8(H):	0.03791703
Atom 3(F):	-0.37239903	Atom 9(O):	-0.23551503
Atom 4(C):	-0.74602541	Atom 10(O):	0.00717219
Atom 5(C):	0.05970390	Atom 11(H):	0.17069472
Atom 6(H):	0.31292266		

Fig .S1. Atomic dipole-corrected Hirshfeld (ADCH) charge distributions for the transition states (TSI) in the U-F system.



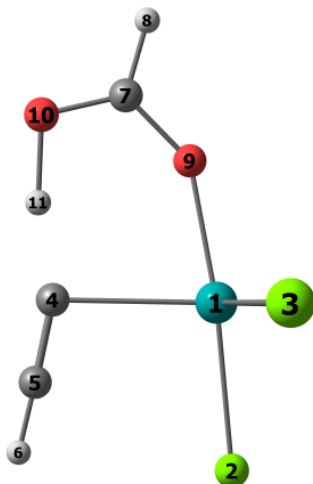
Atom 1(U):	1.17348114	Atom 7(O):	-0.28598542
Atom 2(F):	-0.10371503	Atom 8(C):	0.32024194
Atom 3(F):	-0.26795028	Atom 9(H):	0.18972290
Atom 4(C):	0.30897093	Atom 10(O):	-0.40555452
Atom 5(H):	0.24448632	Atom 11(O):	-0.33329232
Atom 6(O):	-0.25029533	Atom 12(H):	0.40988967

Fig .S2. Atomic dipole-corrected Hirshfeld (ADCH) charge distributions for the transition states (TSII) in the U-F system.



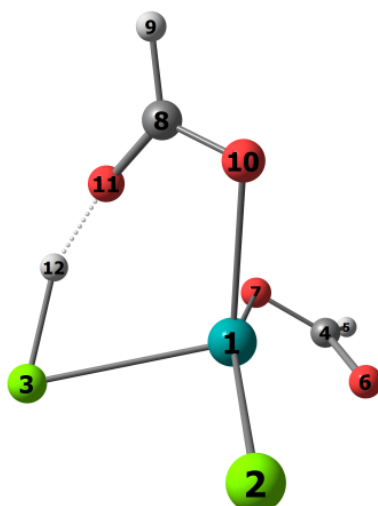
Atom 1(U):	0.98828788	Atom 9(O):	-0.34596689
Atom 2(F):	-0.21263080	Atom 10(O):	-0.32078860
Atom 3(C):	0.31037460	Atom 11(H):	0.33640952
Atom 4(H):	0.22416628	Atom 12(O):	-0.20724525
Atom 5(O):	-0.23683555	Atom 13(C):	0.28130892
Atom 6(O):	-0.29159498	Atom 14(O):	-0.25758228
Atom 7(C):	0.33451553	Atom 15(H):	0.21383424
Atom 8(H):	0.18374738		

Fig .S3. Atomic dipole-corrected Hirshfeld (ADCH) charge distributions for the transition states (TSIII) in the U–F system.



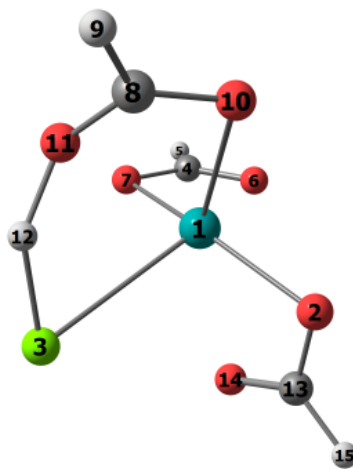
Atom 1(U):	1.13382298	Atom 7(C):	0.28580754
Atom 2(Cl):	-0.05302328	Atom 8(H):	0.15377827
Atom 3(Cl):	-0.27960723	Atom 9(O):	-0.11045185
Atom 4(C):	-0.42859383	Atom 10(O):	0.01188350
Atom 5(C):	-0.69474815	Atom 11(H):	0.23905872
Atom 6(H):	0.74207333		

Fig .S4. Atomic dipole-corrected Hirshfeld (ADCH) charge distributions for the transition states (TSI) in the U–Cl system.



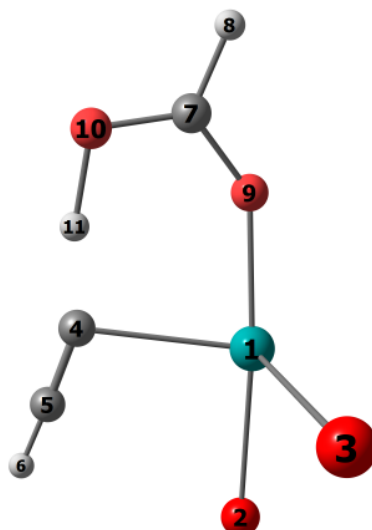
Atom 1(U):	0.72053956	Atom 7(O):	-0.19870574
Atom 2(Cl):	-0.01614838	Atom 8(C):	0.43172345
Atom 3(Cl):	-0.06446700	Atom 9(H):	0.15439812
Atom 4(C):	0.29052299	Atom 10(O):	-0.30051591
Atom 5(H):	0.20502590	Atom 11(O):	-0.32954548
Atom 6(O):	-0.14546385	Atom 12(H):	0.25263632

Fig .S5. Atomic dipole-corrected Hirshfeld (ADCH) charge distributions for the transition states (TSII) in the U–Cl system.



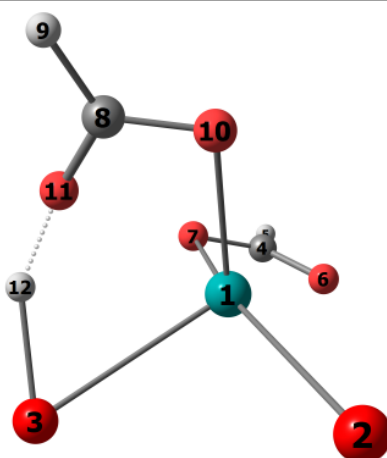
Atom 1(U):	1.03399815	Atom 9(H):	0.21578555
Atom 2(O):	-0.50937258	Atom 10(O):	-0.21315293
Atom 3(Cl):	-0.05607538	Atom 11(O):	-0.15449959
Atom 4(C):	0.31987095	Atom 12(H):	0.06334375
Atom 5(H):	0.23484121	Atom 13(C):	0.42388433
Atom 6(O):	-0.20125952	Atom 14(O):	-0.53272293
Atom 7(O):	-0.28484167	Atom 15(H):	0.40332748
Atom 8(C):	0.25687318		

Fig .S6. Atomic dipole-corrected Hirshfeld (ADCH) charge distributions for the transition states (TSIII) in the U–Cl system.



Atom 1(U):	0.96947232	Atom 7(C):	0.22507100
Atom 2(Br):	0.00959517	Atom 8(H):	0.21481140
Atom 3(Br):	-0.24580440	Atom 9(O):	-0.08994967
Atom 4(C):	0.26934517	Atom 10(O):	-0.04914772
Atom 5(C):	-1.38922040	Atom 11(H):	0.11182021
Atom 6(H):	0.97400691		

Fig .S7. Atomic dipole-corrected Hirshfeld (ADCH) charge distributions for the transition states (TSI) in the U–Br system.



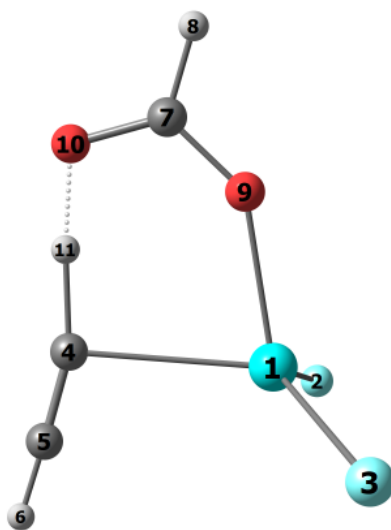
Atom 1(U):	0.58135242	Atom 7(O):	-0.16138390
Atom 2(Br):	0.01527640	Atom 8(C):	0.20880507
Atom 3(Br):	-0.00065690	Atom 9(H):	0.23221792
Atom 4(C):	0.26434618	Atom 10(O):	-0.18561140
Atom 5(H):	0.21212075	Atom 11(O):	-0.22740758
Atom 6(O):	-0.12571803	Atom 12(H):	0.18665907

Fig .S8. Atomic dipole-corrected Hirshfeld (ADCH) charge distributions for the transition states (TSII) in the U–Br system.



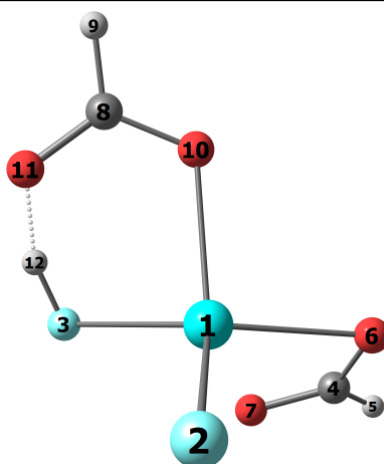
Atom 1(U):	0.94811602	Atom 8(C):	0.25643084
Atom 2(O):	-0.47134335	Atom 9(H):	0.21224821
Atom 3(Br):	0.03765687	Atom 10(O):	-0.20657048
Atom 4(C):	0.30983178	Atom 11(O):	-0.12730303
Atom 5(H):	0.23740617	Atom 12(H):	-0.00189856
Atom 6(O):	-0.18067489	Atom 13(C):	0.42118518
Atom 7(O):	-0.28657621	Atom 14(O):	-0.52030493
		Atom 15(H):	0.37179636

Fig .S9. Atomic dipole-corrected Hirshfeld (ADCH) charge distributions for the transition states (TSIII) in the U–Br system.



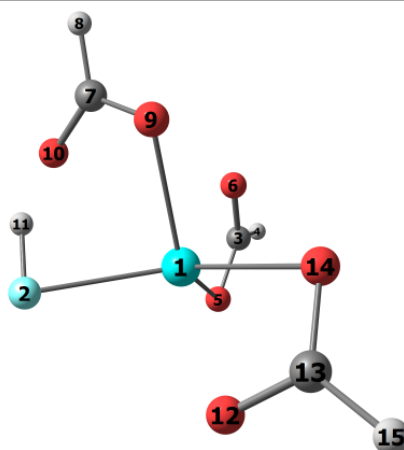
Atom 1(Th):	1.22132263	Atom 7(C):	0.26022228
Atom 2(F):	-0.16496037	Atom 8(H):	0.19590671
Atom 3(F):	-0.16490652	Atom 9(O):	-0.29343574
Atom 4(C):	-0.28418791	Atom 10(O):	-0.18000661
Atom 5(C):	-0.11608184	Atom 11(H):	0.20724296
Atom 6(H):	0.31888440		

Fig .S10. Atomic dipole-corrected Hirshfeld (ADCH) charge distributions for the transition states (TSI) in the Th–F system.



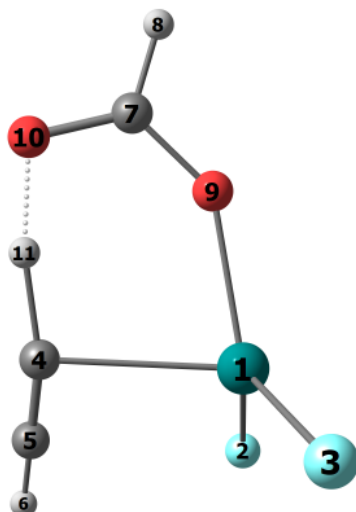
Atom 1(Th):	1.24660408	Atom 7(O):	-0.28799317
Atom 2(F):	-0.15466226	Atom 8(C):	0.35765283
Atom 3(F):	-0.35281485	Atom 9(H):	0.18009437
Atom 4(C):	0.27268556	Atom 10(O):	-0.32699210
Atom 5(H):	0.22625751	Atom 11(O):	-0.42797522
Atom 6(O):	-0.27137951	Atom 12(H):	0.53852276

Fig .S11. Atomic dipole-corrected Hirshfeld (ADCH) charge distributions for the transition states (TSII) in the Th–F system.



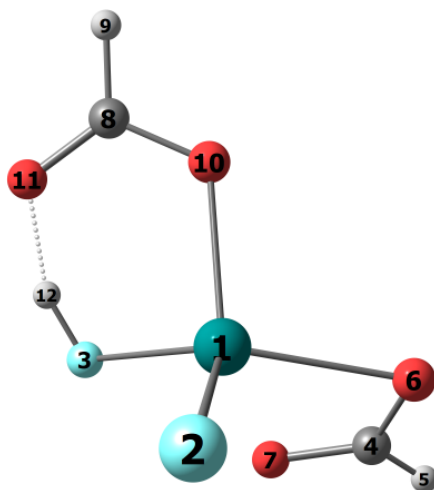
Atom 1(Th):	1.12270336	Atom 8(H):	0.19329390
Atom 2(F):	-0.19698180	Atom 9(O):	-0.32923409
Atom 3(C):	0.30690421	Atom 10(O):	-0.34051246
Atom 4(H):	0.22158416	Atom 11(H):	0.33490186
Atom 5(O):	-0.27249700	Atom 12(O):	-0.24295876
Atom 6(O):	-0.32703411	Atom 13(C):	0.27509778
Atom 7(C):	0.33207428	Atom 14(O):	-0.29051536
		Atom 15(H):	0.21317403

Fig .S12. Atomic dipole-corrected Hirshfeld (ADCH) charge distributions for the transition states (TSIII) in the Th–F system.



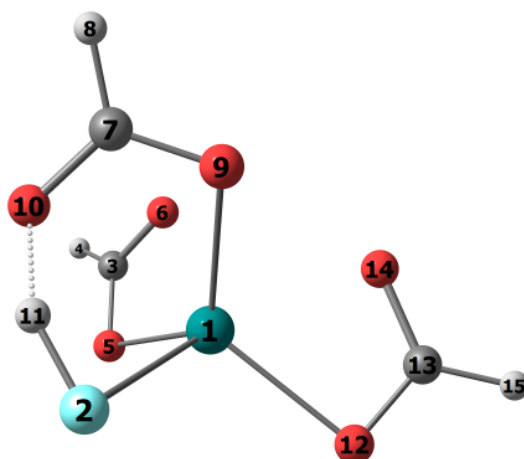
Atom 1(Np):	1.22356304	Atom 7(C):	0.26296042
Atom 2(F):	-0.17272610	Atom 8(H):	0.19839496
Atom 3(F):	-0.19214686	Atom 9(O):	-0.25085368
Atom 4(C):	-0.22096277	Atom 10(O):	-0.16618412
Atom 5(C):	-0.25001221	Atom 11(H):	0.18124706
Atom 6(H):	0.38672025		

Fig .S13. Atomic dipole-corrected Hirshfeld (ADCH) charge distributions for the transition states (TSI) in the Np–F system.



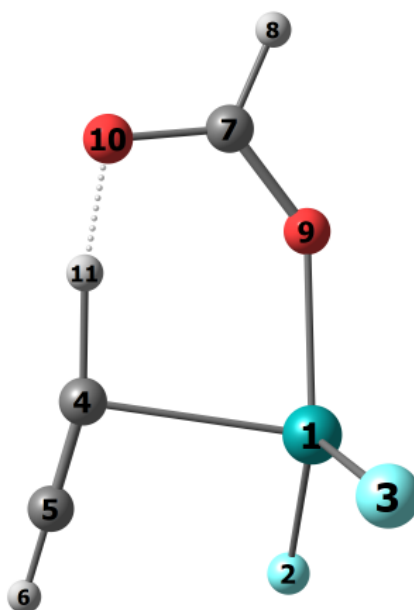
Atom 1(Np):	1.12688077	Atom 7(O):	-0.29612242
Atom 2(F):	-0.13488878	Atom 8(C):	0.33249364
Atom 3(F):	-0.30897784	Atom 9(H):	0.18924143
Atom 4(C):	0.34084013	Atom 10(O):	-0.30104790
Atom 5(H):	0.20712037	Atom 11(O):	-0.36410544
Atom 6(O):	-0.27405581	Atom 12(H):	0.48262186

Fig .S14. Atomic dipole-corrected Hirshfeld (ADCH) charge distributions for the transition states (TSII) in the Np–F system.



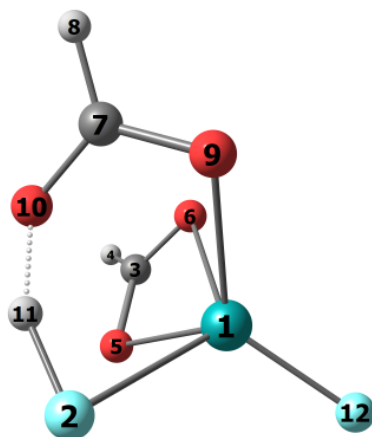
Atom 1(Np):	0.91416641	Atom 9(O):	-0.35395136
Atom 2(F):	-0.23131083	Atom 10(O):	-0.39414751
Atom 3(C):	0.23370221	Atom 11(H):	0.41635799
Atom 4(H):	0.15280805	Atom 12(O):	-0.18728835
Atom 5(O):	-0.15239514	Atom 13(C):	0.28311587
Atom 6(O):	-0.21453464	Atom 14(O):	-0.24537174
Atom 7(C):	0.40653291	Atom 15(H):	0.20504745
Atom 8(H):	0.16726869		

Fig .S15. Atomic dipole-corrected Hirshfeld (ADCH) charge distributions for the transition states (TSIII) in the Np–F system.



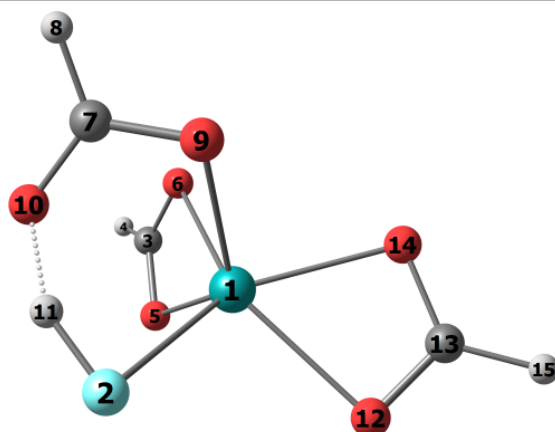
Atom 1(Pu):	1.30496539	Atom 6(H):	-0.07168759
Atom 2(F):	-0.17495941	Atom 7(C):	0.30117009
Atom 3(F):	-0.26270641	Atom 8(H):	0.15870024
Atom 4(C):	-0.49775096	Atom 9(O):	-0.25609998
Atom 5(C):	0.54917054	Atom 10(O):	-0.11411743
		Atom 11(H):	0.06331552

Fig .S16. Atomic dipole-corrected Hirshfeld (ADCH) charge distributions for the transition states (TSI) in the Pu–F system.



Atom 1(Pu):	1.36160045	Atom 7(C):	0.42868218
Atom 2(F):	-0.26118475	Atom 8(H):	0.16663645
Atom 3(C):	0.17772570	Atom 9(O):	-0.29556464
Atom 4(H):	0.45531028	Atom 10(O):	-0.36381566
Atom 5(O):	-0.46801166	Atom 11(H):	0.37843076
Atom 6(O):	-0.47694260	Atom 12(F):	-0.10286650

Fig .S17. Atomic dipole-corrected Hirshfeld (ADCH) charge distributions for the transition states (TSII) in the Pu–F system.



Atom 1(Pu):	0.95276179	Atom 9(O):	-0.34924331
Atom 2(F):	-0.25410529	Atom 10(O):	-0.40239037
Atom 3(C):	-0.12287947	Atom 11(H):	0.40396815
Atom 4(H):	0.29808358	Atom 12(O):	-0.22469445
Atom 5(O):	-0.06815794	Atom 13(C):	0.31301481
Atom 6(O):	-0.10060834	Atom 14(O):	-0.25056359
Atom 7(C):	0.46298660	Atom 15(H):	0.19615034
Atom 8(H):	0.14567749		

Fig .S18. Atomic dipole-corrected Hirshfeld (ADCH) charge distributions for the transition states (TSIII) in the Pu–F system.

Input

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Guess=Mix Nosymm

Basis set H, C, O, N

Web Link: <http://www.basissetexchange.org/basis/cc-pvdz-dk/format/gaussian94/?version=0&elements=1,6,7,8,9>

API Link: <http://www.basissetexchange.org/api/basis/cc-pvdz-dk/format/gaussian94/?version=0&elements=1,6,7,8,9>

Basis set: Th, U, Np, Pu

Web Link: <http://www.basissetexchange.org/basis/cc-pvdz-dk3/format/gaussian94/?version=1&elements=90,92,93,94>

API Link: <http://www.basissetexchange.org/api/basis/cc-pvdz-dk3/format/gaussian94/?version=1&elements=90,92,93,94>

ECP: Th, U, Np, Pu

Web

Link: <http://www.basissetexchange.org/basis/stuttgart%20rsc%201997%20ecp/format/gaussian94/?version=0&elements=90,92,93,94>

API

Link: <http://www.basissetexchange.org/api/basis/stuttgart%20rsc%201997%20ecp/format/gaussian94/?version=0&elements=90,92,93,94>

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10.1021/ci600510j

		Formic	
6	2.061242000	-0.052983000	0.000000000
1	0.948407000	-0.132824000	0.000000000
8	2.654418000	0.976750000	0.000000000
8	2.682392000	-1.236275000	0.000000000
1	2.033187000	-1.950460000	0.000000000
		CH₂	
6	0.000000000	0.000000000	0.603019000
1	0.000000000	0.000000000	1.674168000
6	0.000000000	0.000000000	-0.603019000
1	0.000000000	0.000000000	-1.674168000
		HF	
9	-1.376819000	1.488618000	-0.360884000
1	-0.976233000	2.055324000	0.242664000
		HCl	
17	-1.319418000	-0.002023000	-0.451420000
1	-0.515815000	0.503285000	0.422563000
		HBr	
35	-1.305314000	0.000575000	-0.384399000
1	-1.249185000	0.593471000	0.890642000
		I (UF) System	
92	0.165827000	0.740683000	0.641037000
9	-1.419091000	1.329318000	-0.326825000
9	1.768400000	1.330869000	-0.296004000
6	0.175791000	-2.560335000	-0.079102000
1	0.179102000	-3.615786000	-0.304739000
6	0.172120000	-1.357616000	0.179251000
		II (UF) System	
92	0.019860000	0.790650000	0.328724000
9	-1.860249000	1.183384000	-0.121904000
9	1.445937000	1.803948000	-0.583053000
6	0.487696000	-2.485712000	-0.530866000
1	0.635655000	-3.518941000	-0.797596000
6	0.319682000	-1.307689000	-0.223715000
6	0.360511000	1.035956000	3.811878000
1	1.286866000	1.023257000	4.412896000
8	0.398426000	0.967722000	2.588089000
8	-0.773334000	1.122496000	4.412593000
1	-0.697451000	1.170510000	5.379290000
		TSI (UF) System	
92	-0.382395000	0.943431000	0.615629000
9	-0.822632000	0.466961000	-1.225231000
9	1.494034000	1.402701000	0.248689000
6	-0.028446000	-1.221740000	1.562771000
6	-0.247929000	-1.892813000	0.553992000
1	-0.434102000	-2.501899000	-0.319363000
6	0.388693000	0.921352000	3.747638000

1	0.535666000	1.610975000	4.593448000
8	-0.029867000	1.436841000	2.635079000
8	0.607475000	-0.279630000	3.877392000
1	0.332592000	-0.815190000	2.828335000

III (UF) System

6	1.708027000	0.020801000	-0.283586000
1	0.637133000	-0.205771000	-0.416876000
8	2.119785000	1.209122000	-0.148203000
8	2.575817000	-0.904733000	-0.260784000
92	4.281640000	0.537677000	0.034795000
9	4.597171000	0.676644000	-1.868764000
9	4.027387000	0.555787000	1.953382000
6	4.254268000	3.251930000	0.761498000
1	4.213295000	3.276062000	1.840269000
6	4.279577000	3.285597000	-0.451328000
1	4.277336000	3.384722000	-1.526928000

IV (UF) System

6	1.330549000	-0.085941000	-0.265322000
1	0.233014000	-0.145402000	-0.351731000
8	1.916229000	1.014830000	-0.026008000
8	2.062298000	-1.113535000	-0.398570000
92	3.934457000	0.056913000	-0.049431000
9	4.110639000	0.533926000	-1.902182000
9	3.812171000	-0.424543000	1.805515000

V (UF) System

6	1.687377000	0.546299000	0.097815000
1	0.639707000	0.884941000	0.166094000
8	2.645999000	1.333587000	0.353368000
8	1.964764000	-0.638739000	-0.238517000
92	4.217154000	-0.310923000	-0.051671000
9	4.372470000	0.094667000	-1.939158000
9	4.076365000	-0.699582000	1.842915000
6	5.091408000	2.739435000	0.912849000
1	4.050264000	3.070936000	1.081338000
8	5.339352000	1.601719000	0.525596000
8	6.059329000	3.559466000	1.123022000
1	5.756686000	4.429446000	1.425785000

TSII (UF) System

92	3.890958000	0.492800000	-1.048328000
9	3.053850000	-0.236476000	-2.636247000
9	3.174770000	2.705398000	-0.973708000
6	6.038770000	0.130841000	0.435711000
1	6.879820000	0.032847000	1.141518000
8	5.914206000	-0.578145000	-0.584610000
8	5.121619000	1.016327000	0.653941000
6	1.288518000	0.511453000	0.324043000

1	0.427647000	0.067319000	0.848979000
8	2.398636000	-0.153046000	0.327589000
8	1.185278000	1.593914000	-0.258211000
1	2.239799000	2.431357000	-0.661405000

VI (UF) System

6	1.869840000	0.447196000	0.422169000
1	1.074079000	0.374138000	1.181812000
6	5.552138000	0.163634000	0.551325000
1	6.193598000	0.057640000	1.441550000
8	2.056587000	1.513335000	-0.238444000
8	2.631433000	-0.531226000	0.173858000
8	5.483249000	-0.692403000	-0.347717000
8	4.828295000	1.231141000	0.416775000
92	3.816239000	0.592233000	-1.392730000
9	3.012066000	-0.189996000	-2.972715000
9	3.587431000	3.038659000	-1.607416000
1	2.942449000	3.381697000	-1.021940000

VII (UF) System

6	1.839368000	0.298633000	0.488470000
1	1.030861000	0.112910000	1.214292000
6	5.536261000	0.130346000	0.573593000
1	6.215960000	-0.060426000	1.419976000
8	1.975354000	1.425892000	-0.077844000
8	2.672146000	-0.605211000	0.179863000
8	5.419648000	-0.637097000	-0.399317000
8	4.811259000	1.206647000	0.568199000
92	3.754651000	0.738696000	-1.258315000
9	2.964766000	-0.002786000	-2.858196000

VIII (UF) System

6	1.647613000	0.543380000	0.134708000
1	0.966235000	0.974059000	0.887159000
6	5.199411000	1.010224000	-0.180792000
1	5.900346000	1.616046000	0.417576000
8	2.330436000	1.309266000	-0.626477000
8	1.777461000	-0.696332000	-0.008039000
8	4.584387000	0.034566000	0.332957000
8	4.990760000	1.268805000	-1.402959000
92	3.440483000	-0.435584000	-1.591787000
9	4.284366000	-2.054141000	-2.283372000
6	3.124928000	2.226625000	-3.386580000
1	3.471547000	2.803059000	-2.508392000
8	3.048225000	1.001182000	-3.356299000
8	2.798788000	2.854019000	-4.460446000
1	2.901755000	3.814645000	-4.380900000

TSIII (UF) System

92	3.883335000	0.378988000	-1.146372000
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9	2.925646000	2.392737000	-1.623795000
6	5.899629000	0.336151000	0.573556000
1	6.666206000	0.259513000	1.362100000
8	6.176713000	0.466693000	-0.637303000
8	4.648527000	0.296525000	0.893166000
6	1.502653000	0.483305000	0.382928000
1	0.746283000	0.242269000	1.147088000
8	1.886122000	-0.398876000	-0.433334000
8	2.017396000	1.640404000	0.368730000
1	2.354314000	2.225584000	-0.714307000
8	3.570157000	-0.259565000	-3.185030000
6	3.467913000	-1.527203000	-2.918763000
8	3.649572000	-1.876209000	-1.740193000
1	3.225909000	-2.230718000	-3.731532000

IX (UF) System

6	1.330549000	-0.085941000	-0.265322000
1	0.233014000	-0.145402000	-0.351731000
8	1.916229000	1.014830000	-0.026008000
8	2.062298000	-1.113535000	-0.398570000
92	3.934457000	0.056913000	-0.049431000
9	4.110639000	0.533926000	-1.902182000
9	3.812171000	-0.424543000	1.805515000

X (UF) System

6	1.430958000	0.494440000	0.634723000
1	0.495737000	0.645357000	1.198500000
6	5.927296000	0.297481000	0.556349000
1	6.899409000	0.360621000	1.071715000
8	2.041734000	1.464056000	0.090491000
8	1.945574000	-0.656920000	0.497588000
8	5.296228000	-0.799232000	0.456949000
8	5.382718000	1.317966000	0.034348000
92	3.645450000	0.125075000	-0.767923000
6	3.529190000	-0.393622000	-3.361609000
1	3.447582000	-0.607536000	-4.439502000
8	3.617336000	0.793985000	-2.922132000
8	3.532252000	-1.321790000	-2.496075000

I (UCI) System

92	0.164701000	0.624050000	0.834886000
17	-1.700050000	1.455408000	-0.454121000
17	2.053049000	1.457614000	-0.417625000
6	0.174935000	-2.605730000	-0.061465000
1	0.178291000	-3.648740000	-0.340523000
6	0.171224000	-1.415469000	0.252466000

II (UCI) System

92	0.065807000	0.908387000	0.310425000
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17	-2.293770000	0.665000000	1.045894000
17	2.299011000	1.671527000	-0.414544000
6	0.519489000	-2.319916000	-0.595185000
1	0.650211000	-3.346646000	-0.893927000
6	0.365794000	-1.147700000	-0.257057000
6	0.260070000	0.893508000	3.656253000
1	0.808647000	0.352421000	4.445777000
8	0.590124000	0.787516000	2.478496000
8	-0.726655000	1.653154000	3.973912000
1	-0.915130000	1.668329000	4.926293000

TSI (UCI) System

92	-0.444852000	0.984445000	0.712549000
17	-1.037406000	0.289949000	-1.576313000
17	1.883587000	1.511453000	0.212857000
6	-0.006004000	-1.148687000	1.553496000
6	-0.282602000	-1.851831000	0.578876000
1	-0.507216000	-2.486304000	-0.266727000
6	0.363963000	0.891151000	3.806855000
1	0.474214000	1.564268000	4.670845000
8	-0.136405000	1.401204000	2.721023000
8	0.690734000	-0.288467000	3.879826000
1	0.415077000	-0.796191000	2.825091000

III (UCI) System

6	1.681574000	-0.017012000	-0.238038000
1	0.606932000	-0.253606000	-0.302748000
8	2.101070000	1.169218000	-0.102509000
8	2.567210000	-0.928034000	-0.297371000
92	4.239068000	0.508852000	-0.077443000
17	4.770784000	0.622541000	-2.478320000
17	4.208393000	0.488157000	2.386393000
6	4.303723000	3.279793000	0.776031000
1	4.286058000	3.336210000	1.853097000
6	4.317875000	3.213232000	-0.438071000
1	4.317332000	3.367067000	-1.508773000

IV (UCI) System

6	1.261521000	-0.088068000	-0.277408000
1	0.165251000	-0.144286000	-0.373999000
8	1.858816000	0.989976000	0.030572000
8	2.008937000	-1.098471000	-0.467230000
92	3.834602000	0.040450000	-0.052576000
17	4.308373000	0.643863000	-2.375906000
17	3.961858000	-0.507216000	2.328818000

V (UCI) System

6	1.466619000	0.689321000	0.046168000
1	0.414522000	1.018137000	0.060733000
8	2.418912000	1.484066000	0.308006000
8	1.776515000	-0.508542000	-0.235172000

92	3.979459000	-0.162939000	-0.004063000
17	4.972723000	-0.202294000	-2.265037000
17	4.674820000	-1.290881000	2.079266000
6	5.002850000	2.858914000	0.844130000
1	4.019091000	3.359346000	0.913820000
8	5.080610000	1.666469000	0.539965000
8	6.074041000	3.514617000	1.078791000
1	5.916983000	4.444360000	1.310456000

TSII (UCI) System

92	3.812080000	0.504177000	-1.090908000
17	3.267741000	-0.412371000	-3.289058000
17	3.114696000	3.048373000	-1.559291000
6	5.817153000	0.211841000	0.580603000
1	6.612974000	0.182577000	1.343391000
8	5.866579000	-0.422552000	-0.492535000
8	4.762404000	0.936962000	0.784190000
6	1.477397000	0.382283000	0.456930000
1	0.635386000	0.147678000	1.127629000
8	2.039864000	-0.522393000	-0.213816000
8	1.915318000	1.574107000	0.410690000
1	2.292279000	2.383909000	-0.488554000

VI (UCI) System

6	1.873047000	0.449199000	0.446350000
1	1.052926000	0.368968000	1.178729000
6	5.578465000	0.107008000	0.587076000
1	6.229358000	-0.027241000	1.466455000
8	2.073823000	1.512644000	-0.213201000
8	2.657443000	-0.521809000	0.229303000
8	5.465963000	-0.742514000	-0.317509000
8	4.892214000	1.197238000	0.462836000
92	3.840678000	0.573471000	-1.326770000
17	2.933780000	-0.628992000	-3.271126000
17	3.732392000	3.498989000	-1.725037000
1	2.717315000	3.599086000	-0.910579000

VII (UCI) System

6	1.841671000	0.312435000	0.501147000
1	1.011352000	0.089109000	1.190655000
6	5.562427000	0.132160000	0.619422000
1	6.243980000	-0.104749000	1.452438000
8	1.993786000	1.466040000	-0.006116000
8	2.690679000	-0.570538000	0.174723000
8	5.440376000	-0.582800000	-0.393430000
8	4.839725000	1.207609000	0.668430000
92	3.784681000	0.827399000	-1.173894000
17	2.811596000	-0.169061000	-3.182654000

VIII (UCI) System

6	1.634459000	0.555628000	0.155174000
1	0.943322000	0.964169000	0.910855000
6	5.189385000	1.062929000	-0.158858000
1	5.896461000	1.664119000	0.436356000
8	2.294057000	1.337405000	-0.607606000
8	1.800719000	-0.681305000	0.008955000
8	4.566009000	0.092780000	0.356561000
8	4.976389000	1.320980000	-1.381709000
92	3.437677000	-0.384126000	-1.565790000
17	4.359350000	-2.502003000	-2.479457000
6	3.129893000	2.261397000	-3.378398000
1	3.509173000	2.853113000	-2.524525000
8	3.027700000	1.038260000	-3.310297000
8	2.789475000	2.862909000	-4.460643000
1	2.912674000	3.823565000	-4.414261000

TSIII (UCI) System

92	3.842735000	-0.062615000	-1.624405000
8	3.147104000	-1.064139000	-3.395560000
17	3.039026000	2.401820000	-2.527002000
6	5.920985000	-0.224480000	-0.007451000
1	6.790525000	-0.208588000	0.669725000
8	5.644847000	-1.207063000	-0.736768000
8	5.139076000	0.793320000	-0.076847000
6	1.229435000	0.046054000	-0.573057000
1	0.147541000	0.114761000	-0.372844000
8	1.796201000	-1.015469000	-0.861345000
8	1.977157000	1.106129000	-0.483672000
1	2.145271000	1.936795000	-1.348830000
6	3.969034000	-0.496493000	-4.227566000
8	4.757961000	0.341155000	-3.760183000
1	3.933956000	-0.775426000	-5.293219000

IX (UCI) System

6	1.449009000	0.434199000	0.586247000
1	0.505381000	0.458082000	1.156882000
6	6.033180000	0.178466000	0.657022000
1	6.943530000	0.025080000	1.259530000
8	1.943400000	1.475620000	0.073159000
8	2.085323000	-0.651323000	0.418105000
8	5.012742000	-0.588263000	0.829330000
8	5.928730000	1.080435000	-0.200294000
92	3.768607000	0.279566000	-0.757756000
6	3.423766000	-0.332260000	-3.313669000
1	3.265711000	-0.540099000	-4.384558000
8	3.100114000	0.801580000	-2.817027000
8	3.917343000	-1.180921000	-2.528098000
17	4.096147000	3.217033000	-0.887575000
1	2.832606000	3.530627000	-0.893162000

I (U_{Br}) System

92	-0.813726000	0.237614000	0.148443000
35	-2.238379000	2.299741000	-0.608472000
35	1.444353000	1.445569000	-0.111435000
6	0.611582000	-2.805588000	0.093582000
1	1.036826000	-3.797036000	0.040410000
6	0.124268000	-1.679064000	0.160017000

II (U_{Br}) System

92	0.499458000	0.532687000	0.361798000
35	-2.068875000	0.849812000	0.688824000
35	1.211601000	3.071179000	0.709505000
6	0.396622000	-2.709993000	-0.619817000
1	0.401679000	-3.734139000	-0.957357000
6	0.388747000	-1.542673000	-0.238040000
6	0.372889000	0.762786000	3.611520000
1	0.633165000	0.345834000	4.598783000
8	0.774450000	0.227262000	2.580298000
8	-0.356085000	1.817775000	3.538323000
1	-0.630053000	2.165053000	4.402499000

TSI (U_{Br}) System

92	-0.478597000	0.981312000	0.742724000
35	-1.096286000	0.293797000	-1.720151000
35	2.004265000	1.537408000	0.237348000
6	0.009932000	-1.149703000	1.554047000
6	-0.300784000	-1.857883000	0.592859000
1	-0.548485000	-2.507612000	-0.234126000
6	0.356549000	0.889133000	3.818560000
1	0.452997000	1.553035000	4.691073000
8	-0.195224000	1.388210000	2.753553000
8	0.744935000	-0.273607000	3.865008000
1	0.463787000	-0.783101000	2.817484000

III (U_{Br}) System

6	1.705450000	-0.006581000	-0.273142000
1	0.632295000	-0.240534000	-0.365145000
8	2.124043000	1.180923000	-0.138913000
8	2.589145000	-0.919569000	-0.298481000
92	4.257879000	0.522301000	-0.075832000
35	4.723819000	0.569080000	-2.659715000
35	4.148901000	0.419112000	2.547838000
6	4.310879000	3.287521000	0.755274000
1	4.303607000	3.354354000	1.831700000
6	4.317467000	3.232734000	-0.459300000
1	4.304067000	3.384549000	-1.529853000

IV (U_{Br}) System

6	1.246209000	-0.104842000	-0.286859000
1	0.147907000	-0.113582000	-0.374654000

8	1.875679000	0.959767000	0.035562000
8	1.944819000	-1.142026000	-0.498378000
92	3.810052000	-0.027895000	-0.065108000
35	4.363928000	0.740706000	-2.492354000
35	4.010763000	-0.475880000	2.494063000

V (U_{Br}) System

6	1.492595000	0.713704000	0.054179000
1	0.434340000	1.023087000	0.057621000
8	2.428960000	1.514708000	0.317467000
8	1.820050000	-0.485463000	-0.220804000
92	4.008746000	-0.176616000	0.002818000
35	4.937516000	-0.182645000	-2.452932000
35	4.635806000	-1.375639000	2.253667000
6	4.996370000	2.854667000	0.839000000
1	4.006526000	3.343477000	0.899029000
8	5.089083000	1.663587000	0.540635000
8	6.060291000	3.525063000	1.080004000
1	5.886863000	4.452646000	1.306379000

TSII (U_{Br}) System

92	3.825382000	0.476813000	-0.921459000
35	3.102627000	-0.416041000	-3.267868000
35	3.126999000	3.142891000	-1.519661000
6	5.949492000	0.169644000	0.595079000
1	6.798890000	0.142906000	1.297650000
8	5.894683000	-0.510891000	-0.448092000
8	4.938398000	0.940891000	0.847329000
6	1.422479000	0.410191000	0.499547000
1	0.425923000	0.346474000	0.965572000
8	1.967837000	-0.566945000	-0.045344000
8	2.089546000	1.516038000	0.541776000
1	2.257997000	2.415185000	-0.301425000

VI (U_{Br}) System

6	1.863375000	0.440548000	0.467318000
1	1.025437000	0.359842000	1.179409000
6	5.607956000	0.088816000	0.616116000
1	6.255672000	-0.029447000	1.500148000
8	2.091523000	1.509664000	-0.171709000
8	2.641487000	-0.538777000	0.257100000
8	5.490419000	-0.776343000	-0.269493000
8	4.928012000	1.183915000	0.471452000
92	3.850402000	0.546743000	-1.282618000
35	2.888631000	-0.637350000	-3.425435000
35	3.715585000	3.554107000	-1.852949000
1	2.688904000	3.684330000	-0.882812000

VII (U_{Br}) System

6	1.826149000	0.308665000	0.508170000
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1	0.978803000	0.081397000	1.175335000
6	5.592478000	0.133434000	0.636640000
1	6.275274000	-0.080834000	1.474745000
8	1.992715000	1.465929000	0.014704000
8	2.682043000	-0.574684000	0.197187000
8	5.453403000	-0.609957000	-0.349062000
8	4.881351000	1.223275000	0.657674000
92	3.793502000	0.818819000	-1.137989000
35	2.744555000	-0.158439000	-3.326684000

VIII (UBr) System

6	1.548146000	0.382084000	0.372998000
1	0.890036000	0.736920000	1.183244000
6	5.155580000	1.083820000	-0.116712000
1	5.921315000	1.626842000	0.462174000
8	2.118051000	1.238282000	-0.402128000
8	1.768367000	-0.827638000	0.163700000
8	4.570230000	0.074291000	0.366141000
8	4.833122000	1.454894000	-1.286117000
92	3.305497000	-0.252349000	-1.501161000
35	4.437024000	-2.359369000	-2.656179000
6	3.240000000	2.340363000	-3.531772000
1	4.007906000	2.885039000	-2.952184000
8	2.880620000	1.211213000	-3.208701000
8	2.718125000	2.894860000	-4.566866000
1	3.072721000	3.780568000	-4.740082000

TSIII (UBr) System

92	3.846184000	-0.050478000	-1.627471000
8	3.150287000	-1.081908000	-3.387937000
35	3.044110000	2.555043000	-2.554566000
6	5.920691000	-0.228382000	-0.006618000
1	6.786423000	-0.229771000	0.675588000
8	5.638600000	-1.202668000	-0.746867000
8	5.151127000	0.796892000	-0.071382000
6	1.236446000	0.025411000	-0.575636000
1	0.152023000	0.082921000	-0.386297000
8	1.814196000	-1.028228000	-0.876553000
8	1.976415000	1.087229000	-0.468498000
1	2.103193000	1.980803000	-1.303163000
6	3.969468000	-0.525236000	-4.227339000
8	4.749648000	0.329644000	-3.774863000
1	3.942045000	-0.825512000	-5.287421000

IX (UBr) System

6	1.454606000	0.412083000	0.589943000
1	0.520936000	0.429683000	1.177143000
6	6.022994000	0.167612000	0.652795000
1	6.927639000	0.010239000	1.262881000
8	1.925331000	1.454282000	0.057816000

8	2.102147000	-0.667638000	0.423832000
8	4.979938000	-0.558768000	0.853304000
8	5.949892000	1.037171000	-0.241206000
92	3.761182000	0.275733000	-0.773762000
6	3.424461000	-0.362533000	-3.325020000
1	3.269556000	-0.581661000	-4.394127000
8	3.080889000	0.769417000	-2.838065000
8	3.934445000	-1.196200000	-2.533927000
35	4.155822000	3.302946000	-0.832803000
1	2.795749000	3.695458000	-0.880669000

I (ThF) System

90	0.167442000	0.741262000	0.556714000
9	-1.486469000	1.503501000	-0.296412000
9	1.834662000	1.510086000	-0.264406000
6	0.175635000	-2.678784000	-0.070377000
1	0.177425000	-3.740279000	-0.264717000
6	0.173456000	-1.468653000	0.152817000

II (ThF) System

90	0.010622000	0.959444000	0.172065000
9	-1.937284000	1.501648000	-0.129322000
9	1.529016000	2.006441000	-0.710417000
6	0.543305000	-2.657160000	0.015400000
1	0.512138000	-3.364791000	-0.825696000
6	0.348711000	-1.345713000	0.082534000
6	0.370968000	0.975685000	3.706728000
1	1.279647000	1.134954000	4.310983000
8	0.414185000	0.965130000	2.478521000
8	-0.758675000	0.792712000	4.304161000
1	-0.689034000	0.817230000	5.271380000

TSI (ThF) System

90	0.132957000	0.916470000	0.444709000
9	-1.616748000	1.443566000	-0.428995000
9	1.875521000	1.336842000	-0.499372000
6	0.085105000	-1.372823000	1.567161000
6	0.054535000	-2.145784000	0.614136000
1	0.027334000	-2.853180000	-0.202655000
6	0.185655000	0.908005000	3.752486000
1	0.220807000	1.610107000	4.600534000
8	0.186053000	1.419100000	2.558845000
8	0.147828000	-0.301606000	3.938750000
1	0.114040000	-0.889708000	2.772780000

III (ThF) System

6	1.469913000	-0.068208000	-0.311448000
1	0.397768000	-0.288806000	-0.442841000
8	1.887814000	1.127530000	-0.223692000
8	2.329021000	-0.997236000	-0.241876000

90	4.105698000	0.493916000	0.011412000
9	5.046030000	0.797884000	-1.764134000
9	4.637798000	0.664935000	1.965847000
6	4.229966000	3.291607000	0.763667000
1	4.170509000	3.300361000	1.842296000
6	4.308697000	3.331613000	-0.446510000
1	4.388224000	3.434241000	-1.519247000

IV (ThF) System

6	1.050576000	-0.004883000	-0.268871000
1	-0.048046000	0.003102000	-0.355960000
8	1.695128000	1.047376000	0.041512000
8	1.725077000	-1.059541000	-0.474918000
90	3.738770000	0.017404000	-0.062159000
9	4.693004000	0.785281000	-1.660495000
9	4.460333000	-0.062593000	1.816881000

V (ThF) System

6	1.517528000	0.718551000	0.053798000
1	0.475948000	1.081615000	0.069427000
8	2.485076000	1.492343000	0.316704000
8	1.777158000	-0.487003000	-0.229201000
90	4.096212000	-0.258398000	-0.013566000
9	4.795033000	-0.507218000	-1.905456000
9	4.563139000	-1.392364000	1.607205000
6	5.030213000	2.914131000	0.858435000
1	4.011005000	3.343647000	0.895398000
8	5.207208000	1.732636000	0.571079000
8	6.041425000	3.659309000	1.119201000
1	5.797201000	4.573327000	1.334039000

TSII (ThF) System

90	3.793447000	0.437749000	-0.893604000
9	3.678797000	-0.089735000	-2.835064000
9	3.095436000	2.672546000	-0.506583000
6	6.201356000	0.163978000	0.311055000
1	7.176941000	0.042731000	0.808760000
8	5.425651000	-0.826825000	0.130019000
8	5.807604000	1.293568000	-0.106868000
6	1.045327000	0.486040000	0.293579000
1	0.109522000	0.089785000	0.719552000
8	2.134360000	-0.160328000	0.500111000
8	1.036966000	1.511619000	-0.410738000
1	2.108463000	2.393461000	-0.440947000

VI (ThF) System

6	1.206248000	0.258653000	0.476419000
1	0.231548000	0.191410000	0.986677000
6	6.016769000	0.319203000	0.355236000
1	7.016564000	0.276549000	0.817317000

8	1.729744000	1.377467000	0.200541000
8	1.838948000	-0.788324000	0.136849000
8	5.392452000	-0.743623000	0.050900000
8	5.454666000	1.424480000	0.101612000
90	3.577905000	0.384120000	-0.873326000
9	3.531322000	0.167577000	-2.881235000
9	3.534263000	2.793889000	-1.394696000
1	3.516977000	3.724647000	-1.369768000

VII (ThF) System

6	1.242078000	0.258477000	0.525129000
1	0.263692000	0.243087000	1.031917000
6	6.026934000	0.222095000	0.396856000
1	7.030429000	0.194418000	0.851349000
8	1.828457000	1.351695000	0.255603000
8	1.823180000	-0.816330000	0.179743000
8	5.423228000	-0.843938000	0.064595000
8	5.432789000	1.322717000	0.176836000
90	3.600863000	0.298154000	-0.809307000
9	3.548624000	0.377230000	-2.821999000

VIII (ThF) System

6	1.500038000	0.668830000	-0.033458000
1	0.669053000	1.045586000	0.587807000
6	5.412997000	1.022539000	-0.173357000
1	6.101526000	1.657164000	0.408912000
8	2.395901000	1.429603000	-0.468676000
8	1.560979000	-0.577418000	-0.316647000
8	4.915707000	-0.026259000	0.341895000
8	5.101582000	1.311464000	-1.361229000
90	3.551500000	-0.507800000	-1.460892000
9	4.275192000	-2.189385000	-2.345789000
6	3.083886000	2.180523000	-3.288720000
1	3.526860000	2.776576000	-2.468660000
8	3.030906000	0.952695000	-3.231499000
8	2.621660000	2.780999000	-4.325293000
1	2.718952000	3.744703000	-4.278037000

TSIII (ThF) System

90	3.791092000	0.306652000	-1.174745000
9	2.585537000	2.214199000	-1.816178000
6	5.815908000	0.249722000	0.634145000
1	6.664365000	0.191394000	1.335298000
8	5.961014000	0.757662000	-0.525518000
8	4.669940000	-0.180521000	0.947836000
6	1.554350000	0.680172000	0.626727000
1	0.890630000	0.555754000	1.497121000
8	1.810792000	-0.293784000	-0.129001000
8	2.100603000	1.806783000	0.415522000
1	2.191727000	2.217851000	-0.823453000

8	3.944586000	-0.354088000	-3.406267000
6	3.641202000	-1.555936000	-3.136350000
8	3.474140000	-1.857571000	-1.916009000
1	3.524488000	-2.308689000	-3.932189000

IX (ThF) System

6	1.323154000	0.483297000	0.738593000
1	0.390006000	0.537446000	1.322453000
6	6.049077000	0.234712000	0.599843000
1	7.014042000	0.197692000	1.130516000
8	1.873163000	1.525943000	0.277306000
8	1.882659000	-0.628790000	0.505220000
8	5.384402000	-0.822457000	0.378406000
8	5.564506000	1.328940000	0.189301000
90	3.651068000	0.295571000	-0.714864000
6	3.554631000	-0.332241000	-3.374528000
1	3.517567000	-0.591893000	-4.444711000
8	3.608688000	0.873105000	-2.991755000
8	3.544813000	-1.232519000	-2.482215000
9	3.699958000	2.791302000	-1.140627000
1	3.247854000	3.527714000	-0.794802000

X (ThF) System

6	1.322047000	0.503771000	0.663298000
1	0.387673000	0.654169000	1.227180000
6	6.025423000	0.291925000	0.548898000
1	6.996172000	0.355340000	1.065898000
8	1.926882000	1.477986000	0.120919000
8	1.833406000	-0.649489000	0.532822000
8	5.400018000	-0.807712000	0.456526000
8	5.491727000	1.315545000	0.023612000
90	3.629285000	0.134580000	-0.727211000
6	3.543059000	-0.399652000	-3.392020000
1	3.508926000	-0.615533000	-4.471779000
8	3.608066000	0.791694000	-2.961244000
8	3.518781000	-1.332745000	-2.533478000

I (NpF) System

93	0.166416000	0.711996000	0.651525000
9	-1.387061000	1.338715000	-0.336180000
9	1.736647000	1.342596000	-0.307024000
6	0.175514000	-2.557954000	-0.075173000
1	0.178372000	-3.611312000	-0.311696000
6	0.172262000	-1.356908000	0.192166000

II (NpF) System

93	0.087882000	0.816436000	0.299677000
9	-1.722197000	1.394493000	-0.222661000
9	1.552789000	1.766964000	-0.612442000
6	0.363364000	-2.495582000	-0.361740000

1	0.446050000	-3.549527000	-0.569454000
6	0.267753000	-1.293749000	-0.124254000
6	0.338745000	1.167874000	3.750306000
1	1.063251000	1.720745000	4.373924000
8	0.426823000	1.170509000	2.527819000
8	-0.608741000	0.513273000	4.323147000
1	-0.592120000	0.574145000	5.292016000

TSI (NpF) System

93	0.136307000	0.952022000	0.551172000
9	-1.294155000	0.483622000	-0.723505000
9	1.900710000	1.398409000	-0.176033000
6	0.262278000	-1.209571000	1.510983000
6	-0.227000000	-1.860480000	0.590454000
1	-0.646034000	-2.433788000	-0.225108000
6	0.196053000	0.888682000	3.760273000
1	0.063118000	1.560049000	4.623788000
8	-0.006641000	1.404706000	2.581289000
8	0.523866000	-0.279069000	3.908831000
1	0.504587000	-0.833593000	2.716235000

III (NpF) System

6	1.627852000	0.012354000	-0.249831000
1	0.552554000	-0.210277000	-0.345981000
8	2.057521000	1.195651000	-0.114003000
8	2.503293000	-0.907027000	-0.267850000
93	4.173433000	0.522922000	0.033154000
9	4.739368000	0.891237000	-1.814142000
9	4.313333000	0.584182000	1.989977000
6	4.168313000	3.156088000	0.697099000
1	4.015341000	3.171094000	1.766905000
6	4.339125000	3.278554000	-0.499102000
1	4.481303000	3.393060000	-1.562751000

IV (NpF) System

6	1.200340000	-0.092043000	-0.278074000
1	0.104786000	-0.140312000	-0.385239000
8	1.801125000	0.983333000	0.033180000
8	1.942850000	-1.106472000	-0.460228000
93	3.778691000	0.034976000	-0.064694000
9	4.423326000	0.516485000	-1.839441000
9	4.148241000	-0.359719000	1.806768000

V (NpF) System

6	1.574668000	0.705893000	0.048384000
1	0.528757000	1.055402000	0.050592000
8	2.539838000	1.491444000	0.280541000
8	1.863791000	-0.501705000	-0.190074000
93	4.081408000	-0.193322000	-0.031574000
9	4.678968000	-0.427947000	-1.890235000

9	4.550778000	-1.160514000	1.614843000
6	5.005741000	2.856125000	0.851169000
1	3.990007000	3.292424000	0.884992000
8	5.175662000	1.680354000	0.532686000
8	6.021282000	3.580573000	1.144718000
1	5.786245000	4.491847000	1.381021000

TSII (NpF) System

93	3.780370000	0.318072000	-0.852705000
9	3.772984000	-0.355373000	-2.689266000
9	3.268190000	2.569838000	-0.485992000
6	6.110640000	0.230036000	0.339450000
1	7.097809000	0.146993000	0.822065000
8	5.363083000	-0.791075000	0.168382000
8	5.649816000	1.326367000	-0.079463000
6	1.023119000	0.540104000	0.208979000
1	0.105759000	0.101659000	0.634781000
8	2.123386000	-0.153419000	0.331113000
8	1.029672000	1.613720000	-0.380476000
1	2.289046000	2.467665000	-0.447596000

VI (NpF) System

6	1.790965000	0.463325000	0.431051000
1	1.017793000	0.409708000	1.214276000
6	5.564318000	0.247715000	0.524019000
1	6.268382000	0.053713000	1.349903000
8	1.992933000	1.508750000	-0.246422000
8	2.528713000	-0.535780000	0.161301000
8	5.545356000	-0.488319000	-0.512479000
8	4.742177000	1.208861000	0.566350000
93	3.738008000	0.519549000	-1.344255000
9	3.101190000	-0.315056000	-2.992098000
9	3.656596000	2.935572000	-1.577118000
1	3.100973000	3.378009000	-0.967999000

VII (NpF) System

6	1.868062000	0.310822000	0.447279000
1	1.056850000	0.130769000	1.170643000
6	5.520101000	0.159169000	0.608207000
1	6.244672000	-0.129136000	1.386941000
8	2.010315000	1.429839000	-0.134979000
8	2.703883000	-0.590449000	0.142166000
8	5.394704000	-0.516024000	-0.463914000
8	4.776803000	1.173675000	0.726987000
93	3.774070000	0.738948000	-1.263903000
9	2.870813000	-0.100008000	-2.768707000

VIII (NpF) System

6	1.584223000	0.507437000	-0.102768000
1	0.755043000	0.793332000	0.565859000

6	5.318122000	1.109172000	-0.173349000
1	5.958035000	1.761205000	0.443075000
8	2.438959000	1.337206000	-0.495896000
8	1.697373000	-0.703355000	-0.495559000
8	4.782798000	0.068302000	0.314739000
8	5.090805000	1.357960000	-1.388697000
93	3.632679000	-0.423406000	-1.529807000
9	4.427862000	-2.057441000	-2.279771000
6	3.050726000	2.193223000	-3.232773000
1	3.390102000	2.777327000	-2.357534000
8	3.089753000	0.963635000	-3.237784000
8	2.614859000	2.810334000	-4.270365000
1	2.635402000	3.774890000	-4.173015000

TSIII (NpF) System

93	3.724626000	0.312371000	-1.405166000
9	2.632646000	2.290002000	-1.660136000
6	5.427507000	0.352362000	0.593765000
1	6.128986000	0.458115000	1.436722000
8	5.561340000	1.052993000	-0.469066000
8	4.462126000	-0.452962000	0.613666000
6	1.849150000	0.666196000	0.633877000
1	1.269833000	0.422855000	1.538652000
8	1.827821000	-0.109468000	-0.364140000
8	2.567712000	1.707643000	0.595397000
1	2.505052000	2.288251000	-0.613502000
8	4.102582000	-0.515140000	-3.388070000
6	3.659045000	-1.690264000	-3.107848000
8	3.302309000	-1.883305000	-1.922807000
1	3.599640000	-2.470049000	-3.884406000

IX (NpF) System

6	1.428316000	0.481266000	0.664267000
1	0.511461000	0.509778000	1.275886000
6	5.966637000	0.175210000	0.549674000
1	6.947390000	0.072018000	1.042223000
8	1.974637000	1.549726000	0.237277000
8	1.987311000	-0.604425000	0.354385000
8	5.115243000	-0.755590000	0.554177000
8	5.637348000	1.247393000	-0.053082000
93	3.682467000	0.434025000	-0.746563000
6	3.558836000	-0.325865000	-3.270914000
1	3.486535000	-0.633963000	-4.326785000
8	3.469201000	0.894316000	-2.925343000
8	3.737281000	-1.164800000	-2.343230000
9	3.758194000	2.882768000	-1.032747000
1	3.044731000	3.425967000	-0.781090000

X (NpF) System

6	1.401053000	0.492115000	0.616729000
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1	0.465671000	0.642839000	1.179822000
6	5.943725000	0.285803000	0.505335000
1	6.914402000	0.349839000	1.023419000
8	2.014677000	1.456357000	0.066404000
8	1.924777000	-0.655474000	0.481992000
8	5.308805000	-0.807936000	0.404292000
8	5.397883000	1.301453000	-0.023498000
93	3.629307000	0.132765000	-0.727250000
6	3.545904000	-0.381137000	-3.301830000
1	3.511785000	-0.596578000	-4.382180000
8	3.607614000	0.805268000	-2.856591000
8	3.525862000	-1.305432000	-2.433223000

I (PuF) System

94	0.215169000	0.730553000	0.697642000
9	-1.328495000	1.151531000	-0.373845000
9	1.709473000	1.389064000	-0.316113000
6	0.145445000	-2.516756000	-0.079334000
1	0.119358000	-3.562659000	-0.347577000
6	0.181199000	-1.324601000	0.232845000

II (PuF) System

94	0.054342000	0.884015000	0.323329000
9	-1.779661000	1.212070000	-0.258524000
9	1.496434000	1.706246000	-0.705307000
6	0.434041000	-2.397730000	-0.379501000
1	0.554507000	-3.446462000	-0.596331000
6	0.296899000	-1.199928000	-0.128240000
6	0.349044000	1.045805000	3.769037000
1	1.271719000	1.223727000	4.349290000
8	0.363724000	1.037316000	2.543544000
8	-0.755199000	0.846462000	4.396538000
1	-0.662250000	0.874060000	5.362500000

TSI (PuF) System

94	-0.134257000	0.953118000	0.602454000
9	-1.181776000	0.376397000	-0.946930000
9	1.747244000	1.199010000	0.243730000
6	0.130215000	-1.172948000	1.500660000
6	-0.208759000	-1.830248000	0.518987000
1	-0.511591000	-2.409478000	-0.342021000
6	0.295787000	0.932264000	3.750388000
1	0.300806000	1.613345000	4.617125000
8	-0.072687000	1.448925000	2.611831000
8	0.612649000	-0.241799000	3.866284000
1	0.435458000	-0.797596000	2.695871000

III (PuF) System

6	1.691388000	0.018563000	-0.268452000
1	0.621388000	-0.228285000	-0.364642000

8	2.108200000	1.209685000	-0.239639000
8	2.575098000	-0.892473000	-0.171352000
94	4.208936000	0.542459000	-0.011312000
9	4.684283000	0.839771000	-1.871492000
9	4.165498000	0.563274000	1.927092000
6	4.201071000	3.128032000	0.709614000
1	4.038385000	3.125185000	1.777879000
6	4.372640000	3.260780000	-0.485760000
1	4.515545000	3.393454000	-1.547610000

IV (PuF) System

6	1.287241000	-0.082549000	-0.295061000
1	0.195012000	-0.129399000	-0.432420000
8	1.883018000	0.992249000	0.024945000
8	2.033063000	-1.096566000	-0.459372000
94	3.833162000	0.037257000	-0.019588000
9	4.137802000	0.496026000	-1.856873000
9	4.030059000	-0.380771000	1.850640000

V (PuF) System

6	1.677042000	0.593003000	0.012442000
1	0.627760000	0.931695000	0.000589000
8	2.624576000	1.372718000	0.314697000
8	1.983172000	-0.598807000	-0.283214000
94	4.149390000	-0.264478000	0.007776000
9	4.340174000	0.133548000	-1.877488000
9	4.212166000	-0.779850000	1.875094000
6	5.054642000	2.762866000	0.831146000
1	4.027185000	3.167461000	0.881304000
8	5.254604000	1.586359000	0.542144000
8	6.054436000	3.529044000	1.077371000
1	5.792000000	4.437017000	1.295201000

TSII (PuF) System

94	3.433003000	-0.159302000	-1.159963000
9	2.769741000	1.857184000	-1.771094000
6	5.332695000	0.263370000	0.518831000
1	6.169657000	0.424138000	1.217275000
8	5.254283000	0.890136000	-0.581088000
8	4.404199000	-0.568035000	0.767468000
6	1.866957000	0.880579000	0.864649000
1	1.376860000	0.931909000	1.849504000
8	1.609963000	-0.059911000	0.061638000
8	2.734086000	1.747792000	0.539813000
1	2.728902000	2.067158000	-0.692234000
9	4.079638000	-1.498744000	-2.388612000

VI (PuF) System

6	1.837151000	0.419139000	0.394828000
1	1.053774000	0.380914000	1.169030000
6	5.500123000	0.366771000	0.537533000

1	6.216676000	0.251367000	1.367125000
8	2.044913000	1.454277000	-0.296638000
8	2.568102000	-0.592596000	0.148658000
8	5.496492000	-0.441574000	-0.448123000
8	4.650886000	1.293357000	0.501650000
94	3.722524000	0.420795000	-1.402284000
9	2.813772000	-0.136947000	-3.011056000
9	3.784343000	2.815528000	-1.558124000
1	3.358649000	3.155017000	-0.796073000

VII (PuF) System

6	1.364909000	0.234268000	0.414186000
1	0.355477000	0.203527000	0.855584000
6	5.941698000	0.234885000	0.466199000
1	6.938010000	0.205850000	0.936205000
8	1.970126000	1.331171000	0.203405000
8	1.976426000	-0.825453000	0.069476000
8	5.332800000	-0.823116000	0.114548000
8	5.338103000	1.329357000	0.237376000
94	3.648502000	0.311388000	-0.769697000
9	3.354223000	0.405726000	-2.676561000

VIII (PuF) System

6	1.645297000	0.602200000	0.119986000
1	0.933594000	1.001329000	0.861816000
6	5.196784000	0.986830000	-0.175549000
1	5.898687000	1.577378000	0.435408000
8	2.340035000	1.376833000	-0.601726000
8	1.791292000	-0.642947000	-0.040745000
8	4.551637000	0.018372000	0.324920000
8	5.000993000	1.237107000	-1.395222000
94	3.435902000	-0.399514000	-1.550151000
9	4.333215000	-1.884397000	-2.426705000
6	3.138424000	2.167556000	-3.362998000
1	3.515777000	2.751728000	-2.503158000
8	3.090164000	0.940756000	-3.331689000
8	2.752109000	2.787086000	-4.420409000
1	2.842832000	3.749502000	-4.347420000

TSIII (PuF) System

94	3.635937000	0.126248000	-1.298860000
9	2.636261000	2.093693000	-1.737411000
6	5.409816000	0.344366000	0.603089000
1	6.158175000	0.436657000	1.406000000
8	5.528650000	0.915734000	-0.526709000
8	4.383075000	-0.374343000	0.756957000
6	1.835246000	0.768941000	0.729794000
1	1.282872000	0.588724000	1.665688000
8	1.800161000	-0.107098000	-0.195750000
8	2.522608000	1.808884000	0.580270000

1	2.514379000	2.218050000	-0.699442000
8	4.023965000	-0.417711000	-3.401295000
6	3.729390000	-1.640162000	-3.215333000
8	3.439551000	-1.964453000	-2.027766000
1	3.720288000	-2.367931000	-4.042293000

IX (PuF) System

6	1.421435000	0.496501000	0.654644000
1	0.507522000	0.523302000	1.270346000
6	5.954106000	0.185455000	0.512818000
1	6.943883000	0.065321000	0.982629000
8	2.009830000	1.555954000	0.283671000
8	1.937323000	-0.595649000	0.279767000
8	5.064414000	-0.714678000	0.596216000
8	5.643496000	1.225906000	-0.136448000
94	3.664951000	0.390130000	-0.723545000
6	3.577618000	-0.301808000	-3.234032000
1	3.540673000	-0.594511000	-4.296050000
8	3.395262000	0.897564000	-2.865623000
8	3.827791000	-1.142208000	-2.320695000
9	3.774603000	2.835673000	-1.020216000
1	3.042681000	3.360871000	-0.785349000

X (PuF) System

6	1.422231000	0.481151000	0.602773000
1	0.494612000	0.612009000	1.182860000
6	5.920258000	0.278321000	0.499713000
1	6.895259000	0.320240000	1.011331000
8	2.141301000	1.468362000	0.257791000
8	1.832695000	-0.660903000	0.241526000
8	5.153344000	-0.724253000	0.596160000
8	5.501009000	1.235423000	-0.221075000
94	3.632853000	0.184932000	-0.738956000
6	3.546904000	-0.382972000	-3.277758000
1	3.495866000	-0.617870000	-4.353094000
8	3.380710000	0.797646000	-2.841835000
8	3.774422000	-1.272207000	-2.406015000