

Supporting Information for:

**Nitrogen Reduction by Multimetallic Trans-Uranium Actinide Complexes: A Theoretical
Comparison of Np and Pu to U**

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Relative Spin State Energies Obtained at the PBE/L1 Level

Table S1: Relative energies (kcal/mol) of various spin-states of the optimized complexes. N/A implies we were not able to converge to the lowest HS state. For K₃-Pu-N(N₂)-Pu, the lowest HS state that we obtained was far away in energy from the LS state.

	Rel. Energy	Ground		Rel. Energy	Ground
K ₃ U-N-U	+1.1	HS	K ₃ U-N(N ₂)-U	-1.7	LS
K ₃ -Np-N-Np	-0.7	LS	K ₃ -Np-N(N ₂)-Np	+1.2	HS
K ₃ -Pu-N-Pu	+3.8	HS	K ₃ -Pu-N(N ₂)-Pu	-25.4	N/A
K ₃ -Np-N-Np[NH]	-1.3	LS	K ₃ -Np-N(N ₂)-Np[NH]	+1.9	HS
K ₃ -Pu-N-Pu[NH]	+1.8	HS	K ₃ -Pu-N(N ₂)-Pu[NH]	-1.5	LS
K ₃ -Np-N-Np[CH ₂]	+0.2	HS	K ₃ -Np-N(N ₂)-Np[CH ₂]	+2.2	HS
K ₃ -Pu-N-Pu[CH ₂]	+1.8	HS	K ₃ -Pu-N(N ₂)-Pu[CH ₂]	-11.2	LS

On the Use of Mulliken Spin Densities

There are some shortcomings to using the Mulliken population analysis approach. Most of these shortcomings are however associated with incomplete basis sets. Hirshfeld charges¹ and spins do not as sensitive to basis sets as their Mulliken counterparts.² The L1 basis sets used in our all-electron calculations with Priroda are rather extended and possess several polarization functions on the various atoms e.g. 6 G functions on the actinides and 3 D functions on oxygen. Crucially, despite their ‘shortcomings’ the Mulliken populations will most likely correctly reproduce the number of electrons involved in the reduction of the actinide centers. It is the Δe that ultimately matters. To illustrate, we considered the truncated K₃U-N-U and K₃U-N(N₂)-U complexes. The obtained results are shown in Table S2.

Table S2: Comparison of Mulliken and Hirshfeld spin densities on the actinide centers obtained from all-electron PBE/L1 calculations and calculations with Stuttgart relativistic effective core pseudopotentials.

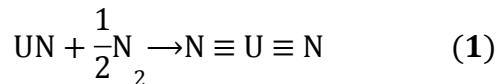
	Gaussian 16: Stuttgart RECP & def2-tzvp		Priroda AE-PBE/L1	
	Mulliken	Hirshfeld	Mulliken	Hirshfeld
K ₃ U-N-U LS	2.88 & -2.88	2.75 & -2.75	2.87 & -2.87	2.62 & -2.63
K ₃ U-N-U HS	2.85 & 2.85	2.81 & 2.82	2.81 & 2.81	2.72 & 2.73
K ₃ U-N(N ₂)-U LS	1.24 & -1.23	1.17 & -1.17	1.17 & -1.13	1.10 & -1.04
K ₃ U-N(N ₂)-U HS	1.24 & 1.22	1.15 & 1.16	1.12 & 1.14	1.04 & 1.05
Δe LS	~ 1.64	~ 1.58	~ 1.70	~ 1.52
Δe HS	~ 1.61	~ 1.66	~ 1.69	~ 1.68

To summarize, the Mulliken spin densities are quite close to the Hirshfeld spin densities and yield similar #s of electrons involved in the N₂ → N₂⁴⁻ transformations.

On the Use of the PBE Exchange-Correlation Density Functional

CASSCF/CASPT2 is often used to account for strong correlation effects. We have however used the PBE exchange-correlation density functional to treat the systems of interest because Pure DFT functionals like PBE correct for static correlation effects, in an indirect manner. DFT also accounts for dynamical correlation in efficiently. We therefore expect that DFT will be able to predict the redox reactivities of actinide complexes correctly. We illustrate with three examples:

First, we considered reaction **1** below in which uranium nitride, UN is converted to UN₂.



This reaction involves a three-electron transfer from U to N, U(III) to U(VI). Also this reaction involves N₂ and is therefore a N₂-induced redox transformation just like the K₃U-N-U → K₃U-N(N₂)-U transformation. The results obtained with CASPT2, PBE and CASSCF are presented in Table S3 below. The CASSCF and CASPT2 calculations were performed at the DKH2/ANO-RCC-VTZP level (using the MOLCAS software 8.1 package³) while PBE calculations were performed with L1 basis sets in Priroda. For CASSCF and CASPT2, we used CAS(11/14) for UN and CAS(14/14) for UN₂. CCSDT (*iterative* treatment of singles, doubles and triples) calculations were performed with Stuttgart small-core ECPs and associated valence basis sets, cc-pVTZ basis sets on nitrogen and the MRCC⁴ code while freezing 10/11 core orbitals during the correlation step. The CASPT2 calculations were performed without the IPEA shift (IPEA = 0.0 eV). We note that the use of the IPEA shift has been recently questioned.⁵ The results are presented in Table S3. We also examined the effect of correlating the 5d orbitals in the second-order perturbation step.

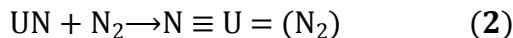
Table S3: Dependence of CASPT2 results for **1** on frozen and correlated orbitals.

	5d orbitals	CASSCF	CASPT2	PBE	CCSDT
CASPT2 with no IPEA shift	Frozen	-25.6	-57.4	-55.3	-55.4
CASPT2 with no IPEA shift	Correlated		-58.8		

CASPT2, PBE and CCSDT are clustered in a range of 3-4 kcal/mol. These results indicate that the PBE exchange-correlation functional is sufficient to study the systems of interest in our manuscript. To perform analogous CASSCF/CASPT2 calculations on the large complexes studied

in this manuscript will require CAS(16/32) for $K_3U\text{-}N\text{-}U$ and CAS(24/32) for $K_3U\text{-}N(N_2)\text{-}U$. These calculations are intractable with modern machines. The Np and Pu analogues will require even larger active space sizes.

Second, we considered **2** below in which the uranium nitride, UN is converted to UN_3 .



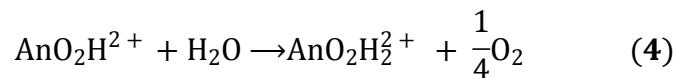
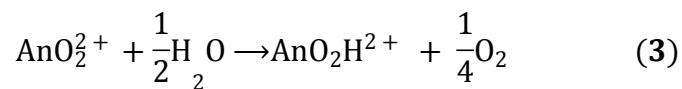
This reaction involves a 2-electron transfer from a U(III) center to N_2 . In UN_3 , U is in the +5 oxidation state (like in $K_3U\text{-}N(N_2)\text{-}U$) and the overall species is of doublet character. Importantly, this reaction is comparable to one half of the $K_3U\text{-}N\text{-}U \rightarrow K_3U\text{-}N(N_2)\text{-}U$ transformation. For UN_3 , we used an active space of 13 electrons in 14 orbitals in the CASSCF and CASPT2 calculations while employing ANO-RCC-VTZP basis sets and the DKH2 Hamiltonian. The PBE calculations were performed with Priroda using L1 basis sets.

Table S4: Calculated energetics (kcal/mol) for **2** using CASSCF, CASPT2 and PBE.

	CASSCF	CASPT2	PBE
2	152.5	-14.5	-11.2

Again, we find that PBE is within 3-4 kcal/mol of the CASPT2 results. CCSDT calculations on UN_3 are beyond the capabilities of our computational resources.

Lastly, we consider the water-induced reduction of actinyl complexes (**3** & **4**). The reaction energies were calculated at the CASPT2, CASSCF, CCSD(T), MC-PDFT and KS-DFT levels. The details of MC-PDFT have been previously provided.⁶ All the calculations were performed with ANO-RCC-TZVP basis sets while using the DKH2 Hamiltonian.



In these reactions, the actinyl (where $An = U$, Np and Pu) dications are reduced to the +5 oxidation state (**3**) and then to the +4 oxidation state (**4**). We ensured that we converged to the same electronic states for the different species with all the methods. **3** & **4** are redox reactions just as the title reactions in our manuscript are redox reactions.

Our results are presented below. PBE has a MAD of 3.2 kcal/mol from CASPT2 and performs as well as CCSD(T) and MC-PDFT. Given that the perturbative triples in CCSD(T) ameliorates some of the multireference characters in the complexes, it is actually questionable to use CASPT2 as the reference benchmark. The best we can say is that CASPT2, CCSD(T) and PBE are clustered in a range of 3.2-4.0 kcal/mol. PBE does better than CASSCF. We obtained similar PBE results with the L1 basis sets in Priroda.

Table S5: Deviations (given in kcal/mol) for CASSCF, CCSD(T), MC-PDFT and KS-DFT from CASPT2 for the energetics of the water-induced reduction of actinyl groups (reactions **3** and **4**).

	CASSCF	CCSD(T)	MC-PDFT	KS-DFT				
			ft-PBE	LSDA	BLYP	PBE	B3LYP	PBE0
MSD	7.4	-3.2	-2.7	2.3	-3.0	-0.7	-4.7	-3.2
MAD	7.9	4.0	3.0	3.7	3.4	3.2	4.7	3.4

As such, we have used PBE in our studies of the bis-actinide nitride complexes

Plutonium-NH Species

Reactant:

Reactant -LS

94	1.635745310	-0.478219290	-1.160842660	1	4.065950810	-3.432481640	-5.649489200
94	-1.690437950	0.403501610	1.108562070	1	3.475151040	-1.992223640	-4.768168980
19	0.511630590	-2.555215240	1.739361890	1	2.680175740	-3.572244060	-4.529832780
19	1.287613630	2.761603760	0.792558030	6	2.874804060	-1.700800470	-7.456477100
19	-1.650308810	0.430007560	-2.701739460	1	3.765253200	-2.181526230	-7.891854460
14	0.185671690	-1.993826470	-4.531907850	6	2.170994180	-1.460876360	-8.269419980
14	3.837646140	-3.273469180	0.660890860	1	3.182530480	-0.757945380	-6.976575460
14	3.262836300	3.049010980	-1.870454980	6	3.617387840	-4.142949710	3.370387310
14	-0.382008090	2.887484060	3.896513140	1	2.894675270	-3.548179210	4.584705290
14	-4.007014520	2.568669740	-1.132262090	1	3.161485520	-4.093673700	5.504607820
7	0.849099450	-1.051182200	-3.253485770	1	3.172690980	-2.489937030	4.716111210
8	-1.325812340	-1.288917800	-4.887846230	1	1.800165710	-3.613295430	4.464479200
8	0.005745340	-3.625878800	-4.233590500	6	3.208975800	-5.608734600	3.174057600
8	1.027736640	-1.904341180	-5.976062080	1	3.516094210	-6.214592340	4.042426290
7	2.731731990	-2.319962120	-0.250002780	1	2.116272710	-5.697135290	3.065855090
8	3.166948700	-3.356572390	2.223821130	1	3.674535230	-6.012231520	2.263693020
8	3.940003520	-4.872041470	0.167239740	6	5.133723580	-4.039508940	3.579307760
8	5.434118600	-2.767604730	0.746286480	1	5.419160530	-4.598487670	4.485854090
7	2.932051450	1.468447980	-1.282995620	1	5.686672590	-4.451950400	2.723429250
8	4.150034010	4.020850280	-0.810460470	1	5.437067760	-2.989046880	3.710823010
8	1.743749210	3.790034960	-1.867722940	1	4.799888190	-5.543551980	-0.786164170
8	4.078939710	3.201670320	-3.326620470	6	4.102700550	-6.875237600	-1.092924820
7	-2.240928600	-1.440944750	2.422111720	1	4.691445500	-7.468860460	-1.810456600
8	-1.720817360	-4.099008820	2.269817470	1	3.980329360	-7.462442550	-0.168631000
8	-4.395946800	-3.407698490	2.519141890	1	3.103304210	-6.692299960	-1.518657690
7	-1.026269090	2.101975760	2.507880560	6	6.171992010	-5.795293940	-0.144751770
8	0.241517150	1.869425170	5.061319170	1	6.832114410	-6.337971330	-0.841128550
8	-1.424998050	3.900434200	4.723195660	1	6.641119400	-4.837974530	0.125563760
8	0.823276930	3.929120440	3.290496460	1	6.058385830	-6.402778890	0.767853150
7	-3.345971290	1.195997260	-0.342038440	6	4.948640390	-4.716933140	-2.069989020
8	-5.670746460	2.815271940	-1.103825860	1	5.581480150	-5.249185890	-2.798741660
8	-3.321588950	3.993671750	-0.588069770	1	3.965533860	-4.541466150	-2.534690470
8	-3.510407120	2.451658510	-2.762563300	1	5.414467720	-3.742788210	-1.854090010
7	-0.020471930	-0.079286150	-0.006493460	6	6.059204700	-1.465410010	0.727859120
6	-2.156248510	-1.445520100	-6.078303430	6	7.455800840	-1.663490160	1.334910920
6	-1.667007270	-0.453052720	-7.140811030	1	8.021860730	-0.718099510	1.321744560
1	-2.288196480	-0.513588580	-8.049628890	1	7.378295910	-2.011098060	2.376925830
1	-1.715523180	0.579440810	-6.757543430	1	8.016799420	-2.415598810	0.758136140
6	-0.621724200	-0.676935150	-7.402118000	6	6.182613260	-1.002798440	-0.729815370
6	-3.585249490	-1.108711390	-5.634477760	1	6.678063540	-0.021179790	-0.794946280
1	-4.285510730	-1.174860670	-6.483255020	1	6.776133290	-1.729340940	-1.307424360
1	-3.921620080	-1.810165150	-4.852962900	1	5.183017110	-0.929669660	-1.190580610
1	-3.641008720	-0.083698770	-5.232017200	6	5.259285460	-0.459850030	1.564844910
6	-2.114710000	-2.876655330	-6.627307530	1	5.766541600	0.519538110	1.587472780
1	-2.777271630	-2.956575330	-7.504917810	1	4.247182380	-0.317305640	1.147823350
1	-1.094737170	-3.149627270	-6.933060120	1	5.160103140	-0.817943220	2.602648720
1	-2.455230880	-3.597164690	-5.869006850	6	5.577343730	4.240506260	-0.679041230
6	-0.540195960	-4.417765530	-3.153771790	6	6.349449590	2.925826170	-0.841266490
6	-1.414421420	-3.580153410	-2.216856770	1	7.430218670	3.089238960	-0.697149180
1	-1.822505460	-4.207630700	-1.408423390	1	6.008488800	2.193098110	-0.092014950
1	-0.833261710	-2.763939470	-1.750849430	1	6.193066680	2.507310510	-1.848278590
6	-2.263803410	-3.141241160	-2.767091590	6	5.784336680	4.797695330	0.734439530
6	-1.372853820	-5.531721420	-3.804781290	1	5.201741450	5.722833270	0.870265550
1	-1.750076240	-6.230552350	-3.040283950	1	5.452929690	4.065192340	1.488208100
1	-2.236883350	-5.110291690	-4.342111940	1	6.847910790	5.026049720	0.912535560
1	-0.758095980	-6.096193230	-4.523443640	6	6.032833400	5.265636360	-1.727201380
6	0.639814600	-5.032683080	-2.392208710	1	5.496245870	6.218348500	-1.586198670
1	0.291763220	-5.714464890	-1.599256880	1	7.113352140	5.463360200	-1.632328800
1	1.278017140	-5.601166900	-3.086768250	1	5.824038270	4.887083080	-2.738932460
1	1.245081660	-4.242549340	-1.920395380	6	1.386313170	5.182659440	-2.109800110
6	2.203858590	-2.622204540	-6.430196030	6	1.418434070	5.934882650	-0.771343210
6	1.752578720	-3.929222650	-7.098013860	1	1.170362290	6.999689450	-0.914734500
1	2.621574750	-4.497265970	-7.468576880	1	0.677818220	5.519454230	-0.067143590
1	1.204282050	-4.548655180	-6.371995920	1	2.425118650	5.866877450	-0.329182700
1	1.090524860	-3.714022200	-7.952181580	6	2.327917210	5.865125140	-3.109569840
6	3.165087520	-2.920660230	-5.273109240	1	1.981797190	6.894960040	-3.297182370
1	3.262836300	3.049010980	-1.870454980	1	3.356421640	5.909362070	-2.721962180
1	2.04282050	-4.548655180	-6.371995920	1	2.341900780	5.324287120	-4.067443980
6	-0.038495470	-5.148834250	-2.670123280	1	-0.416605490	6.171520530	-2.835116280

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1	4.226543960	4.310968750	-5.697048740	1	-0.958297730	2.773421070	7.113403640
1	5.746519910	3.445756110	-5.331289080	6	-3.419698730	4.765970760	5.684815260
6	2.484908810	2.297223450	-4.962621380	1	-2.899975830	5.721670210	5.859007850
1	2.390281310	1.722590100	-5.899052290	1	-3.902510740	4.807837350	4.696216110
1	1.934569560	1.762129370	-4.170427280	1	-4.198975070	4.644592540	6.454066140
1	2.005909830	3.278518240	-5.107713280	6	1.440111560	5.098995530	3.909982730
6	4.642868080	1.101517560	-4.423728710	6	1.689123230	4.882437490	5.407233830
1	4.622875550	0.551082330	-5.378304210	1	2.187300220	5.767880730	5.835520550
1	5.694741620	1.234147010	-4.122661640	1	0.741812460	4.720731700	5.941217730
1	4.132502980	0.495438680	-3.657127450	1	2.336699860	4.007559430	5.572949200
6	-5.220534420	-3.138150980	1.363941630	6	0.524013000	6.307969750	3.682928600
6	-6.314423490	-4.215680560	1.370970570	1	0.968483740	7.220775500	4.113339640
1	-7.015002500	-4.062954560	0.534158540	1	0.369890640	6.474616540	2.603754080
1	-5.869319280	-5.218480750	1.276531990	1	-0.454891900	6.127672790	4.152367670
1	-6.881534220	-4.174838590	2.314287470	6	2.775695380	5.294149640	3.184264050
6	-5.848640400	-1.749347910	1.522563570	1	3.309888880	6.174578870	3.577825860
1	-6.511508390	-1.518824230	0.673538040	1	3.422274750	4.411240570	3.320353510
1	-6.442587230	-1.701846910	2.449600320	1	2.616166450	5.451486820	2.104577710
1	-5.057127920	-0.983191350	1.575841250	6	-6.820455470	1.953587920	-0.941459960
6	-4.405386140	-3.218791380	0.068409050	6	-6.656512090	0.638153690	-1.716189600
1	-5.051221010	-3.043151970	-0.808755150	1	-7.577589710	0.036403830	-1.647844320
1	-3.600265880	-2.463322400	0.066999700	1	-6.450574610	0.836146510	-2.779422330
1	-3.945680740	-4.214641450	-0.037284020	1	-5.829084580	0.034315570	-1.310653830
6	-1.621559060	-5.535078980	2.515532620	6	-7.039837460	1.679513370	0.553014950
6	-0.770453010	-6.091261200	1.367238190	1	-7.906393180	1.015755670	0.704904020
1	-1.262348380	-5.897212450	0.400744540	1	-6.151472970	1.202313220	0.994459220
1	0.230943220	-5.629773560	1.346798830	1	-7.231612260	2.622628840	1.088504680
1	-0.632438730	-7.179482960	1.475492600	6	-8.012537430	2.741941850	-1.503565490
6	-2.995512520	-6.217628340	2.509979420	1	-8.950238570	2.180202380	-1.365837040
1	-3.508722260	-6.051401870	1.550339580	1	-8.102590790	3.708972020	-0.984800970
1	-2.867220140	-7.303496420	2.651505730	1	-7.878759150	2.936899260	-2.579581500
1	-3.637541960	-5.832702080	3.315280950	6	-3.750781500	4.947778640	0.418139710
6	-0.924910550	-5.764536150	3.863274640	6	-2.492460130	5.737698530	0.796288450
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1	-1.511006210	-5.305148440	4.672307690	1	-2.058649930	6.213609110	-0.097285450
6	-3.700466590	-2.975443280	5.638888290	6	-4.329395090	4.248555480	1.652628390
6	-4.758955960	-4.087350970	5.676139580	1	-4.599419180	4.996011630	2.416192090
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1	-5.307220850	-4.113784160	4.722967280	1	-3.597631240	3.553606070	2.093752140
1	-4.275276230	-5.065282420	5.832585010	6	-4.800916080	5.892884580	-0.186138240
6	-2.873161520	-2.982227260	6.930627920	1	-5.128271950	6.629625550	0.565652260
1	-3.512201540	-2.7883387910	7.806942440	1	-4.380984980	6.439154960	-1.044893580
1	-2.382359310	-3.959796160	7.063735280	1	-5.675739200	5.316196950	-0.522669080
1	-2.089492210	-2.208886580	6.884474450	6	-3.834139160	3.273232880	-3.924173890
6	-4.366043280	-1.606207130	5.446535120	6	-3.954974210	4.757825760	-3.567532080
1	-5.066215370	-1.399728670	6.272371940	1	-4.127883340	5.346172310	-4.484400150
1	-3.610341060	-0.804260830	5.433141550	1	-4.799651370	4.927426280	-2.884484390
1	-4.930355610	-1.577361290	4.501039080	1	-3.035949140	5.118708070	-3.082783650
6	1.136860560	0.735830880	5.071299090	6	-2.676744380	3.070729820	-4.910148330
6	0.286758340	-0.523295360	5.275329340	1	-2.837837390	3.656086740	-5.830186900
1	0.922033290	-1.418331810	5.373983860	1	-1.726032130	3.395217790	-4.457973980
1	-0.312768980	-0.426820070	6.194767090	1	-2.590018050	2.011082830	-5.203626480
1	-0.402248750	-0.671527560	4.426944090	6	-5.146199070	2.775348510	-4.542720930
6	1.949578890	0.637216140	3.775398630	1	-5.369362550	3.325575250	-5.472099420
1	2.554426930	1.548019380	3.627385670	1	-5.080798590	1.702237630	-4.786700710
1	2.637372600	-0.223429360	3.814281240	1	-5.978095670	2.929248020	-3.839795260
1	1.282204260	0.501998290	2.904300840	14	-2.823026530	-2.982173340	2.921633010
6	2.075181890	0.937176920	6.269803450	8	-2.756513450	-3.250919380	4.576164360
1	2.687147590	1.843309490	6.136017610	1	1.372919080	-0.284214270	-3.728161910
1	1.490107690	1.048125870	7.196325520	1	3.840520990	1.023545060	-1.045779670
1	2.752563670	0.0749007730	6.384091070	1	-3.973634180	0.374609690	-0.420645290
6	-2.420183620	3.604326080	5.738113890	1	2.608979120	-2.835170950	-1.147688600
6	-3.130102730	2.275941280	5.449842210	1	-2.479602560	-0.801885900	3.211242900
1	-2.409167460	1.443439190	5.477568410	1	-1.631772460	2.808660350	2.034383350

Reactant -HS								
94	1.761410260	-0.660350840	-1.171231740	1	2.484073980	-3.007692450	-5.652658880	
94	-1.682293490	0.438596490	0.991855600	6	1.381547760	-0.900708820	-8.193902330	
19	0.596480970	-2.398177800	1.993561320	1	2.074068150	-1.233072910	-8.983766840	
19	1.525820870	2.529453150	0.876499430	1	0.403899020	-0.681482810	-8.651941850	
19	-1.077420130	1.045982930	-2.767937050	1	1.768674770	0.032406700	-7.752682790	
14	-0.018564680	-1.816082690	-4.550991410	6	3.656473130	-4.155644050	3.689674980	
14	3.827004000	-3.431990940	0.920991040	6	2.916719710	-3.517324040	4.871536250	
14	3.411793760	2.870788590	-1.839595900	1	3.195170650	-4.006440230	5.819313620	
14	-0.375975100	2.905089790	3.831199530	1	3.167026210	-2.446485180	4.949718950	
14	-3.912531500	2.609103600	-1.363435830	1	1.825082710	-3.619255140	4.750941730	
7	0.951597360	-0.984160180	-3.403552770	6	3.301715300	-5.644838190	3.586435920	
8	-1.597941170	-1.256338050	-4.271487280	1	1.364527820	-6.188359350	4.478512500	
8	0.004518840	-3.498264200	-4.543060500	1	2.211114330	-5.779641800	3.512083410	
8	0.293406560	-1.427174360	-6.153426450	1	3.761704170	-6.079606910	2.687745580	
7	2.686794690	-2.594937150	-0.048463940	6	5.168468260	-3.982159170	3.883999270	
8	3.172569270	-3.456306680	2.501770490	1	5.477872230	-4.469394400	4.823605550	
8	4.020030100	-5.051514370	0.532266990	1	5.734291580	-4.428635570	3.054302690	
8	5.389988600	-2.822080420	0.992710260	1	5.432868450	-2.914663850	3.945105150	
7	3.157716400	1.282332020	-1.259213300	6	4.960901470	-5.741022210	-0.327271180	
8	4.235755700	3.896313360	-0.773059490	6	4.312129140	-7.097198010	-0.634441490	
8	1.850808720	3.535393460	-1.861799640	1	4.972368220	-7.712811200	-1.265837560	
8	4.237965070	3.080604590	-3.285575700	1	4.109738120	-7.643410550	0.300692040	
7	-2.190873300	-1.408317930	2.436040100	6	3.355641350	-6.952443430	-1.161883410	
8	-1.554732720	-4.046737970	2.391123050	6	6.280815170	-5.942225710	0.431626500	
8	-4.255311200	-3.461626260	2.242855190	1	7.002840450	-6.500938340	-0.186250130	
7	-0.994791300	2.202000450	2.393647790	1	6.714360090	-4.965379470	0.692872410	
8	0.099568870	1.808414550	5.000031290	1	6.104999810	-6.512317840	1.358152600	
8	-1.380392920	3.965636170	4.648912310	6	5.206629980	-4.964932370	-1.627558600	
8	0.934490140	3.869201590	3.317991780	1	5.894687110	-5.525365100	-2.281335780	
7	-3.235975360	1.193240820	-0.680744910	1	4.262805280	-4.807024760	-2.171068950	
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7	0.150911310	0.034006920	-0.005196530	1	7.823844980	-0.563593120	1.447381480	
6	-2.823520530	-1.527534660	-5.015779070	1	7.242546730	-1.806853100	2.594743910	
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1	-3.763486610	-0.844488650	-6.862599160	6	6.057352290	-1.133899880	-0.604860090	
1	-2.771564150	0.392767370	-6.045881530	1	6.458199660	-0.116185780	-0.739701380	
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1	-3.938479400	-1.704865100	-3.156563760	1	5.476325250	0.533081830	1.574046460	
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6	-2.970342010	-3.012309580	-5.372691900	1	4.956453290	-0.763667590	2.688407560	
6	-3.930551150	-3.170972470	-5.890999960	6	5.652606930	4.173396700	-0.627534740	
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1	-0.264361510	-3.023463010	-1.844466140	1	5.208433730	5.645951420	0.913241010	
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1	0.779839270	-1.455531350	5.466737410	1	-1.693842850	3.776763990	-4.710724760
1	-0.479330680	-0.434873470	6.207574820	1	-2.474117370	2.331068520	-5.430820080
1	-0.525806760	-0.758452390	4.454398870	6	-5.07343040	2.966711020	-4.727152400
6	1.837502220	0.536071090	3.801039790	1	-5.342339940	3.556842650	-5.619106450
1	2.480229040	1.421318180	3.657537950	1	-4.965119070	1.912881540	-5.031575330
1	2.492229120	-0.348588300	3.867804360	1	-5.891769550	3.045412480	-3.997161220
1	1.183026810	0.424209100	2.916555110	14	-2.776327590	-2.964717270	2.869081810
6	1.914975490	0.924228160	6.283806680	8	-2.942996690	-3.219624780	4.519250940
1	2.526653040	1.827741910	6.134123320	1	1.815051280	-0.716630570	-3.907360990
1	1.313062770	1.061616940	7.195661280	1	4.085481700	0.879919380	-1.042373580
1	2.592251930	0.067664770	6.437419750	1	-3.661742150	0.357544970	-1.115828540
6	-2.433922610	3.710736510	5.614039340	1	2.262253410	-3.325848950	-0.647488990
6	-3.208381570	2.430587530	5.273544850	1	-2.498650970	-0.792263120	3.211926870
1	-2.539050340	1.556633230	5.315805520	1	-1.404874560	2.993305200	1.859606230
1	-4.027113890	2.277570180	5.995872540				
1	-3.639329440	2.492177180	4.262019830				

Product

Product - LS				6	4.736851090	1.276469900	6.572724890
94	0.074987500	-0.036578500	-1.876524450	1	5.731041360	0.801461860	6.593710850
94	-0.017739910	0.182994130	1.688738170	1	4.511611770	1.650673000	7.584927550
14	-2.920450940	-2.222551190	-3.022790020	1	4.765146870	2.126132460	5.874191740
14	3.650066240	0.418748130	3.285969260	6	2.280114920	0.907562730	6.143233190
7	-2.020765350	-0.878034950	-2.482885200	1	2.249838300	1.793207090	5.489102940
8	-4.254431410	-2.568506510	-2.022276650	1	2.024380190	1.220968050	7.168644340
8	-3.521355470	-2.258304060	-4.586224600	1	1.519514280	0.192691350	5.794498620
8	-1.912081290	-3.534378590	-2.689640920	6	3.803849610	3.214905360	2.594793350
7	2.107125270	0.004158920	2.673511570	6	4.937783240	4.178624100	2.975038570
8	4.781966210	-0.334382450	2.246653120	1	4.892740650	4.412180500	4.050386060
8	4.017409600	-0.211341420	4.794603740	1	4.858828590	5.120352280	2.407766600
8	3.984033460	2.051499230	3.426249390	1	5.916786290	3.721588340	2.760314270
6	-5.599697870	-2.028918980	-2.037264730	6	2.444861750	3.849732420	2.918072430
6	-6.199758890	-2.371469000	-0.668076500	1	1.625656970	3.174120700	2.625868680
1	-6.179065350	-3.461102790	-0.505015210	1	2.319351690	4.801089310	2.373729950
1	-7.246054210	-2.031196200	-0.601244720	1	2.365358320	4.056857290	3.997067520
1	-5.627783310	-1.886138860	0.140727040	6	3.889565980	2.857834250	1.108914980
6	-5.578618620	-0.506354950	-2.231951560	1	4.850665860	2.368274980	0.888650860
1	-4.963788430	-0.026614470	-1.452065050	1	3.815972660	3.765716510	0.487827210
1	-6.599028720	-0.092343620	-2.171070570	1	3.065749230	2.183993080	0.818029120
1	-5.164666360	-0.243418750	-3.218534300	7	0.373289830	-0.998814850	-0.004978550
6	-6.409790330	-2.707837760	-3.150833330	7	0.160710270	1.922682180	0.065028550
1	-5.938377150	-2.521965110	-4.127341260	7	-0.898230880	1.541563100	-0.373667330
1	-7.444301330	-2.326851830	-3.168370380	14	3.214503820	-1.546902940	-3.356878310
1	-6.443103030	-3.796903450	-2.984262500	14	-2.284519930	2.964573920	3.545926650
6	-3.129577330	-1.539603770	-5.788694080	7	1.538161770	-1.384914570	-3.134396300
6	-3.645956330	-0.098074980	-5.703256310	8	4.014408090	-2.588767720	-2.258512260
1	-4.737298080	-0.087065930	-5.549076810	8	3.780570000	-2.017243850	-4.867369560
1	-3.422763840	0.447151490	-6.634706030	8	3.840299650	-0.057570690	-2.867738360
1	-3.155572640	0.430542920	-4.870345650	7	-1.044989460	1.944478500	2.965381230
6	-1.608548080	-1.543815370	-5.974758260	8	-2.291691430	4.423659990	2.627627690
1	-1.113981900	-1.061576870	-5.116019490	8	-2.086756020	3.532712290	5.113113880
1	-1.336233280	-0.989880040	-6.887829500	8	-3.821699570	2.298987370	3.538064870
1	-1.227724650	-2.571752600	-6.067655650	6	4.195793940	-4.026973570	-2.296605370
6	-3.815374850	-2.282091700	-6.942562570	6	4.602738140	-4.433522420	-0.873647880
1	-3.468889870	-3.327007000	-6.985475570	1	5.500354120	-3.875977900	-0.558407200
1	-3.586926800	-1.797715880	-7.905233360	1	4.832041510	-5.510473410	-0.822629850
1	-4.907971570	-2.285855320	-6.801560340	1	3.786506190	-4.231136770	-0.158524580
6	-2.010790480	-4.923956970	-3.109410180	6	2.888263290	-4.731079580	-2.681773200
6	-3.464600280	-5.410767220	-3.160456200	1	2.076345920	-4.421875390	-2.002827250
1	-3.955182790	-5.284480070	-2.183099990	1	3.000173080	-5.826339160	-2.615576130
1	-3.491320930	-6.479095280	-3.432644580	1	2.597808560	-4.481427170	-3.714507430
1	-4.040152110	-4.846769700	-3.911231850	6	5.320053260	-4.377746340	-3.281065640
6	-1.355890440	-5.074611560	-4.488119460	1	5.065993170	-4.011405880	-4.286483780
1	-1.923731030	-4.509451350	-5.241906270	1	5.478520030	-5.468281480	-3.319512580
1	-1.332184420	-6.133984340	-4.792631290	1	6.262669130	-3.900011100	-2.967242710
1	-0.321186900	-4.696657810	-4.464920450	6	3.153009590	-2.001170890	-6.178812900
6	-1.223962890	-5.727204230	-2.067240600	6	2.229156450	-3.220235740	-6.304806160
1	-0.191904980	-5.349590770	-1.990568700	1	2.789273310	-4.149957540	-6.114895110
1	-1.187200600	-6.793554470	-2.342606750	1	1.797700740	-3.277370080	-7.317479290
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6	6.179577370	-0.668704230	2.495218640	6	2.356335980	-0.711826150	-6.412561340
6	6.813462580	-0.880977200	1.114766010	1	1.583850030	-0.601534850	-5.634922730
1	6.298932440	-1.689025130	0.566241880	1	1.869666190	-0.741334510	-7.400988350
1	7.873747490	-1.166842380	1.211259370	1	3.016027520	0.168455870	-6.378825770
1	6.760079350	0.042128370	0.514945450	6	4.308140000	-2.111332470	-7.182599620
6	6.236213180	-1.969240710	3.307979870	1	4.989219510	-1.251756860	-7.079662210
1	5.720610080	-1.829483560	4.269508230	1	3.924294970	-2.131109870	-8.215055520
1	7.280805100	-2.269118220	3.494825520	1	4.885261380	-3.032671310	-7.004542440
1	5.735541480	-2.785330990	2.759948330	6	5.130028680	0.551535630	-3.152223350
6	6.908007390	0.464081330	3.229492240	6	6.266463860	-0.479357950	-3.149962290
1	6.848483340	1.400814160	2.653120380	1	6.324458360	-0.999149180	-2.181141620
1	7.971391430	0.204627370	3.362902370	1	7.229610220	0.025607460	-3.333333100
1	6.461621010	0.635927860	4.219363120	1	6.112173450	-1.231738310	-3.939034370
6	3.673186900	0.265509410	6.120420010	6	5.061461260	1.256888690	-4.512940380
6	3.697520950	-0.975949010	7.021135340	1	4.921782740	0.519581220	-5.316869940
1	2.944427330	-1.705962480	6.684424360	1	5.993256240	1.812592150	-4.708628990
1	3.482004760	-0.703897690	8.066820100	1	4.220932550	1.968520710	-4.531714510
1	4.688646000	-1.455620560	6.980556570	6	5.349564100	1.583708010	-2.042617150

1	4.514482940	2.300538230	-2.016681830	1	2.060801060	2.734974860	-5.541389550
1	6.287783730	2.140154480	-2.202202620	6	-0.500746670	2.391080760	-6.492833120
1	5.411688930	1.085806540	-1.061945280	1	-0.285280440	1.652152220	-5.704554720
6	-2.801802920	5.734172250	3.019395070	1	-0.166016050	1.990716090	-7.463772580
6	-2.960303450	6.543431340	1.722406620	1	-1.589965400	2.540198380	-6.535306430
1	-1.983442100	6.706794280	1.232052550	6	-0.198112860	4.792368730	-7.199604780
1	-3.378975120	7.540134550	1.936029110	1	-1.285094810	4.964412930	-7.154781670
1	-3.648746900	6.037536800	1.021884410	1	0.063541510	4.486380670	-8.225108190
6	-1.774595750	6.419022050	3.930681170	1	0.310817170	5.743464260	-6.975455500
1	-1.635123220	5.821496040	4.842496710	6	-3.134896410	4.203083550	-3.350373620
1	-2.108425620	7.433939070	4.204193190	6	-2.856619720	5.703693130	-3.173580480
1	-0.802624980	6.500699180	3.415045350	1	-2.637180390	5.957369850	-2.122680280
6	-4.165389410	5.627227140	3.714252500	1	-3.737414880	6.290484430	-3.483339340
1	-4.901643390	5.141517150	3.054233510	1	-1.995536730	6.016159150	-3.784475510
1	-4.539450250	6.632688250	3.969849550	6	-3.511738930	3.920091630	-4.811871250
1	-4.081388710	5.036773210	4.636768100	1	-2.709389130	4.261660120	-5.480413040
6	-2.280303440	2.870751380	6.386388680	1	-4.442549140	4.446018800	-5.081042680
6	-1.320672950	3.563541300	7.363008200	1	-3.663915190	2.839774000	-4.960087500
1	-0.278369460	3.424520880	7.034306060	6	-4.289685840	3.767050790	-2.438439190
1	-1.429078400	3.148085360	8.377647730	1	-4.478412910	2.687620180	-2.551033850
1	-1.531964070	4.644090450	7.402780170	1	-5.213903890	4.314042500	-2.685762230
6	-3.737349960	3.073907390	6.827582050	1	-4.057906400	3.958177150	-1.377000200
1	-3.960184940	4.147966540	6.933520610	6	-3.486686770	4.925747660	2.706626410
1	-3.921908670	2.585732750	7.798572980	6	-3.929593450	-5.436663710	1.329604410
1	-4.416953820	2.644244690	6.076061710	1	-4.368755340	-4.621551070	0.729601490
6	-1.953980140	1.375384620	6.301935750	1	-4.691551980	-6.226802910	1.431902950
1	-2.634972950	0.868329500	5.599560490	1	-3.071974550	-5.860112090	0.780476710
1	-2.062770830	0.908477330	7.294222990	6	-4.680983530	-4.319667420	3.456289420
1	-0.921719170	1.226442030	5.950743700	1	-4.343968070	-3.903875440	4.417571400
6	-4.667746520	1.673398260	2.554721150	1	-5.455093770	-5.082740380	3.642147620
6	-6.106304400	2.066306900	2.923886240	1	-5.130604140	-3.506045440	2.862814320
1	-6.331296050	1.749829800	3.954318440	6	-2.869119920	-6.077180290	3.508945560
1	-6.830686340	1.588564700	2.244122160	1	-2.010662140	-6.509179630	2.970744200
1	-6.235655440	3.158581340	2.861439600	1	-3.616200550	-6.873402640	3.663274700
6	-4.501137970	0.152062660	2.655253610	1	-2.523106530	-5.724312500	4.490429140
1	-3.468008720	-0.150485560	2.419229720	6	-1.501212810	-3.168386960	6.329803210
1	-5.185293400	-0.362175780	1.958970410	6	-2.610207900	-2.643189060	7.250495950
1	-4.729937790	-0.191802300	3.676734800	1	-2.909857570	-1.628428190	6.944920880
6	-4.339717160	2.154381750	1.136263040	1	-2.266565760	-2.611128460	8.296843180
1	-4.442338020	3.250548750	1.076437250	1	-3.494070710	-3.298320820	7.191417040
1	-5.033949250	1.706011650	0.406406230	6	-1.098644760	-4.593117150	6.737332130
1	-3.312686040	1.868042030	0.848537400	1	-1.980522260	-5.253889180	6.748912970
19	3.209563230	-1.145373430	0.083641130	1	-0.653722830	-4.595861080	7.745971480
14	-0.363670130	3.498815670	-3.387076320	1	-0.364645570	-4.993230860	6.021686080
14	-1.372949700	-3.141206560	3.487078940	6	-0.283850990	-2.237560540	6.378550450
7	0.323990330	1.963406310	-3.167876110	1	0.504585700	-2.601434680	5.700722200
8	0.074126950	4.741017360	-2.280532980	1	0.124596640	-2.196018300	7.401535080
8	-0.146452520	4.238869490	-4.887506710	1	-0.565518360	-1.218441280	6.073706020
8	-2.001360820	3.390983410	-2.963673190	6	0.985294030	-4.656580830	2.737295150
7	-1.103287680	-1.558533350	2.884670930	6	1.146213290	-6.145832000	3.078328210
8	-2.518044330	-3.870324490	2.446017310	1	1.384554990	-6.267478870	4.146785960
8	-2.083672940	-3.202585500	5.002999430	1	1.957132780	-6.599286440	2.484794590
8	-0.037368530	-4.147433360	3.614412630	1	0.213694900	-6.692893930	2.867960400
6	1.309483900	5.495847640	-2.214763540	6	2.292368880	-3.912291680	3.040488160
6	1.406528860	6.024126930	-0.775787630	1	2.188412390	-2.840932340	2.808074180
1	0.522961400	6.640504640	-0.531075290	1	3.125123240	-4.322067820	2.443726270
1	2.297949770	6.659834040	-0.648358450	1	2.555428030	-4.008046730	4.106120730
1	1.483364420	5.187580180	-0.059245710	6	0.613036490	-4.488307810	1.260021940
6	2.523264150	4.606129990	-2.513274880	1	-0.341518010	-4.996201730	1.047297050
1	2.508835030	3.719207590	-1.860981330	1	1.385562520	-4.945682010	0.618508370
1	3.460153710	5.163879900	-2.346307970	1	0.536522270	-3.418341430	0.988957040
1	2.511238470	4.267710670	-3.560699030	19	-1.374961780	4.202146330	0.030805540
6	1.233452910	6.671029530	-3.199596570	19	-2.121376950	-2.491977680	0.126293840
1	1.069342550	6.291795140	-4.218986280	1	1.043682600	-2.283606080	-3.244881350
1	2.162200230	7.265108480	-3.175670770	1	-2.604750640	-0.026017840	-2.466744160
1	0.390988020	7.334066120	-2.939573380	1	1.196775310	1.845736710	-3.700630460
6	0.217268490	3.712784290	-6.190032210	1	1.875600980	-0.887002120	3.154102030
6	1.739192530	3.514698520	-6.249671980	1	-1.625383050	-0.939909460	3.531222370
1	2.259251570	4.454002960	-6.003150160	1	-0.168766220	2.342366940	3.348953050
1	2.049461600	3.201045800	-7.259642850	Product -HS			

94	0.011060920	0.042832800	-1.757038920	1	5.487829320	0.989658700	6.687676620
94	-0.116196850	0.057426480	1.619566060	1	4.198964800	1.776758350	7.641375680
14	-2.936585860	-2.167532670	-3.065573880	1	4.472576520	2.259306320	5.936532610
14	3.484335110	0.471601640	3.324854010	6	2.049701650	0.914990800	6.149179300
7	-2.029784470	-0.823706140	-2.537662870	1	1.996517060	1.806953450	5.504521140
8	-4.251653260	-2.530523100	-2.038743850	1	1.749231330	1.202694640	7.169905450
8	-3.584883790	-2.199850530	-4.609607380	1	1.338944690	0.165020210	5.769913140
8	-1.919972790	-3.480749380	-2.760630830	6	3.554244540	3.254375050	2.552867540
7	1.990459660	-0.069995770	2.687307680	6	4.731742180	4.181299070	2.889046000
8	4.691057960	-0.198301090	2.313298380	1	4.707662450	4.453348380	3.956037460
8	3.874239670	-0.112527380	4.846109080	1	4.685878530	5.105735010	2.290217430
8	3.666094950	2.127395840	3.448589550	1	5.689898200	3.679039960	2.680917840
6	-5.599297040	-1.994873690	-2.023180360	6	2.225991830	3.965630510	2.843747600
6	-6.167949890	-2.339243810	-0.640806870	1	1.371638210	3.307220920	2.617106230
1	-6.138496180	-3.428698950	-0.477196960	1	2.135649480	4.880564120	2.232973740
1	-7.214702850	-2.005276080	-0.552324210	1	2.171196750	4.257069390	3.905058010
1	-5.584168310	-1.847910640	0.156239200	6	3.619126810	2.823919630	1.084313460
6	-5.587579980	-0.472332240	-2.216261930	1	4.535041360	2.241560220	0.897218840
1	-4.957947490	0.009171670	-1.449544720	1	3.642956900	3.711035520	0.429461430
1	-6.608035050	-0.062203710	-2.132063900	1	2.731833990	2.229179950	0.807412440
1	-5.197509520	-0.207202090	-3.211773850	7	0.244118020	-1.165722850	0.064346150
6	-6.432127210	-2.676570840	-3.117893730	7	0.371564070	1.520072650	-0.022500770
1	-5.980446630	-2.492832160	-4.104059940	7	-0.956971860	1.211994040	-0.135441220
1	-7.466704290	-2.295409840	-3.115142410	14	3.346211590	-1.399025000	-3.181816390
1	-6.462759360	-3.765280500	-2.947710430	14	-2.067324600	2.828644270	3.607479700
6	-3.218794420	-1.482520880	-5.821223620	7	1.701119130	-1.271281710	-2.750085270
6	-3.752317020	-0.047465430	-5.731506750	8	4.231660280	-2.407780790	-2.123825480
1	-4.841445830	-0.050408730	-5.562046220	8	3.764199330	-1.908038970	-4.723442770
1	-3.549738980	0.498434930	-6.667187880	8	3.982973850	0.115795480	-2.811260580
1	-3.257534750	0.489558520	-4.906607380	7	-0.918685110	1.659231250	3.106129190
6	-1.700340600	-1.470970370	-6.025436640	8	-1.889385850	4.235689870	2.644030490
1	-1.204809410	-0.981827410	-5.171212040	8	-1.835904550	3.394538650	5.168737340
1	-1.444697560	-0.915486930	-6.942275300	8	-3.662782630	2.327857610	3.578183820
1	-1.310766010	-2.495293970	-6.119340790	6	4.443099890	-3.843073800	-2.143927030
6	-3.913267040	-2.235161780	-6.963058210	6	4.976092320	-4.203085590	-0.750827630
1	-3.552698310	-3.274861450	-7.014265310	1	5.890505830	-3.628220020	-0.531287760
1	-3.709036570	-1.746516080	-7.929031220	1	5.219376690	-5.276391120	-0.689041470
1	-5.003103820	-2.255042680	-6.803082410	1	4.224891410	-3.982271710	0.027232480
6	-2.016847510	-4.868215120	-3.185895720	6	3.124248850	-4.583534120	-2.403091950
6	-3.449730030	-5.404308710	-3.072558790	1	2.368019530	-4.294175160	-1.654130220
1	-3.829018820	-5.308017670	-2.043615850	1	3.271156600	-5.674845710	-2.340880410
1	-3.473186790	-6.469360010	-3.357642500	1	2.733941820	-4.350599630	-3.406539380
1	-4.128272540	-4.852584340	-3.741912850	6	5.488772890	-4.195466600	-3.210877920
6	-1.522982790	-4.993421100	-4.632674290	1	5.141314030	-3.867676510	-4.201670050
1	-2.197810660	-4.451965270	-5.311831830	1	5.672445220	-5.282454150	-3.231287450
1	-1.494328580	-6.051861580	-4.939959830	1	6.441101410	-3.685813720	-2.991520420
1	-0.508804830	-4.574559330	-4.729252270	6	3.000691320	-1.939341600	-5.961395100
6	-1.085874150	-5.648367480	-2.250058320	6	2.013088820	-3.111671650	-5.912967350
1	-0.062098670	-5.244410160	-2.302889160	1	2.546984700	-4.060528750	-5.741059650
1	-1.055626620	-6.714619290	-2.527755810	1	1.4611127810	-3.193674520	-6.863398040
1	-1.433278780	-5.577481630	-1.206571320	1	1.283922730	-2.954431970	-5.102641250
6	6.090413170	-0.490952370	2.598690790	6	2.247142020	-0.623886650	-6.184543080
6	6.776503670	-0.627581950	1.233823210	1	1.554099420	-0.435205730	-5.348831320
1	6.308135740	-1.429053560	0.637215490	1	1.665050300	-0.672207850	-7.119153710
1	7.843111740	-0.878554530	1.355383580	1	2.949757370	0.219529600	-6.259073920
1	6.708847090	0.317009990	0.669555290	6	4.037218690	-2.162421080	-7.069660820
6	6.164696690	-1.818377390	3.365474960	1	4.764089400	-1.334895020	-7.086936530
1	5.617314570	-1.729706680	4.315699290	1	3.545709910	-2.216971720	-8.054080430
1	7.212219840	-2.092432540	3.574392580	1	4.586286800	-3.102066460	-6.898896040
1	5.707290460	-2.628467730	2.772670300	6	5.257854770	0.712702330	-3.182580410
6	6.750130650	0.637302250	3.399974470	6	6.391319620	-0.320417990	-3.209267210
1	6.684367290	1.591492190	2.853699300	1	6.496018180	-0.812663240	-2.230138940
1	7.815326220	0.408287290	3.569872460	1	7.344070290	0.177437580	-3.455185250
1	6.256957540	0.758580760	4.374670950	1	6.198101870	-1.093856060	-3.969069300
6	3.473531520	0.344660730	6.161412490	6	5.113492530	1.374463920	-4.558874390
6	3.539299010	-0.893296670	7.065065240	1	4.929092970	0.611839190	-5.329924260
1	2.831696340	-1.660291730	6.711939730	1	6.032919480	1.921899740	-4.823979240
1	3.286455750	-0.631952850	8.105127650	1	4.273405400	2.087030090	-4.553752310
1	4.553890830	-1.322580100	7.047683110	6	5.540134060	1.776920710	-2.117262910
6	4.470811010	1.410902840	6.637569390	1	4.712038750	2.500576560	-2.069523640

1	6.470928000	2.321754680	-2.344937530	6	-0.656066220	2.292862160	-6.570372950
1	5.651753990	1.307699320	-1.126863030	1	-0.415176300	1.553818260	-5.789755520
6	-2.281551970	5.603439400	2.973917770	1	-0.390659310	1.877711840	-7.556575670
6	-2.302349160	6.380702460	1.649006860	1	-1.740321780	2.478523990	-6.550690420
1	-1.294814210	6.425944250	1.198302760	6	-0.304995320	4.677431260	-7.313657600
1	-2.625504940	7.420535780	1.817441500	1	-1.384783130	4.878466980	-7.231891650
1	-3.009905570	5.925071160	0.933491110	1	-0.087830160	4.360294950	-8.346176840
6	-1.229035720	6.211917500	3.910110490	1	0.237241740	5.615302120	-7.113146090
1	-1.190463600	5.638688480	4.847084180	6	-3.125107930	4.114076620	-3.304155130
1	-1.467761010	7.265105040	4.134006490	6	-2.847223740	5.584203360	-2.957652930
1	-0.233095460	6.173428370	3.437932720	1	-2.594511070	5.706239240	-1.891173180
6	-3.676813890	5.656625340	3.609561900	1	-3.741099070	6.195952230	-3.164667800
1	-4.431087380	5.226503300	2.931596760	1	-2.008853510	5.978410220	-3.552475990
1	-3.955724650	6.702892800	3.818530690	6	-3.529382450	4.000194080	-4.780728640
1	-3.694701680	5.093726880	4.552728960	1	-2.735399950	4.406303700	-5.423557760
6	-2.198700290	2.820626280	6.449276400	1	-4.458809130	4.562129240	-4.970134210
6	-1.213285270	3.419263600	7.461360340	1	-3.699249050	2.944996900	-5.045885700
1	-0.181371560	3.136591630	7.199722620	6	-4.252837830	3.568966540	-2.419285310
1	-1.432144250	3.058555800	8.479081130	1	-4.460594920	2.516624770	-2.669162700
1	-1.283960590	4.518710490	7.456806550	1	-5.177854100	4.151829830	-2.559083760
6	-3.637178840	3.235768390	6.790604770	1	-3.973532490	3.613545450	-1.354213950
1	-3.716736390	4.333386540	6.847169100	6	-3.537464290	-5.053934350	2.597850650
1	-3.940493710	2.818082340	7.764583470	6	-3.962492820	-5.550478070	1.210097050
1	-4.324903030	2.869589370	6.013694560	1	-4.419915150	-4.735106300	0.624237210
6	-2.076041450	1.292613740	6.432988840	1	-4.706205540	-6.359785040	1.294988070
1	-2.765051640	0.856830310	5.692032900	1	-3.093192870	-5.943334520	0.656315810
1	-2.322276770	0.881776710	7.425617440	6	-4.744374370	-4.474286920	3.347785400
1	-1.049491500	0.992952240	6.173804620	1	-4.419635810	-4.067679260	4.317166110
6	-4.561995580	1.751577290	2.610159040	1	-5.509101270	-5.250391410	3.517544120
6	-5.966574730	2.226325010	3.012088830	1	-5.201381990	-3.658450270	2.763149440
1	-6.192359150	1.912734590	4.043403890	6	-2.909399310	-6.207690150	3.388280270
1	-6.730416610	1.800316250	2.341319440	1	-2.042538150	-6.622072680	2.849825070
1	-6.030226460	3.324993720	2.961829470	1	-3.647286850	-7.015137760	3.527849650
6	-4.482067980	0.222499700	2.704529530	1	-2.573399190	-5.864284760	4.376625530
1	-3.472275000	-0.138363330	2.451573640	6	-1.600711390	-3.297876630	6.260799810
1	-5.205185320	-0.247252880	2.016249970	6	-2.711977660	-2.761210060	7.171883090
1	-4.716049830	-0.112713930	3.727783570	1	-2.994296040	-1.741050210	6.867751810
6	-4.233491210	2.218478570	1.188306020	1	-2.378588350	-2.738021000	8.221731710
1	-4.269960710	3.319162690	1.134767280	1	-3.603985700	-3.403977460	7.101068890
1	-4.972306300	1.817842520	0.474202580	6	-1.220561520	-4.728990140	6.666648860
1	-3.232820110	1.872030880	0.872434390	1	-2.110832650	-5.378430510	6.663988580
19	3.178732580	-0.903423810	0.094195930	1	-0.788809230	-4.741499980	7.680883330
14	-0.361910100	3.401042070	-3.495584550	1	-0.482334500	-5.134900940	5.958797740
14	-1.448866830	-3.264739600	3.418429860	6	-0.372799840	-2.382119770	6.323638730
7	0.297063120	1.849253400	-3.271333630	1	0.417878610	-2.751618050	5.651655850
8	0.146241890	4.634775360	-2.415254250	1	0.026618910	-2.348856200	7.350389740
8	-0.170538210	4.133684490	-5.000578160	1	-0.640305190	-1.358379780	6.021186980
8	-1.979604410	3.270933720	-3.033725660	6	0.921508480	-4.769632230	2.693096160
7	-1.173253930	-1.673811200	2.826779530	6	1.115152890	-6.248342990	3.061282520
8	-2.581240150	-3.980856580	2.359373370	1	1.353369950	-6.345752080	4.132225350
8	-2.171398210	-3.319976060	4.927694040	1	1.937811230	-6.692783700	2.477343930
8	-0.116253280	-4.270731240	3.560812000	1	0.196107580	-6.820392940	2.858082400
6	1.349227220	5.442773420	-2.444089390	6	2.210525980	-3.990556340	2.985124560
6	1.519558240	5.997664540	-1.022428240	1	2.082970150	-2.928637510	2.724310560
1	0.621046360	6.563856090	-0.721234480	1	3.053826920	-4.394415360	2.399591600
1	2.381017180	6.683337140	-0.968714720	1	2.470802150	-4.056584450	4.053587220
1	1.697597780	5.179879020	-0.302569380	6	0.547172250	-4.633480530	1.213554630
6	2.571950850	4.591729570	-2.809939330	1	-0.399076980	-5.160393190	1.009979250
1	2.639491570	3.723399670	-2.135059580	1	1.327927370	-5.089426960	0.581209500
1	3.498289370	5.184038380	-2.722472730	1	0.454254580	-3.570121250	0.923804510
1	2.497591620	4.227721280	-3.846297750	19	-0.965084180	3.852154090	0.019276260
6	1.164834980	6.600577580	-3.435087070	19	-2.238967850	-2.562515540	0.066519080
1	0.946982950	6.202317950	-4.436709770	1	1.288042420	-2.213043960	-2.647886840
1	2.071643440	7.226499950	-3.478849890	1	-2.622316900	0.022265920	-2.494353940
1	0.319732900	7.237573710	-3.124235860	1	1.281264430	1.799450620	-3.574380120
6	0.118057160	3.590799510	-6.315512690	1	1.859790570	-1.014260970	3.094806190
6	1.628015780	3.340114110	-6.435223760	1	-1.631946200	-1.050284910	3.514557080
1	2.189877370	4.265788310	-6.232053170	1	-0.058281810	1.804718600	3.661644260
1	1.884200120	2.996406120	-7.450700930				
1	1.947651480	2.563125950	-5.723748440				

Neptunium-O Species

Reactant -LS

93	1.605526210	-0.460533780	-1.279645510	1	3.201319720	-1.194066560	-4.785085490
93	-1.707579410	0.430043430	1.180551280	6	2.342419320	-0.955325810	-7.407919770
19	0.450785010	-2.645929600	1.586700980	1	3.294300700	-1.121583880	-7.936945760
19	1.380345650	2.603029420	0.947650180	1	1.532218450	-0.895768250	-8.152312620
19	-1.935892370	-0.015073510	-2.528620620	6	2.395217670	0.008488360	-6.877727900
14	0.121625460	-2.234525210	-4.362527540	6	3.663769850	-4.570363800	2.917260370
14	3.937484810	-2.677279210	0.820466080	1	2.830942450	-4.526091510	4.202842800
14	3.325384950	2.891198450	-2.046082620	1	3.143400840	-5.320304840	4.900539730
14	-0.364720480	2.554731060	4.078212030	1	2.953702190	-3.553432750	4.707191780
14	-3.949761760	2.516541380	-1.144445900	1	1.761484030	-4.675212570	3.982711810
8	0.544838750	-1.329370490	-3.079947700	6	3.475129450	-5.907800190	2.190228290
8	-1.543599660	-1.941688060	-4.530678330	1	3.838226960	-6.745240130	2.808539660
8	0.441088850	-3.870152400	-4.226521650	1	2.408857670	-6.081547280	1.969501450
8	0.772012530	-1.787810730	-5.831067820	1	4.028938900	-5.893892600	1.239369770
8	2.738993110	-1.897892430	0.044898270	6	5.143451150	-4.353002150	3.258852550
8	3.136149610	-3.506888290	2.067724380	1	5.487988900	-5.151853630	3.935953810
8	4.729604180	-3.867652520	-0.037397540	1	5.763668730	-4.372833970	2.351226150
8	5.154480230	-1.700141700	1.421165330	1	5.291658870	-3.383942280	3.759258190
8	2.527346090	1.590656950	-1.482521440	6	5.824574260	-3.771965010	-0.987312900
8	4.981774350	2.752462560	-2.176959610	1	5.744533320	-5.047594720	-1.833853360
8	3.078133410	4.062147860	-0.840776240	1	6.566431210	-5.079981010	-2.566675820
8	2.823493500	3.431574220	-3.548307020	1	5.815697140	-5.937072390	-1.187565850
8	-2.208216590	-1.647992250	1.923011090	1	4.786129040	-5.088074540	-2.373777390
8	-1.798597650	-4.157246990	2.530892530	6	7.151331450	-3.724916870	-0.216208830
8	-4.335960730	-3.416941460	1.608772800	1	8.001869430	-3.656140520	-0.913945310
8	-0.720385520	1.785661850	2.691471480	1	7.164358530	-2.852649650	0.454168120
8	-0.259489720	1.575082830	5.430494130	1	7.274168270	-4.638284430	0.387987100
8	-1.415955600	3.769259960	4.526873460	6	5.673673930	-2.531217970	-1.874971240
8	1.096241310	3.347494250	3.729951440	1	6.478689320	-2.495272060	-2.627172180
8	-3.123353790	1.378111700	-0.327667050	1	4.705325500	-2.545533260	-2.401475830
8	-5.473862870	2.866175120	-0.560617240	1	5.726747540	-1.613897530	-1.267475070
8	-3.204473570	3.999955280	-1.325209750	6	5.142731070	-0.380708490	2.018117050
8	-4.026041710	1.923555750	-2.734060040	6	6.280994720	-0.376110940	3.047857600
7	-0.040449940	-0.022233740	-0.033446900	1	6.380304970	0.618514880	3.511906130
6	-2.412399220	-2.276548780	-5.653686060	1	6.086594970	-1.112728160	3.843878380
6	-2.348350120	-1.127384090	-6.668010010	1	7.234098870	-0.634866380	2.560554310
1	-3.008035980	-1.324733490	-7.529128000	6	5.420773120	0.646722290	0.916566860
1	-2.667159690	-0.179398390	-6.203586030	1	5.477928630	1.668227770	1.329462830
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1	-3.853672000	-3.238176920	-4.336517250	1	3.828413980	0.916679790	3.170755510
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6	-2.007845160	-3.597553150	-6.320215290	6	3.606253050	-0.823668360	3.502854050
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1	-2.018550380	-4.422756100	-5.591855300	1	5.782272560	0.541344310	-4.651643620
6	0.385370310	-4.780030720	-3.101111630	1	4.922032810	0.215419680	-3.118430770
6	-0.685853000	-4.359342120	-2.088931750	1	4.176539710	1.268250040	-4.357901890
1	-0.726122390	-5.078904510	-1.253353070	6	7.124997250	1.808775810	-2.592581670
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6	0.041712700	-6.153699510	-3.693201320	1	7.833472480	1.432518810	-3.347699480
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6	1.767969990	-4.818557700	-2.441394000	1	5.063524630	3.640126260	-4.705831860
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1	2.039532990	-3.830797750	-2.034015510	1	5.585805660	6.048934500	0.295011060
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6	1.969912330	-3.435388810	-7.152055330	6	5.701722290	4.405666290	-0.418973230
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6	3.160953520	-2.142233940	-5.344462700	6	3.173848490	6.145443350	-2.620135170
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6	1.571193980	4.693196520	-5.129537870	1	-1.855750030	4.696558160	7.011141330
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1	0.696126830	4.756432780	-2.514352900	6	1.704906290	4.481663820	4.418754570
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6	-6.119290980	-3.455319320	0.044606040	1	1.514194810	6.656890570	4.370693830
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6	-3.870778660	-2.582737780	-0.667018390	1	3.735527980	5.277448960	4.513928340
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1	-0.366984280	0.459143540	7.772157860				
1	-1.413754090	-0.467070860	6.655038690				
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1	-4.441239800	2.447379770	5.395579680				
				Reactant -HS			
				93	1.603685100	-0.459133920	-1.286370500
				93	-1.713036550	0.433338980	1.177763290
				19	0.452941410	-2.634404100	1.586873310
				19	1.381118540	2.601189130	0.948695050
				19	-1.940919060	-0.018193970	-2.531928090

14	0.108661480	-2.240231700	-4.360733410		1	3.150795050	-5.298697730	4.908820510
14	3.938238630	-2.669788640	0.818670670		1	2.957977400	-3.532901450	4.709337670
14	3.322984370	2.894236620	-2.042902090		1	1.767215640	-4.659384730	3.989426310
14	-0.366636560	2.549004970	4.079651110		6	3.481441110	-5.895985570	2.201080910
14	-3.948145870	2.519905560	-1.156573930		1	3.846244360	-6.730253870	2.822692220
8	0.532063220	-1.331473580	-3.080943690		1	2.415295320	-6.072221410	1.981780990
8	-1.558436680	-1.954781210	-4.524213960		1	4.034611810	-5.885368650	1.249809780
8	0.437123030	-3.874177080	-4.224603120		6	5.148087690	-4.334310720	3.262204360
8	0.752114620	-1.791715460	-5.832006080		1	5.494173570	-5.129911170	3.942348400
8	2.739036060	-1.893049950	0.041903080		1	5.767772530	-4.356991620	2.354270030
8	3.138426780	-3.496058680	2.069194860		1	5.295362820	-3.362961640	3.758423340
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8	3.097881360	4.058744910	-0.826730770		1	4.787765260	-5.096424560	-2.365036250
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8	-1.793254970	-4.151565500	2.542203060		1	7.163314070	-2.839684350	0.448222100
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8	-0.099950350	-4.192087030	3.715422330	1	0.640026870	-6.700884330	3.271555700
6	1.142722270	5.0485328700	-2.143929850	6	2.238353970	-3.614509250	3.485202370
6	1.139361870	5.622736040	-0.720862850	1	2.000898090	-2.585884860	3.171220680
1	0.312091360	6.342827950	-0.602545700	1	3.204405250	-3.900215260	3.035475830
1	2.082556980	6.153652340	-0.511401300	1	2.359747870	-3.622756450	4.579583850
1	1.030000240	4.815206680	0.022698110	6	0.989630730	-4.596562670	1.536007480
6	2.252590660	4.001170430	-2.279669130	1	0.140276140	-5.232327440	1.232216890
1	2.077732630	3.177707580	-1.570321510	1	1.901659490	-5.007198500	1.073357410
1	3.234911990	4.455909390	-2.067951870	1	0.852573100	-3.569711880	1.153848600
1	2.280638680	3.579662460	-3.295680140	19	-1.719532220	3.478790270	-0.231128610
6	1.309459940	6.181272000	-3.164970680	19	-1.606559570	-2.960064840	-0.206409560
1	1.228060800	5.788857770	-4.188900110				
1	2.288564180	6.673280640	-3.042899230				
1	0.519544280	6.938254550	-3.026140520				
6	0.112867490	3.483551480	-6.211924750				
6	1.613907740	3.207217560	-6.063424450				
1	2.148174510	4.128462900	-5.781118130				
1	2.035049880	2.841859010	-7.014112320				
1	1.785159900	2.442410500	-5.290316480				
6	-0.632726660	2.207034350	-6.610941460				
1	-0.519226950	1.442838620	-5.827478230				
1	-0.233031150	1.808424970	-7.557760460				
1	-1.705649060	2.414215070	-6.745169720				
6	-0.123465430	4.591348540	-7.246420390				
1	-1.200004070	4.804282660	-7.343370540				
1	0.263298170	4.288791730	-8.232527310				
1	0.385894520	5.518287140	-6.938445120				
6	-3.399520700	4.280971480	-3.546667590				
6	-2.918638340	5.737107310	-3.504176140				
1	-2.588733630	6.017352100	-2.490624400				
1	-3.735820910	6.415074680	-3.802406200				
1	-2.072659850	5.886725560	-4.193627120				
6	-3.842926060	3.906567620	-4.967074010				
1	-3.007478070	4.045577780	-5.668856190				
1	-4.684627770	4.539471310	-5.293558810				
1	-4.161147210	2.852622860	-4.998796300				
6	-4.565130130	4.074590680	-2.569673330				
1	-4.838652030	3.007811080	-2.526305350				

Neptunium-NH Species

Reactant:

Reactant -LS

93	1.683954470	-0.470214330	-1.186430750
93	-1.720147380	0.408486470	1.117778660
19	0.498681330	-2.582506870	1.659658300
19	1.270677450	2.746509370	0.786707530
19	-1.600433740	0.471097370	-2.704586180
14	0.168959500	-1.985909620	-4.542292910
14	3.854347730	-3.290189710	0.674623690
14	3.276976670	3.095325020	-1.859381480
14	-0.371807270	2.907530000	3.896915960
14	-4.023565230	2.546621530	-1.166926270
7	0.866502450	-1.028591900	-3.291873310
8	-1.346159460	-1.279219230	-4.872270280
8	-0.016828870	-3.615853770	-4.232042170
8	0.989663890	-1.909653460	-5.999209340
7	2.767082580	-2.342043040	-0.264809060
8	3.149309260	-3.355638220	2.220614760
8	3.967580160	-4.893814110	0.199482250
8	5.453564980	-2.791057400	0.775626510
7	2.965447820	1.511917870	-1.267196450
8	4.182666790	4.077837380	-0.827438950
8	1.754269760	3.828744460	-1.828288900
8	4.062600310	3.246410380	-3.332794580

7	-2.216202400	-1.479003230	2.424098220		1	6.859399120	-6.360359140	-0.807095500
8	-1.709865240	-4.137549890	2.258621840		1	6.667057190	-4.859505550	0.158746390
8	-4.382109460	-3.430604790	2.523229040		1	6.084246890	-6.423590710	0.801497180
7	-1.041194830	2.142847620	2.507703380		6	4.975601300	-4.740644410	-2.038621220
8	0.231375040	1.875472350	5.059671590		1	5.609884070	-5.272754100	-2.766201250
8	-1.394207060	3.940434730	4.723925980		1	3.992379660	-4.568490160	-2.505169870
8	0.855613730	3.922145890	3.291235290		1	5.440872230	-3.765634730	-1.824286690
7	-3.378439580	1.159380480	-0.388644400		6	6.079696850	-1.488262280	0.766881670
8	-5.687429660	2.790015720	-1.163621490		6	7.466689260	-1.689007430	1.394919360
8	-3.343551070	3.958805850	-0.581646770		1	8.034078900	-0.744272740	1.392341990
8	-3.497145280	2.460368590	-2.789118320		1	7.372634770	-2.038320150	2.435005450
7	-0.026467660	-0.007279210	-0.066495440		1	8.035755580	-2.440603230	0.825472350
6	-2.205817710	-1.447101080	-6.039396320		6	6.225976650	-1.024518940	-0.688351090
6	-1.741817380	-0.464657860	-7.122695740		1	6.724619460	-0.043753720	-0.744349370
1	-2.383292750	-0.534657840	-8.016572070		1	6.826346140	-1.751464960	-1.258403560
1	-1.782214210	0.571546510	-6.748908220		1	5.233689550	-0.946812920	-1.165028500
1	-0.702456940	-0.690448370	-7.405406470		6	5.270565780	-0.479148580	1.590822500
6	-3.623174210	-1.104919630	-5.563907970		1	5.781213680	0.498278240	1.619088170
1	-4.342924220	-1.171997850	-6.396203290		1	4.265780650	-0.333507450	1.158285990
1	-3.943734080	-1.802825420	-4.772634590		1	5.153963920	-0.835064420	2.627448340
1	-3.666621850	-0.078749370	-5.162953510		6	5.615260430	4.263468940	-0.703773540
6	-2.177917840	-2.882466560	-6.578491930		6	6.355274640	2.928694980	-0.853226590
1	-2.863360710	-2.968868850	-7.437671970		1	7.439968810	3.068123500	-0.713169090
1	-1.166147990	-3.157224180	-6.908996630		1	5.999063430	2.211639390	-0.095824690
1	-2.497433280	-3.597765720	-5.806207640		1	6.188230800	2.503126890	-1.855822470
6	-0.531567150	-4.393690000	-3.127329540		6	5.841713320	4.833079920	0.701750270
6	-1.400417250	-3.548016530	-2.192390310		1	5.281738140	5.773536400	0.827404280
1	-1.788409880	-4.164001600	-1.365346800		1	5.495669830	4.118743680	1.466198450
1	-0.821522120	-2.716820470	-1.749925380		1	6.911174440	5.038380820	0.872429060
1	-2.263004740	-3.127379000	-2.736111490		6	6.089427850	5.264571040	-1.766927010
6	-1.362686770	-5.528393240	-3.743597690		1	5.577947840	6.231966410	-1.633042080
1	-1.724993310	-6.213704590	-2.959927140		1	7.175337210	5.435741690	-1.682580610
1	-2.236201170	-5.125546670	-4.279934070		1	5.861976800	4.880383370	-2.772474620
1	-0.751689310	-6.103354120	-4.457156000		6	1.390608390	5.222527490	-2.056454410
6	0.667293920	-4.980288660	-2.372801680		6	1.423998520	5.961159890	-0.710688550
1	0.338289810	-5.659062520	-1.569067310		1	1.169089650	7.025900700	-0.842137960
1	1.304884820	-5.548281980	-3.068501720		1	0.689919040	5.533824870	-0.006748380
1	1.267199360	-4.177452930	-1.915437230		1	2.433112340	5.894817860	-0.273808350
6	2.151313410	-2.641210080	-6.469067410		6	2.327596270	5.917994390	-3.051649140
6	1.675859480	-3.943759390	-7.128623350		1	1.977862390	6.948632650	-3.227781280
1	2.532576750	-4.520822170	-7.513472430		1	3.356536890	5.960862630	-2.664865160
1	1.133175670	-4.557382390	-6.393476400		1	2.341470090	5.387015200	-4.015027460
1	1.001898940	-3.721659500	-7.971607440		6	-0.035377160	5.189075970	-2.613408200
6	3.126765070	-2.949213330	-5.326081960		1	-0.418320720	6.211956110	-2.765556850
1	4.015000960	-3.473029130	-5.715783150		1	-0.047325740	4.668641750	-3.584622860
1	3.458027820	-2.023723410	-4.828571900		1	-0.715096150	4.659391180	-1.925531620
1	2.645856330	-3.592735230	-4.573172990		6	3.912779190	2.518621350	-4.578206620
6	2.817664000	-1.728131540	-7.505778320		6	4.617815960	3.377229720	-5.637203630
1	3.697150280	-2.218792110	-7.952337590		1	4.560894340	2.898035020	-6.627682210
1	2.105432890	-1.482046300	-8.309444500		1	4.147028750	4.371119880	-5.700187370
1	3.141824220	-0.787759860	-7.031639190		1	5.678660190	3.511732790	-5.373134230
6	3.576199020	-4.128955110	3.385099110		6	2.431447280	2.348098680	-4.936941820
6	2.808972000	-3.536840960	4.573030850		1	2.318282570	1.784114460	-5.877944850
1	3.056175900	-4.072522090	5.504053580		1	1.899823820	1.801757310	-4.139981710
1	3.068268740	-2.474096750	4.704869590		1	1.946186630	3.329355740	-5.060617970
1	1.719575550	-3.617664560	4.421083460		6	4.606251800	1.155708420	-4.457841360
6	3.196949240	-5.602336420	3.188493860		1	4.559155980	0.609124160	-5.413887830
1	3.482970490	-6.194631990	4.073235300		1	5.666229290	1.290526880	-4.187855110
1	2.110251860	-5.708687120	3.043248510		1	4.121724650	0.542614320	-3.679138120
1	3.699482370	-6.007813710	2.299064080		6	-5.209065630	-3.150705670	1.371986300
6	5.083900050	-3.999857320	3.638018550		6	-6.309165020	-4.222027170	1.378070230
1	5.351553100	-4.549306920	4.555705790		1	-7.013810660	-4.059813910	0.546476950
1	5.668371710	-4.407398990	2.800827500		1	-5.870258300	-5.226665660	1.274553610
1	5.365951830	-2.943793970	3.772883060		1	-6.870185280	-4.184058110	2.325085790
6	4.826552500	-5.565898960	-0.753461440		6	-5.829517280	-1.759079170	1.537422440
6	4.128804300	-6.897305050	-1.060235670		1	-6.492188530	-1.522555750	0.689791540
1	4.717780650	-7.492202650	-1.776564130		1	-6.422598030	-1.712003330	2.465027670
1	4.004366030	-7.483736430	-0.135736040		1	-5.035802200	-0.994865380	1.592937340
1	3.130043850	-6.713365260	-1.487360970		6	-4.399590690	-3.231511750	0.072959220
6	6.198648700	-5.817112030	-0.111724180		1	-5.047585420	-3.049121440	-0.801189570

1	-3.589545880	-2.481554340	0.070855780	1	-6.426104230	0.824386550	-2.871477130
1	-3.946053010	-4.229619680	-0.038144980	1	-5.840926790	0.006962050	-1.396539230
6	-1.618303360	-5.575848270	2.497211530	6	-7.087065630	1.636334240	0.455225330
6	-0.766982350	-6.130314910	1.348369520	1	-7.953984360	0.967942980	0.583048970
1	-1.255883310	-5.931398510	0.381292440	1	-6.205891420	1.158725890	0.910606770
1	0.236272830	-5.672631410	1.332756580	1	-7.293855250	2.573567220	0.995440810
1	-0.633350380	-7.219453700	1.452583750	6	-8.021107800	2.715495620	-1.610521130
6	-2.996226220	-6.250103750	2.484051470	1	-8.960201770	2.151136660	-1.494854190
1	-3.506013810	-6.075734310	1.523945900	1	-8.122922980	3.678175030	-1.085865920
1	-2.874641570	-7.337475580	2.619869720	1	-7.867708800	2.919008910	-2.682270840
1	-3.638049960	-5.865836850	3.289912200	6	-3.794050650	4.899314700	0.428825340
6	-0.926592120	-5.816858910	3.845253540	6	-2.544918670	5.686079620	0.842433250
1	-0.812977610	-6.896853860	4.035679270	1	-2.797470240	6.460362600	1.585330380
1	0.077444720	-5.363179160	3.854327600	1	-1.794762520	5.016769040	1.295354930
1	-1.513957170	-5.362410000	4.656094960	1	-2.094513500	6.174207100	-0.036179990
6	-3.666602060	-3.007581120	5.642524190	6	-4.398051150	4.181614760	1.640329860
6	-4.743873130	-4.100979530	5.681948530	1	-4.680298510	4.916330450	2.411805670
1	-5.449895070	-3.922153440	6.509492340	1	-5.296054350	3.618468770	1.349163100
1	-5.297110790	-4.115780430	4.731431680	1	-3.678423670	3.474529310	2.082855130
1	-4.276350340	-5.087506990	5.833596910	6	-4.832806160	5.851768410	-0.183507870
6	-2.832064570	-3.032521430	6.929363410	1	-5.177876700	6.576042200	0.572439930
1	-3.462922650	-2.831532560	7.809982530	1	-4.395432290	6.412277450	-1.024174660
1	-2.356425500	-4.018381240	7.056132150	1	-5.699063770	5.279021870	-0.547841160
1	-2.036462510	-2.271648090	6.881156430	6	-3.799428180	3.300487940	-3.943147990
6	-4.308843110	-1.626031680	5.457656330	6	-3.914207600	4.780618590	-3.566656740
1	-4.999450750	-1.408650140	6.288751590	1	-4.064297180	5.384316720	-4.477545670
1	-3.538855390	-0.8377749840	5.440408630	1	-4.770482180	4.947609420	-2.897540280
1	-4.879879810	-1.584733980	4.516478090	1	-3.001690000	5.126086360	-3.058925350
6	1.114724560	0.732871820	5.074597590	6	-2.630500480	3.102354260	-4.916226230
6	0.251791250	-0.512852900	5.306769790	1	-2.776829020	3.697788120	-5.832214870
1	0.876639570	-1.413527060	5.418368960	1	-1.683936720	3.418223970	-4.449151930
1	-0.340169770	-0.390354030	6.227913070	1	-2.545100060	2.045002040	-5.218220790
1	-0.443101220	-0.672088040	4.465516200	6	-5.106764920	2.821259230	-4.586000780
6	1.910267550	0.608650890	3.770483060	1	-5.315217100	3.388800550	-5.508329870
1	2.526305690	1.508851790	3.605133000	1	-5.044523430	1.752193530	-4.847579670
1	2.585765220	-0.261625820	3.809703950	1	-5.945982380	2.968018340	-3.890334870
1	1.232581080	0.473465110	2.907047810	14	-2.803833820	-3.019812580	2.921205040
6	2.070177320	0.937740920	6.258979300	8	-2.732907080	-3.295731510	4.573615480
1	2.694460320	1.832120440	6.104741040	1	1.481330090	-0.354162250	-3.793969920
1	1.497609610	1.071340180	7.190308470	1	3.886530630	1.064938270	-1.089794660
1	2.735680680	0.066955170	6.378323400	1	-4.013370570	0.348405650	-0.489088500
6	-2.397938250	3.662689050	5.735947870	1	2.818236140	-2.762688980	-1.218539100
6	-3.113712360	2.333612410	5.464923970	1	-2.501401180	-0.838921640	3.198881630
1	-2.398237040	1.497354760	5.509153530	1	-1.661587540	2.857167360	2.070883930
1	-3.897461060	2.162451790	6.221195570				
1	-3.582480810	2.335434170	4.467971730				
6	-1.715963770	3.631070000	7.111170800				
1	-1.235282780	4.599813800	7.322923090				
1	-2.453868020	3.431072140	7.905328640				
1	-0.947589060	2.843447720	7.130060110				
6	-3.391075620	4.828536710	5.659886480				
1	-2.867434260	5.784115190	5.822591060				
1	-3.867508260	4.857819310	4.667656080				
1	-4.175937840	4.722648290	6.425757370				
6	1.496948870	5.080742340	3.906593140				
6	1.724246290	4.873873410	5.408645350				
1	2.242698600	5.749797700	5.832345010				
1	0.767247060	4.744623290	5.933984480				
1	2.345195660	3.983208630	5.590715410				
6	0.613655250	6.309851840	3.658149660				
1	1.075578090	7.215651720	4.084922080				
1	0.474681700	6.469967620	2.575984200				
1	-0.374130680	6.158325140	4.119431490				
6	2.844801040	5.234015800	3.193523640				
1	3.396339420	6.106027310	3.581901540				
1	3.467537900	4.337076890	3.348120500				
1	2.701691960	5.380677320	2.110175420				
6	-6.838694550	1.924578390	-1.031939120				
6	-6.657554090	0.616446460	-1.815346900				
1	-7.580605430	0.015216480	-1.774475650				
				Reactant -HS			
	93	1.674089740	-0.514506510	-1.189816990			
	93	-1.761288030	0.442435500	1.128108640			
	19	0.535244680	-2.443742740	1.872601300			
	19	1.323849760	2.691432550	0.804831050			
	19	-1.660772540	0.417220390	-2.697710600			
	14	0.137404270	-1.939630860	-4.610193720			
	14	3.775128730	-3.360227270	0.728924100			
	14	3.337935170	3.047294090	-1.826679240			
	14	-0.360539790	2.944973540	3.884686160			
	14	-4.086669620	2.490964490	-1.204276010			
	7	0.821238370	-0.993609000	-3.349354050			
	8	-1.385126260	-1.247048900	-4.945133070			
	8	-0.043411390	-3.573469960	-4.304729640			
	8	0.953307200	-1.860266420	-6.070177280			
	7	2.629756730	-2.455837310	-0.176259120			
	8	3.154602380	-3.426547870	2.317547600			
	8	3.904083730	-4.965892340	0.267864080			
	8	5.357272140	-2.803186090	0.772026770			
	7	3.034092820	1.463589800	-1.242833890			
	8	4.222814970	4.038251890	-0.782387650			
	8	1.805248140	3.764866030	-1.818347010			
	8	4.140795850	3.215421830	-3.291544630			
	7	-2.199494820	-1.427082250	2.550561650			
	8	-1.653945730	-4.066362670	2.328772800			

8	-4.339241840	-3.412110730	2.585712130		1	6.050503030	-6.462496940	0.818481050
7	-1.039541430	2.235864850	2.475738800		6	4.856254540	-4.800908440	-1.998721890
8	0.197350040	1.856015770	5.021896480		1	5.482977290	-5.327701860	-2.736680640
8	-1.354636120	3.982068320	4.742184750		1	3.862493910	-4.639896890	-2.444915800
8	0.902095590	3.938741230	3.314495120		1	5.310588660	-3.818942870	-1.795615710
7	-3.465488250	1.091848940	-0.436131180		6	5.932077760	-1.481383220	0.708205220
8	-5.748826880	2.752386590	-1.232149260		6	7.339736810	-1.603195900	1.309705960
8	-3.400907400	3.889628820	-0.586814540		1	7.867786730	-0.637036500	1.261496730
8	-3.529488480	2.431237460	-2.818773970		1	7.283978050	-1.919985300	2.362871170
7	-0.023104510	-0.013320360	-0.016096160		1	7.925892570	-2.350646080	0.752398270
6	-2.231990460	-1.406482190	-6.122880520		6	6.027409650	-1.058779660	-0.763953820
6	-1.767747730	-0.404855560	-7.188363260		1	6.470282620	-0.054682190	-0.862898330
1	-2.400271330	-0.468698230	-8.089086010		1	6.657643120	-1.770390490	-1.320818700
1	-1.821556220	0.625568810	-6.800935000		1	5.025154380	-1.057037520	-1.226301720
1	-0.723895050	-0.617562530	-7.464560010		6	5.100045020	-0.482936900	1.522621900
6	-3.656596340	-1.084405270	-5.655035690		1	5.558582830	0.520112060	1.501124550
1	-4.368611460	-1.142945940	-6.494595170		1	4.075366560	-0.400292710	1.120543750
1	-3.977978960	-1.798793720	-4.878882180		1	5.033121890	-0.808158170	2.573614020
1	-3.711044540	-0.065887510	-5.236360460		6	5.650043810	4.259339580	-0.656996430
6	-2.184685460	-2.833735220	-6.682029640		6	6.425247400	2.945598710	-0.817476160
1	-2.861103820	-2.914990100	-7.548830280		1	7.506077420	3.112050210	-0.677412220
1	-1.166719140	-3.092453200	-7.006441050		1	6.089494510	2.214296130	-0.064110450
1	-2.503697020	-3.563407780	-5.923168620		1	6.267171750	2.523728180	-1.822956760
6	-0.553303960	-4.359510630	-3.207438010		6	5.862418310	4.822282680	0.753417710
6	-1.335871380	-3.507447850	-2.203818270		1	5.276539860	5.745396590	0.888591850
1	-1.719698740	-4.133511020	-1.382662710		1	5.537583750	4.091535720	1.511678180
1	-0.703810480	-2.718293770	-1.758403070		1	6.925919950	5.055871800	0.925045470
1	-2.199325930	-3.028937820	-2.696427840		6	6.100989490	5.280759940	-1.710933970
6	-1.470874640	-5.431767080	-3.813610410		1	5.568938190	6.235601370	-1.567620050
1	-1.815305230	-6.133106490	-3.035896640		1	7.182915440	5.475127930	-1.625482850
1	-2.357077250	-4.970185130	-4.276953240		1	5.881919490	4.900683290	-2.719887170
1	-0.931053530	-6.001209350	-4.586335490		6	1.430427530	5.155831270	-2.043315480
6	0.649345110	-5.033112060	-2.535063070		6	1.430407590	5.884573300	-0.691702940
1	0.336711630	-5.678053330	-1.697858370		1	1.170933820	6.948513240	-0.819808530
1	1.195434440	-5.646547970	-3.268536670		1	0.685010870	5.446521960	-0.006323490
1	1.339390950	-4.269617140	-2.142589720		1	2.430832920	5.822188370	-0.234710440
6	2.135462260	-2.565843770	-6.528140750		6	2.377074460	5.867735850	-3.017273580
6	1.691942910	-3.875334680	-7.196564960		1	2.020162560	6.895932850	-3.193145480
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1	1.022119130	-3.663691810	-8.045531890		6	0.014470530	5.113767140	-2.625579090
6	3.106499130	-2.859480950	-5.377498590		1	-0.374674380	6.134233840	-2.777984680
1	4.009730450	-3.359755400	-5.763588480		1	0.023097350	4.598656140	-3.599516110
1	3.411006170	-1.930796820	-4.869852670		1	-0.672309350	4.575084620	-1.951807890
1	2.635593480	-3.519601500	-4.632908880		6	4.009972380	2.480904490	-4.534517080
6	2.794104120	-1.636721000	-7.555640340		6	4.735266260	3.330281990	-5.587225060
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1	3.096669490	-0.692269590	-7.075275790		1	5.793174030	3.458650200	-5.308819860
6	3.651406090	-4.173631240	3.470523720		6	2.533687270	2.315128740	-4.916075000
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6	3.296422000	-5.657572330	3.310655740		1	4.665025390	0.566106000	-5.352343060
1	3.640660630	-6.232800510	4.185852930		1	5.748313700	1.245300400	-4.104369320
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1	3.762313650	-6.061910930	2.400905590		6	-5.141966460	-3.120923070	1.421352270
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1	5.488660420	-4.537492730	4.563859460		1	-6.916663000	-4.036093950	0.537034740
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6	4.745953050	-5.625972280	-0.709861280		6	-5.778881870	-1.736736590	1.590117140
6	4.057325180	-6.966255900	-0.998474150		1	-6.431306790	-1.499589800	0.734541920
1	4.638634620	-7.556713990	-1.724628510		1	-6.387229220	-1.705086220	2.508363140
1	3.957194450	-7.550589400	-0.069769560		1	-4.995355470	-0.963733630	1.665101340
1	3.048653720	-6.795094530	-1.407429840		6	-4.303549430	-3.176871970	0.138649210
6	6.135586220	-5.858753060	-0.099656670		1	-4.933030120	-2.984432320	-0.746790690
1	6.786540070	-6.396379300	-0.808452700		1	-3.497185870	-2.423791020	0.165761390
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6	-2.892135020	-6.211915530	2.483685140	1	-9.021369410	2.137886950	-1.608273200
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1	-3.552180160	-5.857866160	3.288822730	6	-3.863674330	4.817171050	0.429800160
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1	-3.546142720	-0.855541030	5.551445260	1	-4.782296450	4.929628560	-2.905073240
1	-4.871086850	-1.601648900	4.602447850	1	-3.009750870	5.096511900	-3.033781240
6	1.117319080	0.745015330	5.038109090	6	-2.623823330	3.101289810	-4.919777080
6	0.298168590	-0.521636020	5.313900470	1	-2.753614500	3.707337330	-5.831321070
1	0.953819200	-1.400053710	5.428851250	1	-1.683680890	3.408257150	-4.434441620
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6	1.739991360	4.914575930	5.430766290	8	3.857059930	-0.135247430	4.856872070
1	2.241762410	5.799442100	5.855928650	8	3.662768380	2.100651130	3.451153460
1	0.777942240	4.775151630	5.944023380	6	-5.556510900	-1.989452710	-2.018686710
1	2.371411760	4.033808880	5.625381970	6	-6.108118480	-2.334051480	-0.629541450
6	0.639713930	6.329512370	3.655844520	1	-6.083062030	-3.424235100	-0.469249150
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1	0.507342840	6.474715430	2.570652720	1	-5.509924780	-1.848273950	0.160205450
1	-0.350203990	6.179182520	4.112696850	6	-5.537918940	-0.466578210	-2.208179770
6	2.881204550	5.263398100	3.223681960	1	-4.889956070	0.007745930	-1.452526110
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1	6.305388190	-1.444248710	0.628372770	1	1.683126740	-0.668254190	-7.130076400
1	7.845595910	-0.883818130	1.326125780	1	2.975479380	0.217938210	-6.275151320
1	6.702900670	0.302959880	0.638671300	6	4.042411230	-2.178412200	-7.074064370
6	6.186514590	-1.805522590	3.361166930	1	4.775409030	-1.356510340	-7.099759740
1	5.647941570	-1.708031310	4.315469760	1	3.548246460	-2.237376530	-8.056912300
1	7.236269040	-2.076343040	3.562549410	1	4.584962170	-3.120678790	-6.897027600
1	5.724043850	-2.621757690	2.780882980	6	5.290126160	0.719292460	-3.204341200
6	6.770174910	0.651532080	3.365351800	6	6.422993250	-0.314934170	-3.198759890
1	6.700735010	1.598653620	2.807462780	1	6.518704530	-0.786851200	-2.208731650
1	7.836423050	0.423796700	3.529639960	1	7.378547740	0.176379850	-3.447095310
1	6.284408200	0.785360430	4.342393730	1	6.235419500	-1.104111380	-3.943683310
6	3.494530650	0.345775410	6.160765390	6	5.160704970	1.352128060	-4.595714630
6	3.555624630	-0.893548630	7.062598760	1	4.981878630	0.573362300	-5.351775250
1	2.844615200	-1.657101690	6.708844550	1	6.084208500	1.891516050	-4.863179270
1	3.303843990	-0.632212820	8.102870290	1	4.322418830	2.066698600	-4.614391080
1	4.568406710	-1.326994920	7.044775760	6	5.561897800	1.805644510	-2.158581770
6	4.496951510	1.407234090	6.636090120	1	4.733713700	2.530515860	-2.135381860
1	5.512347930	0.981667350	6.682576210	1	6.495514970	2.344962430	-2.387698950
1	4.229234160	1.772675450	7.641122190	1	5.661613180	1.358025720	-1.156855540
1	4.500411530	2.256691930	5.936340950	6	-2.290468170	5.612891350	2.974776380
6	2.072975690	0.921752400	6.149488070	6	-2.305604080	6.376813040	1.642450300
1	2.022380070	1.813708860	5.504710030	1	-1.297705950	6.407959810	1.191618860
1	1.774387750	1.210899990	7.170335570	1	-2.621218200	7.421044300	1.798683640
1	1.358002980	0.174901790	5.771780650	1	-3.014147780	5.916446120	0.931279990
6	3.568738920	3.258713640	2.555552380	6	-1.243047310	6.229049180	3.911747290
6	4.754902610	4.174271200	2.892055890	1	-1.205778550	5.659340910	4.851070150
1	4.737711480	4.440595740	3.960618710	1	-1.485964360	7.282198010	4.131071890
1	4.713536290	5.102254700	2.298587220	1	-0.245358320	6.191977160	3.443076330
1	5.708045890	3.665712270	2.676910720	6	-3.688269150	5.668522940	3.604579350
6	2.247429800	3.977853400	2.856865510	1	-4.438973580	5.232509600	2.926472760
1	1.387203800	3.324544670	2.637541090	1	-3.969733360	6.715785510	3.805141500
1	2.157425890	4.893807620	2.247699760	1	-3.709268600	5.111799900	4.551464450
1	2.202198070	4.269016650	3.918688350	6	-2.204928650	2.834810600	6.461730560
6	3.625420090	2.834010890	1.084947840	6	-1.213834490	3.427343560	7.472048850
1	4.533575980	2.240266750	0.894425630	1	-0.184097180	3.138264110	7.208442060
1	3.662314670	3.723959160	0.434509550	1	-1.432767000	3.068242380	8.490359920
1	2.729412420	2.253622260	0.804230730	1	-1.277410140	4.527226210	7.467339110
7	0.230764240	-1.194639380	-0.010761980	6	-3.640073850	3.259406870	6.806176490
7	0.444291650	1.445046960	0.012644410	1	-3.712114070	4.357707110	6.860268610
7	-0.975328890	1.150629140	-0.125133560	1	-3.943642950	2.845944600	7.781896810
14	3.363884460	-1.381772770	-3.189738860	1	-4.332641530	2.896658200	6.031860590
14	-2.070480760	2.837980570	3.619923770	6	-2.091870480	1.305959590	6.446096950

1	-2.784196990	0.874575180	5.705678300	1	-3.119417500	-5.938057210	0.654924390
1	-2.339823360	0.896753480	7.438999420	6	-4.751659920	-4.469347950	3.357916600
1	-1.067529510	0.999400900	6.185827620	1	-4.420614160	-4.062512680	4.325071110
6	-4.568652110	1.762116420	2.625063020	1	-5.515359370	-5.245329490	3.532703720
6	-5.970276990	2.251514360	3.020429060	1	-5.212185460	-3.653336890	2.776262470
1	-6.200837510	1.947851280	4.053669710	6	-2.915635890	-6.202477160	3.386105920
1	-6.736277180	1.826923830	2.351218360	1	-2.053875990	-6.617422140	2.839855770
1	-6.024445010	3.350219280	2.961638670	1	-3.652504650	-7.009706760	3.532179930
6	-4.503683470	0.232787850	2.730522230	1	-2.571231350	-5.858492190	4.371372300
1	-3.498394780	-0.140121590	2.478018300	6	-1.594655530	-3.282720630	6.248121540
1	-5.232323970	-0.235027540	2.046733370	6	-2.701736300	-2.742718250	7.162263060
1	-4.739172180	-0.092233310	3.756736350	1	-2.986590610	-1.724395040	6.854458510
6	-4.234358950	2.215055230	1.199861930	1	-2.363073750	-2.713743240	8.210236410
1	-4.258519610	3.315710590	1.138091250	1	-3.593498610	-3.386665290	7.099425070
1	-4.977974470	1.817275970	0.489003860	6	-1.212440220	-4.712312220	6.657198610
1	-3.237828560	1.855986560	0.884545280	1	-2.102511210	-5.362013370	6.659023960
19	3.192597460	-0.898734160	0.085415810	1	-0.777626860	-4.721682850	7.670158640
14	-0.402604270	3.377571810	-3.457994130	1	-0.476107400	-5.120137730	5.948419900
14	-1.456950370	-3.256759090	3.404965740	6	-0.366574520	-2.366354600	6.301921960
7	0.250555980	1.819916260	-3.208217990	1	0.421305950	-2.739071080	5.628400960
8	0.098958080	4.606569710	-2.375512430	1	0.036669840	-2.328275230	7.327014030
8	-0.159381390	4.092500920	-4.961462270	1	-0.635737430	-1.344197180	5.995457270
8	-2.026788010	3.240779550	-3.043714170	6	0.907679380	-4.769957530	2.668908020
7	-1.191802020	-1.667091080	2.807764080	6	1.111117810	-6.239624290	3.066685810
8	-2.595214710	-3.976258320	2.354640720	1	1.365569590	-6.312555530	4.135869300
8	-2.171518740	-3.310035060	4.917854230	1	1.926381890	-6.694664580	2.480598700
8	-0.118974430	-4.255386540	3.540807990	1	0.190761710	-6.818308290	2.890132370
6	1.302587760	5.416577010	-2.400177310	6	2.198363020	-3.980834670	2.925070400
6	1.464241900	5.979232950	-0.980801110	1	2.062705250	-2.925488890	2.642529110
1	0.560493480	6.538947700	-0.684074950	1	3.034089790	-4.395181330	2.336089870
1	2.320531070	6.671482050	-0.930227510	1	2.473749040	-4.023251780	3.990964040
1	1.649393110	5.167641930	-0.255876190	6	0.512150830	-4.666821570	1.192396930
6	2.527583810	4.563882890	-2.754144760	1	-0.438249010	-5.195015980	1.014038750
1	2.589708700	3.697414370	-2.076205180	1	1.283322440	-5.138418480	0.559658700
1	3.453138040	5.156497320	-2.660202400	1	0.417977480	-3.610436190	0.878573530
1	2.461848590	4.197939530	-3.790413040	19	-0.922414850	3.765813910	0.086051350
6	1.123393400	6.569824460	-3.397264710	19	-2.274179710	-2.538338530	0.063688970
1	0.912368230	6.167688710	-4.398623240	1	1.311592300	-2.180596490	-2.631446970
1	2.030677710	7.195327670	-3.437557540	1	-2.585145330	0.044931510	-2.581509780
1	0.277064260	7.208696170	-3.093787250	1	1.236594270	1.762595290	-3.507633560
6	0.129445100	3.546714970	-6.274656390	1	1.872738130	-1.017372540	3.133078060
6	1.636204040	3.273844670	-6.382144230	1	-1.671311300	-1.043303520	3.481315840
1	2.209542250	4.192102590	-6.177231570	1	-0.069317510	1.820790140	3.682264870
1	1.895315780	2.923432750	-7.394493890				
1	1.939590770	2.494749260	-5.666024980				
6	-0.664025920	2.262096060	-6.533711350				
1	-0.437467260	1.516290010	-5.755458000				
1	-0.403804360	1.844356670	-7.520148910				
1	-1.745035520	2.465836650	-6.515418190				
6	-0.269744460	4.639963340	-7.275353000				
1	-1.347745620	4.853932450	-7.204913780				
1	-0.045034790	4.321702100	-8.305852250				
1	0.282165740	5.570471210	-7.067284490				
6	-3.165575020	4.098756220	-3.297209470				
6	-2.892400650	5.549566890	-2.875414930				
1	-2.657251840	5.616434660	-1.800312200				
1	-3.782753530	6.171266260	-3.066641810				
1	-2.044164520	5.972025710	-3.435721240				
6	-3.537164630	4.053688250	-4.785913550				
1	-2.725361300	4.479284030	-5.393316790				
1	-4.456929750	4.632651400	-4.970839720				
1	-3.711063080	3.012779310	-5.100898780				
6	-4.309893970	3.514934950	-2.460094130				
1	-4.519658060	2.478753300	-2.768384180				
1	-5.229248430	4.110219120	-2.583972680				
1	-4.044212580	3.502392290	-1.391029360				
6	-3.549719130	-5.048925830	2.600031320				
6	-3.984695370	-5.545847020	1.215349010				
1	-4.446504560	-4.730472840	0.632889210				
1	-4.727492940	-6.355376890	1.305745550				

Plutonium-O Species

94	1.613863300	-0.504439710	-1.274301870
94	-1.716584200	0.419946570	1.164044050
19	0.469844670	-2.631123200	1.645463070
19	1.392307600	2.556530580	0.954104500
19	-1.908658420	0.041724250	-2.557214410
14	0.095415280	-2.207993600	-4.386236470
14	3.938395150	-2.679867040	0.879710390
14	3.327223680	2.855016880	-2.038539520
14	-0.368965350	2.543056330	4.063006190
14	-3.926232360	2.549428270	-1.170418810
8	0.521011980	-1.325111020	-3.092958440
8	-1.570003010	-1.910081160	-4.548699060
8	0.414745440	-3.846946780	-4.271112050
8	0.742062990	-1.750751480	-5.855257040
8	2.732893910	-1.920088700	0.100847140
8	3.152974930	-3.485110450	2.153939480
8	4.721644140	-3.890719950	0.039496900
8	5.166019040	-1.693970150	1.446628940
8	2.574643270	1.536028180	-1.465111140
8	4.985620180	2.757483520	-2.192122860
8	3.068645200	4.027214770	-0.835551470
8	2.795631470	3.385730020	-3.536053480
8	-2.180809750	-1.662758670	1.947798340
8	-1.773748000	-4.166916470	2.572100620

8	-4.302989360	-3.426669290	1.618808620	1	7.274476290	-4.638645800	0.442604970
8	-0.741233320	1.795597420	2.672483160	6	5.629494340	-2.592869580	-1.844004400
8	-0.269237450	1.550489360	5.408813240	1	6.426132700	-2.567928610	-2.605483680
8	-1.405538660	3.763981500	4.532368310	1	4.656539870	-2.628001350	-2.360789910
8	1.101770600	3.324195040	3.725914870	1	5.681997010	-1.661560890	-1.258093660
8	-3.085934110	1.410305250	-0.373780340	6	5.164302120	-0.360960460	2.011701440
8	-5.450185530	2.883758940	-0.573500530	6	6.309647710	-0.335993200	3.033321540
8	-3.195066530	4.041719930	-1.342330790	1	6.417362410	0.668536550	3.474180680
8	-4.011161260	1.973938470	-2.766939800	1	6.119145760	-1.054231740	3.846871210
7	-0.024910320	-0.018746470	-0.028420310	1	7.258680000	-0.607983270	2.545294030
6	-2.444285890	-2.233906690	-5.670171400	6	5.438567410	0.639366550	0.884472130
6	-2.372075670	-1.084178910	-6.683283980	1	5.512151200	1.668898820	1.274161030
1	-3.035493260	-1.274336860	-7.543162440	1	6.391864110	0.397351880	0.388996620
1	-2.681763160	-0.134106800	-6.216919760	1	4.636623730	0.619095500	0.129002910
1	-1.338032760	-0.973151270	-7.043950430	6	3.834563160	-0.044646360	2.705405900
6	-3.853360970	-2.355395060	-5.076649390	1	3.858477040	0.970687030	3.137021900
1	-4.595569400	-2.553670630	-5.867245010	1	3.000322020	-0.106784680	1.985347790
1	-3.891127410	-3.184508870	-4.351101980	1	3.639803440	-0.759318830	3.521285060
1	-4.148425080	-1.426537150	-4.561500330	6	5.797187680	2.216028700	-3.267531280
6	-2.053151320	-3.557405130	-6.339445480	6	5.145259140	0.968195060	-3.874603930
1	-2.764571860	-3.788334880	-7.149380170	1	5.792903480	0.536211870	-4.654952090
1	-1.042541460	-3.496452480	-6.768789390	1	4.977676300	0.202794230	-3.099545340
1	-2.071660160	-4.383781680	-5.612538140	1	4.176589930	1.225254160	-4.331218090
6	0.371945190	-4.766762900	-3.154344090	6	7.142808130	1.855935210	-2.626959780
6	-0.688247750	-4.357932120	-2.125865720	1	7.585658650	2.744867400	-2.149944680
1	-0.719166080	-5.086317770	-1.297802010	1	7.005067690	1.081935620	-1.856242240
1	-0.463362620	-3.359900930	-1.712596130	1	7.846009220	1.477887280	-3.386132280
1	-1.687150090	-4.321844780	-2.589441620	6	5.987636340	3.298406310	-4.339594320
6	0.023053820	-6.135575720	-3.754981070	1	6.493427610	4.177665720	-3.908997010
1	0.017830430	-6.914754620	-2.975463240	1	6.605219490	2.917542380	-5.169443720
1	-0.972642870	-6.107522430	-4.225930250	1	5.008789820	3.609963220	-4.734179170
1	0.761966350	-6.412213380	-4.523332830	6	3.733070090	5.317556080	-0.681932290
6	1.761778400	-4.812189090	-2.509242250	6	5.027798210	5.101316390	0.111796260
1	1.796965840	-5.549647570	-1.689957960	1	5.552420390	6.057104560	0.275464120
1	2.514573680	-5.097061660	-3.261273580	1	4.806792350	4.657556940	1.097113730
1	2.036196060	-3.829524530	-2.091614620	1	5.690205760	4.415144730	-0.437650500
6	2.031851760	-2.059189160	-6.446417890	6	4.038861080	5.971705150	-2.035452610
6	1.932837710	-3.407372080	-7.174112430	1	4.497063390	6.961192740	-1.873401570
1	2.896017550	-3.667044070	-7.643068930	1	4.735571060	5.355466190	-2.621529040
1	1.655363890	-4.198307170	-6.461180770	1	3.117316980	6.106867030	-2.622228170
1	1.166563680	-3.358494530	-7.964644580	6	2.756210790	6.198803390	0.103149450
6	3.132963240	-2.103204640	-5.380081970	1	3.188298270	7.196383900	0.286103120
1	4.114242000	-2.283524310	-5.848599860	1	1.814429940	6.327694970	-0.455365480
1	3.179763000	-1.149483560	-4.831193560	1	2.524362900	5.750367910	1.0826714430
1	2.940487380	-2.913635430	-4.659513200	6	1.459024520	3.464109590	-4.088716300
6	2.303932990	-0.929770800	-7.446866250	6	1.479560400	4.647377710	-5.066086620
1	3.254271540	-1.098744770	-7.977795230	1	0.507894780	4.748625700	-5.576716760
1	1.491281100	-0.876511340	-8.189029840	1	1.690517300	5.586848520	-4.530448390
1	2.357135060	0.038019820	-6.924117390	1	2.262275930	4.498438850	-5.826492660
6	3.690068450	-4.531496310	3.018079690	6	0.412966940	3.702395760	-2.995333940
6	2.867543260	-4.466446420	4.309501750	1	-0.593142050	3.808842150	-3.431702980
1	3.183831750	-5.251160860	5.016160740	1	0.393042560	2.859068740	-2.283716790
1	2.996533490	-3.486941970	4.798831750	1	0.645788710	4.624656050	-2.438759670
1	1.795939890	-4.616107160	4.099642510	6	1.168489750	2.162120310	-4.844161430
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6	-1.658719950	-4.434904190	6.601098400					

1	-0.574197590	-4.993196150	-4.999110590	6	2.968993560	-1.777971770	-6.000986850
6	-1.270634620	-6.121686580	-2.578175520	6	1.921823070	-2.891863210	-5.886764650
1	-0.205982570	-5.838704120	-2.615709470	1	2.410638530	-3.858758920	-5.684455250
1	-1.369752440	-7.164778480	-2.919999730	1	1.352337740	-2.983169970	-6.825860260
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6	6.031709970	-0.442534990	2.470709500	6	2.298214900	-0.430586400	-6.277419870
6	6.756505230	-0.492491750	1.119921270	1	1.625493360	-0.162516580	-5.447871800
1	6.292911350	-1.238584580	0.451678750	1	1.709481470	-0.477718000	-7.207946600
1	7.813612140	-0.774561770	1.254141710	1	3.054602020	0.361890520	-6.383332560
1	6.725156160	0.493256300	0.626823550	6	3.984252800	-2.112257690	-7.100651240
6	6.055227690	-1.825227470	3.134461140	1	4.749503360	-1.323040290	-7.171188220
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6	6.690949900	0.608548160	3.371395110	6	6.619428010	-0.427796000	-3.226395760
1	6.654131410	1.603364700	2.899877590	1	6.664935020	-0.824867590	-2.200218760
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1	6.180437800	0.668038720	4.342958920	1	6.342445080	-1.252021100	-3.903285480
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1	-0.442790770	-2.031954410	7.301406660	O	-1.588500000	-1.210628000	-2.731306000
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N	-1.168639000	0.914814000	-0.218155000	N	-0.029909000	-0.023852000	-0.035566000
O	1.867305000	-0.716636000	-2.897441000	H	0.811092000	-1.841701000	-3.822384000
O	-1.148091000	1.521204000	2.833663000	H	3.604946000	-2.272605000	0.024823000
K	3.291373000	-0.512341000	-0.072184000	H	3.357835000	1.840284000	-1.889729000
O	-0.180532000	1.795118000	-3.250937000	H	-1.000298000	2.141226000	3.504327000
O	-0.936281000	-1.825753000	2.496043000	H	-2.851559000	-1.931176000	2.536948000
K	-1.719346000	3.479670000	-0.225083000	H	-3.882338000	1.910831000	-0.271611000
K	-1.621128000	-2.952391000	-0.196303000	K3-U-N-U			
H	2.141829000	-0.276087000	-3.705676000	U	1.598999000	-0.477246000	-1.282309000
H	-0.755145000	1.757490000	-4.019288000	U	-1.709197000	0.415288000	1.193320000
H	-1.595117000	-1.656221000	-3.579600000	K	0.453905000	-2.669984000	1.587547000
H	2.352910000	0.055962000	3.254253000	K	1.410304000	2.592834000	0.956423000
H	-0.724601000	1.977723000	3.564754000	K	-1.976533000	-0.037333000	-2.528366000
H	-1.496533000	-1.738836000	3.271112000	O	0.516025000	-1.314744000	-3.086130000
K3-Np-N-Np				O	2.770432000	-1.846491000	0.074185000
Np	1.616955000	-0.475819000	-1.277970000	O	2.543425000	1.560511000	-1.519026000
Np	-1.704148000	0.437908000	1.165843000	O	-2.227434000	-1.673657000	1.880226000
K	0.462116000	-2.627512000	1.601943000	O	-0.702773000	1.781800000	2.685622000
K	1.412951000	2.566535000	0.973853000	O	-3.142630000	1.373491000	-0.289016000
K	-1.909392000	0.037448000	-2.567972000	N	-0.036083000	-0.078050000	-0.004640000
O	0.525631000	-1.352391000	-3.059148000	H	3.249304000	1.896507000	-2.072244000
O	2.752785000	-1.906232000	0.049904000	H	3.624482000	-2.252534000	-0.082180000
O	2.548426000	1.570349000	-1.478466000	H	0.885923000	-1.700895000	-3.881456000
O	-2.211538000	-1.640913000	1.906754000	H	-3.976850000	1.834748000	-0.198791000
O	-0.726711000	1.787093000	2.687526000	H	-2.969098000	-1.947775000	2.422254000
O	-3.063732000	1.414490000	-0.379837000	H	-1.087769000	2.176767000	3.469805000
N	-0.001196000	-0.022109000	0.002372000	K3-U-N3-U			
H	3.204506000	1.933332000	-2.073574000	U	0.042299000	0.041921000	-1.826356000
H	3.643284000	-2.254218000	0.001474000	U	-0.055106000	0.032131000	1.518641000
H	0.822496000	-1.871967000	-3.806348000	O	-1.500390000	-1.290909000	-2.781822000
H	-3.945236000	1.776903000	-0.286556000	O	2.040484000	0.220141000	2.399503000
H	-2.901544000	-1.935133000	2.502208000	N	0.531185000	-1.127948000	-0.140072000
H	-1.115722000	2.259192000	3.424746000	N	0.154280000	1.484030000	-0.116687000
N	K3-Pu-N3-Pu			N	-1.195038000	0.858469000	-0.206920000
Pu	0.041068000	0.049379000	-1.853900000	O	1.927976000	-0.628038000	-2.893882000
Pu	-0.058799000	0.046032000	1.567190000	O	-1.096156000	1.551565000	2.839779000
O	-1.584149000	-1.231481000	-2.714024000	K	3.318599000	-0.536870000	-0.059148000
O	2.062817000	0.284885000	2.351672000	O	-0.270959000	1.778556000	-3.255023000
N	0.492062000	-1.066526000	-0.144115000	O	-0.995517000	-1.820723000	2.476785000
N	0.080648000	1.572767000	-0.121579000	K	-1.680643000	3.439570000	-0.204532000
N	-1.142812000	1.034299000	-0.222017000	K	-1.569741000	-3.010466000	-0.213035000
O	1.868326000	-0.740560000	-2.902797000	H	2.185457000	-0.253704000	-3.739224000
O	-1.159165000	1.548654000	2.843732000	H	-2.019361000	-1.172335000	-3.577055000
K	3.302659000	-0.462223000	-0.097640000	H	-0.410631000	1.741522000	-4.203108000
O	-0.190295000	1.815448000	-3.256071000	H	-1.477239000	-1.800145000	3.306233000
O	-0.937088000	-1.843411000	2.481611000	H	-1.137667000	1.602286000	3.796590000
K	-1.773570000	3.591709000	-0.239374000	H	2.278893000	0.734712000	3.171707000
K	-1.614076000	-2.951601000	-0.191143000	K3-Np-N3-Np[CH2]			
H	2.136375000	-0.290811000	-3.708595000	Np	0.020985000	0.072664000	-1.895601000
H	-1.640372000	-1.589899000	-3.600404000	Np	-0.110043000	0.070050000	1.384692000
H	-0.690547000	1.770416000	-4.074278000	C	-1.758233000	-1.077568000	-3.274419000
H	2.364999000	0.437869000	3.246867000	C	2.031754000	-0.112584000	2.755285000
H	-1.476682000	-1.754901000	3.271155000	H	1.367340000	-1.984442000	-3.308348000
H	-0.811833000	2.004064000	3.613978000	H	-2.374031000	-0.155533000	-3.344196000
H	K3-Pu-N-Pu			H	1.113090000	2.042797000	-3.700066000
Pu	1.606421000	-0.478771000	-1.276006000	H	1.931195000	-1.222818000	2.825128000
Pu	-1.692852000	0.431919000	1.167886000	H	-0.959612000	-1.212994000	3.575640000
K	0.461463000	-2.635941000	1.612170000	H	0.068849000	2.335612000	3.052907000
K	1.419308000	2.569383000	0.971161000	H	1.498991000	-0.448498000	-4.221522000
K	-1.921208000	0.010634000	-2.543257000	H	-1.097678000	-1.098954000	-4.168067000
O	0.503690000	-1.341713000	-3.066061000	H	-0.336405000	1.363579000	-4.499770000
O	2.721436000	-1.910234000	0.084683000	H	1.384779000	0.280058000	3.575353000
O	2.552016000	1.575458000	-1.444574000	H	-0.938024000	1.135798000	3.880574000
O	-2.172689000	-1.658474000	1.918272000	H	-2.401910000	-1.302525000	2.566241000
N				N	0.428551000	-1.116757000	-0.226173000

N	0.187709000	1.507423000	-0.205390000	H	-2.191683000	-1.309492000	-3.425432000
N	-1.180072000	0.961509000	-0.329932000	H	2.013217000	-1.152062000	-3.732378000
C	1.846583000	-0.983516000	-3.313811000	H	-0.892317000	-2.447140000	3.336873000
C	-0.933101000	1.848707000	3.025567000	H	2.416611000	0.496951000	3.419879000
K	3.314230000	-0.604700000	-0.064461000	H	-1.685830000	1.654246000	3.763846000
C	0.011539000	1.942917000	-3.621324000	K3-Np-N-Np[NH]			
C	-1.386194000	-1.746795000	2.693207000	Np	1.677368000	-0.502434000	-1.188257000
K	-1.536893000	3.586056000	-0.211547000	Np	-1.762035000	0.440234000	1.133265000
K	-1.719407000	-3.011278000	-0.201036000	K	0.523298000	-2.471119000	1.836618000
H	-0.464956000	2.923492000	-3.594922000	K	1.312775000	2.692182000	0.804477000
H	-2.427475000	-1.939512000	-3.334483000	K	-1.668996000	0.401948000	-2.693259000
H	2.928093000	-1.119657000	-3.396633000	H	1.318017000	-0.221853000	-3.844594000
H	-1.467459000	-2.805839000	2.943448000	H	3.961601000	1.034629000	-1.061451000
H	3.059317000	0.170725000	2.992846000	H	-4.116920000	0.295432000	-0.536631000
H	-1.747846000	2.565573000	3.110148000	H	2.361645000	-3.078636000	-0.964323000
K3-Np-N-Np[CH2]				H	-2.476215000	-0.816135000	3.327992000
Np	1.725654000	-0.397079000	-1.120515000	H	-1.582288000	2.997806000	2.031402000
Np	-1.652255000	0.418265000	1.147458000	N	0.824237000	-0.988051000	-3.345014000
K	0.453751000	-2.730030000	1.860207000	N	2.644946000	-2.445597000	-0.192243000
K	1.015521000	2.931267000	0.610696000	N	3.040473000	1.474566000	-1.239294000
K	-1.584756000	0.496646000	-2.585813000	N	-2.199738000	-1.438837000	2.542311000
H	2.179849000	-3.229451000	-0.422169000	N	-1.047376000	2.231619000	2.486501000
H	-2.557642000	-2.0874045000	0.527425000	N	-3.470252000	1.092506000	-0.424973000
H	-4.038350000	0.233831000	-0.805994000	N	-0.021772000	-0.006838000	-0.013628000
H	1.147490000	-0.086349000	-3.974997000	H	0.808788000	-1.767442000	-3.992007000
H	3.552952000	1.737152000	-0.173828000	H	3.222600000	2.156688000	-1.968881000
H	-1.599623000	3.162346000	2.128792000	H	3.577551000	-2.745769000	0.068051000
H	-4.204950000	1.173465000	0.676977000	H	-2.852735000	-2.213676000	2.585524000
H	2.006645000	-1.556174000	-3.546910000	H	-4.052610000	1.919640000	-0.493903000
H	3.568313000	-2.274592000	-0.884236000	H	-1.041697000	2.458043000	3.474073000
H	-3.400705000	-1.288886000	1.870440000	K3-Pu-N3-Pu[CH2]			
H	4.022597000	1.097476000	-1.734447000	Pu	0.004573000	0.070528000	-1.906527000
H	-2.091833000	1.957140000	3.317445000	Pu	-0.123685000	0.081828000	1.413320000
C	0.998118000	-1.073740000	-3.474432000	C	-1.755580000	-1.093050000	-3.278521000
C	2.867291000	-2.440018000	-0.024721000	C	2.021255000	-0.069998000	2.749126000
C	3.220494000	1.696999000	-1.240606000	N	0.381401000	-1.097797000	-0.213323000
C	-2.508860000	-1.929431000	1.636318000	N	0.146081000	1.544322000	-0.208393000
C	-1.196103000	2.332887000	2.759094000	N	-1.164686000	1.043562000	-0.332893000
C	-3.639108000	1.133698000	-0.288160000	C	1.891100000	-0.974845000	-3.240625000
N	-0.018485000	0.291693000	-0.166948000	C	-0.953138000	1.900858000	3.017849000
H	0.319889000	-1.671713000	-4.087058000	K	3.276855000	-0.668355000	-0.072971000
H	3.282428000	2.707045000	-1.654723000	C	0.001142000	1.946646000	-3.617199000
H	3.460152000	-2.879177000	0.781474000	C	-1.459257000	-1.725907000	2.665150000
H	-2.703046000	-2.894674000	2.111417000	H	1.405603000	-1.972989000	-3.229181000
H	-3.930569000	2.019405000	-0.859344000	H	-2.366375000	-0.168952000	-3.360791000
H	-0.529645000	2.774976000	3.503669000	H	1.104813000	2.036977000	-3.666482000
K3-Np-N3-Np[NH]				H	1.848360000	-1.166636000	2.875829000
Np	0.016863000	0.026219000	-1.705652000	H	-1.146389000	-1.132373000	3.555811000
Np	-0.088680000	0.066259000	1.613405000	H	0.039510000	2.405221000	2.991515000
H	1.308053000	-2.177729000	-2.655007000	H	1.521880000	-0.431358000	-4.135720000
H	-2.581221000	0.036359000	-2.581644000	H	-1.082071000	-1.123398000	-4.161874000
H	1.207814000	1.745745000	-3.543599000	H	-0.335096000	1.368912000	-4.500417000
H	1.873798000	-1.021262000	3.128091000	H	1.391620000	0.412862000	3.532822000
H	-1.724338000	-1.034890000	3.456038000	H	-0.912769000	1.202464000	3.883211000
H	-0.062126000	1.848194000	3.663766000	H	-2.486974000	-1.357127000	2.434862000
N	-2.011228000	-0.825960000	-2.552809000	K	-1.563198000	3.658271000	-0.191090000
N	2.005044000	-0.085911000	2.700776000	K	-1.730876000	-3.007812000	-0.192731000
N	0.241629000	-1.191558000	-0.007249000	H	-0.483200000	2.921564000	-3.571679000
N	0.434316000	1.450124000	0.011212000	H	-2.425902000	-1.954567000	-3.331837000
N	-0.982513000	1.143597000	-0.126680000	H	2.969504000	-1.113843000	-3.357210000
N	1.721671000	-1.235568000	-2.764850000	H	3.062548000	0.157816000	2.986245000
N	-0.917206000	1.691053000	3.102889000	H	-1.491609000	-2.779550000	2.947541000
K	3.197386000	-0.899250000	0.084050000	H	-1.788320000	2.593996000	3.095671000
N	0.232472000	1.814417000	-3.214057000	K3-Pu-N-Pu[CH2]			
N	-1.216007000	-1.652351000	2.798621000	Pu	1.736465000	-0.374634000	-1.112250000
K	-0.948078000	3.759320000	0.089311000	Pu	-1.658098000	0.451771000	1.160651000
K	-2.272534000	-2.533747000	0.061111000	K	0.437629000	-2.675032000	1.822652000
H	-0.331516000	1.947973000	-4.047592000				

K	1.022804000	2.923857000	0.628354000	N	3.157853000	1.282199000	-1.259247000
K	-1.565474000	0.460849000	-2.556833000	N	-2.190885000	-1.408313000	2.436031000
C	0.991990000	-1.061866000	-3.473530000	N	-0.994793000	2.201907000	2.393603000
C	2.844464000	-2.478610000	-0.069996000	N	-3.235944000	1.193219000	-0.680706000
C	3.229731000	1.742771000	-1.172177000	N	0.150952000	0.033995000	-0.005235000
C	-2.529158000	-1.879320000	1.718049000	H	-1.075354000	2.459645000	3.369748000
C	-1.184623000	2.423995000	2.728039000	H	-3.964553000	1.897470000	-0.679805000
C	-3.640079000	1.076066000	-0.342193000	H	-2.809938000	-2.210353000	2.473005000
H	2.128066000	-3.263643000	-0.414643000	H	3.625899000	-2.922759000	0.146068000
H	-2.631278000	-1.996890000	0.608460000	H	0.527302000	-1.715850000	-3.962162000
H	-4.005490000	0.185740000	-0.899170000	H	3.334444000	1.939689000	-2.012155000
H	1.151758000	-0.086475000	-3.992474000				
H	3.539970000	1.808829000	-0.100791000				
H	-1.542836000	3.279153000	2.108001000				
H	-4.237771000	1.073373000	0.603217000				
H	1.994695000	-1.555799000	-3.536802000				
H	3.527547000	-2.374603000	-0.952243000				
H	-3.407323000	-1.248741000	2.014726000				
H	4.055690000	1.152748000	-1.635296000				
H	-2.101629000	2.089587000	3.275712000				
N	0.013307000	0.224242000	-0.080060000				
H	3.285920000	2.746731000	-1.602947000				
H	0.306974000	-1.664897000	-4.073987000				
H	3.442995000	-2.893314000	0.744988000				
H	-2.693903000	-2.863705000	2.163114000				
H	-0.498432000	2.818500000	3.482220000				
H	-3.939499000	1.971748000	-0.894587000				
K3-Pu-N3-Pu[NH]							
Pu	0.011087000	0.042794000	-1.757068000				
Pu	-0.116203000	0.057395000	1.619602000				
N	-2.029779000	-0.823709000	-2.537657000				
N	1.990475000	-0.070001000	2.687354000				
N	0.244114000	-1.165728000	0.064353000				
N	0.371533000	1.520115000	-0.022478000				
N	-0.956978000	1.212020000	-0.135437000				
N	1.701133000	-1.271270000	-2.750073000				
N	-0.918671000	1.659234000	3.106176000				
H	1.288038000	-2.213043000	-2.647901000				
H	-2.622312000	0.022269000	-2.494434000				
H	1.281258000	1.799446000	-3.574402000				
H	1.859771000	-1.014301000	3.094708000				
H	-1.631965000	-1.050181000	3.514451000				
H	-0.058259000	1.804726000	3.661607000				
K	3.178763000	-0.903390000	0.094211000				
N	0.297066000	1.849267000	-3.271302000				
N	-1.173271000	-1.673843000	2.826804000				
K	-0.965084000	3.852154000	0.019276000				
K	-2.238988000	-2.562600000	0.066560000				
H	-1.684404000	1.601593000	3.769697000				
H	-0.947438000	-2.534130000	3.309797000				
H	2.332424000	0.503114000	3.450493000				
H	2.070660000	-1.208421000	-3.691939000				
H	-2.226304000	-1.258953000	-3.431662000				
H	-0.237490000	1.931332000	-4.131986000				
K3-Pu-N-Pu[NH]							
Pu	1.761305000	-0.660341000	-1.171270000				
Pu	-1.682257000	0.438608000	0.991870000				
K	0.596474000	-2.398176000	1.993565000				
K	1.525703000	2.529598000	0.876512000				
K	-1.077524000	1.046017000	-2.767925000				
H	1.815051000	-0.716635000	-3.907364000				
H	4.085484000	0.879922000	-1.042379000				
H	-3.661766000	0.357569000	-1.115851000				
H	2.262269000	-3.325860000	-0.647486000				
H	-2.498657000	-0.792284000	3.211941000				
H	-1.404861000	2.993360000	1.859677000				
N	0.951712000	-0.984178000	-3.403554000				
N	2.686782000	-2.594912000	-0.048437000				

Cs₃-U Species

Reactant -LS

92	1.63911019	-0.41306888	-1.28785678
92	-1.67840200	0.47140709	1.17280793
55	0.45288238	-2.91483253	1.51854274
55	1.61498215	2.75562243	1.08253108
55	-2.02415086	0.09239164	-2.79611096
14	0.44111974	-2.56678965	-4.24382703
14	4.23851381	-2.40880455	0.72832789
14	3.27707145	2.87288740	-2.44781278
14	-0.45025422	2.27111551	4.34762000
14	-4.00540511	2.78202153	-0.86789211
8	0.74121489	-1.60849649	-2.95666342
8	-1.18352257	-2.27817855	-4.62566004
8	0.72693904	-4.19515444	-3.98089332
8	1.26209807	-2.20662877	-5.64835745
8	3.00279935	-1.63811252	-0.01063281
8	3.50428990	-3.32082501	1.95167348
8	5.06410591	-3.53056374	-0.18567482
8	5.42156584	-1.39942526	1.34663228
8	2.52637203	1.58195148	-1.78586462
8	4.92722215	2.75088129	-2.64432276
8	3.07977436	4.10898757	-1.30702615
8	2.69659095	3.31730998	-3.95275528
8	-2.47594503	-1.55568456	1.73829716
8	-2.29175399	-4.13832647	2.26644109
8	-4.73120347	-3.14527536	1.35672042
8	-0.75519847	1.55540190	2.91232327
8	-0.41187753	1.22775090	5.65532077
8	-1.50980519	3.47524118	4.80182294
8	1.02842021	3.07038160	4.12777480
8	-3.08988280	1.64894362	-0.12932865
8	-5.43283242	3.18761871	-0.10985711
8	-3.26291299	4.24609216	-1.17988283
8	-4.31032545	2.17059467	-2.41789479
7	-0.03033316	0.06136738	-0.08009502
6	-1.91121833	-2.62639845	-5.83782037
6	-1.65972404	-1.53821287	-6.89092456
1	-2.20618886	-1.76028097	-7.82266961
1	-2.00004737	-0.55576457	-6.52186008
1	-0.58325589	-1.47392587	-7.10963573
6	-3.39468988	-2.65912920	-5.44552997
1	-4.02052752	-2.91939804	-6.31459628
1	-3.56861884	-3.40781650	-4.65511485
1	-3.73162511	-1.67557714	-5.07513166
6	-1.49637974	-4.00128719	-6.37744437
1	-2.09415830	-4.24998805	-7.26988995
1	-0.43311335	-4.00726898	-6.65662346
1	-1.66081907	-4.78249436	-5.61919096
6	0.45703588	-5.03458571	-2.83270127
6	-0.79776974	-4.56901706	-2.08352931
1	-0.99781097	-5.22714654	-1.22047778
1	-0.66805646	-3.53449953	-1.72096642
1	-1.67894109	-4.59202398	-2.74466882
6	0.24573399	-6.44861646	-3.38995168
1	0.07945167	-7.16976266	-2.57297029
1	-0.62808505	-6.47256459	-4.06051290

1	1.13145445	-6.76649086	-3.96234231	6	3.76987152	5.38775181	-1.21474154
6	1.68159256	-5.00599000	-1.91025126	6	5.11095391	5.17273340	-0.50000195
1	1.52768398	-5.65321799	-1.02927973	1	5.65785265	6.12486145	-0.39879293
1	2.57376646	-5.37243036	-2.44312437	1	4.94793198	4.76232309	0.51094111
1	1.89138010	-3.97889557	-1.56729671	1	5.72657826	4.45980464	-1.06869251
6	2.58716336	-2.58198543	-6.10708201	6	3.99152602	6.01472645	-2.59716099
6	2.49858222	-3.94288057	-6.81153372	1	4.47955194	6.99755499	-2.49010378
1	3.49067654	-4.25469427	-7.17742721	1	4.63126249	5.37316337	-3.21996268
1	2.12202637	-4.70347097	-6.11058081	1	3.03176318	6.15777203	-3.11750897
1	1.81588925	-3.88499451	-7.67481067	6	2.86066649	6.29945821	-0.37957089
6	3.57396118	-2.64294613	-4.93812605	1	3.30963318	7.29995439	-0.26932720
1	4.59216101	-2.85677581	-5.30204065	1	1.87480796	6.41178991	-0.86011389
1	3.58608109	-1.68045695	-4.40202181	1	2.71072523	5.88947197	0.63408747
1	3.28245292	-3.43290699	-4.22814598	6	1.34527536	3.39995956	-4.46826955
6	3.00059541	-1.48835441	-7.09881810	6	1.37071896	4.50993752	-5.52765479
1	3.98626733	-1.71177683	-7.53753373	1	0.38573569	4.60936109	-6.01245079
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6	-0.26643011	-2.09950465	6.30265098		1	-1.13591126	-5.80311894	-2.87126013
1	0.64222973	-2.42518764	5.77308643		1	-2.49577487	-6.92048331	-3.20180136
1	-0.01449188	-1.91592384	7.35941199		1	-2.55775589	-5.83426520	-1.78668948
1	-0.61450484	-1.15795411	5.85488384		6	6.03283573	0.32190404	3.18701610
6	1.76517227	-4.42559262	3.07280217		6	6.86024465	0.37760975	1.89225086
6	2.26948207	-5.77215002	3.61042153		1	6.70026783	-0.51594869	1.26547203
1	2.41442945	-5.71547039	4.70096064		1	7.93609313	0.41592636	2.12842565
1	3.23257790	-6.04078874	3.14600827		1	6.60387053	1.27574299	1.30582165
1	1.54509616	-6.57404022	3.39796505		6	6.30072949	-0.99638576	3.92648640
6	2.79137955	-3.32451037	3.36504181		1	5.67119419	-1.05146927	4.82643098
1	2.40945668	-2.33596790	3.06208047		1	7.36170269	-1.07492231	4.21687039
1	3.73778924	-3.52757583	2.83302362		1	6.05584457	-1.85743002	3.28188797
1	3.01676493	-3.28217419	4.44265176		6	6.41935718	1.51981066	4.06433140
6	1.48614395	-4.52392126	1.56924445		1	6.23112090	2.46671776	3.53562407
1	0.67786447	-5.24638380	1.37198254		1	7.49293881	1.46845975	4.31087811
1	2.38720536	-4.87378186	1.04047216		1	5.84565220	1.52325288	4.99965775
1	1.19769048	-3.54271974	1.15524950		6	3.20285263	0.50379376	6.55784863
55	-0.97958771	3.37108295	0.08023824		6	3.33116166	-0.76999417	7.40247370
7	-1.21794775	0.20516273	-0.02499267		1	2.66087848	-1.55335291	7.01737109
					1	3.06933588	-0.56515971	8.45304399
					1	4.36556382	-1.14845400	7.36877103
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Product -HS

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1	1.43503177	1.23502287	7.59317463	1	-3.93088534	6.75070352	1.59553100
1	1.09615508	0.25616753	6.13449081	1	-4.05962663	5.12783227	0.86172074
6	3.03736974	3.57976957	3.14803562	6	-2.13885660	6.01585006	3.62474618
6	3.93416412	4.72894760	3.63124321	1	-1.88685373	5.52534179	4.57603629
1	3.74154991	4.93949678	4.69508240	1	-2.57408208	7.00832036	3.82783841
1	3.73612642	5.64679110	3.05287652	1	-1.20591537	6.15886739	3.05397046
1	4.99769437	4.46759773	3.51330387	6	-4.43970654	4.97546496	3.59944996
6	1.56373570	3.96111046	3.33044672	1	-5.14584029	4.35470036	3.02587129
1	0.89826655	3.11328278	3.09938695	1	-4.90474298	5.96074414	3.77007670
1	1.30164697	4.82437136	2.69286434	1	-4.26758424	4.49806087	4.57259471
1	1.36743496	4.25112977	4.37540387	6	-2.13085513	2.75610513	6.40218987
6	3.34470227	3.25616434	1.67807104	6	-1.09183368	3.49334660	7.25568573
1	4.40493930	2.98282910	1.55476555	1	-0.07480576	3.21336973	6.94468887
1	3.14839714	4.13886761	1.04719245	1	-1.21736850	3.24384978	8.32153271
1	2.73254817	2.41360435	1.31073275	1	-1.20356827	4.58326542	7.13649047
55	-2.60302935	-2.54574746	0.10987037	6	-3.54795297	3.17777552	6.81684540
7	1.07189959	-1.03799930	0.02903149	1	-3.65506589	4.27346881	6.77250550
7	1.41167953	0.39878530	-0.09146004	1	-3.75501958	2.85683177	7.85125862
14	3.01792023	-1.51311383	-3.55238833	1	-4.28870303	2.71149668	6.15030162
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8	1.52987429	-1.05337772	-3.07354199	1	-2.72703425	0.72078445	5.94278183
8	3.83318886	-2.58139669	-2.51835246	1	-2.07750664	0.93659585	7.59860174
8	3.14608678	-2.26669161	-5.03982523	1	-0.97145835	0.94218405	6.19451027
8	3.96705655	-0.13243853	-3.47232849	6	-4.58814003	0.90431833	3.04082034
8	-1.14547464	1.59858998	2.81265166	6	-6.01068611	1.11307279	3.57562424
8	-2.50088428	3.85885180	2.54815378	1	-6.05296481	0.86811008	4.64890283
8	-1.87371451	3.17298659	5.03579405	1	-6.72766073	0.46653303	3.04300886
8	-3.74147459	1.74599275	3.85602564	1	-6.32178775	2.16189689	3.44446524
6	3.89125482	-4.03094299	-2.46439942	6	-4.15932416	-0.55545882	3.24040706
6	4.71641621	-4.37976214	-1.21366245	1	-3.11277157	-0.70411391	2.93006386
1	5.70756488	-3.90193718	-1.27014310	1	-4.81238315	-1.23393039	2.66287776
1	4.85585400	-5.47131105	-1.15054584	1	-4.23737875	-0.84295129	4.30126945
1	4.21175616	-4.06363577	-0.28636690	6	-4.51036015	1.29766847	1.56413807
6	2.47504480	-4.61369186	-2.36131817	1	-4.76262513	2.36248649	1.43609587
1	1.94861584	-4.18765728	-1.49225629	1	-5.23131662	0.70729825	0.97553910
1	2.50700387	-5.71179567	-2.25537638	1	-3.49977025	1.11776555	1.15586785
1	1.89229866	-4.37058914	-3.26310875	55	3.93525840	-1.08656424	0.21377351
6	4.62682715	-4.59328878	-3.68980016	14	-0.18647673	3.48361062	-3.27082596
1	4.12349612	-4.28243132	-4.61329862	14	-0.87572304	-3.37129729	3.38331809
1	4.66431168	-5.69367287	-3.64213423	8	0.07108385	1.99386261	-2.66263133
1	5.66236532	-4.21535547	-3.71884257	8	0.48222507	4.70705452	-2.30738031
6	2.31626062	-2.39877785	-6.21374355	8	0.33788118	3.85257580	-4.80864563
6	1.17730164	-3.38105036	-5.91233883	8	-1.83459996	3.75165232	-3.07708956
1	1.59130443	-4.36138578	-5.62514423	8	-0.69082453	-1.95986594	2.57785938
1	0.54111166	-3.52542010	-6.80065829	8	-1.85249945	-4.32463470	2.37351699
1	0.55218193	-3.00320346	-5.08766137	8	-1.73731071	-3.31519412	4.81091752
6	1.77416417	-1.03357806	-6.63470869	8	0.53984124	-4.16426022	3.78035568
1	1.18718641	-0.59296373	-5.81599634	6	1.79620844	5.32396933	-2.31916744
1	1.12881735	-1.12690204	-7.52300273	6	1.88353501	6.12574631	-1.01297355
1	2.60642540	-0.35355069	-6.87188852	1	1.05412455	6.84942793	-0.95386191
6	3.22785315	-2.96415687	-7.31325138	1	2.83172078	6.68460691	-0.95471379
1	4.05755894	-2.26858053	-7.51600246	1	1.83439475	5.46157198	-0.13364466
1	2.66053003	-3.11215942	-8.24604888	6	2.89138608	4.25338587	-2.36602425
1	3.65396782	-3.93266332	-7.00653510	1	2.78218447	3.53689912	-1.53569618
6	5.30782416	0.18128447	-3.91129476	1	3.89080951	4.71609041	-2.30156367
6	6.33649324	-0.81131899	-3.35106116	1	2.83259144	3.68695424	-3.30715727
1	6.28296784	-0.85016463	-2.25097200	6	1.91545643	6.28555585	-3.50999978
1	7.35654487	-0.50059508	-3.63217690	1	1.76035292	5.74198653	-4.45242721
1	6.16104927	-1.82623551	-3.73830853	1	2.91137584	6.75794670	-3.52379541
6	5.37422260	0.19159136	-5.44491381	1	1.15595003	7.08091406	-3.43822152
1	5.16453828	-0.81265638	-5.84263431	6	0.71321444	3.10399002	-5.98821196
1	6.37346547	0.50763038	-5.78728060	6	2.13719651	2.56627717	-5.80978954
1	4.62920985	0.89466408	-5.84906008	1	2.83990974	3.39843017	-5.64152753
6	5.58640685	1.58680499	-3.36180736	1	2.45603378	2.02781705	-6.71674242
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1	6.59272271	1.93227511	-3.64973710	6	-0.27618130	1.96593074	-6.23070331
1	5.51662049	1.58856447	-2.26110084	1	-0.29705907	1.29338582	-5.35919696
6	-3.12249242	5.14376926	2.83285189	1	0.00893750	1.38156545	-7.11884517
6	-3.41486120	5.78510648	1.46860011	1	-1.28926986	2.36566181	-6.38435661

6	0.66940626	4.10463892	-7.15034175	14	-1.831602680	1.363775100	4.321413430
1	-0.34030093	4.53282824	-7.25216061	8	1.433825540	2.895017960	-0.316031320
1	0.93410750	3.60693483	-8.09689927	8	3.110669450	4.105421330	1.288331520
1	1.37971843	4.92912675	-6.97939759	8	1.507947680	5.678818860	-0.372876080
6	-2.71587311	4.77846728	-3.59470155	8	3.574432400	4.372107180	-1.350297530
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1	-1.71809808	6.43074704	-2.57089873	8	-3.890478760	2.181845740	-3.561598750
1	-2.75275128	6.92648990	-3.94420140	8	-1.868497890	2.183442560	-5.264392460
1	-1.16313466	6.16737346	-4.24566021	8	-2.449712010	-0.154103860	-4.085545790
6	-3.13781717	4.40412067	-5.02216152	8	1.522243150	-0.123273950	-2.889024390
1	-2.26266736	4.40708606	-5.68948198	8	1.958804460	-0.746115630	-5.589070780
1	-3.87546130	5.12513902	-5.41182794	8	1.735615160	-2.608444470	-3.718326510
1	-3.58911849	3.39935640	-5.03323411	8	3.976005920	-0.926949670	-3.883272260
6	-3.94220360	4.77288238	-2.67321125	8	-1.894735980	-2.768462700	0.630635220
1	-4.38339888	3.76360187	-2.63625631	8	-2.020961400	-5.444953190	1.437978740
1	-4.70589597	5.48065020	-3.03426455	8	-2.152436490	-4.692654010	-1.122990380
1	-3.65950430	5.06593536	-1.64866450	8	-4.247365970	-4.240803410	0.687048610
6	-2.61629970	-5.52756953	2.67330401	8	0.976916090	-1.668352780	2.844414760
6	-2.92783710	-6.18004313	1.31887168	8	3.367542340	-2.954109030	2.159770660
1	-3.56324497	-5.52697818	0.69688865	8	2.654081980	-2.869785560	4.700690640
1	-3.47220178	-7.12828847	1.45852824	8	3.317145100	-0.555968740	3.327058640
1	-1.99639224	-6.39205163	0.76874313	8	-1.559476100	0.519815020	2.949574130
6	-3.91768888	-5.13069263	3.38485100	8	-0.449885170	2.323130020	4.508044810
1	-3.68402461	-4.61801385	4.32864797	8	-1.926842100	0.460317690	5.721000130
1	-4.53643797	-6.01932009	3.59345451	8	-3.244464220	2.253945090	4.289910330
1	-4.50990213	-4.44429553	2.75647507	7	0.085204380	-0.192003700	0.019146610
6	-1.81094309	-6.50955277	3.53146357	6	4.274476750	4.852597300	1.767893460
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1	-2.40577392	-7.41839908	3.72025836	1	3.278301300	5.370611120	3.634627200
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6	-1.31496510	-3.14880336	6.18589830	1	4.164328990	3.816414270	3.686247090
6	-2.55979221	-2.68684140	6.94762855	6	4.269489160	6.304479570	1.273042150
1	-2.92332420	-1.72900680	6.54453561	1	4.336893030	6.349152740	0.177848930
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1	0.02309227	-4.86232086	6.13234439	1	5.555513670	4.091930530	0.191103350
6	-0.20794302	-2.09464168	6.26612770	6	0.258474380	6.151153050	0.182171540
1	0.69061704	-2.43582154	5.72863548	6	0.156915700	5.797522600	1.669089390
1	0.06201671	-1.89074668	7.31496535	1	0.124522150	4.705080390	1.808025340
1	-0.55688674	-1.15957348	5.80450639	1	-0.761223250	6.224310600	2.106085230
6	1.74532521	-4.45476019	3.03359126	1	1.022499590	6.196607150	2.221264800
6	2.20090852	-5.84562109	3.49645922	6	0.282622760	7.675326010	0.002811630
1	2.33162401	-5.85927467	4.59009621	1	1.129130740	8.113572100	0.555267170
1	3.15983864	-6.11902482	3.02659951	1	-0.651118870	8.126224350	0.375632240
1	1.45202221	-6.60684253	3.22690322	1	0.393400530	7.929694930	-1.062852530
6	2.79647827	-3.40230652	3.40833102	6	-0.909663180	5.541371200	-0.600546750
1	2.44843410	-2.38805823	3.15172953	1	-0.836653240	5.802933060	-1.668388450
1	3.74888001	-3.60483813	2.88679098	1	-1.872877680	5.913995540	-0.216182140
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6	1.49432176	-4.45728129	1.52213925	6	3.584239750	4.984756230	-2.671159580
1	0.68620107	-5.16101169	1.26334151	6	3.798513950	6.498644070	-2.533274020
1	2.405333787	-4.78121397	0.99195223	1	2.990777900	6.941428470	-1.932275200
1	1.22016049	-3.45115492	1.16166063	1	3.806293890	6.973539680	-3.527846550
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92	0.474644230	1.208419140	-1.474577540	6	2.277197730	4.696609040	-3.417594430
92	-0.784500720	-1.108661790	1.667454200	1	2.100975640	3.609336570	-3.480128080
19	-0.547886690	-2.354293190	-1.971681150	1	2.322206930	5.098102940	-4.443007960
19	1.576653440	1.645727700	2.320862730	1	1.428234440	5.163704130	-2.895539280
14	2.353849730	4.244607800	-0.220745470	6	-4.702535900	2.251942730	-2.365770170
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6	5.03373473	0.52439965	-2.29568108	6	5.41979551	-1.37366054	4.19727917
1	4.07116111	0.98101368	-2.01479913	1	5.00445355	-1.49564280	5.20860580
1	5.46812243	1.10404964	-3.12508926	1	6.48342998	-1.09683014	4.28373070
1	5.71334458	0.59752880	-1.43044773	1	5.34927169	-2.33899456	3.67432857
6	-2.34692025	-5.73825698	2.70612106	6	4.76020599	1.04274385	4.18294630
6	-2.61914866	-4.49548159	3.56053717	1	4.29248257	0.95028671	5.17692231
1	-3.49263008	-3.94752738	3.17432420	1	4.25095500	1.84674369	3.62737080
1	-1.74390609	-3.82351105	3.54812214	1	5.81051058	1.34863562	4.31994119
1	-2.81891188	-4.77913078	4.60667898	6	5.25297653	-0.14362200	2.00985794
6	-1.12544149	-6.49590758	3.23819171	1	4.71333956	0.63049700	1.43879559
1	-0.91083317	-7.36644973	2.59789509	1	5.15124700	-1.10094635	1.47796240
1	-1.30484101	-6.85073734	4.26562642	1	6.31972059	0.13598147	2.04732505
1	-0.24014418	-5.84206699	3.24002029	6	-0.07459915	3.08967544	5.68016625
6	-3.57672817	-6.65708984	2.68491034	6	0.85165469	4.20037852	5.17761982
1	-3.36468935	-7.56305822	2.09453860	1	0.32872990	4.85178750	4.45892619
1	-4.43179931	-6.13076619	2.23540790	1	1.73990907	3.77584338	4.68317950
1	-3.84323998	-6.96770150	3.70838606	1	1.20362466	4.82177130	6.01742724

6	0.67317167	2.17127492	6.65291003	8	-1.87184766	0.46680544	5.67833997
1	0.01927971	1.34293365	6.96164619	8	-3.21577254	2.29516358	4.32381120
1	0.99753355	2.73049993	7.54637389	7	0.08466386	-0.04086877	-0.01455248
1	1.56717544	1.74604530	6.16816373	6	4.28638358	4.89515196	1.79790367
6	-1.30043531	3.71079210	6.36176877	6	4.17298015	4.92344999	3.32491833
1	-1.85254611	4.35633544	5.66161487	1	3.24586516	5.43206160	3.63256135
1	-0.97535981	4.32247366	7.21930084	1	5.02663013	5.46482128	3.76474006
1	-1.98479835	2.93218171	6.72860508	1	4.16989080	3.90311216	3.73918509
6	-3.01764466	-0.31233701	6.25943679	6	4.27081697	6.33462929	1.26791652
6	-2.39394088	-1.33638122	7.21471576	1	4.37016693	6.35337500	0.17433447
1	-1.78922711	-0.82247043	7.97886415	1	5.11096967	6.89839505	1.70534596
1	-1.74168164	-2.02882325	6.66119919	1	3.33314294	6.84214150	1.54208207
1	-3.17893022	-1.91896899	7.72323463	6	5.56648198	4.17573979	1.35719203
6	-3.92038986	0.65725454	7.03576738	1	5.59513760	3.15230013	1.76493136
1	-4.30020381	1.43796986	6.36075353	1	6.45890597	4.71554637	1.71455948
1	-3.35193858	1.13653976	7.84906699	1	5.60125614	4.11376759	0.25859735
1	-4.77202547	0.11807161	7.48198383	6	0.25978882	6.13170243	0.21778192
6	-3.81151884	-1.03039733	5.16150422	6	0.18618818	5.82211059	1.71587340
1	-4.25438869	-0.30470166	4.46186435	1	0.16284754	4.73476896	1.89121836
1	-4.62497213	-1.62666429	5.60585695	1	-0.72662110	6.25693854	2.15607133
1	-3.15478888	-1.70786158	4.59235949	1	1.05873994	6.24154906	2.24133754
6	-3.90629864	2.91713079	3.21361595	6	0.26553901	7.65008007	-0.00844375
6	-4.81362493	3.94620938	3.90175466	1	1.12027672	8.11119605	0.51157543
1	-5.51208286	3.43980989	4.58618332	1	-0.66306913	8.10528749	0.37165093
1	-5.39801031	4.50986670	3.15687758	1	0.35080910	7.87278521	-1.08350895
1	-4.21055357	4.65906433	4.48608271	6	-0.91680514	5.48847173	-0.52493250
6	-4.74981115	1.91055328	2.42092149	1	-0.85355345	5.69884046	-1.60453604
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1	-5.31627120	2.41964629	1.62419073	6	3.56848108	4.97732410	-2.65414809
6	-2.90033135	3.62144632	2.29894936	6	3.76612139	6.49486851	-2.52691513
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94	0.52950518	1.23529969	-1.48087021	1	2.25509632	4.67142872	-3.38255501
94	-0.86442492	-1.10282250	1.65221214	6	2.09750867	3.58195312	-3.45402223
19	-0.63782657	-2.25229070	-2.03382262	1	2.27718426	5.08003245	-4.40583084
19	1.43773928	1.61838843	2.34133721	1	1.40673938	5.12056269	-2.84437189
14	2.37665346	4.23995150	-0.18401073	6	-4.68051743	2.17833925	-2.30118591
14	-2.36212003	1.43003805	-3.77173753	6	-4.46444777	0.97328303	-1.38225587
14	2.32867441	-1.04638922	-3.97009897	1	-4.70071645	0.04033794	-1.91601230
14	-2.60117541	-4.21216937	0.34797196	1	-5.11581632	1.04116715	-0.49653636
14	2.44106137	-2.06081205	3.20462387	1	-3.41735621	0.92523991	-1.04087285
14	-1.79531676	1.40847672	4.29811682	6	-4.30496252	3.48329382	-1.58695394
8	1.47882926	2.87470123	-0.28419970	1	-4.46453739	4.34324979	-2.25667855
8	3.14037812	4.12104645	1.31726668	1	-3.24641685	3.45980813	-1.28544005
8	1.50360724	5.65663236	-0.34581532	1	-4.92332821	3.62578722	-0.68552926
8	3.58215525	4.37299943	-1.33062900	6	-6.13882701	2.23311414	-2.77672558
8	-1.33437704	1.64777324	-2.51466492	1	-6.40857086	1.29907318	-3.29404021
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8	-1.86297207	2.11628290	-5.20848073	1	-6.82156976	2.37140858	-1.92309863
8	-2.39264869	-0.23550321	-4.03623944	6	-1.95774836	3.49087138	-5.66999043
8	1.55561120	-0.12527210	-2.86078195	6	-1.66024956	4.47397820	-4.53150953
8	1.96395413	-0.74657639	-5.56779632	1	-2.41047395	4.38149687	-3.73125744
8	1.74171069	-2.61079538	-3.69674264	1	-1.67594390	5.51003507	-4.90726079
8	3.99222683	-0.93324829	-3.87744892	1	-0.66591204	4.27219922	-4.10271606
8	-1.92199818	-2.73846575	0.48739938	6	-3.36084185	3.73093168	-6.24482566
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8	-4.26025480	-4.22921897	0.59081544	1	-3.44845169	4.76028863	-6.62915261
8	0.89665618	-1.72926038	2.80774697	6	-0.90124640	3.62717141	-6.77296935
8	3.31345666	-2.95754708	2.09912748	1	-1.09350131	2.90030308	-7.57759763
8	2.62936339	-2.88490387	4.64334642	1	0.10393216	3.43808357	-6.36594313
8	3.22326160	-0.55713754	3.25760378	1	-0.92135115	4.64048048	-7.20513603
8	-1.52761734	0.63004992	2.89554399	6	-2.96543311	-0.94950972	-5.17490593
8	-0.42302331	2.38229199	4.51067268	6	-4.38233808	-0.45363035	-5.49138563

1	-5.04358591	-0.57907180	-4.61920543	1	-3.65268253	-6.86185172	-0.24585417
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1	-2.40034386	-1.41539331	-7.22871035	6	-5.28956323	-3.28624579	0.21075199
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6	2.66116602	1.59790784	-5.76064938	1	-5.08632758	-3.67625028	-1.92204188
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6	1.98413066	-3.80390620	-4.51003829	6	2.66892857	-5.27643310	2.67687032
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1	4.16430037	-3.70425445	-4.41462152	1	4.76381348	-4.01674113	0.21482604
1	3.46305894	-2.94163218	-5.86789112	1	4.34751012	-5.72795321	0.52277096
1	3.51778374	-4.72197339	-5.73306536	6	1.94265276	-2.78935746	5.91194603
6	1.89156325	-4.98973901	-3.54509336	6	0.65858571	-3.62552083	5.83920927
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1	2.02242866	-5.94211402	-4.08476880	1	0.12440157	-3.60819722	6.80312916
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6	4.877795920	-0.89174107	-2.72784435	6	2.90500897	-3.39019203	6.94595008
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6	-3.92306056	2.99091124	3.27094754		1	-1.149682740	-6.454740080	-2.760052700
6	-4.87498077	3.96014931	3.98511045		1	-2.065587850	-5.418859900	-3.892458790
1	-5.55142430	3.40470040	4.65344761		1	-0.584975700	-6.250910270	-4.445604480
1	-5.48303020	4.51680166	3.25408650		6	1.192317690	-4.991410640	-2.754377440
1	-4.30505072	4.68285954	4.59014777		1	1.146497300	-5.660746640	-1.878738750
6	-4.72345573	1.97251384	2.44929864		1	1.670090400	-5.536606370	-3.583766360
1	-5.42153647	1.42086073	3.09923230		1	1.825649790	-4.129530330	-2.492438240
1	-4.04005825	1.25340254	1.97204582		6	1.392480060	-2.547328420	-7.033543950
1	-5.30784000	2.47964081	1.66446726		6	0.865442940	-3.888146950	-7.566657560
6	-2.94857588	3.76227828	2.37659803		1	1.626502780	-4.389363130	-8.187087920
1	-2.36214330	4.47475966	2.97799001		1	0.598761870	-4.544396880	-6.724422380
1	-3.49330571	4.32485678	1.60119341		1	-0.032231990	-3.725418100	-8.184726940
1	-2.25262633	3.06817544	1.87751402		6	2.674620560	-2.768527110	-6.218530680
					1	3.456753200	-3.213613030	-6.855181480
					1	3.052104820	-1.814237020	-5.818500720
					1	2.486288240	-3.453626250	-5.376457150

Plutonium-CH₂ Species

Reactant -LS

94	1.759346950	-0.357309010	-1.087412850		6	1.668182250	-1.581125060	-8.193430770
94	-1.664716220	0.423797480	1.192986950		1	2.435004680	-1.988162320	-8.871795030
19	0.413061540	-2.694849280	1.767676270		1	0.745786820	-1.406776340	-8.770123280
19	0.918998910	2.985204970	0.558555610		1	2.019142580	-0.611308560	-7.804695590
19	-1.529527790	0.494874960	-2.555113260		6	3.302996870	-4.168372700	3.827059960
14	-0.015772370	-2.044362630	-4.607769460		6	2.353646850	-3.608795380	4.894022470
14	3.916488760	-3.320429070	1.167247260		1	2.502061280	-4.125079530	5.856403500
14	3.433656580	3.463447050	-1.892107570		1	2.536356720	-2.533403590	5.048452980
14	-0.135924790	3.139592050	4.011949440		1	1.298700310	-3.750923140	4.602639690
14	-4.149048820	2.599613900	-1.91518250		6	3.056253700	-5.669270060	3.630921980
6	1.027424310	-1.085495110	-3.426186090		1	3.281537140	-6.218718770	4.559906090
8	-1.574264770	-1.351993610	-4.537810660		1	2.004600050	-5.861402380	3.368942320
8	-0.068903320	-3.704381500	-4.352387060		1	3.689906210	-6.048216620	2.817197760
8	0.353012710	-1.922531920	-6.245506150		6	4.755214020	-3.924119240	4.257738560
6	2.844331770	-2.493029800	-0.084613830		1	4.946366950	-4.429858970	5.218744420
8	2.981869670	-3.446599100	2.593976050		1	5.462058230	-4.312754740	3.510384400
8	4.336570080	-4.927070790	0.886719980		1	4.946156880	-2.847550560	4.389509790
8	5.404056420	-2.588261300	1.436052130		6	5.334967150	-5.519103740	0.024656800
6	3.198765240	1.795100060	-1.138893050		6	4.823255610	-6.931809840	-0.287967370
8	4.587437890	4.476132290	-1.193533460		1	5.536844190	-7.476369400	-0.927017740
8	1.994575670	4.334438210	-1.594124360		1	4.681674630	-7.501346390	0.644586430
8	3.857845260	3.467664760	-3.518302460		1	3.853100460	-6.877148160	-0.808556440
6	-2.563649090	-1.899070090	1.752807590		6	6.666629700	-5.586553310	0.787117740
8	-1.677085420	-4.576994510	1.960883100		1	7.447826420	-6.061256930	0.170768810
8	-4.446912300	-4.238539800	2.091881630		1	6.990829350	-4.571470020	1.061126240
6	-1.230009530	2.436223970	2.713290400		1	6.545597040	-6.177647400	1.709333780
8	0.257041980	2.053438020	5.237076910		6	5.506371460	-4.727251870	-1.279557560
8	-0.647008150	4.494694530	4.866806920		1	6.246440490	-5.222245230	-1.929509370
8	1.244157150	3.712865560	3.190252000		1	4.550891530	-4.666630410	-1.824454990
6	-3.622138600	1.058113770	-0.333772780		1	5.861233120	-3.705428610	-1.071197710
8	-5.792564990	2.863928350	-1.491380320		6	5.857093060	-1.221001430	1.529032760
8	-3.628868020	3.988868560	-0.403283140		6	7.146548430	-1.261603270	2.362521410
8	-3.318826810	2.582872360	-2.683449740		1	7.579293350	-0.252867270	2.460437480
7	-0.007805600	0.209928140	-0.091771400		1	6.939802940	-1.653715180	3.370464570
6	-2.696238520	-1.517298930	-5.458757400		1	7.889204610	-1.916923010	1.880929430
6	-2.519138680	-0.543160100	-6.630343520		6	6.168109820	-0.711551540	0.116149270
1	-3.363638940	-0.622049530	-7.334776360		1	6.577875490	0.310572570	0.146060480
1	-2.474076940	0.496697850	-6.266285800		1	6.905675300	-1.369510110	-0.370016340
1	-1.581396240	-0.767941530	-7.159193300		6	5.254482110	-0.694900140	-0.499348190
					6	4.813348490	-0.332336080	2.213983810

1	5.166663330	0.711099210	2.269661680	1	-5.550566170	-4.403754120	6.074242940
1	3.862289490	-0.352945820	1.655655930	1	-5.320865120	-4.736789790	4.324167860
1	4.616655690	-0.686820430	3.238741770	1	-4.225795030	-5.471922960	5.530396740
6	6.026623700	4.515828470	-1.334772720	6	-3.073027750	-3.171557210	6.461033160
6	6.616395630	3.114729520	-1.544430770	1	-3.751116730	-2.992251300	7.310785280
1	7.715904270	3.168244050	-1.603053060	1	-2.474897570	-4.072201060	6.673853730
1	6.342497790	2.453349210	-0.707723870	1	-2.386210760	-2.315270980	6.370162220
1	6.240475040	2.670525010	-2.479813500	6	-4.664008520	-2.084347120	4.847019980
6	6.554225560	5.115249230	-0.024366280	1	-5.380993470	-1.867887780	5.655733180
1	6.110378140	6.109733210	0.144113530	1	-3.985278860	-1.221641050	4.746825910
1	6.283477220	4.468300590	0.825829250	1	-5.228946730	-2.201380450	3.908681200
1	7.650766980	5.221105160	-0.053457260	6	0.694402470	0.679446830	5.210786960
6	6.380991360	5.424330150	-2.521444040	6	-0.539613270	-0.231885640	5.211229720
1	5.985978940	6.439789910	-2.354787350	1	-0.252756160	-1.295376240	5.270520410
1	7.474044310	5.495525540	-2.646931430	1	-1.181559020	0.002030620	6.075495470
1	5.938902000	5.020961200	-3.444994330	1	-1.136817910	-0.089728150	4.293872350
6	1.726435440	5.760289140	-1.777388570	6	1.579725460	0.388387380	3.993309130
6	2.171966090	6.515593820	-0.519650030	1	2.461276590	1.048819250	3.985348540
1	1.975345840	7.596042450	-0.622164470	1	1.938296900	-0.654048180	4.014284510
1	1.618589020	6.160556320	0.365969650	1	1.025719940	0.552548640	3.051051790
1	3.248411690	6.360273650	-0.352189270	6	1.494456180	0.472269050	6.505572690
6	2.440557020	6.326856660	-3.011127150	1	2.375710330	1.132846190	6.520661320
1	2.177629290	7.390711840	-3.133747970	1	0.867961880	0.711131550	7.379292040
1	3.531860200	6.245682120	-2.905775000	1	1.837075160	-0.571680010	6.595576740
1	2.136775350	5.788725830	-3.921883570	6	-1.590451650	4.639558360	5.952929320
6	0.208988570	5.875073900	-1.959778780	6	-2.747059580	3.636214030	5.840961660
1	-0.088165590	6.928050840	-2.094519690	1	-2.371310360	2.601990930	5.901925700
1	-0.113711220	5.308472920	-2.847957730	1	-3.464553680	3.789849790	6.663621190
1	-0.333723170	5.481583460	-1.083493870	1	-3.280719800	3.763921780	4.885761380
6	3.361857120	2.770485170	-4.680591140	6	-0.844999250	4.445740780	7.281753340
6	3.827844490	3.593980640	-5.889997100	1	-0.037155450	5.189177510	7.375644240
1	3.495633380	3.127662360	-6.831607270	1	-1.530110380	4.568894740	8.136682400
1	3.416155260	4.614239930	-5.839158150	1	-0.402450300	3.438804900	7.317172600
1	4.926919800	3.663770790	-5.901599940	6	-2.128768900	6.072398140	5.842661430
6	1.830674580	2.689022430	-4.658674060	1	-1.300732670	6.795870960	5.910095240
1	1.455208460	2.128848910	-5.531227190	1	-2.632072730	6.214153410	4.872485430
1	1.487820900	2.182737960	-3.740435120	1	-2.848154850	6.285216580	6.649694410
1	1.392045510	3.699342580	-4.676315270	6	2.308689640	4.582391770	3.691712260
6	3.985926030	1.369457080	-4.735658440	6	2.688158810	4.233339760	5.137262200
1	3.677771450	0.839879190	-5.652057840	1	3.516610740	4.881159060	5.468296920
1	5.085069130	1.444716560	-4.727781110	1	1.834605890	4.381094190	5.814201390
1	3.671285300	0.765022760	-3.870473650	1	3.017591730	3.185439150	5.213296830
6	-5.319348560	-4.152369630	0.940982130	6	1.841314830	6.040447390	3.601640000
6	-6.313603310	-5.313314850	1.092061520	1	2.635825000	6.724216660	3.943349400
1	-7.045683550	-5.308907500	0.268689360	1	1.591002410	6.302460960	2.560956610
1	-5.781958190	-6.277424020	1.084308550	1	0.945016920	6.181757060	4.222505240
1	-6.858158680	-5.223695250	2.045088790	6	3.512987720	4.343189530	2.772541630
6	-6.072337780	-2.813687590	0.966160940	1	4.368517010	4.961627080	3.089601830
1	-6.780209520	-2.751419240	0.123119040	1	3.822169610	3.284827050	2.807041840
1	-6.641020950	-2.713154550	1.904267310	1	3.286806420	4.611322230	1.727367990
1	-5.366334660	-1.971742360	0.890414500	6	-6.937927120	1.984280770	-1.594409620
6	-4.539782480	-4.300268690	-0.372502190	6	-6.644939860	0.773909150	-2.491371650
1	-5.229362490	-4.283841360	-1.232783090	1	-7.549619160	0.153743320	-2.605828780
1	-3.817813660	-3.478028600	-0.495299480	1	-6.320265890	1.099524520	-3.491340980
1	-3.985040430	-5.251124910	-0.391892520	1	-5.853743010	0.146274440	-2.051941700
6	-1.434494950	-5.989999240	2.242471870	6	-7.360922830	1.514037140	-0.195062200
6	-0.292224880	-6.404342870	1.305551810	1	-8.265317580	0.886755360	-0.254810610
1	-0.592949550	-6.267697240	0.254388090	1	-6.558333390	0.920806290	0.270645220
1	0.618699700	-5.810708120	1.488978270	1	-7.582755500	2.378854130	0.449922090
1	-0.030664780	-7.464730980	1.453841650	6	-8.052882190	2.838133900	-2.215995380
6	-2.670722280	-6.849197710	1.945807990	1	-8.981368460	2.253887230	-2.318230730
1	-2.972727980	-6.741572060	0.892132590	1	-8.257813830	3.716373840	-1.583951870
1	-2.436373380	-7.910587380	2.130113620	1	-7.752780910	3.193491080	-3.214806900
1	-3.520657260	-6.557611000	2.579117560	6	-4.267347170	4.881354940	0.544067820
6	-1.018718120	-6.161291220	3.709107830	6	-3.152677180	5.799089970	1.063391190
1	-0.765819910	-7.214082840	3.916747860	1	-3.559714610	6.549293290	1.760879740
1	-0.135838160	-5.544950340	3.940990350	1	-2.384096440	5.218094400	1.598265250
1	-1.831928370	-5.844901360	4.377401300	1	-2.675971170	6.328207810	0.222961100
6	-3.866303120	-3.357176380	5.161574230	6	-4.878945670	4.083803100	1.703879780
6	-4.804028280	-4.567496450	5.279843020	1	-5.312130710	4.763696290	2.455703850

1	-5.678566310	3.420508850	1.339041540	6	-2.721964760	-0.709535870	-6.517233760
1	-4.105911940	3.471665610	2.195814630	1	-3.598517220	-0.834184210	-7.174384670
6	-5.346202620	5.725044480	-0.153010130	1	-2.702298730	0.336627090	-6.169254150
1	-5.841712700	6.385998300	0.576683110	1	-1.804422820	-0.902230530	-7.091768580
1	-4.894346790	6.356014460	-0.934696430	6	-4.020821590	-1.356670550	-4.456142520
1	-6.096656310	5.069456950	-0.617453910	1	-4.952517910	-1.494837390	-5.028979790
6	-3.380287950	3.495528730	-3.819805250	1	-4.055035680	-2.022609820	-3.577493310
6	-3.505019560	4.956847890	-3.373848530	1	-4.001761270	-0.310532350	-4.106801780
1	-3.456294200	5.617992730	-4.2255400150	6	-2.871917020	-3.124356770	-5.814218780
1	-4.465068350	5.128823810	-2.866116280	1	-3.783108440	-3.265986710	-6.418782390
1	-2.694075930	5.226991980	-2.681787340	1	-1.997897770	-3.376130600	-6.431919540
6	-2.062619980	3.297483720	-4.579982920	1	-2.908262990	-3.820972050	-4.962572320
1	-2.012376330	3.962768970	-5.457174120	6	-0.010787020	-4.578923210	-3.245817750
1	-1.203709020	3.525130220	-3.927638170	6	-0.739877680	-3.919508000	-2.069467720
1	-1.968741330	2.261165660	-4.948417050	1	-0.751825190	-4.586863060	-1.191875060
6	-4.567721920	3.120845770	-4.714885610	1	-0.252305380	-2.969807820	-1.789570840
1	-4.590877410	3.762164660	-5.611730000	1	-1.784134170	-3.695884430	-2.342331050
1	-4.494769890	2.071936180	-5.045827970	6	-0.745725820	-5.859512730	-3.668218420
1	-5.511242830	3.255213100	-4.165497110	1	-0.745543110	-6.598021800	-2.849805710
14	-2.947605100	-3.555790440	2.461134360	1	-1.790721560	-5.635562920	-3.934811880
8	-2.875608470	-3.612458730	4.136862790	1	-0.252611840	-6.307625090	-4.545094910
1	2.115519970	-3.269454130	-0.421769460	6	1.442551040	-4.910803520	-2.881091930
1	-2.787026310	-1.964912330	0.657842570	1	1.490086800	-5.598840140	-2.020318940
1	-3.961892910	0.172084040	-0.913465780	1	1.944795720	-5.388697920	-3.737230970
1	1.310093270	-0.154947780	-3.972131070	1	1.995007650	-3.995405070	-2.617739860
1	3.469826530	1.892671450	-0.059411190	6	1.254517310	-2.444906910	-7.132245100
1	-1.612410030	3.277520240	2.090162390	6	0.764920670	-3.802623330	-7.658062050
1	-4.239656360	1.028709590	0.598368270	1	1.512048060	-4.254859700	-8.330921870
1	1.980574590	-1.673803050	-3.393855810	1	0.582268260	-4.484094960	-6.813550260
1	3.530655940	-2.413931880	-0.966042960	1	-0.175015160	-3.676447730	-8.219288480
1	-3.395358030	-1.271496210	2.167745540	6	2.589963610	-2.612313860	-6.393446610
1	4.043977490	1.197948450	-1.558187920	1	3.356568350	-3.007685650	-7.079845350
1	-2.134563840	2.090596100	3.274970000	1	2.940763430	-1.645597170	-5.999012560
1				1	2.484070210	-3.317684920	-5.553776350
Reactant -HS							
94	1.736431210	-0.374627790	-1.112241980	6	1.416797420	-1.449494740	-8.288908320
94	-1.658107230	0.451749650	1.160598560	1	2.163935150	-1.807734770	-9.015151360
19	0.437583470	-2.675033630	1.822635790	1	0.456202560	-1.313391360	-8.811074860
19	1.022792270	2.923855060	0.628352840	1	1.739979930	-0.468873660	-7.903141630
19	-1.565478780	0.460842160	-2.556833310	6	3.358176150	-4.202130850	3.811740630
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1	3.130465410	-5.446471890	-2.607194500	1	-3.437932570	1.493807700	1.444175480
1	2.826252120	-4.075383600	-3.706267300	19	3.276825900	-0.668096010	-0.072645070
6	5.543103840	-4.124657870	-3.136836090	14	-0.778208170	3.602341390	-3.602495570
1	5.364179590	-3.764269030	-4.160225860	14	-1.720352390	-3.414649090	3.361149720
1	5.654195510	-5.221470460	-3.152742220	6	0.001136410	1.946665860	-3.617175890
1	6.488313700	-3.683083090	-2.780539830	8	-0.170634960	4.632302790	-2.385638550
6	3.971797110	-1.635032640	-6.171677030	8	-0.794962950	4.512761470	-5.025183980
6	2.983194720	-2.804143500	-6.281790060	8	-2.373388730	3.443439970	-3.054489920
1	3.463047530	-3.746433040	-5.972424740	6	-1.459489940	-1.725858040	2.664637600
1	2.639196610	-2.920268940	-7.322632850	8	-2.561045880	-4.274184350	2.150724820
1	2.104543020	-2.624082730	-5.641894530	8	-2.720979500	-3.505787320	4.710628890
6	3.305226710	-0.335997230	-6.647623810	8	-0.352466290	-4.243433370	3.870601230
1	2.420098330	-0.103177980	-6.035827930	6	1.065137390	5.384660710	-2.279946260
1	2.981203030	-0.438056520	-7.696116170	6	1.188715670	5.775026250	-0.800475970
1	4.004798050	0.510889020	-6.582540350	1	0.315581160	6.371697230	-0.485785810
6	5.221287730	-1.919676010	-7.016698990	1	2.090833740	6.385255570	-0.630311300
1	5.939902590	-1.089530910	-6.928344130	1	1.262252780	4.874010120	-0.167382260
1	4.954150540	-2.041468800	-8.078507000	6	2.272666500	4.527974250	-2.680423070
1	5.715159380	-2.841436170	-6.670584990	1	2.300877370	3.606882200	-2.076653440
6	5.648092020	0.924087300	-2.952822670	1	3.208609190	5.087232840	-2.515205730
6	6.790950520	-0.098509740	-2.918923040	1	2.227071630	4.249616400	-3.744545070
1	6.800096240	-0.642808240	-1.962152970	6	0.965885310	6.645227190	-3.149190370
1	7.761324050	0.411500650	-3.039598970	1	0.805585540	6.372322980	-4.202411660
1	6.676640670	-0.829212550	-3.734866560	1	1.884042040	7.250226540	-3.067652920
6	5.627774680	1.660312420	-4.298558420	1	0.111493550	7.263006160	-2.826067090
1	5.547885720	0.937219730	-5.122541450	6	-0.363302760	4.266253390	-6.386101130
1	6.551037060	2.247278010	-4.435077820	6	1.155421020	4.047272840	-6.437572930
1	4.765576910	2.345788690	-4.341336390	1	1.686275830	4.918609240	-6.022392240
6	5.800376250	1.939369470	-1.813822520	1	1.488249340	3.906037760	-7.478837980
1	4.956666580	2.648005430	-1.821040580	1	1.432066610	3.151642690	-5.859189240
1	6.738354070	2.509187590	-1.917459490	6	-1.085828290	3.054578790	-6.992995860
1	5.819801250	1.427318370	-0.838385710	1	-0.847423860	2.138668430	-6.431118460
6	-2.471622650	5.855948740	2.562047630	1	-0.770199490	2.910129570	-8.039063360
6	-2.761756230	6.417045020	1.162225800	1	-2.176612450	3.198751480	-6.978750430
1	-1.866436490	6.373368140	0.517327780	6	-0.736871210	5.538045610	-7.161158170
1	-3.058203480	7.476321590	1.227146350	1	-1.824666080	5.706684390	-7.118851200
1	-3.590381720	5.867622770	0.681746820	1	-0.435951440	5.453947560	-8.217602050
6	-1.261494180	6.576540330	3.170649200	1	-0.235058730	6.414554300	-6.721366580
1	-1.035767920	6.149872520	4.158250060	6	-3.567699180	4.220678190	-3.331218470
1	-1.461756710	7.655935130	3.275225270	6	-3.291816840	5.728175300	-3.246402050
1	-0.377124520	6.448203300	2.523832110	1	-2.912154460	6.006473090	-2.249324370
6	-3.717522220	6.03459920	3.439412850	1	-4.218167130	6.297223030	-3.432014850
1	-4.581975390	5.511880770	2.999850480	1	-2.541215510	6.024290360	-3.995901170
1	-3.966111350	7.105705330	3.522739520	6	-4.101855100	3.852445350	-4.721744150
1	-3.541834310	5.632621070	4.446238470	1	-3.384097460	4.164243210	-5.492944340
6	-1.788748390	3.646164480	6.364077970	1	-5.065636040	4.351782540	-4.915108020
6	-0.671916670	4.422765160	7.074546800	1	-4.250224600	2.762543670	-4.792730430
1	0.309982990	4.131847930	6.668459100	6	-4.591938360	3.803960160	-2.266511640
1	-0.681476070	4.220157870	8.157556660	1	-4.715240100	2.708969400	-2.264881580
1	-0.804292160	5.505456710	6.919817790	1	-5.571071700	4.270153890	-2.462618470
6	-3.164414110	4.070169560	6.901064500	1	-4.274461300	4.117821970	-1.257230890
1	-3.293033380	5.160388750	6.805246810	6	-3.533280760	-5.355342320	2.286374640
1	-3.266881020	3.803194770	7.965687880	6	-3.707411340	-5.930114690	0.876514410
1	-3.958012970	3.569919860	6.325817200	1	-4.052630900	-5.149355430	0.177816140
6	-1.587538980	2.137525950	6.567725100	1	-4.453848360	-6.741356170	0.872217800

1	-2.753934840	-6.343270110	0.506875680	8	4.415463130	-4.879239730	0.844625210
6	-4.863155570	-4.781046080	2.792944170	8	5.435943160	-2.542030930	1.488455070
1	-4.721650280	-4.336984870	3.788397040	6	3.222169820	1.641534680	-1.274358420
1	-5.627789950	-5.573212580	2.850965260	8	4.593144080	4.319520640	-1.214457760
1	-5.225941850	-3.996782410	2.109371770	8	2.004042200	4.190226600	-1.622231430
6	-3.020233760	-6.447723570	3.232079560	8	3.861745180	3.414171250	-3.587043260
1	-2.068810140	-6.863562730	2.864663920	6	-2.521450590	-1.903928680	1.679134370
1	-3.753777360	-7.268768170	3.292735770	8	-1.696826880	-4.580162930	2.027080200
1	-2.859773230	-6.041810290	4.240925320	8	-4.466344830	-4.192352590	1.957205580
6	-2.459673910	-3.278823830	6.115280330	6	-1.154095720	2.381208450	2.727860890
6	-3.803022420	-2.849686600	6.720607280	8	0.205630720	2.096727540	5.346034290
1	-4.154840210	-1.922434890	6.241093320	8	-0.665908830	4.518421760	4.811089370
1	-3.706658410	-2.674886760	7.804151090	8	1.304887870	3.656032330	3.273535100
1	-4.560158330	-3.633104330	6.557595570	6	-3.655794340	1.134952120	-0.189326670
6	-1.980499060	-4.594241470	6.747267180	8	-5.789263900	2.954632020	-1.375596330
1	-2.747069320	-5.376623740	6.626336690	8	-3.554216300	4.054387380	-0.407855780
1	-1.787375170	-4.462701010	7.824616340	8	-3.366292180	2.528928160	-2.623933270
1	-1.055525980	-4.927956310	6.253510000	7	-0.001909330	0.181855070	-0.096334890
6	-1.412119590	-2.176518710	6.329754980	6	-2.840494100	-1.762902270	-5.288172090
1	-0.453383830	-2.458137730	5.865112510	6	-2.819814470	-0.780879610	-6.466548650
1	-1.240237670	-2.021397450	7.407402680	1	-3.703036150	-0.926439750	-7.110279470
1	-1.754142980	-1.224047700	5.895119220	1	-2.830214950	0.260344890	-6.103605850
6	0.873194270	-4.721388770	3.278260000	1	-1.906152290	-0.932539840	-7.059249900
6	0.936031980	-6.234670730	3.535473210	6	-4.060387520	-1.501853140	-4.394069010
1	0.848498260	-6.441093330	4.613656830	1	-4.995845920	-1.674799850	-4.951028000
1	1.890273570	-6.652831230	3.174091210	1	-4.050842010	-2.172923450	-3.518892520
1	0.113451920	-6.751374640	3.016251440	1	-4.079284230	-0.457188110	-4.039375660
6	2.028286000	-4.025063980	4.008410460	6	-2.875932770	-3.209446750	-5.797078070
1	1.980687500	-2.934148110	3.865884100	1	-3.790024810	-3.372109030	-6.391876740
1	3.005945740	-4.377210450	3.639143920	1	-2.002875550	-3.424853870	-6.429703240
1	1.969295500	-4.235291320	5.087962920	1	-2.878896360	-3.918636520	-4.954886870
6	0.938485730	-4.446137880	1.770566530	6	0.095943510	-4.630115460	-3.363374210
1	0.128846540	-4.989587440	1.252986630	6	-0.711294200	-4.085765600	-2.180284110
1	1.896419440	-4.806095810	1.359173140	1	-0.688629830	-4.791461950	-1.333588400
1	0.846486290	-3.368715360	1.552613450	1	-0.305368550	-3.116743700	-1.839653080
19	-1.563207330	3.658262730	-0.191099490	1	-1.763581880	-3.932352770	-2.470135110
19	-1.730752870	-3.007801520	-0.192251770	6	-0.515536310	-5.948951760	-3.858065610
1	1.405600130	-1.972987270	-3.229180820	1	-0.476183180	-6.717217100	-3.068622030
1	-2.366375990	-0.168952650	-3.360790750	1	-1.567550680	-5.801386370	-4.149211700
1	1.104813000	2.036981260	-3.666481790	1	0.038571170	-6.318929730	-4.735087360
1	1.848406210	-1.166641800	2.875842080	6	1.564251630	-4.850279980	-2.975916440
1	-1.146387610	-1.132398130	3.555826660	1	1.651086750	-5.565692660	-2.141118120
1	0.039516720	2.405208370	2.991513770	1	2.125973200	-5.248062490	-3.836167790
1	1.521886030	-0.431358300	-4.135721800	1	2.029525630	-3.902202160	-2.663087140
1	-1.082070860	-1.123397840	-4.161873770	6	1.203834640	-2.326596770	-7.185356550
1	-0.335093720	1.368909770	-4.500416500	6	0.727495970	-3.671990790	-7.753010400
1	1.391639390	0.412870220	3.532832580	1	1.468817010	-4.084159340	-8.457233920
1	-0.912771610	1.202465880	3.883212310	1	0.573992680	-4.388563120	-6.932144790
1	-2.486988160	-1.357161150	2.434869170	1	-0.225522500	-3.541648440	-8.290866680
				6	2.554636900	-2.497136690	-6.476341000
				1	3.315317710	-2.854830790	-7.189353720
				1	2.896881740	-1.539539310	-6.053572140
				1	2.475103520	-3.233246540	-5.660630100
				6	1.327731410	-1.286323430	-8.306698060
				1	2.068892160	-1.603610000	-9.057653900
				1	0.356255310	-1.149123920	-8.808106150
				1	1.639695060	-0.314692730	-7.890245720
				6	3.376863780	-4.265659320	3.811300620
				6	2.470009480	-3.725978090	4.924545170
				1	2.634861820	-4.279493090	5.863311690
				1	2.680095660	-2.660495170	5.111021330
				1	1.404138240	-3.834542240	4.660652250
				6	3.090176780	-5.750610180	3.557328800
				1	3.322370490	-6.346409440	4.455544290
				1	2.029033790	-5.907651660	3.310373540
				1	3.698311940	-6.106873660	2.714003760
				6	4.844312600	-4.073658800	4.215767270
				1	5.045245590	-4.627815640	5.147672810
				1	5.523870280	-4.443909320	3.434765730
				1	5.063828160	-3.009330630	4.392122100

Uranium-CH₂ Species

Reactant	-LS		
92	1.737476810	-0.438083730	-1.119860440
92	-1.644675390	0.404330060	1.198545810
19	0.455442280	-2.709504390	1.900084750
19	1.091051350	2.890965000	0.646357170
19	-1.657734500	0.387346340	-2.527477500
14	-0.067233110	-2.061233510	-4.646479550
14	3.966815050	-3.294972110	1.193295120
14	3.442753610	3.341629200	-1.964124030
14	-0.114522260	3.122419920	4.054204150
14	-4.148034020	2.652509820	-1.111926130
6	0.949179100	-1.063976080	-3.472041450
8	-1.673065710	-1.517507990	-4.444966060
8	0.056291860	-3.727403120	-4.491111440
8	0.188253260	-1.814187700	-6.291319370
6	2.871100760	-2.442969910	-0.025708000
8	3.039749250	-3.491338330	2.614801770

6	5.434194740	-5.416519220	-0.030945060	6	-5.955493620	-2.826728930	0.599256600
6	4.955894700	-6.826771610	-0.401553530	1	-6.577374380	-2.804922220	-0.311136690
1	5.688364670	-7.331642470	-1.051556330	1	-6.611053010	-2.668538000	1.470263970
1	4.816561550	-7.433387810	0.507650570	1	-5.235381820	-1.994738710	0.548851600
1	3.991067040	-6.773440380	-0.931636340	6	-4.318235820	-4.401692910	-0.495173190
6	6.760997380	-5.485449560	0.739726680	1	-4.919109120	-4.432654570	-1.419390360
1	7.556249330	-5.919541030	0.111620560	1	-3.575906840	-3.594219600	-0.593605640
1	7.061804620	-4.475064150	1.054548160	1	-3.776066580	-5.355983100	-0.403855960
1	6.645991800	-6.114593570	1.637216040	6	-1.484494960	-5.973228890	2.411558000
6	5.597783730	-4.569793950	-1.300965480	6	-0.414527440	-6.505196880	1.449760620
1	6.354166390	-5.021469490	-1.963509510	1	-0.780204640	-6.460086060	0.411308900
1	4.645840590	-4.508202680	-1.851534160	1	0.515149600	-5.916355630	1.516628790
1	5.927425600	-3.549256540	-1.049340450	1	-0.164114980	-7.552831340	1.683663210
6	5.859789530	-1.173385750	1.669985910	6	-2.760691510	-6.813464520	2.269273590
6	7.117846010	-1.234143490	2.548840840	1	-3.132328890	-6.785656800	1.233580290
1	7.531774440	-0.224794440	2.705055120	1	-2.539902460	-7.861938770	2.529125390
1	6.881584010	-1.670698680	3.531720500	1	-3.558081370	-6.447536880	2.932099980
1	7.887229290	-1.858130430	2.067552150	6	-0.989365920	-6.023835780	3.862637920
6	6.213980640	-0.591499240	0.296555240	1	-0.782507880	-7.063001280	4.167372580
1	6.605540910	0.433636710	0.394754070	1	-0.059229240	-5.445733660	3.980474860
1	6.982099140	-1.211955120	-0.191965880	1	-1.744899370	-5.590783830	4.534142160
1	5.324465420	-0.558158590	-0.353001020	6	-4.088055110	-3.232265550	5.028123160
6	4.774614120	-0.336342920	2.355519860	6	-5.032840400	-4.437435730	5.141194510
1	5.113115580	0.705962600	2.482225320	1	-5.829984800	-4.238394720	5.876193320
1	3.847418510	-0.334968910	1.757256010	1	-5.487313090	-4.650376220	4.162618270
1	4.539789430	-0.746045790	3.351320150	1	-4.473053120	-5.327892600	5.471062380
6	6.033096460	4.374038130	-1.357270340	6	-3.382539580	-2.980523010	6.366167340
6	6.626529910	3.001286150	-1.699705470	1	-4.115299850	-2.758200800	7.158357600
1	7.725285810	3.066267990	-1.759561870	1	-2.803110610	-3.869229200	6.664392670
1	6.362342660	2.261327020	-0.928783950	1	-2.688384680	-2.130136190	6.277077920
1	6.246505640	2.645757210	-2.670483370	6	-4.859433910	-1.978634270	4.595552580
6	6.565159720	4.854167370	-0.000591180	1	-5.624783550	-1.719557930	5.345280500
1	6.119114210	5.827770670	0.259529890	1	-4.174307630	-1.121275020	4.489590590
1	6.301378060	4.132014340	0.789236380	1	-5.365308170	-2.147098220	3.631645470
1	7.661272820	4.966252820	-0.024850900	6	0.638453800	0.722074830	5.431140410
6	6.376396700	5.388686590	-2.458024270	6	-0.593200380	-0.190480060	5.371727380
1	5.976701480	6.382785470	-2.199201920	1	-0.312136490	-1.247133340	5.518785470
1	7.468435340	5.477460570	-2.581213710	1	-1.310174840	0.090676810	6.159657400
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6	1.712851680	5.616097850	-1.764410830	6	1.625240230	0.371618370	4.312622730
6	2.076610880	6.320898270	-0.452023390	1	2.505460230	1.033233180	4.345709750
1	1.872142630	7.402780670	-0.517325610	1	1.975856840	-0.668186830	4.420743400
1	1.478991940	5.924590610	0.386485880	1	1.150775370	0.476043390	3.320105960
1	3.145313200	6.173782210	-0.231847940	6	1.321236260	0.587421110	6.800385950
6	2.478454990	6.255816480	-2.929278960	1	2.195577670	1.254794910	6.859202210
1	2.193432420	7.317333910	-3.017730110	1	0.619250970	0.863721810	7.602936330
1	3.563961820	6.197121500	-2.765624470	1	1.658308300	-0.448199180	6.971192330
1	2.241028030	5.753503580	-3.878854560	6	-1.644384590	4.719178830	5.857292730
6	0.204891730	5.706545250	-2.023045640	6	-2.791515720	3.703225000	5.766628740
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1	-0.373038460	5.244689740	-1.204921160	1	-3.299310700	3.775583540	4.791909100
6	3.359718480	2.787895560	-4.787865220	6	-0.940291890	4.607271900	7.217649380
6	3.865030140	3.656988350	-5.948548830	1	-0.136826260	5.357742850	7.292110250
1	3.530544130	3.249032530	-6.915988200	1	-1.651989410	4.778932100	8.041931710
1	3.483910830	4.685720020	-5.850704500	1	-0.498112080	3.605537410	7.327059730
1	4.965735460	3.692978630	-5.944570610	6	-2.185036550	6.139907510	5.647149000
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6	3.941486430	1.373184350	-4.906353100	6	2.680865780	4.220329840	5.256705090
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6	-6.707949740	0.839263150	-2.319010520	1	-4.474726450	-1.482158120	0.359632020
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6	-2.124122840	-4.684889750	6.761176270		1	-3.99203765	-0.29024990	-4.08858177
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1	-1.961590230	-4.562833120	7.844679170		1	-3.79629155	-3.25644434	-6.39068479
1	-1.195694440	-5.050075220	6.296729930		1	-2.01172769	-3.37587380	-6.40930974
6	-1.459552860	-2.287196480	6.370807880		1	-2.91926299	-3.80748598	-4.93430044
1	-0.491620370	-2.607629770	5.952635100		6	0.01454041	-4.58838107	-3.29486110
1	-1.330386590	-2.129222420	7.454042640		6	-0.73896546	-3.96710745	-2.11354365
1	-1.745492680	-1.327346290	5.912834520		1	-0.74063515	-4.65088319	-1.24827496
6	0.870884190	-4.801703040	3.363596320		1	-0.27544292	-3.01240899	-1.80985203
6	1.037973940	-6.299728940	3.659940870		1	-1.78602767	-3.76312669	-2.39082481
1	0.934262510	-6.486948160	4.740253170		6	-0.68596003	-5.87819151	-3.74663879
1	2.030096550	-6.654695700	3.335460340		1	-0.67995186	-6.62868831	-2.93928870
1	0.269489430	-6.887131150	3.132370670		1	-1.73194619	-5.67289686	-4.02399003
6	1.946279430	-4.001459320	4.109261450		1	-0.17156889	-6.30234096	-4.62324798
1	1.818979790	-2.920759730	3.938635340		6	1.47237907	-4.89052817	-2.92461783
1	2.959039870	-4.282593160	3.774795090		1	1.52988020	-5.59240829	-2.07580543
1	1.873215950	-4.193741350	5.191315650		1	1.99307579	-5.34032049	-3.78499649
6	0.960116420	-4.555805070	1.851901840		1	1.99817499	-3.96610137	-2.63953586
1	0.190060930	-5.148393080	1.327365920		6	1.23751048	-2.40855820	-7.16194949
1	1.944363710	-4.875040540	1.470591930		6	0.74671438	-3.76507257	-7.68972028
1	0.823084990	-3.488000430	1.609753590		1	1.48697664	-4.20999450	-8.37486877
19	-1.484798020	3.569351190	-0.185227220		1	0.57705205	-4.45207469	-6.84706974
19	-1.672538320	-3.115427040	-0.186582600		1	-0.20095170	-3.63890598	-8.23789382
1	1.394745020	-1.931524180	-3.358342010		6	2.58201707	-2.57452686	-6.43974277
1	-2.354597550	-0.156166180	-3.447906030		1	3.34265314	-2.96302760	-7.13658137

Neptunium-CH₂ Species

Reactant -LS

93	1.75016825	-0.39583208	-1.11697611
93	-1.67139490	0.41831462	1.14506117
19	0.45084245	-2.67599057	1.88756588
19	0.98862197	2.92941730	0.65136786
19	-1.54925377	0.50233039	-2.58387258

14	-0.04178289	-2.04560341	-4.63956835
14	3.92651844	-3.34685833	1.11116542
14	3.43776405	3.41313009	-1.85320180
14	-0.15779504	3.05927909	4.08355216
14	-4.12403349	2.66211244	-1.21954328
6	1.00546111	-1.05349503	-3.48947068
8	-1.62902195	-1.44265626	-4.46073622
8	0.01601982	-3.71219132	-4.44288991
8	0.22427853	-1.85501925	-6.29126783
6	2.79094162	-2.52419451	-0.09001254
8	3.06102770	-3.44536092	2.58308881
8	4.31154932	-4.96083867	0.82411375
8	5.43212426	-2.63192443	1.30943197
6	3.22070185	1.72814515	-1.13294851
8	4.53831580	4.44490836	-1.09695593
8	1.96947803	4.24181500	-1.58936484
8	3.91644467	3.45035226	-3.46307824
6	-2.52670826	-1.91284826	1.65840243
8	-1.67625361	-4.55091676	2.13260644
8	-4.45373266	-4.20001630	2.04098517
6	-1.21132067	2.31397801	2.77493677
8	0.28422068	1.98697402	5.30207582
8	-0.74157715	4.38421545	4.93880605
8	1.19763450	3.70586361	3.27561199
6	-3.63121231	1.12711151	-0.33162010
8	-5.76209769	2.97945477	-1.49117358
8	-3.53154139	4.04568692	-0.47400401
8	-3.32690728	2.58090216	-2.72716172
7	0.00750638	0.21795652	-0.10742077
6	-2.79776560	-1.66182266	-5.30890063
6	-2.73251229	-0.70517059	-6.50644334
1	-3.61611660	-0.83077495	-7.15382610
1	-2.70689744	0.34271547	-6.16405239
1	-1.82099087	-0.90230217	-7.08884110
6	-4.01356425	-1.33905937	-4.42987700
1	-4.95068722	-1.48192547	-4.99260837
1	-4.03878112	-1.99806020	-3.54579610
1	-3.99203765	-0.29024990	-4.08858177
6	-2.88234181	-3.11588194	-5.79013169
1	-3.79629155	-3.25644434	-6.39068479
1	-2.01172769	-3.37587380	-6.40930974
1	-2.91926299	-3.80748598	-4.93430044
6	0.01454041	-4.58838107	-3.29486110
6	-0.73896546	-3.96710745	-2.11354365
1	-0.74063515	-4.65088319	-1.24827496
1	-0.27544292	-3.01240899	-1.80985203
1	-1.78602767	-3.76312669	-2.39082481
6	-0.68596003	-5.87819151	-3.74663879
1	-0.67995186	-6.62868831	-2.93928870
1	-1.73194619	-5.67289686	-4.02399003
1	-0.17156889	-6.30234096	-4.62324798
6	1.47237907	-4.89052817	-2.92461783
1	1.52988020	-5.59240829	-2.07580543
1	1.99307579	-5.34032049	-3.78499649
1	1.99817499	-3.96610137	-2.63953586
6	1.23751048	-2.40855820	-7.16194949
6	0.74671438	-3.76507257	-

1	2.76523584	-4.07826784	5.87700286	1	1.52562183	2.23181317	-3.80772510
1	2.80008687	-2.49458371	5.05254959	1	1.51264688	3.75611859	-4.73607173
1	1.50055756	-3.67529432	4.69476482	6	4.04328107	1.35736973	-4.69438743
6	3.13751269	-5.65731596	3.63795211	1	3.77186837	0.84977416	-5.63450145
1	3.40396607	-6.20644146	4.55618743	1	5.14205449	1.40004793	-4.62475537
1	2.06683827	-5.82134501	3.44223449	1	3.66325181	0.75054166	-3.85730681
1	3.70937751	-6.06062022	2.79067019	6	-5.20959445	-4.24108794	0.80879719
6	4.92087191	-3.95718802	4.14362536	6	-6.22074018	-5.38363354	0.98541663
1	5.15190343	-4.45759387	5.09870696	1	-6.86563576	-5.47455394	0.09671143
1	5.57128829	-4.37644582	3.36266142	1	-5.69641981	-6.33947611	1.13902766
1	5.15111041	-2.88565882	4.24968497	1	-6.85832332	-5.19247862	1.86276479
6	5.28331872	-5.57387848	-0.05461181	6	-5.95383535	-2.91054212	0.62047339
6	4.75159891	-6.98600209	-0.33453676	1	-6.58251106	-2.94046222	-0.28489829
1	5.44528724	-7.54593361	-0.98201479	1	-6.60450885	-2.71218343	1.48697244
1	4.62752973	-7.54076086	0.60932714	1	-5.24006786	-2.07761005	0.52066570
1	3.77011775	-6.93047223	-0.83290747	6	-4.30624831	-4.52298145	-0.39886041
6	6.63375897	-5.64456273	0.67369645	1	-4.90714970	-4.59834571	-1.32038109
1	7.39316310	-6.13564109	0.04313313	1	-3.56907781	-3.71627891	-0.53351909
1	6.97563685	-4.62941654	0.49270900	1	-3.75858787	-5.46915666	-0.26509194
1	6.53184866	-6.22278395	1.60634809	6	-1.44518517	-5.92411786	2.57129034
6	5.42705255	-4.79959999	-1.37246486	6	-0.38296733	-6.48541485	1.61741375
1	6.14701620	-5.30754394	-2.03481471	1	-0.76223543	-6.48370180	0.58267524
1	4.45883183	-4.73910890	-1.89379395	1	0.54332778	-5.88822510	1.64917632
1	5.79396618	-3.77796210	-1.18574696	1	-0.12104230	-7.52126641	1.88826347
6	5.90808364	-1.26935644	1.34569196	6	-2.71479044	-6.78125592	2.48264477
6	7.23046705	-1.30630050	2.12574009	1	-3.10168512	-6.79964836	1.45246078
1	7.68120892	-0.30185555	2.17456930	1	-2.48004442	-7.81592712	2.78255834
1	7.06107727	-1.66415839	3.15321301	1	-3.50605149	-6.39560300	3.14173364
1	7.94302022	-1.98677082	1.63365790	6	-0.93119391	-5.90618146	4.01667025
6	6.16633234	-0.80714238	-0.09341796	1	-0.70884152	-6.92826762	4.36503986
1	6.57034686	0.21715824	-0.11717320	1	-0.00665969	-5.31264278	4.09720447
1	6.88783377	-1.47979135	-0.58362701	1	-1.68425663	-5.45192671	4.67715540
1	5.23069015	-0.81685179	-0.67610016	6	-4.09672207	-3.10212290	5.06403420
6	4.90564196	-0.34861287	2.05055681	6	-5.05178239	-4.29494626	5.21656774
1	5.27625842	0.69015920	2.06779646	1	-5.85423716	-4.06094985	5.93530779
1	3.93223610	-0.36560455	1.53161731	1	-5.49813688	-4.54400667	4.24288181
1	4.74530223	-0.67663475	3.09053727	1	-4.50121783	-5.17517975	5.58675123
6	5.98170172	4.51318408	-1.17514285	6	-3.40168604	-2.80364415	6.39793531
6	6.60640501	3.12586395	-1.37289880	1	-4.13933019	-2.54311011	7.17374489
1	7.70630440	3.19973166	-1.38187626	1	-2.83368375	-3.68517391	6.73656653
1	6.30734764	2.45112243	-0.55566706	1	-2.69739087	-1.96495701	6.28192452
1	6.28049440	2.68460591	-2.32833094	6	-4.85512891	-1.86059341	4.57603650
6	6.44174083	5.10911050	0.16180750	1	-5.62511296	-1.56613705	5.30766488
1	5.96987266	6.09206474	0.32177071	1	-4.16148060	-1.01378400	4.44441352
1	6.15258522	4.44739760	0.99434406	1	-5.35339871	-2.06244038	3.61449600
1	7.53591565	5.23984217	0.17788252	6	0.79300065	0.63691168	5.26979455
6	6.36936574	5.44015806	-2.33692488	6	-0.39253299	-0.33575131	5.23178273
1	5.95293989	6.44789891	-2.17564303	1	-0.05427618	-1.38379674	5.29992285
1	7.46534122	5.52907536	-2.41736930	1	-1.06743336	-0.13927313	6.08005121
1	5.97074314	5.04099788	-3.28189774	1	-0.97090453	-0.21723819	4.29933759
6	1.66423804	5.66089664	-1.76481846	6	1.71742114	0.40796553	4.06830450
6	1.96334511	6.39157351	-0.45021996	1	2.56179248	1.11565558	4.08368875
1	1.74362260	7.46871507	-0.54056057	1	2.13161027	-0.61365756	4.08703959
1	1.33926184	5.99744575	0.36998092	1	1.16910970	0.54593966	3.11896936
1	3.02471024	6.26609069	-0.18608123	6	1.57376347	0.45712387	6.58015775
6	2.46730046	6.29380521	-2.90821631	1	2.41754610	1.16385344	6.62333256
1	2.17011158	7.34900561	-3.02687218	1	0.91612352	0.64990285	7.44242327
1	3.54570342	6.25428190	-2.69866922	1	1.97065681	-0.56784671	6.66520803
1	2.27736174	5.77174885	-3.85795443	6	-1.70681465	4.47931413	6.01132001
6	0.16722834	5.72471503	-2.08589715	6	-2.81580858	3.42646532	5.87550372
1	-0.16191839	6.77012124	-2.20539678	1	-2.39558965	2.40932404	5.93507690
1	-0.04290346	5.18738864	-3.02463502	1	-3.55056996	3.54187573	6.68914671
1	-0.43683636	5.26464628	-1.28591645	1	-3.34120512	3.53659929	4.91363608
6	3.45727158	2.77481317	-4.65406640	6	-0.97429663	4.30948553	7.35056201
6	4.00246073	3.59670221	-5.83089051	1	-0.20378174	5.08899989	7.46389748
1	3.70225735	3.14970558	-6.79236471	1	-1.67819442	4.39303045	8.19492372
1	3.61759454	4.62781066	-5.78783100	1	-0.48554114	3.32408574	7.38552605
1	5.10234120	3.63492502	-5.78983551	6	-2.30608848	5.88778705	5.90089185
6	1.92486533	2.73500535	-4.70438372	1	-1.51132508	6.64609997	5.98442840
1	1.57713936	2.18969864	-5.59763887	1	-2.80062478	6.01258493	4.92392867

1	-3.04562344	6.06477058	6.69832101	93	-1.63787086	0.43414453	1.16010134
6	2.21058628	4.62797555	3.79069661	19	0.44972460	-2.73140381	1.84585693
6	2.56791198	4.31970030	5.25090199	19	1.07056121	2.90680297	0.63193911
1	3.36217880	5.00561062	5.58894064	19	-1.56744678	0.49804340	-2.57383778
1	1.69265123	4.44602416	5.90374798	14	-0.03957848	-2.06114947	-4.62404511
1	2.93499288	3.28691966	5.35453618	14	3.95881916	-3.29289575	1.20085338
6	1.67977619	6.06130914	3.66337228	14	3.44955513	3.38541471	-1.94150766
1	2.42967679	6.78647281	4.02031459	14	-0.11381767	3.09886383	4.05073066
1	1.45095118	6.29718909	2.61149496	14	-4.14835781	2.63660108	-1.17974570
1	0.75896159	6.16875099	4.25489169	6	1.00875228	-1.07217802	-3.47380440
6	3.44733251	4.42753111	2.90560971	8	-1.63172901	-1.47820688	-4.42577452
1	4.26678941	5.08799880	3.23290824	8	0.04040658	-3.72819689	-4.43509047
1	3.80111007	3.38439790	2.96619848	8	0.20824368	-1.85475484	-6.27636680
1	3.23522531	4.66838878	1.85083063	6	2.87007004	-2.45447945	-0.03126539
6	-6.94214341	2.14025550	-1.53818215	8	3.03121941	-3.46472013	2.62688299
6	-6.71492664	0.88576168	-2.39269975	8	4.40047970	-4.88635607	0.88190663
1	-7.64579819	0.29910343	-2.46544056	8	5.43265865	-2.54246533	1.48486907
1	-6.39817117	1.15866658	-3.41084282	6	3.24071911	1.68888008	-1.24325912
1	-5.94100638	0.24344260	-1.94399726	8	4.60801901	4.37510913	-1.21910210
6	-7.35204160	1.73915671	-0.11370144	8	2.01447066	4.23922581	-1.59029627
1	-8.27719359	1.14016916	-0.13201504	8	3.84717307	3.44869241	-3.57218504
1	-6.56006579	1.13764535	0.35971327	6	-2.50484702	-1.90465511	1.66726619
1	-7.53315607	2.63476581	0.50114290	8	-1.69849819	-4.57678051	2.05762948
6	-8.03694876	3.01313340	-2.16846118	8	-4.46714974	-4.17735763	1.97669162
1	-8.99089450	2.46456243	-2.22198290	6	-1.17496171	2.39429163	2.72633589
1	-8.18888754	3.92440884	-1.56911593	8	0.23929004	2.01913704	5.29246955
1	-7.75038263	3.31410620	-3.18889703	8	-0.63552753	4.46586576	4.87954143
6	-4.10848909	4.97414557	0.47855186	8	1.29124241	3.65861590	3.26113929
6	-2.93899745	5.83420307	0.97547965	6	-3.63079220	1.10466707	-0.30009957
1	-3.29332984	6.60855321	1.67527334	8	-5.79226119	2.92610769	-1.44993413
1	-2.19479561	5.21454692	1.50182711	8	-3.58054814	4.02977486	-0.43458811
1	-2.44776599	6.33086758	0.12393412	8	-3.35508613	2.57061156	-2.69086765
6	-4.74572551	4.21995078	1.65311576	7	-0.00328495	0.27158039	-0.15247230
1	-5.13126486	4.92964034	2.40334188	6	-2.80600715	-1.70669771	-5.26425067
1	-5.58464458	3.59764545	1.30564344	6	-2.76645232	-0.73631853	-6.45189763
1	-4.00131519	3.57123290	2.14254367	1	-3.65512778	-0.86683424	-7.09140847
6	-5.15073506	5.86652144	-0.21311485	1	-2.75181495	0.30814590	-6.09817564
1	-5.59730435	6.56467760	0.51350620	1	-1.85880549	-0.91472750	-7.04630998
1	-4.67834970	6.45852039	-1.01291214	6	-4.01768697	-1.41059350	-4.37043069
1	-5.94433049	5.24618682	-0.65427600	1	-4.95795107	-1.56702830	-4.92422540
6	-3.40745664	3.45259617	-3.89480084	1	-4.02177233	-2.07460582	-3.48981476
6	-3.52678496	4.92798259	-3.49675587	1	-4.01197165	-0.36325384	-4.02403996
1	-3.50150318	5.55916418	-4.40101733	6	-2.87350685	-3.15684992	-5.75961845
1	-4.47568375	5.11401538	-2.97272225	1	-3.79204870	-3.30528114	-6.35121228
1	-2.69977193	5.22341536	-2.83461545	1	-2.00631574	-3.39650704	-6.39156685
6	-2.10231759	3.22842175	-4.67013281	1	-2.88988843	-3.85780620	-4.91078308
1	-2.06743555	3.86402780	-5.56974969	6	0.07680683	-4.60268460	-3.28658588
1	-1.23215805	3.47713495	-4.04098969	6	-0.67416566	-3.99736719	-2.09526155
1	-2.01555362	2.18084888	-5.00770966	1	-0.65137449	-4.68052041	-1.22999000
6	-4.60832098	3.04400889	-4.75605454	1	-0.22687652	-3.03237671	-1.79926214
1	-4.64153501	3.64534193	-5.67986239	1	-1.72854666	-3.81455107	-2.35875414
1	-4.54285846	1.98120384	-5.04129944	6	-0.60062610	-5.90849413	-3.72715603
1	-5.54398277	3.20607760	-4.20095602	1	-0.56765321	-6.65748200	-2.91905284
14	-2.97689410	-3.50521497	2.46893440	1	-1.65431279	-5.72650130	-3.99145292
8	-3.03453710	-3.45491233	4.14458111	1	-0.08812412	-6.32239835	-4.60972992
1	2.02616314	-3.29421122	-0.35369788	6	1.54620393	-4.87227322	-2.93548676
1	-2.55813415	-2.09905761	0.55482787	1	1.63001533	-5.57286701	-2.08777212
1	-4.02493847	0.23094490	-0.86019647	1	2.06613713	-5.31049918	-3.80229581
1	1.12856707	-0.06322692	-3.98972700	1	2.05631222	-3.93650843	-2.65783795
1	3.46362659	1.80600065	-0.04490305	6	1.21753151	-2.39378451	-7.16108128
1	-1.64156205	3.14750951	2.16776700	6	0.72962483	-3.74781509	-7.69783861
1	-4.20628595	1.15796018	0.62891819	1	1.46601390	-4.18134471	-8.39437451
1	2.02029129	-1.51625428	-3.58410950	1	0.57210357	-4.44455989	-6.86079832
1	3.41323690	-2.47287400	-1.02295852	1	-0.22371937	-3.62190496	-8.23608273
1	-3.43251826	-1.28001340	1.86426955	6	2.56930314	-2.55933081	-6.45243478
1	4.07734932	1.13906185	-1.53863268	1	3.32563773	-2.93542783	-7.16062062
1	-2.09344122	1.90608175	3.33377345	1	2.91842914	-1.59576170	-6.04903471
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Reactant -HS

93 1.74129509 -0.40403873 -1.11949956

1	0.37470443	-1.24556676	-8.80692802	1	3.41544830	4.69408571	-5.84088241
1	1.66763363	-0.40139529	-7.91135183	1	4.90774831	3.71900837	-5.95140217
6	3.36664805	-4.22377416	3.83386967	6	1.80160244	2.74752636	-4.73019680
6	2.45939231	-3.66908844	4.93934474	1	1.41354529	2.22178479	-5.61852336
1	2.61781558	-4.21562514	5.88333811	1	1.45538608	2.21592802	-3.82787533
1	2.67544802	-2.60356346	5.11817591	1	1.37699003	3.76376763	-4.71196633
1	1.39385610	-3.77380193	4.67234757	6	3.93236618	1.39719746	-4.87421163
6	3.07891979	-5.71192509	3.60043644	1	3.62086576	0.91953220	-5.81759229
1	3.31006527	-6.29513489	4.50713134	1	5.03264774	1.45131260	-4.85711664
1	2.01763273	-5.87164343	3.35562362	1	3.60002339	0.75678393	-4.04230505
1	3.68693852	-6.08056858	2.76249636	6	5.22483861	-4.16180945	0.74491738
6	4.83397983	-4.02673000	4.23631115	6	-6.25947118	-5.28825991	0.88524445
1	5.03402565	-4.56607740	5.17703270	1	-6.90691172	-5.33625076	-0.00497056
1	5.51378607	-4.40972189	3.46169985	1	-5.75520391	-6.25945098	1.00636596
1	5.05411007	-2.95977311	4.39574702	1	-6.89217371	-5.11282976	1.76939454
6	5.41365998	-5.44288791	0.01227627	6	-5.94092604	-2.81053406	0.60059071
6	4.93050066	-6.85892767	-0.32891597	1	-6.56886578	-2.79723603	-0.30572673
1	5.65836154	-7.37792775	-0.97299218	1	-6.58825979	-2.62716883	1.47287418
1	4.79466689	-7.44779877	0.59239682	1	-5.20972233	-1.98998603	0.52886914
1	3.96292332	-6.81385358	-0.85484687	6	-4.32796254	-4.42387379	-0.47221103
6	6.74426090	-5.50034543	0.77739666	1	-4.93060468	-4.45477486	-1.39523726
1	7.53558450	-5.94719732	0.15330560	1	-3.57223634	-3.63033771	-0.58078107
1	7.04827688	-4.48500621	1.07259033	1	-3.80231016	-5.38635851	-0.37045300
1	6.63271465	-6.11292071	1.68669743	6	-1.49598106	-5.96660274	2.45795788
6	5.57331024	-4.62148732	-1.27497251	6	-0.43216278	-6.51861482	1.50036839
1	6.32404021	-5.08905373	-1.93290362	1	-0.79951356	-6.48332878	0.46197159
1	4.61817772	-4.56697843	-1.82078554	1	0.50302076	-5.93739492	1.55926182
1	5.90867650	-3.59781927	-1.04464522	1	-0.18954399	-7.56535587	1.74616527
6	5.86591878	-1.17248602	1.62583594	6	-2.77853780	-6.79909781	2.32863117
6	7.13331101	-1.21805713	2.49202836	1	-3.15409506	-6.77804226	1.29425018
1	7.55217475	-0.20705844	2.62219016	1	-2.56409435	-7.84657811	2.59764128
1	6.90568320	-1.63277004	3.48633232	1	-3.57064822	-6.42113490	2.99096455
1	7.89564674	-1.85494522	2.01648689	6	-0.99795371	-6.00248329	3.90849864
6	6.20767230	-0.62453407	0.23497641	1	-0.80109995	-7.03924101	4.22767053
1	6.61015162	0.39870247	0.30422532	1	-0.06188287	-5.43200169	4.01638610
1	6.96321722	-1.26330476	-0.24934539	1	-1.74809621	-5.55222468	4.57480782
1	5.31047366	-0.59540373	-0.40369031	6	-4.09389498	-3.18571574	5.03388000
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1	5.13250735	0.73098324	2.39520298	1	-5.85880009	-4.15950247	5.87202748
1	3.85677034	-0.33141569	1.71872202	1	-5.50982110	-4.58384532	4.16234443
1	4.57265199	-0.69656015	3.31333392	1	-4.51721033	-5.27277574	5.48082407
6	6.04546791	4.42880286	-1.37762608	6	-3.39612582	-2.94322634	6.37786097
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1	7.73601708	3.11441660	-1.76725945	1	-2.83386368	-3.84092474	6.68190042
1	6.38210075	2.32713926	-0.90443612	1	-2.68716195	-2.10472018	6.29440932
1	6.24877365	2.67105486	-2.65338301	6	-4.84133871	-1.92023831	4.59279056
6	6.59042430	4.93953571	-0.03721137	1	-5.60981309	-1.64757778	5.33442079
1	6.14556074	5.91803612	0.20594856	1	-4.14074714	-1.07484602	4.49372988
1	6.33522680	4.23463027	0.77084160	1	-5.34021822	-2.08160460	3.62398091
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6	6.37605775	5.41928936	-2.50409608	6	-0.59870248	-0.25271894	5.23952674
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1	5.92471915	5.07549563	-3.44729757	1	-1.15338050	-0.10405788	4.29685335
6	1.72745789	5.66575422	-1.73407812	6	1.58033218	0.32614312	4.11127314
6	2.16610674	6.38823243	-0.45457434	1	2.46979538	0.97556501	4.13507212
1	1.95913328	7.46937012	-0.52443439	1	1.92428376	-0.72061857	4.15382027
1	1.61675598	6.00343187	0.42127370	1	1.06399609	0.48964151	3.14757090
1	3.24459003	6.23930716	-0.29273282	6	1.39085752	0.42062341	6.61764116
6	2.43328811	6.27998125	-2.94950718	1	2.28204396	1.06610192	6.66794066
1	2.15801407	7.34422015	-3.03626079	1	0.73202531	0.67358469	7.46323547
1	3.52569443	6.20829931	-2.84845939	1	1.71104007	-0.62879324	6.72524254
1	2.13405501	5.76928235	-3.87713490	6	-1.60642296	4.62797999	5.93877812
6	0.20823405	5.76453207	-1.91150855	6	-2.76537954	3.62973389	5.80769252
1	-0.10246144	6.81546247	-2.03102409	1	-2.39708699	2.59412754	5.88707550
1	-0.10851189	5.20578474	-2.80691765	1	-3.50150579	3.79480804	6.61142543
1	-0.32707682	5.35053138	-1.04063284	1	-3.27515774	3.75085350	4.83880649
6	3.33384069	2.80545693	-4.75786838	6	-0.89668598	4.44479707	7.28848460
6	3.80766180	3.66931643	-5.93578770	1	-0.08628540	5.18385491	7.39457975
1	3.46173028	3.24794472	-6.89349547	1	-1.60255973	4.58226464	8.12412030

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-2.13324093	6.06248935	5.79842236		Product -LS		
1	-1.30285125	6.78194946	5.87918579	93	0.02207007	0.07879661
1	-2.60982205	6.19540280	4.81365590	93	-0.11090357	0.06838940
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6	2.69568597	4.17171114	5.23792441	6	-1.75595077	-1.05564110
1	3.52086939	4.81414231	5.58718260	8	-3.88391224	-2.58739426
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1	3.01539146	3.12145104	5.32323737	8	-1.83771505	-3.85685022
6	1.89984703	5.98283652	3.67915826	6	2.02744838	-0.09323170
1	2.69171188	6.65972174	4.04016142	8	4.80136772	-0.355527692
1	1.67841718	6.24516766	2.63198118	8	4.16588584	-0.48387831
1	0.98937202	6.13351169	4.27677431	8	4.03138682	1.89831297
6	3.57348674	4.26822741	2.89142068	6	-5.14216938	-1.90730057
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1	3.86751755	3.20565065	2.93045806	1	-5.42257961	-3.11763132
1	3.37388262	4.54281009	1.84216894	1	-6.35970726	-1.59896022
6	-6.95866886	2.06944028	-1.49909020	1	-4.60130195	-1.55477355
6	-6.71700965	0.82986280	-2.37135742	6	-5.05202149	-0.41865497
1	-7.63843592	0.22861048	-2.44563209	1	-4.21592430	0.05924639
1	-6.41188525	1.12151987	-3.38790989	1	-5.98732173	0.09525613
1	-5.92940262	0.19476985	-1.93627852	1	-4.90081056	-0.27911480
6	-7.35325269	1.64351589	-0.07733413	6	-6.25837644	-2.60284323
1	-8.27311345	1.03660368	-0.09697286	1	-6.04562302	-2.56212911
1	-6.55171074	1.04317629	0.38111196	1	-7.23261256	-2.12525762
1	-7.53706621	2.52862323	0.55183525	1	-6.32460890	-3.66366703
6	-8.07143551	2.93229001	-2.11178224	6	-3.86473686	-2.30368170
1	-9.01611982	2.36822291	-2.16915276	6	-4.43938482	-0.88235940
1	-8.23631147	3.83216695	-1.49875733	1	-5.42310120	-0.89040465
1	-7.79440540	3.25274230	-3.12894040	1	-4.56618389	-0.45968806
6	-4.17409373	4.94591203	0.51968848	1	-3.75814926	-0.22760601
6	-3.02353484	5.83553200	1.00844913	1	-2.50390643	-2.27270688
1	-3.39367371	6.59842282	1.71269620	1	-1.79345112	-1.63841219
1	-2.25895867	5.23485167	1.52716975	1	-2.61698278	-1.86225442
1	-2.55243926	6.34842423	0.15513840	1	-2.07803598	-3.28145646
6	-4.78316221	4.17607684	1.69902760	6	-4.83362434	-3.21877738
1	-5.18124398	4.87493359	2.45277798	1	-4.43152794	-4.24296144
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6	-5.24283624	5.81212912	-0.16476759	6	-1.94136283	-5.262123179
1	-5.70237897	6.49745379	0.56600726	6	-1.38106370	-5.77350088
1	-4.79025005	6.41801984	-0.96559988	1	-3.74985531	-5.63144268
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1	-2.74736318	5.22058372	-2.77320075	1	-0.42385446	-5.03901968
6	-2.13066306	3.24780279	-4.62370750	6	-1.01275002	-6.00192500
1	-2.09687509	3.89525551	-5.51489249	1	0.00910572	-5.53919008
1	-1.26450848	3.49501525	-3.98820447	1	-0.97451819	-7.07798467
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1	-4.67121888	3.64846471	-5.63697606	6	6.80681898	-0.84211089
1	-4.56074379	1.98096601	-5.00814917	1	6.23737273	-1.49567678
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14	-2.98027162	-3.51619483	2.42427073	1	6.83859221	0.17345277
8	-3.03484138	-3.51313607	4.10115876	6	6.13569230	-2.23380139
1	2.18181972	-3.24457482	-0.42189007	1	5.63136621	-2.21315473
1	-2.58468475	-2.04003727	0.55834061	1	7.15655017	-2.63100003
1	-4.01293374	0.20817215	-0.83597492	1	5.58081153	-2.91346592
1	1.14662228	-0.08026377	-3.96874923	6	6.96841893	0.13183258
1	3.59387602	1.72419249	-0.18310247	1	6.96927565	1.15220297
1	-1.53935318	3.23662805	2.09071943	1	8.01342200	-0.21123914
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1	2.02053449	-1.54570509	-3.55912367	6	3.86430586	-0.17983676
1	3.57280398	-2.29800574	-0.89291863	6	3.97715560	-1.51405617
1	-3.38073392	-1.25473994	1.93805953	1	3.24292222	-2.23479129
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1	3.79401233	-1.37438624	8.03328922	1	4.68391342	2.33684967	-4.39852117
1	4.98491526	-1.93926608	6.82372995	6	5.71075922	1.97160450	-1.85926506
6	4.90441026	0.82072790	6.73265991	1	4.85305459	2.66315763	-1.87119922
1	5.91686072	0.39119439	6.66318894	1	6.63678310	2.55937141	-1.96958980
1	4.70705162	1.06940450	7.78835010	1	5.74381994	1.47003669	-0.87853229
1	4.87137003	1.74232487	6.13241113	6	-2.41570700	5.80985396	2.56384456
6	2.44884752	0.39339810	6.36859736	6	-2.66769270	6.38305569	1.16174338
1	2.34789465	1.34116355	5.81537963	1	-1.76092559	6.32308992	0.53487996
1	2.24085599	0.59219342	7.43265195	1	-2.94481900	7.44754453	1.22607258
1	1.69556825	-0.31882334	5.99568121	1	-3.49742070	5.85214888	0.66259309
6	3.87935882	3.14170381	2.99686860	6	-1.20877051	6.50954936	3.20245656
6	5.19611844	3.91064486	3.18093595	1	-1.01079329	6.07533753	4.19274473
1	5.41890735	4.03307821	4.25250393	1	-1.39545941	7.59133073	3.30789413
1	5.13413608	4.90902712	2.71759144	1	-0.31289630	6.37082211	2.57398767
1	6.03071507	3.36279504	2.71416449	6	-3.67737812	6.00058344	3.41574828
6	2.72424696	3.91300608	3.64870277	1	-4.53869932	5.49068666	2.95538205
1	1.77988570	3.35488983	3.54827711	1	-3.91451387	7.07434186	3.49940335
1	2.58972328	4.90139894	3.17843153	1	-3.52811228	5.59202676	4.42421512
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6	3.60701707	2.92198087	1.50443158	6	-0.74598573	4.31516114	7.10716900
1	4.43741441	2.36080406	1.04453194	1	0.24185398	4.01705186	6.72119031
1	3.52742374	3.89154206	0.98586062	1	-0.78300867	4.10262519	8.18768113
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7	0.42629340	-1.11017974	-0.22467763	6	-3.23715343	3.99239454	6.87395896
7	0.18615006	1.51337682	-0.21390171	1	-3.35102361	5.08510227	6.78796977
7	-1.17715667	0.96977970	-0.32567797	1	-3.36662653	3.71465580	7.93289583
14	3.65835818	-1.16187249	-3.35783409	1	-4.02346762	3.50806199	6.27555254
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6	1.84261903	-0.99208189	-3.30918660	1	-2.45162062	1.49036117	6.00513073
8	4.22894640	-2.23641409	-2.15857288	1	-1.76089177	1.78806812	7.62400930
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8	4.29133016	0.29686534	-2.77331875	6	-4.70173356	1.90642898	3.10417517
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1	-5.56472603	4.25791188	-2.46037899
1	-4.26172618	4.09413892	-1.26298559
6	-3.55148030	-5.32577167	2.26927422
6	-3.72770490	-5.88759528	0.85454991
1	-4.07274290	-5.10054875	0.16296793
1	-4.47449283	-6.69843114	0.84388487
1	-2.77488279	-6.29828088	0.48033403
6	-4.88065974	-4.759113506	2.78586186
1	-4.73587362	-4.32410900	3.78489791
1	-5.64372489	-5.55311051	2.83962932
1	-5.24733194	-3.96883111	2.11149025
6	-3.03341961	-6.42560911	3.20363341
1	-2.07772534	-6.83057816	2.83530503
1	-3.76234247	-7.25146190	3.25356640
1	-2.87801788	-6.03116228	4.21787249
6	-2.45829499	-3.28200685	6.11170069
6	-3.79084827	-2.82358801	6.71937335
1	-4.11676430	-1.88192678	6.24985723
1	-3.69199068	-2.66367634	7.80498776
1	-4.56849220	-3.58445923	6.54647398
6	-2.01581654	-4.61603865	6.73124977
1	-2.80373516	-5.37574140	6.60316499
1	-1.81992096	-4.49963128	7.80984574
1	-1.10002824	-4.97079108	6.23509213
6	-1.38255910	-2.20982101	6.33931858
1	-0.42949731	-2.51353863	5.87688031
1	-1.21141060	-2.06726270	7.41881658
1	-1.69703913	-1.24540981	5.91010190
6	0.85649383	-4.76339348	3.27720932
6	0.93808400	-6.27331947	3.54881792
1	0.84825779	-6.47052059	4.62854998
1	1.89931158	-6.68223126	3.19577920
1	0.12441078	-6.80587499	3.03130162
6	2.00147657	-4.04532334	4.00223718
1	1.93526315	-2.95583396	3.85564892
1	2.98401874	-4.38225847	3.63138295
1	1.94930416	-4.25321625	5.08259904
6	0.91812186	-4.50141127	1.76714904
1	0.10388948	-5.04471894	1.25679055
1	1.87325253	-4.86860402	1.35591182
1	0.83212291	-3.42516967	1.54042944
19	-1.54466093	3.58343982	-0.20627840
19	-1.72896994	-2.98864215	-0.20264546
1	1.36359587	-1.98760204	-3.31852363
1	-2.37267760	-0.16269788	-3.34674158
1	1.10549577	2.03651200	-3.71839304
1	1.93201478	-1.21642902	2.81869829
1	-1.02817248	-1.17183727	3.56406546
1	0.07055622	2.36262287	3.02507176
1	1.49566164	-0.45232942	-4.23341439
1	-1.09332955	-1.10802443	-4.16292134
1	-0.35548255	1.36453886	-4.50394117
1	1.38580580	0.28312260	3.57507469
1	-0.90866474	1.15936775	3.87837881
1	-2.42185270	-1.32044505	2.49824206

Uranium-NH Species

Reactant -LS

92	1.68131526	-0.49613371	-1.19708214
92	-1.71495933	0.46065475	1.14840030
19	0.53456507	-2.46274315	1.85756400
19	1.40998566	2.69091744	0.86195976
19	-1.66381112	0.38365790	-2.72408171
14	0.18059635	-1.99398779	-4.61037190
14	3.78152722	-3.34452546	0.71424793
14	3.27840635	3.09323062	-1.86887594
14	-0.30972076	2.94334946	3.93686027
14	-4.05279559	2.48742206	-1.20131444
7	0.84895381	-1.05050185	-3.33516331
8	-1.32707197	-1.28376475	-4.96816303
8	-0.01085694	-3.62640800	-4.31599812
8	1.02873379	-1.90930871	-6.05080943
7	2.63398210	-2.43594746	-0.18942132
8	3.15978711	-3.39464014	2.30055542
8	3.88646190	-4.95142869	0.25202329
8	5.37279707	-2.81642071	0.74543571
7	3.00147545	1.48757371	-1.32166818
8	4.20135638	4.05179851	-0.82797453
8	1.75398835	3.81298745	-1.77293421
8	4.03101150	3.29245903	-3.35434104
7	-2.25666562	-1.39002755	2.53177209
8	-1.68463920	-4.03398906	2.34239640
8	-4.37457894	-3.39561247	2.58754550
7	-0.98171325	2.22381272	2.52687651
8	0.23088756	1.87060250	5.09588748
8	-1.30738782	3.99859513	4.76606305
8	0.96171513	3.92296288	3.36503152
7	-3.40761389	1.09674467	-0.43058235
8	-5.71896763	2.71278438	-1.22447911
8	-3.40398747	3.90806403	-0.59746234
8	-3.49114221	2.42630095	-2.81248339
7	0.03972680	0.03531477	0.02687666
6	-2.15084751	-1.41931459	-6.16492413
6	-1.65435758	-0.40852791	-7.20695925
1	-2.27053339	-0.45154399	-8.12015644
1	-1.70322338	0.61673728	-6.80507688
1	-0.60804834	-0.62959687	-7.46688467
6	-3.58176069	-1.08807391	-5.72339529
1	-4.27706525	-1.13530456	-6.57751262
1	-3.92486933	-1.80386375	-4.95795303
1	-3.63657432	-0.07122089	-5.30050240
6	-2.10655080	-2.83991208	-6.74063181
1	-2.76352981	-2.90337053	-7.62370188
1	-1.08427644	-3.10655626	-7.04437633
1	-2.45178943	-3.57469486	-5.99821597
6	-0.58015648	-4.42450483	-3.25543575
6	-1.45186297	-3.58835427	-2.31419151
1	-1.88359817	-4.22208216	-1.52314539
1	-0.86398011	-2.79172039	-1.82249377

1	-2.28437099	-3.12263183	-2.86832987	6	6.08336339	5.27758049	-1.76544383
6	-1.42383247	-5.51748560	-3.92773984	1	5.56929968	6.23686515	-1.58985359
1	-1.81258471	-6.22406051	-3.17623932	1	7.16979649	5.45241428	-1.69684582
1	-2.28058885	-5.07675013	-4.46119435	1	5.83798764	4.92536610	-2.77854265
1	-0.81289418	-6.07707801	-4.65335077	6	1.36938563	5.20802043	-1.95338727
6	0.58324060	-5.06857514	-2.49185362	6	1.40138439	5.90074829	-0.58347621
1	0.21938759	-5.74064114	-1.69781965	1	1.12940391	6.96519626	-0.67683869
1	1.21105982	-5.65035444	-3.18472409	1	0.67875802	5.43766182	0.10966811
1	1.20686032	-4.29163360	-2.02214496	1	2.41484027	5.83649553	-0.15594163
6	2.20882326	-2.62691519	-6.49604151	6	2.29059975	5.94918362	-2.93009763
6	1.76184523	-3.93460391	-7.16559075	1	1.92751802	6.98112000	-3.06712343
1	2.63292121	-4.50202970	-7.53205511	1	3.32172435	5.99051756	-2.54894425
1	1.21012758	-4.55419271	-6.44233234	1	2.30372978	5.45276673	-3.91175837
1	1.10342037	-3.71980168	-8.02266617	6	-0.05988098	5.17366685	-2.50173490
6	3.16420616	-2.92429050	-5.33357583	1	-0.45784577	6.19588735	-2.61446114
1	4.06529646	-3.43879960	-5.70585293	1	-0.07146419	4.68832722	-3.49084682
1	3.47551552	-1.99561238	-4.82957319	1	-0.72667989	4.60936409	-1.82911807
1	2.67654136	-3.57299696	-4.58961115	6	3.85048740	2.59912367	-4.61519066
6	2.88554629	-1.70643728	-7.51933808	6	4.51611271	3.49385533	-5.66969492
1	3.77897938	-2.18753941	-7.94825378	1	4.43413045	3.04230994	-6.67136342
1	2.18673939	-1.46819472	-8.33706065	1	4.03473654	4.48441964	-5.69047472
1	3.19016822	-0.76288167	-7.03882142	1	5.58302429	3.63145332	-5.43309016
6	3.64810156	-4.14305039	3.45625220	6	2.36077498	2.42365263	-4.93505176
6	2.92794581	-3.54003566	4.66836774	1	2.22537325	1.88722900	-5.88912735
1	3.22041893	-4.05875818	5.59592165	1	1.85947751	1.84766789	-4.13921198
1	3.18163670	-2.47267574	4.77354381	1	1.86209941	3.40280232	-5.01360498
1	1.83394788	-3.63488704	4.56381323	6	4.55918226	1.23996680	-4.55448699
6	3.27653032	-5.62346813	3.30110681	1	4.49084708	0.72161738	-5.52474354
1	3.61288236	-6.19913258	4.17910839	1	5.62490384	1.37715861	-4.30929360
1	2.18516716	-5.74242451	3.21087566	1	4.10196808	0.59918074	-3.78216596
1	3.73918990	-6.03691153	2.39378020	6	-5.18012154	-3.14066552	1.41582359
6	5.16403135	-3.99270117	3.63807789	6	-6.25918357	-4.23310218	1.40496966
1	5.48074704	-4.52435687	4.55067936	1	-6.94384124	-4.09442388	0.55263135
1	5.71437628	-4.40616801	2.78094216	1	-5.79826791	-5.22997665	1.32577136
1	5.43884700	-2.93134585	3.74397938	1	-6.84689854	-4.19475767	2.33566790
6	4.72513213	-5.63198549	-0.71395654	6	-5.83187793	-1.76074953	1.55622813
6	4.02491420	-6.96986707	-0.98542311	1	-6.48148859	-1.54459306	0.69309655
1	4.59881726	-7.57273029	-1.70726251	1	-6.44523152	-1.71816967	2.47079226
1	3.92401977	-7.54326476	-0.04999429	1	-5.05474924	-0.98056528	1.62226324
1	3.01593773	-6.79489294	-1.39197226	6	-4.34042969	-3.21530396	0.13535890
6	6.11271321	-5.86951891	-0.10110569	1	-4.97100484	-3.04767981	-0.75428347
1	6.75812465	-6.42191208	-0.80358635	1	-3.54045224	-2.45453159	0.14570798
1	6.58523756	-4.90645734	0.14171985	1	-3.86888742	-4.20655608	0.04048530
1	6.02242283	-6.46148156	0.82422163	6	-1.55371826	-5.47150083	2.56329099
6	4.84093746	-4.82375870	-2.01289816	6	-0.67956986	-5.98609044	1.41272703
1	5.46385375	-5.36275216	-2.74528559	1	-1.16285310	-5.77465983	0.44547106
1	3.84754770	-4.66311628	-2.46065369	1	0.31533213	-5.51023340	1.41520649
1	5.30159071	-3.84214160	-1.82189241	1	-0.52663172	-7.07450552	1.49601960
6	5.98774921	-1.51082053	0.69145283	6	-2.91191994	-6.18425450	2.53411683
6	7.38911525	-1.68132798	1.29644980	1	-3.41892444	-6.01708727	1.57136084
1	7.94687669	-0.73169578	1.25568556	1	-2.76102664	-7.26878285	2.66283905
1	7.32017174	-2.00214469	2.34759671	1	-3.57032149	-5.82415683	3.33788691
1	7.95373734	-2.44330216	0.73644011	6	-0.86436944	-5.70852841	3.91325295
6	6.10230073	-1.08503196	-0.77813047	1	-0.71597574	-6.78664448	4.09020073
1	6.58111608	-0.09693161	-0.87011133	1	0.12431018	-5.22227066	3.93575067
1	6.70766739	-1.81617324	-1.33743847	1	-1.47190588	-5.28505834	4.72613728
1	5.10166937	-1.04243689	-1.24409144	6	-3.70244921	-2.97167198	5.71530306
6	5.18625695	-0.48916850	1.50700796	6	-4.75192123	-4.09224851	5.74205606
1	5.68843055	0.49308864	1.50306842	1	-5.47134879	-3.93284360	6.56199829
1	4.17101807	-0.35636231	1.09243952	1	-5.29415320	-4.11964115	4.78543528
1	5.09193886	-0.82273904	2.55331596	1	-4.26073704	-5.06659793	5.89739096
6	5.63534773	4.23911380	-0.72700788	6	-2.88195577	-2.97579356	7.01121822
6	6.37880252	2.91417054	-0.93659462	1	-3.52732972	-2.79099862	7.88484544
1	7.46546504	3.05485246	-0.81403124	1	-2.38251347	-3.94907164	7.14325967
1	6.04177897	2.17023629	-0.19651194	1	-2.10570399	-2.19460841	6.97205896
1	6.19340967	2.52146651	-1.94934123	6	-4.37815456	-1.60678743	5.52419889
6	5.88836044	4.76206704	0.69208394	1	-5.08498614	-1.40976469	6.34668908
1	5.32732679	5.69511321	0.86086799	1	-3.62902404	-0.79810978	5.51957486
1	5.56089363	4.02064797	1.43894955	1	-4.93746848	-1.57849553	4.57560659
1	6.96020830	4.96650968	0.84841089	6	1.12202111	0.73555174	5.12778642

6	0.26313272	-0.51684046	5.33894823	1	-2.70051964	3.70776407	-5.81877308
1	0.89241164	-1.41444057	5.45375460	1	-1.64080379	3.39842174	-4.41546539
1	-0.34247752	-0.40586449	6.25283214	1	-2.48986038	2.04361663	-5.22792037
1	-0.42358969	-0.67328857	4.48987905	6	-5.06137900	2.81401109	-4.63649835
6	1.94563040	0.61637976	3.84040694	1	-5.25076495	3.39401940	-5.55516445
1	2.56466604	1.51708289	3.69044059	1	-4.99450954	1.74842932	-4.91104822
1	2.61957606	-0.25464517	3.89097690	1	-5.91477201	2.95132860	-3.95624576
1	1.28537225	0.48576273	2.96260373	14	-2.81016384	-2.95032896	3.00523977
6	2.05237719	0.94121413	6.33194238	8	-2.75071801	-3.23677767	4.65641046
1	2.67320090	1.84054311	6.19446437	1	1.38593066	-0.30470628	-3.82640967
1	1.45997942	1.06675599	7.25188036	1	3.93250195	1.03269864	-1.25556384
1	2.72115448	0.07428182	6.46110212	1	-4.08295489	0.31541093	-0.43851926
6	-2.34553626	3.74069955	5.74727017	1	2.40075800	-3.04004992	-1.00247862
6	-3.08201365	2.42659042	5.45736330	1	-2.55818974	-0.76155121	3.30669791
1	-2.38581593	1.57547021	5.52271529	1	-1.50306851	2.99140740	2.05601854
1	-3.88969476	2.27385696	6.19217201				
1	-3.52273087	2.43766475	4.44781341				
6	-1.70105515	3.69453134	7.14015422				
1	-1.20334962	4.65194200	7.36369982				
1	-2.46326289	3.51179422	7.91530934				
1	-0.95182809	2.88919223	7.17890481				
6	-3.31192189	4.92690768	5.64408805				
1	-2.77390398	5.87147387	5.82306956				
1	-3.75823235	4.96636481	4.63812534				
1	-4.12102942	4.83682474	6.38641561				
6	1.60793877	5.07626078	3.98393425				
6	1.81468082	4.86995395	5.48901481				
1	2.33264619	5.74279918	5.91966081				
1	0.84974382	4.74631457	6.00115207				
1	2.42890666	3.97623009	5.67977752				
6	0.74230777	6.31535745	3.72171540				
1	1.21261768	7.21760197	4.14665980				
1	0.61397942	6.46982309	2.63739052				
1	-0.25085508	6.17889600	4.17575745				
6	2.96531535	5.21214689	3.28536263				
1	3.52191197	6.08000219	3.67582081				
1	3.57724180	4.30940254	3.45004602				
1	2.83384601	5.35524754	2.20004423				
6	-6.86980959	1.84310484	-1.13694302				
6	-6.65242580	0.53344620	-1.90848291				
1	-7.57424424	-0.07118412	-1.90426814				
1	-6.37941850	0.74098343	-2.95497066				
1	-5.8503180	-0.07173977	-1.45663812				
6	-7.17374709	1.56074751	0.34118552				
1	-8.04514766	0.89322783	0.44003936				
1	-6.31106776	1.08483290	0.83213533				
1	-7.39906217	2.50096405	0.86867824				
6	-8.03405908	2.62586067	-1.76204221				
1	-8.97477331	2.05898336	-1.67566996				
1	-8.15724117	3.59165859	-1.24780658				
1	-7.84409192	2.82296207	-2.82907435				
6	-3.87735706	4.81966333	0.42819782				
6	-2.65156472	5.64196868	0.84325540				
1	-2.92279329	6.39778347	1.59842811				
1	-1.87516235	4.99219291	1.28010699				
1	-2.22370112	6.15519671	-0.03204973				
6	-4.44834623	4.06500683	1.63376710				
1	-4.74176926	4.77721984	2.42214548				
1	-5.33509712	3.48324786	1.34305816				
1	-3.70519322	3.36775334	2.05406616				
6	-4.94987433	5.74746898	-0.16423795				
1	-5.31598870	6.44721375	0.60482897				
1	-4.53416828	6.33631964	-0.99663651				
1	-5.79718049	5.15210014	-0.53634594				
6	-3.76741742	3.28309801	-3.95989419				
6	-3.88859424	4.75851268	-3.56641701				
1	-4.01923696	5.37351751	-4.47272964				
1	-4.75825966	4.91824963	-2.91284923				
1	-2.98677469	5.09617986	-3.03513593				
6	-2.57772608	3.09606619	-4.91003403				

Reactant -HS

92	1.68893050	-0.49741363	-1.20084785
92	-1.72278689	0.46120766	1.14366804
19	0.53418872	-2.45499809	1.85824700
19	1.40520406	2.69316105	0.85719141
19	-1.65841890	0.38985347	-2.72930621
14	0.17523351	-1.98728737	-4.60981365
14	3.77958707	-3.34379244	0.72370991
14	3.27152104	3.10025146	-1.86725162
14	-0.30381763	2.93670376	3.93000609
14	-4.04736659	2.48910206	-1.21606694
7	0.84756307	-1.04142810	-3.33919939
8	-1.33079143	-1.27416241	-4.97021917
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7	-1.02554534	1.09850679	-0.11154223	1	-3.91882074	2.96108695	7.78633256
14	3.41897338	-1.32441189	-3.20041019	1	-4.30746353	3.00164426	6.03580930
14	-2.05470040	2.86159383	3.62263628	6	-2.11138443	1.35426588	6.46751868
7	1.77376572	-1.17673509	-2.77801820	1	-2.81086187	0.93465905	5.72716155
8	4.28181658	-2.36035277	-2.14914456	1	-2.37618234	0.96229021	7.46308802
8	3.83358602	-1.82526794	-4.74565997	1	-1.09419030	1.01662202	6.21756930
8	4.08240526	0.17314360	-2.81509388	6	-4.58408958	1.82557016	2.66365339
7	-0.93647970	1.66666748	3.11429145	6	-5.97463066	2.33356190	3.07407001
8	-1.85719029	4.25531215	2.64825078	1	-6.19578807	2.03829479	4.11182179
8	-1.80152021	3.43227084	5.17957173	1	-6.75396882	1.91445890	2.41694102
8	-3.66337716	2.39742259	3.61342000	1	-6.01659466	3.43256253	3.00986380
6	4.45337794	-3.80118307	-2.17403093	6	-4.53445313	0.29628037	2.77695051
6	4.98768809	-4.17976701	-0.78629220	1	-3.53804497	-0.08557314	2.50454489
1	5.91666796	-3.62717225	-0.57094551	1	-5.27981920	-0.16767312	2.10892100
1	5.20679462	-5.25865377	-0.73159552	1	-4.75353445	-0.02106221	3.80920740
1	4.24722790	-3.94682837	-0.00133953	6	-4.26264515	2.26430306	1.23133391
6	3.11294671	-4.50570849	-2.42319788	1	-4.27180590	3.36473405	1.16343675
1	2.36996297	-4.19834609	-1.66788231	1	-5.02061971	1.87373314	0.53186962
1	3.23191162	-5.60056923	-2.36306785	1	-3.27574992	1.88699354	0.90663684
1	2.72061076	-4.26256463	-3.42336158	19	3.21614261	-0.90020554	0.08378760
6	5.48109209	-4.17840588	-3.24976745	14	-0.47810018	3.38453035	-3.46924662
1	5.13559628	-3.83853290	-4.23710538	14	-1.47859426	-3.27417358	3.40308317
1	5.63650394	-5.26969694	-3.27434972	7	0.14072716	1.80849062	-3.25304724
1	6.44777693	-3.69372531	-3.03634027	8	0.07101412	4.59274293	-2.38895856
6	3.06979299	-1.85624661	-5.98295709	8	-0.26400397	4.10516922	-4.97411626
6	2.09080525	-3.03624007	-5.94136044	8	-2.09350986	3.28620276	-3.00641140
1	2.63145001	-3.98219700	-5.77507809	7	-1.22977702	-1.68321531	2.80080712
1	1.54002623	-3.11647272	-6.89272133	8	-2.59362108	-4.02013264	2.34731303
1	1.35938319	-2.88909591	-5.13106018	8	-2.20669395	-3.33329418	4.90869697
6	2.30484061	-0.54589795	-6.19798967	8	-0.11772977	-4.23729994	3.55347282
1	1.60310117	-0.37790887	-5.36521328	6	1.30723639	5.35146566	-2.41417204

6	1.50208268	5.88838941	-0.98925012		1	2.08600093	-2.95476940	2.63962211
1	0.62559239	6.48339027	-0.67988968		1	3.03962768	-4.44329919	2.37478168
1	2.38860825	6.54141588	-0.93505778		1	2.47035147	-4.02721174	4.01630939
1	1.65363272	5.05922007	-0.27679602		6	0.52286899	-4.69689655	1.21508436
6	2.49424185	4.45494687	-2.78929989		1	-0.42831711	-5.22348020	1.03538149
1	2.52687332	3.57593990	-2.12552132		1	1.29747381	-5.17988323	0.59544811
1	3.44254106	5.01037534	-2.69443703		1	0.43803745	-3.64311926	0.88899676
1	2.40754878	4.10769874	-3.83057967		19	-0.96972923	3.71709314	0.05251111
6	1.16485203	6.52234990	-3.39637708		19	-2.21299512	-2.63996920	0.02705430
1	0.93362250	6.14083911	-4.40152982		1	1.37667982	-2.12126611	-2.62753758
1	2.09378852	7.11539954	-3.43512854		1	-2.55140735	-0.00435508	-2.65776085
1	0.34292529	7.18653554	-3.08050887		1	1.09372507	1.71514003	-3.63766750
6	0.00115371	3.57406054	-6.29771710		1	1.86093193	-1.03606327	3.10843495
6	1.50785504	3.31564181	-6.44021942		1	-1.76061766	-1.06173325	3.43732910
1	2.07737162	4.23612345	-6.23502816		1	-0.10197460	1.75312254	3.72097970
1	1.74824597	2.98078891	-7.46240937					
1	1.83552106	2.52998915	-5.74189182					
6	-0.78711968	2.28560294	-6.55491006					
1	-0.54204345	1.53313958	-5.78887648					
1	-0.54288106	1.88104776	-7.55087748					
1	-1.86937453	2.47992876	-6.51348666					
6	-0.42749800	4.67414872	-7.27871450					
1	-1.50517183	4.87975967	-7.18235865					
1	-0.22344196	4.36806834	-8.31719683					
1	0.12189028	5.60659637	-7.07282106					
6	-3.22043461	4.15776412	-3.26611643					
6	-2.88847541	5.62645254	-2.96715805					
1	-2.58745300	5.76247133	-1.91551721					
1	-3.77258675	6.25841348	-3.15437988					
1	-2.06434930	5.98219961	-3.60509982					
6	-3.66456085	4.01119986	-4.72828761					
1	-2.87590897	4.37525973	-5.40238521					
1	-4.58242614	4.59301104	-4.91389195					
1	-3.86919031	2.95325460	-4.95717067					
6	-4.33806495	3.66947046	-2.33680770					
1	-4.57139633	2.61272833	-2.54233857					
1	-5.25400617	4.26628371	-2.47739276					
1	-4.03244208	3.74850861	-1.28125976					
6	-3.54920732	-5.09203368	2.59261510					
6	-3.95987172	-5.60986972	1.20816698					
1	-4.41368168	-4.80409238	0.60637842					
1	-4.70200240	-6.42004912	1.29790747					
1	-3.08447413	-6.00837666	0.66799976					
6	-4.76493892	-4.50523671	3.32240750					
1	-4.45128647	-4.08608867	4.29006678					
1	-5.53009927	-5.28054106	3.49380676					
1	-5.21682606	-3.69761009	2.72264450					
6	-2.92456446	-6.23161168	3.40592624					
1	-2.05513298	-6.65442893	2.87813294					
1	-3.66201626	-7.03777887	3.55491270					
1	-2.59466342	-5.87052016	4.39008520					
6	-1.64406171	-3.27026253	6.24378014					
6	-2.76734923	-2.72799257	7.13654413					
1	-3.06037737	-1.71819725	6.80863818					
1	-2.44019705	-2.67716360	8.18737013					
1	-3.65086833	-3.38331791	7.07521761					
6	-1.24636370	-4.68662973	6.68293271					
1	-2.12697264	-5.34911342	6.68730278					
1	-0.82158672	-4.67177048	7.70002920					
1	-0.49693252	-5.09681748	5.98921918					
6	-0.42905847	-2.33641963	6.29245033					
1	0.37124438	-2.71119318	5.63491154					
1	-0.03805975	-2.27302147	7.32103456					
1	-0.70859152	-1.32424728	5.96298421					
6	0.90549946	-4.78254650	2.69627984					
6	1.08848612	-6.24774872	3.11910884					
1	1.33609468	-6.30645579	4.19076165					
1	1.90151398	-6.72200149	2.54524572					
1	0.16237880	-6.81829104	2.94659184					
6	2.20454976	-4.00531484	2.94736157					

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UN MRCC input file

```
unit=angs
basis=atomtype
N:cc-pVTZ
U:RSCBASIS
ecp=atomtype
U:RSCECP-60
calc=CCSDT
mem=110GB
core=10
ccprog=mrcc
charge=0
verbosity=3
scftype=uhf
mult=4
geom=xyz
2
U -0.61364756 0.60687310 -0.17857393
N 0.61364756 -0.60687310 0.17857393
```

UN CASSCF/CASPT2 input file

```
&GATEWAY
Title= UN in C2V symmetry
Coord
2
Angstrom
U -0.61364756 0.60687310 -0.17857393
N 0.61364756 -0.60687310 0.17857393
Group = NoSym
Basis = ANO-RCC-VTZP
End of Input
```

&SEWARD

```
>>COPY /$CurrDir/$Project.RasOrb.1 INPORB
```

&RASSCF &END

```
CHARge
0
LumOrb
NACTEL
9 0 0
Inactive
45
RAS2
12
Spin
4
orblisting
all
ITERation
300 150
CIMX
200
CIROOT
1 1 1
Sdav
500
PRWF
0.01
LEVShft
1.5
SYMMetry
1
End of Input
```

&CASPT2 &END

```
IMAG
0.1
```

```
PROP
IPEAshift
0.0
```

UN3 CASSCF/CASPT2 input file

```
&GATEWAY
Title= UN3 in C2V symmetry
Coord
4
Angstrom
U 0.000000000 0.000000000 -0.077545149
N 0.000000000 0.000000000 -1.848654245
N 0.842600214 0.000000000 1.583457043
N -0.842600214 0.000000000 1.583457043
Group = X XY
Basis = ANO-RCC-VTZP
End of Input
```

&SEWARD

```
>>COPY /$CurrDir/$Project.RasOrb.1 INPORB
```

&RASSCF &END

```
CHARge
0
LumOrb
NACTEL
13 0 0
Inactive
23 4 11 12
RAS2
6 2 2 4
Spin
2
orblisting
all
ITERation
200 100
CIMX
200
CIROOT
1 1 1
Sdav
500
PRWF
0.01
LEVShft
1.5
SYMMetry
1
End of Input
```

&CASPT2 &END

```
IMAG
0.1
PROP
IPEAshift
0.0
```

UN2 MRCC input file

```
unit=angs
basis=atomtype
N:cc-pVTZ
U:RSCBASIS
ecp=atomtype
U:RSCECP-60
calc=CCSDT
mem=110GB
core=11
```

```

ccprog=mrccl
charge=0
verbosity=3
scftype=rhf
scfguess=restart
mult=1
ccmaxit=1000
geom=xyz
3

U    0.000000  0.000000  0.000000
N   -1.741365499  0.000000  0.000000
N    1.741365499  0.000000  0.000000

```

Priroda Sample Input file

```

$system mem=112000 disk=10 $end
$control
task=optimize
theory=DFT
four=1 a137=new
basis=/home/sodoh/bin/PRIRODA/basis4.in
print=charges+bonds
$end
$optimize
tol=1e-5
steps=2000
$end
$dft
functional=PBE
$end
$guess
mix=1
$end
$scf
restrict=0
iterations=300
d1small=1
$end
$molecule
charge=0
multip=1
cartesian
$end

```