

Supporting Information

Accurate prediction of the structure and vibrational spectra of ionic liquid clusters with the generalized energy-based fragmentation approach: critical role of the ion-pair-based fragmentation

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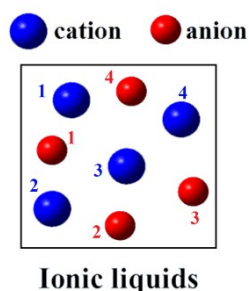
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(1) Automatic ion-pair-based fragmentation procedure for an IL system.



We will take this IL cluster (with 4 cations and 4 anions) as an example to illustrate the procedure, which contains the following four steps:

Step 1: Construct the cation-anion distance matrix of this cluster. Here the distance (in Å) between a cation and an anion is defined as the minimum distance between any atoms of a cation and any atoms of an anion.

		Anions			
		1 ⁻	2 ⁻	3 ⁻	4 ⁻
Cations	1 ⁺	1.3	5.5	7.0	1.5
	2 ⁺	1.4	1.6	6.0	6.5
	3 ⁺	1.5	1.3	2.0	2.1
	4 ⁺	5.0	5.5	2.5	1.5

Step 2: For each cation, label its neighboring anions if the cation-anion distance is less than 4.0 Å.

		Anions			
		1 ⁻	2 ⁻	3 ⁻	4 ⁻
Cations	1 ⁺	1.3	5.5	7.0	1.5
	2 ⁺	1.4	1.6	6.0	6.5
	3 ⁺	1.5	1.3	2.0	2.1
	4 ⁺	5.2	5.5	2.5	1.5

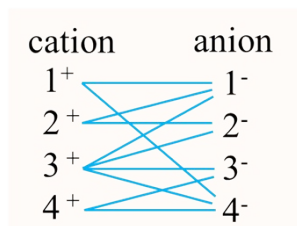
List all labelled cation-anion pairs from the above table:

$1^+—1^-$, $1^+—4^-$;

$2^+—1^-$, $2^+—2^-$;

$3^+—1^-$, $3^+—2^-$, $3^+—3^-$, $3^+—4^-$;

$4^+—3^-$, $4^+—4^-$;



Step 3: Use the above result to search the optimal pairing scheme.

Two conditions should be satisfied in searching the optimal pairing scheme:

- (1) Each cation (or anion) should be paired with one of its neighboring anions (or cations) to form an ion pair;
- (2) Any cation or anion in an IL system should be paired.

There are four pairing schemes, as listed below:

Assignment 1	Assignment 2	Assignment 3	Assignment 4																																								
<table><tr><th>cation</th><th>anion</th></tr><tr><td>1⁺</td><td>1⁻</td></tr><tr><td>2⁺</td><td>2⁻</td></tr><tr><td>3⁺</td><td>3⁻</td></tr><tr><td>4⁺</td><td>4⁻</td></tr></table>	cation	anion	1 ⁺	1 ⁻	2 ⁺	2 ⁻	3 ⁺	3 ⁻	4 ⁺	4 ⁻	<table><tr><th>cation</th><th>anion</th></tr><tr><td>1⁺</td><td>1⁻</td></tr><tr><td>2⁺</td><td>2⁻</td></tr><tr><td>3⁺</td><td>3⁻</td></tr><tr><td>4⁺</td><td>4⁻</td></tr></table>	cation	anion	1 ⁺	1 ⁻	2 ⁺	2 ⁻	3 ⁺	3 ⁻	4 ⁺	4 ⁻	<table><tr><th>cation</th><th>anion</th></tr><tr><td>1⁺</td><td>1⁻</td></tr><tr><td>2⁺</td><td>2⁻</td></tr><tr><td>3⁺</td><td>3⁻</td></tr><tr><td>4⁺</td><td>4⁻</td></tr></table>	cation	anion	1 ⁺	1 ⁻	2 ⁺	2 ⁻	3 ⁺	3 ⁻	4 ⁺	4 ⁻	<table><tr><th>cation</th><th>anion</th></tr><tr><td>1⁺</td><td>1⁻</td></tr><tr><td>2⁺</td><td>2⁻</td></tr><tr><td>3⁺</td><td>3⁻</td></tr><tr><td>4⁺</td><td>4⁻</td></tr></table>	cation	anion	1 ⁺	1 ⁻	2 ⁺	2 ⁻	3 ⁺	3 ⁻	4 ⁺	4 ⁻
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4 ⁺	4 ⁻																																										
$\sum d = 6.4 \text{ \AA}$	$7.5 \text{ \AA}$	$6.7 \text{ \AA}$	$7.1 \text{ \AA}$																																								

$\sum d$ means the sum of the distances between all cation-anion pairs.

Step 4: Obtain the optimal pairing scheme, in which the sum of the distances between all cation-anion pairs is the minimum among all possible pairing schemes.

So the assignment 1 denotes the optimal pairing scheme.

Optimal pairing scheme: $1^+—1^-$, $2^+—2^-$, $3^+—3^-$, $4^+—4^-$; $\sum d = 6.4 \text{ \AA}$

With the above procedure, one can easily achieve the automatic pairing scheme for all cations and anions in an IL cluster or crystal. With each ion-pair as a fragment, one

can achieve the automatic construction of various subsystems in the GEBF approach for a general IL system.

(2) Validation details of the GEBF approach for various IL clusters

Table S1 Ground-state energy deviations (in kcal/mol) between full system calculations and GEBF calculations with different ζ values and two different types of background point charges (with the ion-pair-based fragmentation scheme) for $([\text{EtNH}_3][\text{Cl}])_n$ ($n=10, 20, \text{ and } 30$) at the M06-2X/6-31G** level.

ζ (Å)	NPA charges			ESP charges		
	$n=10$	$n=20$	$n=30$	$n=10$	$n=20$	$n=30$
3	-0.03	1.46	-0.37	-1.15	2.12	0.14
4	0.18	1.92	0.65	0.23	2.30	0.94
5	0.11	0.35	0.86	0.11	0.22	1.36
6	0.11	0.20	0.56	0.11	0.20	-0.74

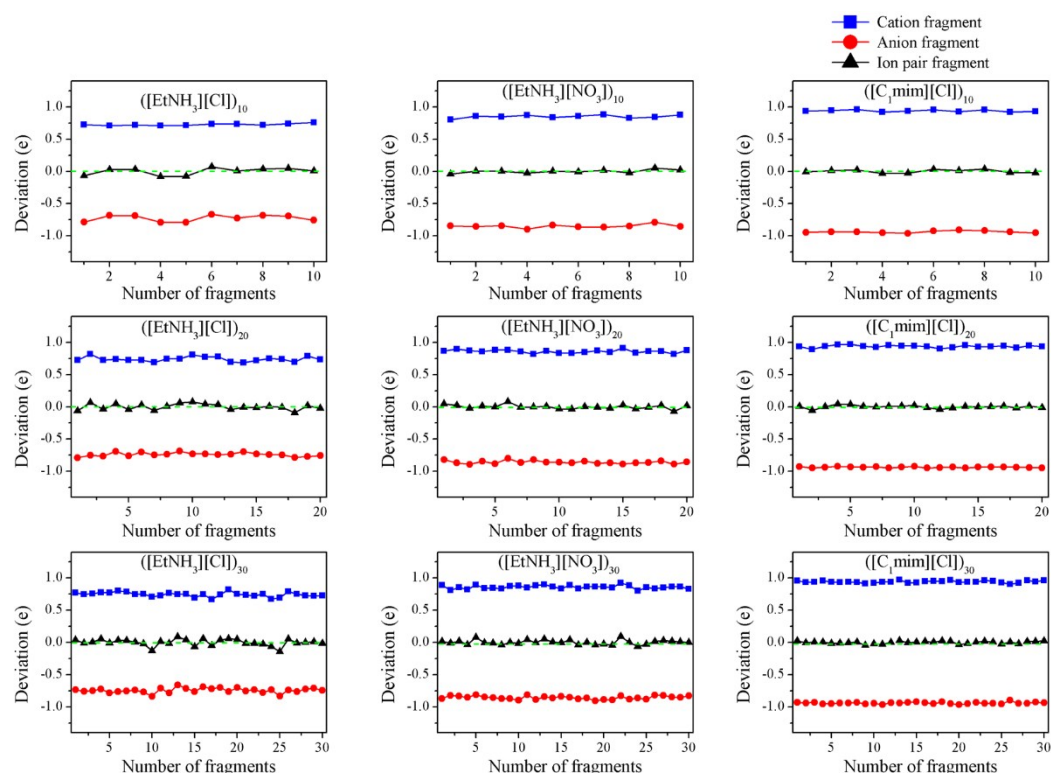


Fig. S1 Charge distributions in various cations, anions and ion pair fragments from GEBF-M06-2X/6-31G** calculations for $([\text{EtNH}_3][\text{Cl}])_n$, $([\text{EtNH}_3][\text{NO}_3])_n$, and $([\text{C}_1\text{mim}][\text{Cl}])_n$ ($n=10, 20, \text{ and } 30$) clusters.

Table S2 Average unsigned errors (AUEs) of the GEBF energies obtained with two different fragmentation schemes (ion-pair-based fragmentation and ion-based fragmentation) at the M06-2X/6-31G** level (relative to the corresponding full system energies) as a function of the $\gamma_{\max}$ value for three IL clusters.^a

$\gamma_{\max}$	AUEs (kcal/mol)		
	$([\text{EtNH}_3][\text{Cl}])_n$ ($n=10,20,30$)	$([\text{EtNH}_3][\text{NO}_3])_n$ ($n=10,20,30$)	$([\text{C}_1\text{mim}][\text{Cl}])_n$ ($n=10,20,30$)
3	2.00 (17.93)	1.21 (13.98)	0.88 (0.52)
4	3.71 (19.62)	6.93 (8.60)	0.45 (2.27)
5	0.23 (22.89)	2.69 (9.49)	0.31 (1.48)
6	0.99 (17.27)	0.51 (6.91)	0.28 (1.13)
7	0.84 (7.78)	0.44 (6.57)	0.16 (0.82)

^aThe GEBF results obtained with the ion-based fragmentation scheme (with $2.0*\gamma_{\max}$) are displayed in the parenthesis.

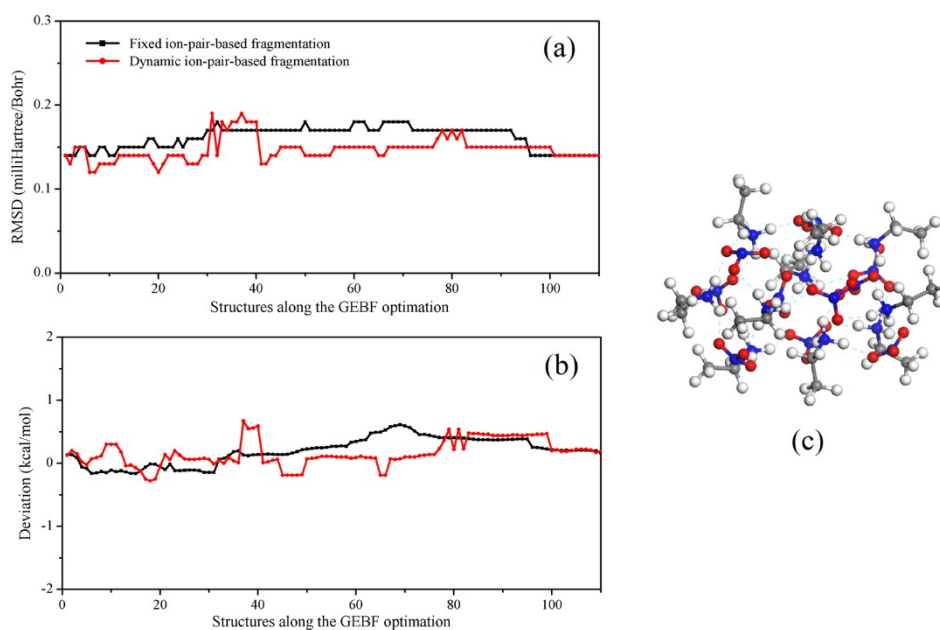


Fig. S2 (a) The root-mean-squared deviations (RMSDs) between energy gradients obtained with conventional calculations and GEBF calculations (with fixed and dynamic ion-pair-based fragmentations) during the optimization of $([\text{EtNH}_3][\text{NO}_3])_{10}$ at the M06-2X/6-31G** level. (b) The corresponding energy deviations obtained from GEBF calculations with fixed and dynamic ion-pair-based fragmentations (relative to the corresponding conventional results). (c) The initial structure of $([\text{EtNH}_3][\text{NO}_3])_{10}$ under study.

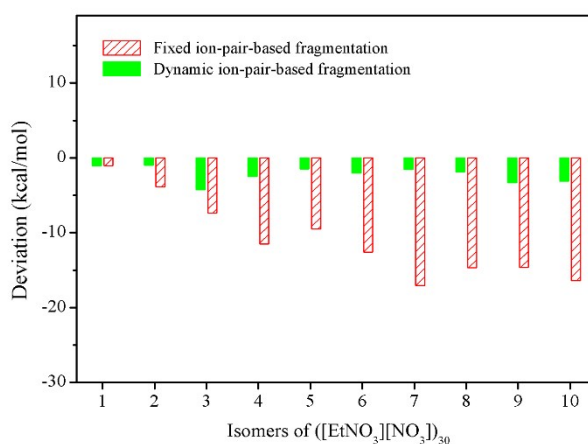


Fig. S3 Ground-state energy deviations between conventional M06-2X/6-31G** calculations and GEBF-M06-2X/6-31G** calculations (with fixed and dynamic ion-pair-based fragments) for ten isomers of $([\text{EtNH}_3][\text{NO}_3])_{30}$, whose geometries were taken out along classical MD trajectories.

(3) Cartesian coordinates of studied IL clusters.

1)	$([\text{EtNH}_3][\text{Cl}])_{10}$	$([\text{EtNH}_3][\text{Cl}])_{20}$	$([\text{EtNH}_3][\text{Cl}])_{30}$
2)	$([\text{EtNH}_3][\text{NO}_3])_{10}$ $\begin{array}{ccccc} \underline{1} & \underline{2} & \underline{3} & \underline{4} & \underline{5} \\ \underline{6} & \underline{7} & \underline{8} & \underline{9} & \underline{10} \end{array}$	$([\text{EtNH}_3][\text{NO}_3])_{20}$ $\begin{array}{ccccc} \underline{1} & \underline{2} & \underline{3} & \underline{4} & \underline{5} \\ \underline{6} & \underline{7} & \underline{8} & \underline{9} & \underline{10} \end{array}$	$([\text{EtNH}_3][\text{NO}_3])_{30}$ $\begin{array}{ccccc} \underline{1} & \underline{2} & \underline{3} & \underline{4} & \underline{5} \\ \underline{6} & \underline{7} & \underline{8} & \underline{9} & \underline{10} \end{array}$
3)	$([\text{C}_1\text{mim}][\text{Cl}])_{10}$	$([\text{C}_1\text{mim}][\text{Cl}])_{20}$	$([\text{C}_1\text{mim}][\text{Cl}])_{30}$
4)	$([\text{C}_1\text{mim}][\text{BF}_4])_{10}$	$([\text{C}_1\text{mim}][\text{BF}_4])_{20}$	$([\text{C}_1\text{mim}][\text{BF}_4])_{30}$
5)	$([\text{C}_1\text{mim}][\text{NO}_3])_{10}$	$([\text{C}_1\text{mim}][\text{NO}_3])_{20}$	$([\text{C}_1\text{mim}][\text{NO}_3])_{30}$
6)	$([\text{n-C}_4\text{NH}_3][\text{NO}_3])_{10}$	$([\text{n-C}_4\text{NH}_3][\text{NO}_3])_{20}$	$([\text{n-C}_4\text{NH}_3][\text{NO}_3])_{30}$
7)	$([\text{n-C}_4\text{mim}][\text{BF}_4])_{10}$	$([\text{n-C}_4\text{mim}][\text{BF}_4])_{20}$	$([\text{n-C}_4\text{mim}][\text{BF}_4])_{30}$

([EtNH₃][Cl])₁₀

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	-0.482004	2.444716	2.968311
H	-0.715659	1.569145	3.574019
H	0.280204	2.094084	2.272469
H	0.016036	3.206552	3.568031
C	-1.649987	3.086049	2.218412
H	-1.919677	2.408205	1.408539
H	-1.204106	4.035609	1.922397
N	-2.814180	3.486168	3.023646
H	-3.554159	3.647799	2.355509
H	-3.023785	2.676415	3.589742
H	-2.640394	4.368454	3.483504
Cl	-3.718699	0.868824	3.735301
C	-8.055582	-2.428805	-2.511561
H	-8.492713	-2.834508	-3.423933
H	-8.084724	-3.142502	-1.688222
H	-8.691062	-1.583513	-2.247461
C	-6.637436	-1.892788	-2.710027
H	-6.691413	-1.217594	-3.564017
H	-6.009675	-2.753851	-2.939346
N	-6.231409	-1.157723	-1.502276
H	-6.381192	-1.555268	-0.585966
H	-5.250147	-0.957171	-1.632669
H	-6.659425	-0.246810	-1.586771
Cl	-6.517418	-1.893537	1.351662
C	-2.761520	-3.221708	0.824170
H	-3.156295	-2.886740	-0.135022
H	-1.863175	-3.833299	0.740314
H	-3.614355	-3.892501	0.928141
C	-2.744801	-2.093943	1.856500
H	-1.737038	-1.718167	1.679569
H	-2.791955	-2.584635	2.828661
N	-3.837123	-1.129788	1.653814
H	-3.797414	-0.536341	0.837515
H	-4.779610	-1.478312	1.755541
H	-3.774200	-0.363317	2.308537
Cl	-3.586109	0.159244	-1.064900
C	-4.757140	3.201335	-4.095737
H	-5.788067	2.847503	-4.086020
H	-4.538253	3.949302	-4.857796
H	-4.142222	2.301539	-4.114213
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H	-5.159651	4.693636	-2.621340
H	-3.679619	4.305968	-2.627601
N	-4.809303	2.842748	-1.534308
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H	-5.651570	2.285526	-1.520527
H	-4.130703	2.137388	-1.285168
Cl	-4.571425	4.280966	0.853127
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H	-10.186752	1.618379	-0.105918
H	-11.206585	0.986064	1.144558

C	-9.195349	0.255326	1.281816
H	-9.259194	-0.607570	0.618918
H	-9.206683	-0.040085	2.330960
N	-7.788784	0.679142	1.205693
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H	-7.225406	-0.159123	1.201458
H	-7.585473	1.083665	0.302849
Cl	-7.302935	1.403269	-1.669472
C	-9.139880	6.960059	6.539623
H	-9.788892	7.686833	7.028175
H	-9.365480	6.877439	5.476430
H	-9.143772	5.971582	6.998969
C	-7.769073	7.624941	6.668705
H	-7.532601	7.485321	7.723545
H	-7.899181	8.687039	6.461052
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C	-6.416576	-0.756604	5.994020
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H	-7.056981	-1.513701	6.446553
H	-6.472586	-0.903699	4.915445
C	-6.319949	0.651625	6.581724
H	-5.585547	0.758322	7.380078
H	-7.242107	1.007184	7.041402
N	-5.752424	1.602409	5.613340
H	-5.070960	1.187959	4.993713
H	-6.600692	1.795250	5.100159
H	-5.610463	2.494935	6.064277
Cl	-5.768362	4.065885	6.943912
C	-9.364570	5.441752	0.545424
H	-9.263409	6.515076	0.706176
H	-10.109357	5.138919	-0.190569
H	-9.872317	4.993047	1.399215
C	-7.965184	4.891826	0.267679
H	-7.364003	5.436424	-0.460396
H	-8.000717	3.846071	-0.037663
N	-7.229165	4.887090	1.541293
H	-7.115053	5.824030	1.900769
H	-7.598490	4.338911	2.304968
H	-6.319143	4.528851	1.289054
Cl	-7.731477	2.516803	3.438889
C	-2.569269	7.072732	1.251710
H	-2.222613	7.719356	0.445605
H	-1.958560	6.170698	1.290033
H	-3.559993	6.723249	0.961142
C	-2.810177	7.964320	2.470264
H	-3.310141	8.913573	2.277773
H	-1.955765	8.303359	3.056041
N	-3.738067	7.302149	3.399990
H	-3.804428	7.846868	4.247916
H	-4.710134	7.205741	3.143297
H	-3.336487	6.429943	3.713182
Cl	-6.634118	7.286180	2.866343
C	-1.785680	4.438953	8.292207
H	-2.483895	3.648064	8.566235

H	-1.357330	4.094031	7.351120
H	-1.068920	4.482438	9.112246
C	-2.466802	5.794098	8.098569
H	-1.743032	6.561775	7.824838
H	-2.793263	6.137758	9.080109
N	-3.482713	5.772935	7.034934
H	-3.061355	5.251237	6.279693
H	-4.336232	5.269520	7.230327
H	-3.790266	6.688639	6.739982
Cl	-4.451229	8.288193	5.979639

Return

([EtNH₃][Cl])₂₀

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	5.715478	2.964621	2.817451
H	6.693830	3.426649	2.949584
H	5.817678	1.950094	3.202666
H	5.374984	2.896526	1.784239
C	4.608481	3.675359	3.596715
H	4.454910	4.647966	3.129221
H	4.898741	3.780534	4.642079
N	3.358861	2.915063	3.752408
H	3.585585	2.081022	4.274971
H	2.753839	3.539575	4.266250
H	2.956472	2.726498	2.845420
Cl	2.737581	2.344463	1.108642
C	4.019673	-1.437350	-0.444038
H	3.778212	-2.193126	0.303358
H	4.759387	-1.976078	-1.036234
H	4.566324	-0.679024	0.116509
C	2.857195	-0.862601	-1.254069
H	2.358078	-1.741970	-1.661122
H	3.228393	-0.370542	-2.153063
N	1.888290	-0.129370	-0.424950
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H	2.267148	0.692803	0.022932
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C	-5.703434	0.105486	0.240781
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H	-6.250962	2.016233	0.938464
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H	-7.280274	-3.296287	4.210441
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H	-7.871216	5.772412	-4.462765

C	-7.633395	3.703426	-3.947750
H	-7.076977	2.883232	-4.401382
H	-8.660731	3.507969	-3.640379
N	-7.057559	3.920061	-2.611590
H	-6.056690	3.801747	-2.545533
H	-7.321832	4.793137	-2.178002
H	-7.647428	3.297944	-2.077619
Cl	-9.952315	4.462238	2.076028
C	-12.040560	-0.157945	1.580565
H	-11.201596	-0.852680	1.540782
H	-12.360432	0.079632	2.595128
H	-12.781134	-0.769451	1.065094
C	-11.673039	1.106555	0.803512
H	-12.552724	1.738560	0.925263
H	-11.610935	0.865000	-0.257569
N	-10.448619	1.852929	1.131479
H	-9.842805	1.678078	0.342482
H	-10.452958	2.844112	1.325479
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Return

([EtNH₃][Cl])₃₀

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H	8.992505	0.214575	13.996399
Cl	7.845141	-4.273345	15.739598
C	4.903958	-7.471706	12.992882
H	3.920819	-7.525141	13.460517
H	4.786384	-6.918115	12.061317
H	4.953535	-8.549801	12.840066
C	5.918650	-6.760297	13.888503
H	6.860812	-6.623946	13.357617
H	6.163968	-7.338019	14.779657
N	5.415985	-5.434167	14.279076
H	6.082342	-4.991160	14.895365
H	5.317847	-4.841096	13.467450
H	4.580532	-5.550201	14.834644
Cl	9.610121	-10.279978	22.257229
C	-3.144127	-15.066415	27.599501
H	-3.630683	-14.277082	27.026511
H	-3.223867	-16.070120	27.181987
H	-3.548234	-15.139954	28.609149
C	-1.630816	-14.848716	27.581075
H	-1.238025	-15.642350	28.216653
H	-1.393822	-13.861985	27.978939
N	-1.067330	-14.789331	26.223578
H	-0.080225	-14.604937	26.331854
H	-0.960378	-15.695831	25.791237
H	-1.331467	-14.046505	25.592277
Cl	-0.305698	-17.618020	25.627784
C	9.171439	-1.382032	19.574054
H	9.905767	-1.466746	20.375107
H	9.456979	-0.508318	18.988229
H	8.281955	-1.041748	20.104267
C	9.091843	-2.586022	18.634951
H	8.722695	-3.398344	19.261020
H	10.086060	-2.816843	18.252389
N	8.012404	-2.266028	17.688243
H	7.277136	-1.947973	18.303323
H	8.309193	-1.596843	16.992392
H	7.770562	-3.058093	17.110105
Cl	5.307187	-2.484593	18.890891
C	5.335872	1.086137	17.482013
H	4.717589	0.194386	17.379022
H	6.294956	0.751264	17.877131
H	4.999633	1.779368	18.253035
C	5.515154	1.584017	16.047504
H	6.345867	2.288581	16.007444
H	4.589605	2.137933	15.890542
N	5.858910	0.457767	15.165895
H	5.044907	-0.139568	15.192169
H	5.961982	0.756169	14.206503

H	6.694378	0.001866	15.503900
Cl	5.142236	-12.584855	23.501601
C	0.457903	-3.446368	17.243127
H	0.503648	-4.453371	16.828455
H	-0.429281	-3.473989	17.875775
H	0.243391	-2.642987	16.538383
C	1.687138	-3.123004	18.092985
H	1.893211	-3.944663	18.778922
H	1.641005	-2.218839	18.699992
N	2.820917	-2.807465	17.210477
H	3.687776	-2.898265	17.720780
H	2.852035	-3.507652	16.483243
H	2.764343	-1.929615	16.714211
Cl	8.754044	-0.114560	15.939407
C	-2.534083	-21.022741	22.622928
H	-1.980339	-20.953696	21.686605
H	-2.802531	-22.023586	22.961080
H	-3.455043	-20.459701	22.471538
C	-1.768554	-20.246452	23.694927
H	-0.850408	-20.797445	23.898674
H	-2.383641	-20.216784	24.594309
N	-1.452417	-18.847226	23.369252
H	-2.065527	-18.064125	23.193326
H	-0.902581	-18.473231	24.129455
H	-0.876360	-18.829275	22.539832
Cl	-3.049791	-16.554789	22.663975
C	14.988917	-7.550118	14.860210
H	14.778376	-6.534252	14.525863
H	14.952769	-7.487045	15.947783
H	16.016700	-7.434675	14.516066
C	14.140361	-8.725312	14.373680
H	14.725393	-9.547679	14.785445
H	14.189597	-8.842808	13.291150
N	12.760936	-8.785886	14.880983
H	12.248336	-9.489876	14.369378
H	12.591022	-8.998409	15.853641
H	12.176348	-8.014305	14.592851
Cl	11.249318	-6.714609	13.601154
C	12.705307	-2.888130	13.152094
H	12.963465	-3.845624	12.699701
H	12.344811	-2.242795	12.351041
H	13.549500	-2.318529	13.540673
C	11.581197	-3.124452	14.161237
H	11.378568	-2.205839	14.711865
H	12.068495	-3.727758	14.927176
N	10.460473	-3.904957	13.614767
H	9.636826	-4.187482	14.126515
H	9.972792	-3.254974	13.014943
H	10.693625	-4.823320	13.264983
Cl	7.773501	-10.027290	14.234425
C	1.853288	-6.061826	24.527517
H	1.454201	-5.770045	23.556078
H	1.003902	-6.680114	24.817968
H	2.017255	-5.221395	25.201973
C	3.228517	-6.714788	24.385295
H	3.506018	-7.037547	25.388748
H	3.945930	-5.977544	24.024892
N	3.362897	-7.848807	23.458049
H	2.874069	-8.694277	23.715590
H	3.201040	-7.684736	22.474696
H	4.367635	-7.948479	23.483862
Cl	3.364925	-6.769855	20.788248
C	-1.947280	-7.766894	24.123097
H	-2.544789	-7.947123	23.229453
H	-2.620631	-7.030601	24.561926
H	-1.003028	-7.244591	23.969191
C	-1.812395	-9.169140	24.717534

H	-2.812465	-9.540038	24.942021
H	-1.344860	-9.034710	25.692951
N	-1.049227	-10.033064	23.803723
H	-0.076859	-9.871952	24.024275
H	-1.121101	-10.996803	24.097222
H	-1.294800	-9.862225	22.839043
Cl	-1.855165	-12.549656	24.806668
C	4.712503	-12.666792	15.960201
H	4.697170	-12.518118	14.880497
H	5.526749	-13.320987	16.271864
H	3.688090	-13.017836	16.084480
C	4.982024	-11.344923	16.679827
H	4.737432	-11.668489	17.691548
H	4.185007	-10.618879	16.519440
N	6.284114	-10.664114	16.609806
H	6.200612	-9.699310	16.896654
H	6.912639	-11.029828	17.310740
H	6.601678	-10.571349	15.655528
Cl	8.628974	-11.999733	17.953415
C	10.447300	-6.557428	17.026716
H	10.342654	-5.777795	16.272182
H	10.785767	-6.178747	17.991154
H	11.284047	-7.219146	16.802922
C	9.111862	-7.288556	17.167777
H	9.271060	-8.102513	17.875046
H	8.766284	-7.594069	16.180185
N	8.082197	-6.415533	17.752125
H	7.904935	-5.550923	17.261078
H	7.238976	-6.958933	17.634674
H	8.243399	-6.296993	18.742106
Cl	4.696541	-3.954434	11.660672

Return

([EtNH₃][NO₃])₁₀ conformer -1

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	-10.723872	2.651617	-0.919558
H	-11.453872	2.350031	-1.670721
H	-10.912973	2.017902	-0.053102
H	-11.049235	3.676220	-0.739481
C	-9.223258	2.571388	-1.201628
H	-8.716182	3.122446	-0.409600
H	-8.969590	3.091389	-2.125398
N	-8.557191	1.259837	-1.207172
H	-9.099866	0.758735	-0.518332
H	-8.720169	0.823035	-2.103131
H	-7.557486	1.353315	-1.097846
N	0.244968	-2.596878	0.686522
O	0.841416	-1.804319	-0.034017
O	0.516917	-2.355169	1.857289
O	-0.922418	-2.877391	0.438329
C	-5.846945	2.312424	3.412040
H	-6.918124	2.126793	3.490889
H	-5.611473	2.509595	4.457878
H	-5.505469	3.203234	2.884829
C	-5.123170	1.123199	2.779793
H	-5.266929	0.219882	3.372625
H	-4.034047	1.150554	2.813884
N	-5.633134	0.797497	1.439011
H	-5.216197	-0.053334	1.089225
H	-6.620330	0.600148	1.520235
H	-5.457583	1.615066	0.872563
N	-3.558267	-2.905684	-3.091702
O	-2.532839	-3.183337	-2.479752
O	-3.374360	-1.895707	-3.761927
O	-4.626172	-3.176062	-2.553606
C	-9.618439	-4.789405	1.523395
H	-10.280931	-3.943705	1.339014
H	-9.264073	-5.143041	0.555166
H	-10.161134	-5.607912	1.996288
C	-8.511345	-4.311594	2.463544
H	-7.722970	-5.063622	2.495446
H	-8.941179	-4.097997	3.442175
N	-7.746062	-3.089652	2.171926
H	-6.992761	-2.938981	2.827621
H	-7.169086	-3.184390	1.348382
H	-8.189558	-2.199727	1.994601
N	-1.232736	2.086902	3.567133
O	-0.287197	2.041925	2.788026
O	-1.379484	1.042085	4.191551
O	-2.265603	2.583228	3.131330
C	-0.162464	-1.932553	5.194991
H	0.577606	-2.514539	4.645728
H	0.128335	-0.882979	5.238936
H	-0.189202	-2.366009	6.194741
C	-1.545878	-2.129585	4.574357
H	-2.404183	-1.903349	5.206994
H	-1.652552	-3.202543	4.414730
N	-1.717972	-1.481302	3.265176
H	-1.070356	-1.826962	2.571481
H	-2.621307	-1.745934	2.899042
H	-1.596146	-0.481949	3.346127
N	-7.774744	0.201255	-4.291009
O	-7.724678	-0.690311	-5.131056
O	-6.747137	0.296077	-3.629112
O	-8.747454	0.242542	-3.545886
C	0.331122	-2.465381	-4.326190

H	-0.655576	-2.889217	-4.512982
H	0.657941	-2.224388	-5.337729
H	0.917637	-3.279950	-3.901245
C	0.176246	-1.206933	-3.471695
H	-0.317980	-0.399541	-4.012028
H	1.159313	-0.821467	-3.201333
N	-0.576006	-1.499545	-2.241925
H	-1.335514	-2.146681	-2.398331
H	0.071873	-1.950324	-1.611725
H	-1.050112	-0.744235	-1.767761
N	-6.256377	-1.856990	-0.389980
O	-6.943327	-2.871375	-0.343068
O	-5.490033	-1.733748	0.559022
O	-6.547965	-0.932034	-1.139985
C	-0.717231	5.109036	1.305429
H	0.067724	4.669339	0.690116
H	-0.320485	6.089083	1.570381
H	-0.616186	4.582381	2.254389
C	-2.131928	5.156898	0.727343
H	-2.031850	5.654035	-0.237509
H	-2.833231	5.785504	1.276094
N	-2.596752	3.769648	0.574645
H	-2.503322	3.375958	1.500052
H	-3.508221	3.633942	0.161234
H	-1.952383	3.406421	-0.113073
N	-4.730353	-3.443793	2.939964
O	-5.307573	-2.463495	3.397029
O	-5.425877	-4.156317	2.224680
O	-3.525148	-3.353019	2.734256
C	-2.741666	-5.854736	1.211046
H	-2.095820	-5.271534	1.867445
H	-3.644504	-6.215335	1.703948
H	-2.199901	-6.709990	0.807152
C	-3.260040	-5.205162	-0.072380
H	-4.062898	-5.737833	-0.582066
H	-2.392433	-5.101073	-0.723935
N	-3.483141	-3.756193	0.048268
H	-4.105067	-3.529521	0.811109
H	-2.621735	-3.334556	0.364974
H	-3.792928	-3.314912	-0.805784
N	-2.759067	0.150537	0.074650
O	-3.437556	1.153702	-0.116105
O	-2.827406	-0.735451	-0.769999
O	-2.243216	-0.129840	1.150922
C	2.329722	0.510387	3.097430
H	1.701689	1.058734	3.799564
H	2.146452	-0.561990	3.164660
H	3.290422	0.628542	3.598622
C	2.281788	0.950275	1.633858
H	3.098661	0.491379	1.076874
H	2.390590	2.023359	1.791187
N	0.978516	0.707633	0.996326
H	0.889419	-0.273309	0.772908
H	0.172393	0.898532	1.574101
H	0.900170	1.303057	0.184272
N	-5.546616	3.278213	-0.859933
O	-4.545266	3.652594	-1.460111
O	-5.483448	3.317823	0.363798
O	-6.079386	2.325807	-1.418640
C	-9.121289	-3.553521	-3.988472
H	-9.175631	-2.888699	-4.850538
H	-9.546346	-4.556504	-4.026582
H	-9.478064	-3.018340	-3.108476
C	-7.641768	-3.752160	-3.657713
H	-7.061177	-4.229356	-4.447205
H	-7.567788	-4.311125	-2.724877
N	-6.935251	-2.521729	-3.269493

H	-7.393465	-2.220300	-2.421388
H	-6.029400	-2.786716	-2.909888
H	-6.836410	-1.847125	-4.014637
N	-9.129330	-0.047578	1.604929
O	-9.508621	-0.504445	0.532321
O	-8.977841	-0.799991	2.560963
O	-8.384155	0.920459	1.501508
C	-4.231985	1.892104	-4.977709
H	-3.689109	2.440894	-5.747263
H	-4.522568	0.964483	-5.470841
H	-5.106015	2.376169	-4.541990
C	-3.377293	1.478608	-3.779224
H	-2.906366	2.318338	-3.268166
H	-2.508503	0.939521	-4.156967
N	-4.221479	0.708415	-2.852944
H	-4.213120	-0.238127	-3.205204
H	-3.929526	0.794754	-1.889924
H	-5.154528	1.089381	-2.919151
N	0.039804	2.250359	-1.463296
O	-0.622690	3.267928	-1.293796
O	-0.459368	1.131637	-1.414662
O	1.136703	2.215602	-0.916780

Return

([EtNH₃][NO₃])₁₀ conformer -2

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	-8.299722	2.448510	-2.649170
H	-9.249803	2.982222	-2.673602
H	-7.605475	3.249447	-2.903375
H	-8.424388	1.657376	-3.388537
C	-7.861396	1.784301	-1.343591
H	-8.635837	1.191332	-0.857043
H	-7.680553	2.547369	-0.586542
N	-6.811065	0.786215	-1.597501
H	-7.085264	0.067403	-2.251889
H	-6.030919	1.257301	-2.032875
H	-6.447387	0.448561	-0.717826
N	-1.069390	-3.280543	1.042472
O	-0.809444	-2.112611	0.775196
O	-1.536126	-3.469257	2.160336
O	-1.674652	-3.863013	0.149463
C	-7.147035	2.957319	2.731405
H	-7.838738	2.176688	2.414765
H	-7.675140	3.579597	3.453884
H	-6.874079	3.699840	1.981566
C	-5.775631	2.591166	3.299757
H	-5.698250	1.974796	4.195413
H	-5.159930	3.470313	3.489791
N	-4.880623	2.060188	2.260111
H	-3.951982	1.878592	2.613310
H	-5.217334	1.175010	1.909132
H	-4.855490	2.804157	1.577486
N	-5.598841	-4.877246	-1.074673
O	-6.747098	-4.447618	-1.075453
O	-5.267283	-5.521500	-0.085693
O	-4.814137	-4.057779	-1.539207
C	-8.739533	-6.078551	1.538720
H	-8.981306	-6.417474	0.531358
H	-7.709891	-6.429211	1.609252
H	-9.289849	-6.698399	2.246563
C	-8.966882	-4.588036	1.792728
H	-9.059280	-4.295211	2.838584
H	-9.950286	-4.335312	1.396311
N	-8.050564	-3.636763	1.145208
H	-8.503931	-2.734546	1.121488
H	-7.206117	-3.571716	1.695460
H	-7.791547	-3.889390	0.202240
N	-1.786048	2.971493	3.055092
O	-2.249929	3.998449	2.572133
O	-2.656479	2.218789	3.478015
O	-0.761380	2.543473	2.535543
C	-0.933591	-1.132256	4.418866
H	-0.509210	-0.634002	5.290499
H	-0.467160	-2.104555	4.260190
H	-0.621476	-0.484728	3.599481
C	-2.451539	-1.215160	4.255150
H	-2.789853	-0.302007	4.744837
H	-2.728166	-2.096175	4.834278
N	-3.034761	-1.437388	2.923118
H	-4.038515	-1.542547	2.962115
H	-2.962790	-0.775370	2.163742
H	-2.713109	-2.334051	2.587505
N	-5.066696	-0.319202	-4.059724
O	-4.189537	0.484414	-3.763296
O	-4.755092	-1.466951	-3.761980
O	-6.257728	-0.028623	-4.068788
C	-0.547969	-1.977222	-2.752425

H	0.086275	-2.663085	-2.190796
H	0.000705	-1.881115	-3.689346
H	-0.414874	-1.013190	-2.261477
C	-1.992942	-2.426264	-2.972095
H	-2.187401	-3.456323	-3.270865
H	-2.437999	-1.802862	-3.747591
N	-2.716684	-2.346404	-1.693948
H	-2.364505	-2.986940	-0.996966
H	-2.617364	-1.438146	-1.263482
H	-3.708755	-2.428834	-1.864540
N	-9.534342	-1.650720	-0.843827
O	-8.948718	-1.036980	-1.728950
O	-9.699134	-2.846342	-1.059247
O	-9.232346	-1.411465	0.320060
C	-0.683524	6.618859	1.260433
H	0.281474	6.510462	0.765328
H	-0.964781	7.631088	1.550928
H	-0.550630	6.185586	2.251752
C	-1.808560	6.112478	0.357265
H	-1.949392	6.660622	-0.574295
H	-2.719881	5.937893	0.929205
N	-1.629752	4.705849	-0.034225
H	-1.796266	4.021719	0.689887
H	-2.485846	4.624566	-0.563938
H	-0.772742	4.463904	-0.510771
N	-5.659618	-3.174042	3.918775
O	-5.852092	-1.978128	3.729517
O	-4.512261	-3.576390	4.076138
O	-6.305686	-3.987763	3.267982
C	-4.461406	-7.078768	2.967509
H	-4.723869	-6.633458	3.927151
H	-5.395034	-7.063036	2.405201
H	-4.137757	-8.092465	3.203664
C	-3.373161	-6.323003	2.204368
H	-3.325473	-6.764008	1.208708
H	-2.381969	-6.372182	2.655168
N	-3.834748	-4.945397	1.974196
H	-4.298176	-4.952853	1.076823
H	-4.461883	-4.472067	2.608830
H	-2.962516	-4.436498	1.955920
N	-2.690362	0.948640	-0.006033
O	-2.476199	0.300161	-1.024211
O	-2.470255	0.403916	1.070027
O	-2.353298	2.124574	-0.087539
C	1.872265	-0.256515	-0.313492
H	1.134530	-1.008340	-0.593858
H	1.985790	0.334680	-1.222172
H	2.724418	-0.875309	-0.032366
C	1.400242	0.426282	0.970574
H	2.098828	1.228531	1.208218
H	1.336209	-0.216988	1.848186
N	0.212286	1.257084	0.720833
H	0.387017	1.827076	-0.094444
H	-0.569152	0.674591	0.455963
H	-0.119497	1.734487	1.546730
N	-4.746826	3.832699	-0.907254
O	-5.266535	2.885790	-1.487206
O	-3.844966	4.500852	-1.400505
O	-4.836147	3.897936	0.313746
C	-6.608416	-4.354849	-4.761156
H	-6.485764	-5.348797	-4.330895
H	-6.940248	-4.753739	-5.719735
H	-5.660514	-3.816721	-4.762252
C	-7.639436	-3.471430	-4.058014
H	-8.543878	-4.019148	-3.793271
H	-7.926068	-2.869391	-4.920272
N	-7.159021	-2.657759	-2.930635

H	-6.872844	-3.357265	-2.260639
H	-6.346353	-2.065207	-3.023118
H	-7.998526	-2.197568	-2.608834
N	-5.186756	-1.321966	0.168868
O	-4.795291	-2.217678	0.908822
O	-5.110272	-1.407164	-1.051774
O	-5.562561	-0.256676	0.645317
C	-2.466529	2.454758	-5.326724
H	-2.912594	3.140425	-6.047132
H	-1.489936	2.147177	-5.700568
H	-3.074598	1.551871	-5.270618
C	-2.476310	3.005544	-3.900407
H	-3.478878	3.418616	-3.789369
H	-1.859576	3.893596	-4.038620
N	-2.151686	2.057525	-2.823504
H	-1.164983	1.875274	-2.708174
H	-2.461990	2.546880	-1.996254
H	-2.726702	1.230531	-2.897925
N	0.509825	3.253469	-1.652665
O	0.335810	2.054166	-1.838317
O	0.789412	3.584163	-0.505691
O	-0.288848	4.000781	-2.206491

Return

([EtNH₃][NO₃])₁₀ conformer -3

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	-9.428957	1.711975	-2.165056
H	-10.150934	2.518915	-2.039766
H	-9.467615	1.476238	-3.228557
H	-9.723252	0.830454	-1.595485
C	-8.039415	2.083261	-1.646249
H	-8.115493	2.519140	-0.650096
H	-7.597683	2.776615	-2.361955
N	-7.249166	0.843418	-1.692464
H	-7.720344	0.074706	-1.237302
H	-7.041404	0.563468	-2.640389
H	-6.339589	1.060803	-1.311001
N	-0.655234	-3.889732	2.024153
O	-0.248608	-2.899781	2.622256
O	-1.589400	-4.342656	2.676280
O	-0.966852	-3.671097	0.858748
C	-5.222773	3.565521	3.907859
H	-5.745918	3.796730	4.835739
H	-4.156535	3.670768	4.108259
H	-5.525262	4.290948	3.152640
C	-5.472560	2.131896	3.438640
H	-6.530358	1.874741	3.493719
H	-5.154659	1.418093	4.198590
N	-4.931154	2.002739	2.077009
H	-3.934057	1.841950	2.070388
H	-5.352233	1.239871	1.566299
H	-5.057826	2.925341	1.686038
N	-2.875588	-2.972734	-1.693314
O	-3.336820	-2.003087	-1.101599
O	-3.529100	-4.009097	-1.737459
O	-2.301861	-2.722367	-2.747463
C	-9.332039	-2.751163	3.954478
H	-9.826239	-3.587298	3.459761
H	-8.608177	-3.234959	4.610272
H	-10.048087	-2.196960	4.561300
C	-8.756041	-1.789942	2.914226
H	-8.334831	-0.991426	3.525007
H	-9.581218	-1.496612	2.265272
N	-7.585150	-2.328925	2.205459
H	-6.861700	-2.828492	2.702604
H	-7.944738	-2.882530	1.441052
H	-7.139814	-1.584659	1.687923
N	-2.101869	0.908262	3.372966
O	-2.875569	0.617507	4.278464
O	-2.262677	1.934530	2.721820
O	-1.374652	0.096494	2.811482
C	-2.664168	-2.161711	6.681551
H	-2.212954	-2.633987	7.554168
H	-3.025491	-1.147047	6.848890
H	-3.567441	-2.741402	6.491400
C	-1.645677	-2.282008	5.547511
H	-1.216232	-3.283117	5.509337
H	-0.720058	-1.728044	5.703886
N	-2.363096	-2.010671	4.292311
H	-1.630974	-2.046152	3.597446
H	-3.019153	-2.695430	3.944758
H	-2.637608	-1.041498	4.366122
N	-5.680489	0.724576	-4.561637
O	-6.084340	1.835689	-4.236969
O	-4.479262	0.777703	-4.801026
O	-5.981118	-0.156177	-3.763532
C	-2.060637	-1.227563	-6.548356

H	-1.339007	-1.434904	-7.338521
H	-2.763043	-2.052906	-6.432015
H	-2.685666	-0.413930	-6.916381
C	-1.341334	-0.751733	-5.285807
H	-0.679397	0.095383	-5.465623
H	-0.677554	-1.516014	-4.881616
N	-2.222078	-0.569640	-4.121774
H	-3.061488	-0.048859	-4.332197
H	-2.374228	-1.446812	-3.644784
H	-1.650758	0.085895	-3.607998
N	-9.010549	-1.761950	-0.672098
O	-8.280684	-1.803084	-1.656314
O	-8.884999	-2.793402	-0.021390
O	-8.852747	-0.724067	-0.038874
C	0.327559	3.294946	1.367228
H	0.915782	3.929152	2.030459
H	0.066800	2.368373	1.878665
H	0.861365	3.293881	0.416886
C	-0.972432	4.056433	1.106452
H	-0.764711	4.968061	0.546194
H	-1.473182	4.211142	2.062179
N	-1.929654	3.414162	0.192640
H	-2.389432	2.581403	0.532074
H	-2.615079	4.013385	-0.244652
H	-1.467831	3.133166	-0.660509
N	-5.602302	-3.803549	3.988562
O	-6.129332	-4.452010	3.091448
O	-5.950279	-2.638879	4.148354
O	-4.392739	-3.997696	3.940185
C	-2.523355	-6.583952	0.474801
H	-2.447822	-6.244415	-0.558209
H	-1.529906	-6.354724	0.860306
H	-2.561533	-7.673220	0.463023
C	-3.665289	-5.971657	1.286542
H	-3.643877	-6.291124	2.328455
H	-4.639631	-6.265404	0.896070
N	-3.752685	-4.503265	1.281402
H	-2.773686	-4.327689	1.456997
H	-3.964493	-4.032310	0.413393
H	-4.326931	-4.098598	2.007064
N	-3.845562	0.744524	-0.911339
O	-4.907137	1.357817	-0.908840
O	-3.221332	0.812283	0.141667
O	-3.139424	1.052798	-1.864970
C	1.324873	-1.085185	0.684510
H	1.226505	-0.628086	1.669134
H	1.226745	-2.166716	0.778122
H	2.274875	-0.823662	0.218461
C	0.077684	-0.762043	-0.138860
H	0.322132	-1.243423	-1.085759
H	0.126774	0.321935	-0.242208
N	-1.176686	-1.082951	0.559292
H	-2.009726	-1.180319	-0.003436
H	-0.941732	-1.942016	1.035636
H	-1.422187	-0.503337	1.349151
N	-4.872193	4.618290	-0.295934
O	-4.595351	4.271979	0.847090
O	-6.000678	4.347587	-0.691304
O	-4.000156	4.530699	-1.153229
C	-5.662424	-3.882496	-4.448248
H	-6.123526	-4.787669	-4.843401
H	-5.745153	-2.972890	-5.043119
H	-4.590153	-4.026082	-4.315140
C	-6.441526	-3.573557	-3.169421
H	-6.635828	-4.405059	-2.491961
H	-7.454439	-3.335448	-3.494090
N	-5.875607	-2.475071	-2.371357

H	-5.802476	-1.702848	-3.018213
H	-6.502312	-2.306899	-1.597369
H	-4.913661	-2.613526	-2.096421
N	-5.035122	-1.361524	1.213852
O	-5.601234	-2.222957	0.550130
O	-4.197155	-1.771746	2.009218
O	-5.795763	-0.446413	1.508930
C	-4.575446	4.934143	-4.784510
H	-4.200587	5.940628	-4.970436
H	-5.205426	4.523555	-5.573586
H	-5.261012	5.077265	-3.949276
C	-3.461601	3.971976	-4.370473
H	-2.591379	4.513939	-4.000218
H	-3.099528	3.369894	-5.203840
N	-4.045020	3.078491	-3.357977
H	-3.491201	2.266348	-3.126012
H	-4.202164	3.685490	-2.566169
H	-4.912344	2.682463	-3.691158
N	-0.457017	1.925955	-2.901903
O	-1.348336	2.273396	-3.668658
O	-0.396693	0.707507	-2.780161
O	-0.302605	2.609402	-1.895854

Return

([EtNH₃][NO₃])₁₀ conformer -4

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	-9.131288	3.198776	-2.586062
H	-8.940823	4.259539	-2.422953
H	-8.718200	3.065890	-3.585962
H	-10.186089	3.062502	-2.824653
C	-8.526247	2.249712	-1.551149
H	-8.878427	1.234146	-1.731962
H	-8.668311	2.488167	-0.497082
N	-7.060826	2.241409	-1.678870
H	-6.551805	1.584249	-1.105164
H	-6.683467	2.040712	-2.593978
H	-6.676821	3.155454	-1.486098
N	-0.069278	-3.399949	3.122905
O	-1.195534	-3.847672	3.307752
O	0.322423	-3.674664	1.994111
O	0.034889	-2.189812	3.289618
C	-6.894933	2.011345	3.563347
H	-7.930529	2.322502	3.700537
H	-6.303321	1.981761	4.478345
H	-6.315057	2.610787	2.861554
C	-7.055549	0.727782	2.748172
H	-7.753683	0.882137	1.925443
H	-7.553817	0.018304	3.408830
N	-5.857293	-0.005305	2.311586
H	-5.250797	-0.262356	3.077215
H	-6.128508	-0.781682	1.725257
H	-5.235073	0.375135	1.612868
N	-2.841320	-3.462917	-2.054065
O	-3.166134	-2.486336	-2.720294
O	-3.748321	-3.962153	-1.397415
O	-1.713031	-3.540633	-1.580779
C	-8.801309	-6.205322	2.347019
H	-9.160434	-5.885063	3.325060
H	-9.588117	-5.822174	1.697225
H	-8.680802	-7.288510	2.330260
C	-7.416856	-5.582195	2.165788
H	-6.990997	-5.905892	1.216070
H	-6.740296	-6.084045	2.857534
N	-7.375091	-4.112132	2.197571
H	-6.562533	-3.699675	1.761992
H	-8.071789	-3.631112	1.646815
H	-7.397749	-3.755676	3.142307
N	-3.053417	1.534166	2.768302
O	-4.082575	2.189133	2.646115
O	-3.066129	0.477375	3.389678
O	-2.306303	1.615056	1.799616
C	-2.655836	-3.996048	6.366634
H	-3.545328	-4.395409	5.879382
H	-1.853778	-4.608313	5.954401
H	-2.623869	-3.993578	7.456162
C	-2.598268	-2.523738	5.958184
H	-1.598724	-2.090549	5.995052
H	-3.174136	-1.790285	6.522561
N	-2.982471	-2.518722	4.538253
H	-3.933810	-2.853647	4.484586
H	-3.149060	-1.580049	4.204724
H	-2.346370	-3.093994	4.004833
N	-5.591143	1.535408	-4.904079
O	-5.784049	2.495091	-5.642234
O	-4.402029	1.282772	-4.745148
O	-6.287571	1.399243	-3.904317
C	-0.476875	-1.565936	-4.645438

H	-0.797432	-2.561578	-4.338776
H	0.250447	-1.846803	-5.407159
H	0.056093	-1.050546	-3.846427
C	-1.663833	-0.743921	-5.148690
H	-2.220923	-1.304957	-5.899015
H	-1.223098	0.124128	-5.638938
N	-2.521068	-0.269823	-4.051320
H	-3.300901	0.287614	-4.369480
H	-2.799536	-1.050230	-3.473807
H	-1.967747	0.404236	-3.541829
N	-8.368999	-1.471764	0.357612
O	-7.957155	-2.528944	-0.106966
O	-7.873466	-0.447576	-0.099072
O	-8.572902	-1.483176	1.566483
C	-1.291790	4.662050	1.874016
H	-0.320740	4.173342	1.794484
H	-1.049995	5.642934	2.283285
H	-1.936682	4.201353	2.622329
C	-2.049974	4.783059	0.551762
H	-1.489657	5.376061	-0.171075
H	-2.986687	5.316264	0.714125
N	-2.341650	3.466754	-0.036545
H	-2.738247	2.832235	0.641834
H	-3.112130	3.409894	-0.687106
H	-1.566924	3.128655	-0.589345
N	-6.154514	-2.329194	4.718288
O	-5.402709	-1.408848	4.416911
O	-5.517700	-3.376832	4.718413
O	-7.251474	-2.341456	4.170926
C	-0.794894	-7.006516	0.362194
H	-1.137744	-6.937470	-0.670175
H	0.214132	-6.675608	0.608091
H	-0.942079	-8.062655	0.588043
C	-1.870976	-6.168625	1.053446
H	-1.858996	-6.368555	2.124886
H	-2.830120	-6.576712	0.734687
N	-1.740752	-4.750523	0.684841
H	-2.420925	-4.237063	1.226897
H	-0.868442	-4.352674	1.002475
H	-1.943787	-4.579095	-0.289576
N	-4.129202	0.776470	-0.470927
O	-3.821207	-0.409538	-0.430954
O	-3.516667	1.395348	-1.333983
O	-5.306140	1.030629	-0.240067
C	0.802259	-0.036685	0.706887
H	0.650619	0.817573	1.366696
H	1.460366	-0.741138	1.215553
H	1.298799	0.367941	-0.175057
C	-0.560986	-0.608659	0.316692
H	-0.351760	-1.501912	-0.271885
H	-1.087491	0.086194	-0.337581
N	-1.455385	-0.813029	1.466527
H	-1.737335	0.076880	1.852100
H	-2.270724	-1.284238	1.101446
H	-0.956667	-1.400649	2.119278
N	-5.163540	5.042208	-1.688483
O	-4.355317	5.680249	-2.353880
O	-4.729631	4.141778	-0.978535
O	-6.220671	4.704053	-2.209252
C	-7.043849	-2.789110	-3.432523
H	-7.525083	-3.465366	-2.725987
H	-7.829868	-2.548650	-4.148382
H	-6.427079	-3.472936	-4.015685
C	-6.249314	-1.632540	-2.825152
H	-7.002320	-0.924744	-2.478588
H	-5.491745	-1.108570	-3.407943
N	-5.603252	-2.049345	-1.571071

H	-4.820951	-2.684358	-1.501329
H	-5.125005	-1.257859	-1.164956
H	-6.287819	-2.370155	-0.901333
N	-4.399440	-3.229316	1.768575
O	-5.334791	-2.628268	1.251919
O	-4.437935	-4.452402	1.693382
O	-3.285786	-2.722274	1.692683
C	-2.272225	2.863248	-6.243908
H	-1.664667	3.085346	-7.121202
H	-1.617877	2.602561	-5.412060
H	-3.049395	2.150354	-6.519390
C	-2.937591	4.088190	-5.615700
H	-3.680398	4.511785	-6.291648
H	-2.292685	4.961967	-5.522378
N	-3.626090	3.863913	-4.335267
H	-2.924037	3.564068	-3.673969
H	-3.938709	4.775688	-4.033545
H	-4.483233	3.347946	-4.473777
N	-0.566565	2.545310	-2.709626
O	-0.531712	2.295612	-1.509829
O	-1.135276	3.595422	-2.986950
O	-0.823634	1.484106	-3.267153

Return

([EtNH₃][NO₃])₁₀ conformer -5

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	-8.646476	1.668037	-4.158894
H	-7.995335	1.983997	-4.973931
H	-8.501272	0.600708	-3.992086
H	-9.685353	1.849860	-4.434170
C	-8.431513	2.499240	-2.893693
H	-9.322323	2.293042	-2.300362
H	-8.346398	3.554709	-3.152227
N	-7.225730	2.045054	-2.184015
H	-6.847080	2.726801	-1.542187
H	-7.402896	1.181683	-1.690759
H	-6.400995	2.118098	-2.762442
N	-0.838619	-4.280910	2.376436
O	-1.857010	-4.514441	3.017856
O	-0.602462	-3.078883	2.425810
O	-0.785408	-4.843098	1.288232
C	-6.274598	2.498398	3.308821
H	-7.281559	2.913648	3.267609
H	-6.215171	2.127881	4.332191
H	-5.533317	3.293028	3.224163
C	-6.094820	1.395256	2.265462
H	-6.080547	1.820092	1.261764
H	-6.995228	0.825935	2.496197
N	-4.865025	0.656570	2.590715
H	-5.049021	0.195725	3.470413
H	-4.688249	-0.009962	1.852755
H	-4.088810	1.298249	2.514299
N	-3.013468	-3.467134	-1.982929
O	-4.132215	-3.848301	-1.657058
O	-2.961322	-2.338270	-2.458349
O	-2.062623	-3.690799	-1.242021
C	-9.004317	-4.884222	2.924161
H	-8.069481	-5.324114	2.576775
H	-8.733377	-4.599142	3.940734
H	-9.852240	-5.568892	2.905365
C	-9.127852	-3.563168	2.164295
H	-9.596788	-2.839527	2.831036
H	-9.638423	-3.686895	1.209251
N	-7.881329	-2.807834	1.965567
H	-7.922219	-2.093908	1.252308
H	-7.612340	-2.320771	2.808487
H	-7.152730	-3.485706	1.793134
N	-1.578039	0.858356	3.068379
O	-2.386189	1.741044	2.802236
O	-1.999562	-0.045959	3.780845
O	-0.815126	0.610866	2.141131
C	-2.616017	-1.923935	6.892514
H	-3.666226	-2.017186	7.169036
H	-2.062015	-2.239187	7.776708
H	-2.418557	-0.868897	6.702762
C	-2.212810	-2.786637	5.696266
H	-2.420234	-3.820251	5.973245
H	-1.123990	-2.748636	5.662718
N	-2.908214	-2.465580	4.440409
H	-3.894442	-2.379850	4.640671
H	-2.592706	-1.570613	4.094591
H	-2.702173	-3.092455	3.675769
N	-5.047396	1.771028	-4.448302
O	-5.522477	2.761466	-3.903870
O	-3.932795	1.854883	-4.951997
O	-5.495340	0.662319	-4.177771
C	-2.499182	-1.317666	-5.559641

H	-3.141861	-0.638356	-6.119643
H	-1.879513	-1.905431	-6.236873
H	-3.054697	-2.142845	-5.114015
C	-1.746360	-0.466539	-4.536566
H	-1.208763	0.402618	-4.915582
H	-1.050220	-1.202419	-4.134111
N	-2.552092	0.048312	-3.418726
H	-1.944330	0.532968	-2.773875
H	-3.266503	0.712130	-3.681523
H	-3.016215	-0.703065	-2.928702
N	-8.728250	-1.078359	-0.547136
O	-8.272082	-2.199047	-0.744738
O	-8.801496	-0.792559	0.642834
O	-8.287271	-0.168276	-1.240217
C	0.498252	3.546402	0.718163
H	0.900674	2.939681	1.529364
H	0.916707	3.324733	-0.263600
H	0.867625	4.501351	1.091976
C	-1.016792	3.750245	0.748662
H	-1.328003	4.569711	0.100803
H	-1.397138	3.894932	1.759851
N	-1.651856	2.539498	0.205866
H	-1.303512	2.275497	-0.704661
H	-1.536100	1.769718	0.849403
H	-2.652709	2.668879	0.246544
N	-6.021514	-1.793914	4.724148
O	-7.062025	-1.519076	4.136886
O	-5.084550	-1.027062	4.531498
O	-5.731421	-2.966930	4.931404
C	-3.688094	-7.595694	1.347618
H	-2.925841	-7.447352	2.112513
H	-4.666105	-7.435266	1.801335
H	-3.613087	-8.653535	1.095734
C	-3.389166	-6.600159	0.226282
H	-4.217658	-6.772334	-0.460781
H	-2.565181	-6.960674	-0.389491
N	-3.198037	-5.213743	0.679230
H	-3.955751	-4.861133	1.246359
H	-2.271268	-5.169901	1.078326
H	-3.091769	-4.623958	-0.133765
N	-4.089969	0.868799	-0.929157
O	-4.949584	0.044891	-1.221246
O	-3.173174	0.365658	-0.289304
O	-3.896226	1.778507	-1.727887
C	0.694276	-2.533267	-0.690627
H	1.236685	-2.925757	0.169515
H	0.059886	-3.329165	-1.080751
H	1.376935	-2.252648	-1.492706
C	-0.045568	-1.272104	-0.243480
H	-0.363793	-0.709796	-1.121342
H	0.493087	-0.527281	0.342343
N	-1.281326	-1.613740	0.477649
H	-1.770311	-2.291326	-0.089688
H	-1.058425	-2.012494	1.378432
H	-1.892124	-0.833761	0.674264
N	-4.858169	3.918283	0.070364
O	-4.214446	3.321380	0.926169
O	-5.697487	3.269155	-0.543846
O	-4.380900	4.744398	-0.699587
C	-6.730830	-3.619323	-3.885276
H	-7.747294	-3.888870	-3.598490
H	-6.578644	-3.920005	-4.921871
H	-5.945461	-4.249405	-3.467793
C	-6.417415	-2.145736	-3.624215
H	-7.255983	-1.517547	-3.924685
H	-5.620455	-1.794219	-4.279494
N	-6.129882	-1.996689	-2.189311

H	-5.399547	-2.675004	-2.026214
H	-5.865710	-1.059783	-1.920013
H	-6.858635	-2.198507	-1.519767
N	-4.794802	-2.660612	1.725281
O	-5.535474	-1.754885	1.359030
O	-3.595468	-2.420552	1.809213
O	-5.197410	-3.818576	1.715195
C	-2.787245	6.592955	-3.238270
H	-2.781023	7.381260	-3.991022
H	-3.378596	6.740766	-2.334635
H	-1.794657	6.371637	-2.845984
C	-3.271981	5.388661	-4.046075
H	-2.716742	5.173908	-4.959141
H	-4.331819	5.537459	-4.252717
N	-3.235595	4.073291	-3.388566
H	-2.284714	3.794630	-3.192928
H	-3.720394	3.954843	-2.510477
H	-3.634164	3.412204	-4.039878
N	-0.482441	2.695056	-2.653247
O	-0.890326	2.431407	-3.778945
O	-0.424107	1.704635	-1.933012
O	-1.061865	3.696516	-2.247757

Return

([EtNH₃][NO₃])₁₀ conformer -6

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	-8.859009	2.492121	-2.664868
H	-9.216783	1.803911	-1.899057
H	-8.442490	3.441870	-2.329327
H	-9.596436	2.796133	-3.407754
C	-7.927645	1.677392	-3.562987
H	-7.620858	2.308792	-4.396843
H	-8.616693	0.898411	-3.889332
N	-6.851865	1.143645	-2.713486
H	-6.174435	0.629024	-3.257871
H	-6.538251	1.832960	-2.045211
H	-7.239723	0.489158	-2.049171
N	-6.692381	-5.431985	0.278202
O	-6.831140	-5.396739	1.495815
O	-5.578347	-5.737395	-0.132562
O	-7.242431	-4.491122	-0.283313
C	-6.487241	1.448505	3.624607
H	-7.460623	1.087770	3.292196
H	-5.941613	0.602124	4.041776
H	-6.608461	2.043401	4.529871
C	-5.729857	2.269687	2.580638
H	-4.824797	2.760788	2.938108
H	-6.383812	3.079407	2.256914
N	-5.426458	1.445116	1.400862
H	-4.979496	2.025435	0.705480
H	-4.742613	0.722405	1.574488
H	-6.296982	1.057264	1.066409
N	-2.393645	-3.371611	-1.324015
O	-1.936706	-2.237631	-1.415520
O	-2.927287	-3.695781	-0.268924
O	-2.899358	-3.818883	-2.347381
C	-8.985946	-4.208935	3.667115
H	-10.070273	-4.318755	3.650593
H	-8.510636	-5.162370	3.436592
H	-8.685523	-4.023741	4.698401
C	-8.659671	-3.119991	2.644575
H	-9.082799	-2.193488	3.032718
H	-9.268817	-3.317749	1.762570
N	-7.208372	-2.974254	2.453969
H	-6.870756	-3.856252	2.095926
H	-6.991700	-2.207364	1.833458
H	-6.848952	-2.762401	3.373771
N	-1.476246	1.588755	3.266729
O	-0.865492	0.571262	2.958890
O	-2.180023	1.562186	4.270256
O	-1.447186	2.494097	2.440540
C	-2.034847	-1.389350	7.262886
H	-3.034407	-1.707183	7.559471
H	-1.330139	-1.966868	7.861184
H	-1.961816	-0.366920	7.633565
C	-1.717146	-1.589331	5.780686
H	-1.567762	-2.645390	5.555915
H	-0.825304	-1.020048	5.518703
N	-2.775842	-1.057339	4.908913
H	-3.637011	-1.580119	4.980935
H	-2.889229	-0.065676	5.063342
H	-2.667949	-1.140766	3.908163
N	-4.781085	0.711926	-5.395177
O	-3.594242	0.723059	-5.702349
O	-5.007804	-0.101643	-4.506482
O	-5.338469	1.767033	-5.113841
C	-1.805237	-2.754972	-5.371932

H	-2.843228	-2.776341	-5.703922
H	-1.217265	-3.073255	-6.232795
H	-1.552446	-3.511483	-4.629040
C	-1.429051	-1.398371	-4.775308
H	-1.419843	-0.590836	-5.507361
H	-0.391598	-1.462117	-4.447091
N	-2.438911	-1.101422	-3.747765
H	-2.403281	-0.225229	-3.246651
H	-3.281285	-0.981807	-4.292006
H	-2.428656	-1.785070	-3.004380
N	-7.757005	-0.222847	0.071597
O	-7.288349	-0.700315	1.098954
O	-7.795276	1.001296	0.016067
O	-7.543268	-0.769357	-1.004842
C	-0.611600	5.749094	-0.611746
H	-0.908145	5.322248	-1.569851
H	-1.302327	6.585754	-0.506881
H	0.402246	6.148261	-0.641474
C	-0.809697	4.701474	0.484196
H	-1.225955	5.209684	1.353996
H	0.157591	4.214344	0.607308
N	-1.910328	3.755657	0.243600
H	-2.842693	4.143646	0.227479
H	-1.862511	3.377800	-0.691834
H	-2.008478	3.134407	1.033862
N	-5.568540	-2.730863	5.187151
O	-5.276968	-3.727694	4.535700
O	-6.503978	-2.019549	4.837776
O	-4.755310	-2.240493	5.962567
C	-2.516207	-6.773097	1.711988
H	-3.257785	-7.166989	1.016998
H	-1.667012	-6.442992	1.113659
H	-2.257501	-7.686630	2.247365
C	-3.082738	-5.706713	2.649917
H	-2.302629	-5.038062	3.013833
H	-3.699088	-6.054711	3.478839
N	-3.920712	-4.835624	1.811559
H	-3.269346	-4.494522	1.119121
H	-4.683012	-5.229290	1.278618
H	-4.297272	-4.041592	2.309371
N	-3.877001	0.921491	-1.257831
O	-3.369984	1.001402	-2.371215
O	-3.145528	1.151366	-0.301179
O	-4.645683	-0.008459	-1.040124
C	1.243035	-1.395941	1.506396
H	2.112485	-1.964287	1.176032
H	1.602136	-0.463429	1.941790
H	0.587693	-1.860385	2.243227
C	0.458200	-1.134441	0.220514
H	0.366027	-2.067969	-0.334579
H	0.987065	-0.401842	-0.389158
N	-0.782740	-0.414679	0.545865
H	-0.600360	0.384677	-0.043937
H	-1.623500	-0.732640	0.085297
H	-0.867313	-0.072523	1.492373
N	-4.819316	3.886934	-0.922840
O	-3.829554	4.034306	-1.631169
O	-4.478934	3.844215	0.254186
O	-5.674553	3.099591	-1.312375
C	-6.339999	-3.825464	-3.553270
H	-7.140043	-4.220538	-2.927213
H	-6.734493	-3.533656	-4.526575
H	-5.575028	-4.601887	-3.562570
C	-5.803236	-2.590269	-2.829379
H	-6.649501	-1.920468	-2.982033
H	-4.908834	-2.158896	-3.278893
N	-5.441665	-2.787571	-1.417225

H	-4.660621	-3.427642	-1.397737
H	-5.214433	-1.852161	-1.111488
H	-6.277074	-3.198869	-1.026040
N	-3.722595	-1.466301	1.892503
O	-2.944773	-2.222796	2.463279
O	-4.716658	-2.058908	1.487867
O	-3.807515	-0.374703	2.444117
C	-3.679364	4.778922	-5.655073
H	-3.412132	5.321802	-6.561698
H	-4.605900	4.279596	-5.938458
H	-4.173069	5.360174	-4.876291
C	-2.715053	3.706456	-5.147371
H	-1.723610	4.020825	-4.821316
H	-2.495076	3.004826	-5.951999
N	-3.164407	3.031187	-3.920206
H	-3.416444	3.579033	-3.109995
H	-3.981076	2.476216	-4.132710
H	-2.385775	2.494889	-3.564935
N	-0.337081	2.091842	-2.250354
O	-0.530248	1.195507	-3.064201
O	-1.012263	3.114312	-2.292302
O	0.133824	1.787102	-1.160190

Return

([EtNH₃][NO₃])₁₀ conformer -7

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	-8.202564	0.018112	-2.730205
H	-8.662508	0.715510	-3.430339
H	-7.120182	0.062074	-2.851110
H	-8.566179	-0.980413	-2.972757
C	-8.370094	0.348329	-1.246719
H	-9.373536	0.207753	-0.844921
H	-8.204754	1.410400	-1.065696
N	-7.536114	-0.521997	-0.403599
H	-7.812624	-0.453097	0.565367
H	-7.546850	-1.478650	-0.727329
H	-6.578101	-0.227090	-0.527453
N	-7.358414	-3.729040	-2.156129
O	-7.398348	-3.282042	-3.297038
O	-7.368645	-2.947542	-1.211548
O	-6.650570	-4.728164	-2.094622
C	-8.907396	4.570305	2.043757
H	-9.342181	3.797867	1.409406
H	-9.697797	5.070561	2.603319
H	-8.549658	5.237038	1.259162
C	-7.709426	4.037144	2.830172
H	-8.193078	3.619243	3.713087
H	-6.964960	4.755468	3.173513
N	-7.118374	2.855375	2.183706
H	-6.570922	3.175934	1.397806
H	-6.407419	2.331686	2.674005
H	-7.833977	2.193470	1.919330
N	-2.279314	-3.957053	-2.493428
O	-1.826816	-3.975908	-3.632712
O	-3.487986	-4.093688	-2.340068
O	-1.669605	-3.133238	-1.820628
C	-7.284196	-2.751180	5.004858
H	-7.758496	-2.961945	5.963355
H	-7.995184	-2.979502	4.210839
H	-6.531611	-3.531912	4.894528
C	-6.643755	-1.367491	4.890486
H	-5.709600	-1.400684	5.451157
H	-7.264170	-0.504413	5.131904
N	-6.271624	-1.286341	3.469650
H	-7.004581	-1.219790	2.777954
H	-5.889235	-0.379505	3.242655
H	-5.594326	-1.928061	3.082916
N	0.662580	0.760756	2.333771
O	0.421287	0.878345	1.137516
O	0.606999	-0.383399	2.770685
O	0.166371	1.656772	3.007574
C	-0.788207	1.095441	6.750847
H	-0.779545	0.748435	7.784100
H	0.244220	1.187850	6.413720
H	-1.338256	2.036442	6.758862
C	-1.512053	-0.081829	6.096688
H	-2.396819	0.159602	6.685754
H	-1.126105	-1.038135	6.449709
N	-1.747225	0.035557	4.649361
H	-2.368574	-0.736271	4.453638
H	-2.392566	0.767177	4.387892
H	-0.896700	-0.052764	4.111860
N	-3.927774	-0.819100	-5.226430
O	-3.040784	-0.054018	-4.864524
O	-3.413381	-1.920897	-5.383016
O	-5.032615	-0.745650	-4.700116
C	-0.086733	-1.504809	-6.308140

H	0.686364	-1.024715	-6.908083
H	0.042648	-2.578655	-6.443102
H	-1.002785	-1.195272	-6.811265
C	0.132699	-1.143567	-4.838720
H	0.465421	-0.115739	-4.693929
H	0.838075	-1.828940	-4.368817
N	-1.002404	-1.382750	-3.934190
H	-1.169575	-2.377384	-3.880743
H	-0.972954	-0.885680	-3.055467
H	-1.833537	-0.926550	-4.282327
N	-8.930756	0.213161	2.220611
O	-8.609441	0.739030	3.280467
O	-8.878525	1.036993	1.314163
O	-8.395205	-0.852661	1.937265
C	-2.076279	4.764074	0.179640
H	-3.101235	5.121553	0.278497
H	-1.501547	5.650146	-0.089915
H	-1.935916	4.260813	-0.776983
C	-1.748293	3.945897	1.428981
H	-2.390636	4.383907	2.192946
H	-0.695739	4.061255	1.687673
N	-2.104382	2.523266	1.314253
H	-1.649776	2.121641	0.506707
H	-2.002174	2.049690	2.200469
H	-3.093404	2.554597	1.111881
N	-4.555634	1.524414	4.277580
O	-5.638361	1.511873	3.702582
O	-4.533260	0.784771	5.255078
O	-3.506077	1.685689	3.664802
C	-4.146425	-5.762023	1.011757
H	-3.402024	-5.566594	0.239892
H	-3.665057	-5.487940	1.950513
H	-4.576109	-6.760138	1.096828
C	-5.418293	-4.953409	0.754201
H	-6.088402	-4.940567	1.613788
H	-6.003949	-5.523015	0.032636
N	-5.212944	-3.587282	0.248861
H	-4.829454	-2.908215	0.890660
H	-4.729466	-3.638759	-0.636406
H	-6.168758	-3.421395	-0.032212
N	-4.465814	-0.087027	0.397571
O	-5.292830	-0.743323	1.020785
O	-4.594628	0.112974	-0.805127
O	-3.339317	-0.092239	0.881361
C	1.237422	-2.575041	0.420210
H	1.734260	-3.511573	0.673507
H	1.221991	-2.485820	-0.666023
H	1.631612	-1.630420	0.794918
C	-0.228610	-2.564409	0.854353
H	-0.093368	-2.566873	1.935927
H	-0.730449	-3.438148	0.438617
N	-0.948717	-1.389040	0.340742
H	-1.802764	-1.163145	0.830308
H	-0.360450	-0.620421	0.629302
H	-1.128118	-1.368596	-0.652986
N	-5.434177	3.486739	-0.149159
O	-4.692183	3.313294	0.811277
O	-5.350009	2.722571	-1.104166
O	-6.576125	3.903019	0.011285
C	-5.381540	-4.700242	-6.833117
H	-5.387372	-3.651429	-7.129865
H	-5.171038	-5.468942	-7.576683
H	-6.459475	-4.551646	-6.769275
C	-4.756032	-4.880800	-5.449651
H	-3.674537	-4.860841	-5.584077
H	-5.104980	-5.781824	-4.945181
N	-5.053594	-3.746655	-4.561387

H	-4.515711	-3.788919	-3.707575
H	-4.685948	-2.869027	-4.900070
H	-6.020134	-3.603570	-4.305600
N	-3.342988	-2.827629	3.392600
O	-2.605240	-2.438413	2.494094
O	-3.273903	-2.133496	4.400808
O	-4.459844	-3.073446	2.950692
C	-5.210580	2.619647	-4.698543
H	-5.563391	3.189562	-5.558091
H	-5.423620	1.560247	-4.841321
H	-5.940630	2.998923	-3.983505
C	-3.772183	2.895307	-4.259376
H	-3.659965	3.942356	-3.977959
H	-3.089999	2.666533	-5.078148
N	-3.358738	2.048755	-3.129662
H	-3.469453	1.060034	-3.303657
H	-2.392360	2.131748	-2.848016
H	-3.873072	2.380422	-2.326196
N	-0.476905	1.349330	-2.025949
O	-1.141064	1.983512	-1.213679
O	-0.432161	0.140017	-1.829392
O	-0.740727	1.733582	-3.159892

Return

([EtNH₃][NO₃])₁₀ conformer -8

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	-8.942845	-2.031665	-4.064188
H	-10.026009	-1.931068	-3.995367
H	-8.718467	-1.390392	-4.916552
H	-8.712004	-3.093841	-4.145392
C	-8.451239	-1.378000	-2.772334
H	-8.827618	-1.913609	-1.900805
H	-8.758113	-0.336945	-2.671677
N	-7.010149	-1.506054	-2.506436
H	-6.793182	-1.262659	-1.550515
H	-6.606864	-2.393804	-2.769801
H	-6.430040	-0.898841	-3.067566
N	-6.131541	-4.757265	-2.364121
O	-5.085635	-5.383875	-2.235602
O	-6.171635	-3.904126	-3.243679
O	-6.778045	-4.559349	-1.341410
C	-6.276502	5.683356	-0.064942
H	-7.301070	5.321076	-0.149292
H	-6.417241	6.747166	0.126373
H	-5.834415	5.506560	-1.045453
C	-5.607834	5.197339	1.221337
H	-6.255237	5.380130	2.078982
H	-4.685500	5.774776	1.158355
N	-5.278796	3.763819	1.196952
H	-6.041883	3.320026	0.706190
H	-4.423415	3.733081	0.660783
H	-5.140040	3.284039	2.074824
N	-0.670039	-2.947564	-2.636951
O	-1.019794	-2.164724	-3.513256
O	-1.543823	-3.746309	-2.318230
O	-0.222939	-2.384593	-1.643854
C	-7.385114	1.769545	3.419283
H	-8.365289	1.977221	2.990066
H	-7.633352	1.827074	4.479080
H	-6.657082	2.567204	3.271600
C	-6.854910	0.344245	3.260397
H	-7.572875	-0.402812	3.598822
H	-6.001917	0.169338	3.916073
N	-6.365816	-0.082188	1.940253
H	-5.488295	0.335746	1.665682
H	-6.243431	-1.074410	2.083836
H	-7.119440	-0.027130	1.270090
N	-0.398146	-0.846103	2.291654
O	-0.411775	-0.793216	1.066871
O	-0.745647	0.152246	2.912637
O	-0.707614	-1.927427	2.779551
C	-3.393902	-1.247990	6.809677
H	-3.883432	-0.340186	7.162315
H	-4.144083	-2.008565	6.593218
H	-3.115161	-1.655060	7.781633
C	-2.196986	-1.189995	5.860009
H	-1.753219	-2.185520	5.850120
H	-1.641646	-0.325476	6.223747
N	-2.697062	-0.754229	4.547045
H	-3.052393	0.190513	4.510961
H	-1.928996	-0.903346	3.908345
H	-3.510509	-1.294389	4.288912
N	-4.566078	-0.254195	-4.592212
O	-3.919428	-1.115366	-5.178134
O	-5.753089	-0.415758	-4.331483
O	-4.063956	0.752280	-4.104404
C	0.285959	1.125725	-1.897716

H	0.991436	1.954011	-1.963632
H	-0.200294	1.232970	-0.928099
H	0.868586	0.209011	-1.988708
C	-0.804183	1.124581	-2.969831
H	-0.457542	0.919547	-3.982699
H	-1.416269	2.020899	-2.869504
N	-1.844569	0.164897	-2.569274
H	-2.731668	0.239653	-3.046312
H	-1.665224	-0.776149	-2.249325
H	-2.061158	0.584099	-1.676269
N	-7.907258	1.324509	-0.472672
O	-7.508110	1.270192	-1.630604
O	-8.108828	0.243520	0.069460
O	-7.584447	2.357027	0.104196
C	0.534946	4.151110	2.086729
H	1.420062	4.412677	2.666602
H	0.634109	4.563732	1.082732
H	-0.282100	4.631749	2.624801
C	0.221286	2.654878	2.059375
H	0.296425	2.295194	3.085573
H	0.691892	2.046557	1.286992
N	-1.237964	2.606597	1.880211
H	-1.491916	1.721322	1.465607
H	-1.807330	2.594848	2.714347
H	-1.485136	3.290604	1.179397
N	-3.670122	2.542837	4.359696
O	-2.444775	2.502848	4.361052
O	-4.151956	1.430980	4.545935
O	-4.169810	3.288889	3.524955
C	-7.687371	-6.705326	1.753476
H	-8.213365	-6.218170	2.574517
H	-8.299170	-6.643170	0.853509
H	-7.507525	-7.741530	2.039899
C	-6.290758	-6.117581	1.548855
H	-5.859627	-6.551899	0.646860
H	-5.737187	-6.296230	2.470671
N	-6.107974	-4.685411	1.267220
H	-6.513430	-4.011768	1.901185
H	-5.226556	-4.279951	0.986496
H	-6.639877	-4.510807	0.426570
N	-4.636190	-2.107768	-0.336207
O	-4.339434	-1.740793	-1.467729
O	-3.905772	-2.898850	0.250099
O	-5.829156	-2.137665	-0.055111
C	1.112795	-4.082907	1.162221
H	1.413776	-3.405458	0.363113
H	1.186646	-3.395969	2.005288
H	1.760056	-4.959866	1.152459
C	-0.349461	-4.414084	0.862271
H	-0.696302	-4.784125	1.827088
H	-0.468318	-5.049443	-0.015392
N	-1.211440	-3.244824	0.630612
H	-1.066594	-2.518811	1.317652
H	-0.861399	-2.944370	-0.267886
H	-2.208787	-3.301058	0.481489
N	-2.648842	4.391227	-1.059069
O	-2.502079	3.951942	0.076081
O	-3.286042	5.428736	-1.202690
O	-3.023015	3.522964	-1.839576
C	-2.606007	-4.486972	-6.034578
H	-1.647419	-4.085797	-5.705538
H	-2.354364	-5.428821	-6.522117
H	-2.914369	-3.870715	-6.879114
C	-3.483887	-4.585011	-4.786557
H	-3.191472	-5.454760	-4.198229
H	-4.488418	-4.822920	-5.136437
N	-3.645311	-3.337397	-4.024164

H	-3.808169	-2.475489	-4.524853
H	-4.486755	-3.473497	-3.482362
H	-2.873444	-3.149006	-3.400601
N	-5.691954	-2.905572	3.798469
O	-6.503587	-2.582382	2.938307
O	-5.478991	-4.089915	4.033109
O	-4.780959	-2.157214	4.134806
C	-7.021837	4.154530	-3.585641
H	-7.039250	5.002721	-4.270016
H	-7.537954	3.382266	-4.156020
H	-7.617223	4.410668	-2.709280
C	-5.572921	3.885735	-3.177924
H	-5.097008	4.732521	-2.683394
H	-4.996940	3.827476	-4.101477
N	-5.412564	2.582576	-2.514672
H	-5.307615	1.807772	-3.154019
H	-4.515866	2.635350	-2.052886
H	-6.132463	2.450791	-1.818627
N	-3.495316	0.985882	0.471260
O	-2.582155	0.913006	-0.343543
O	-3.225831	1.110896	1.660724
O	-4.655567	1.158732	0.114868

Return

([EtNH₃][NO₃])₁₀ conformer -9

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	-9.431042	-0.141205	-2.877336
H	-10.200862	-0.737366	-3.367304
H	-9.523337	0.737267	-3.515983
H	-8.466984	-0.639384	-2.979852
C	-9.704062	0.052822	-1.385473
H	-9.392954	-0.883803	-0.922822
H	-10.716888	0.386128	-1.159224
N	-8.709350	0.985120	-0.833016
H	-7.729889	0.786122	-0.978467
H	-8.574875	1.848397	-1.339741
H	-8.913449	1.137203	0.144386
N	-5.137956	-0.578816	-3.534587
O	-4.280762	-1.352634	-3.122882
O	-5.963695	-0.969640	-4.352198
O	-5.385691	0.456423	-2.926324
C	-7.601786	5.866853	1.790323
H	-8.370973	5.755202	2.554513
H	-7.447063	6.927071	1.990571
H	-8.037932	5.825342	0.792247
C	-6.418960	4.953446	2.113508
H	-6.352407	4.966360	3.201398
H	-5.455120	5.266549	1.712160
N	-6.830188	3.559756	1.884685
H	-6.054090	2.936933	2.057495
H	-7.653773	3.284703	2.400586
H	-7.162793	3.349665	0.954450
N	-1.445256	-4.029013	-1.272662
O	-2.135615	-3.190839	-1.841823
O	-2.001120	-4.438077	-0.259371
O	-0.226466	-3.917055	-1.201313
C	-8.200407	-2.323276	3.896590
H	-9.101590	-1.960976	3.401910
H	-7.935017	-3.160782	3.251413
H	-8.478025	-2.595211	4.914961
C	-7.074241	-1.291916	3.973329
H	-6.165256	-1.721325	4.394582
H	-7.336194	-0.462736	4.630551
N	-6.707419	-0.719262	2.668971
H	-7.535224	-0.354670	2.219626
H	-6.092447	0.080996	2.707652
H	-6.148379	-1.371138	2.137341
N	0.802022	-4.663697	3.188746
O	-0.195150	-4.849406	3.877393
O	1.278148	-3.534311	3.159281
O	0.746573	-5.146277	2.063082
C	-0.407852	-0.822123	4.055281
H	-0.707782	0.057721	4.624505
H	0.343441	-1.438759	4.548655
H	0.064803	-0.413826	3.161977
C	-1.606188	-1.713821	3.728622
H	-2.097069	-2.153851	4.596672
H	-1.117178	-2.545044	3.220647
N	-2.595480	-1.200125	2.768800
H	-2.228010	-0.729060	1.954453
H	-3.217367	-1.972395	2.576561
H	-3.104448	-0.410499	3.139669
N	-2.394235	2.523622	-3.654714
O	-3.001494	3.585168	-3.568501
O	-1.815323	2.378651	-4.725657
O	-2.283501	1.771128	-2.693170
C	3.321692	-1.892583	0.972765

H	2.942487	-0.871169	1.004651
H	3.421487	-2.221427	2.007175
H	4.357100	-1.985689	0.645102
C	2.502443	-2.745403	0.003555
H	3.068749	-3.658536	-0.179711
H	2.428830	-2.151504	-0.907470
N	1.160572	-2.876981	0.591698
H	0.585239	-3.206071	-0.170399
H	1.165633	-3.538804	1.354630
H	0.745555	-2.013430	0.911292
N	-9.179933	1.563849	2.261416
O	-9.330000	2.384039	1.362614
O	-8.462326	1.875871	3.205216
O	-9.014197	0.416479	1.862480
C	-3.595885	4.429885	-0.589855
H	-3.210138	5.428684	-0.794061
H	-4.316681	4.044376	-1.310922
H	-4.106801	4.632278	0.351476
C	-2.384247	3.524902	-0.364508
H	-1.752794	4.020297	0.373022
H	-1.731573	3.603931	-1.233916
N	-2.635497	2.149003	0.091140
H	-3.072326	1.904801	0.968435
H	-3.141163	1.578710	-0.571558
H	-1.709034	1.747168	0.108286
N	-3.876616	1.840287	3.037555
O	-4.327368	2.817776	2.450688
O	-2.770022	1.476627	2.655094
O	-4.682755	0.936428	3.227963
C	-6.872850	-3.963502	-0.366982
H	-6.784001	-4.591777	0.519289
H	-7.320584	-3.005661	-0.102074
H	-7.613109	-4.520026	-0.941785
C	-5.637815	-3.721633	-1.235331
H	-5.965038	-3.010387	-1.993720
H	-5.205343	-4.589638	-1.732960
N	-4.599454	-2.870102	-0.634879
H	-5.010278	-1.973715	-0.416214
H	-4.076900	-3.363271	0.074925
H	-3.904818	-2.654004	-1.335510
N	-5.625452	0.241965	-0.238287
O	-4.796544	-0.392893	0.404321
O	-6.059922	1.304902	0.191221
O	-6.503791	-0.578112	-0.481329
C	-2.719384	-7.981234	2.553390
H	-3.762696	-7.712215	2.718403
H	-2.672866	-8.999502	2.167300
H	-2.101960	-7.939732	3.450701
C	-2.169581	-7.003921	1.513959
H	-2.830186	-6.951903	0.648514
H	-1.228551	-7.432914	1.169684
N	-2.090031	-5.643754	2.068449
H	-1.391507	-5.615248	2.797387
H	-1.775065	-5.022641	1.336933
H	-3.019172	-5.319469	2.295688
N	-7.913868	4.016102	-1.749959
O	-7.222903	4.858302	-2.312401
O	-7.630267	3.557206	-0.649023
O	-8.304804	3.105062	-2.471244
C	-0.859018	-1.998319	-5.238253
H	-1.765343	-2.180451	-5.815752
H	0.030218	-2.152276	-5.849529
H	-0.886487	-2.831344	-4.535818
C	-0.755613	-0.741347	-4.373864
H	-0.845653	0.172816	-4.960634
H	0.195387	-0.734555	-3.841273
N	-1.720262	-0.694043	-3.264335

H	-2.613585	-1.131689	-3.439095
H	-1.223641	-1.254410	-2.586502
H	-1.940622	0.161547	-2.774939
N	-4.782796	-3.769640	2.268874
O	-5.216347	-2.669915	1.943737
O	-4.503463	-4.660469	1.474222
O	-3.901082	-3.693767	3.117344
C	-6.148475	3.566610	-6.168077
H	-5.123895	3.889103	-6.353368
H	-6.643555	3.178968	-7.058431
H	-6.695352	4.441409	-5.816290
C	-6.135051	2.425912	-5.150005
H	-5.342346	1.714101	-5.380313
H	-7.099961	1.955585	-4.960692
N	-5.890116	3.000496	-3.818202
H	-5.027392	3.513503	-3.705813
H	-6.689846	3.564872	-3.569178
H	-5.787115	2.189149	-3.225574
N	-0.464650	-0.432037	-0.328392
O	-1.652363	-0.130530	-0.367179
O	-0.112262	-1.039881	-1.333094
O	-0.023336	-0.625294	0.798981

Return

([EtNH₃][NO₃])₁₀ conformer -10

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	-9.596499	-0.265152	2.320083
H	-9.992950	0.747858	2.388916
H	-10.275302	-0.897347	2.892495
H	-8.604066	-0.267519	2.770829
C	-9.672572	-0.669535	0.847491
H	-10.670704	-1.012151	0.574643
H	-9.053295	-1.566193	0.871994
N	-8.935868	0.269152	-0.012727
H	-7.999764	0.539744	0.252959
H	-8.970105	-0.189191	-0.912088
H	-9.512614	1.098033	0.007776
N	-8.713050	-0.854027	-3.088190
O	-7.960831	-1.325961	-3.933483
O	-8.929379	0.350625	-3.159544
O	-8.545455	-1.343911	-1.976884
C	-6.303043	6.048991	0.486580
H	-5.667698	6.910747	0.282099
H	-6.531785	5.648196	-0.500913
H	-7.177081	6.547674	0.905475
C	-5.584340	5.126728	1.471840
H	-5.534037	5.715580	2.387713
H	-4.598390	4.814146	1.127898
N	-6.191249	3.804889	1.691489
H	-7.171071	3.578631	1.597381
H	-5.907044	3.320235	0.852180
H	-5.675281	3.293192	2.392947
N	-1.271319	-4.274298	-1.973544
O	-0.793932	-3.325568	-1.361099
O	-2.038188	-4.047710	-2.902871
O	-1.403326	-5.281792	-1.287538
C	-6.770223	-2.050441	4.169134
H	-7.160769	-1.038890	4.280217
H	-7.305835	-2.712653	3.488917
H	-6.853264	-2.660314	5.068722
C	-5.264994	-1.931753	3.928220
H	-4.855078	-2.937012	3.830628
H	-4.797801	-1.570554	4.844389
N	-5.011608	-1.196304	2.679721
H	-5.212808	-0.221208	2.849444
H	-4.038427	-1.138625	2.415732
H	-5.478862	-1.530593	1.849043
N	-1.476664	-2.888107	3.212304
O	-0.284101	-2.603836	3.204528
O	-1.945975	-3.397066	2.200481
O	-2.191191	-2.081893	3.797578
C	-0.549354	0.720625	5.416856
H	-0.674539	-0.225199	5.943968
H	0.062263	1.228323	6.162690
H	-1.471043	1.299647	5.474514
C	0.152964	0.655608	4.060256
H	1.101581	0.125587	4.145712
H	0.509046	1.660936	3.835262
N	-0.639536	0.113519	2.945839
H	-0.153793	0.223204	2.067134
H	-0.740227	-0.891426	2.952697
H	-1.575164	0.487741	2.877583
N	-3.551796	1.353184	-3.701250
O	-2.661104	1.878501	-3.042625
O	-4.732235	1.588809	-3.468611
O	-3.313648	0.397334	-4.431121
C	2.173142	-5.051257	0.509149

H	2.305834	-4.692774	-0.511626
H	2.996746	-4.679883	1.118951
H	2.227973	-6.129776	0.361192
C	0.813134	-4.765459	1.146752
H	0.874682	-4.929153	2.222631
H	0.143674	-5.472187	0.656387
N	0.415292	-3.380667	0.850246
H	-0.310954	-2.977514	1.424820
H	1.116669	-2.656088	0.794090
H	0.013002	-3.384094	-0.076172
N	-5.622653	1.150204	0.121818
O	-5.049234	2.171992	-0.239037
O	-5.884647	0.349515	-0.768874
O	-6.477067	1.224115	0.997940
C	-0.138042	3.857529	-0.355274
H	0.177539	4.785906	0.120778
H	0.722937	3.231139	-0.121927
H	-0.220042	3.992112	-1.433821
C	-1.529421	3.377176	0.058452
H	-2.347080	4.081917	-0.092789
H	-1.436225	3.197561	1.129504
N	-1.940096	2.087792	-0.518327
H	-2.238543	2.154505	-1.480917
H	-1.307475	1.331141	-0.300679
H	-2.819810	1.662825	-0.262189
N	-3.741909	2.229854	3.356950
O	-4.544906	1.341548	3.093919
O	-3.980989	3.394083	3.056140
O	-2.593241	1.811357	3.264759
C	-5.158151	-3.078332	-4.084475
H	-5.217907	-4.021095	-3.540666
H	-5.991094	-2.997257	-4.782854
H	-4.172056	-3.019348	-4.545166
C	-4.920351	-1.953717	-3.076242
H	-5.085071	-0.964489	-3.503318
H	-3.963525	-1.937557	-2.554397
N	-5.964364	-1.994595	-2.040768
H	-6.900802	-2.091850	-2.406451
H	-5.821961	-2.664929	-1.298828
H	-5.985820	-1.192994	-1.426704
N	-3.027493	-0.879120	-0.134005
O	-3.797460	-1.832268	-0.092353
O	-2.367179	-0.563302	-1.117529
O	-2.688674	-0.251227	0.863005
C	-3.942563	-7.188454	0.502048
H	-3.981388	-7.015082	-0.573375
H	-3.626198	-8.187734	0.801134
H	-4.995693	-7.009730	0.719019
C	-3.235253	-6.009416	1.170944
H	-2.150674	-6.117868	1.176165
H	-3.525345	-5.792948	2.199092
N	-3.396825	-4.750143	0.428001
H	-3.039592	-4.698528	-0.515302
H	-4.371515	-4.495157	0.356871
H	-2.931002	-4.054284	0.992704
N	-9.522644	3.469049	0.215929
O	-10.159459	2.614850	-0.390607
O	-8.589813	4.008535	-0.368757
O	-8.950003	3.022465	1.203715
C	0.209172	-0.829871	-5.118069
H	-0.496687	-0.495533	-5.878387
H	1.109804	-0.253634	-5.329999
H	0.453919	-1.873151	-5.317483
C	-0.379971	-0.568333	-3.731581
H	-0.803218	0.434838	-3.782663
H	0.380592	-0.679789	-2.958780
N	-1.508765	-1.482481	-3.499207

H	-2.180053	-1.161999	-4.182407
H	-1.331082	-2.476066	-3.462921
H	-1.872744	-1.242191	-2.588229
N	-6.475126	-3.421867	0.617642
O	-6.021688	-3.831011	1.680690
O	-6.446160	-2.197208	0.667136
O	-5.776180	-3.878666	-0.280069
C	-6.755701	4.341688	-3.528983
H	-6.865460	5.160653	-4.239862
H	-6.798956	4.917745	-2.604653
H	-5.788858	3.890405	-3.751825
C	-7.847381	3.271346	-3.507969
H	-7.984617	2.805576	-4.483840
H	-8.869490	3.582569	-3.292252
N	-7.562599	2.348082	-2.398769
H	-8.199819	1.585747	-2.580141
H	-6.621948	1.980302	-2.395074
H	-7.757646	2.828726	-1.532145
N	1.324420	-0.451312	0.407437
O	1.509632	-0.865158	1.546517
O	1.554163	-1.206963	-0.530266
O	0.331460	0.250146	0.249121

Return

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	2.912879	-2.267734	1.420391
H	3.753549	-2.458484	2.087466
H	2.278743	-1.585480	1.986519
H	3.230956	-1.561712	0.653280
C	2.169709	-3.485275	0.869815
H	1.488528	-3.928023	1.596497
H	2.915317	-4.204642	0.531172
N	1.373308	-3.095566	-0.303945
H	0.882854	-3.910968	-0.642581
H	0.659725	-2.443111	-0.012049
H	1.988838	-2.847413	-1.065288
N	-4.929258	-1.225914	2.589065
O	-5.449129	-2.315520	2.375599
O	-3.721570	-1.034417	2.677914
O	-5.674208	-0.256240	2.500425
C	-2.501315	-5.733029	1.152376
H	-3.425376	-5.643448	0.581247
H	-2.003422	-6.511499	0.574286
H	-2.668153	-5.994867	2.197223
C	-1.741814	-4.420584	0.956196
H	-1.445036	-4.301717	-0.085866
H	-0.794372	-4.345419	1.489866
N	-2.702389	-3.385199	1.367433
H	-3.095855	-3.569891	2.279119
H	-2.155720	-2.563502	1.582061
H	-3.443999	-3.078884	0.754012
N	-1.328731	-1.547146	-2.125784
O	-1.179730	-2.551195	-1.438209
O	-1.884070	-1.786325	-3.192306
O	-0.290611	-0.959603	-2.408936
C	-7.797037	-3.712265	-0.406556
H	-6.736714	-3.957298	-0.467973
H	-8.274426	-4.115211	0.486661
H	-8.217436	-4.183985	-1.294725
C	-7.787463	-2.200250	-0.633624
H	-8.784517	-1.839153	-0.885798
H	-7.204420	-1.891534	-1.501296
N	-7.271657	-1.592383	0.602614
H	-6.326042	-1.919277	0.740640
H	-7.184692	-0.588246	0.537449
H	-7.864020	-1.892405	1.363661
N	-8.975311	-1.160723	3.109834
O	-8.525743	-1.411733	4.222470
O	-9.098740	-2.093286	2.323597
O	-8.491456	-0.105295	2.716093
C	-3.260506	-4.006929	9.039041
H	-2.638300	-4.466332	9.807097
H	-4.264141	-4.060499	9.460880
H	-3.171388	-4.482918	8.062520
C	-2.909189	-2.536214	8.812289
H	-2.022303	-2.463350	8.182827
H	-2.837605	-2.033853	9.776970
N	-3.876896	-1.731344	8.050996
H	-3.991674	-1.855158	7.055206
H	-4.793296	-1.741705	8.475502
H	-3.567211	-0.784210	8.215715
N	-7.323234	-1.985933	9.178548
O	-7.978880	-0.979458	9.423928
O	-7.534842	-2.331888	8.021563
O	-6.127730	-1.875682	9.426921
C	4.450321	3.138477	-10.527828

H	3.522618	3.701826	-10.427309
H	5.116946	3.788940	-11.094051
H	4.432481	2.095356	-10.843551
C	4.922236	3.195843	-9.074609
H	4.728816	4.195995	-8.686814
H	5.990266	3.002736	-8.973998
N	4.142586	2.427439	-8.091990
H	4.489693	2.650774	-7.170177
H	3.174053	2.666999	-8.249009
H	4.180690	1.439242	-8.297207
N	4.098525	3.401197	-4.910128
O	3.408404	2.851566	-4.058827
O	3.493478	3.896763	-5.854273
O	5.021175	2.657897	-5.225243
C	-6.562750	-5.505011	5.355766
H	-7.191473	-6.394280	5.310941
H	-5.918036	-5.630479	4.485880
H	-5.911649	-5.565670	6.227826
C	-7.382293	-4.218675	5.248390
H	-7.733068	-4.010085	6.259106
H	-8.255386	-4.350230	4.609249
N	-6.579532	-3.074498	4.789834
H	-7.286568	-2.362581	4.674190
H	-5.850882	-2.758572	5.413821
H	-6.158623	-3.181018	3.877918
N	0.421454	-6.068027	-1.579569
O	0.826873	-5.891572	-0.436076
O	-0.777366	-6.301481	-1.686365
O	0.885076	-5.230301	-2.345301
C	-8.877731	3.480754	3.641236
H	-8.610343	3.991731	2.716299
H	-9.634496	2.742427	3.376131
H	-9.350819	4.221235	4.286197
C	-7.690704	2.756484	4.277035
H	-7.827730	2.179725	5.191733
H	-6.888572	3.440540	4.554073
N	-7.103847	1.825815	3.300668
H	-7.845987	1.162045	3.131145
H	-7.110060	2.194731	2.360475
H	-6.241257	1.336474	3.491939
N	-2.750952	1.311326	9.374105
O	-3.302174	0.455252	10.057015
O	-3.369136	2.366681	9.289556
O	-2.637147	0.843045	8.246791
C	3.581354	-4.167111	-6.697450
H	4.386658	-4.671992	-7.231006
H	2.699230	-4.773966	-6.901616
H	3.454437	-3.229721	-7.239014
C	3.738405	-3.994774	-5.186332
H	4.738897	-3.599216	-5.011262
H	3.774110	-5.018195	-4.812923
N	2.672262	-3.189530	-4.570896
H	2.769058	-3.055921	-3.574462
H	2.762384	-2.245162	-4.917519
H	1.772975	-3.534408	-4.874940
N	3.972618	-1.784680	-2.201901
O	3.574790	-0.648927	-2.436157
O	3.184921	-2.721742	-2.134636
O	5.062282	-2.024060	-2.710235
C	-2.525065	3.591397	0.463095
H	-2.385209	4.069418	1.432649
H	-1.711257	3.809555	-0.228442
H	-3.529828	3.656914	0.045649
C	-2.143555	2.150112	0.802198
H	-1.206876	2.206367	1.356785
H	-1.998879	1.525024	-0.078957
N	-3.158596	1.403450	1.561163

H	-2.956276	0.416303	1.629776
H	-3.173808	1.779663	2.498357
H	-4.060721	1.586621	1.145568
N	-0.450025	-0.890086	1.369947
O	-0.243770	-2.046628	1.720580
O	-1.222966	-0.252452	2.076390
O	0.553989	-0.356869	0.910914
C	-4.770865	6.461363	6.912994
H	-4.229401	6.380756	5.970433
H	-5.738320	6.134931	6.531454
H	-4.803035	7.485850	7.283794
C	-4.154183	5.555375	7.979169
H	-4.681616	5.805386	8.899717
H	-3.090818	5.733910	8.138798
N	-4.376878	4.140336	7.644632
H	-4.149275	3.900217	6.690358
H	-3.736206	3.448278	8.006151
H	-5.363073	3.927989	7.595355
N	-6.592922	1.732040	-0.130900
O	-5.373816	1.613079	-0.078882
O	-7.169135	0.903847	-0.827427
O	-7.180590	2.615114	0.483838
C	-10.778674	0.063632	7.765541
H	-11.839084	0.161754	7.533156
H	-10.773352	-0.598361	8.631473
H	-10.496160	1.085067	8.020407
C	-9.901073	-0.060372	6.519636
H	-10.079196	0.724770	5.784842
H	-10.056017	-1.051682	6.093730
N	-8.499393	0.018665	6.958825
H	-8.339525	-0.665831	7.684087
H	-7.874307	-0.239899	6.208816
H	-8.297697	0.916357	7.375440
N	-1.494253	2.540986	-3.631853
O	-0.271045	2.582693	-3.560455
O	-1.883485	2.487746	-4.793206
O	-1.996736	1.707328	-2.886467
C	-6.207083	2.493912	11.520037
H	-6.928704	2.702746	12.309816
H	-5.237553	2.840460	11.877829
H	-6.624172	3.043004	10.675859
C	-6.368884	1.032515	11.100534
H	-7.415100	0.729307	11.060583
H	-5.711933	0.424999	11.722980
N	-5.843822	0.898199	9.733014
H	-6.271274	0.003878	9.539179
H	-6.357932	1.584702	9.199625
H	-4.841347	0.961783	9.627646
N	-5.355665	0.241905	5.845515
O	-5.506547	0.727541	6.961072
O	-4.351621	-0.441484	5.678324
O	-6.400464	-0.309465	5.517704
C	2.097000	-0.889742	-10.901518
H	1.712870	-1.413717	-11.776730
H	1.915679	0.182189	-10.980176
H	3.168342	-1.047751	-10.777591
C	1.328670	-1.255400	-9.631161
H	1.244883	-2.338880	-9.546600
H	0.375887	-0.742470	-9.762332
N	2.088129	-0.763661	-8.471310
H	2.132025	0.245374	-8.475810
H	1.763804	-1.251081	-7.648306
H	3.068784	-1.003972	-8.497110
N	-8.067169	3.153930	7.846561
O	-7.115927	3.720289	7.319824
O	-7.792430	2.237208	8.612862
O	-8.923355	2.872037	7.015563

C	-6.216708	1.637390	-3.866272
H	-6.998548	1.534023	-4.618697
H	-5.487512	2.332584	-4.282298
H	-6.663736	2.217421	-3.058912
C	-5.640363	0.265436	-3.514973
H	-5.352639	-0.335121	-4.377901
H	-6.522276	-0.234404	-3.114364
N	-4.540232	0.366428	-2.543709
H	-4.856671	0.737338	-1.659180
H	-4.251864	-0.598730	-2.470130
H	-3.747115	0.919508	-2.835546
N	-4.157104	-2.464578	-1.584019
O	-4.141758	-1.671850	-0.648913
O	-4.797312	-2.242723	-2.605777
O	-3.964990	-3.652875	-1.351383
C	2.506373	3.123405	-1.028991
H	2.036819	3.908295	-1.621922
H	2.466274	3.610042	-0.054477
H	3.556559	3.056839	-1.313209
C	1.619245	1.881741	-0.933527
H	0.618491	2.259324	-0.723705
H	1.932919	1.163070	-0.176415
N	1.528892	1.177951	-2.222076
H	1.394451	1.756723	-3.038805
H	2.368688	0.640803	-2.384292
H	0.747788	0.551494	-2.089682
N	-0.084216	-3.523278	-6.497523
O	0.701000	-2.805838	-7.107271
O	-1.228042	-3.082473	-6.518255
O	0.273434	-3.947485	-5.404267
C	0.536929	5.493689	-4.686394
H	0.171347	5.023524	-3.773490
H	0.207221	6.526833	-4.795967
H	1.593265	5.627886	-4.453483
C	0.228085	4.647382	-5.921797
H	0.702246	5.209265	-6.726508
H	-0.854056	4.528926	-5.976915
N	0.873441	3.325922	-5.888586
H	0.755875	2.847813	-6.770453
H	1.871759	3.411822	-5.761768
H	0.506748	2.678924	-5.205190
N	0.997228	2.671377	-9.033410
O	1.415631	3.763060	-8.664296
O	-0.004033	2.335259	-8.410854
O	1.792329	1.772190	-9.283116
C	0.554331	-1.048923	5.205199
H	0.704647	-0.646235	4.203527
H	0.630537	-2.135464	5.163710
H	1.438623	-0.775500	5.780845
C	-0.788837	-0.458700	5.635754
H	-0.731265	0.629652	5.652341
H	-0.733539	-0.839268	6.655660
N	-1.862565	-0.962319	4.765514
H	-1.784614	-0.617247	3.819497
H	-1.882734	-1.969132	4.843119
H	-2.757174	-0.591618	5.052490
N	5.638253	-0.600756	-7.775893
O	5.641389	-1.378190	-6.827914
O	4.764391	-0.569122	-8.635218
O	6.055815	0.515676	-7.489018
C	7.254467	0.542620	-2.799615
H	8.268263	0.837555	-2.528817
H	6.764976	1.513472	-2.722509
H	6.718037	-0.214397	-2.227541
C	7.178242	0.194050	-4.286400
H	7.511207	-0.843576	-4.310168
H	7.777832	0.914254	-4.843084

N	5.752398	0.274813	-4.638943
H	5.174834	-0.370891	-4.119726
H	5.201782	1.120063	-4.688678
H	5.560603	-0.023722	-5.584560
N	-3.403545	2.406773	4.831176
O	-2.391731	2.017298	4.258797
O	-3.314747	3.518135	5.341142
O	-4.448020	2.254661	4.207469
C	-3.731480	-4.505591	-4.784296
H	-3.335080	-4.206742	-5.754686
H	-3.881151	-3.540756	-4.299741
H	-4.703809	-4.967486	-4.955556
C	-2.725279	-5.391613	-4.049200
H	-2.298987	-6.201187	-4.641624
H	-3.262042	-5.896863	-3.246263
N	-1.495825	-4.668001	-3.690497
H	-1.710621	-3.793648	-3.232818
H	-0.831044	-4.963282	-2.989801
H	-1.000021	-4.402259	-4.529342
N	-2.983477	-3.934258	5.046481
O	-1.830809	-3.589618	4.810566
O	-3.677347	-4.336497	4.119214
O	-3.538372	-3.172923	5.831043
C	-2.610873	-0.212247	-7.578928
H	-1.819720	0.527283	-7.702503
H	-3.462541	0.255366	-8.072994
H	-2.315912	-1.174744	-7.996898
C	-2.572334	-0.313112	-6.053745
H	-3.359962	-1.016030	-5.782364
H	-2.961045	0.634057	-5.679750
N	-1.250412	-0.639809	-5.497299
H	-0.777159	-1.349577	-6.038002
H	-0.766277	0.226948	-5.311703
H	-1.372871	-0.939039	-4.540447
N	2.251110	0.349787	-5.518615
O	2.590604	-0.810653	-5.721589
O	2.516259	1.105121	-6.447185
O	1.124010	0.527451	-5.070108

Return

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	-0.701381	-4.517037	1.613790
H	-0.179626	-5.356387	2.073532
H	-1.027636	-4.703597	0.590632
H	-1.623809	-4.333944	2.164883
C	0.161085	-3.287919	1.902343
H	1.106365	-3.304753	1.359885
H	0.236429	-2.990553	2.948287
N	-0.363621	-2.127022	1.166923
H	-0.680739	-2.320297	0.227678
H	-1.214122	-1.997437	1.696031
H	0.183679	-1.278377	1.185969
N	-3.895404	-1.632167	0.973037
O	-4.447714	-1.848360	-0.099945
O	-3.152721	-2.527766	1.359562
O	-4.697601	-1.288761	1.834215
C	-5.243424	-6.296157	0.339391
H	-5.341219	-6.530711	1.399354
H	-6.267083	-6.345525	-0.031804
H	-4.623723	-7.122383	-0.009063
C	-4.578389	-4.934850	0.545340
H	-3.665097	-4.952133	1.140066
H	-5.204890	-4.196136	1.045238
N	-3.944141	-4.471423	-0.698366
H	-3.597390	-3.527011	-0.609199
H	-3.224574	-5.117045	-0.990761
H	-4.601364	-4.476224	-1.465266
N	-1.766327	-1.500713	-1.882957
O	-2.571433	-1.646327	-2.796015
O	-1.591056	-2.493633	-1.185485
O	-0.760856	-0.926772	-2.286313
C	-9.527147	-2.359794	0.606331
H	-9.393810	-1.320039	0.307616
H	-10.510599	-2.756647	0.354475
H	-9.652492	-2.272481	1.685574
C	-8.255156	-3.059293	0.126143
H	-8.185052	-3.086128	-0.961270
H	-8.219993	-4.103922	0.435357
N	-7.085127	-2.225740	0.442468
H	-6.881625	-2.309561	1.428196
H	-6.186033	-2.568503	0.135476
H	-7.261261	-1.284280	0.121953
N	-7.143408	-3.229985	3.618379
O	-6.394645	-3.793192	2.827666
O	-6.940142	-3.290621	4.825890
O	-7.519431	-2.155204	3.163925
C	0.696791	-1.245114	8.040379
H	1.063632	-0.220217	7.984576
H	1.518481	-1.652575	8.629362
H	0.742975	-1.615676	7.016342
C	-0.638557	-1.566048	8.712457
H	-0.687890	-1.152924	9.719927
H	-0.825623	-2.631846	8.843534
N	-1.723237	-0.971529	7.916306
H	-2.637079	-1.263359	8.232261
H	-1.793450	0.030794	8.018859
H	-1.650567	-1.230329	6.942734
N	-4.292355	-2.465465	9.000016
O	-3.956993	-2.906219	7.906241
O	-3.561523	-1.770180	9.696822
O	-5.461933	-2.098706	9.025523
C	6.513164	3.179560	-7.308809

H	6.667752	3.514934	-6.283272
H	7.294343	3.492322	-8.001658
H	5.638380	3.707880	-7.687929
C	6.241778	1.676639	-7.382434
H	7.049277	0.994255	-7.117111
H	6.072690	1.563269	-8.453254
N	4.920674	1.242680	-6.902635
H	4.240348	1.727301	-7.470437
H	4.702276	0.256579	-6.900164
H	4.708966	1.488407	-5.946131
N	4.536908	3.059540	-3.822313
O	4.205064	3.934380	-4.614531
O	5.276321	2.216170	-4.317360
O	3.598445	2.624438	-3.164249
C	-3.346023	-5.450453	4.558425
H	-2.365918	-5.541602	4.090253
H	-3.456249	-6.203413	5.338811
H	-4.119957	-5.593335	3.804296
C	-3.702131	-4.113804	5.209883
H	-3.011167	-3.800864	5.992658
H	-4.678498	-4.236166	5.678748
N	-3.890613	-3.097572	4.163179
H	-3.057421	-2.878957	3.635829
H	-4.612707	-3.387553	3.519292
H	-4.409311	-2.327522	4.560767
N	-1.061187	-6.045525	-1.938710
O	-1.328536	-5.272163	-2.851679
O	0.054675	-5.800869	-1.493657
O	-1.922181	-6.384798	-1.134559
C	-8.015516	2.239748	3.072371
H	-7.276861	3.007604	2.842407
H	-8.675191	2.139467	2.210471
H	-8.635834	2.598616	3.893663
C	-7.254317	1.044134	3.645890
H	-7.995768	0.291251	3.913316
H	-6.752386	1.138398	4.608843
N	-6.180563	0.594669	2.746514
H	-6.424309	0.507035	1.770293
H	-5.403045	1.237965	2.788178
H	-5.742658	-0.278477	3.003333
N	-2.348741	2.439959	9.102689
O	-3.400237	2.892944	9.541134
O	-2.037555	2.805519	7.974591
O	-2.369489	1.217425	9.192442
C	2.209978	-4.871608	-3.515516
H	2.481950	-5.341599	-2.570402
H	1.556444	-5.633345	-3.940663
H	3.118895	-4.942901	-4.112916
C	1.835869	-3.399781	-3.337724
H	1.544987	-2.885265	-4.253563
H	2.808605	-2.982727	-3.077049
N	0.820637	-3.478909	-2.276176
H	0.346496	-4.370650	-2.285587
H	1.294988	-3.171924	-1.439007
H	0.131611	-2.763704	-2.460089
N	2.370361	-0.941674	-0.412156
O	2.697073	-0.302300	-1.405905
O	1.615231	-0.397910	0.386076
O	2.250806	-2.155460	-0.536681
C	-6.346093	5.130524	-0.899790
H	-5.967956	5.965999	-0.310643
H	-7.108548	5.558618	-1.550558
H	-6.939290	4.523758	-0.215646
C	-5.266715	4.348325	-1.648753
H	-4.775729	5.074735	-2.296333
H	-5.680700	3.547572	-2.261543
N	-4.403801	3.619100	-0.706706

H	-3.595701	3.220361	-1.162866
H	-4.098479	4.114971	0.118515
H	-4.932735	2.837350	-0.347269
N	-2.209266	1.479110	0.188586
O	-1.757975	0.566989	0.872289
O	-1.702674	2.595470	0.201990
O	-2.755163	1.241820	-0.883218
C	-4.797670	5.549275	7.903295
H	-5.330007	6.500167	7.880432
H	-5.431421	4.797405	8.373562
H	-3.883862	5.657723	8.487499
C	-4.484489	4.974397	6.521530
H	-3.588430	5.495592	6.184585
H	-5.359352	5.264595	5.939723
N	-4.204951	3.531483	6.582355
H	-4.051960	3.076672	5.693625
H	-3.403368	3.232606	7.119232
H	-5.010805	3.120007	7.031114
N	-6.995116	0.764597	-0.678692
O	-7.647185	0.562176	0.339594
O	-5.876105	1.255957	-0.581443
O	-7.245885	-0.004952	-1.599553
C	-8.686027	-3.386226	7.500925
H	-8.016092	-3.876552	8.207230
H	-9.679519	-3.655550	7.859446
H	-8.429877	-3.916047	6.583440
C	-8.476510	-1.877761	7.364985
H	-8.652318	-1.299499	8.272070
H	-9.089029	-1.293005	6.678706
N	-7.108004	-1.520224	6.961005
H	-6.351788	-1.879273	7.526090
H	-6.896659	-1.917962	6.056993
H	-6.890722	-0.540876	6.843677
N	-2.322620	2.845299	-3.545907
O	-1.151115	3.142785	-3.751224
O	-2.748415	1.715757	-3.760168
O	-3.204849	3.682711	-3.699175
C	-5.149381	1.725256	12.332712
H	-5.554244	1.558796	13.330949
H	-4.389617	2.505543	12.377551
H	-5.944494	2.239254	11.792618
C	-4.831465	0.398731	11.641986
H	-5.659873	-0.266306	11.886049
H	-3.942564	-0.132859	11.981643
N	-4.911857	0.445599	10.173933
H	-4.547362	-0.382818	9.725638
H	-5.802868	0.495807	9.700987
H	-4.361078	1.126192	9.670410
N	-4.327873	-0.038210	5.860078
O	-5.052471	-0.879233	5.339776
O	-4.161611	1.016776	5.258050
O	-4.248364	-0.010693	7.083187
C	2.805084	-3.548019	-8.345744
H	2.782539	-4.202539	-9.217062
H	3.879841	-3.593168	-8.169795
H	2.193903	-3.971816	-7.548903
C	2.523728	-2.077771	-8.657277
H	1.632163	-1.955755	-9.272356
H	3.403372	-1.664477	-9.150748
N	2.320021	-1.337087	-7.402793
H	2.289348	-0.340247	-7.562382
H	1.447350	-1.437191	-6.904271
H	3.135417	-1.393606	-6.809466
N	-7.327725	1.559313	7.825893
O	-7.104276	0.993514	8.890325
O	-7.984661	1.000523	6.954534
O	-6.309351	2.101317	7.410897

C	-6.074313	1.501562	-4.297539
H	-5.327655	2.232349	-4.608265
H	-6.639058	1.854948	-3.434821
H	-6.816152	1.437460	-5.093570
C	-5.510081	0.101275	-4.055297
H	-5.143146	-0.312325	-4.994654
H	-6.306664	-0.637792	-3.969649
N	-4.582871	0.038798	-2.915025
H	-4.989270	0.245763	-2.013856
H	-4.330001	-0.938984	-2.905071
H	-3.764724	0.602791	-3.095707
N	-5.864218	-3.824138	-3.031527
O	-5.350984	-2.966540	-3.741593
O	-5.452682	-4.975247	-3.124605
O	-6.020696	-3.639802	-1.829608
C	0.865501	3.817734	-1.150055
H	-0.172727	4.066769	-0.930593
H	1.521566	4.567441	-0.707767
H	1.056234	3.905853	-2.219613
C	1.214103	2.393657	-0.716091
H	1.065983	2.139340	0.333425
H	2.301161	2.337238	-0.659330
N	0.452054	1.481194	-1.582423
H	0.738952	1.686773	-2.528746
H	0.724696	0.535360	-1.356232
H	-0.549556	1.570006	-1.677245
N	-1.099444	-2.639932	-6.903554
O	-2.023346	-2.323848	-6.162221
O	-0.358215	-1.825831	-7.442901
O	-0.667055	-3.782169	-6.796736
C	1.052407	6.003205	-6.677727
H	2.108955	6.256701	-6.764593
H	0.509939	6.890517	-6.351373
H	0.698393	5.638104	-7.641820
C	0.915437	4.955118	-5.572922
H	-0.058173	4.473098	-5.484376
H	1.027785	5.354249	-4.564869
N	1.751262	3.745140	-5.607449
H	2.076871	3.380816	-6.491387
H	2.622517	4.012902	-5.172341
H	1.527435	2.903618	-5.095743
N	2.333456	1.864099	-8.536961
O	1.486407	1.233675	-7.913945
O	3.093802	0.995721	-8.950325
O	2.883414	2.796587	-7.961559
C	-0.720830	2.901226	4.903497
H	0.145270	2.316170	5.212818
H	-1.440053	2.529080	5.633103
H	-0.291431	3.893791	5.039633
C	-0.988520	2.487079	3.456201
H	-0.176307	2.150258	2.812026
H	-1.477995	3.315628	2.944324
N	-1.980815	1.402253	3.504621
H	-2.857646	1.836479	3.755050
H	-2.020152	0.954729	2.600036
H	-1.837652	0.664822	4.179751
N	5.287934	-1.767646	-5.445710
O	6.226414	-1.114141	-5.003827
O	4.946027	-1.480024	-6.587397
O	4.368641	-1.857749	-4.639572
C	6.290612	1.263979	-1.432904
H	5.423218	1.227766	-0.773801
H	7.107432	1.123499	-0.724969
H	6.115484	2.249990	-1.863267
C	6.143954	0.117619	-2.433999
H	6.378133	-0.844325	-1.978011
H	6.909997	0.403424	-3.154827

N	4.802773	-0.023708	-3.021453
H	4.092968	-0.211016	-2.327773
H	4.584835	0.827762	-3.519049
H	4.693972	-0.725346	-3.739760
N	-4.195377	3.589885	2.460282
O	-4.147537	3.626507	3.684801
O	-4.598723	4.542427	1.802215
O	-4.193867	2.451161	2.005990
C	-3.385736	-6.024182	-6.846829
H	-3.784815	-7.003361	-7.111486
H	-2.297118	-5.987473	-6.806041
H	-3.616460	-5.342935	-7.665834
C	-3.906443	-5.545109	-5.491397
H	-3.921684	-6.329907	-4.735118
H	-4.903197	-5.143124	-5.673028
N	-3.150728	-4.419594	-4.920475
H	-3.821073	-3.895393	-4.376460
H	-2.321195	-4.693140	-4.413379
H	-2.821893	-3.773015	-5.623258
N	-1.315754	-1.454716	4.765439
O	-1.260849	-2.444803	5.486404
O	-1.271841	-0.356051	5.307732
O	-1.891582	-1.414471	3.683830
C	-2.796699	1.904625	-6.839872
H	-2.834177	2.863374	-7.357073
H	-3.321517	2.273009	-5.958419
H	-3.397643	1.096056	-7.256023
C	-1.415162	1.353333	-6.485930
H	-0.761945	2.141692	-6.111902
H	-0.955597	1.001423	-7.409542
N	-1.333082	0.215823	-5.556857
H	-1.583699	-0.688026	-5.931486
H	-0.342788	0.236087	-5.359352
H	-1.867464	0.435069	-4.728323
N	1.724741	0.625676	-4.630532
O	2.647352	1.044425	-5.320833
O	1.232525	-0.445857	-4.966115
O	0.905066	1.407036	-4.160761

Return

([EtNH₃][NO₃])₂₀ conformer -3

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	2.668712	-1.712497	1.877781
H	3.288550	-1.476018	1.012923
H	3.154808	-2.302056	2.655104
H	2.073337	-0.908690	2.310822
C	1.629230	-2.737956	1.424184
H	0.883743	-2.999520	2.175139
H	2.230872	-3.632262	1.261880
N	1.026385	-2.416438	0.121476
H	0.567880	-3.256906	-0.200218
H	0.315689	-1.700731	0.068818
H	1.688925	-2.220342	-0.615198
N	-4.628835	-1.081861	1.593259
O	-4.246401	-2.018255	2.286069
O	-4.837209	-1.262156	0.398625
O	-4.848398	0.014857	2.095332
C	-2.616116	-6.065229	1.801114
H	-2.122407	-7.035166	1.741342
H	-2.299450	-5.611982	2.740470
H	-3.686690	-6.244922	1.899512
C	-2.224834	-5.189481	0.610398
H	-2.332373	-5.667505	-0.363269
H	-1.163180	-4.979589	0.740537
N	-2.824608	-3.852312	0.737246
H	-2.474409	-3.356476	-0.069977
H	-3.821068	-3.956071	0.609177
H	-2.645142	-3.414493	1.629551
N	-1.056928	-2.308534	-2.475613
O	-0.195996	-1.465946	-2.703464
O	-0.855821	-3.138147	-1.595628
O	-1.860487	-2.518936	-3.377334
C	-10.076912	-3.147285	-0.491757
H	-9.644052	-3.845580	-1.208078
H	-11.036834	-3.538940	-0.155220
H	-10.383435	-2.204833	-0.945550
C	-9.085875	-2.979114	0.660374
H	-8.619854	-3.870559	1.080195
H	-9.567359	-2.593167	1.558882
N	-7.989299	-2.031449	0.408795
H	-7.423602	-2.382373	-0.350771
H	-8.390058	-1.111451	0.294360
H	-7.337688	-1.838950	1.156088
N	-8.771300	-1.374104	3.650669
O	-7.967991	-1.017972	2.795719
O	-8.299172	-2.110732	4.509477
O	-9.985044	-1.204524	3.616849
C	-1.453853	-2.692959	9.294002
H	-1.114894	-1.798089	9.815936
H	-2.443476	-2.973502	9.654617
H	-0.892888	-3.584016	9.575848
C	-1.410926	-2.311412	7.813995
H	-1.690066	-3.152201	7.178972
H	-0.425104	-1.988721	7.479146
N	-2.461174	-1.319042	7.538275
H	-3.324020	-1.613489	7.972899
H	-2.205657	-0.455185	7.994961
H	-2.646750	-1.237776	6.548802
N	-5.561327	-2.442540	8.296611
O	-6.644902	-1.876562	8.389399
O	-4.604446	-1.963084	8.894588
O	-5.364785	-3.083714	7.270285
C	5.617429	4.365066	-7.423719

H	6.358740	3.971573	-6.728219
H	6.387495	4.841567	-8.030386
H	4.884550	5.100946	-7.092858
C	4.817106	3.270658	-8.130540
H	5.366221	2.608540	-8.799997
H	4.103053	3.670564	-8.850473
N	4.222000	2.402696	-7.102760
H	3.533048	1.772861	-7.488446
H	4.973117	1.904377	-6.647128
H	3.762766	2.989490	-6.420942
N	3.161978	4.735160	-4.384424
O	3.871486	4.496152	-3.413575
O	2.077219	5.296584	-4.278693
O	3.297941	4.015287	-5.367466
C	-5.517331	-5.347769	4.593058
H	-5.320948	-5.440721	5.661184
H	-6.232467	-6.164963	4.498859
H	-4.782756	-5.617696	3.834349
C	-6.200642	-4.015303	4.284090
H	-7.124802	-4.038721	4.861568
H	-6.420368	-3.893686	3.223416
N	-5.538996	-2.760707	4.674032
H	-6.289868	-2.111690	4.861302
H	-5.122003	-2.886227	5.585329
H	-4.946461	-2.298147	3.999465
N	1.299542	-5.691561	-1.448368
O	1.652909	-4.928240	-2.340303
O	1.116801	-5.163216	-0.357253
O	0.493955	-6.509112	-1.879316
C	-8.089986	3.631947	3.061749
H	-7.140753	4.145423	2.908781
H	-8.575018	3.507360	2.093594
H	-8.691120	4.376542	3.583589
C	-8.073366	2.261861	3.740297
H	-9.045915	1.776928	3.824488
H	-7.893590	2.458350	4.797261
N	-7.086135	1.366172	3.118238
H	-7.070385	1.382965	2.108500
H	-6.152414	1.616643	3.410692
H	-7.283626	0.391085	3.292317
N	-2.139165	1.715940	8.483862
O	-2.874905	2.636796	8.821185
O	-2.278820	1.475803	7.289748
O	-2.312471	0.694164	9.138855
C	4.618765	-4.591924	-4.023499
H	4.433744	-5.015727	-3.036455
H	4.012853	-5.195625	-4.699159
H	5.653499	-4.709591	-4.345337
C	4.164548	-3.139935	-4.176002
H	4.366504	-2.679879	-5.143298
H	4.716506	-2.606746	-3.401953
N	2.764496	-2.919545	-3.782143
H	2.654503	-3.382857	-2.891445
H	2.415049	-1.972014	-3.769086
H	2.247827	-3.440529	-4.476210
N	2.738485	-0.003913	-1.318649
O	2.779256	0.676123	-2.337944
O	2.117899	0.343154	-0.319903
O	2.931453	-1.208482	-1.440515
C	-4.752697	4.261928	-0.836398
H	-4.483507	5.009083	-1.582988
H	-5.821138	4.046215	-0.834511
H	-4.463204	4.738367	0.100245
C	-3.869477	3.040970	-1.095291
H	-2.857530	3.398862	-1.284963
H	-4.116293	2.518277	-2.019398
N	-4.055678	2.032685	-0.040525

H	-3.429572	1.263663	-0.232087
H	-3.925125	2.356236	0.907299
H	-4.994565	1.661406	-0.013274
N	-1.458988	0.277274	-0.055165
O	-1.339372	-0.831997	0.453052
O	-1.489351	1.200368	0.751093
O	-2.163589	0.311479	-1.057883
C	-3.437272	5.692067	6.807941
H	-3.582978	6.725778	7.121490
H	-2.457884	5.293923	7.073232
H	-3.567385	5.716465	5.726009
C	-4.636218	4.862654	7.268856
H	-5.657708	5.094820	6.967595
H	-4.592155	5.100763	8.331617
N	-4.490129	3.445136	6.903970
H	-5.355771	2.926670	6.859738
H	-4.234132	3.362387	5.930463
H	-3.807489	2.986943	7.490624
N	-7.485437	1.146876	-0.138754
O	-6.895985	2.020300	0.487946
O	-8.459361	0.593737	0.359830
O	-6.786142	0.433446	-0.849444
C	-10.394883	0.301189	8.582467
H	-11.453978	0.154073	8.794066
H	-9.810786	-0.064975	9.426774
H	-10.276328	1.384027	8.543641
C	-9.894225	-0.193244	7.224999
H	-10.207828	0.579225	6.522827
H	-10.096650	-1.206410	6.877698
N	-8.428124	-0.075678	7.248788
H	-8.104523	0.768697	7.698692
H	-8.088921	-0.850376	7.800950
H	-7.945253	-0.099285	6.362008
N	-2.349982	1.858473	-4.659842
O	-1.745792	1.954117	-5.722331
O	-2.696364	0.742711	-4.288128
O	-2.094642	2.661876	-3.769662
C	-4.150552	1.342695	11.992780
H	-4.417994	2.374532	11.764989
H	-4.169420	1.019929	13.033725
H	-3.098334	1.263738	11.719461
C	-5.007356	0.460651	11.084084
H	-6.020040	0.184738	11.378093
H	-4.558927	-0.532830	11.086472
N	-4.975349	0.977883	9.707390
H	-5.226934	0.220469	9.088414
H	-5.516357	1.813243	9.535392
H	-4.066843	1.312363	9.419571
N	-5.267062	0.122920	6.011269
O	-4.303675	-0.549365	5.660564
O	-6.370749	-0.085699	5.519914
O	-5.313126	0.368449	7.211548
C	2.764362	-2.494495	-10.236295
H	3.071325	-3.275050	-10.932433
H	1.788673	-2.788106	-9.849096
H	2.627158	-1.581129	-10.815121
C	3.768245	-2.338144	-9.093660
H	4.716739	-1.814724	-9.214031
H	3.931673	-3.375876	-8.802965
N	3.116528	-1.545467	-8.039730
H	3.720796	-1.300054	-7.268540
H	2.914608	-0.651001	-8.463122
H	2.255271	-1.985875	-7.749253
N	-7.338680	3.020614	8.589506
O	-7.906774	1.987007	8.924175
O	-6.529007	3.467118	9.394577
O	-7.108829	3.029565	7.385278

C	-5.658128	-2.234016	-4.471036
H	-4.786521	-2.597384	-5.015431
H	-6.352241	-1.872902	-5.229919
H	-6.166798	-3.106294	-4.060563
C	-5.362531	-1.071139	-3.523312
H	-6.288892	-0.826287	-3.003694
H	-4.970860	-0.163671	-3.982871
N	-4.444524	-1.506934	-2.459739
H	-4.764120	-2.420305	-2.170410
H	-3.444285	-1.591559	-2.571365
H	-4.632407	-0.913939	-1.664027
N	-5.562143	-4.141158	-0.852745
O	-4.499042	-3.842892	-1.385594
O	-6.364068	-3.281388	-1.200288
O	-5.571421	-4.573719	0.294374
C	0.951673	3.601780	-1.029744
H	0.074078	3.871619	-0.442281
H	1.474752	3.012993	-0.276206
H	1.518291	4.522123	-1.171219
C	0.714938	3.015236	-2.421779
H	1.631612	2.953643	-3.008308
H	-0.014896	3.545587	-3.033473
N	0.202039	1.638983	-2.339901
H	1.079572	1.162642	-2.187801
H	-0.396672	1.527097	-1.534217
H	-0.118282	1.337840	-3.249191
N	0.791932	-4.240013	-6.488644
O	1.329869	-3.412069	-7.215424
O	1.417142	-4.330756	-5.437952
O	-0.421353	-4.363721	-6.363297
C	-0.959078	4.540908	-7.695210
H	-0.180380	4.623196	-8.453470
H	-1.646059	5.381540	-7.792657
H	-1.515719	3.619991	-7.868879
C	-0.178428	4.547069	-6.380528
H	-0.915348	4.616354	-5.580373
H	0.522116	5.376653	-6.284990
N	0.621245	3.335138	-6.144757
H	0.019037	2.644515	-5.719921
H	0.957652	2.944948	-7.013481
H	1.396751	3.580055	-5.545835
N	1.607781	1.208014	-8.818858
O	2.703669	0.730437	-9.090935
O	1.488058	2.261198	-8.202786
O	0.670366	0.429068	-8.686296
C	0.020149	0.492146	4.015462
H	0.391272	0.150561	3.049187
H	0.134692	-0.366720	4.676771
H	0.683645	1.280539	4.370863
C	-1.361905	1.118934	3.828635
H	-1.328017	2.049157	3.261506
H	-1.849242	1.272355	4.791476
N	-2.262507	0.083853	3.298197
H	-2.281105	-0.792841	3.799357
H	-3.214352	0.370365	3.119304
H	-1.929378	-0.127946	2.368538
N	5.408653	0.114133	-5.314560
O	5.772853	1.282887	-5.381242
O	5.125519	-0.470256	-6.354465
O	4.857476	-0.204410	-4.266795
C	5.326810	2.600530	-0.641472
H	4.506922	1.948887	-0.339403
H	6.041568	2.692225	0.176339
H	4.984585	3.617059	-0.835512
C	6.035515	2.122437	-1.909149
H	6.526187	1.172602	-1.696652
H	6.803546	2.765427	-2.339024

N	5.094150	2.108856	-3.039409
H	4.315557	1.465825	-3.019266
H	4.753075	3.050524	-3.169901
H	5.554371	1.854999	-3.901879
N	-3.819680	3.421455	3.501654
O	-3.531414	2.786890	2.493038
O	-4.994187	3.385300	3.851369
O	-2.967891	3.460779	4.382554
C	-2.368042	-6.918500	-4.180585
H	-2.131368	-7.062440	-5.234799
H	-3.377866	-7.249372	-3.937934
H	-1.663638	-7.486128	-3.572543
C	-2.201457	-5.420713	-3.922274
H	-2.746373	-5.206801	-3.002813
H	-2.735719	-4.929952	-4.735795
N	-0.806697	-5.018025	-3.684937
H	-0.842123	-4.010403	-3.625419
H	-0.449867	-5.337098	-2.795575
H	-0.111332	-5.268717	-4.373211
N	-1.764946	-3.207636	4.221466
O	-1.678663	-2.111088	4.762959
O	-2.813694	-3.828772	4.353351
O	-1.292926	-3.248753	3.090722
C	-2.917961	-1.659881	-7.343945
H	-3.172373	-1.304115	-8.342346
H	-3.734366	-1.219272	-6.771716
H	-3.013827	-2.745082	-7.308627
C	-1.538596	-1.065173	-7.058434
H	-1.314700	-0.085691	-7.481028
H	-0.900940	-1.795516	-7.556523
N	-1.335709	-1.108726	-5.602144
H	-0.366637	-0.867296	-5.451443
H	-1.913780	-0.457097	-5.090955
H	-1.555433	-2.046589	-5.298444
N	1.560805	0.345363	-5.220016
O	0.572994	0.886635	-4.735937
O	2.585494	1.016269	-5.274538
O	1.368167	-0.717180	-5.800507

Return

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	1.501311	-2.914254	2.338406
H	2.561168	-2.686149	2.451410
H	1.320687	-3.988679	2.371367
H	1.012458	-2.497005	3.218762
C	0.849653	-2.318665	1.090024
H	1.466838	-2.510631	0.212339
H	0.825949	-1.237647	1.227632
N	-0.528457	-2.746653	0.804576
H	-0.973520	-2.231969	0.058172
H	-0.582838	-3.726796	0.566955
H	-1.053388	-2.658546	1.662938
N	-4.003243	-2.439594	0.769522
O	-5.086371	-2.626994	0.226576
O	-3.718777	-3.511730	1.291707
O	-3.082680	-2.184309	0.001102
C	-3.430393	-7.177557	1.052833
H	-2.476329	-7.509328	0.643210
H	-3.175256	-6.440253	1.814008
H	-3.838949	-8.137439	1.368759
C	-4.194664	-6.584903	-0.131435
H	-5.217339	-6.350328	0.163879
H	-4.147094	-7.223267	-1.013665
N	-3.666084	-5.277963	-0.551376
H	-4.213897	-4.893636	-1.307876
H	-3.771542	-4.639725	0.224273
H	-2.695555	-5.465853	-0.758429
N	-1.067314	-1.939492	-2.816023
O	-1.080188	-1.414323	-1.708274
O	-1.643849	-3.012433	-2.955597
O	-0.052712	-1.791415	-3.488133
C	-10.555386	-2.885244	0.653170
H	-10.592572	-3.316839	1.653391
H	-10.297788	-1.844471	0.849474
H	-11.492835	-3.068217	0.127993
C	-9.429573	-3.478501	-0.194434
H	-9.492183	-3.146135	-1.230635
H	-9.427813	-4.566216	-0.264958
N	-8.090283	-3.191442	0.341980
H	-7.866402	-2.209327	0.415665
H	-7.876553	-3.532086	1.268469
H	-7.468304	-3.520263	-0.382670
N	-8.378769	-3.001901	3.920689
O	-7.760147	-3.372376	4.912218
O	-7.998682	-3.566945	2.901211
O	-8.606965	-1.800418	3.834421
C	-0.488663	-2.577216	6.926570
H	0.575227	-2.787859	6.817633
H	-1.001129	-3.316202	7.542507
H	-1.009290	-2.547845	5.969394
C	-0.635637	-1.163569	7.490346
H	0.044192	-0.538819	6.911019
H	-0.290656	-1.165213	8.524312
N	-2.037016	-0.749260	7.322042
H	-2.673888	-1.212470	7.954443
H	-2.150453	0.214510	7.602002
H	-2.359390	-0.785735	6.365567
N	-4.807436	-2.455645	8.467832
O	-5.748801	-1.757541	8.827775
O	-3.665768	-2.153063	8.796640
O	-4.994069	-2.985925	7.378315
C	6.274417	2.082795	-9.102475

H	5.404856	1.505866	-9.417303
H	6.692626	2.677192	-9.914814
H	7.043878	1.470186	-8.632645
C	5.839093	3.205374	-8.160059
H	5.100486	3.839679	-8.650178
H	6.702314	3.740758	-7.764693
N	5.016107	2.809457	-7.006896
H	4.123273	2.557800	-7.406415
H	5.576498	2.017639	-6.725674
H	4.950085	3.565102	-6.340006
N	4.159594	5.209153	-5.546866
O	3.368919	4.449877	-4.997860
O	3.999475	5.534691	-6.717961
O	5.287701	4.846894	-5.231875
C	-4.767671	-5.649033	4.854651
H	-5.834518	-5.789690	4.680999
H	-4.202655	-6.371265	4.265382
H	-4.434190	-5.765557	5.885821
C	-4.557274	-4.267505	4.234206
H	-4.790893	-4.336698	3.171787
H	-3.492061	-4.052165	4.150240
N	-5.262471	-3.141017	4.864733
H	-5.021011	-2.385138	4.239877
H	-6.239365	-3.359177	4.999584
H	-4.925975	-2.978640	5.803085
N	-0.424526	-5.767746	-0.555322
O	-0.878333	-5.231867	0.449650
O	-1.279410	-6.122551	-1.359289
O	0.656488	-5.370374	-0.975537
C	-8.812359	2.488877	4.512573
H	-8.164798	2.249867	5.356160
H	-8.435038	3.446499	4.153840
H	-9.824513	2.646786	4.885010
C	-8.663709	1.418178	3.431210
H	-9.181907	1.911634	2.608974
H	-9.164508	0.523377	3.800847
N	-7.226722	1.194643	3.209984
H	-6.721460	1.050309	4.072525
H	-7.242087	0.513380	2.464500
H	-6.930269	2.095919	2.863693
N	-2.919628	2.512745	8.246188
O	-2.983803	2.584904	7.023997
O	-3.004660	1.382926	8.714542
O	-3.483627	3.356606	8.933850
C	3.748781	-3.883085	-1.588415
H	3.256127	-3.348377	-0.776331
H	2.936531	-4.405650	-2.093663
H	4.387908	-4.507609	-0.964247
C	4.460635	-2.850274	-2.462718
H	5.042426	-3.422307	-3.185489
H	5.215590	-2.371870	-1.838802
N	3.552209	-1.926498	-3.159312
H	3.151838	-1.318308	-2.459377
H	4.070751	-1.253873	-3.705929
H	2.810629	-2.245309	-3.766369
N	3.195193	0.441926	-0.891669
O	2.632490	-0.624853	-1.111718
O	2.476211	1.434961	-0.886766
O	4.238952	0.486126	-1.533300
C	-4.073704	4.336557	-0.980865
H	-4.270796	5.134007	-0.264396
H	-3.269975	3.655425	-0.701256
H	-3.764162	4.712435	-1.956057
C	-5.445977	3.670896	-1.088592
H	-5.269616	3.071042	-1.981437
H	-6.312074	4.330748	-1.139283
N	-5.684358	2.814420	0.083357

H	-6.639370	2.487938	0.121600
H	-5.218361	1.919812	0.032137
H	-5.376283	3.121788	0.994792
N	-3.440812	0.690468	0.873943
O	-3.904150	0.751462	-0.259491
O	-4.305594	0.967310	1.697707
O	-2.316402	1.151823	1.034974
C	-4.751177	5.773779	7.044959
H	-4.868967	6.779530	7.448309
H	-3.702113	5.512089	7.183108
H	-4.858744	6.063285	5.999629
C	-5.804152	4.751824	7.474717
H	-6.778295	5.172158	7.224790
H	-5.630666	4.433948	8.502801
N	-5.636130	3.462753	6.786309
H	-6.356578	2.891010	7.203640
H	-5.793227	3.636726	5.803887
H	-4.736223	3.012585	6.873578
N	-7.596797	0.111032	0.224161
O	-7.843538	1.243746	0.623101
O	-7.672216	-0.793402	1.048411
O	-6.959068	-0.103308	-0.800747
C	-8.475814	-4.011047	7.900583
H	-7.487462	-4.118942	8.347370
H	-9.177021	-4.586624	8.504835
H	-8.783587	-4.556155	7.008265
C	-8.948821	-2.557064	7.894299
H	-9.006192	-2.203430	8.923741
H	-9.980151	-2.434718	7.563406
N	-7.973472	-1.660542	7.254936
H	-7.058008	-1.666786	7.681535
H	-7.931241	-1.924796	6.281034
H	-8.226985	-0.682888	7.259790
N	-2.035852	1.551712	-4.637344
O	-1.337592	2.272375	-5.341725
O	-1.611392	0.422959	-4.416377
O	-2.507969	2.079934	-3.636763
C	-5.226926	1.803625	11.821976
H	-6.092417	2.428683	11.602140
H	-5.176525	1.719697	12.907571
H	-4.298712	2.344008	11.636220
C	-5.382610	0.465389	11.098976
H	-6.138879	-0.140467	11.598071
H	-4.463702	-0.117533	11.036458
N	-5.557840	0.746472	9.665754
H	-5.524890	-0.074291	9.078079
H	-6.407263	1.187918	9.343718
H	-4.775959	1.261721	9.287230
N	-5.312704	0.151144	5.793122
O	-5.700164	0.381747	6.933198
O	-4.911976	1.149444	5.204999
O	-5.950872	-0.531063	4.999138
C	4.690358	-2.759683	-9.099826
H	5.387684	-2.885238	-9.928121
H	4.518802	-3.783392	-8.767126
H	3.838539	-2.254252	-9.554846
C	5.297747	-1.849902	-8.031548
H	5.686705	-0.896151	-8.388158
H	6.048815	-2.353965	-7.423341
N	4.415321	-1.405366	-6.941799
H	4.955365	-0.911226	-6.245897
H	3.629864	-0.922485	-7.354090
H	4.024254	-2.232319	-6.513646
N	-8.267792	1.221995	8.469123
O	-8.272002	0.435919	9.409944
O	-8.722769	0.830031	7.400275
O	-7.368930	2.055123	8.501036

C	-5.031510	-0.631042	-4.437207
H	-4.872709	-1.637068	-4.825528
H	-4.670413	0.106749	-5.153708
H	-6.109015	-0.746561	-4.554417
C	-4.636089	-0.336201	-2.989950
H	-5.266861	0.450007	-2.575097
H	-3.599779	-0.000568	-3.028830
N	-4.704628	-1.502112	-2.095637
H	-5.512978	-2.107498	-2.108940
H	-3.913772	-2.094168	-2.305672
H	-4.508103	-1.204267	-1.150774
N	-6.496659	-4.380685	-2.470954
O	-7.005233	-5.005603	-1.546884
O	-6.843991	-3.205775	-2.515925
O	-5.303802	-4.635800	-2.593771
C	-0.107555	3.427762	-1.827090
H	0.979074	3.409466	-1.743402
H	-0.332881	3.775971	-2.835098
H	-0.500451	4.227728	-1.199566
C	-0.639603	2.082619	-1.331754
H	-1.703297	1.845241	-1.349235
H	-0.396610	2.004790	-0.272038
N	0.037374	0.967885	-2.012128
H	-0.188417	1.173750	-2.974800
H	1.044543	0.957410	-1.937306
H	-0.402574	0.063330	-1.920876
N	2.640035	-3.811433	-5.734880
O	2.226648	-3.333965	-6.785694
O	1.966527	-3.634398	-4.725860
O	3.827275	-3.578430	-5.536769
C	-0.066435	4.708408	-8.204636
H	-0.009473	3.863439	-8.890846
H	0.105933	5.668516	-8.691034
H	-0.944750	4.731482	-7.559554
C	1.126799	4.509489	-7.269507
H	1.315065	5.458866	-6.768171
H	1.987251	4.163928	-7.842489
N	0.980670	3.424945	-6.286526
H	1.001879	2.543980	-6.780036
H	1.728714	3.302094	-5.619114
H	0.070283	3.455837	-5.850247
N	2.025174	1.013140	-8.533684
O	2.468964	-0.047628	-8.108361
O	2.892078	1.867816	-8.678884
O	0.998156	1.436859	-8.015252
C	-0.732922	3.137739	4.253388
H	-0.372737	2.317416	3.632553
H	-0.839019	2.754413	5.268230
H	-0.084875	4.006349	4.136543
C	-2.140348	3.471185	3.757599
H	-2.090830	3.837345	2.732136
H	-2.640511	4.180516	4.416983
N	-3.002524	2.279691	3.728683
H	-2.612846	1.529866	3.175498
H	-3.264543	1.779708	4.566217
H	-3.895337	2.511820	3.317462
N	6.138178	0.609098	-4.892923
O	6.265522	0.592849	-6.112184
O	5.593382	-0.384561	-4.425039
O	6.116595	1.639679	-4.229211
C	5.528144	3.446150	-0.923025
H	6.400792	2.992084	-1.392504
H	5.873405	4.313295	-0.360037
H	5.058794	2.671758	-0.316290
C	4.483565	3.895153	-1.945322
H	4.745740	4.780504	-2.524560
H	3.592057	4.131825	-1.364548

N	4.150520	2.804173	-2.874130
H	3.979671	1.933850	-2.390965
H	3.461092	3.246448	-3.465046
H	4.977697	2.543803	-3.391900
N	-5.997940	4.223219	2.978994
O	-4.865755	3.914264	2.624336
O	-5.982657	4.232805	4.204861
O	-6.935938	3.676570	2.409424
C	-1.026658	-7.091119	-4.253748
H	-1.084366	-7.781628	-5.095156
H	-2.019099	-6.991883	-3.814074
H	-0.395398	-7.527340	-3.479589
C	-0.430736	-5.736549	-4.638270
H	-1.117243	-5.096504	-5.192481
H	0.350594	-5.894522	-5.381686
N	-0.018387	-4.968080	-3.453674
H	0.342741	-5.450900	-2.643384
H	0.544830	-4.244435	-3.877024
H	-0.802256	-4.413871	-3.139826
N	-2.073843	-1.220395	3.958672
O	-1.444618	-0.218601	4.280481
O	-2.889438	-1.664214	4.759238
O	-1.482414	-1.963771	3.183637
C	-1.806355	-1.065710	-7.651592
H	-2.196408	-1.896779	-8.239201
H	-1.629179	-0.242201	-8.343360
H	-2.526426	-0.737745	-6.901901
C	-0.466066	-1.466117	-7.034225
H	0.295877	-1.796524	-7.740180
H	-0.690180	-2.277568	-6.341825
N	0.130139	-0.478283	-6.121776
H	-0.396847	-0.067871	-5.364182
H	1.012766	-0.608519	-5.648375
H	0.340750	0.285548	-6.748119
N	2.713970	0.876396	-4.766507
O	1.891013	1.296063	-3.960470
O	2.392922	-0.265308	-5.077178
O	2.989952	1.617501	-5.703349

Return

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	0.094349	0.606625	2.397600
H	0.464861	0.515207	3.418611
H	-0.584440	1.437733	2.206273
H	0.963519	0.842177	1.783468
C	-0.335135	-0.704895	1.739344
H	-1.201763	-1.170953	2.208220
H	0.446431	-1.461032	1.813582
N	-0.624747	-0.524358	0.308480
H	-0.849611	-1.462951	0.010856
H	-1.391652	0.116655	0.163367
H	0.144323	-0.301495	-0.307120
N	-4.951098	-0.859249	1.683156
O	-4.492648	-1.429504	0.699434
O	-4.413148	-1.053510	2.767567
O	-6.155627	-0.648698	1.594529
C	-5.908670	-6.263026	0.478560
H	-5.862079	-7.312969	0.189514
H	-6.401062	-5.988558	1.411468
H	-6.583239	-5.797552	-0.240043
C	-4.598680	-5.489366	0.326181
H	-4.171606	-5.501786	-0.676592
H	-3.775680	-6.012066	0.813579
N	-4.610572	-4.046518	0.612345
H	-5.144981	-3.718263	-0.179333
H	-5.224709	-3.817549	1.380791
H	-3.686767	-3.639240	0.640766
N	-1.171874	-0.579933	-3.499089
O	-0.362820	-0.888175	-4.367129
O	-0.780456	0.246219	-2.682180
O	-2.072169	-1.369883	-3.237315
C	-9.714359	-3.602975	0.275063
H	-9.316083	-3.837936	1.262114
H	-10.738260	-3.909738	0.061469
H	-9.304576	-4.337174	-0.418573
C	-9.480776	-2.101055	0.109184
H	-9.905712	-1.439506	0.864090
H	-9.898695	-1.799109	-0.851165
N	-8.049092	-1.768323	0.050777
H	-7.671505	-2.427422	-0.614893
H	-7.840008	-0.832721	-0.267082
H	-7.460482	-1.899117	0.861043
N	-6.136469	-3.351717	3.296231
O	-6.691025	-3.289753	4.387883
O	-5.205915	-4.149916	3.301237
O	-6.814861	-3.262274	2.278951
C	0.357314	-0.342519	9.558017
H	0.929624	-0.455600	10.478764
H	1.110041	-0.126298	8.799893
H	-0.217073	0.579739	9.645301
C	-0.638830	-1.496072	9.436139
H	-1.035818	-1.688969	10.432778
H	-0.113978	-2.375653	9.063353
N	-1.709081	-1.010844	8.551292
H	-1.402283	-0.644239	7.661587
H	-2.457233	-1.687499	8.501222
H	-2.158870	-0.158779	8.854237
N	-4.172400	-3.675815	8.698550
O	-3.511220	-2.796267	9.239210
O	-3.978320	-4.000834	7.532457
O	-5.270607	-3.960437	9.163318
C	7.794268	0.468186	-9.413864

H	6.928344	0.392399	-10.071536
H	8.763066	0.489071	-9.912959
H	7.846889	-0.407521	-8.766973
C	7.477091	1.735291	-8.619078
H	7.344727	2.566283	-9.311922
H	8.309918	2.122191	-8.031876
N	6.244194	1.668278	-7.819505
H	5.442328	1.587729	-8.428293
H	6.364524	0.916287	-7.156082
H	6.021213	2.465703	-7.241152
N	5.110811	4.458179	-6.505884
O	4.254545	4.441647	-5.628608
O	4.640377	4.402263	-7.636654
O	6.079903	3.736812	-6.297157
C	-1.804202	-5.430444	3.851743
H	-1.431916	-6.444125	3.999914
H	-2.517183	-5.633837	3.052751
H	-1.035578	-4.752964	3.479805
C	-2.519244	-4.935256	5.109259
H	-1.748344	-4.735250	5.853444
H	-3.103813	-5.740750	5.553733
N	-3.117659	-3.607357	4.903289
H	-2.569093	-2.880776	4.465962
H	-4.023696	-3.733832	4.475267
H	-3.451374	-3.253779	5.788568
N	-1.076480	-4.075560	0.085684
O	-1.448116	-5.101992	-0.472349
O	-1.776287	-3.673669	1.008630
O	-0.491080	-3.220499	-0.569490
C	-9.359941	-1.593169	3.976749
H	-8.875532	-2.134314	3.163970
H	-9.124452	-2.075732	4.925315
H	-10.421659	-1.532668	3.737595
C	-8.659935	-0.238868	3.859695
H	-9.222720	0.480172	4.454971
H	-8.731840	0.007325	2.800300
N	-7.237444	-0.192011	4.231401
H	-6.766749	-0.652648	3.465660
H	-6.980407	0.764488	4.429242
H	-7.082004	-0.711829	5.083298
N	-3.755854	1.100859	10.314153
O	-4.890896	1.551375	10.422746
O	-3.332939	1.046095	9.164710
O	-3.539156	0.111646	11.005222
C	3.826063	-1.567472	-1.799478
H	3.457325	-1.175639	-0.851533
H	4.571207	-2.362934	-1.789432
H	4.227765	-0.757698	-2.408576
C	2.813807	-2.265134	-2.708569
H	2.251945	-3.044155	-2.193267
H	3.297520	-2.752317	-3.555194
N	1.955035	-1.145416	-3.124001
H	1.823272	-0.487627	-2.368983
H	2.473482	-0.599507	-3.797272
H	1.062405	-1.502169	-3.433901
N	2.539034	1.299548	-1.078053
O	2.663855	2.376546	-0.505714
O	2.711281	1.416675	-2.286228
O	1.662682	0.495000	-0.781765
C	-8.101436	4.937508	0.359654
H	-8.611815	4.167798	-0.219276
H	-8.476509	4.982576	1.382097
H	-8.269563	5.909436	-0.104233
C	-6.643662	4.476295	0.363796
H	-6.012157	5.098862	0.997603
H	-6.227475	4.420026	-0.642048
N	-6.506481	3.029542	0.591674

H	-5.568112	2.656615	0.613761
H	-6.887567	2.741443	1.481546
H	-7.100085	2.633710	-0.123205
N	-2.981454	2.158216	0.494096
O	-2.623594	1.066603	0.065851
O	-2.953561	2.217852	1.718327
O	-3.962283	2.660423	-0.043341
C	-5.463550	4.541888	7.808685
H	-5.941697	5.484044	8.076670
H	-4.499839	4.497704	8.316041
H	-5.209240	4.368769	6.763000
C	-6.446031	3.435267	8.193345
H	-7.363672	3.615558	7.633408
H	-6.690244	3.485864	9.254429
N	-6.109447	2.047251	7.841258
H	-6.868193	1.514678	8.242217
H	-6.028929	1.971571	6.837321
H	-5.286992	1.785780	8.365950
N	-8.269707	1.304706	-1.381023
O	-8.018914	2.439112	-1.772560
O	-7.979235	0.297646	-2.017054
O	-8.307236	1.090727	-0.174425
C	-6.411918	-6.032629	6.177925
H	-6.015755	-5.794370	5.190814
H	-5.550082	-6.343046	6.768671
H	-6.911830	-7.000262	6.134624
C	-7.386191	-5.006015	6.756454
H	-7.744122	-5.329424	7.733895
H	-8.341515	-4.818600	6.266219
N	-6.699210	-3.726553	6.990705
H	-5.894324	-3.852149	7.587768
H	-6.289501	-3.381659	6.134383
H	-7.255927	-2.941679	7.297525
N	-1.176631	2.681518	-6.377042
O	-1.126173	1.580772	-5.839560
O	-0.418211	3.458532	-5.807725
O	-1.037005	2.612826	-7.593127
C	-7.888196	-1.727559	11.740119
H	-7.884597	-2.745332	11.349962
H	-8.169692	-1.916046	12.776137
H	-8.671927	-1.214055	11.183182
C	-6.557005	-0.975582	11.722776
H	-5.846209	-1.504809	12.357431
H	-6.669950	0.077220	11.981523
N	-5.986029	-1.021406	10.367886
H	-6.478188	-0.635228	9.574951
H	-5.172439	-0.456293	10.564912
H	-5.634499	-1.923262	10.079475
N	-5.024747	-0.870311	6.607803
O	-4.969857	-1.941205	6.013454
O	-5.164681	-0.823273	7.824882
O	-5.060471	0.202089	6.014711
C	4.752599	-3.900303	-6.736266
H	4.007319	-3.995405	-5.946574
H	4.862181	-4.879508	-7.202365
H	5.665088	-3.539746	-6.261435
C	4.044565	-3.115100	-7.840795
H	3.064100	-3.529353	-8.075707
H	4.538651	-3.096266	-8.812198
N	3.710620	-1.726239	-7.489529
H	4.569413	-1.283712	-7.195006
H	3.309585	-1.196396	-8.250146
H	3.054527	-1.632650	-6.727373
N	-8.315283	-0.709978	7.967141
O	-8.284271	0.474569	8.281723
O	-7.990704	-1.602157	8.742862
O	-7.951740	-0.938395	6.818778

C	-5.111238	0.600811	-4.078068
H	-5.503200	1.347189	-4.768999
H	-5.998791	0.026138	-3.813307
H	-4.347488	-0.066219	-4.477890
C	-4.632018	1.152648	-2.735062
H	-5.421356	1.364357	-2.013797
H	-4.093985	2.093466	-2.851167
N	-3.893683	0.096665	-2.025412
H	-3.823781	0.447335	-1.080825
H	-4.491563	-0.714614	-2.092256
H	-2.978520	-0.194479	-2.338159
N	-5.833798	-2.933202	-2.091211
O	-6.721064	-3.522460	-1.484077
O	-5.863959	-1.711472	-1.993542
O	-4.720961	-3.427929	-2.232333
C	1.032538	4.810092	-3.017348
H	1.987211	4.464361	-2.620904
H	1.251582	4.768164	-4.084288
H	0.974616	5.807256	-2.580987
C	0.008798	3.733573	-2.655541
H	-0.987456	3.992749	-3.013881
H	-0.087196	3.689543	-1.570670
N	0.295748	2.530096	-3.451245
H	-0.379778	1.801039	-3.271692
H	0.251898	2.759423	-4.433888
H	1.137797	2.073581	-3.130862
N	0.857455	-3.534998	-5.534681
O	1.625290	-2.676372	-5.954521
O	0.891695	-3.831602	-4.345593
O	-0.280558	-3.369674	-5.959736
C	0.405943	5.128071	-8.851927
H	0.333147	4.535943	-9.764168
H	0.215130	6.171031	-9.104757
H	-0.326604	4.804059	-8.112676
C	1.838450	5.124837	-8.317368
H	1.997172	5.921771	-7.590867
H	2.549780	5.390365	-9.099419
N	2.108355	3.842611	-7.648870
H	2.974865	3.953970	-7.142056
H	1.372524	3.596974	-7.002097
H	2.339218	3.094351	-8.286765
N	2.852479	0.588864	-9.605037
O	3.877496	0.119166	-10.086494
O	2.650688	1.797076	-9.554243
O	2.232824	-0.060942	-8.770258
C	-2.283122	2.514167	6.031986
H	-2.925273	2.066273	6.790361
H	-1.898051	3.502635	6.282488
H	-1.373660	1.921222	5.935048
C	-2.941269	2.453282	4.653227
H	-2.407397	3.020785	3.890980
H	-3.973264	2.803877	4.640207
N	-3.033625	1.041141	4.251769
H	-3.089379	0.971847	3.245693
H	-2.213968	0.466172	4.384710
H	-3.863806	0.635032	4.659170
N	6.355241	-0.557097	-5.699285
O	6.201404	-0.909250	-6.863501
O	5.397099	-0.675493	-4.943625
O	6.825286	0.563427	-5.536314
C	6.153867	2.032692	-1.902894
H	6.833067	1.270616	-2.285029
H	6.743909	2.610116	-1.191184
H	5.297499	1.588801	-1.395259
C	5.617187	2.893851	-3.046669
H	6.498071	3.364080	-3.483736
H	4.895680	3.652390	-2.743115

N	4.910898	2.063260	-4.034149
H	4.602536	2.489542	-4.896295
H	5.451567	1.284555	-4.382567
H	4.186609	1.731145	-3.413499
N	-6.751717	3.120719	4.139661
O	-5.873904	3.973077	4.062158
O	-6.946947	2.493352	5.174731
O	-7.036626	2.468835	3.141188
C	-1.911663	-6.201304	-4.342800
H	-2.709118	-6.686718	-4.905417
H	-1.755801	-6.797100	-3.443448
H	-0.922155	-6.080498	-4.783686
C	-2.447051	-4.853374	-3.858769
H	-3.153412	-4.956187	-3.035006
H	-2.973634	-4.293364	-4.631555
N	-1.476228	-4.022420	-3.130168
H	-0.637489	-3.821714	-3.655844
H	-1.749713	-3.054000	-3.043746
H	-1.333073	-4.354433	-2.187101
N	-0.753142	-1.288972	5.536934
O	-1.545077	-1.081644	4.624285
O	-0.899574	-2.329331	6.168825
O	-0.274346	-0.371844	6.194738
C	-2.451494	-1.285110	-6.822901
H	-2.780753	-0.416820	-6.252146
H	-2.296567	-1.925767	-5.954767
H	-3.302659	-1.645808	-7.400409
C	-1.182456	-1.235259	-7.674310
H	-1.241071	-0.556027	-8.524786
H	-0.970786	-2.194355	-8.146993
N	0.056986	-0.694112	-7.095704
H	0.363950	-1.190281	-6.271271
H	0.808979	-0.781790	-7.764225
H	0.014276	0.271057	-6.801214
N	2.713810	1.237410	-5.833677
O	3.698473	1.413565	-6.542538
O	2.583622	0.140458	-5.301863
O	2.238162	2.186816	-5.220927

Return

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	1.148474	-4.516336	2.267700
H	1.200049	-5.275756	1.487494
H	0.384186	-4.729064	3.015170
H	2.076745	-4.675425	2.816429
C	1.200059	-3.113574	1.661533
H	1.952952	-3.058916	0.875234
H	1.472818	-2.366207	2.406614
N	-0.109374	-2.835494	1.051701
H	-0.308855	-3.589048	0.409467
H	-0.811473	-2.828231	1.777721
H	0.096885	-1.957511	0.597055
N	-3.660890	-3.470107	1.124217
O	-4.491401	-3.346938	2.017613
O	-4.118034	-3.555810	-0.010133
O	-2.539837	-3.797198	1.497482
C	-1.937952	-7.817097	-0.211771
H	-2.750964	-8.369938	-0.682384
H	-1.034082	-7.739185	-0.815965
H	-1.631616	-8.449733	0.621314
C	-2.645287	-6.526703	0.203443
H	-2.166743	-6.117022	1.092968
H	-3.685152	-6.739440	0.451482
N	-2.640980	-5.527165	-0.875790
H	-3.120174	-4.672397	-0.631157
H	-1.719613	-5.206600	-1.137366
H	-3.056706	-5.791997	-1.757343
N	-1.204265	-2.595730	-2.984910
O	-1.752983	-3.635473	-2.637177
O	-0.331911	-2.052623	-2.316248
O	-1.889815	-1.906616	-3.732050
C	-7.789123	-4.334655	-0.556731
H	-8.068456	-5.386110	-0.489537
H	-8.444720	-3.830148	-1.266496
H	-6.820913	-4.236231	-1.047631
C	-7.529274	-3.569838	0.741489
H	-6.967289	-4.309283	1.312010
H	-8.464727	-3.545384	1.300444
N	-6.741276	-2.343024	0.546996
H	-7.295280	-1.728242	-0.031988
H	-6.694784	-1.881607	1.444232
H	-5.821523	-2.370103	0.130556
N	-7.003379	-0.963976	3.418356
O	-6.878563	-2.180255	3.508703
O	-7.835735	-0.425635	4.139777
O	-7.100835	-0.438710	2.314873
C	0.040396	-2.241057	7.540290
H	1.095671	-2.420993	7.745519
H	-0.479120	-3.112779	7.938165
H	-0.030408	-2.265972	6.452877
C	-0.469333	-0.936352	8.153284
H	0.120345	-0.028161	8.028516
H	-0.528829	-1.112702	9.227277
N	-1.875089	-0.727583	7.773670
H	-1.927641	-0.306039	6.857352
H	-2.469953	-1.536175	7.662245
H	-2.184926	-0.038273	8.443709
N	-4.614611	-2.451431	8.405272
O	-3.522220	-2.848762	8.015548
O	-5.649473	-2.623882	7.770923
O	-4.522242	-1.321035	8.870835
C	5.182527	5.573234	-5.489083

H	5.530870	4.837795	-4.763902
H	5.913132	6.114474	-6.090227
H	4.468826	6.275105	-5.057680
C	4.096734	4.889239	-6.320375
H	4.434517	4.334580	-7.195793
H	3.309817	5.567352	-6.650565
N	3.523070	3.707884	-5.657690
H	2.773253	3.352174	-6.233316
H	4.157657	2.925009	-5.724822
H	3.112123	3.977671	-4.775399
N	1.563122	5.287427	-3.451333
O	0.609655	4.539706	-3.264546
O	2.701466	4.931573	-3.167401
O	1.453759	5.945852	-4.479726
C	-4.889237	-5.250431	5.003640
H	-5.491611	-4.992061	5.874554
H	-5.594848	-5.323954	4.176109
H	-4.612154	-6.296911	5.130940
C	-3.755925	-4.224165	4.988667
H	-3.064654	-4.497029	4.191303
H	-3.149105	-4.218587	5.894116
N	-4.249553	-2.856157	4.767927
H	-4.802818	-2.910070	3.924664
H	-4.784010	-2.480600	5.538258
H	-3.457471	-2.259939	4.574970
N	1.020654	-5.063693	-1.610911
O	-0.078452	-5.064966	-1.067735
O	1.678451	-4.068797	-1.327075
O	1.162936	-5.537613	-2.732620
C	-9.134707	2.250041	3.061690
H	-9.982475	2.821375	2.683581
H	-9.152926	1.357471	2.436322
H	-9.421293	1.850240	4.034381
C	-7.827597	3.036285	3.167157
H	-7.942950	3.833490	3.901499
H	-7.512967	3.493338	2.228962
N	-6.847990	2.134538	3.792508
H	-6.488470	1.366213	3.244309
H	-6.014286	2.697570	3.882130
H	-7.319148	1.718642	4.583167
N	-1.916278	2.358866	9.026574
O	-1.899696	1.337583	9.704648
O	-3.028406	2.871637	8.969015
O	-1.333064	2.233241	7.955521
C	4.222983	-3.636570	-3.658232
H	4.208720	-3.428261	-4.728047
H	5.268296	-3.918876	-3.532834
H	3.550580	-4.479858	-3.500624
C	3.860539	-2.494813	-2.708039
H	4.279840	-1.528687	-2.988907
H	4.218077	-2.665673	-1.692621
N	2.428458	-2.158684	-2.707440
H	2.258008	-1.297880	-2.207377
H	2.132547	-1.979033	-3.656262
H	1.911610	-2.941542	-2.333138
N	1.763664	0.097271	0.091875
O	0.830971	-0.680269	0.260969
O	2.521301	-0.135668	-0.843433
O	1.734491	1.271587	0.442880
C	-5.775865	3.976114	-0.879871
H	-4.861304	4.245711	-1.408071
H	-6.546917	3.835979	-1.637461
H	-6.049479	4.678041	-0.092130
C	-5.426131	2.563298	-0.411386
H	-6.050621	2.298514	0.441844
H	-4.450168	2.494613	0.069112
N	-5.424262	1.546576	-1.474454

H	-4.781887	1.750016	-2.226828
H	-5.128342	0.614097	-1.223428
H	-6.357294	1.454588	-1.850074
N	-3.558189	-0.700344	-0.047508
O	-2.628862	-0.083995	0.461943
O	-3.574777	-0.614369	-1.270377
O	-4.607666	-0.487782	0.549562
C	-4.070265	6.074255	6.593825
H	-4.209559	6.213514	5.521769
H	-4.610899	6.930367	6.997420
H	-3.048561	6.189367	6.955723
C	-4.725859	4.733606	6.926539
H	-5.765765	4.586872	6.634712
H	-4.816185	4.726426	8.012765
N	-3.895281	3.607128	6.473736
H	-4.348602	2.717942	6.628484
H	-3.761422	3.704197	5.477362
H	-3.017727	3.586374	6.973302
N	-7.818452	-0.368691	-1.906327
O	-8.302819	-1.029120	-0.994023
O	-8.070374	0.831134	-1.900785
O	-6.658846	-0.616905	-2.217422
C	-10.094769	-1.142052	6.812968
H	-10.227242	-0.398249	7.598658
H	-9.976554	-0.611461	5.868194
H	-10.929308	-1.840966	6.869217
C	-8.810687	-1.956859	6.971289
H	-8.539254	-2.597965	6.132595
H	-8.680974	-2.501770	7.906353
N	-7.713852	-0.976722	6.960089
H	-7.697058	-0.451717	6.097426
H	-7.658739	-0.238781	7.647480
H	-6.799553	-1.403901	6.919156
N	-3.335009	1.186730	-4.394005
O	-2.122443	1.366528	-4.414749
O	-3.808469	0.056085	-4.417538
O	-3.900554	1.964047	-3.633076
C	-5.230013	2.990950	11.089053
H	-6.189362	3.428485	10.812803
H	-5.372378	3.201173	12.149071
H	-4.488984	3.665907	10.660788
C	-4.847585	1.536155	10.814898
H	-5.387966	0.793224	11.401535
H	-3.871135	1.343382	11.259290
N	-4.884762	1.170131	9.390650
H	-4.842100	0.162428	9.337601
H	-5.781701	1.464290	9.031384
H	-4.137386	1.532691	8.816125
N	-4.613275	0.545566	5.964386
O	-5.133707	-0.564024	5.996570
O	-4.581500	1.184428	4.918479
O	-4.046281	1.027289	6.938828
C	5.170988	-1.185427	-8.362611
H	5.810797	-1.895300	-8.886849
H	4.420105	-0.907699	-9.102302
H	5.819855	-0.391940	-7.991868
C	4.444176	-1.737078	-7.135718
H	5.232133	-1.910343	-6.402776
H	3.970681	-2.713957	-7.233745
N	3.614776	-0.714021	-6.480515
H	4.170605	0.055878	-6.136410
H	2.927190	-0.400611	-7.150664
H	3.099985	-1.098781	-5.701381
N	-7.563389	2.293095	7.878971
O	-7.569863	2.250080	6.653743
O	-6.824370	3.110110	8.416942
O	-7.492483	1.156727	8.333631

C	-5.922542	-3.481943	-4.837502
H	-5.912613	-4.373178	-5.464958
H	-5.944795	-2.667753	-5.561864
H	-6.916140	-3.475148	-4.389375
C	-4.785171	-3.401280	-3.818816
H	-3.895134	-3.603657	-4.414616
H	-4.850634	-4.096926	-2.982221
N	-4.569193	-2.070523	-3.230359
H	-5.422541	-1.649921	-2.891253
H	-3.827216	-1.960687	-2.553968
H	-4.351371	-1.487840	-4.026057
N	-3.572406	-6.922502	-3.701995
O	-3.497538	-6.308969	-4.760790
O	-4.429113	-6.512007	-2.926996
O	-2.449505	-7.097409	-3.242020
C	-1.347406	2.875701	-1.345131
H	-0.630084	3.682996	-1.197402
H	-1.595498	2.966201	-2.402657
H	-2.257751	3.052688	-0.772377
C	-0.638614	1.521160	-1.319160
H	-0.447416	1.364411	-0.257571
H	0.344951	1.662413	-1.767208
N	-1.301181	0.469098	-2.105296
H	-0.731708	-0.355002	-2.234369
H	-2.078751	0.168541	-1.535077
H	-1.637807	0.737362	-3.018980
N	1.274178	-2.781412	-6.154667
O	1.292720	-2.063432	-7.148265
O	0.166825	-3.124170	-5.755468
O	1.938434	-2.366725	-5.211335
C	-2.604372	4.479229	-5.520247
H	-3.115894	5.393565	-5.820973
H	-2.808777	4.483053	-4.449592
H	-3.100102	3.647708	-6.021171
C	-1.164102	4.461585	-6.033231
H	-0.714866	5.440880	-5.868098
H	-1.154023	4.374158	-7.119672
N	-0.420468	3.419789	-5.308309
H	-0.942717	2.621057	-4.977576
H	0.282557	3.049068	-5.931543
H	0.030258	3.848126	-4.512399
N	1.013641	1.945725	-7.527014
O	1.929351	1.159568	-7.311355
O	1.233976	3.108904	-7.208356
O	-0.164036	1.610696	-7.464511
C	-0.610562	2.313667	4.343913
H	-1.259735	2.949083	4.946344
H	0.404762	2.710152	4.347949
H	-0.365530	1.378344	4.847133
C	-1.030145	2.089441	2.890809
H	-0.170803	1.547112	2.496461
H	-1.213778	3.028585	2.368901
N	-2.237923	1.249960	2.910488
H	-2.136644	0.617950	3.691772
H	-3.075131	1.814720	2.925616
H	-2.242369	0.752080	2.031741
N	5.416613	1.130673	-4.613488
O	5.170066	1.934795	-3.721480
O	5.016877	1.594163	-5.675780
O	5.459326	-0.091736	-4.530016
C	4.811571	2.339727	-0.375076
H	5.340487	1.740592	-1.116281
H	5.615050	2.902724	0.099852
H	4.297160	1.751602	0.384916
C	3.842522	3.293045	-1.075056
H	4.457127	3.971527	-1.666684
H	3.378582	3.954622	-0.343500

N	3.042332	2.539888	-2.052958
H	2.376603	1.878840	-1.678900
H	2.478268	3.184127	-2.588576
H	3.735652	2.063771	-2.612170
N	-4.120748	4.282851	3.352445
O	-3.129358	4.363685	4.069165
O	-3.967123	3.267449	2.682791
O	-5.263716	4.394557	3.781655
C	0.596610	-6.373198	-6.362641
H	1.300619	-6.681607	-5.589753
H	1.075188	-5.464604	-6.728045
H	0.541996	-6.993372	-7.257349
C	-0.774792	-6.165696	-5.719181
H	-1.224120	-7.114468	-5.425863
H	-1.608808	-5.867210	-6.354338
N	-0.708593	-5.207731	-4.604838
H	-0.419050	-4.344707	-5.042393
H	-1.655445	-5.190177	-4.253751
H	-0.031672	-5.589650	-3.959845
N	-1.307130	-1.420592	4.046654
O	-1.902843	-0.777853	4.904026
O	-0.580981	-0.853734	3.237669
O	-1.526830	-2.625292	3.987437
C	-1.579734	-1.025623	-8.710306
H	-1.352367	-0.002157	-9.008501
H	-2.265477	-1.410001	-9.465363
H	-0.739609	-1.689862	-8.912982
C	-2.039829	-1.032429	-7.252188
H	-2.496407	-1.953896	-6.890891
H	-2.776698	-0.276616	-6.980398
N	-1.086359	-0.573316	-6.230450
H	-0.520979	0.134166	-6.677569
H	-1.547851	-0.317591	-5.369213
H	-0.533265	-1.405956	-6.085885
N	1.696537	0.874362	-4.367348
O	2.689981	0.346900	-3.879567
O	0.604428	0.410681	-4.058519
O	1.723213	2.098769	-4.423834

Return

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	1.227553	-2.686947	1.818578
H	2.184748	-2.210316	2.030003
H	1.566911	-3.674986	1.507587
H	0.587611	-2.788048	2.695134
C	0.506062	-2.017705	0.648361
H	1.225977	-1.831215	-0.148535
H	0.015576	-1.061956	0.832937
N	-0.535047	-2.906935	0.110585
H	-0.151824	-3.764196	-0.261361
H	-1.356896	-2.967100	0.694576
H	-0.937846	-2.538262	-0.739082
N	-2.872156	-4.551004	2.233427
O	-4.095425	-4.490990	2.288987
O	-2.183848	-3.645931	1.775003
O	-2.486456	-5.678295	1.944419
C	-2.127719	-8.730811	-1.448370
H	-1.061451	-8.777403	-1.227008
H	-2.561556	-9.721715	-1.314224
H	-2.399799	-8.381324	-2.444328
C	-2.687577	-7.900545	-0.292922
H	-2.163468	-8.301108	0.574810
H	-3.736790	-8.087134	-0.063932
N	-2.542447	-6.440486	-0.397831
H	-2.712051	-5.971157	0.480272
H	-1.619759	-6.108298	-0.639490
H	-3.226476	-6.059088	-1.035594
N	-0.948701	-1.574811	-3.185472
O	-0.303186	-0.534977	-3.257092
O	-0.595845	-2.496004	-2.457481
O	-1.816085	-1.812443	-4.018691
C	-7.951530	-4.585540	0.408321
H	-8.109214	-5.664072	0.410472
H	-8.796037	-4.224462	0.995289
H	-8.032917	-4.253506	-0.626682
C	-6.560212	-4.473171	1.032377
H	-5.922097	-4.943897	0.284495
H	-6.508450	-4.959627	2.006430
N	-6.102570	-3.086271	1.208202
H	-5.210388	-3.221698	1.661822
H	-5.992783	-2.492117	0.398865
H	-6.728557	-2.658274	1.875329
N	-7.856690	-2.347531	4.338146
O	-8.064442	-1.235642	4.811030
O	-7.546183	-2.437848	3.155563
O	-7.332843	-3.219239	5.022826
C	-1.917358	-1.739987	10.714641
H	-1.324289	-1.131863	11.397689
H	-2.697923	-2.326753	11.198920
H	-1.124549	-2.380966	10.329023
C	-2.376186	-0.701397	9.690607
H	-1.526265	-0.142219	9.299386
H	-2.780606	0.091343	10.319978
N	-3.216026	-1.244509	8.611931
H	-2.686652	-1.745834	7.912976
H	-4.020648	-1.751578	8.951880
H	-3.664745	-0.505230	8.090186
N	-6.021014	-1.806059	10.370489
O	-5.621943	-2.477982	9.425852
O	-7.179266	-1.404824	10.347313
O	-5.186840	-1.023077	10.811134
C	4.644266	3.831685	-9.652904

H	4.522809	4.146599	-10.689329
H	5.729481	3.801753	-9.555382
H	4.282387	2.803520	-9.648254
C	3.897106	4.661165	-8.608128
H	2.913400	4.911332	-9.005418
H	4.486626	5.545133	-8.364885
N	3.657005	3.994837	-7.318865
H	4.549135	3.706434	-6.943328
H	3.101282	4.577448	-6.709081
H	3.171037	3.116240	-7.428422
N	2.320475	4.987692	-4.615182
O	3.354554	4.331117	-4.563540
O	1.444394	4.647862	-3.827735
O	1.979478	5.317811	-5.745588
C	-4.148887	-6.409173	5.059719
H	-3.603138	-6.220302	4.135280
H	-3.290130	-6.436576	5.730453
H	-4.710967	-7.338725	5.149716
C	-5.111338	-5.253518	5.335385
H	-5.328171	-5.359989	6.398281
H	-5.946641	-5.285598	4.635858
N	-4.627482	-3.869959	5.210929
H	-5.374717	-3.205732	5.354262
H	-4.110981	-3.609038	6.038726
H	-4.117184	-3.669936	4.362585
N	0.679114	-5.503456	-1.278267
O	-0.030422	-5.652810	-0.289668
O	1.174976	-4.384027	-1.342095
O	0.312484	-6.051070	-2.312084
C	-9.371442	1.891945	3.171706
H	-9.844920	1.418254	2.311744
H	-9.628000	1.363360	4.089789
H	-9.807454	2.890603	3.145707
C	-7.842920	1.923691	3.192996
H	-7.442762	2.370945	4.102907
H	-7.397511	2.517100	2.394513
N	-7.150159	0.630225	3.088742
H	-7.455591	0.312832	2.179857
H	-6.200266	0.970110	3.040974
H	-7.323363	0.061306	3.905095
N	-3.120301	2.851592	8.899413
O	-3.517894	1.978674	8.135862
O	-3.133828	2.646496	10.108061
O	-2.748203	3.894115	8.372380
C	4.462042	-2.206552	-4.023893
H	4.774701	-1.216969	-3.690620
H	5.207087	-2.999573	-3.959660
H	4.213213	-2.080222	-5.077565
C	3.275544	-2.604768	-3.145550
H	3.670321	-2.739683	-2.138550
H	2.883129	-3.549145	-3.522727
N	2.115256	-1.702192	-3.199673
H	2.445937	-0.768285	-3.003288
H	1.686220	-1.793774	-4.109421
H	1.391313	-1.842142	-2.509441
N	3.276785	0.741791	-0.952878
O	3.238802	1.926241	-1.267063
O	4.090957	0.130617	-1.636008
O	2.284697	0.068123	-0.697911
C	-5.791955	4.172264	-2.181304
H	-6.637523	3.537107	-2.445295
H	-6.212523	5.177855	-2.184391
H	-4.972395	4.065321	-2.891928
C	-5.099644	3.863318	-0.853487
H	-5.869313	3.847922	-0.081818
H	-4.291102	4.567820	-0.658458
N	-4.599918	2.480105	-0.824520

H	-3.927177	2.350828	-1.566684
H	-4.023665	2.401285	0.001203
H	-5.244779	1.709449	-0.926229
N	-2.632033	0.037356	0.240123
O	-2.735933	-0.970762	-0.449789
O	-2.377315	1.122635	-0.270137
O	-2.532050	-0.067791	1.457507
C	-3.119354	4.818729	5.232349
H	-2.806327	4.225914	4.372881
H	-3.199956	5.845999	4.876936
H	-2.298995	4.718153	5.942981
C	-4.499831	4.498321	5.806336
H	-5.315386	4.758880	5.131740
H	-4.701867	5.106585	6.687980
N	-4.599687	3.048902	6.036676
H	-5.444113	2.846217	6.552393
H	-4.599935	2.644630	5.111115
H	-3.872835	2.689888	6.639083
N	-6.668098	-0.410637	-0.718608
O	-6.169313	-1.485847	-1.031997
O	-7.112201	-0.163196	0.397017
O	-6.327166	0.538528	-1.415694
C	-9.818556	-2.611098	7.308798
H	-9.706052	-2.747148	6.233190
H	-9.201387	-3.398690	7.741117
H	-10.882387	-2.641772	7.544220
C	-9.201819	-1.238864	7.581655
H	-9.647616	-0.666387	8.395064
H	-9.372248	-0.614847	6.704354
N	-7.739968	-1.344752	7.706636
H	-7.464084	-1.787182	8.571646
H	-7.362230	-1.881188	6.938749
H	-7.485496	-0.368215	7.748107
N	-2.564198	2.137133	-3.309591
O	-2.709634	3.252525	-2.821918
O	-3.477033	1.354250	-3.071053
O	-2.039210	2.049636	-4.414041
C	-5.856064	2.266628	12.824562
H	-4.784652	2.121552	12.962868
H	-6.313839	2.924815	13.563029
H	-6.295184	1.286442	13.010327
C	-6.241378	2.620540	11.387857
H	-5.806078	3.615082	11.290382
H	-7.330231	2.570651	11.384803
N	-5.678735	1.778575	10.320914
H	-5.656149	0.804309	10.586234
H	-6.169928	2.032092	9.475598
H	-4.722893	2.090963	10.226688
N	-4.952269	-0.643207	5.580413
O	-5.092311	-1.523978	6.421666
O	-4.059766	0.153728	5.847636
O	-4.943170	-1.069075	4.430791
C	4.344496	-1.189734	-9.513244
H	4.481200	-1.490868	-10.551864
H	5.232857	-0.581146	-9.344318
H	4.415065	-2.092544	-8.906569
C	3.074029	-0.428662	-9.133081
H	2.129498	-0.969199	-9.194552
H	2.961754	0.451369	-9.766359
N	3.214674	0.083312	-7.761242
H	2.516357	0.809062	-7.685481
H	2.926158	-0.574036	-7.050783
H	4.040741	0.579293	-7.458396
N	-7.270083	2.283041	7.691692
O	-6.711426	3.182421	8.309830
O	-7.307243	2.336180	6.467408
O	-7.623417	1.252376	8.253794

C	-5.381029	-1.421113	-5.324057
H	-5.223106	-0.426552	-5.741203
H	-6.242744	-1.800707	-5.873106
H	-4.585349	-2.068228	-5.693159
C	-5.620315	-1.669809	-3.834515
H	-5.787448	-2.679896	-3.460496
H	-6.589891	-1.196877	-3.678453
N	-4.437367	-1.221275	-3.083986
H	-4.519817	-1.360627	-2.087049
H	-3.688375	-1.861662	-3.305378
H	-4.179322	-0.245160	-3.110665
N	-4.057744	-4.924999	-2.741660
O	-3.664323	-6.079381	-2.866941
O	-3.714708	-4.045284	-3.523646
O	-4.069756	-4.589279	-1.562582
C	0.721601	3.305251	0.302379
H	0.976442	4.296456	0.677437
H	-0.311353	3.069699	0.558546
H	1.357165	2.471833	0.601669
C	0.765366	3.441109	-1.219945
H	1.694534	3.841484	-1.625466
H	0.049720	4.215655	-1.495677
N	0.649918	2.132856	-1.882507
H	-0.243796	1.696792	-1.705806
H	0.886021	2.073761	-2.862744
H	1.297423	1.443670	-1.527741
N	1.017069	-2.642986	-6.326082
O	0.945502	-2.960272	-5.144015
O	0.011084	-2.676068	-7.026065
O	1.868275	-1.783187	-6.524247
C	-1.969671	6.008118	-6.396836
H	-2.838706	6.653982	-6.271386
H	-1.828946	5.736980	-7.443154
H	-1.111605	6.668961	-6.273906
C	-1.926204	4.715156	-5.581852
H	-2.771379	4.065080	-5.808081
H	-2.002185	5.021598	-4.538578
N	-0.619898	4.040155	-5.624051
H	-0.520572	3.261733	-4.988210
H	-0.497673	3.695602	-6.565563
H	0.187864	4.574131	-5.336841
N	0.655752	2.055333	-8.577457
O	0.247141	0.925742	-8.332227
O	1.868004	2.187131	-8.450378
O	0.008346	3.013367	-8.169888
C	-0.398155	0.346666	5.422982
H	-0.994780	0.702601	6.262892
H	0.517658	0.937594	5.436787
H	0.031654	-0.631588	5.638349
C	-1.096834	0.356409	4.062984
H	-0.548769	0.211803	3.131956
H	-1.462584	1.375127	3.934375
N	-2.167159	-0.652436	4.084793
H	-2.427480	-0.708720	3.110543
H	-1.992689	-1.593437	4.407559
H	-2.978956	-0.228320	4.510483
N	5.752747	1.793865	-6.642091
O	5.236483	1.721091	-7.751709
O	5.287631	1.034236	-5.799650
O	5.822366	2.896436	-6.110523
C	7.137332	2.302763	-2.770944
H	6.921073	1.360030	-2.268365
H	7.404680	2.016283	-3.788075
H	8.020594	2.781864	-2.348558
C	5.930042	3.210665	-3.007601
H	6.072655	4.093533	-3.630742
H	5.589056	3.622777	-2.057868

N	4.771258	2.461342	-3.517084
H	4.345363	1.957311	-2.752449
H	4.092954	3.142175	-3.827682
H	4.836288	1.862539	-4.327828
N	-4.542145	2.122755	2.332064
O	-4.836833	2.212491	3.518733
O	-5.188112	1.361620	1.620393
O	-4.236277	3.158817	1.752325
C	-1.060471	-6.886591	-5.365012
H	-0.211586	-7.322158	-4.837968
H	-1.228506	-7.317608	-6.351972
H	-2.036688	-7.032115	-4.902492
C	-0.838479	-5.374467	-5.410213
H	-1.605556	-5.014947	-6.096098
H	0.094542	-4.963061	-5.795331
N	-1.084478	-4.808643	-4.074860
H	-0.820348	-3.842809	-3.942580
H	-2.015951	-5.070521	-3.785243
H	-0.415156	-5.122906	-3.386858
N	-1.990046	-3.058034	6.221514
O	-2.067100	-3.195831	5.005722
O	-2.721997	-3.671147	6.990550
O	-1.652398	-1.957579	6.643494
C	-2.406241	-0.923894	-7.804420
H	-1.424126	-1.080702	-8.250470
H	-3.193079	-0.683738	-8.519480
H	-2.820775	-1.789421	-7.287579
C	-2.224080	0.221651	-6.808234
H	-3.076702	0.307873	-6.134660
H	-1.975307	1.218770	-7.171503
N	-1.190610	-0.298799	-5.899986
H	-0.305875	-0.373628	-6.381383
H	-1.030578	0.330169	-5.126107
H	-1.362048	-1.194377	-5.465650
N	1.763017	1.446080	-4.816847
O	2.482363	0.735158	-4.123877
O	2.162868	1.732099	-5.939963
O	0.697576	1.887175	-4.400498

Return

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	1.546200	-5.663266	2.395352
H	0.685096	-5.680846	3.063401
H	2.410614	-6.070940	2.919463
H	1.458096	-6.253481	1.483220
C	1.690227	-4.247858	1.835246
H	2.309177	-4.306060	0.939917
H	2.060553	-3.513974	2.551048
N	0.379166	-3.769632	1.370209
H	-0.188497	-3.611338	2.190453
H	0.549866	-2.874394	0.934881
H	-0.003944	-4.472407	0.754227
N	-2.774038	-3.860745	1.418498
O	-3.464690	-3.317426	2.273414
O	-3.277920	-4.056162	0.318047
O	-2.183932	-4.786674	1.963939
C	-3.757738	-7.225447	-0.248885
H	-3.821192	-6.448023	0.512486
H	-4.412459	-8.080476	-0.080463
H	-2.760723	-7.665947	-0.253365
C	-3.848092	-6.588880	-1.636134
H	-4.875099	-6.230742	-1.707505
H	-3.663682	-7.390149	-2.351719
N	-2.833033	-5.524226	-1.633359
H	-1.939593	-5.994388	-1.604858
H	-2.835471	-5.025360	-2.511554
H	-2.879228	-4.777795	-0.954531
N	-1.107603	-2.171986	-2.906397
O	-1.417031	-3.338041	-2.688120
O	-1.933902	-1.273592	-3.021271
O	-0.200928	-2.066093	-3.724811
C	-8.007959	-4.287622	1.012706
H	-8.339584	-5.325501	1.043232
H	-8.300578	-3.993214	2.020574
H	-8.566851	-3.841098	0.190297
C	-6.483808	-4.263164	0.893511
H	-6.088739	-4.684971	-0.030664
H	-6.079848	-4.915174	1.667978
N	-5.861944	-2.957478	1.162420
H	-4.880022	-3.106110	1.346363
H	-6.027978	-2.371099	0.357006
H	-6.285139	-2.547898	1.982938
N	-6.652196	-3.039584	4.227183
O	-6.390031	-4.199812	3.930171
O	-6.702421	-2.208714	3.327067
O	-6.341951	-2.631533	5.340879
C	1.064723	0.034364	8.003719
H	1.739895	0.225227	8.837874
H	1.550648	-0.713961	7.377630
H	0.988326	0.928111	7.384460
C	-0.331989	-0.353288	8.490299
H	-0.619390	0.327355	9.291688
H	-0.166773	-1.266084	9.062669
N	-1.435497	-0.477600	7.525591
H	-1.345826	-1.008331	6.670967
H	-2.263981	-0.742897	8.038749
H	-1.433319	0.526966	7.420987
N	-4.187104	-1.046364	9.623785
O	-4.902801	-0.068143	9.439559
O	-2.997590	-0.749542	9.629148
O	-4.505200	-2.014548	8.942235
C	2.408531	6.079270	-6.867820

H	2.856548	6.966097	-7.316059
H	1.759497	5.576325	-7.584688
H	1.906554	6.468156	-5.981881
C	3.554424	5.111694	-6.570217
H	4.218287	5.800052	-6.047198
H	3.833818	4.821674	-7.583097
N	3.139510	3.997967	-5.703442
H	2.865618	4.344518	-4.795155
H	2.334271	3.515453	-6.076094
H	3.906946	3.349442	-5.600689
N	0.974573	4.813894	-2.748518
O	1.394158	4.251127	-1.743372
O	1.688933	4.895605	-3.741538
O	-0.224252	4.820954	-3.005120
C	-3.526557	-5.391109	6.184982
H	-4.440714	-5.148381	6.726737
H	-3.690869	-6.468139	6.218257
H	-2.720906	-5.151342	6.878911
C	-3.373469	-4.888147	4.749212
H	-4.131078	-5.308249	4.087667
H	-2.417822	-5.139772	4.289297
N	-3.482142	-3.423003	4.822585
H	-3.373393	-3.030268	3.898446
H	-4.393632	-3.131739	5.145773
H	-2.731441	-3.050208	5.386120
N	0.453085	-5.609814	-1.415817
O	1.178274	-4.621313	-1.409231
O	-0.210029	-5.775696	-0.398055
O	-0.050692	-5.998431	-2.463796
C	-9.607938	1.196992	2.153034
H	-9.513219	2.282429	2.122166
H	-9.525523	0.836855	1.127554
H	-10.600714	0.933740	2.517992
C	-8.772395	0.370449	3.131060
H	-9.041819	-0.665849	2.927108
H	-9.282897	0.604242	4.065313
N	-7.326696	0.627540	3.043322
H	-7.111260	0.303476	3.975346
H	-7.077513	-0.011981	2.302362
H	-7.045731	1.591862	2.937293
N	-2.014077	3.331268	6.892135
O	-1.684890	2.195319	7.215140
O	-2.095881	3.611227	5.701334
O	-2.818224	4.005756	7.525767
C	4.678626	-2.821615	-2.419910
H	4.289257	-3.714761	-2.908562
H	5.655244	-2.479464	-2.762329
H	4.697908	-2.958532	-1.338716
C	3.648620	-1.697890	-2.538954
H	3.685797	-1.368205	-3.577234
H	3.744963	-0.887426	-1.816483
N	2.298569	-2.249958	-2.348098
H	1.693905	-1.441443	-2.376102
H	2.177986	-2.863404	-3.141346
H	2.036443	-2.730775	-1.499448
N	1.261405	-0.706318	0.700921
O	0.121419	-1.141428	0.581811
O	1.526734	0.397595	0.238264
O	2.096620	-1.568692	0.452320
C	-7.341682	2.184796	-3.815381
H	-8.093433	1.479797	-3.460491
H	-7.848289	2.946740	-4.407741
H	-6.715994	1.573356	-4.465578
C	-6.612953	2.870851	-2.659472
H	-7.332748	3.411943	-2.045296
H	-5.882720	3.622633	-2.958940
N	-5.821789	1.915043	-1.869325

H	-4.961069	1.644038	-2.322996
H	-5.555268	2.355859	-1.000563
H	-6.239876	1.010459	-1.704910
N	-3.854172	-0.381724	0.655920
O	-4.562269	-0.353861	1.656370
O	-4.263775	-0.346979	-0.499110
O	-2.650000	-0.266489	0.855330
C	-3.538938	5.479655	3.565798
H	-3.280575	5.004241	2.619579
H	-3.483887	6.562238	3.451414
H	-2.597349	5.341266	4.097172
C	-4.714018	4.939356	4.381338
H	-5.670938	5.055122	3.872417
H	-4.691885	5.543922	5.288041
N	-4.598264	3.504345	4.683303
H	-5.361257	3.182639	5.261617
H	-4.539474	3.151396	3.738808
H	-3.701585	3.433898	5.142765
N	-7.771305	-0.763654	-0.594595
O	-7.503972	-0.096045	0.398333
O	-7.149295	-1.816707	-0.679794
O	-7.943744	-0.189270	-1.663906
C	-7.863750	-1.653529	9.436837
H	-7.025691	-2.222255	9.839712
H	-7.951220	-0.646037	9.843542
H	-8.763535	-2.219460	9.678101
C	-7.722309	-1.512798	7.920912
H	-8.465621	-0.780066	7.606760
H	-7.909057	-2.457905	7.411012
N	-6.495441	-0.861626	7.436547
H	-6.383421	-0.961804	6.437790
H	-6.556713	0.116326	7.681404
H	-5.787896	-1.332083	7.982578
N	-3.462956	1.658954	-4.105853
O	-2.610697	1.337683	-4.926533
O	-3.668739	1.028104	-3.074951
O	-4.218936	2.567221	-4.432380
C	-3.097552	2.721424	10.680180
H	-2.901268	2.995411	11.716763
H	-2.776626	1.680318	10.714910
H	-2.434033	3.415107	10.163801
C	-4.519007	2.855147	10.132983
H	-4.820826	3.883714	10.330604
H	-5.172384	2.091915	10.555683
N	-4.515512	2.552047	8.693553
H	-4.285831	1.582953	8.525619
H	-5.473924	2.664362	8.395339
H	-3.931401	3.157150	8.134299
N	-4.358401	0.191322	5.414265
O	-3.546181	-0.711293	5.583554
O	-5.139841	0.144529	4.470741
O	-4.371478	1.065829	6.273418
C	5.067392	-0.582338	-8.322594
H	5.302340	-0.546684	-9.386373
H	5.673963	0.008506	-7.636246
H	4.958578	-1.573567	-7.882451
C	3.732634	0.158027	-8.232473
H	2.935918	-0.238811	-8.861649
H	3.964967	1.111248	-8.707332
N	3.136348	0.132220	-6.887997
H	2.229304	0.576448	-6.882355
H	3.057675	-0.833453	-6.602715
H	3.748745	0.632221	-6.259451
N	-7.060233	2.218082	6.728235
O	-7.307654	1.729731	7.825218
O	-6.318574	3.171514	6.518507
O	-7.557668	1.570018	5.814098

C	-6.706305	-1.998008	-4.592563
H	-7.329228	-1.872283	-3.706978
H	-6.427126	-3.041492	-4.738513
H	-7.133625	-1.618144	-5.520572
C	-5.417312	-1.220847	-4.323568
H	-5.830460	-0.212189	-4.327710
H	-4.774530	-1.298244	-5.200461
N	-4.700937	-1.529444	-3.076404
H	-3.750762	-1.188700	-3.110505
H	-5.001008	-1.307240	-2.137958
H	-4.470386	-2.508255	-3.170614
N	-4.191552	-4.542801	-4.439984
O	-3.994863	-3.718920	-5.326329
O	-4.373685	-4.080139	-3.319338
O	-3.331904	-5.416490	-4.412637
C	-2.016302	2.822822	-0.192693
H	-2.046765	3.883850	-0.440467
H	-2.971255	2.464941	-0.577512
H	-2.079163	2.595464	0.871476
C	-0.985859	2.079568	-1.043342
H	-0.038610	2.261641	-0.535729
H	-1.023236	2.597126	-2.001901
N	-1.241484	0.637960	-1.185694
H	-2.102091	0.245003	-1.539302
H	-0.511871	0.147948	-1.683342
H	-1.194447	0.223077	-0.266041
N	2.487975	-2.961485	-6.038711
O	3.484202	-2.311063	-5.742806
O	1.599396	-2.384128	-6.655285
O	2.184039	-3.742315	-5.143724
C	-2.292376	4.438937	-7.187401
H	-2.742582	5.284749	-7.707032
H	-2.869373	3.523215	-7.316357
H	-1.491255	4.116564	-7.852518
C	-1.845279	4.815103	-5.774445
H	-2.716072	5.175909	-5.227052
H	-1.121031	5.626840	-5.706276
N	-1.337884	3.664397	-5.011381
H	-1.057549	3.822012	-4.053952
H	-1.886318	2.822727	-4.906923
H	-0.516049	3.360177	-5.513513
N	0.937250	2.454920	-7.696070
O	0.467450	2.999583	-6.703243
O	0.795169	1.239057	-7.763646
O	2.052956	2.930711	-7.874671
C	-0.155660	1.379144	3.523452
H	0.602564	0.624534	3.732641
H	0.343046	2.141001	4.122590
H	-0.013514	1.641423	2.475070
C	-1.609944	1.143659	3.932654
H	-2.275823	1.919690	3.555187
H	-1.614834	1.074936	5.020474
N	-2.116196	-0.130238	3.399048
H	-3.019913	-0.214662	3.842069
H	-2.372292	0.019104	2.433537
H	-1.595231	-0.988318	3.510381
N	5.050406	1.942792	-4.036765
O	4.575804	1.762716	-5.152741
O	4.741137	1.179127	-3.128886
O	4.857407	3.061252	-3.573220
C	5.050024	1.416821	0.252014
H	4.561324	0.736351	0.949318
H	5.625440	0.909899	-0.522600
H	5.827137	1.951765	0.797937
C	4.074126	2.456399	-0.300022
H	4.675790	3.176546	-0.854539
H	3.677421	3.108966	0.477720

N	3.064785	2.012749	-1.273802
H	2.449919	1.315954	-0.878181
H	2.594086	2.804026	-1.689039
H	3.465783	1.578289	-2.092671
N	-5.252076	2.786559	1.547431
O	-4.163803	2.613546	2.084836
O	-5.165365	3.268265	0.423368
O	-6.194981	3.111205	2.260601
C	0.803578	-6.076307	-6.482195
H	1.358386	-5.310500	-7.024253
H	0.583045	-6.969907	-7.066100
H	1.445842	-6.309678	-5.632998
C	-0.501387	-5.478383	-5.955511
H	-1.273909	-6.205994	-5.706732
H	-0.936842	-4.927192	-6.788977
N	-0.228009	-4.672565	-4.755609
H	0.580224	-4.112388	-4.985956
H	-0.919045	-4.043028	-4.373181
H	0.080631	-5.244544	-3.982510
N	-0.366683	-2.393375	4.964256
O	-1.260036	-2.639585	5.766987
O	0.188601	-1.348839	5.286252
O	-0.619019	-2.419347	3.764787
C	-1.919928	-0.166385	-7.743020
H	-2.787243	-0.679074	-8.158972
H	-1.151274	-0.295886	-8.504924
H	-2.247621	0.860918	-7.583748
C	-1.609771	-0.932440	-6.456629
H	-1.209990	-1.934199	-6.613965
H	-2.552827	-1.079669	-5.930254
N	-0.554896	-0.177628	-5.762844
H	-0.089971	-0.788805	-5.106790
H	0.227564	0.145456	-6.313727
H	-0.844801	0.561607	-5.138674
N	1.230585	1.032937	-3.634292
O	1.891477	0.742636	-4.625262
O	0.264820	1.734585	-3.913693
O	1.095236	0.198019	-2.746785

Return

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	-0.132850	-3.283772	1.185313
H	0.293378	-2.836574	0.287291
H	-0.271883	-4.360295	1.085976
H	0.608994	-3.100221	1.962537
C	-1.434786	-2.529974	1.458428
H	-1.213387	-1.463252	1.424006
H	-1.836560	-2.783291	2.439504
N	-2.428536	-2.808256	0.410163
H	-2.778605	-3.750385	0.509878
H	-3.082841	-2.042390	0.336438
H	-1.871189	-2.845311	-0.431319
N	-4.320486	-5.256303	-0.051305
O	-3.302477	-5.205258	0.629964
O	-4.399767	-6.159310	-0.876756
O	-4.704172	-4.158470	-0.439409
C	-3.170043	-9.619305	-1.152206
H	-4.192212	-9.320520	-1.384580
H	-2.928737	-10.019981	-2.136752
H	-3.181155	-10.519826	-0.538171
C	-2.094691	-8.589839	-0.803410
H	-1.094995	-9.021906	-0.848405
H	-2.130571	-8.206908	0.216480
N	-2.234621	-7.467634	-1.744110
H	-1.398028	-6.901882	-1.755763
H	-2.322478	-7.870292	-2.666199
H	-3.049814	-6.888264	-1.603071
N	-2.171686	-1.566261	-2.705670
O	-2.970734	-1.424869	-3.624694
O	-1.936102	-0.569547	-2.031773
O	-1.660980	-2.633954	-2.385847
C	-8.608537	-4.462121	1.103578
H	-7.900054	-5.290197	1.082541
H	-8.578951	-3.925848	2.052070
H	-9.550996	-5.001802	1.010760
C	-8.597902	-3.597336	-0.157324
H	-9.390565	-2.860171	-0.029376
H	-8.732738	-4.124105	-1.102011
N	-7.290615	-2.943758	-0.323687
H	-6.460687	-3.519283	-0.333221
H	-7.160729	-2.344960	-1.126600
H	-7.260581	-2.426207	0.543111
N	-7.324932	-1.334460	3.108974
O	-6.923027	-1.582017	1.977487
O	-6.599921	-0.582555	3.750904
O	-8.438032	-1.663900	3.503378
C	0.041771	-1.345474	10.336476
H	0.348773	-1.954493	11.186738
H	0.875746	-1.025076	9.712031
H	-0.376003	-0.400485	10.683694
C	-1.053094	-1.958038	9.462475
H	-1.878062	-2.290495	10.092555
H	-0.629658	-2.853980	9.008505
N	-1.511228	-1.082698	8.372643
H	-0.876680	-1.060523	7.587177
H	-2.435505	-1.372389	8.086476
H	-1.555289	-0.147953	8.752657
N	-4.964687	-1.839485	8.279001
O	-5.805024	-2.236046	7.479221
O	-3.817291	-2.259155	8.176848
O	-4.988749	-0.629898	8.477485
C	5.238227	4.568647	-5.023406

H	6.061278	4.908857	-5.651851
H	5.095075	5.333817	-4.260436
H	5.663961	3.647911	-4.624535
C	4.034223	4.328346	-5.934707
H	4.213998	3.594939	-6.720770
H	3.764785	5.289176	-6.373236
N	2.896050	3.711502	-5.236204
H	2.168470	3.650729	-5.934082
H	3.154116	2.758344	-5.024089
H	2.536471	4.361999	-4.552349
N	2.061553	5.082014	-2.489136
O	1.678771	5.755421	-3.439439
O	1.302520	4.185441	-2.138275
O	3.272193	4.898190	-2.428849
C	-5.100323	-4.193135	4.123741
H	-5.944709	-3.518252	3.983586
H	-4.721296	-4.360233	3.115516
H	-5.349366	-5.207230	4.436296
C	-3.988027	-3.502224	4.913223
H	-3.043342	-3.979426	4.652555
H	-4.268822	-3.467028	5.965846
N	-3.859063	-2.058585	4.661993
H	-4.738790	-1.588189	4.819812
H	-3.278688	-1.464217	5.236442
H	-3.640735	-1.856877	3.696722
N	0.467465	-5.682372	-2.679574
O	0.886518	-4.788025	-3.405944
O	-0.235191	-5.252341	-1.771596
O	0.175493	-6.761405	-3.183077
C	-6.326565	3.605838	2.158420
H	-5.756424	4.439645	2.568060
H	-5.816926	3.196435	1.286206
H	-7.311520	3.926148	1.818766
C	-6.430161	2.480018	3.187807
H	-7.152284	1.780414	2.766862
H	-6.623472	2.989741	4.131688
N	-5.185399	1.708461	3.326035
H	-5.334040	1.002297	4.032673
H	-5.017481	1.312065	2.412376
H	-4.468432	2.325056	3.680815
N	-1.431656	2.208683	8.874554
O	-2.012798	1.496276	9.685619
O	-0.948896	1.631256	7.906774
O	-1.938771	3.295197	8.618821
C	3.472146	-3.216036	-1.902086
H	2.935148	-4.163657	-1.860280
H	4.537627	-3.365297	-2.076938
H	3.395498	-2.992391	-0.838033
C	2.608776	-2.277136	-2.745236
H	2.732468	-2.565631	-3.789060
H	3.047559	-1.302077	-2.533510
N	1.154453	-2.292260	-2.524874
H	0.727224	-3.176752	-2.759924
H	0.876107	-1.903577	-1.635183
H	0.795498	-1.551248	-3.109813
N	1.625608	0.166001	0.056288
O	0.650877	-0.197948	-0.592185
O	1.617545	1.320834	0.467837
O	2.726554	-0.193388	-0.345998
C	-6.766898	1.515669	-2.805404
H	-6.128243	2.078448	-3.486213
H	-7.310084	0.750588	-3.360111
H	-7.468549	2.309605	-2.549568
C	-6.107191	1.033598	-1.513028
H	-6.818982	0.386606	-1.000335
H	-5.823605	1.849750	-0.848516
N	-5.011481	0.126746	-1.888367

H	-4.572716	-0.220875	-1.047686
H	-5.305165	-0.651380	-2.461402
H	-4.339370	0.626695	-2.452651
N	-4.462462	-0.405408	1.187369
O	-4.033259	-0.798189	2.266528
O	-4.357254	-1.138033	0.209991
O	-4.735189	0.767247	0.955905
C	-1.352107	6.355147	6.902566
H	-0.623535	5.655115	7.311514
H	-1.099152	6.461553	5.847676
H	-1.121484	7.328322	7.335976
C	-2.770920	5.812928	7.078094
H	-3.527233	6.518057	6.733301
H	-2.964756	5.749888	8.148866
N	-3.096997	4.491372	6.520415
H	-4.056232	4.281778	6.757141
H	-2.975314	4.305927	5.535070
H	-2.564662	3.769025	6.984025
N	-6.939854	-2.160589	-3.337628
O	-7.731165	-1.734256	-2.503874
O	-5.990908	-1.416946	-3.560273
O	-6.722201	-3.357202	-3.183287
C	-8.809777	-0.684530	8.190576
H	-8.230775	-1.540593	8.537002
H	-8.254970	0.102746	8.700955
H	-9.857708	-0.783095	8.473816
C	-8.505157	-0.589265	6.695259
H	-9.165863	0.199882	6.336353
H	-8.833777	-1.492879	6.181848
N	-7.110058	-0.226450	6.402162
H	-7.066092	0.697105	6.808627
H	-6.411844	-0.916997	6.638260
H	-7.036992	0.035557	5.429478
N	-3.501828	3.195650	-3.689344
O	-3.245915	3.367392	-4.875974
O	-3.566632	2.003759	-3.409569
O	-2.826666	3.898996	-2.946016
C	-4.582011	1.199509	11.869635
H	-4.677499	0.180816	11.493806
H	-3.537161	1.476224	12.010410
H	-5.175557	1.470631	12.742731
C	-5.222558	2.054679	10.775914
H	-5.170716	3.095471	11.095545
H	-6.301436	1.902021	10.804486
N	-4.812907	1.755377	9.395174
H	-5.067507	0.825343	9.094647
H	-5.313721	2.422441	8.825691
H	-3.833885	1.987394	9.306938
N	-3.730861	0.716833	6.188661
O	-2.761853	-0.033564	6.156961
O	-4.669658	0.383372	5.474139
O	-3.519599	1.921749	6.270029
C	2.996810	-1.645923	-8.561667
H	3.763179	-1.878421	-7.822260
H	2.323671	-2.491016	-8.705901
H	3.413852	-1.771822	-9.560830
C	2.310710	-0.296665	-8.345774
H	1.503773	-0.103922	-9.052741
H	3.058601	0.441090	-8.636424
N	1.954460	-0.059404	-6.938424
H	1.746458	0.902285	-6.710414
H	1.239773	-0.659014	-6.551397
H	2.691205	-0.331813	-6.303521
N	-6.942879	3.333054	7.682885
O	-7.225226	3.107193	8.854355
O	-5.814826	3.808915	7.618627
O	-7.084221	2.365363	6.943511

C	-4.935179	-4.419431	-6.107658
H	-4.756372	-4.128769	-7.142860
H	-5.998054	-4.360865	-5.873205
H	-4.647129	-5.470287	-6.078848
C	-3.974504	-3.642599	-5.206838
H	-4.185793	-2.573300	-5.199377
H	-2.969678	-3.707651	-5.624202
N	-3.894448	-4.160109	-3.832205
H	-3.342175	-3.464493	-3.351358
H	-4.845238	-4.130044	-3.492802
H	-3.534604	-5.102808	-3.876142
N	-2.743582	-7.548619	-5.048905
O	-3.450657	-6.764208	-4.426153
O	-2.274996	-7.097898	-6.088305
O	-2.158217	-8.305383	-4.282269
C	-0.734454	3.801759	0.399225
H	-1.127700	4.508761	1.129708
H	0.265212	3.487222	0.698952
H	-0.606069	4.517180	-0.413049
C	-1.577782	2.560090	0.107851
H	-2.612959	2.865644	-0.044283
H	-1.594835	1.809065	0.897642
N	-0.995840	1.861161	-1.048299
H	-1.668677	1.212465	-1.431164
H	-0.663825	2.392365	-1.840566
H	-0.267311	1.207825	-0.798303
N	-0.250197	-2.280803	-6.255514
O	0.721497	-2.261241	-5.508183
O	-0.633309	-1.308598	-6.896700
O	-0.561607	-3.366310	-6.732769
C	-1.826889	6.480090	-5.966743
H	-1.901663	5.811427	-6.824297
H	-1.631837	7.508900	-6.269406
H	-2.887062	6.615280	-5.752602
C	-0.891781	6.140924	-4.805545
H	-1.250157	6.621163	-3.895030
H	0.133180	6.484407	-4.945448
N	-0.984139	4.709816	-4.478066
H	-0.297204	4.378400	-3.815961
H	-1.917930	4.582444	-4.114871
H	-0.834285	4.104175	-5.272323
N	0.280605	2.752238	-7.284025
O	1.477743	2.971697	-7.431585
O	-0.243975	3.697597	-6.705934
O	-0.063964	1.633087	-6.920916
C	1.525081	2.137725	4.348659
H	1.648543	1.258114	3.716883
H	2.437235	2.651179	4.652702
H	0.938619	2.773196	3.685079
C	0.603715	1.881813	5.541737
H	0.425248	2.813659	6.078311
H	1.031700	1.233925	6.306702
N	-0.654338	1.217229	5.168280
H	-1.163247	1.529083	4.353504
H	-0.552913	0.239672	4.935483
H	-1.346462	1.263755	5.902378
N	4.473686	0.408728	-4.919930
O	4.067035	-0.713651	-5.199172
O	4.493927	0.651805	-3.718440
O	4.112944	1.340069	-5.630947
C	5.174317	1.696800	-0.405482
H	5.479456	0.961898	-1.150405
H	6.028598	2.253042	-0.019610
H	4.726660	1.109832	0.396497
C	4.144058	2.717722	-0.889349
H	4.675326	3.474764	-1.466185
H	3.587948	3.304968	-0.158607

N	3.158327	2.022118	-1.730960
H	3.570355	1.495578	-2.487985
H	2.694404	1.352630	-1.133747
H	2.561677	2.806886	-1.950613
N	-2.517272	3.301986	3.532940
O	-2.354616	2.122815	3.239384
O	-1.572309	3.858767	4.080766
O	-3.650538	3.740873	3.694689
C	2.149597	-6.745555	-5.662797
H	3.125420	-6.949071	-6.103762
H	1.599700	-7.685785	-5.703783
H	2.312989	-6.472319	-4.620326
C	1.336280	-5.660669	-6.369467
H	1.315786	-5.723571	-7.457457
H	1.971639	-4.776441	-6.318886
N	-0.014739	-5.602519	-5.790495
H	-0.520997	-4.864980	-6.259366
H	-0.541166	-6.463064	-5.741132
H	0.079490	-5.496013	-4.790556
N	-0.203743	-1.907300	5.108276
O	0.027690	-1.450473	6.222199
O	-0.736077	-3.011183	5.074533
O	-0.423117	-1.144228	4.174106
C	-3.361004	1.039794	-7.602507
H	-4.322627	0.945487	-8.106973
H	-2.590195	0.526839	-8.177687
H	-3.016350	2.072821	-7.555955
C	-3.460246	0.434125	-6.202093
H	-3.674662	-0.620596	-6.374395
H	-4.283015	0.951527	-5.708692
N	-2.196033	0.704158	-5.500174
H	-2.176780	0.149510	-4.656316
H	-1.416059	0.601958	-6.133653
H	-1.946783	1.672416	-5.357167
N	0.490524	1.317508	-3.959377
O	0.164342	0.142459	-4.085635
O	-0.423492	2.108462	-3.754333
O	1.635802	1.695611	-4.179496

Return

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	1.000633	-4.123005	1.839897
H	1.921682	-3.725484	1.413580
H	0.793812	-5.157516	1.565827
H	1.352540	-4.279401	2.859605
C	0.011832	-2.992706	1.552607
H	0.346357	-2.001809	1.859717
H	-0.965690	-3.221008	1.977377
N	-0.344701	-2.813179	0.136805
H	-0.774404	-3.561549	-0.387978
H	-0.938705	-2.005075	0.017529
H	0.475116	-2.560896	-0.396443
N	-4.247706	-3.317993	0.744947
O	-3.249299	-3.948512	0.415239
O	-5.206022	-3.468619	-0.004731
O	-4.529733	-3.110208	1.919835
C	-4.022766	-7.638557	-0.487065
H	-4.534374	-6.956614	0.192135
H	-4.767794	-7.902633	-1.237596
H	-3.926891	-8.529867	0.132996
C	-2.780628	-7.013677	-1.123037
H	-2.330108	-7.493969	-1.991629
H	-2.108589	-6.972313	-0.265860
N	-3.060604	-5.639296	-1.566354
H	-2.198194	-5.187913	-1.835801
H	-3.594522	-5.559375	-2.419961
H	-3.486741	-5.093621	-0.830999
N	-1.613214	-2.624503	-2.751332
O	-2.012305	-3.070517	-3.821320
O	-2.368160	-2.589037	-1.785995
O	-0.729460	-1.780619	-2.651771
C	-9.835880	-3.669734	1.035954
H	-9.604645	-4.167903	1.977473
H	-10.380256	-2.726311	1.077277
H	-10.408253	-4.399895	0.463805
C	-8.459004	-3.458723	0.405455
H	-8.590608	-3.055425	-0.598602
H	-7.948267	-4.405912	0.232018
N	-7.434754	-2.696529	1.136082
H	-6.556954	-2.929312	0.694065
H	-7.568343	-1.695493	1.122697
H	-7.511863	-2.931624	2.115308
N	-7.400292	-2.593788	4.287237
O	-8.329455	-2.912094	3.553471
O	-7.646982	-2.065798	5.365869
O	-6.483382	-2.134899	3.615098
C	0.726034	-1.658564	9.536646
H	1.688685	-2.070132	9.839986
H	0.662802	-0.577358	9.413780
H	-0.064215	-1.956617	10.225682
C	0.153607	-2.336042	8.291178
H	-0.158368	-3.377085	8.374845
H	0.939826	-2.397510	7.538728
N	-1.003156	-1.587888	7.775418
H	-1.876395	-1.880042	8.190388
H	-1.000250	-0.588430	7.920936
H	-1.131885	-1.700180	6.779969
N	-4.218944	-2.466745	8.658250
O	-4.720746	-1.589532	9.352344
O	-5.064699	-3.243544	8.228883
O	-3.059529	-2.812037	8.857268
C	4.724008	5.925852	-6.291951

H	5.029655	6.844270	-6.793138
H	4.700328	6.293924	-5.266249
H	5.570110	5.238848	-6.307307
C	3.501917	5.126449	-6.745041
H	3.593774	4.832855	-7.790730
H	2.581506	5.710336	-6.740682
N	3.221885	3.957312	-5.897374
H	4.037955	3.442775	-5.598407
H	2.712403	4.158656	-5.048853
H	2.622967	3.246567	-6.292645
N	2.147362	4.863526	-2.985605
O	2.898092	3.956658	-2.643451
O	1.993133	5.335660	-4.106488
O	1.089439	4.937466	-2.370456
C	-4.971349	-4.629471	4.975654
H	-5.775687	-4.155799	5.538480
H	-5.351954	-4.785338	3.966226
H	-4.812820	-5.595551	5.454882
C	-3.697476	-3.815726	5.205672
H	-2.837560	-4.344196	4.794135
H	-3.524626	-3.748647	6.279787
N	-3.673781	-2.580544	4.407170
H	-2.739628	-2.247240	4.597874
H	-3.936414	-2.869095	3.475579
H	-4.293475	-1.821310	4.651391
N	0.164942	-5.306183	-2.229334
O	-0.453813	-5.755504	-3.187629
O	-0.442281	-5.228778	-1.167089
O	0.826066	-4.313900	-2.514581
C	-8.450351	0.725381	3.220768
H	-8.510870	1.389454	2.358536
H	-8.558804	-0.335254	2.994071
H	-9.307897	0.978001	3.844385
C	-7.222497	1.171506	4.015242
H	-7.289659	0.742922	5.015195
H	-7.180228	2.257804	4.094434
N	-6.011769	0.543300	3.464486
H	-6.073422	-0.450388	3.294529
H	-5.949434	0.913026	2.526660
H	-5.143062	0.684419	3.960000
N	-1.816374	1.827042	7.844867
O	-1.715018	0.799043	8.505185
O	-2.590827	2.689729	8.243701
O	-1.582852	1.771116	6.642612
C	4.022645	-3.889419	-4.640407
H	3.483070	-4.373667	-5.454325
H	5.105342	-3.857608	-4.762293
H	3.856081	-4.509909	-3.759869
C	3.468972	-2.529088	-4.215216
H	3.826761	-1.917697	-5.043642
H	3.891906	-2.160912	-3.280511
N	2.001997	-2.636514	-4.198405
H	1.631787	-1.702033	-4.099462
H	1.673665	-2.830099	-5.133724
H	1.676254	-3.199668	-3.425845
N	2.623053	-0.945030	-1.242072
O	2.065798	-0.643897	-2.291768
O	3.253809	-0.030224	-0.724044
O	2.137975	-1.834593	-0.551816
C	-5.209487	4.501625	-1.579283
H	-4.643917	4.158262	-2.445501
H	-6.238177	4.147064	-1.643960
H	-5.168898	5.590242	-1.616223
C	-4.538733	4.013746	-0.294797
H	-5.051161	4.361914	0.602029
H	-3.578649	4.506328	-0.140849
N	-4.300222	2.563983	-0.223105

H	-3.768989	2.355973	0.610335
H	-5.105246	1.955828	-0.269827
H	-3.718158	2.144520	-0.933987
N	-2.593197	-0.316821	0.775130
O	-3.310645	0.105689	-0.124775
O	-2.840998	0.000219	1.933213
O	-1.412114	-0.386344	0.453747
C	-5.461574	5.541765	6.306359
H	-5.530514	6.552094	6.709575
H	-5.649944	5.630662	5.236446
H	-6.307478	5.044507	6.780999
C	-4.068063	5.016726	6.653204
H	-3.967718	5.262896	7.710290
H	-3.412747	5.707098	6.122122
N	-3.839967	3.644236	6.175620
H	-4.178312	3.491994	5.236234
H	-2.892635	3.301363	6.247037
H	-4.478774	3.001301	6.621331
N	-7.018747	0.690808	-0.564931
O	-6.746004	0.973376	0.596466
O	-7.506565	-0.433705	-0.589017
O	-6.091421	1.012435	-1.299572
C	-9.466067	-1.382742	8.043245
H	-9.406201	-0.301120	7.922368
H	-9.638828	-1.868365	7.082816
H	-10.301055	-1.493869	8.735015
C	-8.174622	-1.962895	8.620682
H	-8.133932	-3.050685	8.676870
H	-8.024118	-1.476033	9.584225
N	-7.048048	-1.522926	7.783366
H	-7.198877	-1.736917	6.807887
H	-7.088604	-0.513747	7.786904
H	-6.157275	-1.867270	8.112078
N	-3.409450	1.889898	-3.363641
O	-3.382807	0.672154	-3.503163
O	-2.813105	2.272015	-2.362923
O	-3.132828	2.527554	-4.373567
C	-2.897744	1.022925	11.728481
H	-3.125919	0.011264	12.064007
H	-1.994716	1.115617	11.125116
H	-2.740336	1.769382	12.507021
C	-4.105584	1.537856	10.945019
H	-3.983270	2.567699	10.609515
H	-5.001105	1.337335	11.533179
N	-4.114729	0.831029	9.654999
H	-3.340637	1.027227	9.036624
H	-4.122554	-0.177607	9.706897
H	-4.922527	1.125298	9.124936
N	-3.818969	-0.023929	5.984281
O	-5.013916	-0.188038	6.203936
O	-3.115367	-0.952007	6.367283
O	-3.700314	0.352152	4.823436
C	2.273021	-0.233158	-9.797613
H	1.600432	-1.084521	-9.693178
H	1.576715	0.592570	-9.944007
H	3.093130	-0.360243	-10.504275
C	2.837993	0.090926	-8.414278
H	3.432208	1.002167	-8.346107
H	3.470751	-0.745599	-8.117727
N	1.811091	0.200981	-7.366804
H	1.271674	-0.640620	-7.222452
H	2.313179	0.486696	-6.538326
H	1.159548	0.971487	-7.410536
N	-6.669693	2.153939	8.065639
O	-7.197477	1.055736	8.201538
O	-5.738890	2.237635	7.272117
O	-6.405821	2.662653	9.149455

C	-6.419491	-0.802908	-3.917979
H	-7.085691	-0.505831	-3.108027
H	-7.061182	-1.256690	-4.673236
H	-5.862856	0.028278	-4.350863
C	-5.455648	-1.893257	-3.448952
H	-4.952035	-2.370561	-4.289580
H	-6.236282	-2.557238	-3.077684
N	-4.611694	-1.360921	-2.368119
H	-3.974989	-2.006746	-1.923577
H	-4.085327	-0.628658	-2.822904
H	-5.054791	-0.808465	-1.648010
N	-4.893749	-5.942750	-4.453950
O	-3.982115	-6.398526	-3.772579
O	-5.859771	-5.455426	-3.877416
O	-4.565378	-5.542283	-5.565200
C	-0.612699	2.896156	-0.236076
H	0.021290	3.668473	0.199451
H	-1.395808	3.281239	-0.889187
H	-1.097978	2.361436	0.580428
C	0.167083	1.899810	-1.094608
H	0.903887	1.514404	-0.389852
H	0.713819	2.423223	-1.878966
N	-0.701182	0.923201	-1.770028
H	-0.136704	0.360762	-2.390614
H	-1.099100	0.267192	-1.113206
H	-1.475896	1.351592	-2.256237
N	0.260433	-2.425392	-7.002291
O	-0.396481	-1.451677	-7.353604
O	1.464215	-2.449628	-6.771218
O	-0.475817	-3.108454	-6.299129
C	-2.425232	5.907427	-4.732641
H	-2.141194	6.460551	-5.627893
H	-2.979854	6.578669	-4.076952
H	-3.171760	5.131519	-4.902235
C	-1.173474	5.353857	-4.051097
H	-1.307088	5.038262	-3.016377
H	-0.317887	6.017880	-4.174150
N	-0.759164	4.141976	-4.774653
H	0.172539	3.993532	-4.414105
H	-1.285664	3.308265	-4.555969
H	-0.573673	4.419978	-5.727758
N	0.578369	3.303300	-7.722461
O	-0.152367	2.318894	-7.715771
O	1.749968	3.119431	-8.033304
O	0.166185	4.304597	-7.147495
C	0.940536	0.898512	2.804974
H	1.077355	-0.100146	3.219779
H	1.904107	1.405232	2.751442
H	0.516585	0.631515	1.836946
C	-0.054713	1.790976	3.547152
H	-0.274162	2.733889	3.046295
H	0.361019	1.777405	4.554665
N	-1.301590	1.064426	3.832217
H	-1.754083	0.920453	2.940801
H	-1.177910	0.174761	4.294060
H	-1.866487	1.605010	4.471561
N	5.122124	1.483554	-5.195011
O	4.309157	1.316758	-6.097418
O	5.421923	0.672603	-4.325784
O	5.399799	2.664691	-5.019255
C	6.698903	1.484243	-1.202165
H	7.564959	1.903428	-0.689983
H	6.133911	0.877659	-0.494394
H	7.112200	0.959665	-2.063620
C	5.647899	2.491147	-1.670540
H	6.089453	3.163382	-2.406222
H	5.430101	3.173913	-0.849264

N	4.421187	1.910445	-2.237819
H	3.946242	1.388101	-1.515543
H	3.809498	2.662596	-2.521026
H	4.669925	1.257999	-2.967575
N	-3.428782	3.769736	2.929419
O	-4.535166	3.499889	3.383482
O	-2.658686	4.133978	3.811097
O	-3.017573	2.966859	2.099135
C	-1.432408	-6.258294	-7.621125
H	-0.756315	-6.950656	-8.122756
H	-1.068632	-5.274232	-7.916742
H	-2.474928	-6.457869	-7.868962
C	-1.133684	-6.273173	-6.121664
H	-0.150570	-5.948209	-5.781096
H	-1.220308	-7.231242	-5.609123
N	-1.940170	-5.302928	-5.365328
H	-1.617534	-4.394553	-5.666758
H	-2.928511	-5.507464	-5.327285
H	-1.572812	-5.426649	-4.432674
N	-0.510386	-2.248834	4.800892
O	-0.796416	-3.248032	5.451173
O	-1.223762	-1.754929	3.934734
O	0.090414	-1.333563	5.352610
C	-3.588459	-1.530722	-7.163766
H	-4.462736	-1.581957	-6.514833
H	-3.013203	-2.436560	-6.972359
H	-4.083838	-1.517227	-8.134599
C	-2.930608	-0.178117	-6.888936
H	-3.667223	0.602478	-6.698750
H	-2.372400	0.041709	-7.798980
N	-2.061945	-0.271740	-5.705509
H	-2.586494	-0.378116	-4.848986
H	-1.270327	-0.845767	-5.958364
H	-1.679494	0.648713	-5.542422
N	0.647733	1.106724	-4.561195
O	1.444393	1.828710	-5.150385
O	0.626989	-0.051322	-4.963159
O	-0.448171	1.583169	-4.287207

Return

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	-3.519066	1.205605	-5.467020
H	-3.022226	2.061202	-5.924407
H	-4.508865	1.162117	-5.921451
H	-3.771527	1.608216	-4.486068
C	-2.818958	-0.150516	-5.374148
H	-2.378608	-0.491175	-6.311242
H	-3.502392	-0.941672	-5.065780
N	-1.690224	-0.076346	-4.433777
H	-1.106596	-0.895436	-4.526345
H	-1.118568	0.723437	-4.665411
H	-1.917327	-0.000519	-3.452566
N	-10.249985	-5.145714	-1.416401
O	-11.165465	-4.584554	-0.824733
O	-9.858982	-4.583517	-2.433322
O	-9.401972	-5.748773	-0.768120
C	2.997870	-7.649835	-0.196845
H	3.819698	-7.042143	0.181849
H	3.006655	-8.635971	0.267439
H	3.092568	-7.739143	-1.279045
C	1.745378	-6.893993	0.247913
H	1.854601	-6.544063	1.274421
H	0.800139	-7.408339	0.074503
N	1.534513	-5.681683	-0.558116
H	2.414513	-5.189562	-0.498818
H	1.189224	-5.914762	-1.478197
H	0.933904	-5.036826	-0.064631
N	0.549062	-1.316353	-7.339060
O	1.722765	-1.580030	-7.102473
O	0.065906	-0.539297	-6.523082
O	-0.233175	-2.207776	-7.649779
C	-8.536664	-10.594626	0.271106
H	-7.767750	-10.997185	-0.388302
H	-8.172164	-10.660739	1.296225
H	-9.443134	-11.186868	0.145958
C	-8.963947	-9.133796	0.125344
H	-9.541029	-9.007212	1.041343
H	-9.648836	-9.043433	-0.717782
N	-7.894606	-8.124065	0.153482
H	-7.149215	-8.370713	-0.481858
H	-8.137900	-7.145771	0.091429
H	-7.496608	-8.223284	1.076440
N	-5.060635	-9.310273	-0.758144
O	-5.542370	-9.879977	0.214709
O	-4.032986	-8.708263	-0.467288
O	-5.924857	-8.780876	-1.448025
C	8.709244	0.305348	-0.726634
H	9.772994	0.416964	-0.516683
H	8.399594	0.838491	-1.625509
H	8.173520	0.873097	0.034129
C	8.283994	-1.158051	-0.602271
H	8.722640	-1.700043	0.235544
H	8.635722	-1.708695	-1.474727
N	6.815903	-1.245365	-0.571885
H	6.520453	-0.812567	-1.435305
H	6.390461	-2.160354	-0.615396
H	6.411970	-0.776957	0.226572
N	0.816605	-2.784895	-3.194829
O	1.335739	-2.895520	-4.299971
O	0.043867	-1.845554	-3.041242
O	1.613245	-3.041462	-2.298942
C	-10.245353	-4.652714	3.726167

H	-11.090913	-5.315310	3.910814
H	-9.538582	-4.753503	4.549828
H	-10.553389	-3.607910	3.766163
C	-9.457960	-4.973307	2.455312
H	-10.094484	-5.138360	1.586005
H	-9.107610	-5.997155	2.586043
N	-8.372584	-4.013584	2.200884
H	-7.858031	-4.160977	1.344374
H	-8.873943	-3.157555	2.011272
H	-7.757663	-3.877635	2.990497
N	-7.045003	-7.765628	3.713528
O	-7.026345	-7.901981	2.495277
O	-7.385860	-6.761227	4.328403
O	-6.103180	-8.095457	4.425747
C	-6.871557	3.465544	0.250703
H	-5.839994	3.341726	0.580318
H	-6.930601	4.533221	0.039328
H	-7.607965	3.334664	1.043593
C	-7.257428	2.441011	-0.816666
H	-6.752601	2.709585	-1.744630
H	-8.287300	2.607951	-1.132254
N	-7.088441	1.026907	-0.448435
H	-6.089453	0.885619	-0.401960
H	-7.514789	0.875114	0.454497
H	-7.592908	0.450535	-1.106774
N	-9.683744	-0.465258	1.446582
O	-9.496863	-1.028748	2.519257
O	-9.824358	-1.160938	0.446916
O	-9.019067	0.564295	1.482647
C	-3.510838	3.759262	4.494883
H	-4.201719	3.718858	3.652771
H	-4.071715	4.242662	5.294783
H	-2.686803	4.365148	4.118095
C	-3.281012	2.441253	5.235068
H	-4.226162	1.928493	5.413583
H	-2.701183	2.584151	6.146922
N	-2.547887	1.358217	4.561717
H	-3.047895	1.214961	3.695940
H	-1.620671	1.563444	4.217840
H	-2.397256	0.479330	5.036025
N	-1.491342	-6.356519	1.216782
O	-0.765958	-7.126992	1.835866
O	-1.193819	-6.160292	0.043730
O	-2.679700	-6.376685	1.517569
C	-7.421803	1.821349	4.541676
H	-7.143149	2.502449	5.345762
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H	-8.443748	1.943599	4.182814
C	-7.130125	0.367712	4.915450
H	-7.931375	0.032914	5.574242
H	-6.144838	0.272331	5.371750
N	-7.081697	-0.471004	3.707952
H	-6.765316	-1.365798	4.053418
H	-7.907436	-0.416348	3.128930
H	-6.323091	-0.063214	3.180386
N	-5.526510	-2.227920	13.667049
O	-6.111855	-2.250849	12.590053
O	-4.758301	-3.133922	13.970516
O	-5.211943	-1.136297	14.128007
C	-4.417568	-6.824461	11.044281
H	-5.271646	-7.499500	10.989747
H	-3.928919	-6.921694	10.074813
H	-3.716892	-7.199496	11.790271
C	-4.745671	-5.378025	11.415780
H	-5.202691	-5.506765	12.396933
H	-5.582150	-5.039776	10.804233
N	-3.495142	-4.613859	11.542540

H	-3.735795	-3.633023	11.554559
H	-2.936065	-4.863458	12.345804
H	-2.971168	-4.760422	10.691616
N	-6.847641	-3.176429	5.483448
O	-7.219908	-4.086868	6.215292
O	-7.260629	-3.152078	4.329358
O	-6.522721	-2.102232	5.977010
C	-1.379007	3.965081	0.930104
H	-1.784772	4.953337	1.146444
H	-1.535482	3.484635	1.895913
H	-0.330807	3.865446	0.648234
C	-2.156856	3.209004	-0.147458
H	-2.162638	3.602119	-1.164083
H	-3.209872	3.248116	0.131339
N	-1.753300	1.797829	-0.245279
H	-2.495440	1.492452	-0.858528
H	-0.905311	1.652481	-0.774324
H	-1.770071	1.282319	0.623092
N	-0.012519	0.657512	2.926774
O	-0.094181	1.752414	3.472298
O	-0.217810	-0.306495	3.655899
O	-0.607364	0.599357	1.856329
C	2.627895	1.626245	5.804780
H	1.693109	2.169310	5.943907
H	2.976793	1.434902	6.819550
H	3.338076	2.286029	5.306353
C	2.579461	0.249450	5.141507
H	3.577712	-0.160500	5.294918
H	2.450239	0.236386	4.059273
N	1.652089	-0.637587	5.860526
H	1.830756	-1.550898	5.468046
H	1.825959	-0.727747	6.851355
H	0.706695	-0.305415	5.734068
N	-1.288487	-0.363750	7.335551
O	-0.507912	0.570460	7.190529
O	-2.024037	-0.573449	6.377391
O	-0.611279	-1.306846	7.729294
C	-6.392330	2.706426	13.899811
H	-6.840123	1.770809	14.234778
H	-5.652977	3.031266	14.631887
H	-7.258013	3.365142	13.969000
C	-5.918942	2.402077	12.478151
H	-5.451687	3.351562	12.216906
H	-6.657553	2.279871	11.685927
N	-5.070519	1.206201	12.360244
H	-4.873156	1.102733	11.375134
H	-4.211672	1.378725	12.862954
H	-5.513370	0.388888	12.755190
N	-3.255985	-4.112793	8.301179
O	-4.254881	-4.798541	8.488346
O	-2.375078	-4.270545	9.139149
O	-3.298679	-3.152821	7.539794
C	0.794019	3.386410	10.205897
H	1.613543	2.994989	9.603177
H	0.824626	4.474694	10.152978
H	1.007624	3.009242	11.206005
C	-0.583698	2.946357	9.709822
H	-0.705808	3.218155	8.661340
H	-1.404699	3.529476	10.126989
N	-0.838378	1.497704	9.690210
H	-0.077590	1.037303	9.211324
H	-0.981521	1.231920	10.654040
H	-1.704093	1.282524	9.216569
N	2.194923	-0.734751	9.483777
O	1.828249	-1.697418	10.148532
O	1.722877	0.367513	9.739245
O	2.405829	-0.912559	8.289215

C	-6.274370	-6.831644	-3.768265
H	-7.146432	-7.481806	-3.698282
H	-5.674318	-7.246033	-4.578401
H	-5.725758	-6.868251	-2.827103
C	-6.780408	-5.398925	-3.938800
H	-7.723002	-5.431148	-4.485222
H	-6.141812	-4.852321	-4.632715
N	-7.112450	-4.673025	-2.703220
H	-7.519609	-3.769042	-2.895926
H	-7.817546	-5.280576	-2.311020
H	-6.284758	-4.717661	-2.126130
N	-5.464085	-5.179974	0.124209
O	-5.002348	-5.161758	-1.011372
O	-6.653877	-5.441776	0.261798
O	-5.212550	-4.122098	0.690516
C	-2.476036	-9.856350	2.280157
H	-1.834927	-10.318381	3.030893
H	-2.963415	-10.601822	1.651799
H	-1.894274	-9.207178	1.625765
C	-3.546878	-9.067570	3.034454
H	-3.188065	-8.412349	3.828203
H	-4.233170	-9.715798	3.579343
N	-4.344885	-8.205709	2.148892
H	-3.705415	-7.434668	2.019767
H	-4.423151	-8.770595	1.315298
H	-5.178513	-7.846391	2.591675
N	-2.471505	-6.997116	6.232022
O	-1.858540	-5.936523	6.182096
O	-3.668472	-6.932308	5.974833
O	-1.892255	-8.072564	6.336710
C	2.628116	1.093813	0.195527
H	2.369561	0.861840	1.228696
H	3.706650	1.128084	0.041610
H	2.176279	2.061414	-0.022857
C	2.251336	-0.029814	-0.770569
H	2.643986	0.095235	-1.779671
H	1.162377	-0.041740	-0.816672
N	2.534054	-1.399286	-0.313994
H	2.028962	-1.464566	0.558198
H	2.461956	-2.195504	-0.931197
H	3.500868	-1.404304	-0.021853
N	5.149653	-0.185336	1.970100
O	6.289823	0.235806	1.809705
O	4.695393	-0.374765	3.092972
O	4.784840	-0.921811	1.060379
C	-5.913580	-8.564546	7.543372
H	-4.904557	-8.428291	7.932482
H	-6.474161	-9.101586	8.308510
H	-5.836220	-9.046226	6.568641
C	-6.692514	-7.249564	7.587258
H	-6.543587	-6.821520	8.578570
H	-7.741372	-7.385207	7.323445
N	-6.062284	-6.374127	6.587128
H	-6.253412	-6.627448	5.628275
H	-6.271548	-5.388302	6.520362
H	-5.056773	-6.282925	6.614157
N	1.863429	-4.143781	4.758780
O	0.816384	-4.468765	5.307560
O	2.127340	-2.951267	4.865261
O	2.670882	-4.950747	4.311679
C	-1.473980	-8.627202	-2.594129
H	-0.885519	-9.128017	-3.362893
H	-0.841849	-8.364876	-1.745780
H	-2.141237	-9.368361	-2.154183
C	-2.218481	-7.378738	-3.068362
H	-2.950807	-7.681153	-3.816923
H	-1.643397	-6.727352	-3.726446

N	-2.827376	-6.563406	-2.006137
H	-2.088203	-6.215431	-1.412306
H	-3.283231	-5.732874	-2.356155
H	-3.486032	-7.088714	-1.449070
N	1.292753	-6.512478	-3.855777
O	2.503625	-6.396546	-3.702720
O	0.721851	-6.365407	-4.930726
O	0.597285	-6.148350	-2.914071
C	-1.449796	-0.974476	16.417586
H	-0.561270	-1.584944	16.256492
H	-1.275888	0.071358	16.164430
H	-1.642829	-0.909897	17.488412
C	-2.581946	-1.689043	15.679025
H	-3.481703	-1.148152	15.972239
H	-2.534729	-2.695601	16.094609
N	-2.509243	-1.499274	14.222130
H	-2.403089	-0.550944	13.891222
H	-1.856650	-2.027426	13.660633
H	-3.327692	-1.967141	13.859720
N	-4.626951	1.838349	8.655408
O	-5.556772	1.528786	7.918740
O	-4.828979	1.688056	9.855272
O	-3.459874	1.966009	8.302266
C	-7.462493	-2.131251	9.281309
H	-7.665063	-2.936062	8.574666
H	-7.976424	-2.626443	10.105178
H	-8.064076	-1.256909	9.032861
C	-5.982495	-1.840637	9.532289
H	-5.489943	-2.766385	9.829749
H	-5.792004	-1.068989	10.278192
N	-5.364005	-1.290864	8.316122
H	-5.712640	-0.350108	8.199801
H	-4.389426	-1.202339	8.566044
H	-5.530583	-1.813371	7.467984
N	5.254219	-4.327629	-0.440564
O	5.464610	-4.052405	0.735473
O	4.129441	-4.687105	-0.770303
O	5.769212	-3.527175	-1.213306
C	2.533169	1.883007	-6.700961
H	1.728425	2.472740	-6.261983
H	3.104676	2.729747	-7.081107
H	2.094779	1.229725	-7.455373
C	3.230333	1.106743	-5.583277
H	3.587110	1.645612	-4.705535
H	4.139556	0.592514	-5.894696
N	2.423243	0.028886	-4.991103
H	1.524262	0.345608	-4.657008
H	2.173674	-0.639182	-5.706296
H	2.928884	-0.398019	-4.228096
N	-7.581736	-1.361326	-2.745376
O	-7.550183	-2.082816	-1.754653
O	-8.082564	-1.990858	-3.670544
O	-7.961089	-0.213357	-2.542064
C	-3.503634	-3.386407	3.943625
H	-3.838041	-3.056901	2.959908
H	-3.490632	-4.472680	4.032750
H	-4.174604	-3.018370	4.719801
C	-2.037364	-2.977391	4.087149
H	-2.028164	-1.888285	4.044002
H	-1.425500	-3.553860	3.393315
N	-1.578979	-3.245817	5.458890
H	-0.624434	-2.933613	5.565991
H	-2.178565	-2.746238	6.099997
H	-1.632300	-4.215274	5.737117
N	0.711825	-3.545107	1.659981
O	0.693938	-4.621094	2.247355
O	0.385120	-3.566626	0.478509

O	1.647264	-2.803884	1.940373
C	-11.982095	-1.698017	-4.060919
H	-12.609461	-2.574517	-4.222967
H	-12.674820	-0.956899	-4.459638
H	-11.096353	-1.740475	-4.694762
C	-11.594404	-1.243720	-2.653385
H	-12.410503	-1.451542	-1.961364
H	-11.435480	-0.166263	-2.697311
N	-10.466012	-2.049052	-2.161434
H	-10.058159	-1.697848	-1.306794
H	-10.670728	-3.033620	-2.255335
H	-9.644313	-1.965182	-2.742704
N	-1.759148	1.614246	12.856331
O	-2.438497	1.126702	13.752913
O	-2.447729	2.179620	12.014141
O	-0.637548	1.228994	12.545411
C	3.025542	-1.907935	13.561985
H	2.466599	-2.769882	13.926306
H	3.591663	-2.060924	12.643180
H	3.902619	-1.781443	14.196679
C	2.030133	-0.754270	13.435265
H	2.382285	0.240728	13.163110
H	1.512957	-0.686562	14.392367
N	0.953276	-1.055040	12.479359
H	0.213655	-0.384900	12.324529
H	1.330652	-1.219371	11.557035
H	0.532070	-1.941123	12.719241
N	-2.696921	-1.271325	10.692335
O	-3.494988	-1.883729	11.393139
O	-1.606979	-0.953907	11.155314
O	-3.227093	-0.759687	9.712427
C	4.301542	-2.985712	-5.684726
H	3.560251	-2.239352	-5.399184
H	5.339692	-2.658777	-5.743542
H	4.066654	-3.287375	-6.705475
C	4.287986	-4.215414	-4.776162
H	5.221784	-4.768670	-4.676017
H	3.468289	-4.853660	-5.106067
N	4.009482	-3.729667	-3.415895
H	4.502748	-2.868702	-3.227413
H	3.052278	-3.413947	-3.351220
H	4.255447	-4.377387	-2.681007
N	-4.204822	0.623633	-1.892298
O	-4.862355	-0.325289	-1.479654
O	-3.035038	0.457552	-2.219558
O	-4.438835	1.696393	-1.346865
C	1.670001	-8.373382	5.458161
H	2.274920	-9.278810	5.409434
H	2.332398	-7.596147	5.839260
H	0.969938	-8.706738	6.224246
C	0.861627	-8.043632	4.202918
H	0.220709	-8.917751	4.087857
H	1.408271	-7.922274	3.267743
N	0.009691	-6.854647	4.358999
H	0.475858	-5.962469	4.441503
H	-0.482686	-6.865192	3.477209
H	-0.761687	-6.858177	5.010967
N	5.468454	-0.642581	-3.224591
O	5.681084	0.255527	-2.417580
O	4.296963	-0.999588	-3.167784
O	6.387090	-1.440837	-3.372820
C	6.223964	-4.601736	4.150435
H	5.557611	-5.404542	4.465992
H	6.698368	-4.940246	3.229320
H	7.147636	-4.469767	4.713918
C	5.480998	-3.272978	4.008146
H	6.251440	-2.519460	3.844653

H	4.999853	-2.841519	4.885894
N	4.471023	-3.231255	2.939478
H	4.378195	-2.228101	2.867610
H	4.961334	-3.522954	2.106047
H	3.655408	-3.750056	3.232253
N	-0.034800	2.452267	-3.483635
O	-1.238335	2.568587	-3.686239
O	0.263430	2.187439	-2.324325
O	0.495882	1.739057	-4.327902
C	1.514739	-5.250324	9.351277
H	2.024341	-6.097896	8.892989
H	2.314056	-4.721079	9.870019
H	0.952085	-5.586288	10.222281
C	0.698002	-4.456970	8.330800
H	-0.013564	-4.993335	7.703037
H	1.348842	-4.036851	7.563984
N	0.089622	-3.330339	9.054966
H	-0.227903	-2.660444	8.369022
H	-0.785459	-3.525320	9.520064
H	0.702727	-2.883533	9.721725
N	-0.408774	-3.915460	13.066775
O	-1.488710	-4.340724	13.461698
O	-0.259896	-3.715978	11.866309
O	-0.107930	-2.988610	13.810762
C	0.194301	-5.489924	-7.868915
H	0.892649	-6.160531	-7.368219
H	-0.000288	-6.104355	-8.747955
H	0.733334	-4.598405	-8.189444
C	-0.997755	-5.083150	-7.002096
H	-1.469781	-6.007749	-6.669820
H	-1.669899	-4.581795	-7.698491
N	-0.548185	-4.189130	-5.923923
H	0.071715	-4.691384	-5.304597
H	-0.253618	-3.290033	-6.277415
H	-1.343929	-3.997831	-5.332066
N	-3.460290	-3.933980	-4.297805
O	-2.628616	-3.033581	-4.323836
O	-3.363682	-4.910395	-5.032895
O	-3.887008	-4.211384	-3.182442
C	-1.849832	-1.642839	0.236701
H	-1.915823	-2.039842	1.249684
H	-0.803112	-1.389071	0.069133
H	-2.347850	-0.676437	0.158304
C	-2.291463	-2.604613	-0.866836
H	-1.678298	-3.505652	-0.882846
H	-2.077627	-2.159361	-1.838497
N	-3.751302	-2.716432	-1.008985
H	-4.169325	-3.108362	-0.177272
H	-4.210233	-1.834893	-1.188908
H	-4.054645	-3.414021	-1.673404
N	-4.510442	0.510642	2.140014
O	-5.665211	0.782531	1.830726
O	-4.310971	-0.296202	3.041286
O	-3.721134	1.444135	2.046959

Return

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	-4.649892	0.024064	-5.956870
H	-5.125307	-0.956371	-5.985653
H	-4.692262	0.416367	-4.940797
H	-5.189601	0.647990	-6.669281
C	-3.177966	-0.272378	-6.245656
H	-2.587831	0.564426	-5.872027
H	-3.003659	-0.421132	-7.311296
N	-2.858339	-1.606780	-5.715512
H	-3.423831	-2.251990	-6.248449
H	-1.875212	-1.809895	-5.604585
H	-3.155657	-1.663162	-4.751912
N	-8.250771	-5.863476	0.637101
O	-7.457116	-5.531650	-0.236443
O	-9.131010	-5.035695	0.844548
O	-8.036687	-6.560916	1.622404
C	1.001088	-10.106689	-4.694726
H	0.141245	-10.454125	-4.121962
H	0.939376	-10.488698	-5.713726
H	1.967065	-10.420038	-4.298745
C	1.132586	-8.596750	-4.493151
H	1.972511	-8.237651	-5.087856
H	1.309117	-8.456203	-3.426763
N	0.106466	-7.692980	-5.035479
H	0.058192	-6.737675	-4.711191
H	0.215558	-7.540191	-6.027878
H	-0.853090	-7.975026	-4.894763
N	0.877223	-1.954272	-6.911982
O	2.007506	-2.152266	-6.480317
O	0.125954	-1.365543	-6.142521
O	0.386556	-2.781019	-7.672779
C	-6.248778	-9.804642	-2.878082
H	-5.842824	-9.328749	-3.770734
H	-5.293024	-9.929681	-2.369160
H	-6.660658	-10.796480	-3.064394
C	-7.164361	-8.866317	-2.091256
H	-7.368068	-9.417136	-1.172996
H	-8.142831	-8.634758	-2.512060
N	-6.458312	-7.621404	-1.751362
H	-7.010719	-6.982887	-1.197068
H	-5.718206	-7.901576	-1.123789
H	-6.121525	-7.097352	-2.546374
N	-6.692425	-5.756954	-4.133686
O	-5.942340	-5.957628	-5.082463
O	-6.267338	-5.140840	-3.162717
O	-7.714557	-6.411145	-3.959452
C	5.740364	-2.909180	-0.828557
H	5.500031	-3.199789	-1.851243
H	5.611035	-1.826884	-0.831601
H	6.810603	-3.112538	-0.792032
C	5.144613	-3.563526	0.418340
H	5.454225	-2.925293	1.245926
H	5.421061	-4.596495	0.629647
N	3.680234	-3.424118	0.417545
H	3.283771	-3.364974	1.344594
H	3.366413	-2.572437	-0.025463
H	3.298510	-4.223462	-0.067672
N	-0.783546	-4.584855	-5.564709
O	-1.343188	-3.774242	-4.834788
O	-1.506017	-5.477626	-5.993746
O	0.371984	-4.841554	-5.245440
C	-5.331206	-9.123827	4.448072

H	-5.620676	-9.772165	3.621050
H	-4.257496	-8.957694	4.535512
H	-5.632311	-9.581859	5.390220
C	-6.058103	-7.802754	4.194638
H	-6.007739	-7.137704	5.056770
H	-7.128480	-7.993333	4.116714
N	-5.627890	-7.169044	2.938783
H	-5.980526	-6.230935	2.813488
H	-4.640580	-6.956917	2.920893
H	-5.948300	-7.622933	2.095324
N	-4.435262	-8.549332	0.542697
O	-5.651650	-8.399761	0.509459
O	-3.836128	-8.681917	1.604080
O	-3.698439	-8.554329	-0.437173
C	-4.396144	1.637844	-0.062450
H	-3.647024	1.540067	0.723273
H	-3.848359	1.142431	-0.864072
H	-4.401524	2.723585	-0.158564
C	-5.852989	1.198298	0.086693
H	-6.507238	1.708560	-0.620194
H	-6.192146	1.587134	1.046838
N	-6.125849	-0.244049	-0.008305
H	-5.739513	-0.692443	-0.826710
H	-5.762475	-0.767586	0.775255
H	-7.121552	-0.400530	0.056418
N	-6.967378	-3.932652	5.694434
O	-7.320883	-4.941450	5.094070
O	-7.142612	-2.859165	5.128753
O	-5.970355	-4.025310	6.401849
C	-3.967074	6.146431	5.552822
H	-4.429363	5.860816	4.607934
H	-4.646667	6.044028	6.398852
H	-3.878869	7.215392	5.358804
C	-2.637266	5.424412	5.772228
H	-2.139785	5.713327	6.698047
H	-1.907897	5.675202	5.002017
N	-2.720552	3.955988	5.747033
H	-1.937400	3.822148	6.370618
H	-3.523216	3.592331	6.240576
H	-2.628447	3.653249	4.787884
N	-2.972776	-7.952577	-3.713520
O	-2.093949	-7.308744	-3.151188
O	-4.070422	-7.414931	-3.809364
O	-2.625053	-8.179933	-4.866982
C	-7.662851	1.173005	5.255950
H	-7.599243	2.243887	5.448991
H	-8.436552	0.967022	4.516316
H	-7.826410	0.716554	6.232167
C	-6.307241	0.702292	4.728131
H	-5.486482	0.639628	5.442643
H	-5.834033	1.358293	3.997491
N	-6.459811	-0.524052	3.930232
H	-7.124816	-0.454366	3.173256
H	-5.512112	-0.659522	3.608339
H	-6.646850	-1.324197	4.517500
N	-6.669195	-0.412945	12.739386
O	-6.263604	0.612050	12.202769
O	-6.852176	-1.333069	11.950104
O	-6.147536	-0.684677	13.815076
C	-6.769099	-4.506882	13.135273
H	-7.463264	-3.843130	13.650702
H	-7.069818	-4.466662	12.088349
H	-6.953314	-5.552890	13.380288
C	-5.380042	-4.076161	13.607334
H	-4.601294	-4.830819	13.497146
H	-5.490527	-3.737242	14.637396
N	-5.002089	-2.914890	12.787308

H	-5.538516	-2.062517	12.863508
H	-4.084107	-2.564465	13.020997
H	-5.000479	-3.314967	11.859928
N	-3.177468	-0.407729	4.392818
O	-3.034871	0.566008	5.123966
O	-3.745380	-0.255455	3.317009
O	-3.127210	-1.527338	4.889837
C	1.554232	3.656962	-1.182188
H	1.411157	4.202411	-0.249389
H	2.467782	3.077420	-1.049303
H	1.826193	4.422472	-1.908916
C	0.299202	2.864449	-1.549153
H	0.538347	2.347010	-2.478220
H	-0.616213	3.432254	-1.715620
N	-0.042931	1.940084	-0.457213
H	-0.460310	2.386562	0.346872
H	-0.798689	1.404085	-0.859252
H	0.587555	1.215953	-0.143808
N	3.219271	0.374520	0.557705
O	2.124397	0.770928	0.174055
O	3.468111	0.383057	1.758156
O	3.563281	-0.613790	-0.081026
C	-0.203791	-1.164598	6.172001
H	0.678857	-1.792888	6.052488
H	-0.838165	-1.327102	5.300644
H	0.124325	-0.129879	6.073027
C	-0.990953	-1.327258	7.472678
H	-0.375704	-1.135303	8.351724
H	-1.476395	-2.289125	7.637774
N	-2.149959	-0.424485	7.547142
H	-2.793322	-0.779241	8.240201
H	-1.954844	0.546272	7.746290
H	-2.723893	-0.410706	6.716172
N	-0.409119	2.512962	7.812598
O	-0.913600	3.577496	8.152219
O	-0.957768	2.130531	6.785074
O	-0.411387	1.641059	8.674488
C	-3.257034	4.434133	10.880824
H	-3.990643	5.085748	11.355498
H	-2.407862	4.702394	11.509347
H	-2.989958	4.865788	9.916229
C	-3.484276	2.924239	10.960975
H	-4.409036	2.684433	10.436178
H	-3.625629	2.633800	12.002015
N	-2.235599	2.235176	10.600645
H	-1.881790	2.337207	9.660162
H	-1.416165	2.474566	11.140386
H	-2.371041	1.239484	10.702394
N	-3.846388	-3.054523	9.419943
O	-4.792532	-3.246329	10.175654
O	-3.879261	-2.048454	8.720070
O	-2.761761	-3.321004	9.925559
C	3.083605	2.693433	10.173317
H	2.852564	2.687355	9.108102
H	2.336103	3.374809	10.579600
H	3.947140	3.341288	10.323949
C	3.131986	1.294730	10.789054
H	3.454591	1.319778	11.829918
H	3.738895	0.545283	10.281029
N	1.797719	0.693162	10.641782
H	1.598405	0.475219	9.675928
H	1.834495	-0.254169	10.990080
H	1.077151	1.102657	11.219014
N	2.107385	-2.325563	11.528576
O	1.685973	-1.900072	10.458789
O	2.976857	-1.638859	12.053489
O	1.232607	-2.863230	12.198467

C	-8.904708	-1.608191	-3.131563
H	-9.497783	-1.710039	-4.040402
H	-9.511942	-1.098285	-2.383658
H	-7.977131	-1.054307	-3.276180
C	-8.727426	-3.018304	-2.567651
H	-8.054395	-3.505148	-3.273422
H	-9.695271	-3.519502	-2.580893
N	-8.103942	-3.151105	-1.241955
H	-8.662733	-2.725145	-0.516413
H	-8.032196	-4.132641	-1.014931
H	-7.139350	-2.854143	-1.203536
N	-5.712533	-3.257834	1.888791
O	-5.907752	-4.316650	2.475199
O	-6.660322	-2.655337	1.397091
O	-4.743526	-2.542189	2.116729
C	0.298227	-9.089507	0.974540
H	0.529026	-10.150770	1.067024
H	1.329429	-8.744513	0.899034
H	-0.077549	-8.724548	1.930415
C	-0.623115	-8.818708	-0.215266
H	-1.513746	-9.407449	0.004420
H	-0.246888	-9.288638	-1.123956
N	-0.941138	-7.410779	-0.498884
H	-1.421591	-6.985771	0.281266
H	-0.027691	-6.999004	-0.625990
H	-1.522748	-7.323557	-1.319994
N	-2.233796	-5.435954	2.627303
O	-1.711192	-6.094018	1.734602
O	-3.036256	-5.996887	3.365197
O	-1.673309	-4.423286	3.031573
C	2.025806	2.844036	2.935700
H	2.826829	2.665294	2.218404
H	1.427719	3.621321	2.460072
H	2.529079	3.307773	3.784090
C	1.304776	1.625434	3.512732
H	0.634728	1.389347	2.686053
H	0.748584	1.948401	4.392756
N	2.141881	0.525032	4.014938
H	2.805097	0.212432	3.320298
H	2.604770	1.046373	4.745717
H	1.587522	-0.191876	4.460840
N	3.325838	0.976745	7.034372
O	2.873359	1.998132	6.529292
O	2.848973	0.518394	8.066647
O	3.632320	0.113141	6.219920
C	-3.188955	-5.968617	6.616179
H	-3.242299	-6.730669	5.838663
H	-2.586107	-6.332396	7.448248
H	-4.183688	-5.959468	7.061740
C	-2.752732	-4.557734	6.220000
H	-1.770575	-4.580493	5.747825
H	-2.744965	-3.822814	7.024943
N	-3.606053	-4.101817	5.111929
H	-3.188464	-3.229288	4.821391
H	-3.539826	-4.764338	4.352468
H	-4.573459	-4.018881	5.390044
N	0.656264	-4.381681	7.269246
O	-0.180789	-5.084850	7.824197
O	1.100445	-3.449417	7.930052
O	0.871308	-4.370166	6.062308
C	-3.393495	-8.153850	-8.294114
H	-2.775790	-7.469698	-8.875901
H	-2.719108	-8.685067	-7.622465
H	-3.953560	-8.822707	-8.947610
C	-4.583590	-7.685318	-7.456265
H	-4.961497	-8.537036	-6.890702
H	-5.401759	-7.305511	-8.068185

N	-4.082920	-6.657846	-6.530267
H	-3.615432	-5.811507	-6.822272
H	-4.831016	-6.361412	-5.919874
H	-3.464929	-7.075204	-5.849091
N	0.773217	-6.626210	-8.570897
O	1.687014	-6.183952	-7.883540
O	0.296805	-5.893143	-9.430386
O	-0.016962	-7.450606	-8.124730
C	-4.248078	2.113042	15.628383
H	-4.868126	2.536520	16.418513
H	-3.247501	2.534794	15.533135
H	-4.749350	2.373619	14.696221
C	-4.126257	0.597969	15.794384
H	-5.095354	0.152543	16.019210
H	-3.473219	0.441751	16.653009
N	-3.579562	0.028169	14.553299
H	-2.648638	0.375617	14.372302
H	-3.540879	-0.961657	14.750396
H	-4.087728	0.203595	13.698259
N	-4.993562	2.002200	7.730488
O	-6.129143	1.617996	7.987237
O	-3.995406	1.343645	8.000793
O	-4.861383	3.116559	7.236717
C	-8.340696	-1.235060	8.876357
H	-8.863751	-0.283347	8.969924
H	-8.929816	-1.791489	8.147368
H	-8.574018	-1.737609	9.815029
C	-6.833039	-1.419306	8.700674
H	-6.425206	-1.360871	7.691537
H	-6.420491	-2.428193	8.693608
N	-6.104282	-0.485929	9.573348
H	-6.209571	0.481809	9.304093
H	-6.447569	-0.550028	10.521054
H	-5.107674	-0.648207	9.596533
N	1.091599	-5.044957	0.179382
O	1.212303	-6.234582	0.450120
O	0.270164	-4.768664	-0.687789
O	1.270364	-4.235771	1.082895
C	2.749902	-0.306121	-3.575094
H	3.216821	0.436732	-2.928366
H	3.441858	-1.075444	-3.917789
H	2.440213	0.240459	-4.465849
C	1.561866	-0.947863	-2.857751
H	0.817144	-0.227032	-2.520272
H	1.892647	-1.622676	-2.068251
N	0.811279	-1.920306	-3.666957
H	0.822359	-1.654795	-4.641370
H	1.459135	-2.693497	-3.717524
H	-0.138574	-2.125228	-3.391481
N	-8.980457	-0.652770	1.481412
O	-8.325476	0.312063	1.859794
O	-9.109044	-1.518427	2.340004
O	-8.648997	-1.039641	0.366270
C	0.232634	-1.484516	1.777080
H	0.591061	-2.076792	2.619006
H	0.527442	-2.067887	0.904803
H	0.830714	-0.579106	1.880195
C	-1.245551	-1.095144	1.811715
H	-1.405025	-0.259554	1.130204
H	-1.331858	-0.787801	2.853920
N	-2.046393	-2.292833	1.515012
H	-1.683482	-3.029175	2.103396
H	-2.986687	-2.088273	1.821773
H	-2.025812	-2.525724	0.532445
N	3.864998	-2.990900	3.893950
O	3.556567	-3.782736	3.010242
O	4.063834	-3.531562	4.976182

O	3.263684	-1.923807	3.946958
C	-10.573967	-5.570132	4.328887
H	-9.853042	-5.842602	5.099683
H	-11.602787	-5.718705	4.656843
H	-10.469676	-6.319127	3.543884
C	-10.254302	-4.149099	3.863784
H	-10.220033	-3.416136	4.669818
H	-10.979344	-3.791026	3.132896
N	-8.962729	-3.920978	3.197721
H	-8.899669	-2.970136	2.863022
H	-8.095780	-4.087046	3.688556
H	-8.957762	-4.426427	2.323309
N	-0.463623	1.685621	13.393373
O	-0.113966	2.200186	12.336945
O	-1.619576	1.510395	13.762353
O	0.430823	1.104066	13.997388
C	1.257471	-1.939654	16.592818
H	0.736079	-1.123446	17.092873
H	0.469836	-2.675946	16.432802
H	2.079592	-2.232027	17.246067
C	1.606528	-1.635197	15.135661
H	2.172631	-2.400850	14.605187
H	2.281910	-0.781395	15.081077
N	0.418656	-1.428654	14.292962
H	-0.293839	-2.067030	14.616885
H	0.239530	-0.446592	14.139440
H	0.695415	-1.639278	13.344730
N	-2.583589	-0.844711	11.454764
O	-1.522622	-0.354378	11.084633
O	-3.671990	-0.307605	11.281625
O	-2.534524	-1.516643	12.479058
C	4.763372	-6.049446	-6.393253
H	4.943695	-6.555425	-5.444797
H	4.188060	-6.496514	-7.203959
H	5.796121	-6.051418	-6.741858
C	4.374831	-4.579436	-6.232165
H	4.884213	-3.966774	-6.975990
H	4.712657	-4.144609	-5.291475
N	2.919733	-4.602376	-6.017681
H	2.475735	-5.191193	-6.707798
H	2.809016	-5.001281	-5.096423
H	2.577381	-3.654442	-6.083384
N	-5.386646	-1.704858	-2.849777
O	-5.545037	-0.498170	-2.701815
O	-4.421569	-2.110791	-3.487681
O	-5.673400	-2.231889	-1.780625
C	2.741972	-6.777451	4.389146
H	3.447533	-6.266738	3.733817
H	3.026417	-6.206431	5.272960
H	2.963410	-7.830297	4.564020
C	1.354467	-6.427619	3.850362
H	0.486677	-6.854269	4.353364
H	1.311320	-6.897916	2.867988
N	1.312238	-4.974827	3.623530
H	2.080049	-4.535749	3.135906
H	0.527703	-4.635710	3.085380
H	1.246696	-4.635196	4.572453
N	2.952409	-4.890551	-2.664943
O	2.709351	-5.530537	-3.682006
O	3.495444	-5.449631	-1.718572
O	3.067417	-3.680360	-2.823961
C	4.330957	-4.645059	7.912600
H	5.083154	-5.164495	8.506306
H	3.323988	-4.953046	8.194130
H	4.556858	-5.101283	6.948791
C	4.343039	-3.136665	8.162482
H	5.357436	-2.897348	7.843382

H	4.274603	-2.812336	9.200860
N	3.428535	-2.437510	7.246673
H	3.363218	-1.452655	7.460902
H	3.639874	-2.647504	6.281614
H	2.483487	-2.791275	7.289510
N	-1.872054	-0.640769	-2.159294
O	-1.635959	-1.464093	-1.282099
O	-1.672236	-0.963370	-3.325088
O	-1.632438	0.494082	-1.762086
C	1.266983	-5.845178	10.897595
H	1.325522	-6.922337	11.053804
H	1.717029	-5.571607	9.943279
H	1.842794	-5.579687	11.784194
C	-0.204393	-5.434484	10.832593
H	-0.587801	-5.766596	11.797373
H	-0.659715	-5.947792	9.985659
N	-0.362379	-3.980210	10.677777
H	0.215304	-3.415349	11.283843
H	-0.096533	-3.642394	9.763826
H	-1.322429	-3.728339	10.864768
N	-2.296793	-2.662132	15.606630
O	-1.485254	-3.282264	14.928460
O	-3.474423	-2.677373	15.265993
O	-1.838576	-1.588767	15.982127
C	-2.479589	-4.140725	-11.517819
H	-2.344940	-3.918347	-12.576364
H	-2.535404	-5.204778	-11.288087
H	-3.458163	-3.757204	-11.229021
C	-1.379482	-3.432911	-10.726236
H	-1.520945	-2.352142	-10.721118
H	-0.372145	-3.451716	-11.142191
N	-1.471371	-3.850212	-9.318665
H	-0.906317	-4.675708	-9.179488
H	-1.212921	-3.104200	-8.688769
H	-2.394307	-4.123258	-9.012500
N	-4.304086	-3.622933	-8.077425
O	-3.980081	-2.638289	-8.732081
O	-4.222822	-3.413019	-6.872266
O	-4.022552	-4.721145	-8.544056
C	-3.977552	-5.096940	-0.996262
H	-3.961586	-6.186448	-1.024841
H	-3.649402	-4.783263	-0.005291
H	-5.013724	-4.758638	-0.996886
C	-3.085678	-4.528705	-2.100577
H	-2.271343	-5.236437	-1.945414
H	-2.809405	-3.564434	-1.674017
N	-3.531593	-4.819193	-3.471933
H	-4.307282	-4.214386	-3.701311
H	-2.698955	-4.620140	-4.007834
H	-3.896116	-5.739115	-3.674339
N	-1.934047	3.227522	2.341388
O	-3.125028	3.511663	2.278906
O	-1.301537	3.701577	3.278553
O	-1.487957	2.209508	1.823964

Return

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	-0.030291	-2.174372	-8.881799
H	-0.590588	-1.614844	-9.630862
H	1.004793	-1.833472	-8.903926
H	-0.174634	-3.187755	-9.256394
C	-0.691453	-2.037802	-7.509919
H	-1.755345	-2.244073	-7.626899
H	-0.604910	-1.028253	-7.108146
N	-0.101033	-2.995580	-6.562339
H	0.257670	-3.861711	-6.938170
H	0.761585	-2.604085	-6.212023
H	-0.633084	-3.225224	-5.735123
N	-10.518424	-3.314040	0.531439
O	-11.076075	-4.377255	0.779784
O	-9.329783	-3.219057	0.816375
O	-11.206857	-2.330231	0.778935
C	3.704731	-6.687823	-0.232257
H	4.208899	-7.535729	0.231393
H	2.902547	-6.491867	0.479221
H	3.314494	-7.184893	-1.120365
C	4.626742	-5.477452	-0.383056
H	5.558452	-5.878883	-0.781641
H	4.922103	-5.093868	0.593532
N	4.080746	-4.369692	-1.182178
H	4.652844	-3.537772	-1.155465
H	3.736975	-4.573549	-2.109736
H	3.232866	-4.033495	-0.748391
N	3.225318	-1.975707	-6.476209
O	3.043918	-3.036357	-7.063741
O	4.216518	-1.861874	-5.763720
O	2.213247	-1.440820	-6.037250
C	-7.724784	-5.819054	-0.842863
H	-8.107180	-4.908198	-1.303530
H	-6.716033	-5.458375	-0.641784
H	-7.741342	-6.558444	-1.643568
C	-8.500158	-6.342211	0.366659
H	-7.935170	-7.260010	0.529558
H	-9.503469	-6.518659	-0.021068
N	-8.401848	-5.475187	1.550908
H	-8.945479	-4.631393	1.438763
H	-8.841506	-5.857107	2.376097
H	-7.405010	-5.361083	1.666635
N	-5.013373	-2.275424	-0.990098
O	-5.369264	-1.370198	-0.243785
O	-5.796399	-2.749958	-1.805428
O	-3.808718	-2.351847	-1.204670
C	4.240022	1.301913	0.760315
H	4.795005	0.363783	0.757611
H	3.664557	1.628045	-0.106044
H	4.912732	2.134635	0.965584
C	3.129978	1.054808	1.782362
H	2.455606	1.911037	1.768473
H	3.387784	0.968356	2.837901
N	2.419063	-0.177794	1.409358
H	1.764202	-0.456977	2.125818
H	2.002899	-0.063239	0.496240
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O	1.347396	-6.490156	-6.148853
O	-0.649872	-5.763630	-6.322692
O	0.774456	-5.102375	-7.619129
C	-5.714711	-3.423648	-5.133563
H	-5.057902	-2.886316	-5.817652
H	-6.529919	-3.838509	-5.726375
H	-6.183334	-2.660952	-4.511640
C	-5.102853	-4.515988	-4.255917
H	-4.723986	-5.288373	-4.925232
H	-5.901078	-5.018707	-3.709830
N	-3.964776	-4.223948	-3.370854
H	-3.879117	-5.036629	-2.777295
H	-3.209013	-4.160284	-4.037839
H	-4.026290	-3.348667	-2.870653
N	-4.243973	2.470854	1.503084
O	-4.212289	3.495638	0.830856
O	-3.993888	2.532821	2.701705
O	-3.885039	1.386475	1.057703

Return

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	-0.774016	-2.585914	-8.624117
H	0.249771	-2.959928	-8.632738
H	-1.527074	-3.373831	-8.637898
H	-0.917588	-1.831556	-9.397702
C	-1.074964	-1.747511	-7.381398
H	-2.069936	-1.325082	-7.241095
H	-0.445026	-0.858140	-7.364161
N	-0.745228	-2.378102	-6.093970
H	-1.401342	-3.137940	-5.983249
H	0.169942	-2.800811	-6.156250
H	-0.902513	-1.750938	-5.318065
N	-5.915889	-5.541274	-0.864332
O	-6.072220	-5.918827	0.291561
O	-5.031827	-4.744217	-1.157948
O	-6.828797	-5.687541	-1.669493
C	6.738198	-2.285647	2.708298
H	7.569726	-1.996601	2.065559
H	6.252552	-1.352396	2.993411
H	7.070508	-2.726929	3.647947
C	5.815152	-3.317008	2.058590
H	6.175381	-4.344776	2.103627
H	5.687462	-3.036887	1.012967
N	4.501221	-3.305094	2.719865
H	3.985007	-2.437117	2.735282
H	3.833021	-3.949417	2.321797
H	4.565615	-3.687429	3.652481
N	2.482003	-2.849911	-6.103671
O	1.714610	-1.953395	-5.771343
O	1.987691	-3.939527	-6.371008
O	3.629244	-2.805680	-5.673604
C	-5.251010	-6.679219	3.604003
H	-5.936471	-7.123196	4.325895
H	-5.224168	-7.222576	2.659470
H	-4.242050	-6.961390	3.904801
C	-5.547171	-5.189106	3.431690
H	-5.227387	-4.694184	4.348691
H	-6.595575	-5.013316	3.190763
N	-5.017795	-4.621144	2.182282
H	-5.225805	-3.670410	1.912214
H	-4.014420	-4.535096	2.105251
H	-5.313209	-5.227371	1.430405
N	-5.578225	-2.334320	-0.011467
O	-4.928508	-2.369650	1.027617
O	-5.177784	-1.540149	-0.855276
O	-6.779928	-2.504645	0.161670
C	3.444406	3.107306	3.266464
H	3.295448	2.667639	4.252672
H	4.450648	3.509863	3.382761
H	2.721917	3.914160	3.143601
C	3.201455	1.994789	2.246110
H	3.816781	1.216682	2.697798
H	3.577495	2.245651	1.254262
N	1.833676	1.454041	2.270898
H	1.412146	1.551159	3.183576
H	1.227969	1.772270	1.527965
H	1.898103	0.468699	2.058652
N	-0.664025	-3.306729	-2.726111
O	-1.834343	-3.365004	-2.365506
O	-0.155051	-3.890938	-3.676228
O	0.168207	-2.655188	-2.104855
C	-9.229382	-7.359112	-0.266544

H	-9.589721	-8.018046	0.523432
H	-9.612273	-7.854881	-1.158569
H	-8.163989	-7.438432	-0.482758
C	-9.575865	-5.871786	-0.191380
H	-10.634983	-5.617292	-0.151362
H	-9.166367	-5.420956	-1.095351
N	-8.874249	-5.126777	0.865283
H	-8.803930	-5.556715	1.776496
H	-7.914990	-4.946677	0.605501
H	-9.360455	-4.242106	0.832687
N	-9.445602	-6.307217	4.633490
O	-8.423349	-6.669388	5.205249
O	-10.088096	-5.407461	5.163319
O	-9.333870	-6.181169	3.419116
C	-3.440479	-1.421251	4.724172
H	-3.622683	-2.495791	4.740421
H	-3.580771	-1.155360	3.676450
H	-2.447995	-1.208206	5.121273
C	-4.541431	-0.670533	5.473951
H	-4.212535	0.314062	5.806366
H	-4.705004	-1.206539	6.408853
N	-5.769521	-0.534520	4.675743
H	-5.675926	0.085542	3.883996
H	-6.314185	-1.330070	4.374843
H	-6.423813	-0.110775	5.317961
N	-11.519530	-2.618158	0.606036
O	-11.597596	-1.539630	1.183755
O	-11.180526	-2.733698	-0.566483
O	-11.379892	-3.594367	1.334455
C	-8.626277	5.901229	3.702498
H	-8.960214	6.833090	4.158809
H	-9.187021	5.967001	2.770114
H	-9.025696	5.161801	4.396624
C	-7.103148	5.948179	3.827862
H	-6.535174	5.897107	4.756784
H	-6.860305	6.898698	3.352846
N	-6.475397	4.888307	3.023847
H	-5.552860	5.173403	2.727630
H	-6.461567	4.023997	3.546224
H	-6.961565	4.719330	2.154831
N	-2.017526	-5.025390	1.181430
O	-0.855654	-5.402666	1.077555
O	-2.372665	-4.335906	2.130938
O	-2.896890	-5.468160	0.450847
C	-9.167801	-5.911685	8.050733
H	-9.383594	-6.103323	9.101832
H	-9.775017	-5.078304	7.697371
H	-9.502137	-6.780736	7.484103
C	-7.661209	-5.650914	8.046112
H	-7.274306	-6.666339	8.131654
H	-7.380092	-4.982680	8.860076
N	-7.071717	-5.063061	6.833360
H	-7.410595	-4.155367	6.548137
H	-6.073566	-4.914964	6.876510
H	-7.320509	-5.727906	6.114900
N	-4.579687	-4.127830	11.010193
O	-3.538589	-4.676571	10.666573
O	-4.623659	-2.903354	11.052646
O	-5.540439	-4.795097	10.643061
C	-4.393517	-8.919155	8.363797
H	-3.590557	-9.656274	8.367026
H	-5.244012	-9.548701	8.625391
H	-4.573367	-8.347252	7.453477
C	-4.389938	-7.725016	9.318711
H	-4.081891	-8.189261	10.255559
H	-5.350952	-7.243691	9.500037
N	-3.288945	-6.775703	9.094076

H	-3.385230	-6.410962	8.157170
H	-3.275179	-5.960693	9.690456
H	-2.348993	-7.142785	9.051174
N	-3.794857	2.030355	2.510585
O	-3.349306	1.575890	3.558450
O	-3.531032	1.358240	1.519760
O	-4.004531	3.237910	2.541012
C	-4.968238	1.597992	-1.865243
H	-5.900488	1.265877	-1.408394
H	-5.128488	1.276564	-2.894371
H	-4.171466	0.984723	-1.444343
C	-4.521746	3.043075	-1.641145
H	-5.303419	3.642533	-2.107768
H	-3.580007	3.222165	-2.159946
N	-4.575514	3.487018	-0.239765
H	-4.531969	4.479648	-0.058411
H	-5.477341	3.190079	0.104673
H	-3.919772	2.928000	0.287116
N	-0.852833	2.250486	-0.011911
O	0.059622	2.541478	0.753483
O	-0.667915	1.544765	-0.997222
O	-1.945976	2.799845	0.067578
C	-0.598621	-3.670502	4.747718
H	-0.099222	-4.354451	4.061486
H	-1.651567	-3.948715	4.702950
H	-0.799842	-2.771804	4.164663
C	-0.225210	-3.447511	6.213555
H	-0.984867	-2.817679	6.676516
H	0.723531	-2.917470	6.129612
N	-0.092398	-4.694038	6.983213
H	0.833276	-5.054895	6.801529
H	-0.063372	-4.414050	7.953195
H	-0.823318	-5.383385	6.879981
N	-4.142646	-4.210420	7.219943
O	-3.102949	-3.911932	7.797014
O	-5.105675	-3.457065	7.309990
O	-4.344808	-5.417717	7.151836
C	-3.477682	3.591645	8.239777
H	-3.175487	2.664305	8.726417
H	-3.208361	4.461131	8.839409
H	-4.527577	3.878680	8.298354
C	-2.726787	3.740592	6.916216
H	-1.643125	3.624896	6.896473
H	-3.080100	4.646093	6.422923
N	-3.162786	2.815169	5.859174
H	-2.772531	2.982703	4.942805
H	-3.044720	1.833173	6.063736
H	-4.127112	2.949833	5.590772
N	-8.539029	-1.311631	6.185448
O	-9.747258	-1.359972	5.983160
O	-7.834293	-2.304195	6.331190
O	-8.009014	-0.210406	6.088166
C	1.358877	1.591950	9.143784
H	0.390557	1.247186	9.506544
H	2.013143	1.434131	10.001181
H	1.322413	2.618274	8.778505
C	1.737293	0.740980	7.931145
H	1.472893	-0.304463	8.090023
H	2.771981	0.911020	7.633478
N	0.927752	1.067129	6.747038
H	1.001209	2.053853	6.544358
H	1.392738	0.677892	5.939335
H	-0.035191	0.777024	6.840197
N	3.933954	-9.569863	6.838155
O	3.427917	-9.668776	5.725852
O	3.138884	-9.586046	7.771256
O	4.835627	-8.740172	6.879098

C	-9.964713	0.075553	-2.268181
H	-9.854727	0.115815	-3.351871
H	-10.905112	-0.439646	-2.072421
H	-9.980708	1.062933	-1.806743
C	-8.789155	-0.617742	-1.578800
H	-7.949077	0.029115	-1.831677
H	-8.527079	-1.524152	-2.124544
N	-8.870975	-0.827855	-0.125185
H	-8.220421	-1.451636	0.330640
H	-9.057748	0.039354	0.357688
H	-9.752831	-1.292401	0.037992
N	-1.793864	-7.104601	5.256871
O	-2.629909	-7.998320	5.183600
O	-0.666696	-7.290537	4.811901
O	-1.741295	-6.657781	6.397338
C	1.638558	-9.061411	2.383196
H	1.053834	-9.961639	2.572369
H	2.485339	-9.068523	1.696893
H	2.030978	-8.771165	3.357806
C	0.567384	-8.079871	1.906744
H	-0.166065	-8.218293	2.701094
H	0.077769	-8.267423	0.951129
N	1.178829	-6.742004	1.916183
H	0.519714	-6.008123	1.699189
H	1.724555	-6.508367	2.733310
H	1.978126	-6.758063	1.298958
N	2.985786	-0.970124	4.515602
O	2.344497	0.037376	4.792673
O	4.115505	-0.699301	4.123854
O	2.925321	-1.865677	5.350710
C	0.352712	5.940782	1.724510
H	0.411588	6.990724	1.437709
H	0.696926	5.896663	2.757792
H	1.128788	5.329687	1.263676
C	-1.127260	5.557067	1.741488
H	-1.603776	5.556742	0.761165
H	-1.628227	6.471420	2.059435
N	-1.482570	4.250974	2.317436
H	-1.124037	4.140092	3.255125
H	-2.490901	4.194914	2.302409
H	-1.254305	3.522790	1.655815
N	5.870021	-5.036481	5.573373
O	6.397371	-5.857509	4.831154
O	5.352600	-5.198515	6.672962
O	5.646538	-3.985082	4.983719
C	-13.232614	-2.937199	5.379152
H	-13.225057	-2.136950	6.119183
H	-14.299560	-3.006574	5.167223
H	-12.731603	-3.772938	5.867646
C	-12.480850	-2.896274	4.048356
H	-12.731307	-1.987658	3.500828
H	-12.917788	-3.644346	3.386864
N	-11.052878	-3.149877	4.294166
H	-10.722083	-2.374697	4.850737
H	-10.826447	-4.072000	4.638432
H	-10.631910	-3.123166	3.376466
N	2.613616	-5.777791	5.019928
O	2.590618	-7.001428	5.092452
O	2.429832	-5.225176	3.941079
O	2.559749	-5.235764	6.118282
C	-2.717665	-8.243049	-1.795375
H	-3.356686	-8.136351	-0.918809
H	-3.182021	-9.023878	-2.397688
H	-1.769752	-8.642662	-1.435001
C	-2.624215	-6.941881	-2.592916
H	-3.640121	-6.630582	-2.836079
H	-2.298045	-7.318797	-3.562269

N	-1.854732	-5.921006	-1.865214
H	-0.889394	-6.163018	-1.693012
H	-1.804457	-5.001138	-2.279236
H	-2.088604	-5.727578	-0.901892
N	1.176079	-6.934771	-2.001749
O	0.370733	-7.594098	-2.649654
O	2.056753	-6.457525	-2.708662
O	0.704219	-6.150760	-1.185813
C	-0.989011	-2.935649	12.705134
H	-1.731914	-3.721363	12.842423
H	-0.088495	-3.549017	12.674292
H	-0.833768	-2.375493	13.627211
C	-1.328198	-2.157455	11.433439
H	-0.450985	-1.576413	11.148855
H	-2.225293	-1.557504	11.586347
N	-1.522508	-3.016970	10.255595
H	-0.649559	-3.520349	10.187264
H	-2.267969	-3.682824	10.400598
H	-1.564333	-2.419139	9.442606
N	-6.503629	3.133481	6.022151
O	-7.481673	3.169139	5.283751
O	-5.993125	2.032576	6.196707
O	-5.794947	4.122514	6.172681
C	-7.463639	-2.088788	9.768457
H	-7.446785	-2.900259	9.040906
H	-7.164649	-2.277568	10.799508
H	-8.547866	-2.011925	9.686959
C	-6.676286	-0.925848	9.163901
H	-6.721757	-0.032412	9.786640
H	-7.082966	-0.489795	8.251449
N	-5.272726	-1.331414	8.992506
H	-5.253118	-2.083201	8.318317
H	-4.654864	-0.575842	8.732785
H	-4.874893	-1.752583	9.819820
N	4.117816	-6.133142	0.964054
O	3.334499	-5.195883	0.859000
O	4.629828	-6.284583	2.067678
O	3.668710	-7.186671	0.526497
C	1.915508	1.894359	-3.335819
H	2.681395	2.344923	-3.967095
H	1.029720	2.320938	-3.806468
H	1.993933	2.172059	-2.284708
C	1.907519	0.365380	-3.336835
H	2.793160	0.192917	-2.725283
H	2.082061	-0.133962	-4.289878
N	0.644741	-0.129983	-2.767758
H	0.161582	0.380438	-2.042411
H	-0.064453	-0.259608	-3.475106
H	0.667526	-1.086470	-2.444162
N	-7.244122	1.722687	1.410445
O	-6.808812	2.528390	0.595322
O	-6.918996	1.970214	2.566343
O	-8.388549	1.298996	1.292764
C	-0.353817	-1.389879	0.687718
H	0.222985	-2.128303	1.244611
H	0.173044	-1.244147	-0.255298
H	-0.211517	-0.524116	1.334483
C	-1.832093	-1.773045	0.612059
H	-2.312307	-1.835057	1.588609
H	-1.902843	-2.660438	-0.016930
N	-2.710745	-0.822443	-0.086631
H	-2.402377	-0.531805	-1.003441
H	-3.518571	-1.422885	-0.170224
H	-2.997980	-0.039080	0.482524
N	0.369572	3.502749	4.935997
O	0.929600	3.659954	6.015225
O	-0.676527	4.087998	4.678634

O	0.491234	2.477720	4.274491
C	-11.092822	2.615705	4.002596
H	-11.432997	2.448870	2.980565
H	-12.005580	2.965827	4.484663
H	-10.403619	3.442671	4.173552
C	-10.482922	1.308860	4.510552
H	-10.848792	0.457800	3.936149
H	-10.584928	1.329273	5.595576
N	-9.050651	1.249714	4.180486
H	-8.522183	2.039038	4.523689
H	-8.718104	0.482927	4.747540
H	-8.895974	1.274371	3.182705
N	-2.150115	0.082651	8.097612
O	-1.473853	0.728545	7.304791
O	-3.360967	0.270957	8.135752
O	-1.617219	-0.906658	8.587883
C	5.154962	-5.543250	10.038681
H	5.449989	-4.745360	9.357189
H	4.532617	-5.174497	10.854038
H	6.125564	-5.910355	10.372247
C	4.520817	-6.766971	9.376709
H	3.921527	-7.341861	10.082722
H	5.320599	-7.417696	9.023147
N	3.677100	-6.501051	8.201435
H	4.246739	-6.068054	7.488605
H	3.316952	-7.326735	7.744664
H	2.899580	-5.915076	8.470128
N	2.180682	-3.048045	9.366258
O	2.610536	-3.903896	8.600869
O	2.892353	-2.049770	9.373093
O	0.997620	-2.914823	9.658988
C	4.712911	-4.110644	-2.498497
H	5.355464	-3.979610	-3.369160
H	5.126945	-3.696778	-1.579046
H	4.763615	-5.168292	-2.239829
C	3.301859	-3.650903	-2.866482
H	2.906868	-4.076964	-3.788737
H	3.292217	-2.587219	-3.104355
N	2.429423	-3.987653	-1.731011
H	2.191426	-4.940235	-1.967750
H	2.870640	-4.106112	-0.830237
H	1.569019	-3.466576	-1.639996
N	-7.998346	-2.176836	2.973767
O	-7.065128	-2.684800	3.585448
O	-7.978538	-0.951210	2.950889
O	-9.023592	-2.684393	2.532936
C	6.651574	-8.919205	2.918292
H	7.380258	-8.679236	3.692588
H	6.770433	-9.765779	2.242063
H	6.653436	-8.066659	2.239129
C	5.295541	-9.139760	3.589389
H	5.247520	-10.030174	4.216250
H	4.553038	-9.247692	2.798732
N	4.873402	-7.881905	4.224559
H	4.727728	-7.123110	3.574091
H	4.041944	-7.935369	4.795453
H	5.554477	-7.365889	4.763041
N	2.887019	-1.107058	0.408404
O	2.772444	-0.283484	-0.492525
O	3.451932	-2.190790	0.311059
O	2.427568	-0.782550	1.497750
C	6.246531	-1.197180	6.433067
H	7.164247	-0.696885	6.742266
H	6.462987	-1.949453	5.674561
H	5.535965	-0.476574	6.028191
C	5.430727	-1.783307	7.585785
H	5.052975	-0.951073	8.179746

H	6.092986	-2.300460	8.280095
N	4.391659	-2.694777	7.082398
H	3.782628	-2.410387	6.328538
H	4.931243	-3.449723	6.683642
H	3.738176	-3.033249	7.774133
N	-2.523470	-0.444206	-3.610720
O	-2.066192	-0.376748	-2.475193
O	-3.648371	-0.905525	-3.768379
O	-1.655724	-0.567883	-4.467923
C	-0.826303	-10.816810	7.139021
H	-0.521813	-10.656640	8.173300
H	-1.703452	-10.184592	7.001142
H	-1.121334	-11.839726	6.905141
C	0.215629	-10.229793	6.186325
H	-0.095252	-10.202745	5.141949
H	1.061669	-10.904460	6.317245
N	0.636873	-8.859629	6.516545
H	1.509213	-8.606962	6.074636
H	0.054237	-8.225051	5.989337
H	0.685180	-8.759087	7.520366
N	-0.042383	-6.794390	9.213825
O	0.933423	-6.697278	8.477994
O	-0.757625	-5.822902	9.432269
O	-0.654390	-7.856575	9.196906
C	2.662060	-7.608118	-5.802464
H	3.207942	-6.748797	-6.191924
H	3.133853	-7.847544	-4.849476
H	2.930418	-8.369120	-6.535240
C	1.168405	-7.307906	-5.673194
H	0.636751	-7.929337	-4.952591
H	0.558370	-7.349829	-6.575524
N	1.010778	-5.997772	-5.023161
H	1.330294	-5.953949	-4.066036
H	1.606852	-5.375567	-5.550094
H	0.043929	-5.778753	-5.216378
N	-2.577321	-5.161031	-6.136102
O	-2.977910	-5.315967	-4.987799
O	-1.395901	-5.487144	-6.167292
O	-2.767977	-4.004783	-6.496405
C	-5.949826	-3.139326	-5.394273
H	-5.341667	-2.262639	-5.617122
H	-5.395833	-3.967804	-5.835651
H	-6.890655	-3.203432	-5.940929
C	-5.887654	-3.457366	-3.900009
H	-6.404612	-4.391524	-3.680459
H	-6.459915	-2.720535	-3.336364
N	-4.464510	-3.406867	-3.531293
H	-4.031526	-4.027689	-4.200027
H	-4.186619	-2.441677	-3.637523
H	-4.309729	-3.619474	-2.556130
N	-4.416840	6.628577	1.121578
O	-5.627270	6.437670	1.082974
O	-4.013319	6.388265	2.254052
O	-3.820344	6.023980	0.237423

Return

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	1.194483	-0.971789	-7.639081
H	2.017423	-1.569555	-7.247232
H	1.500011	-0.660286	-8.637940
H	1.264136	-0.002740	-7.144924
C	0.005831	-1.933449	-7.651623
H	0.235709	-2.839745	-8.211876
H	-0.911120	-1.507969	-8.059382
N	-0.438537	-2.371285	-6.319453
H	0.387263	-2.686474	-5.830771
H	-0.976776	-1.724334	-5.761015
H	-1.102396	-3.125142	-6.424761
N	-6.245371	-3.860270	-0.946781
O	-6.101319	-4.783624	-0.153218
O	-7.391871	-3.491701	-1.176502
O	-5.487589	-3.962101	-1.905151
C	7.271325	-2.361284	7.874351
H	8.194203	-2.186815	8.427484
H	6.814667	-3.274680	8.255495
H	7.482096	-2.760904	6.882393
C	6.408413	-1.124418	8.126117
H	6.959274	-0.244929	7.792724
H	6.230246	-0.900326	9.177849
N	5.261150	-1.121203	7.205455
H	4.604565	-0.381895	7.411414
H	5.337697	-0.889084	6.225475
H	4.817651	-2.027085	7.258258
N	2.039374	-3.967211	-5.060545
O	1.860295	-4.817779	-4.195941
O	1.801641	-2.804987	-4.751036
O	1.602092	-4.213428	-6.179132
C	-4.855200	-8.344015	1.778904
H	-4.583659	-8.156603	0.740038
H	-3.892049	-8.697205	2.147276
H	-5.537804	-9.193536	1.800508
C	-5.334803	-7.079396	2.492038
H	-4.620221	-6.257448	2.448753
H	-5.470614	-7.314323	3.547719
N	-6.580772	-6.477799	1.992554
H	-6.548691	-6.063546	1.071976
H	-7.411848	-7.051540	1.977182
H	-7.003052	-5.759181	2.562964
N	-4.958379	-0.688182	-0.352353
O	-5.181408	-0.561402	-1.551212
O	-4.212057	0.146058	0.147768
O	-5.543936	-1.494138	0.362233
C	3.654195	2.503822	1.646794
H	3.432457	3.319615	0.958743
H	4.026990	3.174983	2.420530
H	4.414167	1.862214	1.200832
C	2.464689	1.631381	2.048991
H	2.780558	1.232634	3.013007
H	2.212638	0.872303	1.308471
N	1.209062	2.316539	2.392214
H	1.408461	3.129432	2.957498
H	0.856566	2.606444	1.491213
H	0.464407	1.719452	2.722480
N	-1.557833	-3.082168	-2.711585
O	-0.632220	-2.288246	-2.585066
O	-1.186056	-4.250139	-2.685075
O	-2.498485	-2.857106	-1.958194
C	-10.882197	-6.260262	-2.680936

H	-11.880332	-5.851529	-2.523567
H	-10.808651	-6.550340	-3.729051
H	-10.838924	-7.209324	-2.146607
C	-9.659349	-5.510473	-2.151501
H	-9.418734	-4.558385	-2.624505
H	-8.748405	-6.108630	-2.129438
N	-9.922016	-5.317008	-0.717130
H	-10.315536	-6.208846	-0.452806
H	-9.044555	-5.087987	-0.272483
H	-10.638455	-4.630399	-0.529021
N	-9.650473	-7.438604	1.824441
O	-9.653195	-7.185720	3.024074
O	-8.609657	-7.739786	1.250797
O	-10.679844	-7.219214	1.195682
C	-4.562652	-2.296931	3.843519
H	-3.498960	-2.117889	3.686665
H	-4.659856	-2.913783	4.736910
H	-4.913473	-3.078235	3.169287
C	-5.430448	-1.038084	3.852163
H	-5.235598	-0.415336	4.725271
H	-6.447959	-1.428630	3.867822
N	-5.305654	-0.177843	2.665465
H	-4.414481	0.296517	2.695349
H	-5.538910	-0.615496	1.785607
H	-6.000299	0.553021	2.723822
N	-11.840192	-2.950495	0.332065
O	-11.098222	-2.160851	0.905668
O	-11.542406	-3.242391	-0.820842
O	-12.149471	-3.937285	0.990600
C	-8.161834	4.421047	6.251835
H	-7.509646	5.275114	6.434373
H	-9.184544	4.763556	6.409483
H	-7.819326	3.562127	6.828936
C	-8.115639	3.779339	4.864781
H	-8.515426	4.440231	4.095696
H	-8.673411	2.848512	4.967498
N	-6.744246	3.431697	4.461959
H	-6.126269	4.130743	4.075258
H	-6.275840	2.756249	5.048871
H	-6.915731	2.878374	3.634599
N	-1.643363	-5.799685	1.085418
O	-0.945053	-5.967643	2.079013
O	-1.124726	-5.191003	0.156119
O	-2.261527	-6.782199	0.690935
C	-7.185219	-5.934795	6.435250
H	-6.653125	-6.518280	7.186597
H	-8.158340	-6.425362	6.413347
H	-6.593795	-6.169717	5.550304
C	-7.071770	-4.426455	6.658589
H	-6.006215	-4.201351	6.613661
H	-7.518836	-4.078834	7.589927
N	-7.760234	-3.614974	5.643032
H	-7.442102	-3.779932	4.698744
H	-8.769818	-3.588727	5.630659
H	-7.464508	-2.659125	5.780875
N	-2.052389	-2.471662	7.880214
O	-3.277692	-2.487174	7.841907
O	-1.511622	-1.450864	7.469583
O	-1.452752	-3.208644	8.655049
C	-4.449271	-5.407814	10.555986
H	-4.141593	-4.508678	11.089832
H	-5.526048	-5.449943	10.392049
H	-4.035346	-6.304364	11.017468
C	-3.944552	-5.453471	9.113414
H	-4.352916	-4.640924	8.512493
H	-4.265688	-6.387528	8.652427
N	-2.480650	-5.551563	9.007540

H	-2.271587	-6.010079	9.882843
H	-2.053564	-6.049560	8.239623
H	-1.968694	-4.681032	8.994162
N	-2.079997	1.206190	2.892854
O	-2.703699	0.185779	3.162731
O	-0.938687	1.330846	3.322907
O	-2.543091	2.141702	2.249863
C	-4.249655	4.024466	-2.082928
H	-3.325084	3.979075	-2.658434
H	-5.053429	3.943946	-2.814752
H	-4.332529	4.890382	-1.426102
C	-4.111726	2.704388	-1.323843
H	-3.726188	1.845337	-1.872926
H	-5.121552	2.432113	-1.016893
N	-3.388786	2.909618	-0.059296
H	-3.783862	3.619344	0.540957
H	-3.306431	2.095613	0.532915
H	-2.388769	3.029571	-0.134647
N	-0.014528	2.382519	-0.970120
O	-1.117402	2.337460	-1.503708
O	-0.020745	2.708182	0.211819
O	0.675282	1.393642	-1.192294
C	-0.030113	-3.709273	3.988160
H	1.030697	-3.883866	4.167881
H	-0.312384	-3.976625	2.969854
H	-0.405953	-2.715652	4.232214
C	-0.800512	-4.690501	4.872196
H	-1.831302	-4.535029	4.553763
H	-0.699408	-4.378383	5.911647
N	-0.503040	-6.102014	4.584129
H	-0.663436	-6.367061	3.622816
H	0.446172	-6.322399	4.849699
H	-1.073740	-6.693799	5.170809
N	-7.837653	-0.783234	6.594884
O	-7.636478	0.389375	6.890844
O	-7.102807	-1.569747	7.181805
O	-8.211014	-1.046583	5.457200
C	-0.883271	2.623911	7.815279
H	-1.893258	2.231029	7.932202
H	-0.664806	2.934007	8.837146
H	-0.991823	3.523219	7.209011
C	0.010904	1.496113	7.299176
H	0.157180	0.647822	7.967836
H	0.984603	1.954207	7.125511
N	-0.422139	0.907015	6.022743
H	-1.286421	0.425499	6.225866
H	-0.705018	1.639862	5.387909
H	0.173752	0.189165	5.635825
N	-11.140325	-3.476104	5.479080
O	-10.310260	-4.341094	5.222448
O	-12.109287	-3.457203	4.728192
O	-10.691809	-2.382950	5.806070
C	4.103302	4.811676	7.071811
H	4.017455	4.458500	8.099428
H	4.719387	5.709781	7.115957
H	3.065210	4.877848	6.746104
C	4.913814	3.742197	6.338923
H	5.871865	3.738659	6.858755
H	5.135396	4.013708	5.306798
N	4.288162	2.412219	6.398599
H	3.465791	2.391443	5.812619
H	4.878161	1.630562	6.151589
H	3.908562	2.154101	7.298253
N	0.879962	-5.642410	7.531168
O	1.540425	-5.302928	6.555660
O	0.305608	-6.724383	7.480911
O	1.232313	-5.172080	8.607140

C	-9.669216	0.402382	-1.149338
H	-10.735342	0.175565	-1.143921
H	-9.390066	1.004389	-0.284605
H	-9.605771	1.033073	-2.036077
C	-8.826294	-0.862914	-1.311662
H	-7.880333	-0.434457	-1.642843
H	-9.183833	-1.562665	-2.067052
N	-8.685991	-1.559791	-0.023827
H	-8.280892	-1.087362	0.771664
H	-9.548911	-1.927321	0.350860
H	-8.044813	-2.335239	-0.111419
N	-3.283934	-6.826050	5.903639
O	-3.948858	-5.798692	5.977714
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O	-2.314278	-6.934361	6.646008
C	-0.665213	-9.561198	2.878046
H	-0.956578	-8.585355	3.266552
H	-1.280466	-10.320816	3.360276
H	0.323205	-9.640283	3.330680
C	-0.752300	-9.437391	1.356557
H	-1.790979	-9.273668	1.069434
H	-0.402102	-10.395980	0.973716
N	0.055112	-8.307559	0.871370
H	-0.140442	-7.406124	1.282798
H	1.054490	-8.288834	1.016264
H	-0.265761	-8.215594	-0.081878
N	3.038409	-9.718073	8.091216
O	2.375837	-9.357530	7.124736
O	2.401055	-9.628025	9.134646
O	4.183317	-9.281099	8.127478
C	-1.783971	7.215157	4.531299
H	-1.842099	7.874872	5.397033
H	-0.694759	7.207147	4.490626
H	-2.217840	7.688289	3.650387
C	-2.394619	5.840043	4.803350
H	-3.484588	5.847823	4.800973
H	-2.286049	5.481250	5.826863
N	-1.934011	4.781920	3.891178
H	-0.930755	4.891658	3.852014
H	-2.162007	3.862379	4.241267
H	-2.424395	4.932077	3.021076
N	4.279945	-4.196858	8.471177
O	4.027762	-5.396566	8.457662
O	4.149637	-3.556852	7.433638
O	4.027996	-3.487573	9.438912
C	-12.709662	-7.415383	4.425532
H	-12.569195	-6.971524	5.411107
H	-13.453129	-8.202463	4.551476
H	-11.787351	-7.970031	4.252880
C	-13.024878	-6.277101	3.454556
H	-13.902342	-5.729690	3.798790
H	-13.243935	-6.678112	2.464958
N	-11.789899	-5.557558	3.106813
H	-11.064862	-6.170990	2.763124
H	-11.914525	-4.854150	2.392820
H	-11.440555	-5.157417	3.965852
N	5.977559	0.249785	4.347525
O	5.218389	0.669401	3.481120
O	6.103881	0.863574	5.401271
O	6.067262	-0.967410	4.463567
C	-4.048456	-7.696065	-2.540867
H	-3.984195	-8.394165	-3.375509
H	-3.534625	-8.168776	-1.703836
H	-5.097237	-7.546989	-2.284088
C	-3.380792	-6.367026	-2.895440
H	-3.892956	-5.999551	-3.784681
H	-2.387541	-6.659267	-3.236245

N	-3.232457	-5.490618	-1.723371
H	-2.695198	-4.672801	-1.973627
H	-4.138737	-5.276625	-1.332264
H	-2.766054	-5.986527	-0.977286
N	-0.015643	-8.452127	-2.638688
O	-0.835028	-8.730525	-1.770253
O	-0.370335	-8.664550	-3.792874
O	0.573786	-7.383071	-2.525692
C	1.157961	-2.637552	11.509442
H	0.672241	-3.608868	11.602832
H	2.193995	-2.825147	11.791476
H	0.807739	-2.101446	12.391505
C	0.924714	-1.839792	10.226081
H	1.517309	-0.938991	10.385737
H	-0.106899	-1.512820	10.095832
N	1.606106	-2.517392	9.112347
H	2.578614	-2.747848	9.258015
H	1.180459	-3.400122	8.867989
H	1.439592	-1.983394	8.271384
N	-3.736332	2.054304	5.809850
O	-3.103298	1.039517	6.079203
O	-3.104936	3.094074	5.657237
O	-4.956338	2.113956	5.915225
C	-5.172957	1.331242	9.983024
H	-5.330106	2.157666	9.289894
H	-6.152576	0.967315	10.292871
H	-4.604713	1.714350	10.830625
C	-4.432492	0.235169	9.216098
H	-4.408541	-0.620141	9.891353
H	-3.405749	0.598839	9.256641
N	-4.942150	0.072078	7.845882
H	-4.164968	-0.195795	7.259084
H	-5.527794	-0.746378	7.760722
H	-5.409930	0.913005	7.539084
N	2.442360	-7.172697	3.063944
O	1.723605	-7.471493	4.011144
O	2.232846	-7.752701	2.004334
O	3.442876	-6.504345	3.299209
C	2.821676	1.884794	-3.305827
H	3.671609	2.369927	-3.785783
H	2.004416	2.598591	-3.409177
H	3.078275	1.902052	-2.246601
C	2.627731	0.474861	-3.864679
H	3.519149	-0.123672	-3.676975
H	2.528168	0.577158	-4.945291
N	1.404374	-0.190158	-3.390350
H	1.399943	-0.118709	-2.382890
H	0.603706	0.334891	-3.711840
H	1.263547	-1.166109	-3.608954
N	-8.145232	1.242476	2.262774
O	-8.219158	0.071124	1.908451
O	-9.172928	1.658103	2.786386
O	-7.068073	1.607002	2.720952
C	-1.249040	-1.781239	1.067657
H	-0.788920	-2.033786	2.022964
H	-2.293926	-1.988597	1.298561
H	-0.814969	-2.612501	0.512061
C	-0.863264	-0.478710	0.365920
H	0.215191	-0.327366	0.319790
H	-1.375883	0.357304	0.841739
N	-1.515146	-0.343432	-0.945793
H	-1.194224	-1.121084	-1.504691
H	-2.495569	-0.168634	-0.777521
H	-1.099686	0.449700	-1.413163
N	1.137565	4.294582	4.794694
O	0.555053	4.727997	5.782574
O	0.608698	4.529626	3.713893

O	1.752757	3.251999	4.988690
C	-12.254722	0.290814	4.281054
H	-12.071596	0.006538	5.317274
H	-11.756062	1.239775	4.083795
H	-13.300188	0.345737	3.977597
C	-11.591423	-0.724636	3.350068
H	-11.558713	-0.358381	2.323966
H	-12.053447	-1.707124	3.446762
N	-10.160336	-0.782753	3.685414
H	-9.676527	0.084185	3.499820
H	-9.951960	-1.100443	4.621230
H	-9.835745	-1.442422	2.992900
N	2.104470	-0.838185	5.719455
O	2.985295	0.005041	5.846707
O	1.332928	-0.834725	4.766676
O	1.670684	-1.276451	6.779091
C	4.571904	-6.106890	11.566334
H	5.020858	-5.496752	10.782579
H	4.660325	-5.467062	12.444345
H	5.055961	-7.070066	11.727834
C	3.064984	-6.310886	11.406900
H	2.627602	-5.313185	11.369622
H	2.632930	-6.689227	12.333337
N	2.646465	-6.949532	10.149595
H	1.703325	-7.274350	10.307965
H	2.581579	-6.248875	9.425047
H	3.268616	-7.704865	9.899594
N	3.745367	1.030850	9.117788
O	2.938461	1.801710	8.610093
O	3.465019	-0.158138	9.013922
O	4.896476	1.211310	8.736397
C	3.608316	-4.930646	-1.543301
H	4.374085	-5.576587	-1.113814
H	3.559080	-5.434435	-2.508636
H	3.980630	-3.911790	-1.650142
C	2.327976	-5.020611	-0.712351
H	2.455379	-4.545190	0.260193
H	2.088459	-6.046995	-0.434380
N	1.136118	-4.505129	-1.403432
H	0.968074	-4.949980	-2.294481
H	0.286367	-4.718098	-0.900772
H	1.240989	-3.512568	-1.558112
N	-7.980184	-3.816687	2.306475
O	-8.703149	-4.315658	1.451241
O	-7.755161	-4.572886	3.244879
O	-8.348446	-2.697147	2.644245
C	5.188416	-3.722368	2.754704
H	5.937576	-2.930734	2.741481
H	5.601790	-4.422399	3.480774
H	5.076335	-4.310597	1.843922
C	3.952200	-3.208811	3.493535
H	4.145195	-3.291058	4.563155
H	3.175375	-3.917931	3.207543
N	3.589957	-1.857495	3.039040
H	3.514326	-1.745096	2.038167
H	2.695527	-1.519251	3.364134
H	4.262312	-1.239171	3.469987
N	2.399439	-1.761903	0.149942
O	1.826864	-2.369667	1.047637
O	3.263916	-0.958591	0.482276
O	1.919179	-1.819777	-0.976591
C	6.039349	-7.748913	4.904557
H	6.411249	-8.585766	5.495715
H	5.244495	-8.172151	4.290408
H	6.870297	-7.396085	4.293707
C	5.396367	-6.640190	5.738311
H	5.566661	-5.761098	5.116782

H	6.033445	-6.269168	6.541165
N	4.041428	-6.856538	6.268571
H	3.276607	-6.980284	5.620624
H	4.106474	-7.666808	6.868014
H	3.755658	-6.077194	6.843948
N	-2.065674	0.092693	-4.379917
O	-2.975360	-0.187357	-3.607182
O	-0.955539	0.221352	-3.875810
O	-2.097407	-0.509473	-5.447374
C	-1.301390	-11.166578	9.077805
H	-0.415124	-11.799956	9.116092
H	-1.526048	-10.667582	10.020478
H	-2.064571	-11.899889	8.817210
C	-1.146587	-10.084990	8.008205
H	-2.147380	-9.661019	7.925979
H	-0.706987	-10.464854	7.085950
N	-0.283315	-9.009150	8.519254
H	-0.614771	-8.702692	9.422758
H	0.671045	-9.332268	8.589205
H	-0.221285	-8.189669	7.932138
N	-1.108871	-7.212603	11.042062
O	-1.898770	-7.848919	10.353414
O	0.080328	-7.374717	10.791858
O	-1.386931	-6.060534	11.355900
C	2.397222	-7.666053	-5.503179
H	2.718553	-8.578490	-6.005481
H	3.104269	-6.839572	-5.574688
H	2.281957	-7.938434	-4.454073
C	1.102845	-7.293884	-6.227001
H	0.496421	-8.197872	-6.170816
H	1.248036	-6.968758	-7.257201
N	0.253934	-6.491289	-5.333115
H	0.187294	-7.195277	-4.611963
H	0.901805	-5.792342	-4.998698
H	-0.719122	-6.263306	-5.479014
N	-2.596360	-4.845764	-5.933113
O	-1.907515	-4.394962	-6.841599
O	-2.237939	-5.963125	-5.577988
O	-2.935670	-4.005696	-5.107140
C	-6.121452	-1.632013	-5.779729
H	-5.677259	-2.363204	-6.455120
H	-7.147892	-1.522844	-6.129876
H	-5.537144	-0.733326	-5.977331
C	-6.115089	-2.171339	-4.349020
H	-6.328805	-3.240182	-4.348393
H	-6.915435	-1.699938	-3.778646
N	-4.795392	-2.180338	-3.699282
H	-4.424694	-1.248846	-3.576791
H	-4.948939	-2.714846	-2.856177
H	-4.027115	-2.677685	-4.126477
N	-5.060736	5.045848	2.056695
O	-5.337425	3.851630	2.037657
O	-3.869759	5.171097	1.794088
O	-5.399816	5.562217	3.115687

Return

Atomic Number	Atomic Coordinates (Angstroms)		
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C	2.387444	-6.011416	-10.033785
H	3.081951	-6.308116	-10.819743
H	1.615873	-6.780518	-10.069306
H	1.913337	-5.101702	-10.402222
C	3.095906	-5.851100	-8.688341
H	3.915358	-5.132676	-8.666736
H	3.594202	-6.806930	-8.526510
N	2.258393	-5.352762	-7.586492
H	2.802770	-5.247339	-6.742312
H	1.798486	-4.458033	-7.676190
H	1.618198	-6.116017	-7.420083
N	-3.952987	-3.698829	-4.185351
O	-2.728026	-3.749191	-4.182185
O	-4.416350	-4.601381	-3.497041
O	-4.443526	-2.588757	-4.011609
C	5.359704	-4.970798	4.553341
H	4.426915	-5.534043	4.580904
H	5.271332	-4.267271	3.725487
H	6.255117	-5.580431	4.432168
C	5.566401	-4.108299	5.798817
H	6.492144	-3.544851	5.682085
H	5.689153	-4.678546	6.719605
N	4.415764	-3.202892	5.940638
H	3.641362	-3.786057	6.224046
H	4.616386	-2.530701	6.667281
H	4.153574	-2.711764	5.097934
N	3.885832	-5.133751	-4.538128
O	3.794695	-3.916958	-4.657224
O	3.891427	-5.829136	-5.547823
O	3.482133	-5.600855	-3.478922
C	-7.906541	-2.972702	-3.778705
H	-7.278421	-2.292094	-4.353456
H	-8.562998	-3.509882	-4.463250
H	-8.599418	-2.294902	-3.280096
C	-7.271410	-3.806157	-2.665242
H	-6.947705	-4.799663	-2.975503
H	-7.987684	-3.984038	-1.863114
N	-6.212656	-3.072423	-1.954949
H	-5.451667	-2.760113	-2.541001
H	-6.586873	-2.389677	-1.311583
H	-5.803715	-3.709453	-1.286323
N	-8.684321	-0.236128	-1.321670
O	-8.583702	0.660647	-0.491763
O	-7.736868	-0.337858	-2.093071
O	-9.549479	-1.098760	-1.219471
C	2.701814	1.667222	0.136727
H	2.899923	2.651031	-0.288682
H	3.391153	1.463110	0.956025
H	3.130843	0.959789	-0.572902
C	1.221823	1.327044	0.314906
H	0.806874	1.046902	-0.653308
H	0.718662	2.239771	0.634057
N	1.100613	0.040555	1.017826
H	1.876340	-0.189423	1.622357
H	0.201450	-0.099813	1.455894
H	1.010326	-0.640713	0.277677
N	0.355669	-4.468572	-4.008728
O	0.246674	-3.266658	-3.792855
O	0.598771	-4.875282	-5.139464
O	0.264621	-5.315259	-3.126738
C	-11.504325	-4.116724	-2.266836

H	-10.674519	-3.679276	-2.821960
H	-11.106560	-5.123619	-2.140169
H	-12.322304	-4.100787	-2.987082
C	-11.718573	-3.355310	-0.958329
H	-12.397730	-3.839738	-0.256777
H	-12.041235	-2.329590	-1.136892
N	-10.521918	-3.118233	-0.136349
H	-9.970314	-2.395798	-0.576715
H	-10.912956	-2.774614	0.729166
H	-10.070925	-3.993406	0.088992
N	-9.186439	-6.647389	-0.133359
O	-9.056634	-7.366426	0.851126
O	-8.132664	-6.160999	-0.528402
O	-9.976007	-5.770539	0.199495
C	-4.554589	-0.924628	1.232572
H	-5.274069	-0.585295	0.487387
H	-3.692546	-1.175209	0.614357
H	-4.925560	-1.830006	1.712959
C	-4.043338	0.194443	2.140395
H	-3.561295	0.999975	1.586453
H	-3.331618	-0.112796	2.906658
N	-5.083764	0.626591	3.086230
H	-5.475292	-0.242136	3.421071
H	-4.763277	1.151806	3.887190
H	-5.814592	1.126294	2.600137
N	-10.939731	-2.336538	3.307251
O	-10.447815	-3.447782	3.469214
O	-10.503852	-1.336665	3.867019
O	-11.356774	-2.111418	2.176556
C	-5.634107	6.239575	5.239848
H	-6.103460	7.209363	5.074565
H	-5.132440	6.290189	6.206217
H	-4.830091	5.914433	4.579590
C	-6.712008	5.155446	5.265058
H	-7.129994	5.164706	4.258429
H	-7.588814	5.292795	5.897866
N	-6.035862	3.870838	5.502651
H	-5.607993	3.808536	6.415419
H	-6.706216	3.117993	5.439798
H	-5.262527	3.762562	4.862081
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O	-4.774561	-4.385477	-0.248392
O	-2.967816	-3.758317	-1.078175
O	-2.975858	-5.243373	0.308930
C	-4.685610	-8.205262	1.546289
H	-4.677837	-8.272925	2.634159
H	-4.514963	-9.236201	1.236218
H	-3.849356	-7.620581	1.162977
C	-5.895283	-7.596745	0.836189
H	-6.716736	-8.310517	0.774188
H	-5.583067	-7.401732	-0.189769
N	-6.174629	-6.215885	1.259309
H	-6.978477	-5.930928	0.718267
H	-6.247406	-6.023842	2.248209
H	-5.368892	-5.661271	1.007730
N	-1.834063	-0.893291	9.149402
O	-1.127982	-0.891304	10.151661
O	-1.702178	-0.014592	8.304671
O	-2.834782	-1.595475	9.056803
C	-4.603775	-3.183242	13.086158
H	-5.252133	-2.609919	13.748753
H	-5.213096	-4.018341	12.740562
H	-3.808308	-3.401344	13.798734
C	-4.171790	-2.353698	11.876577
H	-3.699358	-1.459798	12.283824
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N	-3.103293	-3.087484	11.181081

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H	-2.823931	-2.409786	10.486256
H	-2.395089	-3.293332	11.871135
N	-2.997378	2.397943	5.314372
O	-4.163381	2.022981	5.368375
O	-2.110490	1.552133	5.281021
O	-2.903480	3.350206	4.547916
C	-6.070164	3.951506	-2.760706
H	-5.196379	3.551505	-3.275098
H	-6.844424	3.353104	-3.240849
H	-6.217556	5.017814	-2.932065
C	-6.055881	3.689290	-1.254426
H	-6.979067	4.075948	-0.822774
H	-5.233260	4.253384	-0.814889
N	-6.101961	2.253605	-0.937368
H	-6.126172	2.005631	0.041419
H	-6.775595	1.773647	-1.516987
H	-5.227155	1.973152	-1.357083
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O	-3.296693	3.204262	-0.097290
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O	-3.590302	1.682132	-1.460585
C	0.824436	-1.456324	6.519894
H	1.608363	-1.414276	5.763727
H	0.607743	-0.442449	6.856350
H	1.005160	-1.961112	7.468909
C	-0.420883	-1.731464	5.676496
H	-1.279022	-1.844121	6.339072
H	-0.348325	-2.673742	5.133405
N	-0.691855	-0.668183	4.696778
H	-1.525618	-0.867363	4.162675
H	-0.710862	0.251170	5.114544
H	0.071511	-0.744123	4.039811
N	-4.535667	-2.125927	5.303476
O	-4.767156	-2.536404	6.435288
O	-3.452283	-1.564698	5.183574
O	-5.481202	-1.683717	4.660445
C	1.475414	3.251805	8.647101
H	1.938838	3.131759	7.667853
H	1.124512	4.282915	8.604913
H	2.167810	3.223071	9.488447
C	0.395338	2.169833	8.622327
H	-0.192322	2.060862	9.533854
H	0.727485	1.158735	8.386831
N	-0.612715	2.325247	7.562367
H	-1.075769	1.467022	7.299440
H	-1.302346	3.036890	7.757494
H	-0.290530	2.691803	6.678097
N	-6.017287	-6.555897	4.512155
O	-6.242208	-6.150764	5.647212
O	-7.017181	-6.499349	3.804986
O	-5.030539	-6.002661	4.039573
C	4.212352	3.162668	5.121325
H	3.168326	3.464613	5.204627
H	4.771674	3.205049	6.055917
H	4.747180	3.938549	4.573540
C	4.081424	1.783524	4.474285
H	5.109081	1.482032	4.271495
H	3.553023	1.972075	3.539758
N	3.288929	0.811824	5.243435
H	3.580990	-0.133004	5.038248
H	3.449647	0.918945	6.234796
H	2.306905	1.011440	5.117419
N	-0.480330	-4.757060	9.576102
O	0.344188	-5.661740	9.645378
O	-0.118519	-3.709712	9.051477
O	-1.680657	-5.003645	9.537550

C	-9.616868	2.967800	2.017482
H	-10.559122	3.515634	2.029047
H	-9.104394	3.318126	2.913441
H	-9.062363	3.206853	1.110025
C	-9.992847	1.501738	2.234611
H	-10.741899	1.115183	1.543529
H	-10.503340	1.461649	3.196843
N	-8.832881	0.598025	2.194302
H	-9.124404	-0.259657	2.640950
H	-8.571026	0.344803	1.252277
H	-8.016833	0.925502	2.691217
N	-4.800971	-5.825833	10.389270
O	-5.009673	-4.954377	9.552559
O	-5.206654	-6.970016	10.217974
O	-3.847019	-5.633963	11.135083
C	-2.840579	-7.146370	7.451571
H	-1.958678	-7.725012	7.176755
H	-2.828061	-7.223353	8.538777
H	-3.758149	-7.651950	7.150649
C	-2.878523	-5.736621	6.860799
H	-2.585910	-5.801549	5.812819
H	-2.022254	-5.203173	7.273516
N	-4.101503	-4.946864	7.071619
H	-4.827090	-5.418703	6.551052
H	-4.407638	-4.941593	8.034092
H	-4.130119	-3.995784	6.732903
N	1.272036	-8.766566	10.458873
O	2.350940	-8.341193	10.061255
O	0.361071	-8.557592	9.665432
O	0.966117	-8.397696	11.587334
C	-0.752885	5.158779	0.718042
H	-1.032865	6.164370	0.404201
H	0.292274	5.294603	0.996063
H	-0.727313	4.384642	-0.048874
C	-1.682213	4.813257	1.882003
H	-2.670591	5.189263	1.617754
H	-1.370658	5.479496	2.686464
N	-1.663947	3.403578	2.301896
H	-0.746364	3.220501	2.682192
H	-2.279511	3.286161	3.093978
H	-2.004905	2.835090	1.539879
N	4.217410	-4.677268	8.959537
O	4.430389	-3.483070	8.781749
O	3.973624	-5.373209	7.980093
O	3.525758	-4.953429	9.933410
C	-12.026397	-6.692028	3.143825
H	-11.865831	-7.256690	2.225415
H	-12.861286	-7.206696	3.619406
H	-12.320048	-5.675291	2.882835
C	-10.703415	-6.712221	3.910083
H	-10.424852	-7.645032	4.400354
H	-10.816635	-6.199900	4.865493
N	-9.608356	-6.030558	3.202961
H	-9.787950	-5.045002	3.331506
H	-8.677863	-6.211262	3.551714
H	-9.488792	-6.385541	2.264988
N	2.852619	-1.508687	3.073859
O	3.342715	-0.629252	2.374234
O	1.661413	-1.297687	3.272815
O	3.497609	-1.623715	4.110118
C	-3.746149	-7.925064	-2.386493
H	-4.167109	-8.635173	-3.098278
H	-3.512587	-8.518523	-1.502550
H	-4.618432	-7.276362	-2.306451
C	-2.540650	-7.223490	-3.012918
H	-2.732450	-7.096640	-4.078386
H	-1.662938	-7.869147	-2.983791

N	-2.252907	-5.981779	-2.278616
H	-1.990237	-6.197748	-1.327585
H	-1.496312	-5.623744	-2.843838
H	-2.964816	-5.268698	-2.347918
N	0.608815	-6.879595	-0.197962
O	-0.536760	-7.077821	0.191194
O	0.752959	-7.180757	-1.377623
O	1.125245	-5.808093	0.099119
C	2.546934	-0.920187	11.879159
H	2.321876	-0.078537	11.224122
H	2.327916	-0.739987	12.931613
H	3.626923	-1.053602	11.816502
C	1.841311	-2.118778	11.244088
H	0.784270	-1.914449	11.414426
H	2.147178	-3.009433	11.792977
N	1.928724	-2.411246	9.805108
H	2.015208	-1.490893	9.398205
H	2.795820	-2.885041	9.595917
H	1.172168	-2.960435	9.422858
N	-3.222709	4.008655	7.929074
O	-2.249975	4.479174	7.349870
O	-4.362629	4.237280	7.539985
O	-2.986396	2.876589	8.336086
C	-6.571400	-0.136254	9.233005
H	-7.368559	0.256685	8.601947
H	-6.595943	-1.138401	8.804987
H	-6.976665	-0.173770	10.244169
C	-5.252845	0.599457	8.992206
H	-4.408213	0.295172	9.610355
H	-5.402834	1.664357	9.169948
N	-4.595439	0.371159	7.696237
H	-3.869471	1.073118	7.678201
H	-4.176542	-0.544570	7.618354
H	-5.200096	0.448202	6.890909
N	-1.679819	-1.864701	1.809186
O	-1.245685	-2.422766	0.807604
O	-1.821502	-2.557842	2.810463
O	-1.153302	-0.782068	2.041053
C	4.340206	0.451606	-5.879647
H	4.285245	1.148696	-5.043497
H	5.224127	0.590990	-6.502026
H	3.612548	0.704819	-6.650683
C	4.153810	-1.025144	-5.529925
H	4.830748	-1.477129	-4.804968
H	4.416721	-1.659131	-6.376707
N	2.746944	-1.326833	-5.224060
H	2.185777	-1.151270	-6.045260
H	2.661730	-2.276239	-4.890194
H	2.420899	-0.801264	-4.425579
N	-7.889788	1.313593	5.166575
O	-7.460855	1.915441	6.144773
O	-7.907203	0.090431	5.085045
O	-7.450113	1.870721	4.166890
C	-1.251621	-0.117736	-2.985146
H	-0.947896	-0.437826	-3.981838
H	-1.894492	0.743236	-3.168294
H	-0.419366	0.333262	-2.444727
C	-2.007797	-1.113139	-2.104685
H	-2.875751	-1.509824	-2.631370
H	-2.526240	-0.668481	-1.255217
N	-1.120375	-2.239571	-1.776853
H	-0.793645	-2.674265	-2.627963
H	-0.277521	-1.875641	-1.355840
H	-1.626259	-2.842848	-1.144209
N	0.511262	2.230865	4.116996
O	0.261360	1.449542	3.205865
O	0.895921	1.779318	5.189945

O	0.721881	3.401993	3.821741
C	-8.969463	-2.893368	6.720964
H	-9.971114	-2.835410	6.295011
H	-9.105867	-3.300244	7.722934
H	-8.733851	-1.861151	6.980031
C	-7.985063	-3.467131	5.701359
H	-8.204226	-4.424572	5.228734
H	-6.956120	-3.492129	6.060177
N	-7.897765	-2.546275	4.557574
H	-7.725179	-2.994182	3.668926
H	-8.752732	-2.024672	4.426955
H	-7.246269	-1.829089	4.842702
N	1.128763	-4.775882	4.992876
O	1.512830	-4.999237	3.850212
O	1.960422	-4.475797	5.842211
O	0.217844	-5.535206	5.303889
C	2.702860	-7.088978	14.155068
H	1.749308	-6.993406	14.674401
H	2.506511	-8.076706	13.738005
H	3.504511	-7.198044	14.885521
C	3.069250	-6.133741	13.018793
H	4.017697	-6.337402	12.521733
H	3.260707	-5.163447	13.477021
N	2.075557	-6.015308	11.940651
H	2.452603	-5.647378	11.078930
H	1.725071	-6.899403	11.600599
H	1.346976	-5.454782	12.359077
N	3.783688	-0.043198	8.177602
O	3.119349	0.018185	9.206175
O	4.106467	0.970441	7.568155
O	3.845054	-1.095517	7.551556
C	-1.521005	-7.089273	3.219269
H	-2.302873	-7.390461	3.916455
H	-1.792635	-7.799350	2.438175
H	-0.549947	-7.321081	3.656775
C	-1.557985	-5.574521	3.014323
H	-1.562330	-4.958844	3.913779
H	-2.513003	-5.230866	2.616905
N	-0.555975	-5.060812	2.067793
H	-0.940359	-4.151199	1.855770
H	0.336005	-4.845006	2.489575
H	-0.538177	-5.627894	1.232209
N	-7.245452	-2.812226	1.426054
O	-7.347549	-1.742623	2.016479
O	-7.651228	-2.933872	0.275566
O	-7.378249	-3.838161	2.084004
C	3.679888	-3.537496	0.611736
H	4.647201	-3.420872	1.100413
H	3.383894	-2.494883	0.495779
H	2.896460	-4.078891	1.142050
C	3.768851	-4.231855	-0.747599
H	3.989426	-5.280441	-0.547815
H	4.510967	-3.888110	-1.468156
N	2.484370	-4.259686	-1.463961
H	2.142168	-3.328273	-1.652290
H	2.617421	-4.727698	-2.349038
H	1.750136	-4.707308	-0.934210
N	2.282078	-0.955692	-1.925604
O	3.378580	-1.468134	-2.120959
O	1.564462	-1.494787	-1.090451
O	1.874419	-0.298119	-2.876649
C	1.498087	-8.790484	5.788596
H	1.776457	-9.077216	4.774497
H	1.452665	-9.673889	6.425490
H	0.536888	-8.317952	5.586337
C	2.496751	-7.778600	6.351271
H	2.629814	-7.057538	5.544757

H	3.445336	-8.302875	6.467121
N	1.976247	-7.064278	7.527136
H	1.113270	-6.554716	7.401766
H	1.969141	-7.654238	8.346889
H	2.624511	-6.296225	7.626878
N	1.357884	-2.204091	-8.068388
O	2.472535	-2.679275	-7.881759
O	0.477646	-3.057063	-8.041993
O	1.141096	-1.224846	-7.363293
C	-2.604823	-9.411919	11.258966
H	-2.923609	-10.368771	11.672377
H	-3.433534	-8.943814	10.727728
H	-1.838804	-9.693702	10.536531
C	-2.245587	-8.318323	12.265365
H	-1.535590	-8.626061	13.033025
H	-3.142494	-7.943974	12.758845
N	-1.576544	-7.256610	11.497909
H	-1.270218	-6.618501	12.218382
H	-0.804868	-7.467947	10.881506
H	-2.192946	-6.732131	10.893699
N	-0.550014	-4.437149	13.676137
O	-0.953984	-5.579154	13.487165
O	-1.238125	-3.596379	13.108083
O	0.661805	-4.289990	13.562501
C	3.205813	-9.229200	-5.240603
H	3.534322	-10.267786	-5.201597
H	2.599483	-9.058963	-6.130257
H	4.063411	-8.609542	-5.502612
C	2.405113	-8.951935	-3.967872
H	3.071722	-8.890893	-3.107637
H	1.701928	-9.755915	-3.750509
N	1.713031	-7.654144	-3.943341
H	0.981674	-7.566476	-4.634377
H	1.295745	-7.364418	-3.070397
H	2.479034	-7.033213	-4.161939
N	-0.411515	-7.830382	-6.303198
O	-0.430115	-8.444147	-5.242056
O	0.685238	-7.548367	-6.772960
O	-1.308554	-7.036461	-6.564132
C	-2.907543	-2.190939	-7.109334
H	-3.747768	-1.829995	-7.702495
H	-3.144906	-1.886692	-6.089926
H	-2.107447	-1.555137	-7.488415
C	-2.707790	-3.703814	-7.204990
H	-2.629184	-4.082747	-8.223976
H	-3.474930	-4.379592	-6.826941
N	-1.425931	-4.145378	-6.634291
H	-0.593038	-3.626211	-6.872733
H	-1.399375	-4.055286	-5.628668
H	-1.301089	-5.136633	-6.782374
N	-5.856032	3.641667	2.149502
O	-4.881590	3.464443	2.872088
O	-6.354723	4.718349	1.841054
O	-6.380599	2.664543	1.626880

Return

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	2.007458	-4.161256	-9.747383
H	1.259195	-4.769936	-10.255036
H	2.405605	-3.607572	-10.597685
H	2.644690	-4.952558	-9.352574
C	1.370365	-3.241600	-8.705180
H	0.663769	-2.526712	-9.126793
H	2.115518	-2.492054	-8.438669
N	0.752507	-3.901598	-7.544795
H	1.543523	-4.272152	-7.037761
H	0.387832	-3.101865	-7.047263
H	-0.045086	-4.518183	-7.606182
N	-3.636556	-3.491145	-2.547979
O	-3.194914	-2.385178	-2.839294
O	-3.001123	-4.494753	-2.851410
O	-4.844497	-3.669474	-2.658228
C	5.636374	0.479433	5.711855
H	5.129338	0.271013	4.769742
H	5.630609	1.555715	5.884141
H	6.672516	0.169608	5.575769
C	5.328339	-0.555267	6.794606
H	5.838909	-0.255404	7.709757
H	5.589567	-1.542855	6.414435
N	3.881727	-0.645636	7.045581
H	3.328332	-0.847773	6.225218
H	3.567877	-1.454302	7.562938
H	3.419263	0.066381	7.592626
N	3.721151	-4.618923	-6.276077
O	3.631919	-4.715758	-5.057169
O	3.642375	-3.480647	-6.724626
O	3.058553	-5.473964	-6.853092
C	-7.064259	-6.060149	-3.224152
H	-6.005056	-6.156729	-3.462609
H	-7.373693	-7.069521	-3.495295
H	-7.311396	-5.348503	-4.011924
C	-7.570664	-5.733504	-1.818912
H	-7.019703	-6.467555	-1.230940
H	-8.650915	-5.844081	-1.724407
N	-7.184387	-4.376253	-1.403581
H	-7.521986	-3.740725	-2.112263
H	-7.602314	-4.143072	-0.514164
H	-6.213213	-4.100372	-1.432054
N	-7.976393	-2.130352	-4.059495
O	-6.960186	-2.288180	-4.726945
O	-8.272162	-0.994773	-3.704448
O	-8.149113	-3.024377	-3.238544
C	3.380918	1.366780	0.341569
H	2.313863	1.280248	0.136621
H	3.712666	2.397329	0.468105
H	3.843982	0.990714	-0.570706
C	3.402117	0.378640	1.508176
H	2.727043	0.691177	2.304854
H	4.410524	0.146806	1.850911
N	2.786332	-0.931286	1.245984
H	1.828413	-0.840422	0.939005
H	3.228887	-1.348328	0.439559
H	2.928380	-1.549949	2.031591
N	-0.016743	-4.221941	-3.573543
O	-0.016387	-5.412277	-3.279990
O	0.307060	-3.415711	-2.708545
O	0.363012	-3.984450	-4.714797
C	-12.131521	-1.967990	-3.342551

H	-12.100256	-0.893666	-3.524073
H	-11.438804	-2.532984	-3.966269
H	-13.128867	-2.354321	-3.552672
C	-11.588097	-2.317597	-1.956800
H	-11.357155	-3.380354	-1.883908
H	-12.322474	-1.995409	-1.218569
N	-10.254250	-1.766388	-1.672437
H	-9.576561	-1.679929	-2.416320
H	-10.401542	-0.823716	-1.341114
H	-9.945949	-2.300083	-0.872299
N	-9.777062	-4.528673	1.160262
O	-9.737072	-4.296334	2.363381
O	-8.787320	-5.153429	0.795343
O	-10.172998	-3.641457	0.412492
C	-4.281074	-1.446810	2.840902
H	-5.038406	-0.862056	2.318779
H	-4.786874	-2.225381	3.411949
H	-3.804390	-0.779115	3.558577
C	-3.182495	-1.905808	1.881587
H	-2.415527	-2.344536	2.519850
H	-2.848866	-1.015485	1.348561
N	-3.678171	-2.993667	1.024435
H	-3.872663	-3.824277	1.565137
H	-4.478186	-2.715058	0.474476
H	-2.914012	-3.364329	0.477836
N	-10.974357	0.605433	0.157446
O	-11.791251	-0.245213	0.492349
O	-10.680617	0.659412	-1.031621
O	-10.159123	0.838849	1.042876
C	-5.871131	6.824077	6.661098
H	-5.055718	7.205665	7.275585
H	-6.339892	7.611805	6.071311
H	-6.591990	6.706061	7.470132
C	-5.644712	5.476193	5.975690
H	-5.055318	5.531551	5.060457
H	-6.685742	5.207028	5.797072
N	-4.926438	4.553328	6.868015
H	-5.626464	4.434708	7.586341
H	-4.658500	3.699520	6.399699
H	-4.082453	4.894015	7.305874
N	-4.441398	-6.127077	0.422864
O	-5.210745	-5.174517	0.484572
O	-4.611798	-7.094789	1.156059
O	-3.383780	-5.897545	-0.153186
C	-7.911866	-5.020443	4.754803
H	-7.265765	-4.409306	5.385014
H	-8.572313	-4.205172	4.459436
H	-8.356019	-5.749711	5.432295
C	-6.998387	-5.633523	3.692951
H	-7.450355	-6.535682	3.280721
H	-6.021113	-5.914442	4.085532
N	-6.747114	-4.612406	2.664348
H	-6.411536	-3.707865	2.963164
H	-6.045688	-5.092530	2.118835
H	-7.571470	-4.415117	2.115152
N	-1.530052	-1.345074	8.864696
O	-0.950211	-1.044832	9.902345
O	-1.807014	-2.518022	8.639837
O	-2.469707	-0.600652	8.607869
C	-4.288676	-3.528219	11.812252
H	-4.793003	-3.434526	12.774009
H	-4.449763	-2.604319	11.256769
H	-4.670007	-4.417386	11.310186
C	-2.783968	-3.796248	11.855329
H	-2.642189	-4.683486	12.472425
H	-2.239996	-3.004554	12.370514
N	-2.190162	-4.190663	10.568600

H	-2.788639	-4.910652	10.189731
H	-2.093312	-3.385475	9.966608
H	-1.292162	-4.629285	10.714571
N	-2.149738	4.370837	8.171142
O	-2.420712	5.061091	7.194823
O	-0.998200	3.950079	8.171515
O	-3.085972	3.902949	8.809593
C	-6.152161	0.971350	-4.856153
H	-5.709992	1.600554	-5.628610
H	-6.759712	0.293946	-5.456242
H	-6.879664	1.497004	-4.237666
C	-5.033496	0.387449	-3.992735
H	-4.509529	1.147409	-3.413065
H	-4.297330	0.185447	-4.770780
N	-5.337311	-0.836220	-3.234994
H	-5.823945	-0.664359	-2.366806
H	-5.864512	-1.507148	-3.775378
H	-4.455335	-1.309859	-3.101257
N	-3.954244	0.985895	-0.349497
O	-4.581213	0.737680	0.674406
O	-4.582013	1.756024	-1.067748
O	-3.314885	0.088389	-0.886877
C	-0.489329	-1.988290	5.447729
H	-1.184687	-2.817345	5.579051
H	0.269480	-1.958054	6.229647
H	-0.962215	-1.006409	5.467418
C	0.161159	-2.131990	4.071482
H	1.107008	-1.590645	4.091798
H	-0.524884	-1.737290	3.322043
N	0.472806	-3.549084	3.829488
H	0.908978	-3.556032	2.918551
H	1.263320	-3.867818	4.371333
H	-0.352119	-4.130876	3.796064
N	-2.922998	-4.747763	3.932673
O	-3.082732	-4.220626	5.027975
O	-1.815410	-4.927998	3.438871
O	-3.887392	-4.663575	3.180389
C	-3.382672	0.700335	12.149337
H	-3.059003	1.116506	13.103349
H	-4.447093	0.547227	12.327289
H	-2.841908	-0.183792	11.811704
C	-3.147296	1.755754	11.068351
H	-2.098811	2.039746	10.978202
H	-3.611828	2.706381	11.330300
N	-3.664143	1.397783	9.738475
H	-3.561983	2.163001	9.087242
H	-3.225421	0.602416	9.296871
H	-4.668370	1.297993	9.779317
N	-7.326653	-1.238968	4.650476
O	-7.251199	-2.002313	3.694084
O	-8.312334	-1.300631	5.376910
O	-6.337457	-1.006499	5.336425
C	1.035599	2.824076	5.619619
H	0.895801	3.663262	6.301032
H	1.821253	2.197158	6.041308
H	1.470006	3.152955	4.675569
C	-0.306039	2.091911	5.577424
H	-0.183167	1.204706	4.956240
H	-1.092383	2.684561	5.109953
N	-0.725683	1.773461	6.950861
H	-1.567133	1.229216	6.824931
H	-0.041326	1.273654	7.500360
H	-1.078846	2.625459	7.362535
N	0.608423	-3.921405	8.871310
O	0.409756	-5.071289	8.495312
O	0.592269	-3.737751	10.083369
O	1.510629	-3.261354	8.367890

C	-7.993908	2.897268	-2.082631
H	-8.701994	3.601144	-2.519979
H	-7.047441	3.109211	-2.580006
H	-8.385084	1.916454	-2.352976
C	-7.994652	3.101637	-0.567351
H	-8.972028	2.746777	-0.240378
H	-7.796351	4.084634	-0.140162
N	-7.032382	2.220779	0.112329
H	-7.292277	1.244798	0.108386
H	-6.108059	2.228362	-0.294697
H	-6.992642	2.417933	1.102103
N	-3.402923	-7.251814	10.006992
O	-3.291004	-7.324177	11.225726
O	-3.586787	-6.149521	9.502789
O	-2.736648	-8.069350	9.381860
C	-3.031686	-7.371898	6.273889
H	-2.767410	-8.207043	5.625206
H	-3.577213	-7.834128	7.096593
H	-3.780677	-6.787420	5.739569
C	-1.892312	-6.499648	6.801950
H	-2.152874	-5.679916	7.471463
H	-1.382543	-6.049642	5.950052
N	-0.886766	-7.338721	7.471781
H	-1.369454	-7.894132	8.163612
H	-0.377125	-7.936517	6.836952
H	-0.210730	-6.706800	7.876443
N	1.391082	-8.760239	8.923931
O	1.724235	-8.059644	7.974588
O	0.527212	-9.628891	8.876502
O	1.315677	-8.201821	10.012765
C	-2.947270	4.444946	3.354731
H	-3.415323	4.391493	4.337671
H	-1.952085	4.175874	3.708718
H	-2.968531	5.481841	3.019324
C	-3.477867	3.411948	2.360134
H	-2.670859	3.197818	1.659430
H	-4.346008	3.721932	1.778463
N	-3.748114	2.069662	2.897790
H	-3.985661	1.378726	2.200451
H	-2.818929	1.729834	3.100847
H	-4.377296	1.947767	3.678412
N	4.478679	-2.990323	9.455039
O	3.672775	-3.902661	9.600758
O	4.033125	-1.902946	9.804566
O	4.825508	-2.970905	8.279280
C	-11.174486	-0.219737	4.025281
H	-12.080451	-0.249231	4.630637
H	-10.364265	0.059025	4.699027
H	-11.399085	0.642998	3.398109
C	-10.941631	-1.584888	3.377221
H	-11.787781	-1.860197	2.747668
H	-10.749868	-2.419449	4.051636
N	-9.794079	-1.432586	2.469604
H	-9.492641	-2.291774	2.032535
H	-9.912300	-0.819403	1.675797
H	-8.970181	-1.252127	3.025236
N	0.835849	-6.637393	4.634737
O	1.309098	-5.947830	5.531183
O	0.940757	-6.268613	3.470233
O	0.191854	-7.665880	4.809554
C	-3.084111	-8.955405	-1.643570
H	-2.313850	-9.524973	-1.123580
H	-3.849107	-8.615365	-0.945535
H	-3.506482	-9.727211	-2.287012
C	-2.468299	-7.892055	-2.553463
H	-3.251558	-7.337527	-3.070284
H	-1.785787	-8.379864	-3.249394

N	-1.658828	-6.860913	-1.886123
H	-1.092711	-6.283895	-2.491649
H	-2.216484	-6.327414	-1.234588
H	-0.838971	-7.223888	-1.421167
N	1.213575	-8.326379	-1.068606
O	2.211314	-7.758116	-0.638871
O	0.331669	-8.110714	-0.244709
O	0.747254	-8.144108	-2.187711
C	1.892668	-0.359854	12.780759
H	2.358020	-0.769195	13.677413
H	2.785834	0.076137	12.333247
H	1.159267	0.429527	12.945382
C	1.586010	-1.574688	11.904415
H	0.736661	-2.191588	12.197910
H	2.374252	-2.295827	12.120594
N	1.591241	-1.320439	10.455564
H	2.525758	-1.442271	10.092338
H	0.934356	-1.968596	10.045081
H	1.241129	-0.417128	10.169989
N	-6.575348	2.966643	9.596995
O	-5.754516	3.178595	10.482651
O	-6.670047	3.891152	8.797376
O	-6.482571	1.855007	9.088334
C	-5.343449	-2.587230	8.655868
H	-4.464027	-2.239343	9.197803
H	-5.864953	-1.657786	8.427248
H	-5.902745	-3.330284	9.224338
C	-4.793757	-3.184769	7.360250
H	-5.574733	-3.708203	6.808712
H	-4.015826	-3.909347	7.600897
N	-4.073341	-2.190864	6.549697
H	-4.569488	-1.413795	6.137264
H	-3.260128	-1.709039	6.905548
H	-3.779107	-2.703924	5.730981
N	-0.382819	-3.742840	0.471745
O	-1.099395	-2.887958	-0.036952
O	0.594174	-3.379887	1.117365
O	-0.822324	-4.869509	0.673061
C	2.613547	-0.388218	-5.923871
H	1.590448	-0.576676	-6.249220
H	2.875950	0.669375	-5.951129
H	3.270954	-0.904987	-6.623061
C	2.649853	-0.832691	-4.461350
H	1.974169	-0.241322	-3.843423
H	3.662133	-0.589944	-4.138145
N	2.453459	-2.278634	-4.275555
H	3.038126	-2.958653	-4.740139
H	2.748345	-2.609909	-3.368141
H	1.508962	-2.612880	-4.403243
N	-3.800641	1.116110	6.072087
O	-3.541809	2.310737	5.977489
O	-2.944876	0.302888	5.741314
O	-4.534034	0.635600	6.929013
C	-1.288098	1.806689	-2.356662
H	-0.672040	2.660805	-2.637832
H	-1.824009	1.676505	-3.296849
H	-2.091744	2.086808	-1.675642
C	-0.481129	0.598332	-1.880726
H	-0.269835	0.550816	-0.812458
H	0.359999	0.489747	-2.565425
N	-1.124971	-0.697045	-2.147760
H	-1.205848	-0.995522	-3.109253
H	-0.567459	-1.466140	-1.804581
H	-2.052560	-0.736070	-1.750071
N	-0.349623	1.308314	1.933851
O	-1.141796	1.194896	2.862654
O	-0.099331	2.389885	1.413626

O	0.257558	0.294787	1.606482
C	-9.403660	1.595091	7.743181
H	-9.584657	0.523316	7.661707
H	-9.060496	1.867359	8.741283
H	-10.343734	2.027433	7.400482
C	-8.455378	2.076514	6.644621
H	-8.323519	3.154892	6.556219
H	-8.753038	1.676762	5.675241
N	-7.121991	1.459793	6.719286
H	-7.195328	0.488966	6.450556
H	-6.505794	1.889156	6.043971
H	-6.697083	1.497514	7.634780
N	3.340485	-2.730051	4.141536
O	2.852847	-3.428956	5.022907
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O	3.683279	-1.583825	4.409370
C	3.914288	-7.730382	12.020494
H	3.252515	-7.770015	12.885703
H	3.668096	-8.534487	11.327021
H	4.907433	-8.066705	12.318235
C	3.755557	-6.398039	11.287346
H	4.362617	-6.342069	10.383772
H	4.173182	-5.571294	11.861960
N	2.339166	-6.089839	11.036969
H	1.931631	-6.029182	11.959106
H	2.292611	-5.225913	10.515851
H	1.811771	-6.780551	10.522313
N	1.869233	1.236693	8.744993
O	0.896788	1.093717	9.477785
O	3.023421	0.946653	9.039614
O	1.673704	0.564491	7.738520
C	-0.790528	-9.680907	2.443121
H	0.161076	-9.460041	2.926617
H	-1.110829	-10.467642	3.126170
H	-0.566425	-9.996723	1.424231
C	-1.776187	-8.523764	2.277781
H	-2.374895	-8.277285	3.154648
H	-2.502262	-8.881163	1.547590
N	-1.017853	-7.370401	1.769326
H	-0.242713	-7.109087	2.361754
H	-0.589570	-7.708200	0.919287
H	-1.622905	-6.579026	1.602780
N	-6.728283	-1.191389	-0.161497
O	-6.826084	-0.100365	-0.712112
O	-5.693172	-1.828442	-0.322077
O	-7.687990	-1.941099	-0.302828
C	4.511270	-5.876767	0.626237
H	4.940445	-5.644897	-0.348517
H	5.049813	-5.432033	1.463066
H	4.516407	-6.965215	0.568321
C	3.218886	-5.071227	0.762946
H	3.489846	-4.016198	0.802879
H	2.734721	-5.395883	1.683968
N	2.332846	-5.165647	-0.407463
H	2.887626	-4.643436	-1.070498
H	2.180963	-6.127806	-0.674451
H	1.512018	-4.697289	-0.051116
N	4.062193	-2.323214	-1.378847
O	3.282686	-1.432049	-1.697080
O	4.736505	-2.071011	-0.386490
O	3.773645	-3.454698	-1.752422
C	4.422610	-6.869381	5.905224
H	5.243253	-7.574745	5.774431
H	3.423640	-7.234066	5.666137
H	4.621732	-6.057509	5.205713
C	4.188742	-6.308650	7.308338
H	5.103091	-5.861135	7.697946

H	3.857843	-6.943692	8.130121
N	3.256288	-5.177910	7.182651
H	2.379484	-5.550128	6.846840
H	3.107238	-4.545021	7.955526
H	3.617377	-4.501166	6.525588
N	-0.993599	-0.957862	-5.747263
O	-0.336320	-0.381232	-4.887869
O	-0.416134	-1.699796	-6.534121
O	-2.085611	-1.356414	-5.357722
C	0.410131	-10.126578	12.892605
H	0.564255	-9.351551	13.643391
H	0.512434	-11.039664	13.479042
H	1.241863	-10.024041	12.195605
C	-0.881717	-9.974755	12.088914
H	-1.790762	-10.097630	12.677675
H	-0.999990	-10.784853	11.369295
N	-0.928548	-8.711041	11.337465
H	-1.746751	-8.605940	10.754714
H	-0.815958	-7.945073	11.986090
H	-0.168230	-8.634162	10.677081
N	0.214308	-5.974715	13.467034
O	-0.634048	-6.712407	12.977975
O	-0.115088	-4.822229	13.209446
O	1.422324	-6.172281	13.398179
C	3.018290	-8.674634	-6.118706
H	3.619129	-9.560579	-5.913295
H	2.410205	-8.868797	-7.002241
H	3.781864	-7.959131	-6.423846
C	2.232368	-8.226394	-4.886128
H	2.781580	-8.299615	-3.947457
H	1.427980	-8.961486	-4.859679
N	1.648165	-6.894593	-5.107158
H	0.830644	-7.064067	-5.675522
H	1.227227	-6.431095	-4.314643
H	2.179274	-6.263690	-5.690240
N	-1.215122	-6.351643	-6.967666
O	-0.139889	-6.903781	-7.172833
O	-1.388561	-5.300706	-7.574731
O	-1.624613	-6.423927	-5.814337
C	-4.222437	-3.871362	-7.209272
H	-5.293384	-3.817724	-7.404968
H	-3.754394	-2.997503	-7.662490
H	-3.844696	-4.665314	-7.853518
C	-3.946284	-3.900157	-5.705693
H	-4.590038	-4.640315	-5.230461
H	-4.407459	-3.024746	-5.248447
N	-2.533784	-3.976240	-5.302089
H	-2.560743	-3.979895	-4.292455
H	-2.251438	-4.939491	-5.414024
H	-1.970076	-3.304184	-5.802763
N	-6.718004	2.459701	3.417359
O	-6.247104	1.362021	3.140905
O	-6.359906	2.926937	4.492781
O	-6.952297	3.250520	2.510283

Return

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	0.227949	-3.166189	-10.737680
H	-0.229755	-2.231248	-10.414427
H	0.691588	-3.111692	-11.722651
H	-0.509720	-3.966748	-10.792909
C	1.323871	-3.318350	-9.682386
H	2.056028	-2.527785	-9.846860
H	1.769739	-4.297771	-9.855693
N	0.845306	-3.167362	-8.299628
H	1.516556	-3.343940	-7.565909
H	0.527542	-2.270672	-7.960402
H	0.174927	-3.915942	-8.198034
N	-3.565352	-3.355804	-1.423598
O	-4.038009	-2.551849	-0.627778
O	-2.413589	-3.732599	-1.237744
O	-3.786507	-3.109308	-2.604025
C	6.326953	-3.723941	7.170981
H	6.772252	-4.382057	7.917099
H	5.958260	-4.267263	6.300943
H	7.034706	-2.919033	6.972710
C	5.048818	-3.024523	7.634688
H	4.451862	-2.696469	6.783733
H	5.321547	-2.183748	8.272509
N	4.148262	-3.801125	8.500557
H	4.022759	-4.733894	8.134099
H	4.609011	-3.841669	9.398425
H	3.286940	-3.281213	8.589541
N	3.729670	-3.760362	-6.952007
O	4.130506	-4.228670	-5.892245
O	3.257898	-2.629195	-6.920892
O	3.208745	-4.476213	-7.800105
C	-6.935242	-6.677064	-3.602252
H	-7.040942	-6.091978	-4.515818
H	-5.848869	-6.727814	-3.529328
H	-7.465113	-7.583708	-3.894369
C	-7.371535	-6.020110	-2.292328
H	-7.393661	-6.661215	-1.411082
H	-8.385508	-5.620433	-2.307075
N	-6.425033	-4.987306	-1.843675
H	-6.991240	-4.579198	-1.113637
H	-5.615041	-5.450385	-1.456930
H	-6.261019	-4.251752	-2.516104
N	-7.186955	-3.054185	-4.305329
O	-6.014264	-3.213559	-3.985219
O	-8.093258	-3.812622	-3.979039
O	-7.529905	-1.877322	-4.326663
C	4.082527	-0.281581	2.986721
H	4.181339	-1.360535	3.105863
H	4.913543	0.318934	2.616730
H	3.841768	0.040992	3.999679
C	2.951905	-0.062126	1.981051
H	3.453539	-0.175641	1.020021
H	2.452468	0.902795	2.068164
N	1.972413	-1.151541	2.113762
H	1.343096	-1.053218	1.329930
H	2.431548	-2.047653	2.034523
H	1.368340	-1.081021	2.920126
N	0.647890	-3.967300	-3.578941
O	1.069176	-3.866155	-4.725834
O	-0.572749	-4.009972	-3.472664
O	1.317907	-4.645206	-2.807839
C	-11.188131	-2.976450	-4.430274

H	-11.315423	-4.009841	-4.107783
H	-12.113795	-2.850812	-4.991934
H	-10.279913	-3.055097	-5.027815
C	-11.075388	-1.988773	-3.268541
H	-11.914861	-2.024712	-2.574212
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N	-2.118408	-4.112105	-5.613982
H	-1.586518	-4.132867	-4.755634
H	-1.812876	-4.902660	-6.163321
H	-2.029406	-3.199288	-6.036999
N	-5.604929	4.714601	4.369852
O	-5.795672	4.061244	3.350137
O	-4.818423	5.640770	4.206465
O	-5.593488	4.122771	5.443481

Return

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	4.631377	-6.366386	-7.471010
H	3.655699	-6.832586	-7.333858
H	5.048276	-6.904841	-8.322103
H	5.139997	-6.464639	-6.511972
C	4.304741	-4.927647	-7.872485
H	3.737583	-4.936302	-8.803267
H	5.275474	-4.454625	-8.020898
N	3.585066	-4.190561	-6.822431
H	2.628835	-4.474103	-6.663289
H	4.032356	-4.278709	-5.921176
H	3.490608	-3.197703	-6.981838
N	-3.079901	-1.632444	-3.975355
O	-3.706030	-1.399924	-2.947263
O	-3.487492	-0.991249	-4.937547
O	-1.903533	-1.885889	-3.740831
C	5.471568	-3.955815	4.996637
H	5.609272	-3.019769	5.537890
H	6.516630	-4.155356	4.759720
H	5.009168	-3.768269	4.027558
C	4.707505	-5.016133	5.790220
H	5.160626	-5.191457	6.765946
H	4.683704	-5.997108	5.315645
N	3.288634	-4.628905	5.816716
H	2.603060	-5.148704	6.345767
H	3.127109	-3.752614	6.292240
H	2.982341	-4.536858	4.858691
N	5.144988	-4.113696	-3.483710
O	4.259125	-4.390339	-2.682591
O	5.166956	-2.916547	-3.747204
O	5.118922	-4.852179	-4.461994
C	-8.773927	-5.739408	-2.252123
H	-8.636686	-6.446296	-3.070398
H	-9.240811	-6.150882	-1.357245
H	-9.368251	-4.870750	-2.535515
C	-7.346937	-5.328653	-1.887676
H	-6.828416	-4.968625	-2.776278
H	-6.779704	-6.201901	-1.565521
N	-7.394104	-4.390106	-0.755975
H	-7.417004	-3.405232	-0.978681
H	-8.077119	-4.580926	-0.036824
H	-6.459181	-4.563894	-0.415657
N	-8.385645	-1.432861	-1.977989
O	-9.084806	-2.439792	-1.996443
O	-8.886375	-0.431042	-1.479288
O	-7.194364	-1.616000	-1.753519
C	3.473804	2.617695	1.115993
H	4.435672	2.169473	1.365005
H	3.037049	2.194167	0.211576
H	3.747519	3.656086	0.929111
C	2.403969	2.333432	2.170739
H	1.420924	2.654630	1.826422
H	2.665550	2.913608	3.055651
N	2.256976	0.890910	2.418457
H	1.383257	0.534602	2.778680
H	2.245720	0.461514	1.504349
H	2.940278	0.339899	2.918044
N	1.230516	-2.930030	-3.404540
O	0.966499	-1.743958	-3.567653
O	2.088460	-3.293362	-4.201407
O	1.179973	-3.350332	-2.253946
C	-12.923416	-3.148450	-1.556491

H	-13.116966	-3.862919	-0.756383
H	-13.801346	-2.979222	-2.179951
H	-12.263619	-3.664864	-2.253688
C	-12.226218	-1.912662	-0.986769
H	-12.817360	-1.225669	-0.381218
H	-11.902734	-1.383868	-1.883337
N	-11.011437	-2.235475	-0.222610
H	-10.979160	-3.155396	0.193085
H	-10.205293	-2.255474	-0.830750
H	-10.829686	-1.477931	0.420192
N	-10.662577	-5.247785	1.459008
O	-10.681965	-5.282513	2.684363
O	-9.586813	-5.082153	0.894763
O	-11.611740	-4.707771	0.901737
C	-4.201353	-1.228466	0.434192
H	-3.503398	-0.392597	0.386423
H	-4.004453	-1.979586	-0.330760
H	-5.066979	-0.684809	0.055735
C	-4.806433	-1.553679	1.800192
H	-5.625795	-2.245450	1.604747
H	-5.232285	-0.611474	2.145154
N	-3.727476	-2.127019	2.619321
H	-3.313395	-3.008633	2.352124
H	-3.056974	-1.459393	2.972594
H	-4.264955	-2.349107	3.445090
N	-11.839177	-0.145203	2.534124
O	-11.130416	0.180985	1.588430
O	-12.554294	-1.119470	2.328005
O	-11.310732	-0.087394	3.638877
C	-7.001380	5.296337	6.433758
H	-6.673574	5.181246	7.466907
H	-6.327713	6.126854	6.222771
H	-8.035579	5.632829	6.506602
C	-6.935103	3.949915	5.712234
H	-6.997638	4.057222	4.629333
H	-7.668411	3.250349	6.113439
N	-5.636516	3.289398	5.915283
H	-5.351893	3.179764	6.878128
H	-5.751341	2.327832	5.628393
H	-4.868065	3.803236	5.508400
N	-4.877554	-5.287704	0.607089
O	-4.877542	-4.336806	-0.166777
O	-5.926522	-5.438736	1.223474
O	-4.241487	-6.296117	0.321434
C	-8.402346	-7.699336	4.347104
H	-8.060152	-8.716401	4.155837
H	-8.460490	-7.540893	5.423959
H	-9.469093	-7.707676	4.123318
C	-7.512720	-6.632482	3.708175
H	-7.651903	-6.699828	2.629197
H	-6.433636	-6.667869	3.857929
N	-8.082698	-5.287821	3.883822
H	-8.124298	-4.992891	4.848905
H	-7.669587	-4.521506	3.371766
H	-9.005513	-5.292468	3.473346
N	-2.684382	-2.684806	10.018321
O	-3.430024	-2.569775	9.051956
O	-2.046547	-1.700643	10.375625
O	-2.072292	-3.746942	10.001355
C	-0.140929	-4.167582	13.346569
H	0.056745	-3.624957	14.271006
H	-1.201672	-3.991882	13.167537
H	-0.122607	-5.239138	13.545395
C	0.675499	-3.729066	12.130432
H	1.756711	-3.674383	12.257274
H	0.506984	-2.686718	11.859854
N	0.313135	-4.446451	10.898404

H	0.442046	-5.438361	11.038389
H	-0.630675	-4.267375	10.586546
H	0.916055	-4.039059	10.197961
N	-3.055426	5.022173	5.483068
O	-4.075717	4.958575	4.806284
O	-3.156572	4.341459	6.497698
O	-1.953040	5.052392	4.947431
C	-7.591310	1.213508	-4.773873
H	-8.060083	1.234077	-5.757707
H	-8.303369	0.852365	-4.031816
H	-7.445374	2.213079	-4.364409
C	-6.285143	0.418690	-4.768092
H	-5.649228	0.794765	-5.569516
H	-6.581464	-0.575032	-5.103964
N	-5.845182	0.033810	-3.418225
H	-4.981162	-0.487498	-3.460738
H	-5.536584	0.823168	-2.868878
H	-6.434089	-0.519931	-2.812700
N	-5.093757	2.383389	-1.338125
O	-6.181277	1.969575	-1.724303
O	-4.187592	2.099676	-2.113654
O	-4.888547	2.163104	-0.149664
C	-0.864285	-2.093330	6.649596
H	-0.832148	-1.014439	6.497733
H	-1.547233	-2.371720	7.452206
H	0.076108	-2.250475	7.177863
C	-0.845389	-2.972847	5.399023
H	-1.851228	-2.870757	4.991635
H	-0.794212	-4.052379	5.540764
N	0.136179	-2.594728	4.370727
H	0.335286	-3.227090	3.608772
H	-0.182171	-1.708231	4.006204
H	1.038440	-2.367699	4.763770
N	-4.641123	-4.446705	4.853571
O	-4.802127	-3.235255	4.951255
O	-3.450399	-4.643241	4.637638
O	-5.089295	-5.187507	5.721574
C	-3.026276	1.115782	11.806595
H	-3.025079	1.962990	12.492407
H	-4.013797	0.793481	11.476407
H	-2.447980	0.298894	12.238299
C	-2.277262	1.606455	10.567217
H	-1.259309	1.896327	10.827688
H	-2.802693	2.431895	10.086934
N	-2.258905	0.724643	9.389970
H	-1.697896	1.117089	8.647437
H	-1.957649	-0.186511	9.704840
H	-3.240004	0.756200	9.152170
N	-9.832534	-4.183628	6.184942
O	-10.112781	-5.278863	5.710603
O	-10.748572	-3.384816	6.345721
O	-8.769220	-3.692604	5.822540
C	0.922085	3.951255	5.218224
H	1.018775	4.382069	6.214794
H	1.898915	3.970641	4.734978
H	0.318142	4.804165	4.908547
C	0.155570	2.647593	4.992925
H	0.883075	1.866624	5.214115
H	-0.197875	2.628114	3.962005
N	-1.007911	2.639843	5.892977
H	-0.724390	2.236556	6.774496
H	-1.321297	3.582204	6.076942
H	-1.755723	2.023498	5.608378
N	0.688324	-6.057865	7.595058
O	1.716686	-6.634313	7.931593
O	0.823383	-5.139694	6.793936
O	-0.197496	-5.981655	8.439210

C	-8.948379	3.224027	1.737634
H	-9.980641	3.188357	2.085862
H	-8.240183	3.052260	2.548222
H	-8.860767	4.275040	1.462325
C	-8.557951	2.242239	0.632419
H	-7.585745	2.440285	0.181094
H	-9.340838	2.248407	-0.125967
N	-8.640339	0.836193	1.056786
H	-8.122239	0.501537	1.856585
H	-9.569211	0.755513	1.445098
H	-8.631340	0.124431	0.340256
N	1.194371	-7.489414	12.314964
O	1.919899	-6.512003	12.461090
O	1.717216	-8.342845	11.606893
O	0.060283	-7.187530	11.960300
C	-4.821443	-6.318483	8.823541
H	-4.972183	-5.379057	9.355384
H	-5.384982	-6.080418	7.921405
H	-5.243276	-7.108343	9.445054
C	-3.382481	-6.533456	8.353415
H	-3.253681	-7.493746	7.854062
H	-2.703179	-6.661255	9.196218
N	-2.891282	-5.433548	7.509161
H	-3.403411	-5.295502	6.649645
H	-2.876313	-4.497464	7.888138
H	-1.962190	-5.713995	7.229452
N	-0.994348	-8.546220	5.812794
O	-0.460585	-8.995352	4.804600
O	-1.589138	-7.481413	5.688340
O	-0.376524	-8.852693	6.826423
C	-2.677550	4.272067	1.147408
H	-1.643623	3.927212	1.160451
H	-3.191271	4.167210	0.191795
H	-2.534980	5.308550	1.453150
C	-3.330281	3.437920	2.250123
H	-4.372579	3.688420	2.447518
H	-2.833445	3.634256	3.200232
N	-3.282007	1.982909	2.039286
H	-2.336126	1.634612	2.103306
H	-3.587327	1.605922	2.925153
H	-3.858831	1.550117	1.332132
N	2.691471	-3.299551	8.786961
O	2.368452	-2.321299	9.451610
O	3.667199	-3.094462	8.073540
O	2.561696	-4.400661	9.310212
C	-13.469510	-5.191551	4.182667
H	-12.879340	-5.848315	3.543557
H	-13.076380	-5.384285	5.180866
H	-14.503544	-5.526843	4.102333
C	-13.379740	-3.706632	3.829400
H	-13.993706	-3.213385	4.582960
H	-13.731316	-3.517923	2.815061
N	-11.964391	-3.314947	3.744485
H	-11.964365	-2.425552	3.265866
H	-11.550662	-3.202586	4.658981
H	-11.460191	-4.031901	3.242630
N	1.860318	-5.594636	3.147058
O	2.878708	-6.268102	3.258428
O	2.075804	-4.444048	3.511458
O	0.913676	-6.152717	3.690648
C	-3.859915	-5.020760	-3.098007
H	-4.022732	-4.018823	-2.700877
H	-3.928202	-4.926619	-4.181785
H	-4.452757	-5.849945	-2.711885
C	-2.473629	-5.454486	-2.620581
H	-1.756398	-4.827012	-3.149688
H	-2.313899	-6.411252	-3.117757

N	-2.287136	-5.305329	-1.169094
H	-3.023219	-5.768950	-0.655931
H	-1.377947	-5.706080	-0.987780
H	-2.352563	-4.340943	-0.876212
N	0.662540	-6.566425	-0.356373
O	0.094442	-6.265781	-1.400381
O	1.845970	-6.303384	-0.539073
O	0.217054	-6.130785	0.699485
C	4.729252	0.483857	9.410392
H	4.481938	1.483909	9.766527
H	4.451440	-0.199952	10.212468
H	5.812983	0.493564	9.526733
C	4.178258	0.071275	8.045100
H	4.547019	-0.842973	7.580056
H	4.579823	0.780508	7.321335
N	2.708011	0.053556	8.001528
H	2.412358	-0.081268	7.045227
H	2.406599	-0.680569	8.626278
H	2.215978	0.900897	8.246511
N	-5.744973	1.538563	8.816702
O	-5.478716	2.735005	8.843373
O	-6.432078	1.157694	7.875479
O	-4.758037	0.844245	9.033392
C	-7.118934	-2.300371	8.533796
H	-7.521687	-1.322563	8.797958
H	-8.066390	-2.814183	8.371237
H	-6.596419	-2.633693	9.430442
C	-6.355657	-2.112943	7.222263
H	-7.021046	-1.775822	6.427464
H	-5.969877	-3.087592	6.923375
N	-5.261359	-1.145327	7.395672
H	-5.665945	-0.249084	7.626233
H	-4.550733	-1.422638	8.057646
H	-4.737685	-1.053949	6.536885
N	-0.947054	-3.379876	1.046071
O	0.022175	-2.850461	1.578415
O	-1.875925	-3.825008	1.711000
O	-1.242328	-2.950554	-0.063692
C	3.756430	1.808929	-3.444433
H	4.523521	2.541085	-3.192207
H	3.243768	2.158193	-4.340699
H	3.066115	1.828725	-2.601122
C	4.439313	0.452278	-3.620529
H	4.962233	0.225636	-2.691396
H	5.069775	0.524998	-4.506716
N	3.557126	-0.704177	-3.840076
H	4.070299	-1.496645	-4.198890
H	3.268437	-1.070808	-2.944341
H	2.853015	-0.608645	-4.557851
N	-3.305959	0.482596	5.513952
O	-2.618272	0.420547	6.527023
O	-3.967110	-0.483686	5.150284
O	-3.335883	1.526101	4.871085
C	-0.139017	1.467564	-2.270557
H	0.047246	0.935529	-3.203479
H	-0.877320	2.230654	-2.516937
H	0.687322	1.951236	-1.749667
C	-0.947738	0.413055	-1.514367
H	-1.821984	0.170045	-2.118304
H	-1.363777	0.874483	-0.618769
N	-0.184251	-0.815481	-1.246739
H	0.757041	-0.664497	-0.913163
H	-0.736645	-1.485959	-0.731549
H	-0.086011	-1.363787	-2.089242
N	-0.814406	0.155010	2.537470
O	-1.974998	-0.137373	2.803200
O	-0.676508	1.081939	1.746987

O	0.039247	-0.161450	3.358571
C	-10.973234	-0.250255	7.163134
H	-11.078113	-1.296833	7.449100
H	-11.240948	0.341115	8.038755
H	-11.821215	-0.060179	6.505182
C	-9.659156	0.118272	6.473766
H	-8.960497	-0.145320	7.267802
H	-9.656577	1.196717	6.315501
N	-9.434600	-0.632988	5.229167
H	-9.319444	-1.631086	5.332316
H	-10.093231	-0.518139	4.472123
H	-8.576166	-0.371956	4.765428
N	3.990959	-8.726990	7.154373
O	4.318107	-8.314795	6.047058
O	4.554605	-8.262788	8.139205
O	2.927579	-9.323987	7.280444
C	5.963300	-5.993648	9.857304
H	6.225778	-6.452181	8.903914
H	5.775440	-5.009297	9.428512
H	6.816234	-5.985520	10.535935
C	4.805159	-6.578754	10.666131
H	4.715504	-6.090124	11.636339
H	5.191017	-7.582087	10.846507
N	3.512742	-6.757510	9.986760
H	3.840700	-7.385763	9.267147
H	2.723129	-7.174940	10.458315
H	3.077149	-5.919928	9.627854
N	2.977396	-0.846238	5.080754
O	3.290466	-0.951070	3.900045
O	2.682880	0.308617	5.368238
O	2.593384	-1.812346	5.730559
C	-2.127623	-7.982926	1.469630
H	-1.110440	-8.357269	1.584983
H	-2.698633	-8.884517	1.247859
H	-2.148186	-7.217805	0.693571
C	-2.586500	-7.285559	2.750626
H	-2.819699	-7.941061	3.589693
H	-3.576480	-6.831728	2.796208
N	-1.760897	-6.126734	3.123917
H	-0.998711	-6.598672	3.589155
H	-1.611130	-5.465126	2.375623
H	-2.228082	-5.562407	3.819167
N	-8.547856	-2.619730	2.221670
O	-9.184788	-2.390441	3.243835
O	-8.565651	-1.742145	1.365747
O	-7.519146	-3.277746	2.330505
C	4.948789	-4.844846	1.037450
H	4.495297	-5.810649	0.814584
H	5.907508	-4.865549	0.519251
H	5.128031	-4.758817	2.109165
C	4.138888	-3.642710	0.550860
H	4.827285	-2.904197	0.139998
H	3.696945	-3.098911	1.385766
N	3.110816	-3.880368	-0.474043
H	2.289126	-3.315162	-0.314453
H	3.536549	-3.782086	-1.384643
H	2.668223	-4.768107	-0.283963
N	3.150615	-0.680345	-0.349218
O	3.568616	-1.253236	-1.349292
O	3.742708	-0.646164	0.723785
O	2.159374	0.032185	-0.462431
C	2.228562	-9.243887	2.033936
H	2.491949	-10.013151	1.308016
H	1.153221	-9.151202	1.881780
H	2.665699	-8.247782	1.964740
C	2.542316	-9.682466	3.464687
H	3.622679	-9.586323	3.572726

H	2.337779	-10.703174	3.787829
N	2.050796	-8.678635	4.421020
H	1.049448	-8.669764	4.552640
H	2.406684	-8.846552	5.351207
H	2.355913	-7.748736	4.171436
N	3.314695	-0.870665	-7.285928
O	3.023562	-1.918663	-7.851628
O	4.484086	-0.785882	-6.927580
O	2.426108	-0.674998	-6.464220
C	-0.013288	-10.869579	10.797711
H	-0.230570	-10.383801	11.748978
H	-0.756434	-11.666669	10.819635
H	0.974966	-11.329169	10.782472
C	-0.283366	-10.096725	9.506357
H	-1.259763	-9.641688	9.672759
H	-0.416895	-10.583833	8.540439
N	0.732141	-9.040287	9.377808
H	0.527183	-8.295708	8.726890
H	1.088100	-8.659648	10.242972
H	1.458216	-9.444808	8.803981
N	0.722724	2.470832	8.852109
O	1.184926	1.659720	9.646805
O	-0.470174	2.416174	8.574470
O	1.445678	2.577571	7.867722
C	3.970755	-7.559286	-2.826379
H	3.695588	-7.567160	-1.771713
H	4.332776	-8.542439	-3.127132
H	4.819660	-6.876853	-2.868142
C	2.733422	-7.207446	-3.652851
H	1.867260	-7.854526	-3.514464
H	3.023357	-7.387847	-4.687980
N	2.062639	-5.930029	-3.366324
H	1.320999	-5.756848	-4.029707
H	1.629065	-5.954208	-2.454441
H	2.716909	-5.161034	-3.392366
N	-0.175201	-5.159394	-5.902706
O	-0.972562	-4.232634	-5.994396
O	0.935441	-4.780492	-6.257646
O	-0.188507	-6.015485	-5.025205
C	-0.761668	0.455268	-7.087536
H	-0.942588	0.979495	-8.025915
H	-1.494270	0.830031	-6.372730
H	0.299033	0.636952	-6.914317
C	-0.805262	-1.064297	-7.251435
H	-0.122578	-1.526326	-7.964577
H	-1.824314	-1.349614	-7.512635
N	-0.355973	-1.744785	-6.027132
H	-1.111416	-1.709370	-5.357690
H	-0.192382	-2.735135	-6.139134
H	0.465847	-1.328319	-5.613287
N	-6.529880	0.883663	4.051904
O	-7.299168	0.265929	3.324114
O	-5.986834	1.818338	3.473492
O	-6.814232	0.912342	5.244127

Return

([EtNH₃][NO₃])₃₀ conformer -10

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	2.987735	-5.813764	-8.434350
H	3.683147	-6.248557	-7.716397
H	2.881261	-6.447181	-9.315000
H	3.347289	-4.846165	-8.784453
C	1.573401	-5.651879	-7.876414
H	1.151833	-6.649925	-7.756897
H	0.890472	-5.082565	-8.506960
N	1.640836	-4.854793	-6.641931
H	2.318252	-5.212923	-5.983942
H	2.003269	-3.976284	-6.983932
H	0.709265	-4.852385	-6.251713
N	-3.721593	-2.705395	-1.687424
O	-4.852902	-2.267149	-1.510914
O	-2.807967	-1.889096	-1.642493
O	-3.557595	-3.647690	-2.454406
C	5.971329	-1.354666	4.549692
H	5.336239	-0.607925	4.073101
H	6.838712	-0.825045	4.943707
H	6.148987	-2.188301	3.870286
C	5.388871	-1.947957	5.832887
H	5.186208	-1.372697	6.736271
H	6.181798	-2.506246	6.330562
N	4.336925	-2.948080	5.594132
H	4.849797	-3.804343	5.439614
H	3.786583	-3.243179	6.387946
H	3.609566	-2.762291	4.918461
N	4.424273	-4.873376	-4.434471
O	4.398761	-3.741974	-4.906016
O	4.091445	-4.925219	-3.255652
O	3.935208	-5.704324	-5.191714
C	-7.684142	-6.638723	-3.839283
H	-7.641640	-7.407246	-4.611076
H	-7.533261	-7.177608	-2.903902
H	-8.663680	-6.160612	-3.835172
C	-6.447667	-5.741453	-3.901560
H	-6.401516	-5.052475	-4.744935
H	-5.461607	-6.205715	-3.917210
N	-6.368346	-4.754087	-2.814060
H	-5.559276	-4.151598	-2.864186
H	-7.182151	-4.164376	-2.914370
H	-6.407935	-5.296006	-1.962675
N	-6.754589	-2.013378	-5.128393
O	-7.448611	-2.999855	-4.908681
O	-6.977818	-0.938243	-4.583113
O	-6.061975	-2.070801	-6.138375
C	4.102583	1.666650	2.191014
H	4.567844	0.684562	2.275486
H	4.343776	1.999070	1.181349
H	4.543669	2.424169	2.838862
C	2.616492	1.391114	2.422220
H	2.166799	0.866685	1.579101
H	2.191270	2.394398	2.448808
N	2.124393	0.724441	3.637633
H	2.339757	-0.261476	3.596559
H	2.447320	1.216948	4.458154
H	1.121299	0.832813	3.684073
N	0.618318	-3.986767	-3.078712
O	1.729375	-3.566685	-2.775133
O	0.697708	-4.858374	-3.937243
O	-0.406262	-3.334500	-2.911803
C	-10.659258	-2.978964	-5.542530

H	-11.290433	-2.891642	-6.426890
H	-9.732755	-3.387882	-5.945615
H	-10.917144	-3.837933	-4.923040
C	-10.525629	-1.640954	-4.814714
H	-11.508015	-1.233577	-4.575838
H	-10.184971	-0.895201	-5.532977
N	-9.557369	-1.881484	-3.733762
H	-8.713899	-2.221372	-4.173234
H	-9.396272	-1.044049	-3.192606
H	-9.969682	-2.587740	-3.141055
N	-10.512787	-4.576802	-1.244454
O	-11.100341	-4.461981	-0.174560
O	-10.504652	-3.566914	-1.939533
O	-9.476254	-5.211828	-1.403879
C	-4.002808	-1.016670	2.702338
H	-3.213206	-1.763655	2.620838
H	-3.433579	-0.121726	2.451031
H	-4.374402	-1.117913	3.722028
C	-5.180812	-1.245011	1.754705
H	-4.663712	-1.115695	0.803924
H	-5.949474	-0.496287	1.946203
N	-5.518086	-2.664034	1.945658
H	-4.752116	-3.267086	1.681617
H	-5.754309	-3.043400	2.851406
H	-6.280619	-2.875191	1.317919
N	-10.085627	0.694246	-1.745038
O	-11.082638	0.068042	-2.086965
O	-9.027998	0.498740	-2.333490
O	-9.990882	0.968282	-0.553819
C	-6.985991	3.738865	10.686359
H	-6.812585	2.761303	11.136253
H	-5.977546	4.137194	10.798038
H	-7.615900	4.324208	11.356201
C	-7.344406	3.582067	9.208254
H	-7.549974	4.571755	8.800384
H	-8.318555	3.113353	9.068824
N	-6.338532	2.912626	8.369262
H	-6.347930	1.910784	8.497024
H	-6.586008	3.002408	7.394175
H	-5.376129	3.160275	8.549679
N	-5.584628	-6.433698	0.372072
O	-6.046129	-6.258920	-0.750223
O	-4.771909	-7.313318	0.634432
O	-6.205167	-5.907006	1.288916
C	-9.092837	-7.666555	1.175449
H	-8.007399	-7.740309	1.108475
H	-9.354286	-8.625356	1.623160
H	-9.546850	-7.605711	0.186373
C	-9.413379	-6.459732	2.057873
H	-9.138907	-6.577453	3.106161
H	-10.484477	-6.293619	1.942749
N	-8.811063	-5.260406	1.455650
H	-7.824558	-5.345497	1.256481
H	-9.104958	-5.029273	0.517406
H	-8.897866	-4.435754	2.032290
N	-1.512049	-3.427099	9.868594
O	-0.313496	-3.602212	9.679170
O	-2.188374	-4.330517	10.347653
O	-2.056941	-2.745597	9.007361
C	2.726805	-2.267256	13.007262
H	3.074303	-1.303589	12.634848
H	2.467870	-2.122467	14.056113
H	3.610922	-2.885096	12.850068
C	1.581977	-3.048922	12.362119
H	0.614358	-2.565290	12.495953
H	1.381875	-3.923838	12.980650
N	1.954786	-3.306562	10.962664

H	2.639884	-4.046312	10.903403
H	1.188816	-3.544255	10.348749
H	2.453407	-2.538266	10.536992
N	-3.140607	3.368972	9.684496
O	-2.285302	2.522859	9.448652
O	-3.674024	3.267348	10.783684
O	-3.847838	3.749146	8.758015
C	-4.612228	2.033267	-3.151391
H	-5.005408	2.082134	-4.166833
H	-5.228225	2.687242	-2.534168
H	-3.599413	2.412303	-3.014868
C	-4.696989	0.556909	-2.762774
H	-3.974341	0.413729	-1.959418
H	-4.404438	-0.124589	-3.561570
N	-6.022820	0.135428	-2.284895
H	-6.711329	0.276952	-3.010171
H	-5.997762	-0.873925	-2.258856
H	-6.122248	0.700632	-1.453776
N	-5.269474	2.292983	0.596297
O	-4.172701	2.071710	1.097498
O	-5.827853	1.334187	0.074760
O	-5.949603	3.244320	0.964343
C	-2.577619	-2.485917	5.352852
H	-2.507933	-1.469787	4.964618
H	-3.022979	-3.101322	4.571167
H	-3.244102	-2.557680	6.212358
C	-1.228468	-3.063153	5.782307
H	-0.604645	-2.792610	4.930397
H	-1.264684	-4.122553	6.036200
N	-0.665776	-2.342316	6.934527
H	-1.267321	-2.377200	7.745099
H	0.265816	-2.702583	7.084339
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N	-5.869435	-4.241231	5.101000
O	-6.221388	-4.220357	3.926791
O	-5.495071	-5.289782	5.614293
O	-5.791173	-3.161217	5.675911
C	-2.867298	-1.122830	12.745548
H	-2.925254	-1.103847	13.833841
H	-3.704810	-1.801478	12.583960
H	-1.969208	-1.666464	12.452295
C	-3.062445	0.251055	12.103520
H	-2.305679	1.033894	12.154192
H	-3.934522	0.710220	12.569084
N	-3.299222	0.068832	10.663182
H	-4.251709	-0.175311	10.432395
H	-3.199605	1.026149	10.357042
H	-2.568565	-0.386090	10.134708
N	-8.901282	-1.602307	2.894574
O	-7.820465	-1.172609	3.282220
O	-8.900687	-2.817843	2.734743
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C	-0.348959	3.428561	6.295105
H	-0.931015	4.109589	6.916001
H	0.610373	3.845878	5.989114
H	-1.130080	3.179764	5.576739
C	0.198250	2.248753	7.099130
H	0.881894	2.527557	7.901003
H	0.749308	1.580545	6.437365
N	-1.031977	1.569989	7.534631
H	-1.544217	2.125746	8.204589
H	-1.677109	1.415967	6.772934
H	-0.804476	0.663643	7.917881
N	1.696217	-4.524960	7.503671
O	2.449012	-4.920727	8.386703
O	1.692107	-3.316749	7.295621
O	0.704894	-5.231099	7.356288

C	-9.914793	2.144231	2.422405
H	-10.282211	3.155527	2.596717
H	-10.639454	1.747460	1.711392
H	-9.875835	1.447409	3.259675
C	-8.551304	2.306395	1.749766
H	-7.715625	2.510874	2.419041
H	-8.663331	3.002686	0.918665
N	-8.064281	1.032313	1.198982
H	-8.658506	0.587275	0.514192
H	-7.197651	1.301696	0.755714
H	-7.796374	0.218262	1.733442
N	2.272992	-6.836217	10.808704
O	3.088435	-7.649187	10.387744
O	1.196803	-6.809689	10.222028
O	2.748194	-5.784992	11.223658
C	-3.228266	-8.179051	9.900642
H	-3.274723	-8.573890	8.885731
H	-3.528422	-8.979199	10.577230
H	-3.847374	-7.308978	10.119227
C	-1.819198	-7.727580	10.286053
H	-1.144347	-8.581993	10.337552
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N	-1.278969	-6.563760	9.566666
H	-1.525813	-6.587591	8.587586
H	-1.763034	-5.733369	9.876882
H	-0.314699	-6.581284	9.866626
N	-1.697447	-7.843507	6.678404
O	-1.142371	-7.678227	5.597826
O	-2.273247	-6.877423	7.166472
O	-1.138350	-8.480066	7.564563
C	-2.863838	4.516122	2.977147
H	-1.861116	4.134648	3.169828
H	-3.097770	4.371890	1.922361
H	-2.385493	5.478337	3.159982
C	-3.874394	4.058883	4.029549
H	-4.814468	4.606659	3.963973
H	-3.245134	3.996474	4.917376
N	-4.242740	2.647893	3.836497
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N	4.907456	-2.307838	10.021549
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O	5.083531	-3.428041	10.487615
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C	-13.226417	-2.035400	-0.823629
H	-12.828790	-1.518356	-1.696932
H	-13.160430	-3.114691	-0.961026
H	-14.284825	-1.944446	-0.579497
C	-12.467644	-1.699810	0.460693
H	-12.626731	-2.374028	1.302252
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N	-11.033464	-1.656788	0.136472
H	-10.340057	-1.552570	0.863400
H	-10.845652	-2.427709	-0.488433
H	-10.844226	-0.829150	-0.410616
N	2.333635	-2.650147	2.798279
O	1.195772	-2.879492	3.192926
O	3.000336	-3.679008	2.803814
O	2.886062	-1.661161	3.267115
C	-2.423230	-7.891523	-1.511063
H	-3.108185	-8.598667	-1.043212
H	-2.348896	-8.213759	-2.549686
H	-1.537539	-8.158301	-0.934451
C	-2.725233	-6.400178	-1.360981
H	-2.820071	-6.134634	-0.308084
H	-3.671798	-6.299192	-1.891939

N	-1.731787	-5.675906	-2.168654
H	-1.925169	-4.684626	-2.160494
H	-0.838254	-5.753461	-1.704237
H	-1.533647	-5.980780	-3.110935
N	1.364912	-6.119743	-0.327990
O	2.524822	-6.442137	-0.559824
O	0.456815	-6.740009	-0.869935
O	1.182846	-5.162805	0.416456
C	5.067102	2.008909	9.629589
H	5.469555	2.372534	8.684122
H	5.174075	2.923215	10.213285
H	5.654409	1.261187	10.162583
C	3.609125	1.548335	9.633659
H	2.893414	2.347870	9.442350
H	3.389219	1.092567	10.599069
N	3.500830	0.399432	8.721444
H	2.568264	0.026973	8.613302
H	3.824649	0.683259	7.807835
H	3.968677	-0.390096	9.143185
N	-6.755756	-0.536208	9.571082
O	-7.044552	-1.712399	9.380692
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O	-5.826360	-0.297850	10.334288
C	-5.513349	-4.489453	9.995708
H	-6.526990	-4.188012	10.259839
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C	-5.174095	-4.206625	8.531892
H	-6.043697	-4.460818	7.925856
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N	-4.844402	-2.799921	8.255617
H	-4.797138	-2.776416	7.246997
H	-5.520590	-2.137071	8.607042
H	-4.021892	-2.604295	8.808163
N	-2.333591	-4.314915	1.805386
O	-3.527050	-4.233779	1.536784
O	-2.069615	-5.238701	2.566972
O	-1.472870	-3.989402	0.995277
C	3.158555	0.668842	-5.554823
H	2.875767	1.334440	-4.739280
H	3.909167	0.985514	-6.278979
H	2.241401	0.519469	-6.124573
C	3.661855	-0.648556	-4.964066
H	4.543748	-0.358048	-4.393130
H	4.034800	-1.319279	-5.738109
N	2.638729	-1.255771	-4.098997
H	1.913150	-1.477772	-4.765594
H	2.847162	-2.157591	-3.694799
H	2.310367	-0.685999	-3.332420
N	-4.011812	0.098255	7.065951
O	-3.354592	-0.596802	7.832785
O	-4.985974	-0.299835	6.436978
O	-3.501308	1.161735	6.732077
C	-1.067888	0.354223	0.284395
H	-1.600418	0.893357	1.067878
H	-0.114328	0.851441	0.106640
H	-1.699901	0.238682	-0.596123
C	-0.791939	-1.072275	0.760626
H	-1.803246	-1.306056	1.093349
H	-0.074389	-1.101032	1.580623
N	-0.511594	-1.975388	-0.366156
H	-1.248922	-1.964416	-1.056320
H	0.329530	-1.573359	-0.754723
H	-0.434793	-2.929047	-0.042528
N	-1.010915	0.597713	4.233004
O	-0.355634	0.002307	5.081046
O	-2.161907	0.952645	4.461734

O	-0.486773	1.227829	3.321244
C	-9.930446	-0.202559	6.100444
H	-10.050359	-0.137784	5.018998
H	-10.895813	-0.540925	6.476841
H	-10.051277	0.760976	6.595519
C	-8.746965	-1.077002	6.515851
H	-8.770404	-2.161394	6.407939
H	-8.752366	-0.866921	7.585400
N	-7.502610	-0.654130	5.855093
H	-7.568742	-0.778235	4.854932
H	-7.281704	0.252961	6.240433
H	-6.667177	-1.109799	6.193499
N	4.303891	-6.358061	5.993583
O	4.391966	-7.261447	6.817727
O	4.988741	-5.401603	6.338900
O	3.189905	-6.190983	5.509644
C	7.150581	-6.075508	8.975540
H	7.063081	-6.473523	7.964586
H	7.198052	-5.015959	8.724140
H	8.147448	-6.369813	9.303778
C	5.981247	-6.397831	9.906457
H	6.214184	-5.943671	10.869565
H	6.025863	-7.473042	10.079749
N	4.809210	-5.831280	9.221482
H	4.726462	-6.309993	8.335996
H	4.011538	-6.136544	9.760585
H	4.827282	-4.828652	9.101022
N	3.741200	2.391235	6.021561
O	3.260087	2.782410	4.963928
O	4.103019	1.220276	6.053487
O	3.162037	2.759479	7.037456
C	-5.074241	-8.378996	4.787025
H	-5.449904	-7.677969	5.532369
H	-5.881019	-8.780954	4.174130
H	-4.791998	-9.123061	5.531878
C	-4.002096	-7.680875	3.949783
H	-3.730272	-8.307523	3.100358
H	-3.076962	-7.533476	4.507008
N	-4.494199	-6.383713	3.460860
H	-4.743097	-5.886447	4.303994
H	-3.729326	-5.835782	3.093655
H	-5.163900	-6.403479	2.705075
N	-7.654224	-2.317722	-0.638396
O	-7.725195	-1.218065	-0.101000
O	-7.634439	-2.276814	-1.863553
O	-7.268627	-3.298433	-0.011820
C	5.835503	-3.047029	-0.577715
H	5.569126	-2.107679	-0.093191
H	6.848857	-3.247953	-0.230088
H	5.850744	-2.907919	-1.658695
C	4.865040	-4.100306	-0.042320
H	4.819108	-4.025590	1.044146
H	5.206544	-5.074032	-0.393509
N	3.518160	-3.944235	-0.612755
H	3.347896	-2.951412	-0.539192
H	3.412638	-4.221103	-1.578317
H	2.863531	-4.433547	-0.019345
N	2.394510	-0.730803	-1.105738
O	3.479964	-0.842460	-1.664664
O	2.245814	-1.205224	0.014928
O	1.480996	-0.366063	-1.837539
C	0.354570	-7.872179	2.745882
H	0.485425	-8.871843	3.160190
H	-0.694061	-7.630122	2.918742
H	0.543912	-8.118580	1.701116
C	1.099679	-6.748020	3.466242
H	2.187505	-6.779123	3.404864

H	0.888721	-6.823378	4.532974
N	0.617469	-5.424656	3.041950
H	0.915598	-5.184320	2.107361
H	-0.369602	-5.360096	2.837930
H	1.037062	-4.646494	3.530321
N	0.806109	-1.986623	-6.668542
O	0.052291	-2.835716	-7.131008
O	0.417480	-1.504338	-5.610504
O	1.990476	-2.303357	-6.674133
C	1.703775	-9.580084	6.239615
H	2.307262	-8.997921	5.543203
H	2.080699	-10.586317	6.056520
H	0.713322	-9.622559	5.786515
C	1.699954	-9.042125	7.670847
H	2.641545	-9.193349	8.198710
H	0.912977	-9.426380	8.319781
N	1.579638	-7.579567	7.569423
H	1.665755	-7.194358	8.499100
H	2.312466	-7.056056	7.112259
H	0.726722	-7.281573	7.117943
N	0.436497	-0.633424	9.517073
O	0.823147	-0.297614	8.403156
O	-0.698253	-0.265090	9.799470
O	1.303101	-0.711130	10.380806
C	3.318767	-9.071135	-3.354710
H	3.208946	-9.194032	-2.277242
H	3.402455	-10.066863	-3.790166
H	4.221186	-8.489720	-3.543647
C	2.257436	-8.166813	-3.982101
H	1.417645	-8.861235	-4.007156
H	2.525414	-7.859254	-4.992890
N	2.065690	-6.923214	-3.220172
H	2.948643	-6.508944	-2.957736
H	1.545893	-6.206525	-3.706247
H	1.691264	-7.007005	-2.285890
N	-1.335602	-6.860932	-5.228419
O	-0.684631	-7.132786	-4.225719
O	-2.211170	-6.037331	-4.987301
O	-0.686720	-6.431057	-6.175644
C	-3.467713	-3.555601	-7.238685
H	-2.896834	-3.079483	-8.035872
H	-3.429556	-4.643921	-7.285639
H	-4.424963	-3.255656	-7.665072
C	-3.163175	-3.032528	-5.834586
H	-3.900529	-3.446910	-5.147057
H	-3.203783	-1.946225	-5.754612
N	-1.832085	-3.334744	-5.286220
H	-1.159224	-2.763313	-5.776959
H	-1.760078	-3.200317	-4.287799
H	-1.558167	-4.282804	-5.501281
N	-7.167903	2.694673	5.319254
O	-6.593894	2.010223	4.479541
O	-7.883829	2.038533	6.067589
O	-6.514573	3.569456	5.876920

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([C₁mim][Cl])₁₀

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
N	-7.06183534	-4.89751581	-3.57290937
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C	-5.60926330	-3.33077348	-3.84339962
N	-6.44441074	-3.34613245	-4.88452043
C	-7.31262454	-4.29862096	-4.70121095
C	-6.39255297	-2.44107264	-6.04170917
C	-7.81907123	-6.02540715	-3.01134449
H	-5.54700476	-4.57719526	-2.07979306
H	-4.78548587	-2.66366674	-3.69754031
H	-8.10728807	-4.54972939	-5.37230232
H	-6.77179697	-2.94511034	-6.90601271
H	-5.37958836	-2.14461140	-6.21752209
H	-6.98852766	-1.57471402	-5.84389495
H	-8.83905168	-5.96347537	-3.32868677
H	-7.77504734	-5.98784408	-1.94291459
H	-7.39429886	-6.94588535	-3.35367735
Cl	-6.33079600	-3.16644300	7.15044200
N	-13.30329033	-0.63831956	-5.61809621
C	-13.42743296	-1.11897743	-4.37906647
C	-13.26129246	-2.45156874	-4.45698872
N	-13.04105090	-2.74175275	-5.74109326
C	-13.07057876	-1.63384410	-6.42395398
C	-12.80519261	-4.08452293	-6.29086709
C	-13.41105845	0.77528547	-6.00669917
H	-13.62204553	-0.55220381	-3.49261276
H	-13.29858663	-3.14661193	-3.64432147
H	-12.92627811	-1.55403076	-7.48117422
H	-13.73976262	-4.52553173	-6.56832512
H	-12.32871851	-4.69395440	-5.55163267
H	-12.17541704	-4.01147450	-7.15281097
H	-13.08767215	1.39377784	-5.19566421
H	-14.42900205	1.00305960	-6.24506254
H	-12.79494687	0.95796674	-6.86223114
Cl	-5.77589600	-5.43481400	0.13613800
N	-3.65481833	-1.99615355	1.96630169
C	-3.88555187	-3.22560713	2.43194754
C	-3.86093315	-3.14737615	3.77461138
N	-3.61596156	-1.87266956	4.08562596
C	-3.49504456	-1.19564779	2.98034661
C	-3.50204167	-1.32610430	5.44546886
C	-3.59181413	-1.61140404	0.54894914
H	-4.05737358	-4.10581852	1.84833565
H	-4.00944828	-3.95350843	4.46235578
H	-3.29571342	-0.14637629	2.91555396
H	-4.46538323	-1.00482184	5.78258340
H	-2.83007495	-0.49344268	5.44006632
H	-3.12775550	-2.08221457	6.10358156
H	-3.24023088	-2.43960862	-0.03015190
H	-2.92185498	-0.78519164	0.43310514
H	-4.56750392	-1.32935489	0.21222192
Cl	-11.25477100	-2.45690600	4.36575000
N	-9.16838292	-0.20367493	6.77184955
C	-7.89665630	-0.05250268	7.14799770
C	-7.48153143	1.13045812	6.66040618
N	-8.51314903	1.66359879	6.00225357
C	-9.52027994	0.84264157	6.08190658
C	-8.51216691	2.95809624	5.30569727
C	-10.02600858	-1.35609649	7.08374948
H	-7.31764657	-0.74117414	7.72711665
H	-6.50943161	1.56190605	6.77780189
H	-10.48540747	1.00267849	5.64850642

H	-7.52675712	3.16874652	4.94584724
H	-8.81652292	3.72805578	5.98350636
H	-9.19250272	2.91974265	4.48073043
H	-9.72778702	-1.77957517	8.02002784
H	-9.92938487	-2.09162676	6.31267608
H	-11.04511258	-1.03592004	7.14557374
Cl	-5.16967200	2.03667300	3.59461200
N	-9.37917222	1.67918000	-4.70125518
C	-10.30628928	0.79036157	-4.33778522
C	-10.60319109	1.03811377	-3.04940646
N	-9.84780216	2.07024080	-2.66762138
C	-9.11716459	2.44143972	-3.67904076
C	-9.84192857	2.68364835	-1.33174934
C	-8.75921524	1.78013392	-6.03027963
H	-10.73223690	0.02626572	-4.95392789
H	-11.31027274	0.50860738	-2.44558981
H	-8.41222447	3.24637057	-3.67136974
H	-10.81032182	2.58171796	-0.88823964
H	-9.59608360	3.72153408	-1.41692237
H	-9.11509393	2.19417626	-0.71771932
H	-7.88325834	1.16649614	-6.06277293
H	-8.48915405	2.79768117	-6.22150574
H	-9.45395999	1.44970358	-6.77394160
Cl	-14.56736600	1.93723000	-3.09714300
N	-8.96324449	-5.93690563	2.31945273
C	-7.88160357	-6.01349364	3.09778549
C	-8.30834566	-5.93437734	4.37101083
N	-9.63683672	-5.81203455	4.32918129
C	-10.01107346	-5.81576220	3.08235545
C	-10.52632968	-5.69324426	5.49347234
C	-8.97004121	-5.98174633	0.85015094
H	-6.86805038	-6.11793052	2.77112881
H	-7.69887517	-5.96389902	5.24997319
H	-11.02095354	-5.73239016	2.73869873
H	-11.38624274	-5.11457186	5.22780186
H	-10.00457551	-5.21028962	6.29311485
H	-10.83561740	-6.66841007	5.80698347
H	-8.14855700	-6.57568165	0.50765005
H	-8.87818476	-4.98864545	0.46257523
H	-9.88831870	-6.41355470	0.51073674
Cl	-11.33106300	-4.79823800	-1.87410100
N	-12.29095572	4.75245112	0.36760413
C	-11.44297279	5.78141689	0.30596695
C	-11.25574528	6.05768389	-0.99714303
N	-11.99547453	5.18855389	-1.68928985
C	-12.61154898	4.41048862	-0.84685485
C	-12.09720734	5.12139300	-3.15422774
C	-12.77985519	4.11380088	1.59805298
H	-10.99703915	6.28974386	1.13521119
H	-10.63248983	6.82757054	-1.40179204
H	-13.27673003	3.61509631	-1.11105452
H	-12.28627199	4.11141537	-3.45270790
H	-11.17985904	5.45666942	-3.59119237
H	-12.89956500	5.74722885	-3.48509323
H	-12.03490834	4.19425364	2.36191641
H	-12.98454397	3.08111477	1.40684106
H	-13.67598282	4.60117395	1.92103781
Cl	-9.54160400	-1.98071200	-6.49971400
N	-6.35109514	4.26584761	0.64557977
C	-5.50764747	3.35264639	0.15947303
C	-4.94588624	3.88426972	-0.94110086
N	-5.46436862	5.10499294	-1.09161019
C	-6.30953130	5.31494844	-0.12401676
C	-5.13662731	6.05164032	-2.16740365
C	-7.18534075	4.11285785	1.84620773
H	-5.31503396	2.38244288	0.56753906
H	-4.22136160	3.41745245	-1.57516408

H	-6.88021934	6.20907545	0.01658433
H	-5.98697422	6.66831512	-2.37118921
H	-4.86936187	5.50955078	-3.05035754
H	-4.31498434	6.66611595	-1.86372485
H	-7.43564726	3.08086417	1.97745240
H	-8.08193995	4.68571387	1.73289612
H	-6.64567463	4.46063605	2.70219670
Cl	-8.69729500	5.73540300	-2.56013800
N	-8.11125694	-1.68502972	0.43705393
C	-7.66393469	-0.44576752	0.65096702
C	-7.52985449	-0.30155575	1.98164872
N	-7.89960025	-1.45740383	2.53746072
C	-8.24649756	-2.27780128	1.58812542
C	-7.91282592	-1.75365794	3.97723892
C	-8.40185029	-2.27956278	-0.87557044
H	-7.45228715	0.29240152	-0.09415833
H	-7.19125415	0.57316918	2.49653707
H	-8.58888434	-3.28137015	1.73138873
H	-8.09860966	-0.85341926	4.52491883
H	-6.96555917	-2.15827867	4.26684412
H	-8.68393516	-2.46491331	4.18795427
H	-8.71121192	-1.51221104	-1.55407031
H	-9.18398541	-3.00269438	-0.77432102
H	-7.52186890	-2.75653907	-1.25376066
Cl	-6.34629500	0.35055900	-2.61012100
N	-13.63935894	-2.54158276	0.25301722
C	-14.27495148	-1.41753064	-0.08661964
C	-13.49329202	-0.39221379	0.29639458
N	-12.41233984	-0.92154578	0.87212454
C	-12.52497050	-2.21797084	0.84399390
C	-11.28614875	-0.16848173	1.44262472
C	-14.15725736	-3.90677973	0.08311281
H	-15.22621000	-1.34598593	-0.57131024
H	-13.69957717	0.64950177	0.16540071
H	-11.81338955	-2.90963002	1.24421406
H	-10.85657396	-0.72550945	2.24890222
H	-11.63599904	0.77467619	1.80727649
H	-10.54613391	-0.00645231	0.68696034
H	-14.25992026	-4.37114947	1.04160297
H	-13.47702919	-4.47419088	-0.51708772
H	-15.11179803	-3.86871463	-0.39885197
Cl	-10.01090000	2.83036500	2.23148800

Return

([C₁mim][Cl])₂₀

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
N	-9.17041486	-6.94199291	-1.03894976
C	-8.88594033	-7.69687442	-2.10238028
C	-9.30091550	-7.01831349	-3.18719899
N	-9.82533998	-5.87089466	-2.75130591
C	-9.73658034	-5.84526293	-1.45280248
C	-10.40476832	-4.81534456	-3.59449649
C	-8.89167840	-7.29000634	0.36180540
H	-8.41709086	-8.65864498	-2.09362893
H	-9.22504877	-7.33757902	-4.20563986
H	-10.07560570	-5.04821611	-0.82456689
H	-10.82298819	-5.25300772	-4.47679021
H	-9.64045348	-4.11892586	-3.86970916
H	-11.17260325	-4.30577598	-3.05074890
H	-8.02255386	-7.91237771	0.40852949
H	-9.72880580	-7.81502975	0.77226408
H	-8.72077635	-6.39592156	0.92421688
Cl	-4.44183400	6.77106800	-2.74072700
N	-2.33308027	3.65129254	0.30883162
C	-2.15127027	2.58758601	1.09437450
C	-0.84797958	2.56364494	1.42654353
N	-0.27589816	3.61352517	0.83317390
C	-1.18936314	4.25599081	0.16425003
C	1.14457439	3.98174603	0.92028378
C	-3.60838728	4.06897322	-0.29119420
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Return

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Return

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H	-8.11170381	7.87822953	-4.97952745
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B	-3.35115696	1.92380023	-5.13346362
F	-4.03042051	2.24275318	-6.38584926
F	-2.78796756	3.14312493	-4.56104417
F	-4.30722441	1.34240413	-4.19564241
F	-2.27901755	0.96691554	-5.39131555
N	-8.80546037	-7.45145319	-0.73690794
C	-8.87611838	-8.10886196	0.42257517
C	-10.09188647	-7.85936877	0.94132097
N	-10.72450732	-7.05759441	0.08190650
C	-9.93072862	-6.82393327	-0.92306108
C	-12.08642828	-6.52828864	0.24292839

C	-7.65257741	-7.43831027	-1.64880356
H	-8.11128826	-8.71829668	0.85674871
H	-10.47826749	-8.23258068	1.86670695
H	-10.16615973	-6.21239786	-1.76892256
H	-12.04672105	-5.59339575	0.76187521
H	-12.67509339	-7.22325044	0.80455033
H	-12.52880722	-6.38296036	-0.72044821
H	-7.74327172	-8.24146937	-2.34992780
H	-6.75073102	-7.55688869	-1.08530038
H	-7.62454426	-6.50701764	-2.17493169
B	-12.76919911	2.05917268	-1.33315983
F	-11.84279768	2.96227973	-0.65656890
F	-14.09497795	2.18392076	-0.73454391
F	-12.84012429	2.40627535	-2.74952413
F	-12.29890197	0.68421847	-1.19199923

Return

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
N	-7.86670186	1.69439651	-4.04939183
C	-8.44526026	0.80190626	-3.24293427
C	-8.21678967	-0.41261966	-3.77416834
N	-7.50608859	-0.22267029	-4.88792243
C	-7.30604077	1.05519054	-5.03514739
C	-7.03005715	-1.27744685	-5.79440586
C	-7.86323881	3.15175847	-3.85704026
H	-8.98752708	1.01245102	-2.34487097
H	-8.54271656	-1.35209220	-3.37912426
H	-6.76580586	1.50872665	-5.83972963
H	-7.76832615	-1.46105248	-6.54683054
H	-6.85718006	-2.17480676	-5.23784494
H	-6.11815849	-0.96424387	-6.25835825
H	-6.97015871	3.56488232	-4.27733697
H	-7.90083993	3.37353747	-2.81095032
H	-8.71618906	3.57765888	-4.34281577
B	6.33309096	-2.84466497	1.44154895
F	7.77077824	-2.68484904	1.24382119
F	5.72541682	-3.34522014	0.21200422
F	6.09334279	-3.79410720	2.52445329
F	5.74282619	-1.55448265	1.78591735
N	1.30347694	-6.90144020	-1.67792422
C	1.28468578	-7.24219679	-0.38751148
C	2.55436086	-7.18136815	0.05260071
N	3.30758617	-6.80537933	-0.98321626
C	2.53328464	-6.64197141	-2.01684742
C	4.76424820	-6.60912680	-0.96058056
C	0.13392251	-6.83110086	-2.56566382
H	0.42362011	-7.51232046	0.18738439
H	2.89554202	-7.39391697	1.04422375
H	2.85676492	-6.34166807	-2.99156654
H	5.25192977	-7.52867805	-1.20855819
H	5.06695137	-6.29723416	0.01716943
H	5.03415572	-5.85861100	-1.67386815
H	-0.59907725	-7.54244676	-2.24691666
H	0.43358653	-7.05281615	-3.56863235
H	-0.28404928	-5.84684786	-2.52762062
B	-10.05707301	3.31689003	0.12660563
F	-10.24853306	2.72801537	-1.19557991
F	-11.35785197	3.59028131	0.73058855
F	-9.31440150	2.38585957	0.97112392
F	-9.30750646	4.56340373	0.00029081
N	-2.15458825	5.34491337	-1.23889142
C	-2.74456867	6.51818294	-1.00016550
C	-2.04604575	7.11563791	-0.01802485
N	-1.05197350	6.28799250	0.31133045
C	-1.13594872	5.22616172	-0.43707090
C	-0.03496614	6.53384454	1.34391471
C	-2.58247360	4.35491003	-2.23771730
H	-3.60861919	6.90905840	-1.49568229
H	-2.24869361	8.07221801	0.41646006
H	-0.47219014	4.38777003	-0.39914417
H	0.14190671	7.58585301	1.42700134
H	0.87466067	6.03951055	1.07349392
H	-0.38119365	6.15512943	2.28284801
H	-2.09331290	4.55299380	-3.16851730
H	-3.64223856	4.41804827	-2.37120196
H	-2.32332269	3.37306551	-1.90046980
B	1.40380122	0.01750428	-8.34629531
F	2.67720941	0.70537885	-8.53819159
F	0.89941752	-0.44178742	-9.63712482

F	1.59826335	-1.12923314	-7.46381105
F	0.44031549	0.93565943	-7.74605423
N	2.65159229	0.41373427	-3.65255205
C	3.00956489	1.21310853	-2.64533558
C	3.43455639	0.41878798	-1.64637605
N	3.32244742	-0.84006502	-2.07575705
C	2.84833819	-0.82037132	-3.28797353
C	3.67459472	-2.04429867	-1.30977145
C	2.12462179	0.85249663	-4.95281367
H	2.96664059	2.28219536	-2.63458023
H	3.79403545	0.73574600	-0.68970959
H	2.65136872	-1.68278386	-3.88993128
H	4.69897387	-2.29508581	-1.49048872
H	3.04918761	-2.85693979	-1.61535412
H	3.53194543	-1.85741881	-0.26591929
H	1.46426293	0.10519416	-5.34059276
H	2.93570733	1.00037057	-5.63484546
H	1.59031639	1.77130380	-4.82944917
B	-3.54977442	-0.07855194	-3.50024215
F	-4.62331471	0.63727976	-2.81708787
F	-2.42202094	0.82378497	-3.71359762
F	-3.12063248	-1.20877206	-2.68168152
F	-4.03312844	-0.56649974	-4.78860183
N	-4.28722594	3.68004537	-7.60791166
C	-3.65625041	3.15518773	-6.55471963
C	-2.61144249	2.45461544	-7.03071176
N	-2.62756954	2.58646257	-8.35829665
C	-3.64003513	3.33660928	-8.68449719
C	-1.66458872	1.98750490	-9.29361534
C	-5.45054111	4.57706012	-7.55366428
H	-3.92973228	3.27048792	-5.52670356
H	-1.90187074	1.89846015	-6.45443136
H	-3.89972826	3.62613057	-9.68130774
H	-1.56499387	2.61579454	-10.15397637
H	-2.01372126	1.02213687	-9.59543397
H	-0.71412249	1.88858728	-8.81224451
H	-6.25912020	4.14636971	-8.10647874
H	-5.19124888	5.52358806	-7.97999660
H	-5.74800970	4.71416548	-6.53502864
B	2.33125409	3.17066101	1.12069811
F	3.63830608	3.12576304	0.47171129
F	1.77422940	1.82272603	1.18692636
F	2.47691092	3.70398471	2.47196557
F	1.43557051	4.03017021	0.35218967
N	-0.58665139	4.91044904	6.02745776
C	-0.65166833	6.24350645	6.00875462
C	0.52666969	6.68691977	5.53505234
N	1.27328121	5.61033863	5.27974441
C	0.58274934	4.54952323	5.58378863
C	2.64286098	5.62080222	4.74586582
C	-1.65435646	4.00378632	6.47338197
H	-1.48282866	6.84490262	6.31270223
H	0.81127837	7.70818406	5.39045221
H	0.92282960	3.53985811	5.48464803
H	3.17371466	4.76562033	5.10886075
H	3.14262468	6.51204897	5.06335848
H	2.60914973	5.59234782	3.67678078
H	-1.54735656	3.81481931	7.52111269
H	-1.58644274	3.08113432	5.93580012
H	-2.60643510	4.45544881	6.28782916
B	7.26509691	-6.13249109	-3.99475016
F	8.12380488	-5.11980650	-3.38753891
F	5.87862033	-5.67595243	-3.96560122
F	7.67591305	-6.35289172	-5.37831384
F	7.38204883	-7.38131525	-3.24754587
N	-11.18167059	4.76346074	-3.72594821
C	-11.23781030	5.69374183	-4.68148259

C	-10.51995843	6.74534735	-4.24753497
N	-10.04861352	6.42336840	-3.04097299
C	-10.45952344	5.22397277	-2.74561784
C	-9.20814526	7.27809011	-2.19011862
C	-11.82595944	3.44301002	-3.77270801
H	-11.75529147	5.61749970	-5.61492376
H	-10.35768956	7.66486510	-4.77008410
H	-10.23848632	4.69924433	-1.83969884
H	-8.57040560	6.66510173	-1.58808869
H	-9.83154684	7.87407558	-1.55681941
H	-8.61071204	7.91723460	-2.80612281
H	-12.07454618	3.13207761	-2.77952930
H	-11.15495848	2.73405952	-4.21096053
H	-12.71733453	3.50174660	-4.36168033
B	6.28657934	1.51776315	-3.71376428
F	5.95243561	1.95406814	-2.36114046
F	7.68680807	1.82371529	-3.99185221
F	6.07097706	0.07830095	-3.82800379
F	5.43609692	2.21496848	-4.67406127
N	5.38200404	-1.57905924	-6.71975648
C	6.39014280	-1.93069885	-5.91871853
C	6.32385670	-3.26576241	-5.76802665
N	5.27738493	-3.68637668	-6.48190553
C	4.72357263	-2.65306616	-7.04775204
C	4.82675828	-5.07992387	-6.60775755
C	5.06846648	-0.21117033	-7.15732440
H	7.11333028	-1.27539964	-5.47998729
H	6.98426101	-3.87462757	-5.18660221
H	3.86269368	-2.68196919	-7.68253727
H	4.36450049	-5.22046720	-7.56247195
H	4.12049280	-5.29765812	-5.83400703
H	5.66727268	-5.73600475	-6.51840234
H	5.58934735	0.00027979	-8.06776218
H	5.37309921	0.48338567	-6.40254323
H	4.01473265	-0.12149648	-7.32018533
B	0.09846371	0.92835714	6.11211416
F	-0.74053219	1.11494064	7.29229864
F	-0.59905650	1.43548145	4.93401776
F	1.35213636	1.65609155	6.28624963
F	0.38130662	-0.49308677	5.93589181
N	-4.15775788	-3.97179937	-2.60030247
C	-2.92602220	-4.45492470	-2.42411889
C	-2.89759855	-5.02079759	-1.20409136
N	-4.11289693	-4.86498846	-0.67455508
C	-4.85723503	-4.22990058	-1.53318440
C	-4.53854996	-5.33140658	0.65290740
C	-4.64218684	-3.26777414	-3.79636649
H	-2.11555294	-4.40214614	-3.12071774
H	-2.06021156	-5.50384645	-0.74545644
H	-5.88256928	-3.96218950	-1.38512817
H	-5.58391039	-5.55883993	0.63276812
H	-4.35418647	-4.56486561	1.37631653
H	-3.98738877	-6.21002247	0.91588394
H	-3.82955706	-2.74529582	-4.25629770
H	-5.40220416	-2.56891314	-3.51554005
H	-5.04740697	-3.97666552	-4.48787118
B	-6.17796067	-5.30386810	-8.74437243
F	-7.38549627	-5.89990508	-8.18028156
F	-6.22778600	-5.38940395	-10.20100220
F	-6.09288951	-3.90305892	-8.34174979
F	-5.00567055	-6.02310495	-8.25445701
N	-1.75730466	0.10313726	0.96685539
C	-2.87243880	-0.62691371	1.03836359
C	-3.44240279	-0.35679162	2.22649736
N	-2.65695852	0.52951065	2.84225544
C	-1.64640017	0.79312715	2.06513848
C	-2.89306318	1.10949837	4.17219938

C	-0.81448273	0.12438875	-0.16075653
H	-3.24252427	-1.29903818	0.29258658
H	-4.35218909	-0.77314041	2.60576365
H	-0.84999487	1.47032823	2.29321038
H	-3.94570432	1.16070280	4.35719768
H	-2.47577300	2.09400764	4.21117204
H	-2.42958368	0.49595771	4.91627800
H	-0.35029525	1.08667242	-0.21947319
H	-1.34197898	-0.07326037	-1.07047698
H	-0.06490768	-0.62477869	-0.01310728
B	-6.29205047	-3.04538050	3.28859314
F	-6.93009608	-4.31309183	2.94596421
F	-5.62582521	-2.50135744	2.10885794
F	-7.30382686	-2.10163386	3.75469564
F	-5.30845339	-3.26543936	4.34485507
N	-1.71082420	-2.70444166	-7.90259151
C	-1.30592493	-3.91349221	-8.29742610
C	-2.12361747	-4.29429424	-9.29535174
N	-3.00150121	-3.30551502	-9.47777055
C	-2.73458570	-2.35657483	-8.62753712
C	-4.08571942	-3.29065365	-10.47031753
C	-1.10367988	-1.90192450	-6.83102190
H	-0.48687708	-4.47323232	-7.89647764
H	-2.07883011	-5.21460755	-9.83933881
H	-3.27208055	-1.43566094	-8.53855668
H	-4.90277303	-2.70908231	-10.09733739
H	-4.41512797	-4.29203876	-10.65370539
H	-3.72846170	-2.86002896	-11.38236265
H	-1.23301345	-0.86200276	-7.04724311
H	-0.05932011	-2.12551117	-6.76602743
H	-1.57677518	-2.13412213	-5.89979645
B	-6.54042099	0.65566530	-9.14791751
F	-7.36961431	-0.06687319	-8.18772586
F	-5.97533343	1.84029817	-8.50846778
F	-5.45958978	-0.21174794	-9.60726562
F	-7.35714649	1.06098466	-10.28821024
N	-5.60606542	-7.50248042	-3.49704143
C	-6.45891658	-7.03015447	-4.40872652
C	-5.74124763	-6.75913309	-5.51371534
N	-4.47325156	-7.07466479	-5.24119036
C	-4.41398060	-7.52099834	-4.01974789
C	-3.33664622	-6.94086851	-6.16376760
C	-5.95390703	-7.92931013	-2.13406185
H	-7.51279323	-6.89318952	-4.28430268
H	-6.11557684	-6.36554255	-6.43559682
H	-3.52533295	-7.85111315	-3.52353286
H	-2.60547479	-7.68929597	-5.93982836
H	-2.89943442	-5.97059974	-6.05271843
H	-3.67770661	-7.06531545	-7.17029434
H	-6.79485391	-7.36573059	-1.78751282
H	-5.12034346	-7.76220352	-1.48432627
H	-6.19971676	-8.97069077	-2.13824342
B	-5.91291935	5.96274350	-3.22601929
F	-5.79017759	4.77385630	-2.38752993
F	-7.26274634	6.03165640	-3.77808504
F	-5.65442609	7.15390414	-2.42232053
F	-4.94432863	5.89155666	-4.31614221
N	-10.08312978	-2.29833975	-8.84800982
C	-10.82394095	-1.72101768	-7.89956192
C	-10.88524002	-2.58457011	-6.86999742
N	-10.17988246	-3.66139986	-7.22288649
C	-9.70487221	-3.46787025	-8.41935285
C	-9.97433211	-4.86208288	-6.40010005
C	-9.75081731	-1.71285815	-10.15479670
H	-11.28184993	-0.75520572	-7.94882319
H	-11.40120371	-2.43645185	-5.94439401
H	-9.09892447	-4.16098869	-8.96461503

H	-9.09431856	-4.73954081	-5.80389433
H	-9.85839574	-5.71471876	-7.03609049
H	-10.82067177	-5.00596704	-5.76141983
H	-9.62990688	-2.49447988	-10.87546049
H	-8.84000801	-1.15696931	-10.07533686
H	-10.54065309	-1.06095627	-10.46479553
B	-3.05560092	-9.11523353	-0.30418462
F	-4.12983395	-8.32265533	0.28697155
F	-1.97907457	-8.22935102	-0.73764620
F	-2.54232293	-10.05572448	0.68755760
F	-3.57116963	-9.85320464	-1.45361933
N	0.84702489	-11.07069944	2.20006613
C	-0.12894909	-10.40386650	2.82010426
C	0.43126658	-9.77370051	3.86821576
N	1.73128375	-10.07602343	3.85445113
C	1.96062611	-10.85912863	2.84017705
C	2.73386680	-9.60467999	4.82066283
C	0.69085095	-11.90280639	0.99837194
H	-1.16051391	-10.37588066	2.53727286
H	-0.06983483	-9.14904291	4.57784629
H	2.91433552	-11.26503049	2.57446794
H	2.44830374	-8.64188817	5.18993696
H	3.68704717	-9.53389457	4.33969525
H	2.79602110	-10.29521485	5.63566618
H	-0.29192049	-12.32566478	0.98263838
H	1.41704086	-12.68854121	1.01176934
H	0.83374485	-11.29991647	0.12601369
B	-11.24361255	-0.23047995	-4.42061502
F	-12.59248667	-0.40921041	-4.94992328
F	-10.31554633	0.00493100	-5.52281784
F	-11.22397546	0.91446143	-3.51489067
F	-10.84244199	-1.43210206	-3.69482920
N	-6.80363406	3.03625759	2.13338766
C	-7.41598396	2.15490568	2.92703300
C	-7.21204621	0.93766630	2.39203827
N	-6.48176539	1.11491408	1.28890381
C	-6.24659844	2.38788787	1.15157144
C	-6.02122289	0.05288907	0.38286379
C	-6.76485193	4.49198292	2.33398328
H	-7.96462055	2.37476396	3.81897626
H	-7.56756481	0.00493365	2.77741080
H	-5.68402032	2.83145510	0.35680345
H	-5.87916660	-0.85159779	0.93660038
H	-5.09539344	0.34468379	-0.06723037
H	-6.75389400	-0.10745418	-0.38028339
H	-6.70010254	4.98124917	1.38459486
H	-5.91108052	4.74781356	2.92603801
H	-7.65514534	4.80649522	2.83733074
B	1.12843395	-5.00275176	-5.67701755
F	0.91438828	-5.47436840	-7.04207063
F	1.70381705	-3.66131975	-5.71016700
F	-0.14766445	-4.96756146	-4.96856949
F	2.04319416	-5.90775763	-4.98726233
N	2.73577620	-1.78356355	3.77936292
C	2.60640540	-2.49734501	4.89980328
C	2.52709798	-3.78954429	4.53453103
N	2.61061429	-3.82322187	3.20279799
C	2.73599609	-2.60275103	2.76765125
C	2.56820963	-5.03315093	2.36903317
C	2.85736786	-0.32069167	3.70115006
H	2.57227943	-2.11454806	5.89839904
H	2.41786733	-4.63032758	5.18725363
H	2.82519137	-2.31778271	1.74015930
H	3.56145177	-5.40668109	2.23174369
H	2.14177588	-4.79542688	1.41690729
H	1.97054169	-5.77804049	2.85155655
H	2.33282346	0.12510330	4.52030752

H	2.43737996	0.02332129	2.77910551
H	3.89040365	-0.04569044	3.74710876
B	0.08686576	-3.21925984	0.30292002
F	0.37250238	-2.14530201	1.24980596
F	-0.85960827	-2.74335519	-0.70170320
F	1.32458211	-3.63278803	-0.35179242
F	-0.49001298	-4.35559292	1.01536965
N	-10.87546220	-1.31202799	0.32347856
C	-11.52172221	-2.27017142	-0.34431811
C	-11.02458629	-3.44640712	0.07854919
N	-10.09069339	-3.16863880	0.99088931
C	-10.01691600	-1.87571902	1.12334454
C	-9.28264827	-4.15527394	1.72200063
C	-11.09583817	0.13426227	0.18002929
H	-12.28911996	-2.12941095	-1.07657173
H	-11.32128367	-4.41942503	-0.25327324
H	-9.35482135	-1.35785067	1.78543937
H	-9.02884010	-3.76494407	2.68540194
H	-8.38735205	-4.36022457	1.17304584
H	-9.84357976	-5.05881111	1.83972390
H	-11.84861890	0.45064712	0.87149726
H	-11.41555664	0.34903514	-0.81824413
H	-10.18375205	0.65584117	0.38241937
B	-8.21542375	-4.28869055	-2.19066519
F	-8.24626606	-3.93101560	-3.60584782
F	-8.09593238	-3.07702770	-1.38494409
F	-9.44779717	-4.98780372	-1.83841341
F	-7.07169865	-5.15891642	-1.93345448
N	7.42669545	2.84472083	-0.76150693
C	6.55100449	2.45515186	0.16748248
C	6.68736676	1.12358314	0.30096107
N	7.64189857	0.74290854	-0.55085210
C	8.07425895	1.79645557	-1.18151860
C	8.12320166	-0.63257437	-0.74400415
C	7.62603913	4.22348108	-1.23071137
H	5.87019062	3.08257910	0.70388634
H	6.13569118	0.49016276	0.96377409
H	8.84117355	1.80021615	-1.92766138
H	7.32798090	-1.32005377	-0.54425683
H	8.93607050	-0.82329133	-0.07484239
H	8.45588572	-0.75557803	-1.75350823
H	7.94767050	4.20998067	-2.25114706
H	8.37038257	4.70109287	-0.62842255
H	6.70516945	4.76295592	-1.15410238
B	0.07240034	-6.46378891	5.56038822
F	-0.68765778	-7.41949779	6.36071082
F	-0.54868354	-6.32691378	4.24619103
F	0.08293914	-5.16702596	6.23113255
F	1.44300384	-6.94171856	5.40351837
N	8.66651746	-6.27165186	-0.06833361
C	8.25216796	-6.90357502	1.03194520
C	8.08386007	-8.19663639	0.70157198
N	8.40086776	-8.31268192	-0.58980777
C	8.74946449	-7.13998201	-1.03464326
C	8.36281173	-9.55404283	-1.37622905
C	8.97655518	-4.83841628	-0.17139808
H	8.08560842	-6.46508285	1.99364584
H	7.75791792	-8.98252820	1.35044724
H	9.05592821	-6.92383810	-2.03677230
H	7.39531682	-9.66603930	-1.81929983
H	8.56057005	-10.38814567	-0.73586208
H	9.10484845	-9.51152152	-2.14595442
H	9.73238737	-4.68950137	-0.91398716
H	9.32945132	-4.48100263	0.77338394
H	8.09349978	-4.30151005	-0.44861065
B	4.92787563	-10.61532425	0.98175999
F	5.41189012	-9.24011394	0.90362264

F	5.38555642	-11.22226056	2.22825855
F	3.46834079	-10.62038060	0.94517183
F	5.44571604	-11.37854165	-0.15001401
N	-3.22485788	-4.50025540	5.87494607
C	-3.01863251	-3.32860154	6.48019912
C	-2.13259528	-2.64998567	5.72926881
N	-1.82633937	-3.42907298	4.68960534
C	-2.49609179	-4.54016724	4.79700948
C	-0.89143313	-3.08995911	3.60706512
C	-4.12255473	-5.56485793	6.34571362
H	-3.47182067	-2.99305012	7.38956825
H	-1.74678122	-1.67187430	5.92760737
H	-2.45418517	-5.35755794	4.10778430
H	-0.43914890	-3.98464268	3.23305131
H	-0.13201724	-2.43674554	3.98321835
H	-1.42263786	-2.60164515	2.81695455
H	-4.50112196	-6.10941423	5.50604390
H	-4.93765563	-5.13097023	6.88632327
H	-3.58230966	-6.22910895	6.98744415
B	-3.41611791	5.10382976	3.39372001
F	-3.60774818	4.32350782	2.17471392
F	-2.03245047	4.97512222	3.84147965
F	-3.71182927	6.50795238	3.12427348
F	-4.31244417	4.60873583	4.43441394

Return

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
N	6.55397926	-1.75991165	1.42045529
C	6.40480906	-0.85855532	2.39355061
C	6.60405101	0.35158532	1.84098268
N	6.86846114	0.15023519	0.54825130
C	6.83317161	-1.13014968	0.31587923
C	7.15148258	1.19672672	-0.44453757
C	6.42489877	-3.21651056	1.57062998
H	6.17122280	-1.06020249	3.41808508
H	6.55913473	1.29580922	2.34229599
H	7.00638540	-1.59218902	-0.63354737
H	7.62018304	2.02878650	0.03805767
H	6.23595266	1.51616775	-0.89692473
H	7.80433084	0.80696106	-1.19737895
H	5.40936151	-3.50451072	1.39562946
H	6.71004375	-3.49947566	2.56236270
H	7.06135485	-3.70578865	0.86321963
B	2.42427032	4.21004143	9.95263890
F	2.24707149	2.76084037	9.95655535
F	1.56280241	4.80291932	8.93382872
F	2.06918862	4.74729799	11.26293386
F	3.81801915	4.52911089	9.65723515
N	7.79409282	-5.68764157	11.30790969
C	7.23862890	-4.71000938	12.02715710
C	8.21948932	-3.84117672	12.33133721
N	9.34233149	-4.31622440	11.78803767
C	9.06333855	-5.43049679	11.17550408
C	10.66883826	-3.68779515	11.86784684
C	7.09175787	-6.85633389	10.75855525
H	6.20914755	-4.63222618	12.30826031
H	8.11877106	-2.94070148	12.90045972
H	9.76656343	-6.03918322	10.64648657
H	10.79832984	-3.02174525	11.04049428
H	11.42448674	-4.44476015	11.83800105
H	10.74924982	-3.13944948	12.78313632
H	7.11370876	-7.65347626	11.47197592
H	7.57435983	-7.17118419	9.85696400
H	6.07597977	-6.59501691	10.54685498
B	-7.06583383	-9.03143106	2.22259297
F	-6.56922057	-7.97960429	3.10499790
F	-6.26554529	-10.23869516	2.40603168
F	-8.46063550	-9.31855443	2.54461107
F	-6.96793881	-8.58886906	0.83473238
N	5.32944764	-11.59545050	2.82481351
C	4.45262903	-12.52507741	2.44127036
C	4.19280866	-12.30541649	1.14002571
N	4.90711005	-11.23850439	0.77355269
C	5.59717012	-10.83619495	1.80204367
C	4.98161804	-10.67887022	-0.58370170
C	5.89774185	-11.45365558	4.17308372
H	4.03635022	-13.29865312	3.05216475
H	3.53804336	-12.87757674	0.51646922
H	6.27805529	-10.01080002	1.80567872
H	4.01116033	-10.34383643	-0.88513610
H	5.32545034	-11.43194286	-1.26161129
H	5.66248747	-9.85349587	-0.59229829
H	6.79566089	-12.03121422	4.24423185
H	5.19089462	-11.80267315	4.89657990
H	6.12031709	-10.42385105	4.35982929
B	0.17268472	2.33747059	5.10556594
F	1.39333253	3.12972583	4.98744025
F	-0.31997685	2.00098308	3.77302571

F	0.45847611	1.11023442	5.84300441
F	-0.84109252	3.10894009	5.81879269
N	-11.73824262	-6.87775460	3.39558415
C	-11.42096781	-5.94323096	2.49690564
C	-10.88128605	-6.58054249	1.44236074
N	-10.88638789	-7.88371509	1.73106216
C	-11.40726289	-8.04086585	2.91368620
C	-10.38838967	-8.95898538	0.86120193
C	-12.35650105	-6.63478429	4.70691079
H	-11.56793701	-4.88805179	2.59638031
H	-10.51724508	-6.12883088	0.54328882
H	-11.54214739	-8.97846746	3.41129513
H	-9.59222218	-8.58501727	0.25197812
H	-11.18282787	-9.30802793	0.23515449
H	-10.02765497	-9.76659365	1.46330521
H	-11.59135821	-6.48699116	5.44012124
H	-12.95487866	-7.47844786	4.98090611
H	-12.97332666	-5.76206233	4.65418897
B	-3.11980358	7.25704571	0.45704003
F	-4.21018824	7.71559034	1.31284568
F	-1.84192037	7.64462894	1.04728759
F	-3.17734505	5.80352391	0.33226948
F	-3.24976376	7.86443810	-0.86424177
N	-7.12718362	5.87542943	-1.43095801
C	-7.65061056	5.64590886	-2.63717869
C	-6.62410767	5.58070523	-3.50408076
N	-5.50690274	5.77250020	-2.79931894
C	-5.83302752	5.94829119	-1.55136638
C	-4.14021019	5.78337232	-3.34052993
C	-7.88375500	6.02117061	-0.17906708
H	-8.68902107	5.53491880	-2.87018648
H	-6.69053259	5.40797220	-4.55795956
H	-5.14558000	6.12486782	-0.75064843
H	-3.87930028	6.77976476	-3.63038109
H	-4.08910518	5.13894080	-4.19317202
H	-3.45742237	5.43931640	-2.59198135
H	-8.77850264	5.43685678	-0.23298351
H	-8.13805652	7.05030154	-0.03376745
H	-7.28542304	5.68243605	0.64078266
B	-9.10921513	-3.89675504	-1.49480132
F	-8.59834652	-2.99748658	-0.46430066
F	-7.99516468	-4.60447537	-2.11900376
F	-10.02131656	-4.86265082	-0.88923105
F	-9.82203012	-3.12240720	-2.50667222
N	4.09111177	1.24580964	8.05053751
C	3.74164840	0.33027272	8.95678416
C	4.75511284	0.24309852	9.83700361
N	5.69080207	1.10821454	9.43990699
C	5.27009104	1.70232417	8.36071728
C	6.97790556	1.34919346	10.10786944
C	3.28198914	1.66709877	6.89784690
H	2.82910886	-0.22801583	8.97889664
H	4.80221105	-0.39772845	10.69259055
H	5.80857888	2.44842955	7.81460354
H	6.86324210	2.12776408	10.83283531
H	7.70713371	1.64245756	9.38184015
H	7.30020846	0.45276382	10.59514239
H	3.51260351	1.04919168	6.05528904
H	3.50094866	2.68762394	6.66229912
H	2.24346695	1.57114083	7.13691837
B	3.11598532	-3.64405179	3.64554164
F	2.07455730	-3.73369183	4.66485091
F	2.50062199	-3.62112328	2.32175761
F	3.88785667	-2.42087302	3.84466809
F	4.00090772	-4.80052007	3.75088875
N	-8.49279382	-5.99095937	8.85661190
C	-7.34938734	-5.34470422	8.61873307

C	-7.03089395	-5.57211438	7.33174927
N	-7.99006285	-6.34992923	6.82517789
C	-8.86167653	-6.59063592	7.76164513
C	-8.05170286	-6.84985884	5.44417961
C	-9.21321042	-6.02048101	10.13764113
H	-6.79222487	-4.75754244	9.31851999
H	-6.17215321	-5.20027489	6.81290500
H	-9.74261913	-7.18742275	7.64908681
H	-8.55403225	-7.79448847	5.42890898
H	-7.05892578	-6.96762773	5.06283547
H	-8.58702762	-6.15134186	4.83557307
H	-8.86768786	-6.84740860	10.72219522
H	-10.26208336	-6.12661824	9.95461400
H	-9.03424516	-5.10889203	10.66856147
B	7.51436640	-9.53618321	7.53374536
F	8.93208732	-9.85833148	7.40000182
F	7.16859107	-9.43981978	8.94893316
F	7.24117075	-8.26062606	6.87806222
F	6.71561445	-10.58595546	6.90798444
N	-7.93153252	2.27702528	6.59393403
C	-8.74902574	1.64540768	5.74871866
C	-8.68416640	0.33509888	6.04598147
N	-7.82916444	0.20877443	7.06314804
C	-7.38691731	1.39196490	7.37795277
C	-7.45110342	-1.05239204	7.71691828
C	-7.68761732	3.72612240	6.63283251
H	-9.34287879	2.09563109	4.98090120
H	-9.21659706	-0.45539864	5.55963634
H	-6.68610425	1.60368330	8.15828590
H	-7.50692590	-1.85217117	7.00830772
H	-8.12013589	-1.24783217	8.52877413
H	-6.45106560	-0.97516110	8.08954724
H	-6.86768019	3.96719912	5.98902862
H	-7.45367060	4.02167465	7.63423946
H	-8.56396456	4.24427538	6.30354063
B	-3.23664438	-5.93277023	5.11534320
F	-2.37768559	-6.39084288	4.02724287
F	-4.52254732	-6.62035894	5.04269846
F	-2.59911676	-6.22690334	6.39543810
F	-3.44722895	-4.49297361	4.99599137
N	3.80337374	-8.18199931	5.78635004
C	2.62101044	-8.42370059	5.21607117
C	1.97594443	-9.29982515	6.00713131
N	2.78518133	-9.56491930	7.03498804
C	3.88183235	-8.88036961	6.88213138
C	2.48840607	-10.47534898	8.15030715
C	4.84083374	-7.28022823	5.26542927
H	2.25583305	-8.00102466	4.30344228
H	0.99995231	-9.70674536	5.84354763
H	4.71634279	-8.89018663	7.55174802
H	1.83912011	-11.25523051	7.81102256
H	2.01061996	-9.93080313	8.93776335
H	3.39945959	-10.90270314	8.51396772
H	4.78596392	-7.25278026	4.19719211
H	5.80494435	-7.63550262	5.56403662
H	4.68674482	-6.29600251	5.65588937
B	-7.99327879	3.15437199	2.46885349
F	-6.73253682	3.68223522	1.95553886
F	-7.76778322	1.83354249	3.04864746
F	-8.51577011	4.05310352	3.49398118
F	-8.95702607	3.04860778	1.37724500
N	1.46764267	-6.67791310	0.77547129
C	1.69008622	-6.79267649	-0.53562099
C	3.02140083	-6.72269241	-0.71504362
N	3.56905621	-6.56744941	0.49226844
C	2.61429426	-6.54307236	1.37684659
C	5.00639136	-6.44481381	0.77500858

C	0.15124994	-6.70001740	1.42931382
H	0.95027593	-6.91671566	-1.29863755
H	3.54220021	-6.78047601	-1.64795813
H	2.75055976	-6.42999302	2.43209455
H	5.14810461	-5.84148254	1.64725199
H	5.49612281	-5.98685139	-0.05886054
H	5.42116728	-7.41683380	0.94243560
H	0.18350374	-6.10242486	2.31629136
H	-0.10224480	-7.70715840	1.68682220
H	-0.58570504	-6.30655033	0.76074942
B	1.47487943	-10.19602696	2.01048109
F	2.26464548	-10.95555624	2.97535966
F	0.81386408	-11.11684342	1.09028661
F	0.46891270	-9.40861116	2.71731303
F	2.35209432	-9.30309922	1.25896861
N	12.02652278	-7.02893742	4.38435049
C	12.15281070	-7.05240954	5.71293376
C	11.73371826	-8.26229257	6.12530396
N	11.36501814	-8.93865178	5.03524936
C	11.54973638	-8.17639831	3.99628316
C	10.83954157	-10.31131624	5.01191879
C	12.36788652	-5.89911623	3.50806951
H	12.51789545	-6.25976658	6.33207443
H	11.70197394	-8.61528904	7.13490025
H	11.34231741	-8.44996595	2.98286655
H	9.77360358	-10.28673060	5.10172253
H	11.25355166	-10.86563305	5.82814261
H	11.10898043	-10.78073139	4.08890787
H	11.51226293	-5.26738793	3.39094935
H	12.67176101	-6.26906386	2.55114697
H	13.16811323	-5.33851750	3.94426443
B	-0.53061956	6.40664778	-5.24201438
F	0.25228491	7.62218523	-5.44481684
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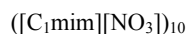
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C	11.24839649	0.49099624	5.37947070
C	11.69918597	-0.76917269	5.51452279
N	11.95087880	-0.95537626	6.81205453
C	11.66672556	0.14437725	7.44800596
C	12.46214310	-2.19238143	7.41975859
C	10.81819032	2.40330053	6.92726351
H	10.95326944	0.96756329	4.46804923
H	11.83092453	-1.48584170	4.73099012
H	11.76845359	0.29378690	8.50262881
H	11.64055251	-2.81606767	7.70420529
H	13.04301476	-1.95092776	8.28531357
H	13.07500553	-2.71055375	6.71209726
H	10.07003692	2.72271783	6.23218024
H	11.66161829	3.05922094	6.86991238
H	10.41636369	2.42485186	7.91871491
B	10.26121740	0.11371440	11.22223659
F	9.56313130	0.68600877	12.36973804
F	9.47176370	-0.98320123	10.66984257
F	10.44588017	1.14210453	10.20247353
F	11.56409343	-0.39005248	11.64689327
N	3.39440445	1.92949595	-3.93864070
C	2.98966426	3.17728828	-3.69199415
C	2.58983456	3.69900892	-4.86563804
N	2.76329703	2.75301233	-5.79117514
C	3.24933568	1.69402421	-5.21069714
C	2.45741826	2.88466762	-7.22296256
C	3.91551734	0.98199808	-2.94285436
H	2.98427668	3.66895258	-2.74166206
H	2.20586266	4.68468343	-5.02660879

H	3.49148823	0.77476128	-5.70182922
H	2.18634772	1.92840960	-7.61917656
H	3.31898890	3.25345604	-7.73929840
H	1.64429118	3.56797449	-7.35260485
H	4.97768699	1.08901249	-2.87035401
H	3.67734310	-0.01720641	-3.24245375
H	3.47084595	1.18451611	-1.99093826
B	7.27061888	2.31448599	5.56815027
F	6.23311941	3.28286031	5.91085951
F	8.24984014	2.94218559	4.68569950
F	7.93424472	1.86045661	6.78678071
F	6.66526985	1.17244150	4.88926201
N	2.37818030	-5.02480890	-6.08170572
C	3.24607615	-5.90427233	-6.58661004
C	2.73607321	-7.12930313	-6.36598872
N	1.57315810	-6.95845730	-5.73347518
C	1.37653414	-5.68177600	-5.57206425
C	0.66808184	-8.03008704	-5.29377518
C	2.52801987	-3.56256003	-6.09832643
H	4.17132355	-5.67793475	-7.07404101
H	3.17841257	-8.06293489	-6.64450962
H	0.52557848	-5.24168385	-5.09551630
H	0.92571074	-8.32883284	-4.29914927
H	0.76042329	-8.86781476	-5.95300642
H	-0.34068405	-7.67364562	-5.30912026
H	1.56121864	-3.10531815	-6.13181025
H	3.09031980	-3.27143280	-6.96085594
H	3.04158836	-3.24657261	-5.21441040
B	-10.37559723	-9.52934824	6.99971595
F	-11.28319373	-8.53004031	6.44360524
F	-9.42561827	-9.94870776	5.97342088
F	-9.65011328	-8.95344348	8.12825789
F	-11.14346448	-10.68519821	7.45357604

Return



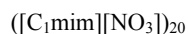
Atomic Number	Atomic Coordinates (Angstroms)		
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N	-4.39628816	1.49132350	4.57163761
C	-5.49536939	1.81644692	5.18883829
C	-3.43763171	2.42998666	3.97098384
C	-7.36956315	0.68302685	6.32756118
H	-5.59296850	-1.34739243	5.40647274
H	-3.49388500	-0.41477259	4.14842569
H	-5.84783998	2.81518827	5.34112063
H	-2.95818016	1.96422876	3.13546724
H	-2.70159843	2.70226248	4.69832121
H	-3.95531536	3.30670766	3.64195976
H	-8.18155743	0.62581399	5.63309314
H	-7.47245066	1.56489300	6.92474649
H	-7.38014393	-0.17960497	6.96053831
N	-4.27577692	-4.00581634	-4.02367492
O	-3.14398944	-4.46779533	-3.83060754
O	-5.26527080	-4.56999860	-3.53969250
O	-4.41807185	-2.97966273	-4.70073504
N	-13.76758795	0.71166046	-4.32151150
C	-14.41716415	-0.43179437	-4.09305256
C	-13.48555905	-1.39463138	-3.97248389
N	-12.29708641	-0.80812387	-4.13110477
C	-12.49008108	0.46213567	-4.34047864
C	-10.99181960	-1.48221637	-4.07830295
C	-14.38928309	2.02912090	-4.51829843
H	-15.47711102	-0.55844348	-4.01975640
H	-13.66338249	-2.43298043	-3.78509260
H	-11.71991880	1.18701755	-4.50263694
H	-10.29950547	-0.96912785	-4.71258559
H	-11.09887157	-2.49337733	-4.41145354
H	-10.62699744	-1.47481625	-3.07244276
H	-14.58813548	2.17778078	-5.55909569
H	-13.72553528	2.79241874	-4.16941360
H	-15.30670413	2.07613222	-3.96963112
N	-3.50554909	1.75499225	-1.35139230
O	-4.63758071	1.29506626	-1.54790635
O	-2.95184114	1.58962389	-0.25699598
O	-2.92722907	2.38029459	-2.24927137
N	-7.20411043	-0.33995734	0.76250448
C	-7.88542545	0.24362129	-0.22586360
C	-9.17051484	-0.13000377	-0.09011814
N	-9.23256393	-0.92968743	0.97677951
C	-8.03564311	-1.04290794	1.47597689
C	-10.44646950	-1.57329782	1.49936117
C	-5.75989256	-0.21080136	1.00429638
H	-7.48551914	0.88627033	-0.98215302
H	-9.98744555	0.15885226	-0.71788337
H	-7.77616009	-1.62251397	2.33715293
H	-10.35607744	-1.69874684	2.55812860
H	-10.57062398	-2.52982834	1.03617691
H	-11.29629617	-0.95980408	1.28415104
H	-5.23912750	-0.97980231	0.47294105
H	-5.56377337	-0.30557114	2.05189241
H	-5.42554796	0.74698546	0.66405777
N	-5.36820416	-3.54757328	3.36848477
O	-6.21237903	-2.86242115	3.95973578
O	-4.23407739	-3.09470221	3.16772031
O	-5.65815742	-4.68559436	2.97799415
N	-3.57908572	-3.06987102	-0.39881772

C	-2.58266988	-2.60843402	0.36004751
C	-1.77271898	-1.89825531	-0.44562666
N	-2.30060232	-1.94891206	-1.67052737
C	-3.38947386	-2.66054326	-1.61993267
C	-1.74645804	-1.30956331	-2.87263177
C	-4.70028368	-3.89945007	0.06552647
H	-2.45288684	-2.77223031	1.40944080
H	-0.87602698	-1.38957781	-0.15911704
H	-4.02808824	-2.87522239	-2.45119069
H	-1.21591462	-0.42343921	-2.59293122
H	-2.54295307	-1.05289295	-3.53943433
H	-1.07715024	-1.98696211	-3.36053311
H	-5.50716293	-3.26814388	0.37417619
H	-4.38135758	-4.50016308	0.89154882
H	-5.02844100	-4.53388921	-0.73117322
N	-7.00859869	2.85107493	2.38313400
O	-6.06416528	3.59971684	2.66459713
O	-7.49525964	2.86981645	1.24539263
O	-7.46637739	2.08369878	3.23941524
N	-7.25285608	-7.07801902	-2.06382244
C	-6.27818323	-7.49411912	-2.87529919
C	-6.85262738	-7.80313493	-4.05173900
N	-8.15958603	-7.56573742	-3.92077849
C	-8.37933130	-7.12913253	-2.71425082
C	-9.17798106	-7.76369389	-4.96221517
C	-7.08304309	-6.63691858	-0.67188034
H	-5.23797438	-7.56783681	-2.63564330
H	-6.35633971	-8.16950174	-4.92602871
H	-9.33535694	-6.85536645	-2.31933134
H	-9.97313161	-7.06166691	-4.82152733
H	-9.56536833	-8.75901915	-4.89765333
H	-8.73673845	-7.61448513	-5.92551059
H	-7.18203356	-7.47718301	-0.01685861
H	-7.83100883	-5.90954944	-0.43446161
H	-6.11247402	-6.20295286	-0.55114572
N	-10.93671804	-0.71946037	5.12482342
O	-9.71332429	-0.90637422	5.12880658
O	-11.70419807	-1.65138610	4.85254655
O	-11.39263160	0.39938069	5.39311245
N	-11.65838627	2.20774351	2.40986539
C	-12.71098947	1.48867582	2.80557903
C	-13.65996636	1.63127172	1.86293104
N	-13.15629942	2.43281439	0.92194116
C	-11.94822790	2.76889798	1.27156086
C	-13.84832423	2.86302932	-0.30154350
C	-10.38753284	2.34302233	3.13618026
H	-12.78571060	0.90915908	3.70194588
H	-14.63326471	1.18677510	1.86671760
H	-11.29613944	3.40606959	0.71146856
H	-13.49575142	3.83153099	-0.58894442
H	-14.90172225	2.90665390	-0.11891852
H	-13.65121546	2.16404598	-1.08733547
H	-9.59192097	2.49644063	2.43734634
H	-10.20147940	1.45188856	3.69847230
H	-10.44415527	3.17919310	3.80139349
N	-11.55753612	-4.24778097	-6.44385851
O	-11.14155659	-4.56241612	-5.32153502
O	-12.75748406	-3.99482739	-6.61055166
O	-10.77356723	-4.18609852	-7.39948881
N	-6.98343579	4.87588060	-0.94367712
C	-5.65756156	4.99028316	-0.84080930
C	-5.12876228	4.42579664	-1.94135564
N	-6.14873737	3.98476096	-2.68079149
C	-7.25814928	4.26649006	-2.06074193
C	-6.03806687	3.29753080	-3.97555910
C	-7.96653822	5.35647310	0.03786458
H	-5.11802927	5.44451424	-0.03613842

H	-4.08852732	4.34561045	-2.17881301
H	-8.24108398	4.03379537	-2.41370056
H	-5.97133829	2.24183215	-3.81443819
H	-5.16066607	3.63664979	-4.48553582
H	-6.90164425	3.51385511	-4.56913910
H	-7.57635623	6.21579023	0.54209731
H	-8.16526933	4.58406200	0.75113935
H	-8.87357688	5.61938836	-0.46519057
N	-10.98807675	-8.27662758	-0.87853242
O	-11.83477264	-8.42896617	0.01115302
O	-11.34514222	-8.01623133	-2.03453662
O	-9.78431539	-8.38468393	-0.61221299
N	-8.08457913	-2.90675845	-5.69871100
C	-8.75160485	-2.03429897	-6.45733689
C	-8.56487304	-0.81841423	-5.91305817
N	-7.78981486	-0.98755097	-4.83959778
C	-7.51177102	-2.25444485	-4.72866144
C	-7.32850899	0.07623437	-3.93602008
C	-8.00955220	-4.35792898	-5.92091178
H	-9.32557098	-2.25923545	-7.33190845
H	-8.96203714	0.10794881	-6.27224865
H	-6.90753510	-2.69089090	-3.96099333
H	-6.39590982	0.46437748	-4.28886235
H	-7.19917418	-0.32302379	-2.95175627
H	-8.05466740	0.86166943	-3.90973411
H	-8.81205592	-4.84005277	-5.40278934
H	-7.07492222	-4.72716345	-5.55344438
H	-8.08706615	-4.56286727	-6.96823698
N	-14.26815045	-0.63767019	-0.72587251
O	-14.43759380	-1.57725328	0.06159937
O	-13.12854657	-0.35750391	-1.11887692
O	-15.23831018	0.02175038	-1.12033494
N	-13.26397504	-4.37855637	-1.78601963
C	-14.59100967	-4.27851350	-1.88896007
C	-14.96998289	-5.09920619	-2.88511399
N	-13.86216220	-5.67393372	-3.35844473
C	-12.84474493	-5.22529344	-2.68152122
C	-13.80132736	-6.64814789	-4.45759502
C	-12.41928310	-3.65532413	-0.82460106
H	-15.23142944	-3.66274324	-1.29264488
H	-15.96924581	-5.26058264	-3.23200598
H	-11.82451282	-5.50801291	-2.83674200
H	-13.89468593	-7.63808724	-4.06236089
H	-12.86464299	-6.55403068	-4.96616793
H	-14.60037123	-6.46145258	-5.14431335
H	-12.97726331	-3.46600962	0.06854878
H	-12.10619955	-2.72626276	-1.25322211
H	-11.55954874	-4.24727310	-0.58931491
N	-10.30289684	2.51527287	-3.69087561
O	-9.75836611	2.36038340	-4.79139435
O	-11.36242659	3.14950804	-3.60851710
O	-9.78790046	2.03592369	-2.67271594
N	-9.14016254	-4.51100839	5.15718574
C	-10.27719495	-5.12354398	5.49417798
C	-10.75935032	-5.69745608	4.37720115
N	-9.90126277	-5.41681389	3.39406359
C	-8.93211020	-4.70042741	3.88617475
C	-10.02895452	-5.84415381	1.99335107
C	-8.27047460	-3.75144767	6.06693036
H	-10.72070895	-5.15253470	6.46749706
H	-11.65937840	-6.26995068	4.29289576
H	-8.09611595	-4.32619788	3.33304290
H	-10.57541386	-5.10641273	1.44378358
H	-10.54933466	-6.77815461	1.95142171
H	-9.05505582	-5.95894806	1.56528103
H	-8.57489930	-2.72572447	6.07788128
H	-7.25690584	-3.81910304	5.73079305

H	-8.34658430	-4.15664060	7.05431299
N	-8.84151693	-3.42025406	-1.12080155
O	-9.51199221	-2.66433865	-1.83543542
O	-9.40615069	-4.25447147	-0.40183573
O	-7.60640817	-3.34194782	-1.12512829

Return



Atomic Number	Atomic Coordinates (Angstroms)		
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N	1.87408159	-7.43182360	-3.55043144
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C	1.41936757	-8.72936356	-5.20796112
N	0.96197660	-9.27494372	-4.07890465
C	1.24678267	-8.47603867	-3.09135849
C	0.25639570	-10.55987148	-3.96925547
C	2.36372921	-6.30150072	-2.74823180
H	2.46623234	-6.86886904	-5.54017331
H	1.34126827	-9.14221810	-6.19200143
H	1.00355553	-8.65023972	-2.06403835
H	0.59277224	-11.21860243	-4.74244296
H	-0.79643609	-10.39847230	-4.07120872
H	0.45925556	-10.99782659	-3.01429668
H	3.23244661	-5.88412099	-3.21300683
H	2.61431611	-6.64344324	-1.76579667
H	1.60081365	-5.55417413	-2.68197618
N	-0.52637822	-5.62194050	7.00124264
O	-1.68103371	-5.66662603	7.44444626
O	-0.19353325	-4.71113779	6.23227759
O	0.29543018	-6.48806368	7.32699951
N	-9.57625161	-3.88295180	-4.25737910
C	-10.31948679	-4.92703206	-3.88435637
C	-9.68524573	-6.03301770	-4.31330621
N	-8.57513294	-5.62870914	-4.93444129
C	-8.52893104	-4.32853296	-4.88920297
C	-7.57454981	-6.50321300	-5.56291396
C	-9.88753069	-2.46977891	-3.99864007
H	-11.24379763	-4.89110307	-3.34653454
H	-10.00900852	-7.04432331	-4.18164993
H	-7.75236286	-3.72163836	-5.30577413
H	-6.82641606	-6.76371248	-4.84364480
H	-7.11743834	-5.99023967	-6.38316230
H	-8.05148400	-7.39222522	-5.91940024
H	-10.94888181	-2.33963372	-3.95988783
H	-9.48257055	-1.86584321	-4.78360858
H	-9.45771562	-2.17522238	-3.06409068
N	-5.85350369	-11.07951438	2.50717639
O	-7.06827668	-10.90980132	2.67204580
O	-5.45087942	-11.88984964	1.66283912
O	-5.04135922	-10.43888466	3.18663969
N	-4.42029743	-6.48383030	-9.34995767
C	-4.24625387	-5.39385716	-10.10046976
C	-2.95944056	-5.02603528	-9.96519845
N	-2.38912560	-5.90324729	-9.13640609
C	-3.28781136	-6.77388508	-8.77725383
C	-0.98460384	-5.88866676	-8.70279600
C	-5.67744402	-7.23004475	-9.19620784
H	-4.98893086	-4.90563138	-10.69627435
H	-2.48363314	-4.18953625	-10.43291809
H	-3.12177877	-7.59814950	-8.11550414
H	-0.39506342	-6.46624750	-9.38378229
H	-0.90990666	-6.30865065	-7.72151189
H	-0.62650570	-4.88048828	-8.68746997
H	-6.23122176	-6.83004163	-8.37265992
H	-5.45981779	-8.26141473	-9.01231954
H	-6.25636523	-7.14183845	-10.09173017
N	-3.34257416	-4.66135863	0.94871661
O	-2.91221178	-4.01370847	-0.01408693
O	-2.97493935	-4.38136593	2.09680279
O	-4.14057071	-5.58900397	0.76343352
N	-1.82536404	-10.30226054	3.89242940

C	-1.42144324	-9.97364895	5.12146524
C	-1.28546477	-8.63555526	5.14481839
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Return

([C₁mim][NO₃])₃₀

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
N	-4.34406248	-3.99702776	-5.79048395
C	-3.94487470	-4.58331561	-6.92122225
C	-2.60010096	-4.60581544	-6.89764286
N	-2.22139439	-4.03245142	-5.75331281
C	-3.28877042	-3.67260769	-5.10072468
C	-0.83441666	-3.83999283	-5.30590369
C	-5.73866272	-3.75822665	-5.39176706
H	-4.57465250	-4.96310020	-7.69842565
H	-1.95653510	-5.00696765	-7.65249452
H	-3.29735505	-3.18667574	-4.14745341
H	-0.77514900	-2.96375701	-4.69466801
H	-0.19761576	-3.72423971	-6.15795279
H	-0.52091006	-4.69188869	-4.73942989
H	-6.36401894	-4.52035302	-5.80768878
H	-6.05404382	-2.80163366	-5.75283872
H	-5.81304144	-3.77886992	-4.32455193
N	2.98040860	1.20931781	-0.65126052
O	3.24857554	1.58813946	0.49601203
O	3.45519845	1.80521923	-1.62652055
O	2.23744940	0.23459349	-0.82327396
N	-0.62765517	-10.51004535	6.70662992
C	0.11336569	-11.06717174	5.74635544
C	1.32443641	-11.31223739	6.27809063
N	1.28395993	-10.89685586	7.54593892
C	0.09757748	-10.41660812	7.78363602
C	2.39117374	-10.96938750	8.51015219
C	-2.02545386	-10.07570284	6.57099871
H	-0.19687300	-11.27859625	4.74438014
H	2.16095264	-11.75571196	5.77961195
H	-0.22990019	-10.00919727	8.71726792
H	1.99662698	-11.07800208	9.49880545
H	2.97196413	-10.07245497	8.45444911
H	3.01086751	-11.81049245	8.27903941
H	-2.20744798	-9.24966884	7.22631127
H	-2.67687703	-10.88483113	6.82763193
H	-2.20947828	-9.77644426	5.56031399
N	-8.02967634	2.78182212	0.54865318
O	-7.51880567	3.52646800	-0.29761504
O	-9.05456544	3.13505626	1.14571782
O	-7.51565655	1.68394261	0.79785904
N	3.60268348	-5.18902991	5.50730049
C	4.65202151	-4.61266898	4.91708966
C	5.50638062	-5.59791255	4.58719981
N	4.95120913	-6.74421613	4.98649421
C	3.80361733	-6.47483267	5.53886859
C	5.53637217	-8.08352385	4.82917739
C	2.42074059	-4.49039745	6.03250501
H	4.78777382	-3.56617886	4.74006271
H	6.45112843	-5.48432011	4.09786290
H	3.13135265	-7.19663904	5.95355948
H	4.75297780	-8.80591789	4.73243781
H	6.13166647	-8.31572966	5.68743438
H	6.15040501	-8.10379323	3.95313205
H	2.58717052	-4.22812974	7.05642476
H	1.56707547	-5.13173278	5.96281877
H	2.24764600	-3.60280115	5.46057099
N	-4.90637921	-2.84623802	3.49191093
O	-3.94767448	-2.28580943	4.03823346
O	-4.80298392	-4.01966951	3.11240866
O	-5.96847739	-2.23323303	3.32508995
N	-8.67832709	0.76191797	4.29214935

C	-8.13871467	-0.25492332	4.96778467
C	-6.86334503	0.08213512	5.23104552
N	-6.66522897	1.29395048	4.70771540
C	-7.77253061	1.68542409	4.14623010
C	-5.40973260	2.05696633	4.75704782
C	-10.06081623	0.82776241	3.79688886
H	-8.62754424	-1.16490621	5.24685078
H	-6.14454160	-0.50869262	5.75938223
H	-7.91563328	2.61925895	3.64386635
H	-4.87246650	1.80254282	5.64671540
H	-5.62874822	3.10430786	4.75986158
H	-4.81411696	1.81943787	3.90046939
H	-10.68727332	1.26638674	4.54526525
H	-10.40775054	-0.15990132	3.57539893
H	-10.09372915	1.42473084	2.90950836
N	-2.59103522	-9.74124965	2.04869221
O	-3.66452225	-10.18411633	1.62072876
O	-1.62313595	-9.62182835	1.28674298
O	-2.48544658	-9.41780766	3.23860605
N	-2.39801501	0.61222779	12.94748810
C	-1.81451571	0.30808853	14.10879906
C	-2.33958830	-0.86115253	14.51705538
N	-3.22682803	-1.23334854	13.59189859
C	-3.24628018	-0.33065289	12.65413095
C	-4.04341910	-2.45520417	13.62617256
C	-2.12848863	1.80882728	12.13731247
H	-1.07071789	0.88458258	14.61803885
H	-2.09298452	-1.39180861	15.41286551
H	-3.86248208	-0.35919303	11.77983088
H	-3.51698774	-3.24978710	13.13995444
H	-4.96987169	-2.27931279	13.12055598
H	-4.23780686	-2.72587814	14.64296924
H	-1.83894598	2.61549257	12.77790103
H	-3.01177855	2.08090496	11.59817190
H	-1.33854574	1.60106910	11.44612905
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O	-1.35045111	-4.71375929	13.22133841
O	0.56146019	-5.18093683	14.07064978
N	-5.38787685	-7.80214961	-0.60166702
C	-4.82034964	-6.85085544	-1.34636384
C	-5.19714771	-5.66886307	-0.82636989
N	-5.98262951	-5.93643390	0.21912567
C	-6.08452115	-7.22887681	0.33677545
C	-6.62380010	-4.94065828	1.08990521
C	-5.24967365	-9.25123466	-0.80645584
H	-4.18637123	-7.00005984	-2.19531155
H	-4.91996933	-4.69885483	-1.18295461
H	-6.65159912	-7.73959784	1.08676613
H	-7.54218707	-5.33740290	1.46947375
H	-6.82413709	-4.05210515	0.52840776
H	-5.97178097	-4.70765065	1.90566048
H	-5.10280056	-9.45196655	-1.84715117
H	-6.13703596	-9.74527107	-0.46968703
H	-4.40858204	-9.61123538	-0.25160349
N	-8.43210954	-3.38194542	-2.90434466
O	-9.37522533	-4.18307585	-2.92377637
O	-8.51941271	-2.30844445	-3.51396709
O	-7.40168943	-3.65431528	-2.27529588
N	-10.23008338	-6.72486055	7.53544657
C	-10.73110026	-5.54531509	7.16223385
C	-10.73591758	-4.75847485	8.25326571
N	-10.23765455	-5.48286157	9.25757252
C	-9.93909977	-6.66556387	8.80290210
C	-10.05673580	-5.02311802	10.64206847
C	-10.03927129	-7.89266443	6.66325347
H	-11.06526957	-5.27676872	6.18187132

H	-11.07467018	-3.74488537	8.30599149
H	-9.52043014	-7.46335228	9.38010334
H	-9.87320628	-3.96898651	10.64673500
H	-9.22411608	-5.53205910	11.08096287
H	-10.94118564	-5.23366437	11.20626693
H	-10.92134856	-8.49810404	6.67980728
H	-9.20629679	-8.46634889	7.01246937
H	-9.85127414	-7.56357336	5.66261770
N	0.75303587	2.98895874	10.30042348
O	1.78469720	2.95343094	10.98311299
O	-0.12797521	3.82055137	10.55327887
O	0.60238015	2.19288895	9.36488267
N	-5.73954724	-4.44625451	6.17391179
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C	-3.68914056	-5.10166333	6.11007115
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C	-5.68952861	-5.56692684	5.51344150
C	-3.98873707	-7.20984143	4.80488772
C	-6.95302743	-3.66299284	6.44752722
H	-4.21172742	-3.26563672	7.12183364
H	-2.62922346	-5.15911765	6.24488063
H	-6.52962530	-6.06843552	5.08027891
H	-3.73830942	-6.99594307	3.78683599
H	-4.76340169	-7.94735909	4.83423782
H	-3.12399659	-7.58039003	5.31461050
H	-6.70035427	-2.62538272	6.51397867
H	-7.38441688	-3.98496244	7.37226939
H	-7.65759298	-3.80850756	5.65549835
N	-11.69451483	-0.93096012	5.82467499
O	-11.15274903	-2.03707623	5.70361216
O	-11.24316236	-0.10554382	6.62880670
O	-12.68763078	-0.65025883	5.14160315
N	1.79655706	-6.58933924	10.75346034
C	2.66020565	-7.10581751	11.63039243
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N	0.64871250	-7.53232020	12.27055016
C	0.58895795	-6.85800090	11.15863174
C	-0.50277007	-8.02236589	13.04180445
C	2.14920790	-5.84371038	9.53666418
H	3.72771997	-7.05440246	11.57870260
H	2.31192910	-8.21760265	13.44983926
H	-0.31105258	-6.56991841	10.65672972
H	-1.33310656	-7.36227839	12.90134116
H	-0.24730610	-8.05818802	14.08024324
H	-0.76605517	-9.00332856	12.70522623
H	1.37869141	-5.13450765	9.31706512
H	2.25088052	-6.52491421	8.71780047
H	3.07473633	-5.32897932	9.68943275
N	-6.17822411	5.16088668	6.17678173
O	-7.11362184	4.40670273	5.88030201
O	-6.18374603	6.33591101	5.78826398
O	-5.23730702	4.74004658	6.86177928
N	-2.07824976	-1.08638855	0.45651006
C	-2.95083814	-0.66673355	1.37525680
C	-4.18059006	-0.86400179	0.86703430
N	-4.01934015	-1.39781076	-0.34568169
C	-2.74379706	-1.52337081	-0.57340756
C	-5.09889983	-1.77919869	-1.26763131
C	-0.61418518	-1.05964634	0.58575743
H	-2.71671426	-0.25231236	2.33355731
H	-5.11090661	-0.63635033	1.34408781
H	-2.31060687	-1.92286064	-1.46652670
H	-4.75869123	-1.67703338	-2.27695056
H	-5.94418107	-1.14236960	-1.10997669
H	-5.37962979	-2.79580100	-1.08704658
H	-0.27777115	-1.97726732	1.02129960
H	-0.32628630	-0.24105761	1.21179484

H	-0.17281853	-0.94115728	-0.38174505
N	-6.76565466	-9.41861214	7.05269213
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O	-5.60089870	-9.77029424	6.82614691
N	-7.59586144	0.79360727	9.40988557
C	-7.12267238	2.03888998	9.32624231
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H	-6.99939174	-0.47428791	10.95620272
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N	-4.87266050	-8.14424053	-5.11507968
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N	0.94704009	5.06530312	-2.03386820
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C	-0.71119895	2.02298422	-1.27788524
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H	0.63918696	3.51683906	0.74008272
H	-0.10831458	3.80164309	-3.35338323
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H	-1.16570458	1.90473727	-0.31645897
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H	-12.15388197	-3.39360449	1.82670326
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H	-7.93445999	-0.19750796	-1.22777329
H	-9.46561670	0.60836897	-0.98454551
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O	-5.82479830	-3.08997187	10.60352065
O	-7.11391738	-3.95537849	12.08142560
N	4.34890858	2.41365915	9.09638237
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C	2.82685941	5.54954356	8.44321127
C	4.41428013	0.94622893	9.03913732
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H	5.31308852	5.36745859	9.82627061
H	2.52774161	2.78787373	8.09885288
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O	4.29604785	-8.00017537	2.18312575
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N	-9.16859783	-8.93383738	-1.77311190
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C	-8.10580068	-9.17682023	-3.63032254
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H	-7.86676887	-7.10719245	-5.29035692
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N	-5.25968779	-9.63275091	10.96213973
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H	-5.21109613	-6.09160847	8.75746589
H	-5.08455902	-7.50102847	7.73246848
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H	-6.41761195	-11.34197645	11.26568485
H	-5.07222789	-11.16481961	12.36642538
N	-9.36038746	-6.81113466	3.04408289
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O	-9.65134918	-7.62371467	2.15711199
O	-10.20519489	-5.99771329	3.43943563
N	-2.02013684	5.30891840	7.47711598
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C	-1.28484253	7.32083134	7.25493287
N	-2.23276938	7.09167136	6.34358624
C	-2.66278294	5.87235742	6.49519566
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H	-0.73650121	8.22984527	7.38876192

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H	-3.73691727	7.85326795	5.11399305
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H	-2.61618234	9.04701392	5.72388516
H	-1.29958056	3.55966773	8.35764087
H	-2.53327437	3.31371612	7.14496758
H	-2.96830438	3.92823961	8.72173342
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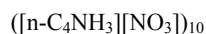
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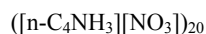
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H	-4.353603	-0.473669	2.924652
N	-6.827076	2.124905	4.569386
O	-7.890960	2.288679	3.982525
O	-6.800673	2.591664	5.702750
O	-6.210957	1.070687	4.459397
C	-9.204207	-0.902042	0.099112
H	-8.500298	-0.934599	-0.732484
H	-8.741958	-1.378829	0.963462
H	-9.954240	-1.646867	-0.166948
C	-9.685399	0.505243	0.453856
H	-10.349698	0.454579	1.316549
H	-10.208681	0.685384	-0.485199
C	-8.595400	1.534472	0.754571
H	-8.054935	1.190434	1.636408
H	-7.846673	1.452233	-0.033303
C	-9.083606	2.939045	1.110479
H	-9.690083	2.759952	1.998291
H	-9.677550	3.393141	0.317304
N	-7.967688	3.846772	1.418049
H	-7.447227	3.472729	2.198633
H	-7.383448	4.091242	0.631285
H	-8.248796	4.786309	1.659605
N	-6.974968	4.637719	-1.682340
O	-7.034234	5.345622	-0.683122
O	-7.138033	3.425529	-1.598197
O	-6.225562	4.920499	-2.610511
C	3.254924	5.002148	1.034346
H	3.778140	4.395376	1.773380
H	3.420738	4.447953	0.110509
H	3.871992	5.888323	1.182738
C	1.748165	5.216228	1.181610
H	1.345491	5.415464	0.188504
H	1.728254	6.119052	1.792030
C	0.904151	4.151895	1.883521
H	1.220802	3.111408	1.811285
H	1.190341	4.333649	2.919455
C	-0.584788	4.357459	1.603081
H	-0.837578	4.140860	0.565159
H	-0.815959	5.409080	1.772646
N	-1.514101	3.504464	2.359795
H	-1.249147	3.722342	3.309758
H	-2.463463	3.816892	2.214192
H	-1.567448	2.496191	2.334499
N	-4.644033	3.974130	2.787181
O	-4.474709	3.117097	1.927007
O	-5.787188	4.416563	2.810126
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C	-12.991416	5.580027	8.002881
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C	-10.802124	5.007786	6.946561
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H	-10.288484	5.923562	7.239185
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N	-8.847280	4.374061	5.573495
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H	-8.162465	3.651984	5.401065
N	-9.500266	6.413877	3.093413
O	-9.958353	5.284649	3.227860
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O	-9.268146	6.743753	4.251160
C	-6.665427	12.067720	4.090338
H	-6.338804	12.132096	3.052420
H	-7.750220	12.086143	4.195151
H	-6.239799	12.927516	4.607728
C	-6.174654	10.718882	4.617234
H	-6.594371	10.642603	5.620288
H	-5.095099	10.852752	4.548387
C	-6.650333	9.568847	3.728984
H	-7.672138	9.719786	3.380801
H	-6.079104	9.680781	2.807426
C	-6.316443	8.197739	4.317561
H	-7.023545	7.856191	5.073503
H	-5.345932	8.204755	4.813705
N	-6.139737	7.142380	3.308188
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H	-5.979082	6.248281	3.749637
N	-5.931706	5.928951	6.435592
O	-5.486272	6.970471	6.904528
O	-5.308871	5.553681	5.448513
O	-6.888967	5.275316	6.834949
C	-0.732183	8.362820	-3.300013
H	-0.226914	7.401870	-3.396848
H	-0.657181	9.046110	-4.145939
H	-0.209534	8.807547	-2.453162
C	-2.235787	8.120127	-3.165410
H	-2.675058	7.555504	-3.987809
H	-2.800580	9.050737	-3.109976
C	-2.543408	7.255069	-1.942756
H	-1.790963	6.476807	-1.815341
H	-2.530371	7.891641	-1.058049
C	-3.926238	6.609112	-2.034194
H	-4.035975	6.061327	-2.970137
H	-4.615182	7.448402	-2.129317
N	-4.232356	5.756309	-0.875376
H	-5.206664	5.498938	-0.807671
H	-3.731811	4.879176	-0.889222
H	-3.866746	6.221082	-0.056587
N	-3.502056	7.586953	1.689135
O	-3.269294	7.784344	2.876541
O	-4.645294	7.345667	1.317832
O	-2.719996	6.783273	1.193599
C	-1.142010	10.696599	6.907238
H	-2.212665	10.861654	6.786595
H	-0.938879	11.334626	7.767331
H	-0.617376	11.118812	6.050152
C	-0.631141	9.283874	7.191950
H	-0.863438	8.922561	8.193743

H	0.427903	9.472002	7.368395
C	-0.992424	8.158283	6.222228
H	-0.742992	8.378048	5.184159
H	-0.518764	7.208409	6.470196
C	-2.460435	7.738552	6.303541
H	-3.037664	8.657573	6.202023
H	-2.673108	7.169845	7.208771
N	-2.865430	6.809212	5.237639
H	-3.019746	7.277619	4.356231
H	-2.307717	5.982887	5.075639
H	-3.777125	6.472427	5.512393
N	-0.967462	4.175615	5.650201
O	-1.090733	4.951389	4.708897
O	-1.479784	4.497622	6.716462
O	-1.260203	3.052237	5.255993

Return



Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	7.495801	6.295293	5.490917
H	7.774125	6.774615	6.429473
H	7.972045	6.678549	4.588472
H	6.410141	6.388624	5.517948
C	7.904476	4.821933	5.496904
H	7.338786	4.396248	6.325691
H	8.930801	4.741314	5.855035
C	7.451617	4.008604	4.283950
H	7.651314	4.473800	3.318645
H	8.172072	3.190707	4.293311
C	5.972247	3.624980	4.330194
H	5.379139	4.531315	4.208216
H	5.633374	3.169492	5.260675
N	5.474766	2.707135	3.293896
H	5.668158	3.202538	2.435249
H	5.970215	1.836267	3.166541
H	4.503101	2.454784	3.404738
N	6.707010	-5.670409	0.158867
O	6.179892	-6.175492	1.143811
O	6.135845	-5.705638	-0.925386
O	6.865010	-4.467378	0.334447
C	-3.320744	-6.839726	0.729531
H	-4.403462	-6.733563	0.662065
H	-3.017561	-7.182667	-0.259697
H	-3.049535	-7.621516	1.439002
C	-2.827082	-5.475436	1.212078
H	-3.377967	-5.375926	2.147345
H	-3.203875	-4.694967	0.551024
C	-1.311475	-5.378878	1.389422
H	-0.972236	-6.172533	2.055103
H	-0.910026	-5.745868	0.444828
C	-0.897705	-3.958258	1.774745
H	-1.320301	-3.671134	2.737592
H	-1.249881	-3.177511	1.100575
N	0.571341	-3.946870	1.699811
H	0.887500	-4.347800	0.828376
H	0.872691	-3.006900	1.913687
H	1.058834	-4.493783	2.395035
N	6.922635	3.569296	0.612961
O	7.406417	2.656508	1.273149
O	5.813890	3.976546	0.941453
O	7.301091	3.738949	-0.540757
C	-0.783180	-1.469755	-4.812706
H	-0.016892	-0.987883	-5.419915
H	-0.592410	-2.534761	-4.680531
H	-1.773470	-1.195287	-5.176151
C	-0.863164	-0.907149	-3.393228
H	-1.432539	-1.709854	-2.924638
H	-1.331188	0.074600	-3.320964
C	0.565820	-0.752481	-2.871765
H	1.082453	-1.691037	-3.072520
H	1.184828	-0.000099	-3.360490
C	0.606740	-0.411476	-1.381838
H	0.067969	-1.167441	-0.810575
H	0.017104	0.495016	-1.245080
N	1.942293	-0.136527	-0.829984
H	2.445792	0.647672	-1.219367
H	1.938990	0.056042	0.161483
H	2.402656	-1.029054	-0.937514
N	5.461898	0.263100	-2.119748
O	5.717327	-0.836621	-1.641789

O	4.321276	0.593266	-1.814714
O	6.304921	1.153077	-2.137904
C	-5.998538	-2.930076	3.470841
H	-6.547248	-2.839049	4.408247
H	-6.682014	-3.439847	2.791802
H	-5.092423	-3.527572	3.571112
C	-5.546560	-1.498315	3.181672
H	-6.489873	-0.957098	3.108572
H	-4.922263	-1.361812	2.298655
C	-4.611697	-0.961058	4.265751
H	-5.170960	-0.860121	5.195879
H	-3.824285	-1.675526	4.505787
C	-3.983965	0.398324	3.956117
H	-4.761226	1.150179	3.819443
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O	-1.220572	-0.765679	3.677949
C	-4.981410	3.358101	-0.133484
H	-5.693249	2.871775	-0.800470
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C	-3.602140	2.702334	-0.207153
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C	-2.609291	3.390127	0.730414
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C	-1.301349	2.598293	0.719030
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H	0.521812	2.842483	1.637785
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H	-0.659958	2.788882	2.696084
N	-3.780725	4.213270	4.437845
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H	-2.052321	10.940671	8.382472
H	-1.595197	10.051618	9.738879
C	-2.129341	8.727980	8.142729
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C	-1.866869	8.758756	6.636740
H	-2.639153	9.363723	6.161668
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C	-1.853068	7.341015	6.064323
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H	-1.170929	6.637412	6.541532
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H	-1.060939	6.299729	4.467427
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C	-5.948484	4.193500	11.877345
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C	-5.901128	4.492611	10.378635
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C	-4.572903	3.968618	9.831742
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H	-5.052801	3.309703	7.793491
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O	-3.628777	8.312857	-2.149523
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H	5.246798	12.452832	4.779827
H	5.075913	10.925454	4.074899
C	3.126183	11.835356	4.504829
H	2.649902	12.807171	4.634562
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C	2.295878	10.981204	3.546258
H	2.612054	11.283684	2.547940
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C	0.782816	11.076809	3.744614
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H	0.182274	10.680429	1.838336
H	0.570415	9.309722	2.846813
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C	6.041572	3.166051	8.773586
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H	6.779187	2.660034	8.150711
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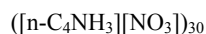
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H	2.639165	6.135059	9.465241
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N	1.625076	7.882058	6.042064
O	0.906636	7.497098	6.957883
O	1.050457	8.393469	5.087419
O	2.548787	7.128115	5.756750
C	11.811781	0.505407	-0.933870
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H	11.024503	-0.453840	0.848181
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C	9.395346	0.463827	-0.204623
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C	8.405823	-0.334774	0.644448
H	8.770551	-0.283683	1.670344
H	8.299522	-1.398018	0.429248
N	7.038756	0.190275	0.505553
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O	2.259003	-3.097460	-1.308637
C	6.476343	-4.581522	7.788309
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H	6.615399	-3.502892	7.715359
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C	6.668581	-5.027797	6.338577
H	6.402638	-6.075609	6.199065
H	7.716177	-5.110926	6.049216
C	5.868973	-4.275197	5.274592
H	4.827211	-4.595509	5.289852
H	5.838020	-3.208853	5.498319
C	6.615033	-4.536862	3.965865
H	6.754375	-5.603943	3.792594
H	7.573430	-4.021548	4.029303
N	5.947760	-4.009400	2.765711
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N	2.406300	2.550371	5.619504
O	2.402102	3.776356	5.623798
O	3.304927	2.046945	4.954593
O	2.116107	2.024490	6.688294
C	1.565201	-3.670410	7.343374
H	0.790792	-3.850551	8.088988
H	2.108277	-4.615348	7.327189
H	2.181672	-2.849086	7.708736
C	1.001498	-3.272758	5.978839
H	0.261625	-2.492354	6.156761
H	0.417757	-4.116838	5.611585
C	1.942618	-2.780700	4.878834
H	2.879015	-3.276163	4.622365
H	1.214473	-2.914543	4.078839

C	2.302089	-1.304377	5.049403
H	2.877597	-1.059223	5.942034
H	1.396064	-0.713792	5.185148
N	3.034609	-0.703623	3.924081
H	3.188779	0.291289	4.004588
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H	2.664052	-0.800389	2.989509
N	-3.135558	0.538683	8.060571
O	-2.989131	0.864254	9.233448
O	-4.070262	0.985264	7.404850
O	-2.080792	0.334305	7.470001
C	6.043961	7.625089	-3.834904
H	6.782728	7.750177	-3.043275
H	6.515450	8.007985	-4.739994
H	5.159526	8.214703	-3.593592
C	5.739339	6.135462	-3.996327
H	6.571814	5.532686	-4.359298
H	4.881057	5.941103	-4.639504
C	5.511650	5.459071	-2.644109
H	6.462450	5.354207	-2.121535
H	4.896246	6.023478	-1.943521
C	4.844318	4.089000	-2.768260
H	5.437042	3.560911	-3.515187
H	3.812721	4.215136	-3.096887
N	4.777543	3.303210	-1.526521
H	4.581718	2.348212	-1.790590
H	5.707186	3.282425	-1.132272
H	4.031550	3.535973	-0.886664
N	2.457932	2.103590	1.788514
O	1.584569	1.532574	1.144889
O	3.542250	1.563704	1.977866
O	2.158418	2.972601	2.599802
C	3.929653	-0.344767	11.207837
H	3.939117	0.328361	12.065106
H	4.305721	-1.328094	11.490221
H	4.722083	0.089680	10.598401
C	2.529291	-0.502286	10.614530
H	1.928164	-0.712254	11.499210
H	2.457162	-1.393259	9.990781
C	2.127812	0.638920	9.679487
H	2.270104	1.621756	10.128804
H	2.839283	0.653848	8.853844
C	0.627000	0.577961	9.393675
H	0.112102	0.629754	10.352996
H	0.413912	-0.317543	8.809923
N	0.176404	1.677620	8.526752
H	0.201605	2.584249	8.971148
H	0.781581	1.834816	7.733563
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N	6.542430	-0.672716	3.922643
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O	6.270552	0.324663	3.263557
O	5.555305	-1.267394	4.340994
C	2.155858	5.624217	-6.083658
H	1.325346	5.513984	-6.780938
H	3.030070	6.016604	-6.603164
H	2.410913	4.630063	-5.716638
C	1.847139	6.568627	-4.921494
H	1.498234	7.529393	-5.300035
H	2.746131	6.749208	-4.332169
C	0.876729	6.046022	-3.861763
H	-0.087525	5.709317	-4.242480
H	1.264286	5.082305	-3.531385
C	0.705657	7.050798	-2.722025
H	0.213245	7.944952	-3.104280
H	1.587125	7.526449	-2.292059
N	-0.232005	6.728054	-1.635532

H	-0.304822	7.475898	-0.960606
H	-1.113102	6.586787	-2.108621
H	0.019065	5.792263	-1.350297
N	-0.408206	7.113254	1.743001
O	-0.356261	5.938951	1.394588
O	0.357087	7.453694	2.638269
O	-1.462225	7.738512	1.777244
C	6.029441	8.225047	2.101518
H	6.850364	8.176757	1.386080
H	5.500514	9.155154	1.893580
H	6.449181	8.126468	3.102618
C	5.181310	7.004832	1.741531
H	5.833644	6.134529	1.813161
H	4.844291	7.073737	0.707234
C	3.997624	6.967574	2.708661
H	4.585389	6.924303	3.625591
H	3.464402	7.917948	2.732408
C	3.169114	5.688379	2.585898
H	3.846618	4.849335	2.744310
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N	2.092365	5.631392	3.586501
H	1.664484	4.721357	3.680600
H	2.473279	5.935348	4.471156
H	1.384421	6.327186	3.399992
N	1.641049	3.603164	-1.039188
O	1.839339	2.508783	-1.555023
O	2.538636	4.159555	-0.416418
O	0.653245	4.224863	-1.414433
C	-2.560595	13.092500	-4.141864
H	-2.988008	12.339719	-4.804237
H	-2.692747	14.111893	-4.504459
H	-1.478516	12.961428	-4.136927
C	-2.986616	12.846631	-2.694143
H	-4.050403	12.979986	-2.497483
H	-2.388527	13.528018	-2.089080
C	-2.694897	11.388936	-2.336563
H	-3.036894	10.789665	-3.180372
H	-1.621034	11.229373	-2.433816
C	-3.114466	11.296240	-0.869181
H	-4.072106	11.776579	-0.668434
H	-2.395981	11.872241	-0.285998
N	-3.264682	9.959206	-0.274525
H	-3.598601	9.281098	-0.944426
H	-2.353691	9.738820	0.101806
H	-3.947838	9.947448	0.469290
N	0.407482	10.150395	-0.443772
O	-0.381442	9.321345	-0.883492
O	-0.038010	11.134636	0.135780
O	1.450185	9.803160	0.099618
C	3.846605	-2.272777	-6.551531
H	2.785138	-2.459512	-6.388682
H	4.057794	-1.203929	-6.518932
H	3.932553	-2.659812	-7.566872
C	4.782923	-2.998119	-5.584563
H	5.823922	-2.867822	-5.880273
H	4.488083	-4.040809	-5.702739
C	4.528969	-2.627630	-4.123027
H	4.774923	-1.584488	-3.924378
H	3.454031	-2.669716	-3.947416
C	5.235639	-3.631284	-3.211359
H	6.319030	-3.657618	-3.328284
H	4.899318	-4.624048	-3.510367
N	5.148583	-3.378713	-1.764822
H	4.203106	-3.552508	-1.455034
H	5.757008	-4.047191	-1.314205
H	5.524798	-2.489682	-1.467860
N	3.682949	-2.097346	1.048721

O	4.737827	-1.505427	1.248570
O	3.650185	-3.321686	1.103437
O	2.615124	-1.558095	1.317110
C	2.878003	-9.686634	-3.182542
H	3.805179	-9.139274	-3.352368
H	3.182301	-10.684650	-3.497929
H	2.206545	-9.133167	-3.838985
C	2.559034	-9.780592	-1.690137
H	3.307785	-10.430324	-1.237015
H	1.668505	-10.408971	-1.676059
C	2.367209	-8.457254	-0.948639
H	1.808120	-7.768160	-1.581623
H	1.776700	-8.649219	-0.052788
C	3.685158	-7.803839	-0.531624
H	4.195550	-7.440712	-1.423667
H	4.303004	-8.424284	0.117539
N	3.502977	-6.543926	0.205443
H	4.406922	-6.158762	0.439178
H	2.913111	-5.917896	-0.323940
H	3.090189	-6.584155	1.126360
N	2.444128	-6.249397	3.225712
O	3.500005	-5.687260	2.957005
O	1.811275	-6.613350	2.240769
O	1.792350	-5.528097	3.972697

[Return](#)



Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
C	-11.506588	16.414424	4.066069
H	-10.869514	15.835402	3.397511
H	-11.775558	15.780585	4.911056
H	-12.437531	16.674257	3.562153
C	-10.928052	17.679907	4.699859
H	-11.653988	18.011831	5.442115
H	-10.869231	18.508571	3.994200
C	-9.502159	17.279217	5.079487
H	-9.667223	16.342209	5.611342
H	-8.902391	16.988816	4.216906
C	-8.732948	18.221790	6.005616
H	-9.090376	18.282259	7.033569
H	-8.656438	19.220109	5.574795
N	-7.373839	17.692168	6.195776
H	-6.939292	17.590000	5.289779
H	-6.757101	18.260679	6.758386
H	-7.429478	16.786389	6.639136
N	-4.669611	19.431563	-0.610872
O	-4.475190	19.782257	-1.769445
O	-5.870169	19.251221	-0.439956
O	-3.939380	19.902776	0.253880
C	1.042729	12.514243	10.086012
H	0.134220	12.659899	10.670388
H	1.241079	11.543480	9.631724
H	1.798497	12.797273	10.818685
C	1.082217	13.514242	8.930035
H	2.100904	13.539217	8.543055
H	0.933297	14.535162	9.281665
C	-0.021028	13.199404	7.919307
H	-0.062519	12.128070	7.722783
H	-0.947553	13.452208	8.434808
C	0.251385	13.574058	6.462164
H	1.266867	13.231032	6.264103
H	0.483815	14.638177	6.420608
N	-0.759723	13.100270	5.504549
H	-1.693597	13.416949	5.722938
H	-0.517834	13.514909	4.615918
H	-0.766505	12.095508	5.402045
N	-0.818572	5.947453	6.171444
O	-0.514026	6.274524	5.029799
O	-1.883757	5.386613	6.403645
O	-0.018279	6.267785	7.043220
C	-2.713657	14.783273	11.840088
H	-3.597017	15.252195	12.273547
H	-2.923110	13.796311	11.427611
H	-1.973237	14.821049	12.639120
C	-2.297884	15.600233	10.616344
H	-1.478728	14.981880	10.249299
H	-1.746756	16.421760	11.074000
C	-3.373506	15.903242	9.572761
H	-3.849912	14.964091	9.291456
H	-4.170106	16.579520	9.882887
C	-2.847245	16.650852	8.347212
H	-1.945680	16.165027	7.974043
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H	-3.451468	16.970818	6.328281
H	-4.395896	16.009204	7.123754
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O	-0.822512	2.031754	7.935510
O	-0.537446	1.387830	6.011743
C	-1.265039	29.190058	7.967028
H	-1.507779	29.128104	6.906207
H	-0.875471	30.188300	8.166652
H	-0.468567	28.497134	8.238300
C	-2.497231	28.775253	8.771690
H	-3.408276	29.354609	8.621878
H	-2.284503	28.944877	9.827187
C	-2.874744	27.314910	8.521244
H	-2.907090	27.026507	7.470588
H	-2.203429	26.591796	8.984432
C	-4.226417	27.001568	9.163614
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H	-5.493332	25.400511	9.620804
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O	-7.622524	26.720671	11.366240
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C	4.883694	20.721594	4.846138
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H	4.201509	21.509624	5.165092
H	5.084935	20.222123	5.793836
C	4.222234	19.670946	3.953698
H	4.930167	18.940568	3.561933
H	3.803917	20.264487	3.140790
C	3.172973	18.776010	4.613987
H	3.577419	18.357434	5.535571
H	2.313468	19.366723	4.930860
C	2.686594	17.670671	3.676170
H	3.535255	16.991987	3.590952
H	2.542433	17.979526	2.640832
N	1.531289	16.892207	4.148510
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H	1.530143	16.082315	3.545040
H	1.735446	16.446693	5.031651
N	-3.640263	12.643197	6.407866
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C	-13.539172	23.717340	11.822521
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H	-13.365978	23.481234	10.772588
H	-14.285879	23.006945	12.177298
C	-12.269532	23.708189	12.674442
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H	-11.751258	24.666367	12.711700
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C	-10.129150	22.696754	13.130918
H	-10.199526	21.973129	13.943022
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H	-8.555084	23.138296	11.910546
H	-8.149514	22.091823	13.108877
H	-9.035646	21.618674	11.770155
N	-3.775259	23.690409	6.485946
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O	-2.799961	24.021244	7.151092
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C	-12.820919	21.199811	3.170229
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H	-12.949258	20.264871	3.715679
C	-11.381528	21.668586	3.385273
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C	-10.815472	22.888787	2.658270
H	-10.929657	23.817363	3.217562
H	-11.116219	23.074173	1.627114
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H	-8.932910	23.531907	2.241609
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O	-3.863415	19.616912	7.034111
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O	-5.457494	18.651404	7.945091
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H	-0.634620	25.527019	2.469978
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H	-6.604398	24.606605	3.768374
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H	2.924085	9.089439	0.403608
H	2.952883	7.501093	-0.263168
C	1.821487	7.773079	1.516952
H	1.250519	6.892618	1.222193
H	2.667753	7.328144	2.040372
C	1.009276	8.764570	2.350678
H	0.065364	8.971928	1.846561
H	1.660623	9.612069	2.564200
N	0.698144	8.167632	3.658616
H	1.602962	8.174291	4.107347
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H	0.361016	7.221588	3.765602
N	2.503066	5.151014	4.729984
O	1.601275	4.362808	4.468107
O	2.805004	6.074938	3.982807
O	3.090782	4.985846	5.793179
C	0.677844	21.995429	3.088216
H	1.510466	22.198895	2.414834
H	0.489393	22.898800	3.668308
H	1.059495	21.294023	3.830155
C	-0.653948	21.628704	2.432713
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C	-1.678581	21.272957	3.510402
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H	-1.785392	22.146223	4.153907
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H	-3.679814	21.600888	2.561570
N	-3.901306	20.257589	4.085840
H	-3.378612	19.656033	4.706340
H	-4.372691	21.016123	4.557563
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N	-9.009296	20.396126	9.808411
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O	-8.524248	19.692033	8.929743
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C	-7.648349	14.254965	-1.544197
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H	-8.167097	13.631278	-2.272219
H	-6.910000	14.769487	-2.159184
C	-8.417934	15.316854	-0.758086
H	-9.191289	14.809684	-0.181197
H	-8.993824	15.838565	-1.522459
C	-7.605623	16.192607	0.196403
H	-7.110303	15.679200	1.020521
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H	-8.593086	15.327836	14.628599
H	-8.010645	16.904769	15.156972
H	-9.265767	16.883268	13.872049
C	-7.261364	16.255414	13.313656
H	-7.547801	15.538937	12.543777
H	-6.416724	15.722645	13.750507
C	-6.794283	17.581867	12.713489
H	-7.559079	18.357787	12.747196
H	-6.068122	17.915718	13.454660
C	-6.455141	17.509003	11.224357
H	-7.244996	16.944381	10.728949
H	-5.554479	16.895310	11.207400
N	-6.287859	18.823588	10.585824
H	-7.164526	19.286747	10.393370
H	-5.547816	19.387875	10.978272
H	-6.005694	18.711403	9.622549
N	-3.307130	24.627687	11.825048
O	-3.902462	25.654589	12.131853
O	-3.362359	23.641893	12.551846
O	-2.554619	24.604072	10.857450

Return

([n-C₄mim][BF₄])₁₀

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
N	-17.20070927	3.92207900	-3.97554518
C	-17.98489639	4.17533609	-2.92542516
C	-17.17410513	4.44705740	-1.88699074
N	-15.92094949	4.35103258	-2.33636335
C	-15.95978504	4.03324439	-3.59822962
C	-14.70354838	4.56746349	-1.54130495
C	-17.66039174	3.57637997	-5.32845262
C	-17.83876630	4.86381231	-6.15461843
C	-18.88067908	5.77068731	-5.47370078
C	-19.05971017	7.05741482	-6.30064811
H	-19.05476603	4.16436609	-2.91214254
H	-17.47615839	4.69333381	-0.89047622
H	-15.10613926	3.88665837	-4.22639709
H	-13.91191478	3.96070361	-1.92873575
H	-14.89107845	4.30103795	-0.52211850
H	-14.42147617	5.59825755	-1.59436439
H	-18.59548809	3.05993970	-5.26635482
H	-16.93598757	2.94674984	-5.80133516
H	-18.17391596	4.61211977	-7.13912766
H	-16.90357593	5.37991534	-6.21730233
H	-18.54507869	6.02296369	-4.48946588
H	-19.81575631	5.25457450	-5.41033011
H	-19.78352847	7.68761983	-5.82756401
H	-19.39541296	6.80502447	-7.28477950
H	-18.12461393	7.57357212	-6.36420110
B	-12.22582788	2.95002478	-4.54757893
F	-13.02066554	3.58018407	-5.59769435
F	-10.96161824	2.48232601	-5.10851294
F	-11.95951616	3.92069941	-3.48999902
F	-12.96152118	1.81687874	-3.99410176
N	-11.10851038	-1.99290018	-4.06288211
C	-12.30417179	-2.53292386	-3.81680619
C	-13.18291317	-1.93102847	-4.63848013
N	-12.49553928	-1.04299184	-5.35992266
C	-11.24653902	-1.09684107	-4.99707083
C	-13.05389501	-0.15471831	-6.38946158
C	-9.84961262	-2.34927626	-3.39257346
C	-9.15960967	-3.48784677	-4.16673688
C	-10.08562230	-4.71775691	-4.20480412
C	-10.38291910	-5.18120177	-2.76658578
H	-12.52217924	-3.29872368	-3.10208323
H	-14.23297815	-2.12678601	-4.70161590
H	-10.45764658	-0.49862772	-5.40285484
H	-13.36253843	0.76491790	-5.93786746
H	-13.89687610	-0.62696767	-6.84897612
H	-12.30860761	0.04455783	-7.13091932
H	-10.05643931	-2.67169633	-2.39344679
H	-9.20580624	-1.49504638	-3.36570471
H	-8.24314428	-3.74651263	-3.67877877
H	-8.95309414	-3.16577166	-5.16598313
H	-9.60596852	-5.50879087	-4.74250704
H	-11.00211146	-4.45926706	-4.69280026
H	-10.86253056	-4.39009570	-2.22897141
H	-9.46649207	-5.43974242	-2.27849317
H	-11.02633697	-6.03570916	-2.79301012
B	-16.95069954	-0.11563123	-5.20051917
F	-15.99775314	0.83800244	-4.64007265
F	-17.53671201	-0.90810057	-4.12339787
F	-18.00691614	0.60739813	-5.90282468
F	-16.26143418	-0.99981877	-6.13579064
N	-11.81029584	-4.90984219	4.38240976

C	-12.32291847	-3.68110215	4.47805204
C	-12.37174534	-3.37744506	5.78754418
N	-11.88680426	-4.43038544	6.44940619
C	-11.55474845	-5.34345719	5.58298714
C	-11.75087534	-4.54015172	7.90898756
C	-11.57443957	-5.64808892	3.13341744
C	-12.82852013	-6.46756569	2.77691591
C	-12.58100143	-7.24184813	1.46897925
C	-13.83599320	-8.05952811	1.11139767
H	-12.63552054	-3.05665712	3.66741343
H	-12.73075137	-2.46558833	6.21689489
H	-11.13741150	-6.29965622	5.82029689
H	-10.92062460	-5.17316844	8.14327636
H	-12.64563631	-4.95865908	8.32006435
H	-11.58723284	-3.56841165	8.32596032
H	-10.74160080	-6.30752505	3.26081446
H	-11.36432683	-4.95645627	2.34447325
H	-13.66101591	-5.80771003	2.64883733
H	-13.03945234	-7.15883240	3.56602383
H	-11.74933936	-7.90262444	1.59775863
H	-12.36883298	-6.55094734	0.67992831
H	-14.66744544	-7.39850320	0.98247121
H	-14.04846703	-8.75025579	1.90041275
H	-13.66407412	-8.59781904	0.20278184
B	-15.92584144	2.97801015	3.04540205
F	-15.33197133	1.77513442	3.62161519
F	-14.92805173	3.67519876	2.23921090
F	-17.05864060	2.60583382	2.20286141
F	-16.38470989	3.85589885	4.11794646
N	-4.23740731	1.33457980	-1.58545897
C	-5.39298025	0.73987293	-1.28109846
C	-6.00691580	1.51843397	-0.37186912
N	-5.20661104	2.56363480	-0.15094942
C	-4.14488337	2.43248988	-0.89258196
C	-5.47803231	3.67433844	0.77283708
C	-3.23792057	0.83544646	-2.54068006
C	-3.54316588	1.39472473	-3.94263169
C	-3.49466830	2.93346461	-3.90228597
C	-2.09303992	3.39167377	-3.45842929
H	-5.76096064	-0.18068036	-1.68357636
H	-6.95599211	1.33484587	0.08688482
H	-3.32504482	3.11920300	-0.92742929
H	-6.07763389	3.32314425	1.58646076
H	-6.00059127	4.45038434	0.25364206
H	-4.55343706	4.05797529	1.15077955
H	-3.27263344	-0.23363458	-2.56752504
H	-2.26304567	1.15315440	-2.23482666
H	-4.51755195	1.07655222	-4.24969610
H	-2.81442258	1.03263667	-4.63743937
H	-4.22423836	3.29510844	-3.20821269
H	-3.70538106	3.32264703	-4.87645600
H	-1.88249388	3.00254078	-2.48414738
H	-2.05965701	4.46079410	-3.43034862
H	-1.36316349	3.03014915	-4.15223685
B	-8.73629768	3.94304723	4.36922245
F	-10.14688626	3.82045640	4.01308193
F	-8.00638313	2.77972849	3.87370249
F	-8.18625680	5.15479349	3.76862124
F	-8.60564414	4.01725639	5.82146788
N	-9.75897684	5.44581540	0.62840961
C	-9.87985156	4.50354655	1.56606459
C	-10.11083595	3.34233273	0.92746027
N	-10.12380644	3.61294058	-0.37959867
C	-9.90982096	4.88722166	-0.53785388
C	-10.34247653	2.63743408	-1.45737207
C	-9.49930468	6.87214496	0.87169987
C	-10.83730814	7.61940914	1.02410917

C	-11.66375961	7.46190401	-0.26573914
C	-13.00119746	8.20999796	-0.11275643
H	-9.80684508	4.64504330	2.62420024
H	-10.25638623	2.38418744	1.38090004
H	-9.86493771	5.39538582	-1.47843428
H	-11.38846225	2.57305015	-1.67332830
H	-9.98229444	1.67825238	-1.14882888
H	-9.81578468	2.95091654	-2.33442161
H	-8.95423774	7.28119071	0.04678459
H	-8.92550526	6.98218795	1.76807599
H	-10.64768658	8.65741278	1.20153999
H	-11.38230448	7.21025681	1.84900168
H	-11.85389759	6.42399425	-0.44318463
H	-11.11864740	7.87074045	-1.09076326
H	-12.81106947	9.24792385	0.06482888
H	-13.54626933	7.80100054	0.71215937
H	-13.57545359	8.10087695	-1.00896613
B	-6.70178158	5.67003445	-1.48638391
F	-6.77771628	5.32826211	-0.06897990
F	-7.09576499	4.51468238	-2.28735673
F	-7.60054959	6.78592469	-1.76675386
F	-5.33308556	6.05127336	-1.82243860
N	-15.46368580	-0.71666054	1.17873706
C	-16.71267383	-0.66185342	0.71093106
C	-16.63445351	-0.25786248	-0.56974522
N	-15.34024525	-0.07879886	-0.84277538
C	-14.65154142	-0.36190568	0.22500273
C	-14.78667557	0.36336765	-2.13075075
C	-15.07210413	-1.11039952	2.54009247
C	-14.83582353	-2.63151411	2.58813685
C	-16.13154952	-3.36520206	2.19531164
C	-17.25408502	-2.98744624	3.17959996
H	-17.60600858	-0.89473301	1.25182135
H	-17.45367646	-0.10853935	-1.24178283
H	-13.58579475	-0.31083948	0.30596788
H	-15.49406668	0.99640749	-2.62452787
H	-14.58320941	-0.48992952	-2.74336469
H	-13.87985076	0.90557555	-1.96184984
H	-15.85173961	-0.84911291	3.22480854
H	-14.17172156	-0.60100213	2.81341531
H	-14.55102138	-2.91676244	3.57926812
H	-14.05613725	-2.89337949	1.90366738
H	-15.96745377	-4.42207631	2.22986638
H	-16.41599251	-3.08060638	1.20395284
H	-16.96978506	-3.27201381	4.17111497
H	-18.15434640	-3.49717430	2.90653579
H	-17.41808625	-1.93064766	3.14500323
B	-7.34102053	-5.69310854	3.24755138
F	-8.40080443	-6.36414226	3.99466605
F	-7.51491127	-4.24702959	3.34864942
F	-6.04309139	-6.06710672	3.80172334
F	-7.40527238	-6.09414789	1.84517481
N	-5.77716390	-2.50861669	5.32052109
C	-5.24808285	-1.61643603	4.48039664
C	-6.08616760	-0.56475035	4.44637197
N	-7.10014815	-0.84850005	5.26685951
C	-6.89395719	-2.02552945	5.78345732
C	-8.25391440	0.02052923	5.54058317
C	-5.19710651	-3.81501955	5.66443052
C	-4.27319272	-3.66121411	6.88697932
C	-5.08678422	-3.13073776	8.08192833
C	-4.16260309	-2.97743520	9.30414721
H	-4.33174377	-1.71843862	3.93741568
H	-5.96333817	0.32907392	3.87113844
H	-7.54053633	-2.51829663	6.47912171
H	-7.95948300	1.04481092	5.44543186
H	-8.60710212	-0.15815932	6.53469586

H	-9.03493474	-0.19253307	4.84091283
H	-4.63155691	-4.18368965	4.83435599
H	-5.98236415	-4.50421482	5.89532553
H	-3.48785416	-2.97208257	6.65611110
H	-3.85119541	-4.61217743	7.13694579
H	-5.87217961	-3.81972107	8.31283414
H	-5.50868732	-2.17972294	7.83213413
H	-3.37724485	-2.28840238	9.07321288
H	-3.74067768	-3.92854656	9.55377490
H	-4.72768415	-2.60890382	10.13463008
B	-2.67678268	-1.26280613	1.33042559
F	-2.32661593	-2.66371726	1.54587948
F	-2.56172976	-0.94532593	-0.08999052
F	-4.04914821	-1.03079211	1.77135370
F	-1.76962442	-0.41139757	2.09447375
N	-8.29703825	3.48267054	-6.80364452
C	-7.00346300	3.78166810	-6.94169081
C	-6.78021537	4.89735588	-6.22406705
N	-7.94470805	5.24392371	-5.67129108
C	-8.84605169	4.37754528	-6.03400483
C	-8.17097684	6.40661259	-4.80062051
C	-8.98520057	2.33725363	-7.41643005
C	-9.53644162	2.74668833	-8.79482536
C	-10.25785452	1.54665017	-9.43603735
C	-10.80931454	1.95550244	-10.81454468
H	-6.28157217	3.23748513	-7.51405054
H	-5.84687197	5.40946506	-6.11674505
H	-9.87605830	4.39771747	-5.74499974
H	-8.44145910	7.25220196	-5.39786888
H	-7.27527567	6.62535120	-4.25764439
H	-8.96088196	6.18857653	-4.11257554
H	-9.79317285	2.02820154	-6.78666372
H	-8.29523792	1.52795023	-7.53439070
H	-8.72847418	3.05539347	-9.42470089
H	-10.22627399	3.55618032	-8.67706257
H	-11.06579326	1.23815398	-8.80600142
H	-9.56803238	0.73715788	-9.55368356
H	-11.31058255	1.12157392	-11.25968056
H	-10.00145016	2.26392342	-11.44473982
H	-11.49905907	2.76505523	-10.69706040
B	-7.14083853	0.07392003	-5.38438025
F	-7.95433178	-0.56994216	-6.41164856
F	-6.27106053	1.06882982	-6.00505890
F	-8.01225490	0.72792040	-4.41251477
F	-6.32571926	-0.93112709	-4.70830351
N	-4.60751937	-4.02165640	-0.37421032
C	-4.58593371	-3.13809931	-1.37447269
C	-5.56688721	-2.24954283	-1.13398766
N	-6.15591757	-2.61928588	0.00542557
C	-5.56168433	-3.69020241	0.44692051
C	-7.28403655	-1.93344439	0.65193360
C	-3.70654603	-5.17356047	-0.22547065
C	-4.32261955	-6.40024966	-0.92336610
C	-3.37854009	-7.60691491	-0.76870694
C	-3.99453014	-8.83319760	-1.46739030
H	-3.91584135	-3.13695289	-2.20869757
H	-5.82585831	-1.40687203	-1.74056110
H	-5.81723906	-4.21536085	1.34349439
H	-6.91111725	-1.19360120	1.32906439
H	-7.87290907	-2.64579717	1.19103650
H	-7.88925212	-1.46171225	-0.09377342
H	-3.56825138	-5.38648284	0.81394550
H	-2.76094644	-4.94672151	-0.67194047
H	-4.46129718	-6.18692117	-1.96264656
H	-5.26801222	-6.62741552	-0.47663297
H	-3.24001206	-7.82060814	0.27057097
H	-2.43309112	-7.37954140	-1.21516595

H	-4.93997959	-9.06054353	-1.02092856
H	-3.33857635	-9.67169000	-1.36014184
H	-4.13310494	-8.61938466	-2.50664633
B	-10.33306900	-2.46111711	8.03063613
F	-9.50174973	-3.46949234	7.37975438
F	-9.59721353	-1.86819284	9.14355588
F	-10.67994029	-1.42044455	7.06713533
F	-11.55341445	-3.08632617	8.53211528
N	-11.36736801	1.98370238	7.18283637
C	-11.84559704	1.28303558	6.15231019
C	-12.45482777	2.15806525	5.33228449
N	-12.32930278	3.36487752	5.88851239
C	-11.67023894	3.23710235	7.00387049
C	-12.84738380	4.62438931	5.33522335
C	-10.62476224	1.43298171	8.32565780
C	-10.89102717	2.29431491	9.57415543
C	-10.11351907	1.71686533	10.77151434
C	-10.37967975	2.57808286	12.02012825
H	-11.76052303	0.22647370	6.00632283
H	-12.94650270	1.93011991	4.40973158
H	-11.41738680	4.03639842	7.66879188
H	-12.10584868	5.06873907	4.70467265
H	-13.08370965	5.29477730	6.13497323
H	-13.72975717	4.42641726	4.76327429
H	-9.57747338	1.43734762	8.10615427
H	-10.94647708	0.42926055	8.50953634
H	-11.93834310	2.29030984	9.79352688
H	-10.56886664	3.29792757	9.39029189
H	-9.06622494	1.72082185	10.55209331
H	-10.43563727	0.71323198	10.95531724
H	-9.83938165	2.17681437	12.85196713
H	-11.42693346	2.57402496	12.23961327
H	-10.05766487	3.58177537	11.83638212
B	-10.77751888	-0.98558536	0.00345257
F	-9.59713260	-0.12858290	0.06536380
F	-10.36902203	-2.38412443	0.09751191
F	-11.67109928	-0.66394148	1.11234984
F	-11.47282821	-0.76567083	-1.26138012

Return

([n-C₄mim][BF₄])₂₀

Atomic Number	Atomic Coordinates (Angstroms)		
	X	Y	Z
N	-13.72288006	-3.50806524	1.17678404
C	-12.93283670	-4.36249525	0.52297001
C	-12.83360410	-5.46657064	1.28488596
N	-13.56623825	-5.25076558	2.37960075
C	-14.09346487	-4.06365882	2.29417039
C	-13.74717028	-6.19357428	3.49270046
C	-14.10892872	-2.16732772	0.71356213
C	-15.50293743	-1.81481769	1.26536737
C	-15.90732278	-0.41074508	0.77885338
C	-17.30116213	-0.05789718	1.33050839
H	-12.46695371	-4.20017196	-0.42662840
H	-12.27401552	-6.34959819	1.05685129
H	-14.73111561	-3.61519027	3.02703060
H	-12.87416750	-6.80480054	3.58786187
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H	-7.73076823	9.28383391	3.97662615
H	-8.76675733	9.43194286	5.37581539
H	-9.29417788	10.04990547	3.82893061
B	-9.84279882	2.75279205	2.19514051
F	-9.19316956	3.66396032	3.13285637
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C	-3.51788291	-9.85432805	-3.88565271
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C	-2.06358298	-9.04836430	-5.23078166
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H	-0.74551971	2.56711374	-2.47958065
H	-4.87081594	6.56634990	-1.54551708
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F	0.73190398	-1.05155572	-8.07610060
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C	-0.03349232	-1.61327206	-3.28207504
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C	-1.79182884	-3.32316571	-2.80938545
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H	3.31351429	-4.43193581	-2.54946848
H	5.00284910	-4.20499564	-0.76405028
H	5.60191018	-2.74595167	-1.51601881
H	5.58298661	-5.48787944	-2.79225710
H	6.99345941	-4.68652136	-2.14308483
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B	-4.14621835	-7.50158865	5.04279486
F	-3.50399641	-8.25437266	6.11628093
F	-5.28124720	-6.75791807	5.58147234
F	-3.18565534	-6.56908934	4.46026274
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N	-2.78762638	-1.91563094	4.86726574
C	-1.86519292	-2.73223684	5.28840883
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H	-2.77219997	0.09470463	5.42710735
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H	0.16044796	-4.05136581	6.32958916
H	0.00710061	-5.55901175	7.19943121
H	-1.76108946	-4.56634578	8.60784769
H	-1.60531092	-3.05798074	7.73974053
H	0.74429433	-2.87697376	8.47689254
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H	-0.32817725	-2.98712239	9.85190120
B	2.60366564	2.05503722	-0.79258589
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Return

([n-C₄mim][BF₄])₃₀

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C	-6.70388308	-1.37219246	0.09493047
C	-4.73244814	-0.74021810	1.43975177
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C	-8.38930456	-3.70654546	-2.16803207
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H	-5.30345663	0.09397747	1.79036570
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H	-8.27266090	-4.61548186	-1.61563482
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H	-9.62456595	-4.60032150	-3.68145473
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H	-10.94598698	-3.13997277	-1.38580683
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F	-0.32612267	4.86095600	-7.80860196
F	-0.43852859	3.08964889	-6.21673531
F	-0.27536693	2.59317859	-8.54295039
F	1.59526784	3.51394212	-7.38649492
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C	-3.59666784	-2.17474983	-2.49508781
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C	-2.19500800	-3.67245614	-3.10006197
C	-1.38300162	-2.14587868	-1.33829487
C	-3.46856630	-4.89183178	-4.82745722
C	-4.95845943	-5.27667596	-4.88949364
C	-5.16233299	-6.36656155	-5.95821050
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H	-1.89116712	-1.71747460	-0.49973800
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H	-4.63717850	-7.97938955	-4.63973751
H	-3.29040988	-7.33848477	-5.55009533
B	-6.82108227	-0.17789341	-4.15554259
F	-7.76961185	0.75695768	-3.55720781
F	-7.43778045	-1.49718726	-4.25949067
F	-6.44896400	0.29172870	-5.48694765
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C	-1.58832346	6.81979062	10.39336330
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C	-0.07915417	8.40307315	9.15228968
C	0.23765739	9.02076592	7.77764761
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H	-1.02632773	6.66097327	8.32604259
H	0.77560140	7.86637691	9.50756551
H	-0.32507087	9.18087475	9.84476309
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